NONEQUILIBRIUM SORPTION OF VOLATILE PETROLEUM HYDROCARBONS BY SURFACTANT-MODIFIED ZEOLITE

by

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ABSTRACT

The sorption process significantly affects the transport of reactive solutes through geologic media. Nonequilibrium sorption complicates breakthrough curve (BTC) predictions because early-time breakthrough and extended tailing occur. These conditions have adversely affected the accuracy of BTC predictions of volatile petroleum hydrocarbons—specifically benzene, toluene, ethylbenzene, and xylenes (BTEX)—through surfactant-modified zeolite (SMZ) columns.

According to our conceptual model, BTEX molecules are kinetically sorbed on bilayer surfactant sites where the solutes must penetrate external surfactant hydrophilic head groups before partitioning into the hydrophobic tail region of the SMZ. Monolayer SMZ sites allow instantaneous sorption because BTEX molecules immediately partition into the hydrophobic surfactant tail groups. Concentration effects on the kinetics of nonequilibrium sorption of BTEX by SMZ were studied by applying a first-order bicontinuum sorption model to batch experiment data. The modeling results indicate that a constituent's distribution coefficient (K_d) is not affected by concentration variations. However, the first-order sorption rate coefficient (k_2) and the fraction of instantaneous sorption sites (F) are both inversely related to the initial BTEX concentration. A 30 to 45% reduction in k_2 and a 35 to 45% reduction in F occurred as the total BTEX concentration increased from 0.25 to 1.5 mmol L^{-1}. According on the batch results, these nonequilibrium parameters are controlled by the total initial BTEX concentration rather than the concentrations of individual compounds. The variation in F was unexpected based upon a conceptual model of BTEX partitioning into surfactant monolayers and

bilayers. The batch-determined kinetic measurements were used to parameterize a nonequilibrium transport model to predict BTEX breakthrough curves for varying input concentrations.

Monolayer SMZ batch tests were run to test our conceptual model, and the results were in agreement with the conceptual model. As hypothesized, only minor variations between the monolayer and bilayer k_2 results were observed. The significant increase (3 to 10 times) in the monolayer F results was anticipated because of the increase in the fraction of surface covered by a surfactant monolayer. The monolayer K_d results, adjusted for partial coverage, agreed with the bilayer K_d results.

The nonequilibrium transport model fully parameterized with values from the batch experiments was not successful in predicting BTEX transport through SMZ laboratory columns. Predicted breakthrough was earlier than the observed breakthrough for each solute, with the degree of overestimation increasing with increasing hydrophobicity. Sensitivity analysis revealed that the retardation factor, R, (calculated from the distribution coefficient) limited the prediction capabilities. When R was inversely fit to the BTC data while retaining values of k_2 and F from the batch studies, the nonequilibrium model provided reasonable agreement for each constituent's transport behavior. On average, R values fitted to the transport results were three times those calculated from the batch-derived K_ds. Aqueous phase surfactant monomers are present in SMZ batch systems due to surfactant wash-off, but are constantly flushed from transport systems. Consequently, the BTEX solubility might increase in the batch systems, producing lower K_d values in SMZ/BTEX batch systems than transport systems.

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THESIS INTRODUCTION

This document contains a manuscript written for submission to a professional journal and supporting appendices. It represents the results of a thesis project that partially fulfills the requirements for the Degree of Master of Science in Hydrology at the New Mexico Institute of Mining and Technology. This study furthered research on surfactant-modified zeolite (SMZ) removal of benzene, toluene, ethylbenzene, and xylenes (BTEX) from produced water. Previous research showed BTEX transport through SMZ columns is characterized by nonequilibrium sorption. These nonequilibrium processes were investigated through laboratory batch and column experiments. A first-order bicontinuum model was fit to kinetic batch sorption data in order to obtain three nonequilibrium sorption parameters: the distribution coefficient (K_d), a first-order sorption rate coefficient (k_2), and the fraction of instantaneous sorption (F). Since produced water contains highly variable organic hydrocarbon concentrations, the effect of initial BTEX concentrations on these nonequilibrium sorption parameters was investigated in batch experiments.

The nonequilibrium sorption conceptual model was investigated through batch experiments with monolayer SMZ. These studies also tested the experimental procedure's accuracy because three tests with identical experimental conditions were conducted. Finally, the monolayer batch experiments tested the sorption capacity of monolayer zeolite versus bilayer zeolite.

The nonequilibrium sorption parameters determined from the batch experiments were used to parameterize a chemical nonequilibrium transport model. The transport

model predictions were compared to column experiment results. Multiple influent concentrations were studied in order to test the nonequilibrium transport model's sensitivity to this variable.

The following manuscript entitled "Nonequilibrium Sorption of Volatile Petroleum Hydrocarbons by a Surfactant-Modified Zeolite" was prepared for submission to a professional journal. The article presents the introduction, methods, results, and conclusions of the research described above.

The appendices contain data from the batch, tritium, and column experiments, as well as discussion and results for unreported topics.

MANUSCRIPT:

NONEQUILIBRIUM SORPTION OF VOLATILE PETROLEUM HYDROCARBONS BY SURFACTANT-MODIFIED ZEOLITE

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The sorption process significantly affects the transport of reactive solutes through geologic media. Nonequilibrium sorption complicates breakthrough curve (BTC) predictions because early-time breakthrough and extended tailing occur. These conditions have adversely affected the accuracy of BTC predictions of volatile petroleum hydrocarbons—specifically benzene, toluene, ethylbenzene, and xylenes (BTEX)—through surfactant-modified zeolite (SMZ) columns.

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nonequilibrium model provided reasonable agreement for each constituent's transport behavior. On average, R values fitted to the transport results were three times those calculated from the batch-derived K_ds. Aqueous phase surfactant monomers are present in SMZ batch systems due to surfactant wash-off, but are constantly flushed from transport systems. Consequently, the BTEX solubility might increase in the batch systems, producing lower K_d values in SMZ/BTEX batch systems than transport systems.

1. INTRODUCTION

Water brought to the earth's surface during the production of oil and gas (produced water) represents a significant waste stream within the United States and the single largest waste stream for the oil and gas industries. Within the United States, approximately 18-21 billion barrels (2.8-3.3 billion m^3) of produced water are annually brought to the ground surface during oil and gas recovery (API, 2000; Sirivedhin and Dallbauman, 2004). Over the lifetime of an individual production well, approximately 10 barrels of water will be produced for every barrel of oil or gas. Since produced water contains high total dissolved solids, heavy metals, organic constituents, radionuclides, and chemicals added during the production process (Stephenson, 1992), approximately 92% of onshore produced water goes through a preliminary oil separation treatment process and is reinjected into the subsurface (API, 2000). Portions of this water maintain backpressures within the producing formations; however, large amounts of wastewater are pumped into surrounding formations.

Because large portions of the western United States are experiencing water shortages, beneficial use of produced water has been widely considered, and numerous produced water treatment technologies have been proposed (see Altare et al., 2007 and Ranck et al., 2005 for reviews). Since organic constituents foul filtration and membrane treatment systems, organic removal is necessary before reversed osmosis/ultrafiltration methods can be successfully applied to produced waters. According to the American Petroleum Institute (API, 2002), volatile one-ring aromatic hydrocarbons—benzene, toluene, ethylbenzene, and xylenes (BTEX)—and low molecular-weight saturated

hydrocarbons are the most abundant petroleum hydrocarbons within produced waters. Total BTEX concentrations in produced waters have been measured up to 578 mg L^{-1} (API, 2002). Benzene, a Class A carcinogen, is usually the most abundant BTEX constituent within produced waters. Benzene concentrations in produced waters have been measured up to 7,000 times the benzene maximum contaminant level (MCL) of 5 μg L^{-1} for drinking water under the U.S. Environmental Protection Agency's National Primary Drinking Water Regulations (EPA, 2003).

Natural zeolites are hydrated aluminosilicate minerals and have rigid, cage-like crystal structures. They are characterized by high negative surface charges and high surface areas and, consequently, have high total and external cation exchange capacities (CEC). Many natural zeolites are mined as aggregates that can be crushed to any desired particle size. This characteristic, combined with their high porosity and rigid structure, make natural zeolites suitable for use as packed-bed sorbents.

The positive head groups of cationic surfactant molecules, for example hexadecyltrimethylammonium (HDTMA), are strongly attracted to the zeolite's negative surface and readily exchange for the original inorganic counterions. A stable surfactant monolayer forms on the zeolite surface, with hydrophobic tail groups exposed to the environment. When the aqueous surfactant concentration approaches the critical micelle concentration, admicelles are formed on the zeolite surface. Monolayer, bilayer, or patchy bilayer surfactant coverage is produced depending upon surfactant concentrations and the surfactant counterion (Li and Bowman, 1997; Sullivan et al., 1998). In this paper, we will use the term "monolayer" to refer to zeolite loaded to or below its external CEC. At this surfactant loading, the zeolite primarily has monolayer coverage but also

may exhibit patchy bilayer coverage. We will use the term "bilayer" to indicate a surfactant loading beyond that required to satisfy the external CEC of the zeolite. At this surfactant loading, the zeolite exhibits monolayer, patchy bilayer, and full bilayer coverage (Figure 1). Nonpolar organic solutes, such as BTEX, have an affinity for the hydrophobic surfactant tail group region formed on the SMZ.

Neel and Bowman (1992) examined the sorption of benzene, toluene, and *para*-xylene (BTX) by SMZ. They reported high sorption affinities, with SMZ distribution coefficients approximately 30 – 45 times those of natural zeolite. Based on linear isotherms, no competition between multiple constituents, and a strong correlation between BTEX sorption and octanol-water partitioning coefficients (K_{ow}), Neel and Bowman concluded that the sorption of BTX onto SMZ occurred primarily via a partitioning mechanism. Neel (1992) and Huddleston (1990) both showed that zeolites modified with long-chain alkyl quaternary amines (cationic surfactants with long tail groups) have the highest organic sorption affinities. Sorption equilibrium in batch systems also occur in less than twenty-four hours (Huddleston, 1990).

Ranck *et al*. (2005) studied the transport of BTEX through SMZ in laboratory and field experiments. Ranck *et al*. (2005) reported no statistically significant loss of sorption capacity over ten sorption/regeneration cycles (approximately 4500 PV). Altare *et al.* (2007) also investigated the long-term stability of SMZ in laboratory columns during extended treatment times. A weakly decreasing trend in sorption capacity over fifty sorption and regeneration cycles indicated that minimal surfactant washed off the SMZ during the transport experiments. Because SMZ was fully regenerated by simply blowing air through the columns, both studies concluded that SMZ presented an effective and

regenerable medium to remove BTEX from produced waters (Altare et al., 2007; Ranck et al., 2005). A pilot field test was also conducted in order to determine the suitability of the SMZ treatment system at larger scales (Katz et al., 2006). Continuous treatment successfully removed BTEX from produced water, and a vapor phase bioreactor (VPB) effectively removed BTEX from the off gas during the regeneration cycle, with carbon dioxide and water as the main byproducts.

Even though BTEX sorption onto SMZ is a rapid partitioning process (Neel, 1992), transport models assuming instantaneous sorption inadequately describe BTEX transport through packed beds of SMZ (Ranck et al., 2005). However, equilibrium models adequately describe the transport of tritium—a nonreactive solute—through SMZ (Altare et al., 2007; Ranck et al., 2005). As a result, the nonequilibrium transport of BTEX is apparently explained by chemical, or sorption-related, nonequilibrium.

The purpose of this research was to investigate the nonequilibrium sorption of BTEX by SMZ and to improve predictions of BTEX transport through SMZ. We began with the conceptual model shown in Figure 1. Monolayer SMZ sites allow instantaneous sorption because BTEX molecules immediately partition into the hydrophobic surfactant tail groups. However, BTEX molecules are kinetically sorbed on bilayer sites because the solutes must penetrate the external surfactant's hydrophilic head groups before partitioning into the hydrophobic region (Pignatello and Xing, 1996). Consequently, BTEX molecules are sorbed in the two domains (equilibrium and kinetic) in parallel and represent monolayer and patchy bilayer surfactant coverage on the bilayer SMZ, respectively. We conducted batch experiments with monolayer and bilayer SMZ in order

to obtain kinetic sorption parameters. Since produced water contains highly variable BTEX concentrations, we investigated competition and concentration effects on kinetic sorption parameters. The nonequilibrium sorption parameters obtained from bilayer SMZ batch experiments were used to parameterize a nonequilibrium transport model. We also conducted column experiments to determine the prediction capabilities of the nonequilibrium model. The sensitivity of model predictions to the batch-derived transport parameters was also determined.

2. MATERIALS AND METHODS

2.1. Surfactant-Modified Zeolite

The zeolite used in these studies was obtained from the St. Cloud mine located near Truth or Consequences, New Mexico. It is a natural clinoptilolite-rich tuff, with a mineral composition of 74% clinoptilolite, 10% quartz/cristobalite, 5% smectite, 10% feldspar, and 1% illite. The clinoptilolite's internal cation exchange capacity is 800 meq kg^{-1}, and the external CEC is 90-100 meq kg^{-1}. The St. Cloud zeolite's external surface area is approximately 15.7 $m^2 g^{-1}$ (Bowman et al., 2000). The clinoptilolite was crushed to 14-40 mesh size (1.4 to 0.4 mm diameter) for this research.

The bilayer SMZ used in batch and column tests was mass-produced at the St. Cloud mine and had a HDTMA-Cl loading of 180 mmol kg^{-1} of zeolite (Bowman et al., 2001). Monolayer SMZ with a surfactant loading of 77 mmol kg^{-1} of zeolite was prepared by the following procedure. Approximately 525 g of raw zeolite was packed into a 30-cm long, 5-cm diameter cast acrylic column (Soil Measurement Systems, LLC, Tucson, AZ). After running carbon dioxide through the column for four hours to remove air, approximately 2000 ml of 20-mmol L^{-1} HDTMA-Cl (Aldrich, Milwaukee, WI) water (Milli-Q, Millipore, Billerica, MA) was circulated through the column at 5 ml min^{-1} with a peristaltic pump for 10 days to allow equilibration to a monolayer configuration. Effluent samples were taken at two-day intervals to monitor the zeolite sorption of HDTMA. A constant effluent concentration of 0.03 mmol L^{-1} was observed after four days. Following equilibration, the monolayer SMZ was removed from the column and allowed to air dry. Electrophoretic mobility analyses showed a net negative charge for

the monolayer zeolite, indicating that the final surfactant loading was less than the external CEC and that coverage was less than a complete monolayer.

2.2. Kinetic Batch Experiments

All BTEX solutions used in batch and column experiments were prepared in a 0.22-mol L^{-1} NaCl solution, simulating the inorganic salt composition of San Juan Basin produced waters (Altare et al., 2007). Batch experiments, prepared in triplicate with appropriate blanks, were conducted as follows. Three grams of SMZ was added to an 11-mL glass headspace vial. Approximately 6 ml of 0.22-mol L^{-1} NaCl solution was also added to the headspace vial. After placing (not crimping) a polytetrafluoroethylene (PTFE)-lined butyl septum on the vial, the vial was gently shaken and allowed to sit overnight to promote saturation of the SMZ by the NaCl solution. The vial was then completely filled with 0.22-mol L^{-1} NaCl solution. Ten microliters of concentrated BTEX solution in methanol was injected into the vial below the air-water interface, and the vial was immediately capped and crimped (procedure adapted from Kolb and Ettre, 1997). The vial was placed on an end-over-end shaker and rotated for a period of 0.5 to 90 min at 9 rpm. The vial was then centrifuged for 2 minutes, and 3 mL of the supernatant solution was transferred into a separate 11-mL glass headspace vial using a rapid open-vial transfer technique (Fuierer, 2001). All procedures were carried out at room temperature (23 ± 2 ^{o}C). The solution was analyzed for aqueous BTEX concentration by gas chromatography.

Numerous batch tests were performed in order to examine the effects of single versus multiple solutes, initial solute concentrations, and surfactant loading (monolayer

versus bilayer) on BTEX sorption kinetics. Six single-solute (e.g. benzene alone, *m*-xylene alone) kinetic batch experiments were performed using bilayer SMZ. An initial aqueous solute concentration of approximately 0.2 mmol L^{-1} was used for each single-solute experiment.

Twelve multiple-solute tests were conducted with initial concentrations of each constituent ranging from 0.05 mmol L^{-1} to 0.5 mmol L^{-1}. For each multiple-solute test, all BTEX constituents were included except for *p*-xylene. *p*-Xylene was not included because it co-elutes with *m*-xylene during the GC analysis. The twelve tests were broken into two subgroups: 1) Four multiple-solute tests with the same initial aqueous concentration for all BTEX constituents (e.g. all constituents at 0.05 mmol L^{-1}); 2) Eight tests with the same initial concentration for four BTEX constituents while the initial concentration of one constituent varied (e.g., benzene, toluene, *m*-xylene, and *o*-xylene at 0.2 mmol L^{-1}, ethylbenzene at 0.35 mmol L^{-1}). These tests investigated the sensitivity of concentration variations of individual constituents on benzene nonequilibrium sorption parameters. For these eight multiple-solute tests, the initial aqueous concentration of benzene was always 0.2 mmol L^{-1}.

A monolayer SMZ, multiple-solute batch test with an initial aqueous concentration of each solute equaling 0.1mmol L^{-1} (total BTEX equaled 0.5 mmol L^{-1}) was replicated three times.

2.3. Column Experiments

Bilayer SMZ was packed into duplicate 11-cm long, 2.5-cm diameter glass columns (Omnifit, Boonton, NJ) to a bulk density of 0.94 g cm^{-3} for BTEX transport

experiments. The columns contained one fixed end piece and one adjustable end piece (both Teflon) in order to eliminate voids. Both end pieces contained removable 100-μm frits (Aldrich, Milwaukee, WI).

Carbon dioxide was passed through each column for 4 hours to displace air and speed saturation. A 0.22-mol L^{-1} NaCl solution was passed through each column using a Model 510 HPLC pump (Waters Corp., Milford, MA) at 8 mL min^{-1} (specific discharge of 1.6 cm min^{-1}), conditions shown to exhibit nonequilibrium BTEX sorption (Altare et al., 2007; Ranck et al., 2005). Tritium tracer tests were conducted with each column in order to determine the hydraulic properties. After column saturation and steady flow conditions were achieved, a 2-pore volume (PV) slug of tritiated water was injected into the column at the same 8 mL min^{-1} flow rate, followed by tritium-free solution for an additional 5 PV. Effluent samples were collected every 0.5 min in 10-mL glass vials using a Retriever II fraction collector (ISCO Inc., Lincoln, NE). One milliliter of each sample was added to 5 mL of scintillation cocktail (ICN Biomedicals, Irvine, CA) in a 7-mL plastic scintillation vial. Samples were gently shaken and tritium was analyzed using a Model LS6500 liquid scintillation counter (Beckman Coulter Inc., Fullerton, CA).

Following the tritium test, a step input of BTEX at a total concentration of 0.60 mmol L^{-1} (approximately 0.12 mmol L^{-1} each of benzene, toluene, ethylbenzene, *m*-xylene, and *o*-xylene) was introduced into the duplicate columns. The influent was held in a 16-L PTFE gas sampling bag (Alltech, Deerfield, IL) to minimize BTEX volatilization losses. Influent samples were taken at 2-h intervals, while effluent samples were taken every 10 min for the first 80 min and at 20-min intervals for the remainder of each experiment. Approximately 250 PV of BTEX solution passed through each column.

The entire process was repeated with freshly packed bilayer SMZ columns and total BTEX concentrations of 0.75 and 0.9 mmol L^{-1}.

2.4. Analytical Methods

All BTEX samples were analyzed by gas chromatography. Samples were loaded into a Model 7694 headspace sampler attached to a Model 5890 GC (Hewlett Packard, Palo Alto, CA). The operating conditions for the headspace sampler were: 70 ^{o}C oven temperature, 90 ^{o}C transfer line temperature, 80 ^{o}C loop temperature, 8.3-min GC cycle time, 3.0-min vial equilibration time, 0.2-min pressurization time, 1.0-min loop fill time, 0.7-min loop equilibration time, and 0.07-min injection time. The operating conditions for the GC were: 35-mL min^{-1} carrier gas (He) flow rate, 40-ml min^{-1} split gas (He) flow rate, 55 ^{o}C oven temperature, 210 ^{o}C injector temperature, and 240 ^{o}C detector temperature. The BTEX compounds were separated using a 10-m long x 0.53-mm diameter x 2.65-μm film thickness HP-5 column and detected with a flame ionization detector. Complete calibration curves—five standards encompassing typical experimental concentrations (0.05, 0.1, 0.2, 0.3, and 0.4 mmol L^{-1})—were prepared prior to and after each experiment's set of 56 samples. In addition, calibration curves with three standards (0.1, 0.2, and 0.3 mmol L^{-1}) were run after every 10-12 samples.

High-performance liquid chromatography (HPLC) was used to analyze HDTMA, following the method of Li and Bowman (1997).

2.5. Data Analysis

Two bicontinuum models, physical (two-region) and chemical (two-site) nonequilibrium, have been widely used to explain nonequilibrium processes. Two-region nonequilibrium occurs between mobile and immobile water zones. Consequently, both sorbing and non-sorbing constituents experience physical nonequilibrium (Gamerdinger et al., 1991). Two-site nonequilibrium results from kinetic limitations during the sorption process (Brusseau and Rao, 1989). Only sorbing solutes experience chemical nonequilibrium. The sorption process is considered to occur in two domains; one domain that allows instantaneous sorption and one domain where sorption is rate-limited.

Since tritium (a non-sorbing solute) transport through SMZ is accurately explained by equilibrium models (Altare et al., 2007), the two-site linear bicontinuum model developed by Selim et al. (1976) was used to explain BTEX transport. This model assumes linear isotherms and first-order mass transfer into the rate-limited domain. Sorption is described by the following expressions (Larsen et al., 1992):

$$S_1 = FK_d C_{aq} \tag{1}$$

$$\frac{dS_2}{dt} = k_2\left[(1-F)K_d C_{aq} - S_2\right] \tag{2}$$

where S_1 represents solute sorbed on sites exhibiting instantaneous sorption (M M^{-1}), S_2 represents solute sorbed on sites exhibiting kinetic/ rate-limited sorption (M M^{-1}), F equals the fraction of instantaneous sorption sites, K_d is the distribution coefficient (L^3 M^{-1}), C_{aq} is the solute's aqueous concentration (M L^{-3}), and k_2 is the first-order kinetic rate coefficient for rate-limited sorption (T^{-1}).

Values of K_d were estimated from the equilibrium data of the batch experiments, while k_2 and F were fit to kinetic batch-experiment data using a least sums-of-squares

method. Similar to previous research (Connaughton et al., 1993; Farrell and Reinhard, 1994; Harmon and Roberts, 1994), early investigation of the bicontinuum model fits to batch data revealed that the single rate coefficient did not fully describe the entire kinetic portion of the sorption curve. Consequently, the fitting algorithm placed a lower weighting on early time data in order to obtain a k_2 estimation based on the kinetic sorption curve as it approached equilibrium. These data provide a more accurate representation of k_2 in our system. The values of K_d, k_2, and F were used to parameterize a nonequilibrium transport model. The following equations describe one-dimensional transport of constituents subject to nonequilibrium chemical sorption in a homogeneous porous medium (Brusseau and Rao, 1991):

$$\beta R\frac{\partial C^*}{\partial p}+(1-\beta)R\frac{\partial S^*}{\partial p}=\frac{1}{P}\frac{\partial^2 C^*}{\partial X^2}-\frac{\partial C^*}{\partial X} \tag{3}$$

$$(1-\beta)R\frac{\partial S^*}{\partial p}=\omega\left(C^*-S^*\right) \tag{4}$$

where:

$$C^*=\frac{C_{aq}}{C_o} \tag{5}$$

$$S^*=\frac{S_2}{(1-F)K_dC_o} \tag{6}$$

$$R=1+\frac{\rho}{\theta}K_d \tag{7}$$

$$P=\frac{vl}{D} \tag{8}$$

$$p=\frac{vt}{l} \tag{9}$$

$$X = \frac{x}{l} \tag{10}$$

$$\beta = \frac{\left(1 + F\left(\rho / \theta\right) K_d\right)}{R} \tag{11}$$

$$\omega = k_2 (1 - \beta) \frac{lR}{v} \tag{12}$$

and C_o is the influent aqueous concentration, p is dimensionless time (pore volumes), R is the retardation factor (-), P is the Peclet number (-), *l* is the length of the column (L), D is the dispersion coefficient ($L^2\ T^{-1}$), *v* is the linear pore water velocity ($L\ T^{-1}$), x is distance (L), ρ is the medium's bulk density ($M\ L^{-3}$), θ is the volumetric water content (-), β is the fraction of instantaneous sorption (-), and ω is the Damkohler number (-), which represents the ratio of hydrodynamic residence time to characteristic sorption time. The optimization program CXTFIT version 2.1 (Toride et al., 1999) was used with Eqs. (3) and (4) in the forward mode to predict solute transport from K_d, k_2, and F values determined in batch studies, and in an inverse mode to estimate these parameters from observed column results.

3. RESULTS AND DISCUSSION

3.1. Bilayer Batch Tests

Six single-solute batch experiments (approximately 0.2 mmol L^{-1} initial concentration) were run, and the bicontinuum model was fit to the data. In order to determine the effect of multiple-solutes, these single-solute results were compared to the multiple-solute results with similar individual initial BTEX concentrations. Figure 2 presents the bicontinuum fit to ethylbenzene single-solute and the corresponding multiple-solute data. The presence of multiple solutes had minimal effect on the ethylbenzene K_d (5 % difference), but noticeably reduced the values of k_2 (30 % decrease) and F (65 % decrease). For all six constituents, sorption equilibrium was reached within 0.5 hr. The bicontinuum model fit all batch experimental data well, with all r^2 values greater than 0.90. Figure 3 presents the relationship between the batch K_d and the octanol-water partition coefficient (K_{ow}) for each BTEX compound from the single-solute and multiple-solute tests. Similar to previous findings (Neel, 1992; Bowman et al., 1995), there is a linear relationship between log K_d and log K_{ow}, and the BTEX distribution coefficients are not significantly affected by the presence of multiple constituents. Figure 4 shows the k_2 results from these batch tests. An inverse relationship between the K_{ow} and k_2 of each constituent is seen. Competition or concentration effects are also seen, with a 5 – 35% decrease in rate coefficients in the multiple-solute results. The inverse relationship between k_2 and K_{ow} is consistent with k_2 versus K_d results involving natural sediments and organic solutes (Ball and Roberts, 1991; Brusseau and Rao, 1991; Karickhoff, 1984). Since BTEX diffusion coefficients

decrease and molecular size increases with increasing K_{ow}, k_2 of the more hydrophobic molecules may be limited by their larger molecular sizes and smaller diffusion coefficients.

F results from the multiple-solute and single-solute batch tests are presented in Figure 5. An inverse relationship is also observed between F and K_{ow}, and F decreased by 10 – 80% during the multiple-solute test.

Twelve additional multiple-solute experiments were run in order to determine concentration effects on the three nonequilibrium sorption parameters. The first set of four experiments contained a concentration of 0.05, 0.10, 0.20, or 0.30 mmol L^{-1} for each of the five constituents (total BTEX concentrations of 0.25, 0.50, 1.00, or 1.50 mmol L^{-1}). Figure 6 shows the concentration effects on K_d. In agreement to the single-solute versus multiple-solute data, initial BTEX concentrations have minimal effects on the K_d of each constituent. Concentration effects on k_2 are presented in Figure 7. As initial aqueous BTEX concentrations increase in the batch systems, the kinetic rate coefficient decreases. Hu and Brusseau (1998) reported that k_2 increased with concentration in batch systems containing natural sediment and 2,4-dichlorophenoxyacetic acid. Since diffusive processes control rate-limited sorption, Hu and Brusseau suggested that increased concentration gradients would increase the rate of sorption. However, similar to our results, Gamerdinger et al. (1991) reported an inverse relationship between concentration and k_2 in batch experiments containing natural sediments and herbicides. Physical and/or chemical interactions between the constituents and the sorbent could cause the decrease in k_2 as concentration increases. Figure 8 shows concentration effects on F. According to the conceptual and numerical models, F should be independent of variations in initial

concentration. However, based on the multiple-solute results, F decreases as concentration increases. Because the determination of F is extremely sensitive to early-time data and a rapid partitioning process is present in the BTEX/SMZ system, these variations in F might be attributed to experimental limitations. Furthermore, a dependence of F on initial concentration is also seen in desorption processes and is not fully explained (Farrell and Reinhard, 1994; Grathwohl and Reinhard, 1993; Pignatello, 1990).

Eight additional multiple-solute batch experiments were run. Because benzene represents the first constituent to break through in transport experiments, the primary purpose of these eight tests was determining the sensitivity of benzene sorption kinetics to variations in individual BTEX constituent initial concentration. Benzene K_d results are seen in Figure 9. Similar to previous results, concentration variations of individual constituents do not significantly affect the K_d of benzene. Consequently, no individual constituent (i.e. toluene, *m*-xylene) is more influential on the benzene K_d than the other BTEX constituents. Figure 10 displays benzene k_2 results from these eight experiments. Increasing each constituent's concentration slightly lowered (<10%) the k_2 of benzene. Even though the benzene k_2 is affected by other constituent's initial concentration, it does not exhibit consistent sensitivity variations between individual constituents. Figure 11 presents the benzene F results from these experiments. An overall decrease in the F of benzene is observed as each constituent's concentration increases. The parabolic nature of the benzene F data is similar to the ethylbenzene, *m*-xylene, and *o*-xylene results seen in Figure 8. Similar to the k_2 results, no individual constituent consistently influences the F of benzene greater or less than any other constituent. Consequently, the k_2 and F

parameters of benzene, and the other BTEX constituents, are apparently affected by the total BTEX initial aqueous concentration.

Based upon the results from the multiple-solute, bilayer SMZ batch experiments, relationships between batch-determined nonequilibrium sorption parameters and total initial BTEX concentrations were developed (Table I). Since K_d does not vary significantly over the tested concentration ranges, Table I presents the average distribution coefficient for each constituent. Linear regressions accurately describe k_2 as a function of total concentration (r^2 greater than 0.89 for all constituents except toluene). Figure 12 shows the linear regression and the *m*-xylene multiple-solute batch test data. Since the slope of the linear regressions decreases with increasing hydrophobicity (Table I), concentration variations within batch systems have the greatest effect on the least hydrophobic constituent, benzene.

F shows a decreasing trend with increasing total BTEX concentrations from 0.2 to 1 mmol L^{-1}. However, when initial BTEX concentrations were greater than 1 mmol L^{-1}, an increasing F is observed with increasing concentration. As previously discussed, these variations in F might result from experimental (early-time sampling) limitations. The data was fit with a 2^{nd}-order polynomial, with reasonable fits for all of the constituents (Table I). The polynomial fit of *m*-xylene to the multiple-solute batch test data is seen in Figure 13.

The relationships in Table I were used with Eqs. (7), (11), and (12) to calculate input parameters for the nonequilibrium transport model for various column conditions (Table II).

3.2. Monolayer Kinetic Batch Tests

A multiple-solute, monolayer batch test was replicated three times. The initial concentration of each BTEX compound was 0.1 mmol L^{-1} (total BTEX concentration of 0.5 mmol L^{-1}). The kinetic sorption results were compared to the identical bilayer, multiple-solute test in order to test our conceptual model, and amongst themselves to test each parameters sensitivity to the experimental procedure. According to the conceptual model, loading the zeolite to a complete surfactant monolayer should have minimal effects on K_d and k_2, but should produce a significant increase in F.

Figure 14 shows that log K_d varies linearly with log K_{ow} for BTEX sorption on monolayer SMZ, with K_d values approximately 20% lower than the bilayer SMZ K_d values. The zeolite was loaded with 77 mmol kg^{-1} of surfactant for the monolayer experiments. Since the external CEC of the St. Cloud zeolite is 90 – 100 mmol kg^{-1}, approximately 80% monolayer coverage of the zeolite was achieved. Li and Bowman (1998) reported a linear decrease in K_d for perchloroethylene sorption by SMZ when surfactant loading was below full monolayer coverage; and a constant K_d above monolayer coverage. The average K_d values from the monolayer batch tests were divided by 0.8 and compared to the bilayer K_d results (Table III). In agreement to Li and Bowman's (1998) results, the adjusted monolayer K_d and bilayer K_d results are nearly identical.

Figure 15 shows the k_2 results from the monolayer and corresponding bilayer batch tests. An inverse relationship between k_2 and K_{ow} is also seen in the monolayer results, similar to the results for bilayer SMZ (see also Figure 4). Since the monolayer SMZ likely contains areas of patchy bilayer (Sullivan et al., 1998; Sullivan et al., 1997),

similar kinetic rate coefficients are expected between monolayer and bilayer results. The k_2 values for monolayer and bilayer systems are similar (Figure 15 and Table III).

The results for F from the monolayer and corresponding bilayer batch tests are presented in Figure 16. F decreases with log K_{ow} for both monolayer and bilayer SMZ. However, F increases from 0.03 – 0.16 for the bilayer system to 0.34 – 0.44 in the monolayer system (Table III). This ~3 to 11 fold increase in F is due to the significantly greater fraction of monolayer surfactant coverage, and the resultant higher proportion of the surface subject to instantaneous sorption.

Parameter sensitivity to the monolayer experimental procedure was also examined from the three replicate monolayer results. Table III presents the average nonequilibrium sorption parameter results and 95% confidence intervals (2σ) from the three replicate monolayer tests. A normal distribution was assumed for the 95% confidence intervals. The bilayer results in Table III present the 0.5 mmol L^{-1} total BTEX multiple-solute batch test parameters. K_d shows strongly reproducible results based on the three replicate results; therefore, K_d is fairly insensitive to slight variations (e.g. time, temperature, human) in the experimental procedure. The 95% confidence intervals of F also indicate that reproducible F results are obtainable. According to Table III, k_2 represents the parameter with the most variability during the replicate monolayer tests. Furthermore, k_2 is also not applicable for the entire kinetic portion of the batch sorption data. For the single-solute results, a 25 – 35% decrease in k_2 was produced after applying the previously discussed modification to the k_2 fitting algorithm. Additionally, k_2 was sensitive to input parameter precision (e.g. initial concentration) for the bicontinuum model. Therefore, not only does k_2 show sensitivity to the experimental procedure, but it

is also sensitive to the data fitting algorithm and input parameters of the numerical model. Consequently, the variations in k_2 between the monolayer and bilayer tests (Figure 15) might result from k_2 imprecision (experimental shortcomings).

3.3. Column Experiments

Tritium transport experiments were run in order to obtain the dispersion coefficient for each column. Representative tritium results from column 2B are seen in Figure 17. CXTFIT version 2.1 (Toride et al., 1999) was used to inversely fit the 1-dimesional advection dispersion, physical equilibrium equation to the tritium breakthrough curve data:

$$R\frac{\partial C^*}{\partial p} = \frac{1}{P}\frac{\partial^2 C^*}{\partial X^2} - \frac{\partial C^*}{\partial X} \tag{13}$$

Flux-averaged effluent concentrations were assumed along with a 3rd-type upper boundary condition and a semi-infinite lower boundary condition. Three parameters were required for the inverse solution: v, R, and D. R and D were calculated from the model fit, while v was specified to the effluent discharge rate. The tritium modeling results and the column characteristics are seen in Table IV. The physical equilibrium model provides a very good fit to the tritium breakthrough data, with all six r^2 values greater than 0.988. Therefore, as seen in previous research (Altare et al., 2007), zones of immobile water (physical nonequilibrium) are not significant in the SMZ columns under these flow conditions.

Figure 18 shows the column 2B breakthrough curves of the BTEX compounds. The compounds break through the column in order of increasing hydrophobicity. The breakthrough curve (BTC) of each constituent was fit with chemical nonequilibrium and

equilibrium models, and the nonequilibrium model, with batch-determined input parameters (Table II), was used to predict BTEX transport. Figure 19 presents benzene effluent data from column 2B, along with the predicted nonequilibrium model and the inversely fit equilibrium and nonequilibrium models. Similar to previous research (Altare et al., 2007), the equilibrium fit model (v and D fixed; R fit) does not adequately describe benzene's early breakthrough and slow approach to complete breakthrough. The nonequilibrium prediction (v, D, R, β, and ω all fixed) also underestimates the time required for complete benzene breakthrough and over-predicts the amount of early-time breakthrough. The nonequilibrium model fit (v and D fixed; R, β, and ω fit) adequately describes the entire benzene BTC of column 2B. Consistent trends between the predicted versus fit models and equilibrium versus nonequilibrium models were observed for all six sets of benzene transport data.

An accurate prediction of the benzene BTC, especially early-time data, is vital because it elutes first from SMZ columns. Therefore, proper regeneration schemes (i.e. timing, length) depend on the early-time breakthrough of benzene. Even though the nonequilibrium model inadequately predicted benzene transport, it provides a conservative estimation of the benzene early-time breakthrough.

Figure 20 shows *m*-xylene transport data from column 2B and the nonequilibrium model prediction, and equilibrium and chemical nonequilibrium model fits. Similar to the benzene results (Figure 19), the equilibrium model does not fit the early-time breakthrough or extended tailing of *m*-xylene. The nonequilibrium prediction model vastly underestimates the time required for the entire *m*-xylene BTC. The

nonequilibrium model provides a good fit to *m*-xylene BTC data. Similar results were obtained for all of the BTEX compounds in the replicated column experiments.

A comparison of the averaged unknown parameters for the nonequilibrium fit and predicted models is seen in Table V. The Peclet number is identical for all scenarios (values provided in Table II). The fit parameters represent transport-determined values, while the predicted parameters represent batch-determined values. According to Table V, the constituents experienced greater retardation during the transport experiments than predicted from batch experiments. Equation (7) was used to calculate K_d values from the transport experiments. Similar to the batch results, the transport-determined K_d values were not concentration dependent and log K_d was linearly related to log K_{ow}.

The transport-determined K_d values are 1.5 – 3.75 times greater than the batch-determined values. Ranck (2003) reported a similar relationship between batch and column K_d for BTEX sorption on SMZ. Since batch-determined distribution coefficients are typically greater than transport-determined distribution coefficients (Maraqa, 2001 and references therein), a BTEX/SMZ-specific process is producing anomalous results. HDTMA is released from the SMZ when exposed to aqueous solutions (Li et al., 2003). Micellular surfactant solutions are known to increase BTEX solubility (surfactant-enhanced remediation); consequently, HDTMA monomers could also produce an increase in BTEX solubility. In column systems, the surfactant wash-off is constantly flushed from the column; however, a static aqueous phase is present in batch systems. Therefore, higher concentrations of surfactant monomers present in batch systems might increase BTEX solubility and produce lower K_d values for the batch system than the column system.

The Damkohler number (ω) is 2 – 4 times greater for the batch-determined values than the transport-determined values. Since ω represents the residence time divided by the characteristic sorption time, it is inversely proportional to the magnitude of nonequilibrium processes present in contaminant transport systems. According to the transport-determined ω, the magnitude of chemical nonequilibrium is greater in the SMZ columns that predicted by the batch-determined values. The transport-determined k_2 of each constituent was calculated by Eqs. (7), (11), and (12). Transport-determined k_2 values range from 0.2 to 1.56 hr^{-1}, while batch-determined values range from 1.87 to 9.27 hr^{-1}. Similar to the batch results, the transport-determined rate coefficients are constituent dependent (Figure 21). The batch-experiment k_2 results appear to have greater initial concentration sensitivity than transport-experiment results.

Table V also reveals that the batch-determined values for the fraction of instantaneous retardation (β) are 0.2 – 0.7 times the transport-determined values. Equations (7) and (11) were utilized to calculate F; and F ranged from 0.2 to 0.4 for all constituents based on transport experiments, but ranged from 0.02 to 0.2 based on batch experiments. Figure 22 also shows that, contrary to batch results, F determined in transport experiments is relatively insensitive to total BTEX concentrations.

The limitations of individual input parameters on the nonequilibrium model prediction were also investigated. One input parameter (R, β, or ω) was inversely fit to benzene and *m*-xylene transport data while the other two input parameters were fixed with the values determined from the batch experiments. The various model fits to column 2B BTC data of benzene are seen in Figure 23. When β was inversely fit to the transport data (R and ω fixed with batch-determined values), the nonequilibrium model

still underestimated the time for early-time and full breakthrough of benzene. Similar results are seen when ω was inversely fit to the transport data. However, when R was inversely fit to the data (β and ω fixed with batch-determined values), the model adequately described the benzene BTC ($r^2 = 0.990$). Therefore, R is constraining the prediction capabilities of the nonequilibrium transport model, which is relatively insensitive to the values of β and ω in our system. Allowing both β and ω to vary while R was fixed with the batch-determined value did not improve the model's fit (Figure 23).

Figure 24 presents the various models fit inversely to *m*-xylene column 2B transport data. When β or ω (or both together) are fit inversely to the data (R fixed to batch-determined value), the nonequilibrium model immensely underestimates the time for early-time and full breakthrough of *m*-xylene. However, the model describes the m-xylene BTC reasonably well when β and ω are fixed but R is inversely fit ($r^2 = 0.929$). These results suggest that the β and ω values obtained from the batch experiments could provide acceptable predictions to BTEX transport data (with varying initial concentrations) if a better understanding of the transport K_d of each solute was obtained.

4. CONCLUSIONS

The first-order bicontinuum model accurately described the sorption process in kinetic batch experiments containing SMZ and volatile hydrocarbons (specifically BTEX). The K_d of each solute did not show competition effects between single-solute and multiple-solute batch experiments. However, a 5 – 35% decrease in k_2 occurred during the multiple-solute test. F also decreased during the multiple-solute test. Chemical or physical interaction or competition could possibly explain the decrease in k_2; however, F should not decrease based on the conceptual and numerical models. Because BTEX partitioning into SMZ is a rapid process, experimental limitations on early-time sampling might cause the variations in F. Additional batch results show an inverse relationship between k_2 or F and the initial total BTEX concentration over the studied concentration ranges. The K_d of each constituent was not affected by solute competition or concentration variations.

According to the conceptual model, BTEX molecules instantaneously sorb within portions of the SMZ covered by a surfactant monolayer, while bilayer surfactant patches kinetically limit BTEX sorption. The monolayer SMZ kinetic batch-test results were in agreement with the conceptual model. The monolayer K_d results, adjusted for partial coverage, agreed very well with the bilayer K_d results. The kinetic rate coefficient was expected to remain constant in both systems, and only minor variations between the monolayer and bilayer k_2 results were observed. Finally, the significant increase (3 to 10 times) in F seen in the monolayer tests was expected because of the increase in the fraction of surface covered by a monolayer of surfactant.

Because the equilibrium model does not accurately fit the BTEX breakthrough data, nonequilibrium processes are present during BTEX transport through the SMZ columns. The nonequilibrium transport model accurately fit transport data for all BTEX constituents when R, β, and ω were allowed to vary. The nonequilibrium transport model, using batch-determined parameters to calculate R, β, and ω, was unable to accurately predict BTEX breakthrough curves through SMZ columns. Complete effluent breakthrough time of each constituent was significantly underestimated with the model prediction. In addition, prediction accuracy decreased with increasing constituent hydrophobicity.

Investigation of each input parameter for the nonequilibrium prediction revealed the value used for R controlled the prediction capability of the nonequilibrium transport model. Adequate BTC predictions for benzene and *m*-xylene were obtained when using β and ω derived from the batch tests and simply adjusting R. A more accurate estimation of the BTEX distribution coefficients in transport systems would significantly improve the prediction of BTEX transport through SMZ columns.

5. RECOMMENDATIONS FOR FUTURE WORK

Since surfactant wash-off likely causes the variation between distribution coefficients in batch and transport systems, future research needs to determine the effect of aqueous-phase surfactant concentrations on BTEX sorption/solubility. BTEX solubility experiments, with varying surfactant concentrations, should be run in order to qualitatively test this hypothesis. Octanol-water partition tests, with surfactant-containing and surfactant-free water, should also be conducted in order to quantitatively determine surfactant wash-off effects on BTEX sorption. For the surfactant-containing water, bilayer and monolayer SMZ batch experiments (without BTEX included) should be initially completed. Aqueous samples should be taken after 90 minutes of shaking and used for the surfactant-containing water in the octanol-water partition tests. Surfactant wash-off might also affect the BTEX chromatographic analysis. Consequently, chromatographic analysis should be conducted with a constant BTEX aqueous concentration but varying surfactant concentrations.

BTEX distribution coefficients in dynamic systems should also be determined. Recirculation column experiments (similar to "circulation-through" experiments in Maraqa, 2001) should be conducted to complete BTEX breakthrough. Since the BTEX-laden water recirculates through the SMZ column in these experiments, aqueous-phase surfactant conditions in these transport experiments should be similar to batch experiment conditions. Distribution coefficients should be calculated when full BTEX breakthrough conditions are reached to determine if batch-determined K_d values can be replicated in the recirculation dynamic experiments. Flow-through column experiments should also be

conducted in order to improve the prediction capabilities of the nonequilibrium transport model. Step-input column experiments should be run to complete BTEX breakthrough. The column effluent should be collected, and an effluent sample should be taken after full BTEX breakthrough is achieved. The flow-through, transport-determined K_d values should be coupled with the batch-determined F and k_2 values in order to parameterize the nonequilibrium transport prediction model. These experiments would likely determine the role of surfactant wash-off in our systems and improve the prediction capabilities of our nonequilibrium transport model.

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Table I. Batch-determined nonequilibrium sorption parameter relationships used to parameterize the nonequilibrium transport model. Standard deviation for K_d is in parentheses.

Constituent	K_d (L/kg)	k_2 (hr^{-1}) Linear Regression	r^2	F Polynomial Regression	r^2
Benzene	7.5 (0.23)	$-2.14(C_o)+9.71$	0.88	$0.058(C_o)^2-0.158(C_o)+0.234$	0.29
Toluene	17.7 (0.39)	$-1.59(C_o)+5.77$	0.59	$0.068(C_o)^2-0.154(C_o)+0.147$	0.64
Ethylbenzene	35.2 (0.53)	$-1.36(C_o)+3.96$	0.89	$0.085(C_o)^2-0.160(C_o)+0.103$	0.76
M-Xylene	37.4 (0.54)	$-1.37(C_o)+3.74$	0.92	$0.108(C_o)^2-0.196(C_o)+0.102$	0.96
O-Xylene	34.4 (0.58)	$-1.25(C_o)+3.76$	0.89	$0.083(C_o)^2-0.159(C_o)+0.103$	0.86

Table II. Input parameters used to predict nonequilibrium BTEX transport.

Column	Total BTEX C_o (mmol L^{-1})	P	Constituent	R	β	ω
1A	0.62	11.3	Benzene	11.7	0.23	5.2
			Toluene	26.3	0.11	7.8
			Ethylbenzene	51.4	0.06	10.5
			M-xylene	54.6	0.04	10.5
			O-xylene	50.3	0.06	9.8
1B	0.59	10.7	Benzene	12.3	0.23	5.7
			Toluene	27.7	0.11	8.4
			Ethylbenzene	54.1	0.06	11.5
			M-xylene	57.5	0.04	11.5
			O-xylene	52.9	0.06	10.7
2A	0.93	13.3	Benzene	12.5	0.21	5.3
			Toluene	28.2	0.10	7.6
			Ethylbenzene	55.0	0.05	9.9
			M-xylene	58.5	0.03	9.8
			O-xylene	53.9	0.05	9.3
2B	0.89	11.9	Benzene	13.0	0.21	5.3
			Toluene	29.5	0.10	7.7
			Ethylbenzene	57.7	0.05	10.0
			M-xylene	61.3	0.03	9.9
			O-xylene	56.5	0.04	9.5
3A	0.78	6.7	Benzene	12.2	0.22	5.4
			Toluene	27.6	0.10	7.9
			Ethylbenzene	54.0	0.05	10.4
			M-xylene	57.3	0.03	10.4
			O-xylene	52.8	0.05	9.8
3B	0.71	8.1	Benzene	12.0	0.22	5.2
			Toluene	27.2	0.11	7.6
			Ethylbenzene	53.0	0.05	10.2
			M-xylene	56.3	0.04	10.2
			O-xylene	51.9	0.05	9.6

Table III. Monolayer versus bilayer SMZ batch experiment results. For monolayer results, average values are reported with 95% confidence intervals. The multiple-solute, bilayer SMZ experiment with total BTEX C_o equaling 0.5 mmol L^{-1} represents the bilayer results.

	K_d (L kg^{-1})		k_2 (hr^{-1})		F	
Constituent	Monolayer [1]	Bilayer	Monolayer	Bilayer	Monolayer	Bilayer
Benzene	7.3 ± 1.0	7.3	5.74 ± 1.2	8.52	0.42 ± 0.05	0.16
Toluene	16.8 ± 1.0	17.5	4.50 ± 1.0	4.96	0.37 ± 0.03	0.09
Ethylbenzene	34.1 ± 1.9	34.7	4.35 ± 1.2	3.4	0.35 ± 0.03	0.04
M-Xylene	36.2 ± 2.0	37.3	4.26 ± 0.8	2.95	0.34 ± 0.03	0.03
O-Xylene	32.5 ± 1.9	34.4	4.30 ± 1.2	3.19	0.35 ± 0.03	0.04

[1] Experimental monolayer K_d values divided by 0.8 to account for ~80% monolayer coverage (see text).

Table IV. Column characteristics and tritium results from the column experiments.

	Column Characteristics					Tritium Results		
Column	Velocity (cm/min)	Mass Zeolite (g)	Porosity (Vv/Vt)	Bulk Density (g/cm^3)	R	D (cm^2/min)	P (vL/D)	Equil. Fit (r^2)
1A	2.65	47.13	61.0%	0.873	1.17	2.57	11.32	0.996
1B	2.62	50.52	60.9%	0.936	1.15	2.75	10.69	0.989
2A	2.62	50.59	61.0%	0.937	1.1	2.17	13.29	0.988
2B	2.77	49.56	57.0%	0.918	1.15	2.56	11.9	0.999
3A	2.63	48.9	60.2%	0.906	1.17	4.32	6.69	0.988
3B	2.67	47.15	60.2%	0.873	1.2	3.55	8.11	0.991

Table V. Nonequilibrium parameters from predicted model (predicted) and fit model (fit). Table presents average values over the six column runs with standard deviations in parentheses.

	R		β		ω	
Constituent	Predicted	Fit	Predicted	Fit	Predicted	Fit
Benzene	12.29 (0.45)	18.22 (1.64)	0.22 (0.01)	0.31 (0.05)	5.36 (0.17)	2.58 (0.69)
Toluene	27.76 (1.06)	58.27 (10.35)	0.10 (0.01)	0.40 (0.11)	7.83 (0.31)	1.60 (0.81)
Ethylbenzene	54.21 (2.11)	199.00 (23.48)	0.05 (0.01)	0.22 (0.09)	10.41 (0.56)	3.36 (1.10)
M-Xylene	57.58 (2.24)	212.83 (24.30)	0.03 (0.01)	0.23 (0.09)	10.37 (0.61)	3.70 (2.08)
O-Xylene	53.05 (2.06)	187.20 (28.39)	0.05 (0.01)	0.22 (0.05)	9.78 (0.50)	3.28 (0.65)

FIGURE CAPTIONS

Figure 1. Conceptual model of benzene partitioning into surfactant-modified zeolite's hydrophobic tail group.

Figure 2. Kinetics of ethylbenzene sorption to bilayer SMZ. A) ethylbenzene alone (single solute), B) ethylbenzene with equal concentrations of benzene, toluene, *o*-xylene, and *p*-xylene (multiple solute).

Figure 3. Relationship between log K_d and log K_{ow} for BTEX compounds in single-solute and 1.0 mmol L^{-1} total BTEX multiple-solute batch experiments.

Figure 4. Relationships between log k_2 and log K_d for BTEX compounds in single-solute and 1.0 mmol L^{-1} total BTEX multiple-solute batch experiments.

Figure 5. Relationship between F and K_{ow} for BTEX compounds in single-solute and 1.0 mmol L^{-1} total BTEX multiple-solute batch experiments.

Figure 6. Initial concentration effects on BTEX constituent distribution coefficients when all constituents have similar initial aqueous concentrations.

Figure 7. Initial concentration effects on BTEX constituent rate coefficients when all constituents have similar initial aqueous concentrations.

Figure 8. Initial concentration effects on the F of BTEX constituents when all constituents have similar initial aqueous concentrations.

Figure 9. Concentration effects of individual BTEX constituents on the benzene K_d. The initial concentration of benzene was 0.2 mmol L^{-1} for all experiments.

Figure 10. Concentration effects of individual BTEX constituents on the benzene k_2. The initial concentration of benzene was 0.2 mmol L^{-1} for all experiments.

Figure 11. Concentration effects of individual constituents on the benzene F. The initial concentration of benzene was 0.2 mmol L^{-1} for all experiments.

Figure 12. *m*-Xylene kinetic batch-experiment k_2 data fit with a linear regression.

Figure 13. *m*-Xylene kinetic batch-experiment F data fit with a polynomial trend line.

Figure 14. K_d results from three replicate monolayer and corresponding bilayer SMZ batch experiments.

Figure 15. Results for k_2 from three replicate monolayer and corresponding bilayer SMZ batch experiments.

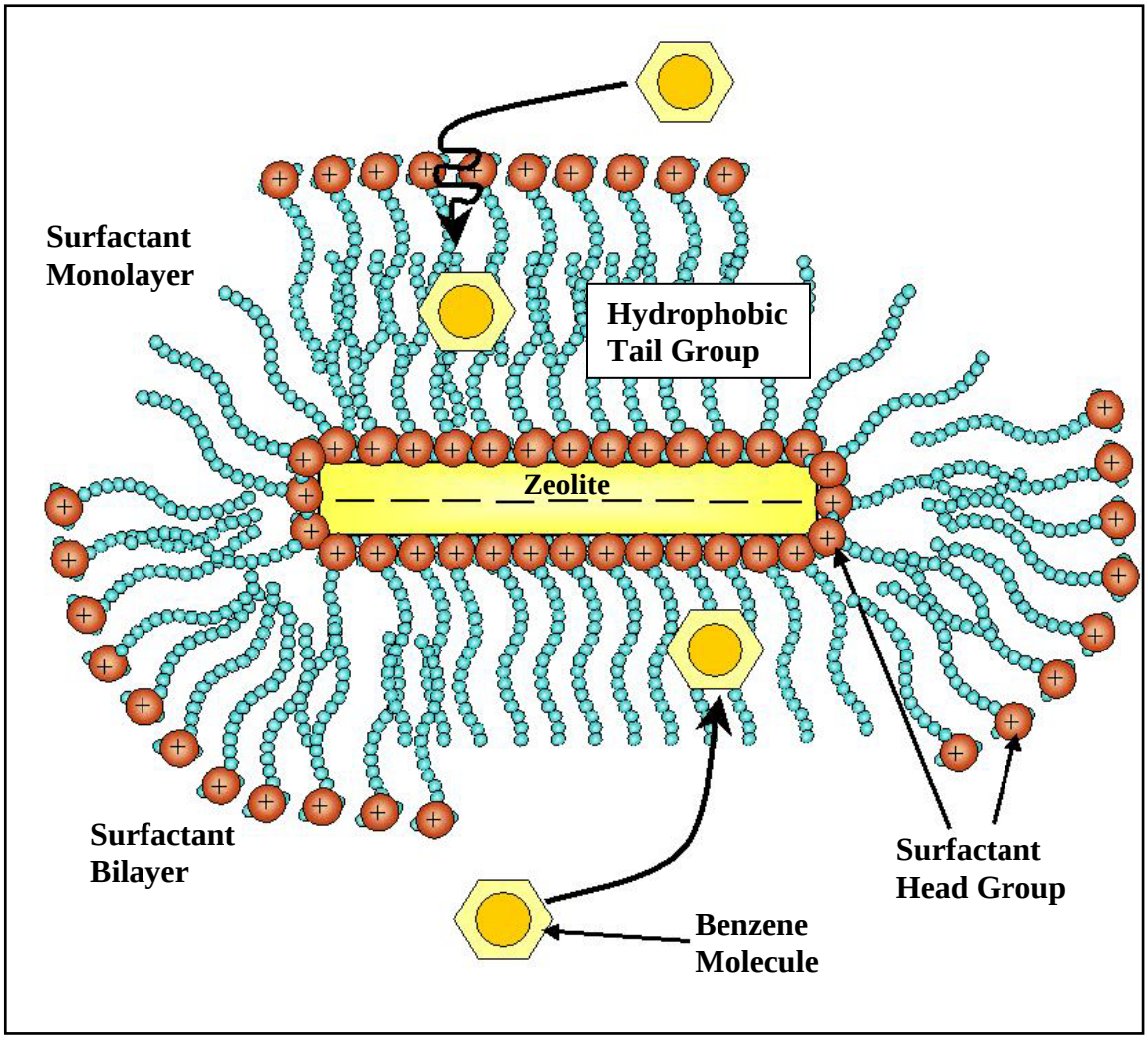

Figure 1. Conceptual model of benzene partitioning into surfactant-modified zeolite's hydrophobic tail group.

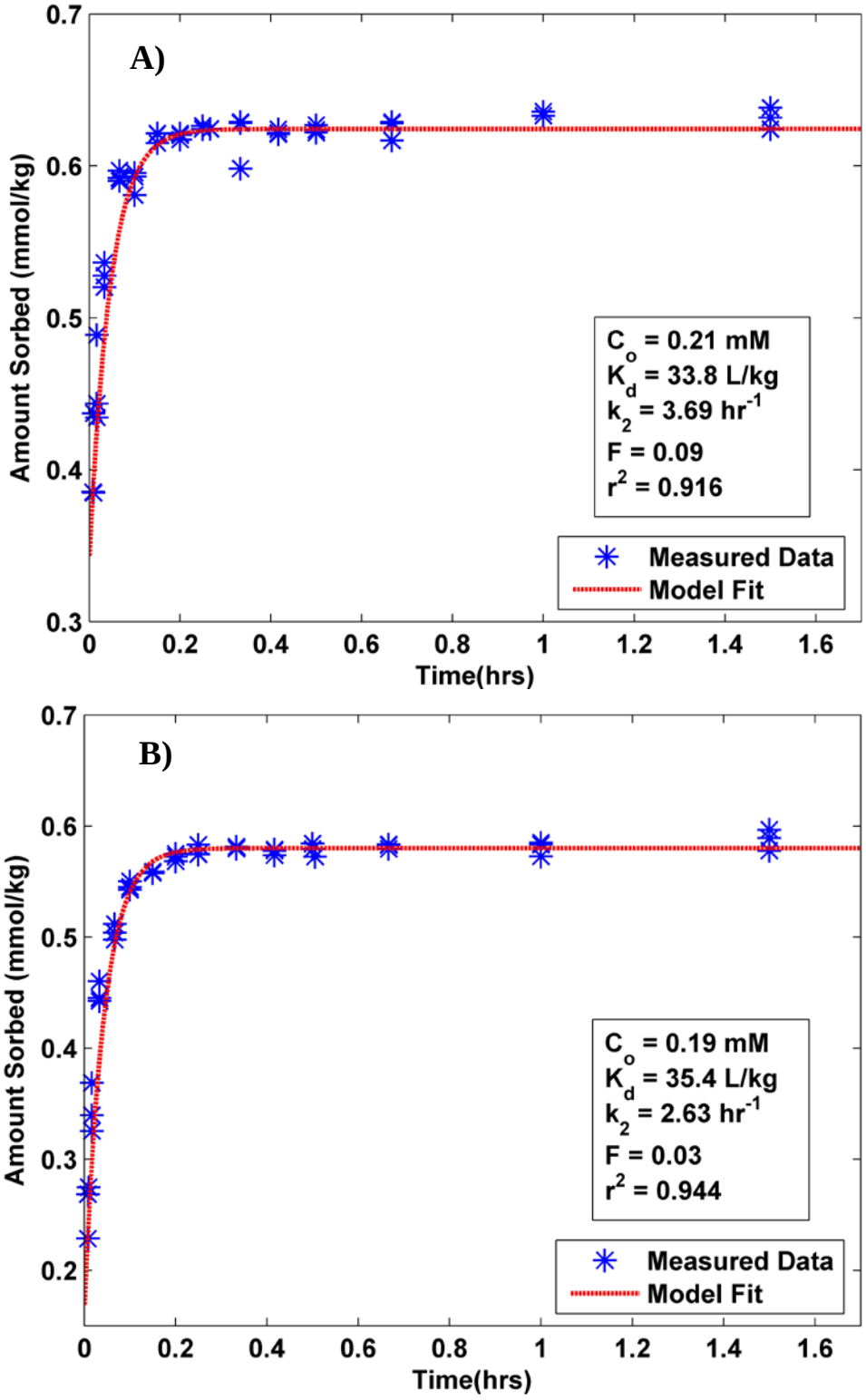

Figure 2. Kinetics of ethylbenzene sorption to bilayer SMZ. A) ethylbenzene alone (single solute), B) ethylbenzene with equal concentrations of benzene, toluene, *o*-xylene, and *p*-xylene (multiple solute).

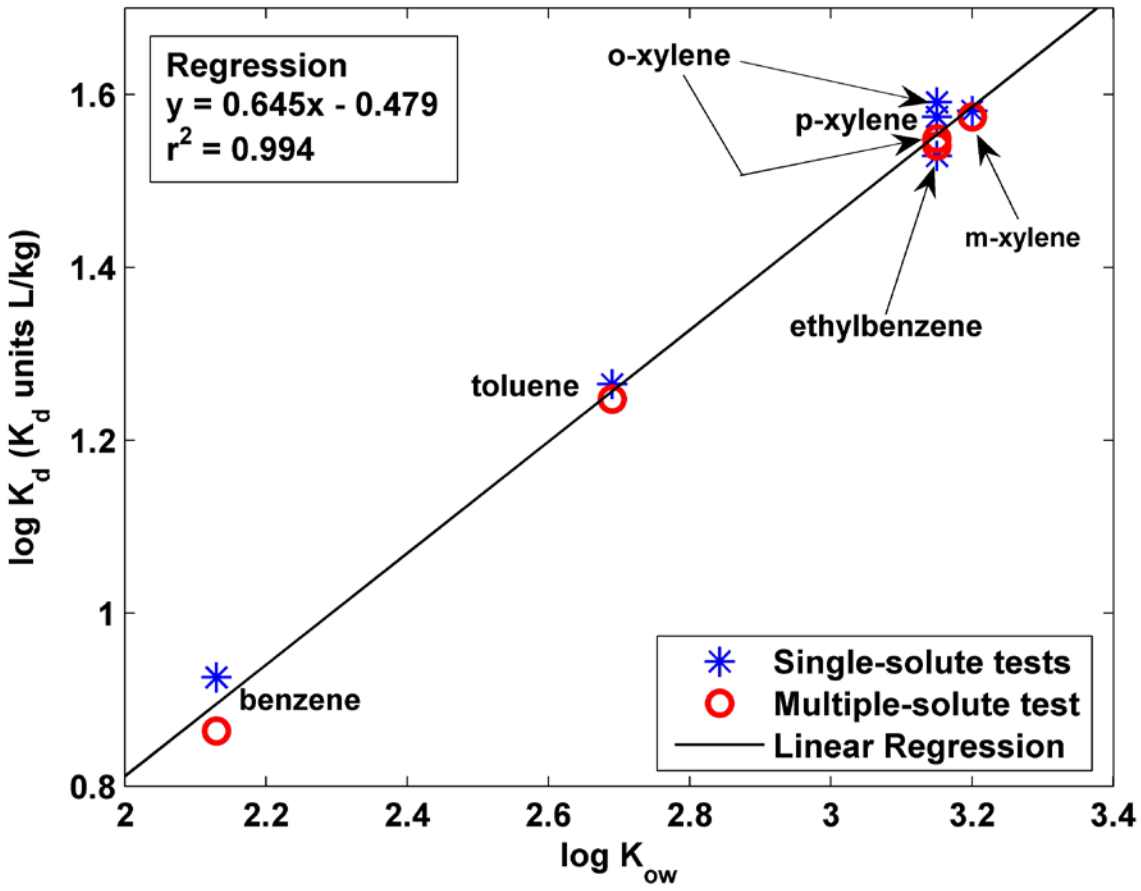

Figure 3. Relationship between log K_d and log K_{ow} for BTEX compounds in single-solute and 1.0 mmol L^{-1} total BTEX multiple-solute batch experiments.

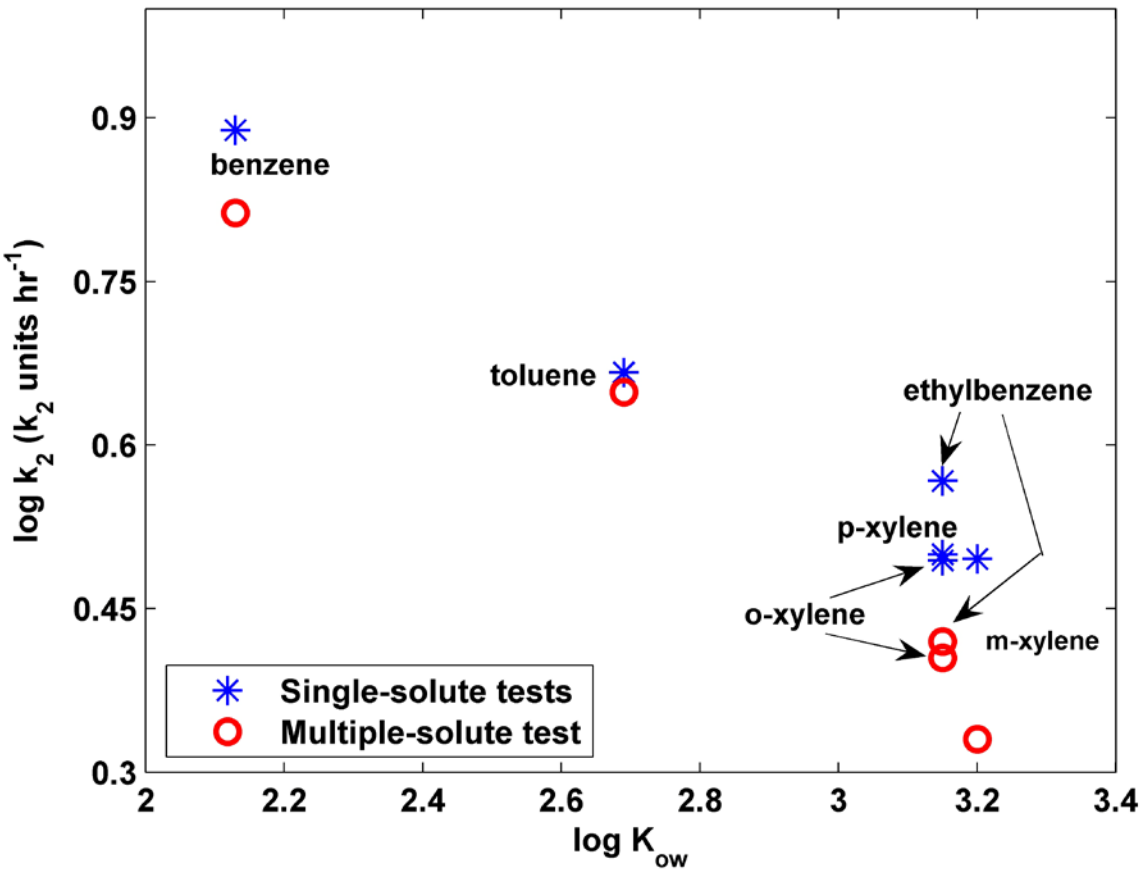

Figure 4. Relationships between log k_2 and log K_d for BTEX compounds in single-solute and 1.0 mmol L^{-1} total BTEX multiple-solute batch experiments.

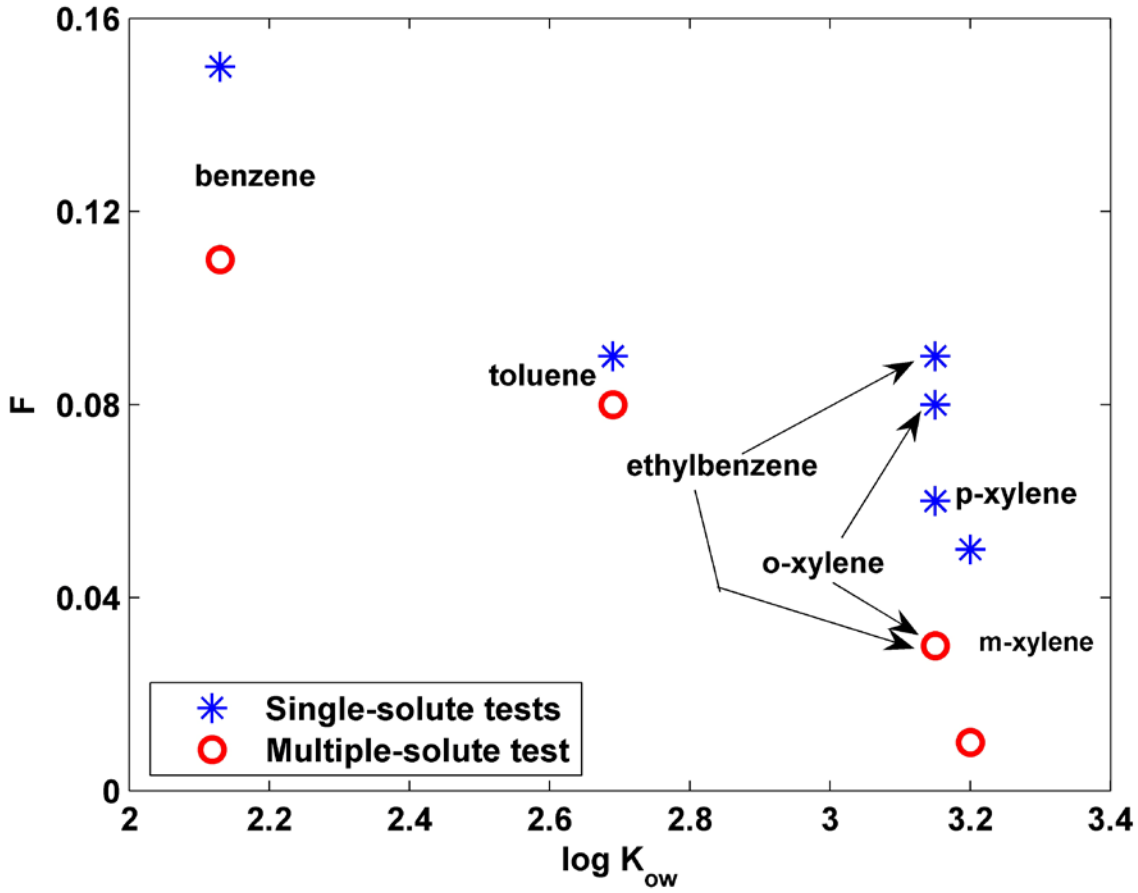

Figure 5. Relationship between F and K_{ow} for BTEX compounds in single-solute and 1.0 mmol L^{-1} total BTEX multiple-solute batch experiments.

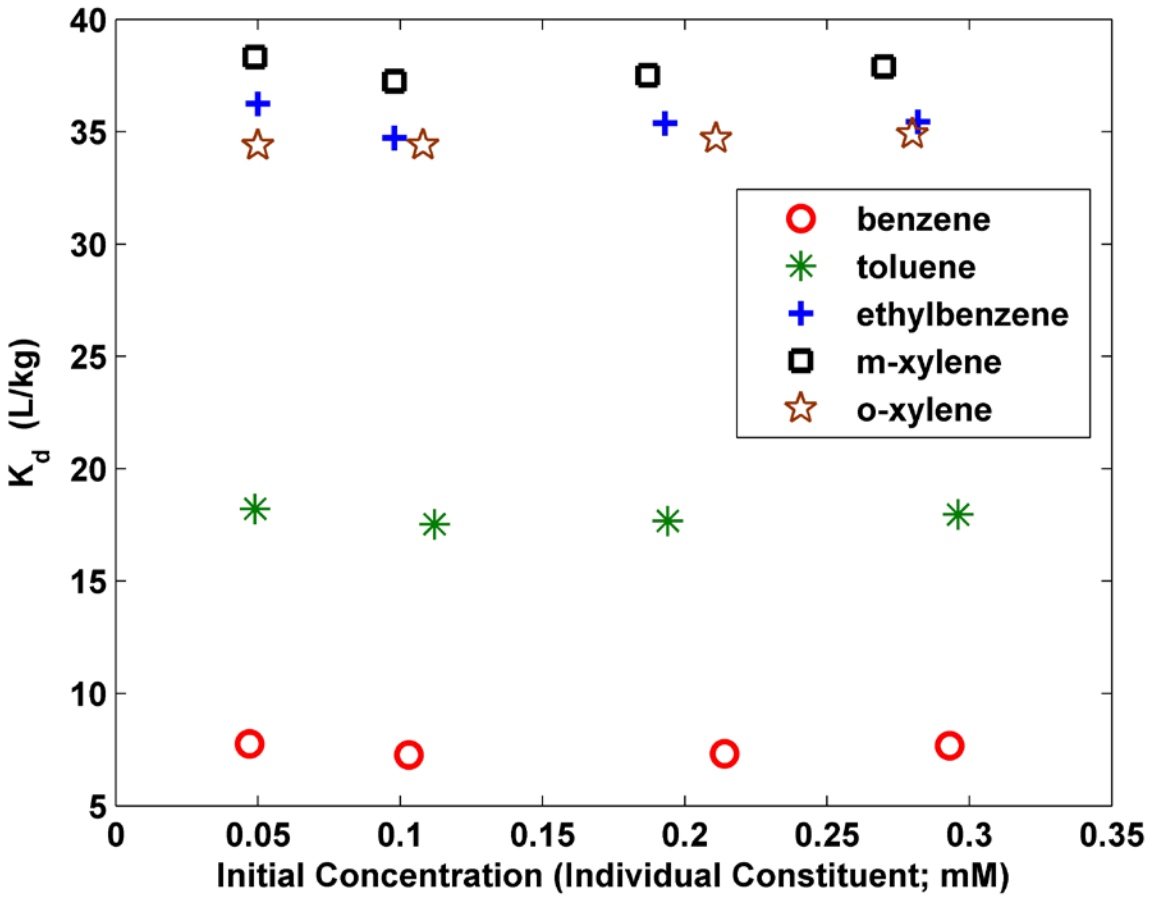

Figure 6. Initial concentration effects on BTEX constituent distribution coefficients when all constituents have similar initial aqueous concentrations.

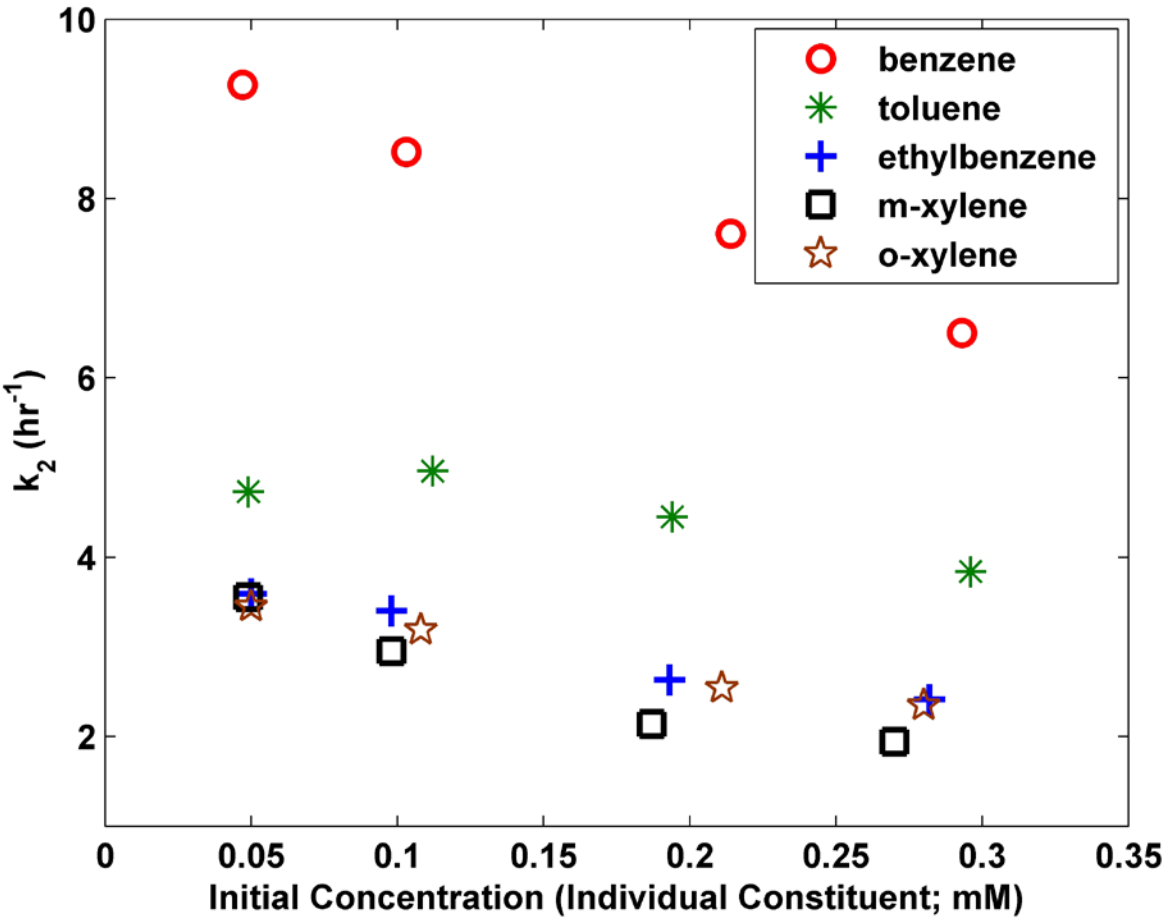

Figure 7. Initial concentration effects on BTEX constituent rate coefficients when all constituents have similar initial aqueous concentrations.

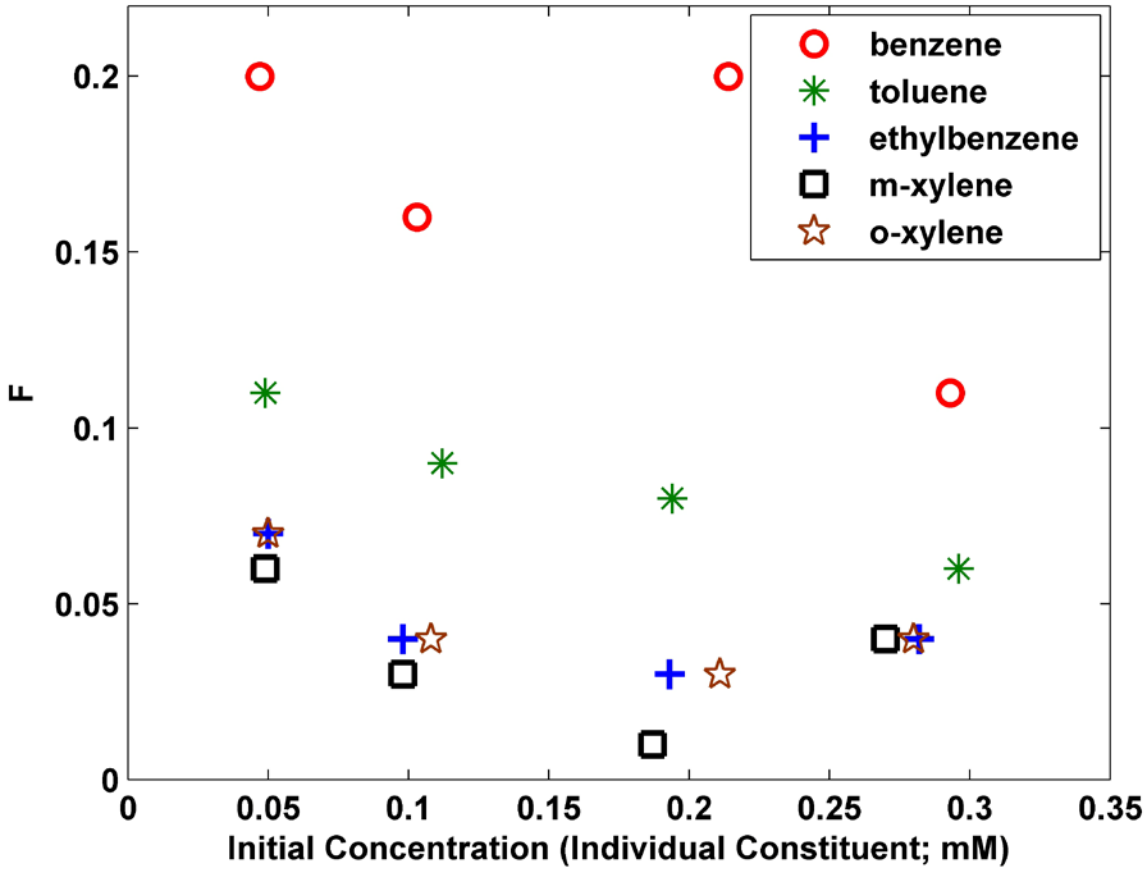

Figure 8. Initial concentration effects on the F of BTEX constituents when all constituents have similar initial aqueous concentrations.

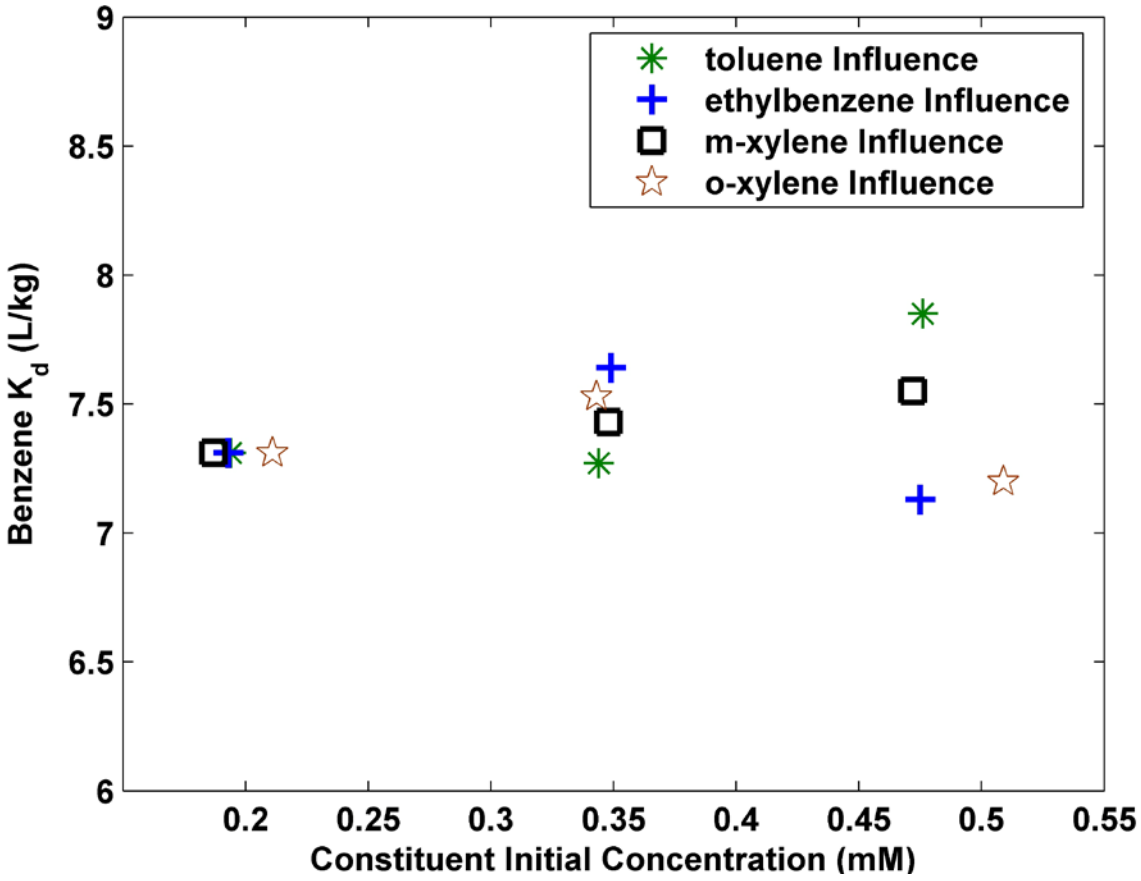

Figure 9. Concentration effects of individual BTEX constituents on the benzene K_d. The initial concentration of benzene was 0.2 mmol L^{-1} for all experiments.

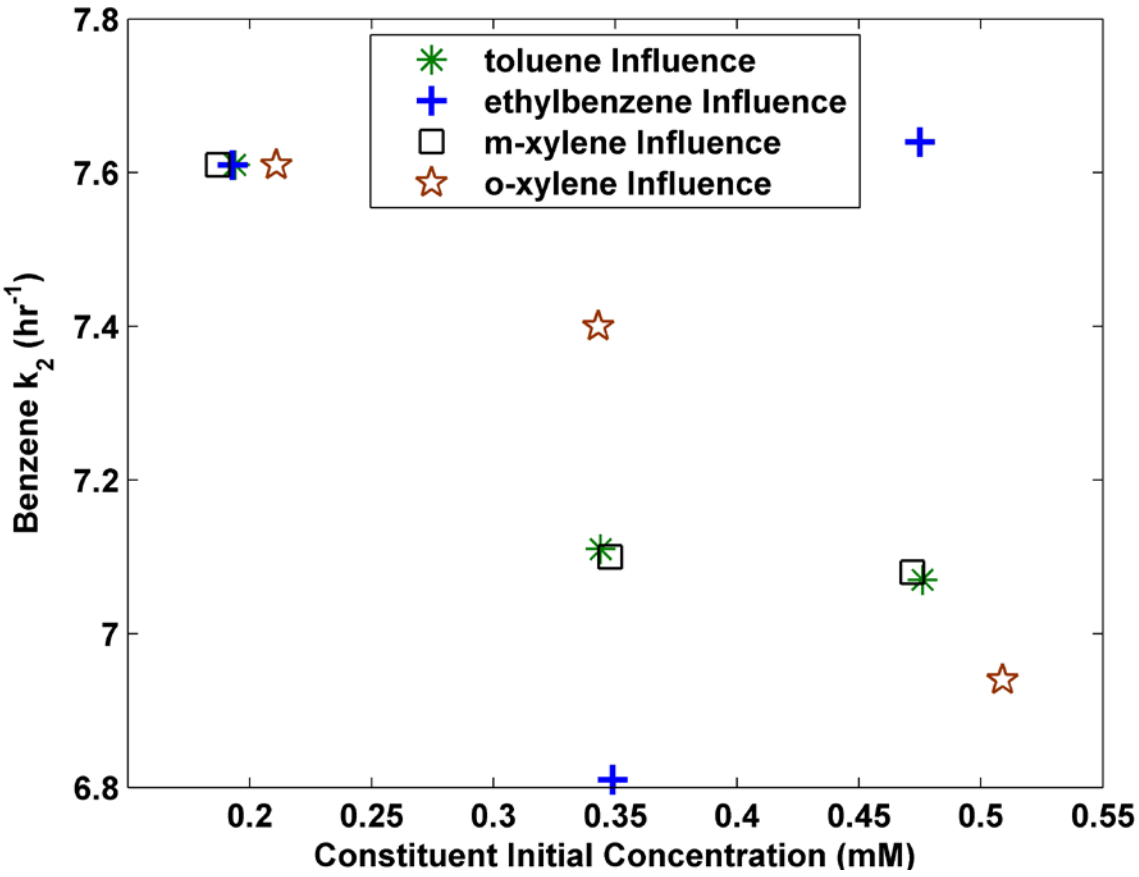

Figure 10. Concentration effects of individual BTEX constituents on the benzene k_2. The initial concentration of benzene was 0.2 mmol L^{-1} for all experiments.

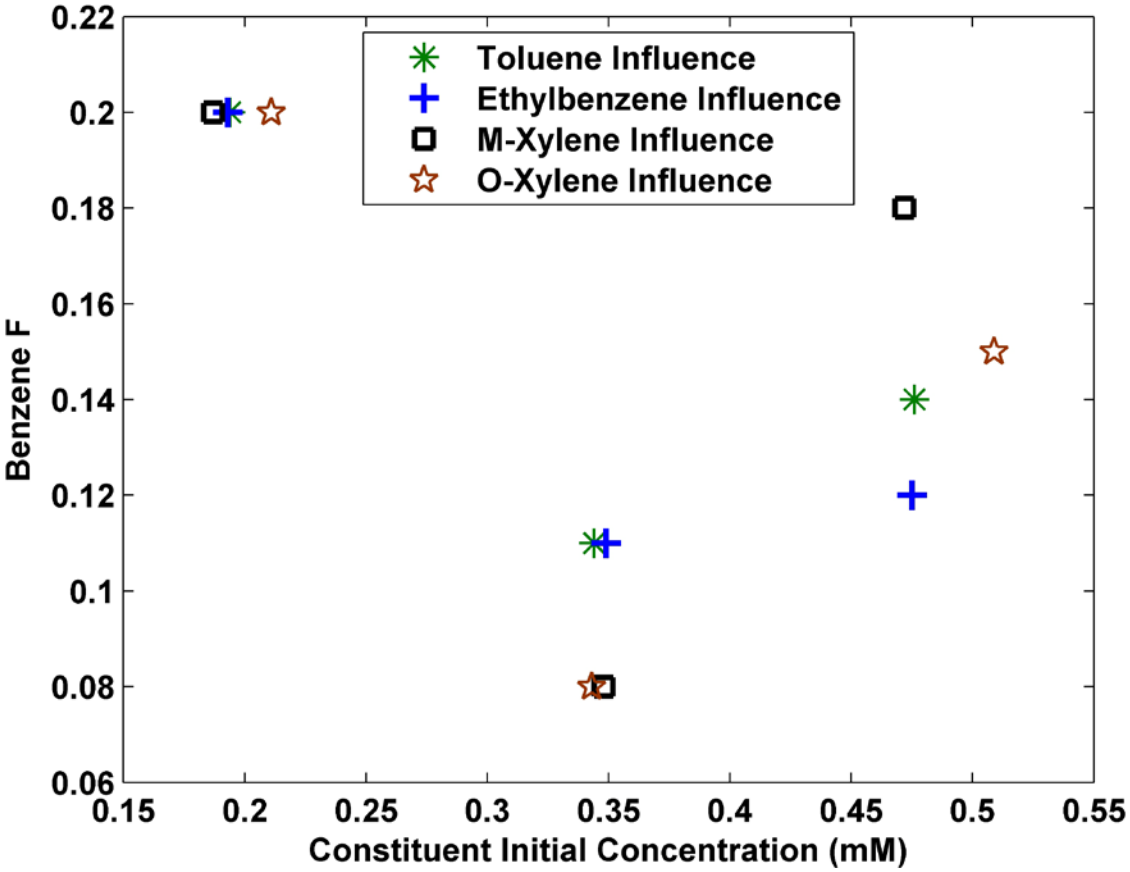

Figure 11. Concentration effects of individual constituents on the benzene F. The initial concentration of benzene was 0.2 mmol L^{-1} for all experiments.

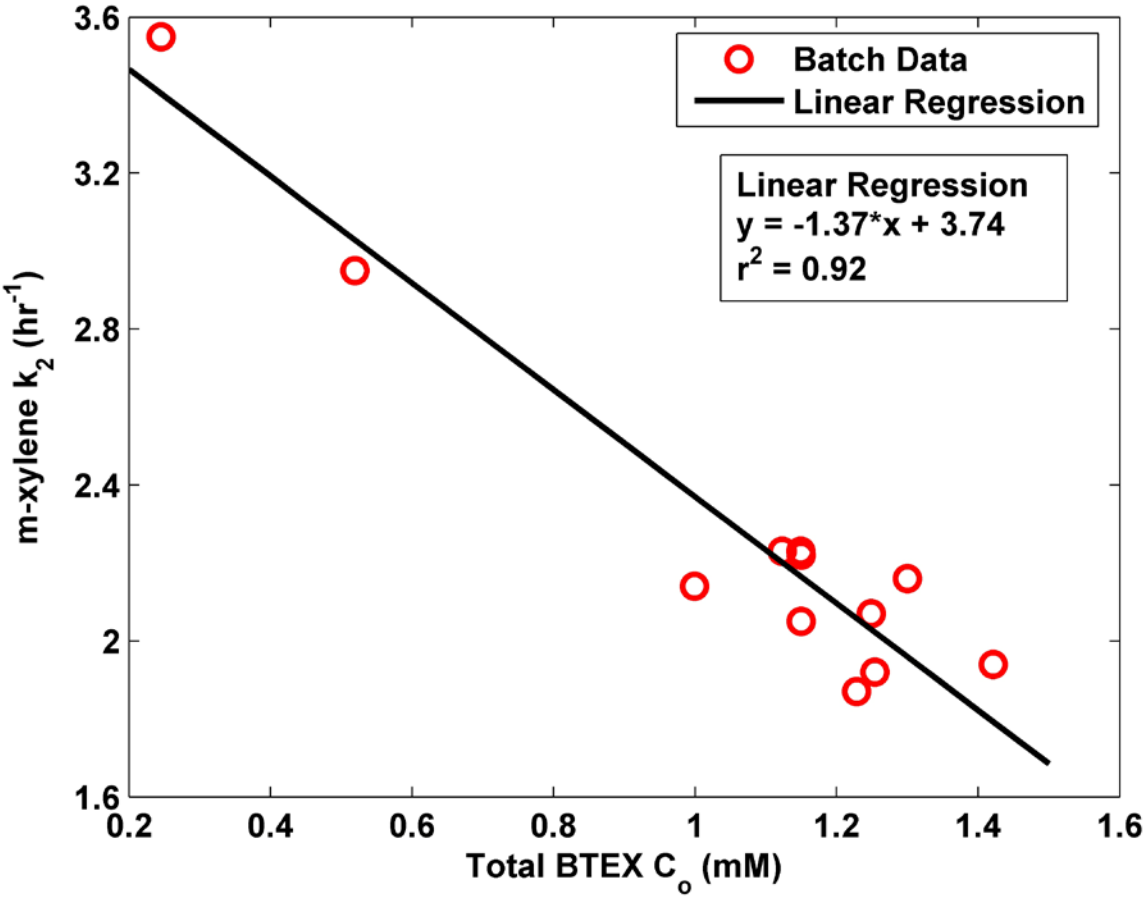

Figure 12. *m*-Xylene kinetic batch-experiment k_2 data fit with a linear regression.

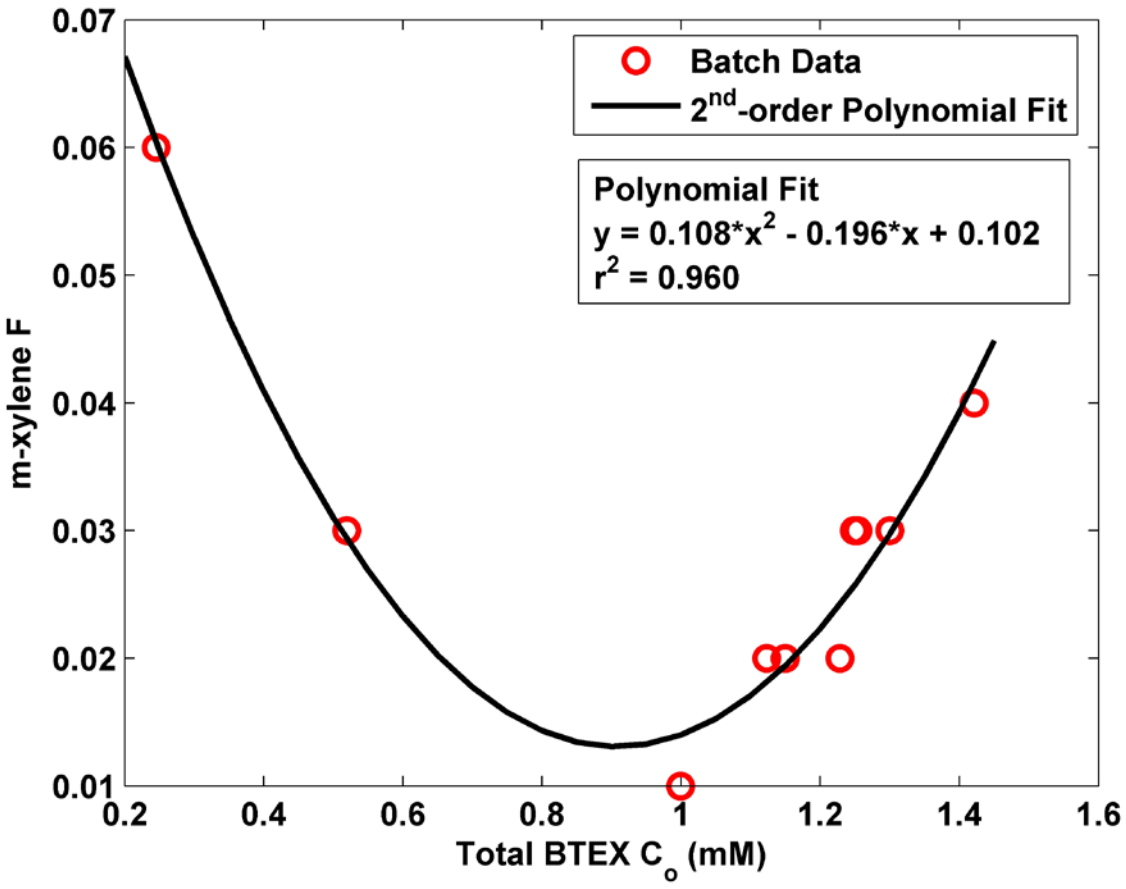

Figure 13. *m*-Xylene kinetic batch-experiment F data fit with a polynomial trend line.

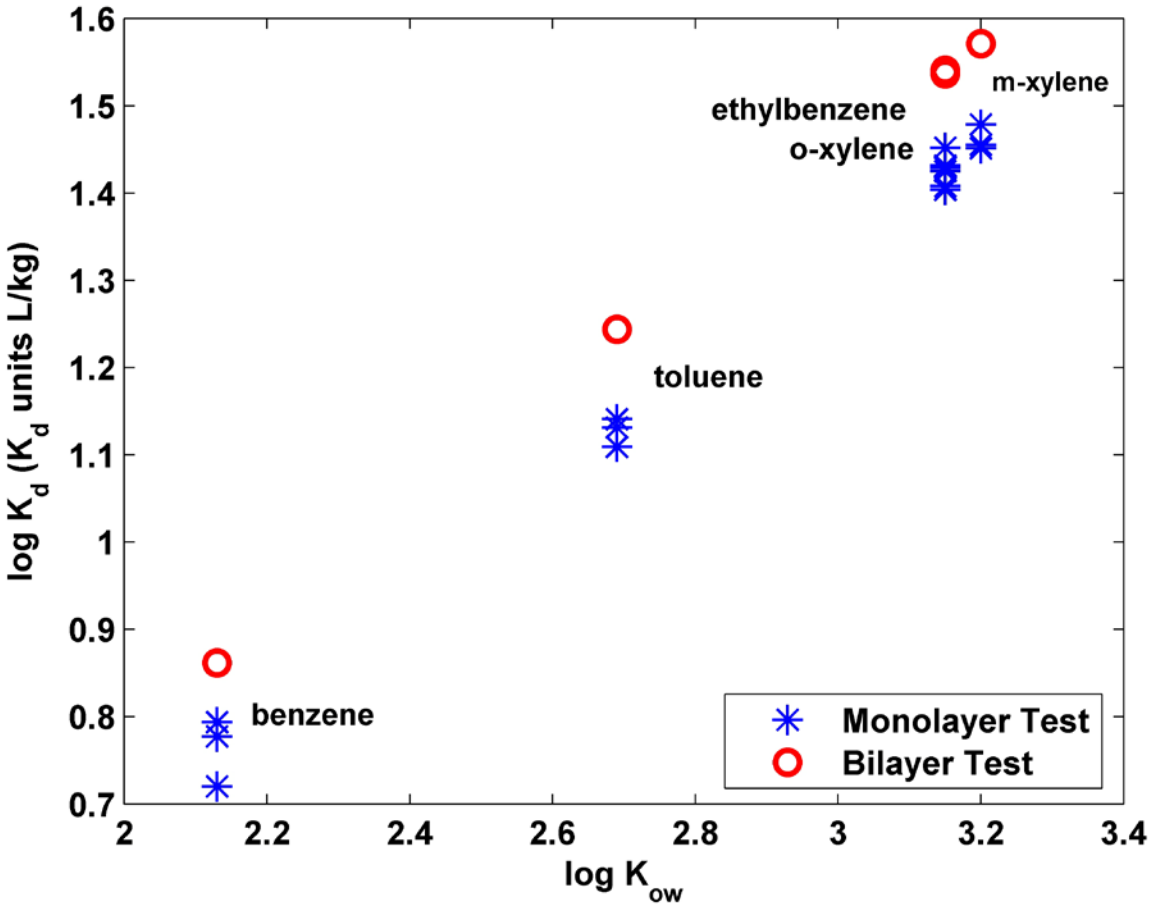

Figure 14. K_d results from three replicate monolayer and corresponding bilayer SMZ batch experiments.

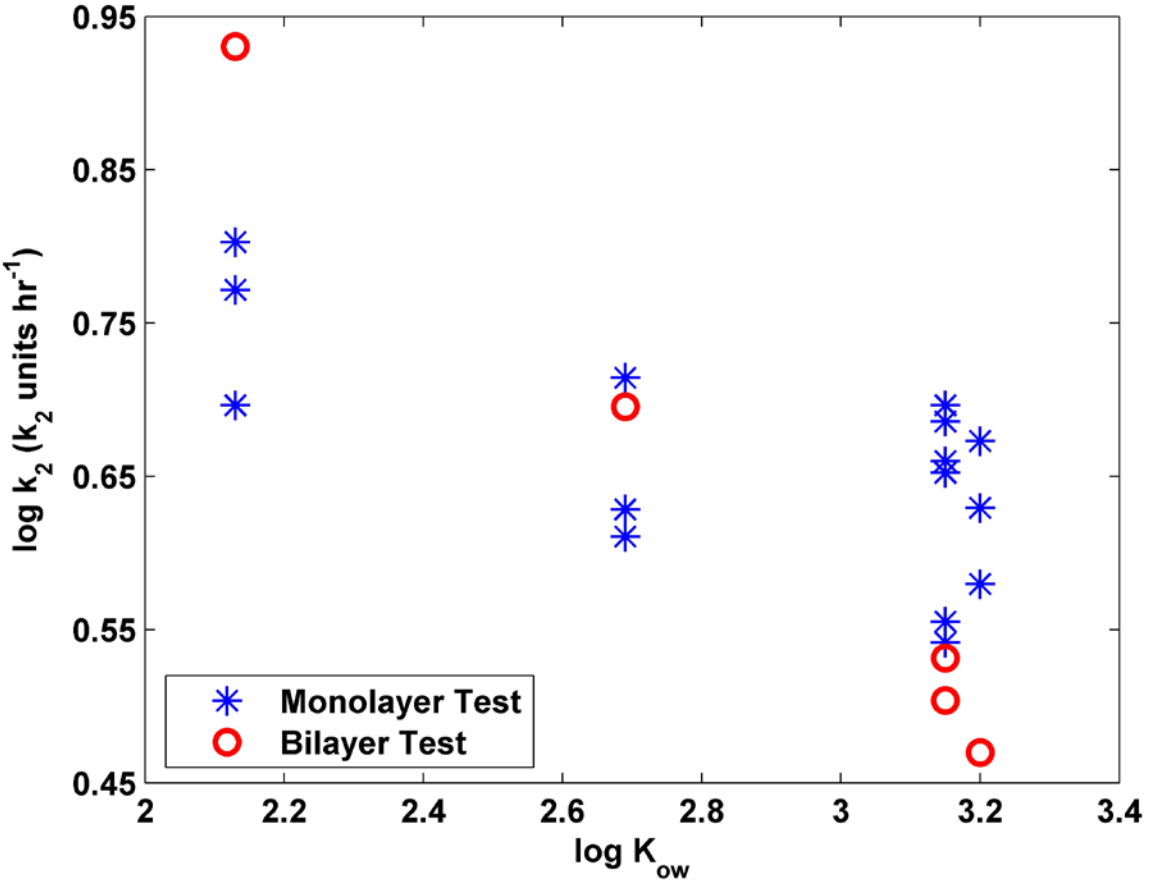

Figure 15. Results for k_2 from three replicate monolayer and corresponding bilayer SMZ batch experiments.

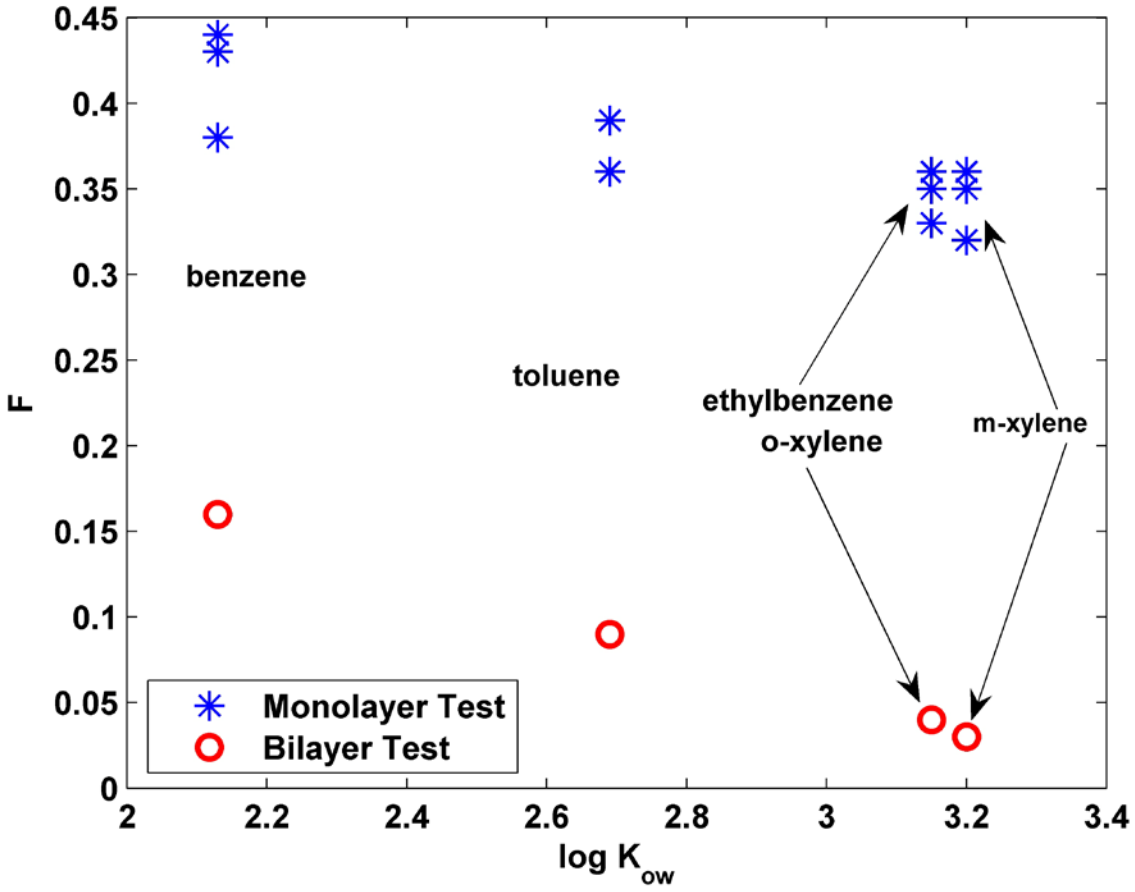

Figure 16. F results from three replicate monolayer and corresponding bilayer SMZ batch experiments.

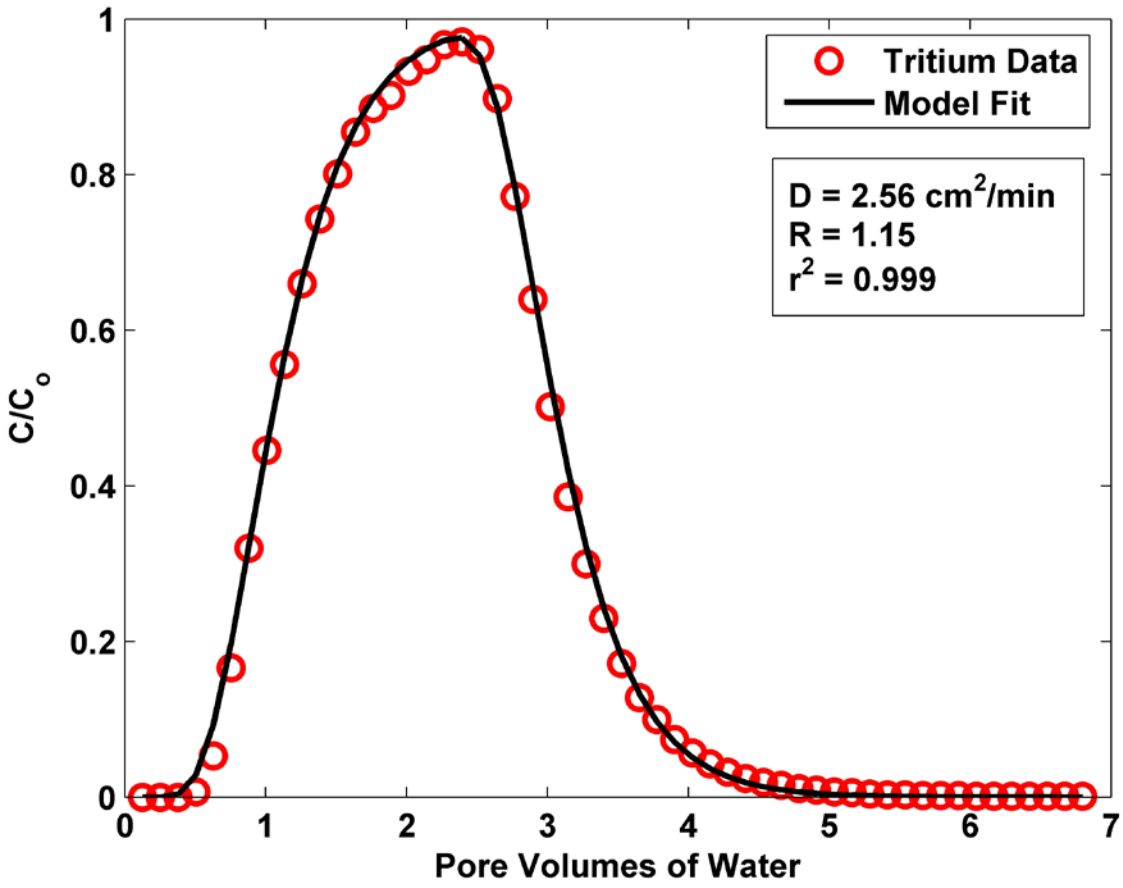

Figure 17. Tritium breakthrough curve for column 2B fitted with the physical equilibrium, 1-D advection-dispersion model.

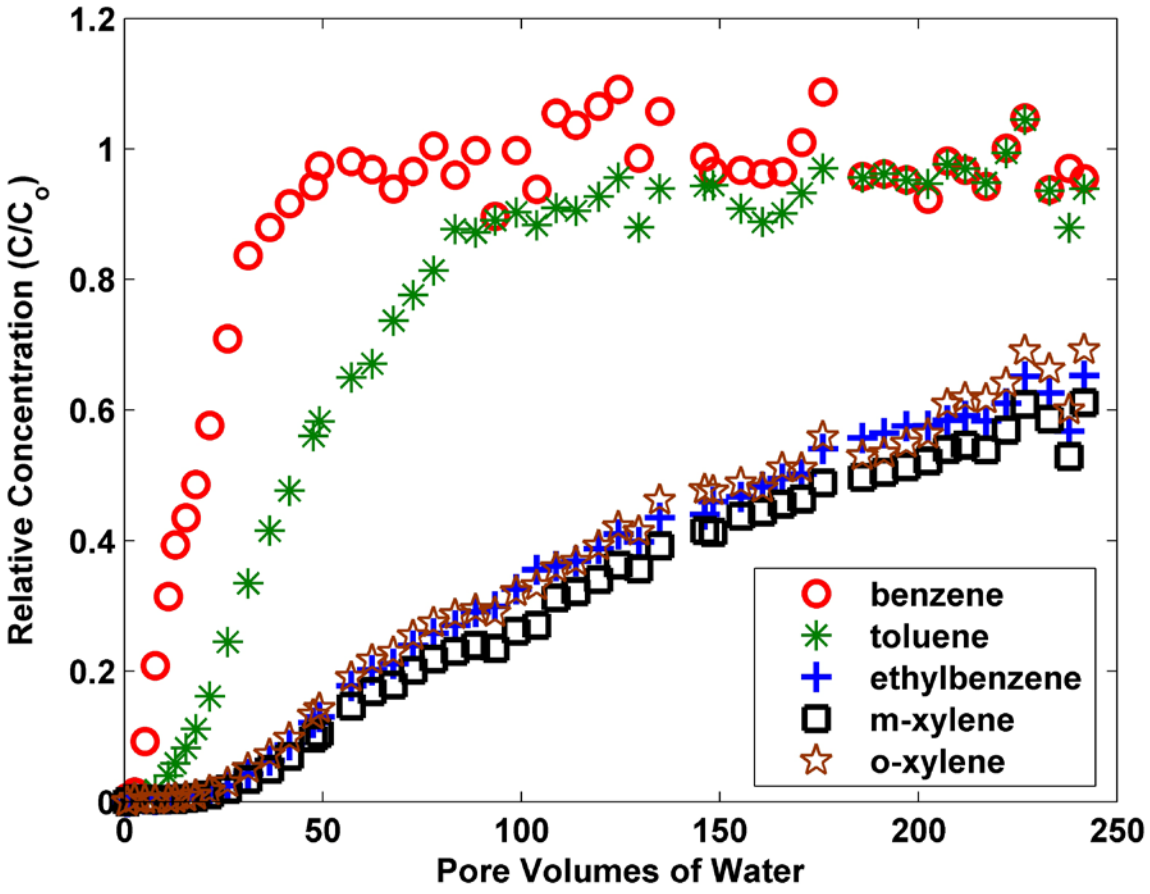

Figure 18. BTEX breakthrough curves for Column 2B.

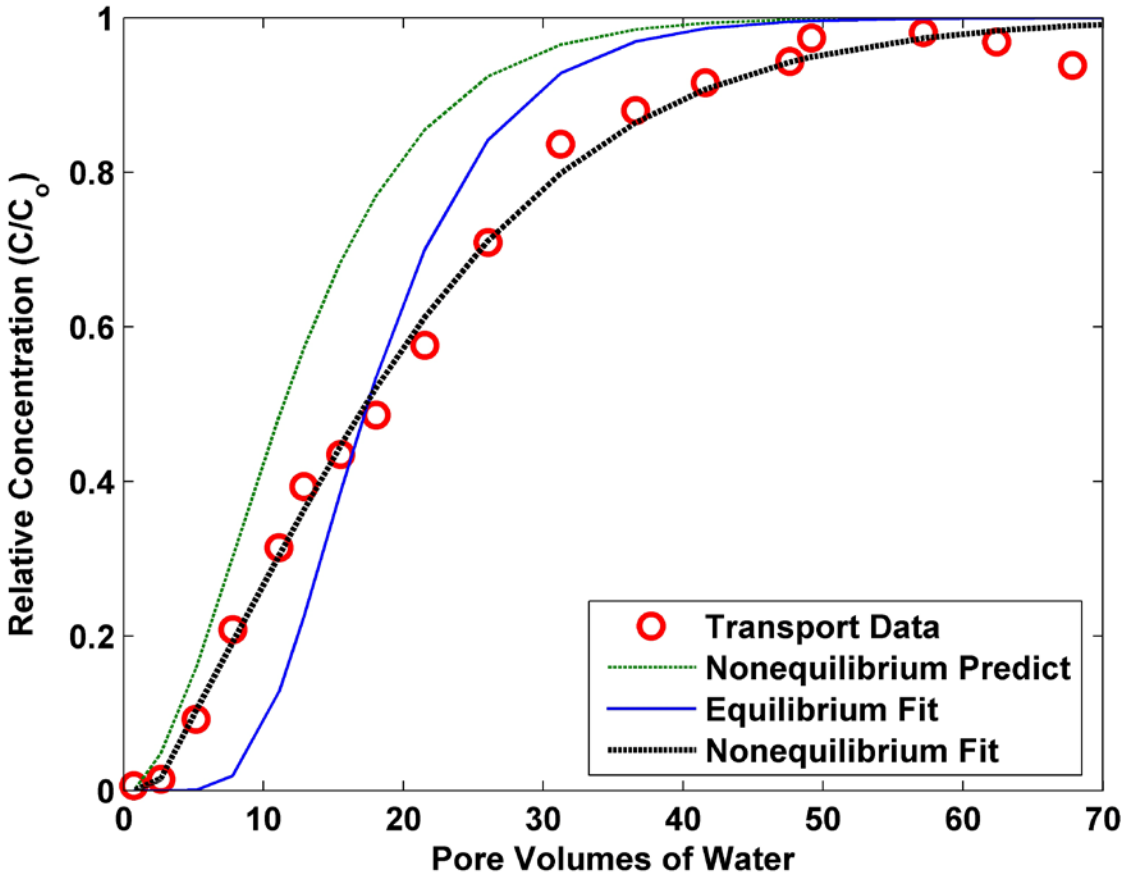

Figure 19. Benzene Column 2B data with nonequilibrium model prediction and equilibrium and nonequilibrium model fits.

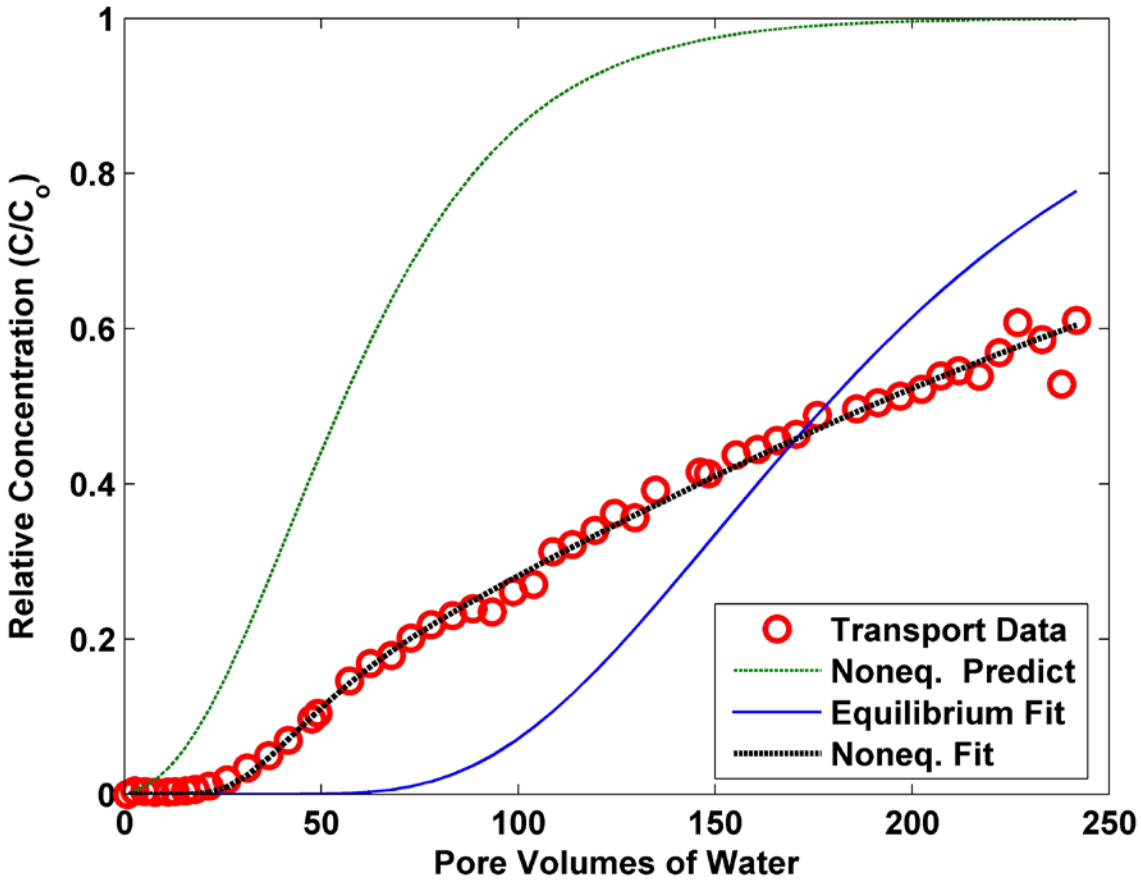

Figure 20. *m*-Xylene Column 2B data with nonequilibrium model prediction and equilibrium and nonequilibrium model fits.

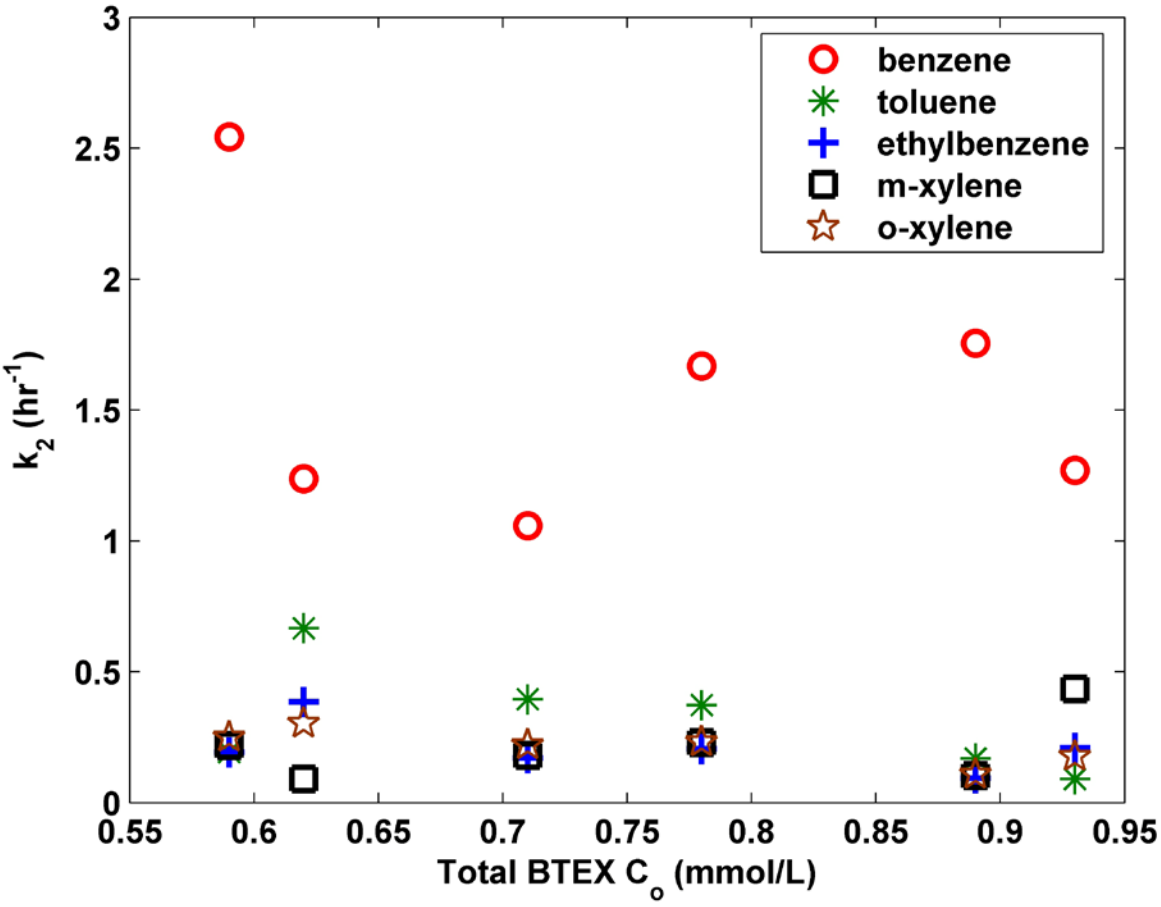

Figure 21. The k_2 calculated from the nonequilibrium model having R, β, and ω inversely fit, termed transport-determined values.

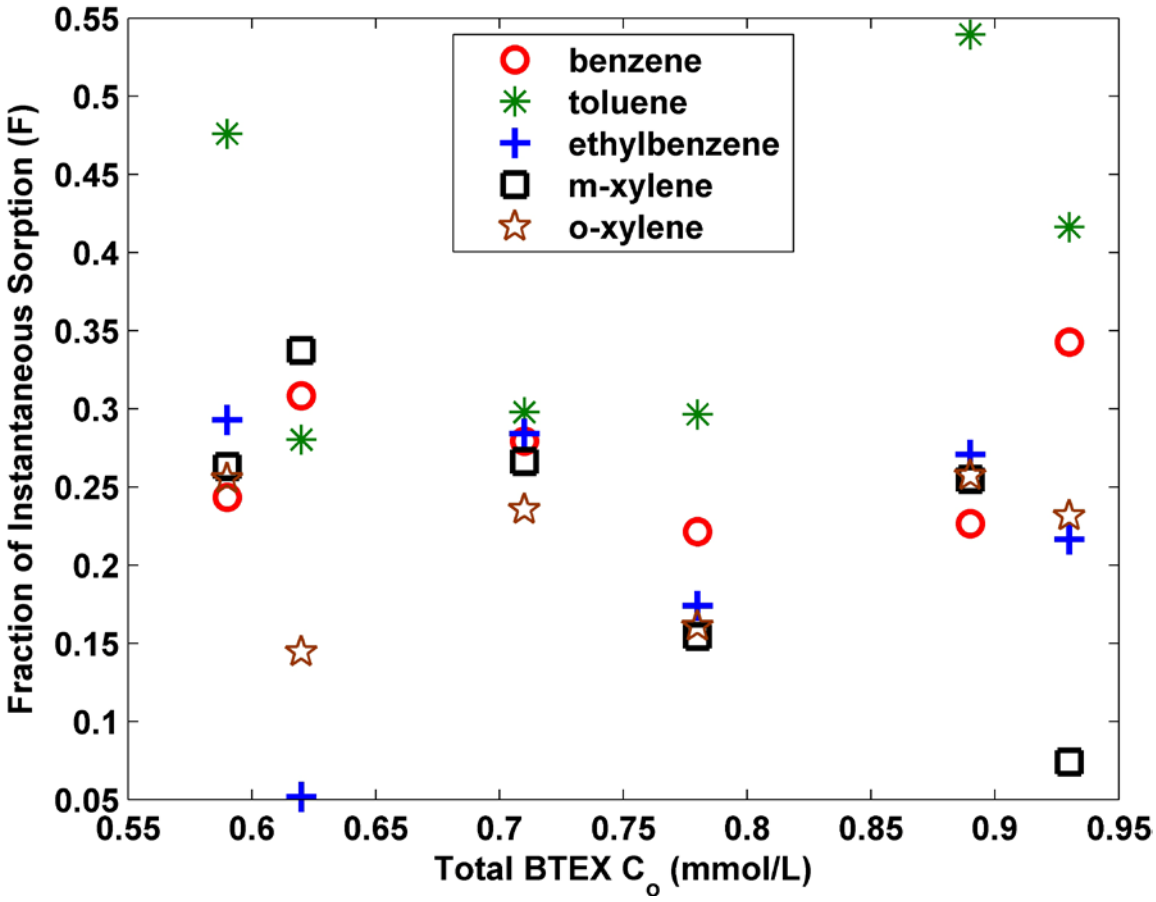

Figure 22. F calculated from the nonequilibrium model having R, β, and ω inversely fit, termed transport-determined values.

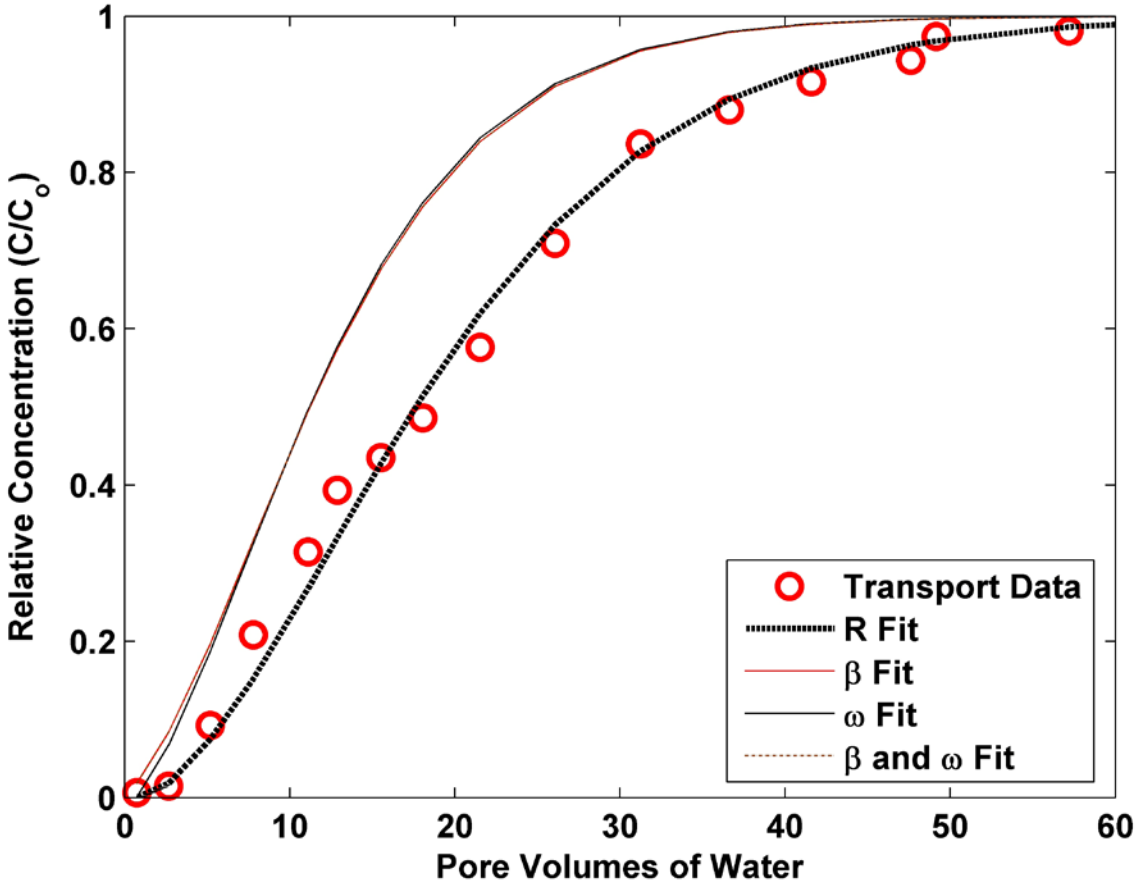

Figure 23. Nonequilibrium prediction model's individual parameter fits to Column 2B benzene data.

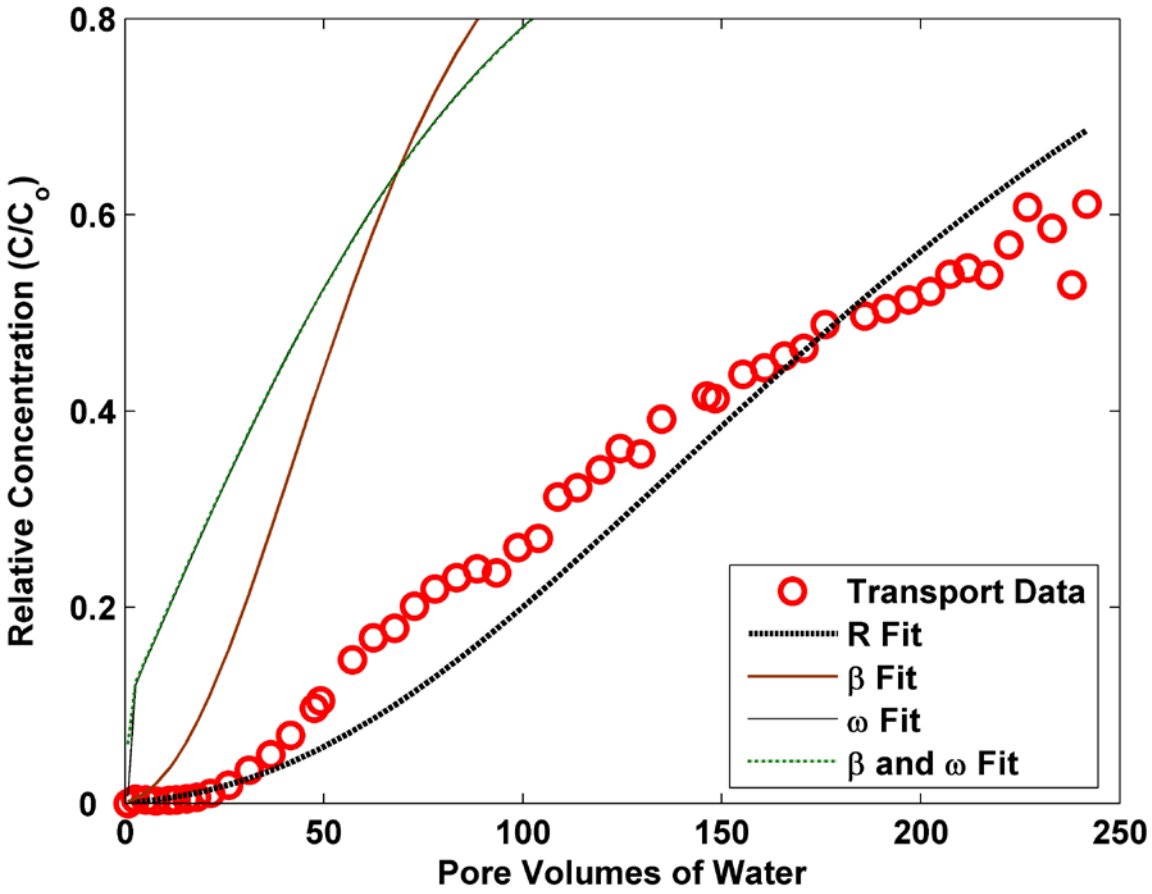

Figure 24. Nonequilibrium prediction model's individual parameter fits to Column 2B *m*-xylene data.

APPENDIX A. SINGLE-SOLUTE AND INITIAL MULTIPLE-SOLUTE BATCH EXPERIMENT RESULTS.

The results from the single-solute batch experiments are contained in this appendix. Six single-solute batch experiments—containing benzene, toluene, ethylbenzene, *m*-xylene, *p*-xylene, and *o*-xylene alone—were conducted. The experimental procedure is discussed in the main text. Tables A-1 through A-6 present the data from the single-solute experiments. Overall results from the single-solute batch experiments can be found in Table A-8.

Table A-1. Data from benzene single-solute batch experiment

Sample	Starting Concentration (mM)	Experiment Time (min)	Final Concentration (mM)	Amount Sorbed (mmol/kg)
0.5-1	0.26	0.5	0.16	0.34
0.5-2	0.27	0.5	0.17	0.30
0.5-3	0.26	0.5	0.17	0.31
1-1	0.26	1	0.15	0.36
1-2	0.27	1	0.15	0.37
1-3	0.27	1	0.17	0.33
2-1	0.26	2.6	0.10	0.53
2-2	0.27	2	0.12	0.49
2-3	0.26	2	0.12	0.47
4-1	0.26	4	0.09	0.56
4-2	0.26	4	0.09	0.55
4-3	0.27	4	0.09	0.56
6-1	0.26	6	0.09	0.57
6-2	0.26	6	0.09	0.57
6-3	0.26	7.2	0.08	0.58
9-1	0.26	9	0.09	0.57
9-2	0.26	9	0.08	0.60
9-3	0.27	10.5	0.08	0.61
12-1	0.26	12	0.08	0.61
12-2	0.26	12	0.08	0.61
12-3	0.27	12	0.08	0.60
15-1	0.27	15	0.07	0.65
15-2	0.26	15	0.07	0.63
15-3	0.24	15	0.07	0.62
20-1	0.26	20	0.08	0.60
20-2	0.25	20	0.08	0.59
20-3	0.27	20.75	0.07	0.62
25-1	0.26	25	0.07	0.63
25-2	0.25	25	0.07	0.61
25-3	0.26	25	0.07	0.62
30-1	0.27	30	0.07	0.62
30-2	0.26	30	0.07	0.65
40-1	0.26	40	0.08	0.61
40-2	0.25	40	0.08	0.60
40-3	0.26	40	0.08	0.61
50-1	0.27	50	0.07	0.63
50-2	0.26	50	0.06	0.66
50-3	0.27	50	0.06	0.67
60-1	0.26	60	0.07	0.62
60-2	0.26	60	0.08	0.61
60-3	0.27	60	0.08	0.62
90-1	0.26	90	0.07	0.62
90-2	0.27	90	0.08	0.62
90-3	0.27	90	0.07	0.63

Table A-2. Data from toluene single-solute batch experiment

Sample	Starting Concentration (mM)	Experiment Time (min)	Final Concentration (mM)	Amount Sorbed (mmol/kg)
0.5-1	0.18	0.5	0.10	0.25
0.5-2	0.18	0.67	0.10	0.29
1-1	0.18	1	0.08	0.33
1-2	0.19	1	0.09	0.32
1-3	0.18	1	0.08	0.33
2-1	0.19	2	0.05	0.44
2-2	0.18	2	0.06	0.39
2-3	0.18	2	0.05	0.42
4-1	0.18	4	0.04	0.45
4-2	0.18	4	0.04	0.47
4-3	0.18	4	0.04	0.46
6-1	0.18	6	0.04	0.47
6-2	0.18	6	0.04	0.47
6-3	0.19	6	0.04	0.48
9-1	0.18	9	0.03	0.50
9-2	0.18	9	0.03	0.50
9-3	0.18	9	0.03	0.49
12-1	0.18	12	0.03	0.49
12-2	0.18	15	0.03	0.49
15-1	0.18	15	0.04	0.48
15-2	0.19	15	0.04	0.49
15-3	0.18	25	0.03	0.50
20-1	0.18	20	0.03	0.49
20-2	0.18	20	0.03	0.50
20-3	0.19	20	0.03	0.50
25-1	0.18	25	0.03	0.51
25-2	0.18	25	0.03	0.51
25-3	0.18	25	0.03	0.51
30-1	0.19	30	0.03	0.50
30-2	0.18	30	0.03	0.51
30-3	0.18	30	0.03	0.51
40-1	0.18	40	0.03	0.51
40-2	0.19	40	0.02	0.52
40-3	0.18	40	0.03	0.52
60-1	0.18	60	0.03	0.51
60-2	0.18	60	0.02	0.52
60-3	0.19	60	0.03	0.52
90-1	0.18	90	0.03	0.51
90-2	0.19	90	0.02	0.52
90-3	0.18	90	0.02	0.52

Table A-3. Data from ethylbenzene single-solute batch experiment

Sample	Starting Concentration (mM)	Experiment Time (min)	Final Concentration (mM)	Amount Sorbed (mmol/kg)
0.5-1	0.21	0.57	0.09	0.38
0.5-2	0.21	0.50	0.09	0.39
0.5-3	0.21	0.60	0.08	0.44
1-1	0.21	1	0.06	0.49
1-2	0.21	1	0.07	0.44
1-3	0.21	1	0.08	0.43
2-1	0.21	2	0.05	0.53
2-2	0.21	2	0.05	0.52
2-3	0.21	2	0.05	0.54
4-1	0.21	4	0.03	0.59
4-2	0.21	4	0.03	0.59
4-3	0.21	4	0.03	0.60
6-1	0.21	6	0.03	0.58
6-2	0.21	6	0.03	0.60
6-3	0.21	6	0.03	0.59
9-1	0.21	9	0.02	0.61
9-2	0.21	9	0.02	0.62
9-3	0.21	9	0.02	0.62
12-1	0.21	12	0.02	0.62
12-2	0.21	12	0.02	0.62
12-3	0.21	12	0.02	0.62
15-1	0.21	16	0.02	0.62
15-2	0.21	15	0.02	0.62
15-3	0.21	15	0.02	0.63
20-1	0.21	20	0.02	0.63
20-2	0.21	20	0.02	0.63
20-3	0.21	20	0.03	0.60
25-1	0.21	25	0.02	0.62
25-2	0.21	25	0.02	0.62
25-3	0.21	25	0.02	0.62
30-1	0.21	30	0.02	0.62
30-2	0.21	30	0.02	0.62
30-3	0.21	30	0.02	0.63
40-1	0.21	40	0.02	0.62
40-2	0.21	40	0.02	0.63
40-3	0.21	40	0.02	0.63
60-1	0.21	60	0.02	0.63
60-2	0.21	60	0.02	0.63
60-3	0.22	60	0.02	0.64
90-1	0.21	90	0.02	0.62
90-2	0.21	90	0.02	0.63
90-3	0.21	90	0.01	0.64

Table A-4. Data from *m*-xylene single-solute batch experiment

Sample	Starting Concentration (mg/L)	Experiment Time (min)	Final Concentration (mg/L)	Amount Sorbed (mg/kg)
0.5-1	0.21	0.5	0.11	0.31
0.5-2	0.21	0.5	0.10	0.34
0.5-3	0.21	0.5	0.11	0.32
1-1	0.20	1	0.08	0.42
1-2	0.21	1	0.08	0.41
1-3	0.21	1	0.08	0.43
2-1	0.21	2	0.05	0.51
2-2	0.21	2	0.05	0.51
2-3	0.21	2	0.05	0.50
4-1	0.21	4	0.03	0.58
4-2	0.21	4	0.03	0.58
4-3	0.21	4	0.03	0.58
6-1	0.21	6	0.03	0.59
6-2	0.20	6	0.03	0.58
6-3	0.21	6	0.03	0.59
9-1	0.20	9	0.02	0.60
9-2	0.21	9	0.02	0.61
9-3	0.21	9	0.02	0.61
12-1	0.21	12.53	0.02	0.60
12-2	0.21	12	0.02	0.61
12-3	0.20	12	0.02	0.60
15-1	0.21	15	0.02	0.61
15-2	0.21	15	0.02	0.61
15-3	0.21	14.18	0.02	0.61
20-1	0.21	20	0.02	0.62
20-2	0.21	20	0.02	0.62
20-3	0.21	20	0.02	0.62
25-1	0.21	25.33	0.02	0.62
25-2	0.21	25.1	0.02	0.62
25-3	0.20	25	0.02	0.62
30-1	0.21	30.7	0.02	0.62
30-2	0.21	30	0.02	0.62
30-3	0.20	30	0.02	0.62
40-1	0.21	40	0.01	0.63
40-2	0.21	40	0.01	0.63
40-3	0.21	40	0.02	0.63
60-1	0.21	60	0.02	0.62
60-2	0.21	60	0.02	0.63
60-3	0.21	60	0.01	0.63
90-1	0.21	90	0.02	0.62
90-2	0.21	90	0.01	0.63
90-3	0.20	90	0.01	0.63

Table A-5. Data from *o*-xylene single-solute batch experiment

Sample	Starting Concentration (mg/L)	Experiment Time (min)	Final Concentration (mg/L)	Amount Sorbed (mg/kg)
0.5-1	0.19	0.5	0.08	0.33
0.5-2	0.19	0.5	0.08	0.34
0.5-3	0.19	0.5	0.08	0.35
1-1	0.19	1	0.07	0.39
1-2	0.19	1	0.07	0.39
1-3	0.19	0.93	0.07	0.40
2-1	0.19	2	0.05	0.45
2-2	0.19	2	0.04	0.48
2-3	0.19	2	0.04	0.47
4-1	0.19	4	0.02	0.53
4-2	0.18	4	0.03	0.52
4-3	0.18	4	0.03	0.51
6-1	0.18	6	0.03	0.52
6-2	0.19	6.38	0.03	0.52
6-3	0.19	6	0.03	0.52
9-1	0.19	9	0.02	0.54
9-2	0.19	9	0.02	0.54
9-3	0.19	9	0.02	0.54
12-1	0.19	12	0.02	0.54
12-2	0.19	12	0.02	0.56
12-3	0.19	12.2	0.02	0.55
15-1	0.18	15	0.02	0.55
15-2	0.19	15	0.02	0.55
15-3	0.19	15	0.02	0.55
20-1	0.18	20.2	0.01	0.56
20-2	0.19	20	0.01	0.57
20-3	0.19	20	0.01	0.56
25-1	0.19	25	0.01	0.56
25-2	0.19	25.27	0.02	0.56
25-3	0.18	25	0.02	0.56
30-1	0.19	30	0.02	0.56
30-2	0.19	30	0.02	0.56
30-3	0.19	30	0.02	0.55
40-1	0.19	40	0.01	0.56
40-2	0.18	40	0.01	0.57
40-3	0.19	40	0.01	0.57
60-1	0.19	60	0.02	0.55
60-2	0.19	60	0.01	0.56
60-3	0.19	60	0.01	0.57
90-1	0.18	90	0.02	0.56
90-2	0.19	90	0.01	0.56
90-3	0.19	90	0.01	0.57

Table A-6. Data from *p*-xylene single-solute batch experiment

Sample	Starting Concentration (mg/L)	Experiment Time (min)	Final Concentration (mg/L)	Amount Sorbed (mg/kg)
0.5-1	0.20	0.5	0.11	0.28
0.5-2	0.19	0.8	0.09	0.33
0.5-3	0.19	0.9	0.09	0.33
1-1	0.20	1	0.09	0.36
1-2	0.20	1	0.08	0.37
1-3	0.19	1	0.07	0.39
2-1	0.19	2	0.05	0.48
2-2	0.19	2	0.05	0.48
2-3	0.20	2	0.05	0.48
4-1	0.19	4	0.03	0.54
4-2	0.20	4	0.03	0.54
4-3	0.20	4	0.03	0.54
6-1	0.20	6	0.03	0.55
6-2	0.20	6	0.03	0.55
6-3	0.19	6	0.03	0.54
9-1	0.20	9	0.02	0.56
9-2	0.20	9	0.02	0.57
9-3	0.20	9	0.02	0.57
12-1	0.19	12	0.02	0.56
12-2	0.20	12	0.02	0.57
12-3	0.20	12	0.02	0.57
15-1	0.19	15	0.02	0.57
15-2	0.20	15	0.02	0.57
15-3	0.20	15	0.02	0.57
20-1	0.19	20	0.01	0.59
20-2	0.19	20	0.01	0.59
20-3	0.20	20	0.02	0.58
25-1	0.19	25	0.02	0.58
25-2	0.19	25	0.02	0.58
25-3	0.19	25	0.02	0.58
30-1	0.20	30	0.02	0.58
30-2	0.19	30	0.02	0.58
30-3	0.19	30	0.02	0.58
40-1	0.20	40	0.01	0.59
40-2	0.20	40	0.01	0.59
40-3	0.20	40	0.01	0.59
60-1	0.19	60	0.02	0.58
60-2	0.20	60	0.01	0.59
60-3	0.19	60	0.01	0.59
90-1	0.20	90	0.01	0.59
90-2	0.19	90	0.01	0.59
90-3	0.20	90	0.02	0.58

Table A-7. Results from the single-solute batch experiments

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum fit (r^2)	Starting Conc. (mM)	Water Added (ml)	Zeolite Added (g)	Log K_{ow} [1]	Solubility (mg/L) [1]
benzene	8.4	7.74	0.15	0.921	0.26	9.87	3	2.13	1850
toluene	18.4	4.64	0.09	0.901	0.18	9.82	3	2.69	470
ethylbenzene	33.8	3.69	0.09	0.916	0.21	9.78	3	3.15	140
m-xylene	38.1	3.13	0.05	0.956	0.21	9.77	3	3.2	173
o-xylene	39.0	3.12	0.08	0.955	0.19	9.76	3	3.15	204
p-xylene	37.5	3.16	0.06	0.939	0.20	9.75	3	3.15	200

[1] Mackay et al., 1992

APPENDIX B. MULTIPLE-SOLUTE BATCH EXPERIMENT DATA.

The data from the multiple-solute batch experiments are presented in this appendix. Four multiple-solute experiments (benzene, toluene, ethylbenzene, m-xylene, and o-xylene) were run with the same initial concentration for each BTEX constituent in order to determine concentration effects on the nonequilibrium sorption parameters. Eight multiple-solute experiments were run in order to determine preferential influences of individual constituents on the nonequilibrium sorption parameters. The experimental procedure is discussed in the main text. The definitions for each experiment are found in Table B-1. Tables B-2 through B-5 represent data from the first four experiments. Tables B-6 through B-13 represent data from the final eight experiments. Tables B-14 through B-25 present the overall results from each experiment.

Table B-1. Multiple-solute kinetic batch experiment definitions. In description field: B = benzene, T = toluene, E = ethylbenzene, M = *m*-xylene, O = *o*-xylene.

Batch Experiment	Description
MSB-0.05	All BTEX constituents' initial aqueous concentrations were 0.05 mM. Total initial aqueous BTEX equaled 0.25 mM.
MSB-0.1	All BTEX constituents' initial aqueous concentrations were 0.1 mM. Total initial aqueous BTEX equaled 0.5 mM.
MSB-0.2	All BTEX constituents' initial aqueous concentrations were 0.2 mM. Total initial aqueous BTEX equaled 1.0 mM.
MSB-0.3	All BTEX constituents' initial aqueous concentrations were 0.3 mM. Total initial aqueous BTEX equaled 1.5 mM.
MSB-0.35T	Initial aqueous concentrations were: B, E, M, and O = 0.2 mM; T = 0.35 mM. Total initial aqueous BTEX concentration equaled 1.15 mM.
MSB-0.35E	Initial aqueous concentrations were: B, T, M, and O = 0.2 mM; E = 0.35 mM. Total initial aqueous BTEX concentration equaled 1.15 mM.
MSB-0.35M	Initial aqueous concentrations were: B, T, E, and O = 0.2 mM; M = 0.35 mM. Total initial aqueous BTEX concentration equaled 1.15 mM.
MSB-0.35O	Initial aqueous concentrations were: B, T, E, and M = 0.2 mM; O = 0.35 mM. Total initial aqueous BTEX concentration equaled 1.15 mM.
MSB-0.5T	Initial aqueous concentrations were: B, E, M, and O = 0.2 mM; T = 0.5 mM. Total initial aqueous BTEX concentration equaled 1.3 mM.
MSB-0.5E	Initial aqueous concentrations were: B, T, M, and O = 0.2 mM; E = 0.5 mM. Total initial aqueous BTEX concentration equaled 1.3 mM.
MSB-0.5M	Initial aqueous concentrations were: B, T, E, and O = 0.2 mM; M = 0.5 mM. Total initial aqueous BTEX concentration equaled 1.3 mM.
MSB-0.5O	Initial aqueous concentrations were: B, T, E, and M = 0.2 mM; O = 0.5 mM. Total initial aqueous BTEX concentration equaled 1.3 mM.

Table B-2. BTEX sorption data from MSB-0.05 batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.064	0.079	0.090	0.088	0.089
0.5-2	0.5	0.060	0.077	0.091	0.089	0.090
0.5-3	0.5	0.060	0.078	0.093	0.092	0.092
1-2	1	0.078	0.096	0.111	0.102	0.108
1-3	1	0.071	0.088	0.102	0.102	0.099
2-1	2	0.084	0.108	0.124	0.122	0.122
2-2	2	0.089	0.112	0.129	0.128	0.128
2-3	2	0.089	0.114	0.132	0.130	0.131
6-1	6	0.103	0.128	0.144	0.142	0.143
6-2	8	0.102	0.128	0.145	0.144	0.144
6-3	6.2	0.103	0.128	0.144	0.143	0.144
9-1	9	0.101	0.128	0.145	0.144	0.145
9-2	9	0.106	0.131	0.147	0.145	0.146
9-3	9	0.103	0.129	0.147	0.145	0.146
12-1	12	0.111	0.134	0.149	0.148	0.149
12-2	12	0.103	0.130	0.147	0.146	0.147
12-3	12	0.108	0.134	0.149	0.148	0.149
15-1	15	0.108	0.129	0.146	0.144	0.144
15-2	15	0.107	0.133	0.148	0.147	0.148
15-3	15	0.110	0.134	0.149	0.148	0.149
20-1	20	0.108	0.137	0.151	0.149	0.151
20-2	20	0.109	0.134	0.150	0.148	0.149
20-3	20	0.108	0.134	0.149	0.147	0.149
25-1	25.2	0.106	0.133	0.148	0.148	0.149
25-2	25	0.110	0.135	0.149	0.149	0.150
25-3	25	0.105	0.132	0.145	0.144	0.144
30-1	30	0.106	0.133	0.149	0.148	0.149
30-2	30	0.108	0.134	0.150	0.148	0.149
30-3	30	0.115	0.138	0.152	0.150	0.152
40-1	40	0.111	0.137	0.152	0.150	0.151
40-2	40	0.111	0.136	0.152	0.150	0.151
40-3	40	0.111	0.135	0.150	0.148	0.150
60-1	60	0.107	0.135	0.151	0.149	0.151
60-2	60	0.109	0.136	0.152	0.150	0.151
60-3	60	0.109	0.135	0.149	0.148	0.149
90-1	90	0.111	0.138	0.153	0.151	0.152
90-2	90	0.112	0.138	0.153	0.151	0.153

Table B-3. BTEX sorption data from MSB-0.1 batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.117	0.157	0.155	0.151	0.166
0.5-2	0.5	0.109	0.151	0.154	0.150	0.164
0.5-3	0.5	0.098	0.134	0.129	0.123	0.137
1-1	1	0.137	0.192	0.195	0.164	0.209
1-2	1	0.132	0.196	0.201	0.173	0.218
2-1	2	0.185	0.250	0.245	0.244	0.265
2-2	2	0.178	0.240	0.238	0.237	0.259
2-3	2	0.163	0.230	0.232	0.231	0.251
4-1	2.4	0.175	0.244	0.242	0.241	0.263
4-2	4	0.190	0.265	0.265	0.265	0.290
4-3	4	0.187	0.262	0.262	0.262	0.286
6-2	6	0.221	0.293	0.283	0.284	0.310
6-3	6	0.212	0.288	0.282	0.282	0.308
9-1	9	0.216	0.286	0.279	0.280	0.306
9-2	9	0.230	0.300	0.287	0.288	0.315
9-3	9	0.224	0.293	0.284	0.285	0.312
12-1	12	0.214	0.289	0.282	0.283	0.309
12-2	12	0.218	0.292	0.283	0.284	0.311
12-3	12	0.239	0.302	0.288	0.288	0.316
15-2	15	0.238	0.304	0.290	0.290	0.318
15-3	15	0.224	0.298	0.288	0.289	0.316
20-1	20	0.232	0.303	0.289	0.290	0.317
20-2	20	0.230	0.302	0.290	0.291	0.318
20-3	20	0.232	0.303	0.290	0.291	0.319
25-1	25	0.227	0.302	0.284	0.291	0.318
25-2	25	0.230	0.303	0.285	0.291	0.319
25-3	25	0.224	0.301	0.284	0.291	0.319
30-1	31.5	0.238	0.308	0.292	0.292	0.319
30-2	30	0.234	0.307	0.293	0.294	0.321
30-3	30	0.237	0.308	0.294	0.294	0.322
40-1	40	0.226	0.304	0.290	0.291	0.318
40-2	40	0.232	0.307	0.294	0.295	0.323
40-3	40	0.233	0.308	0.295	0.296	0.324
60-1	60	0.230	0.305	0.292	0.292	0.321
60-2	60	0.232	0.309	0.295	0.296	0.325
60-3	60	0.236	0.312	0.297	0.298	0.327
90-1	90	0.233	0.307	0.292	0.293	0.322
90-2	90	0.231	0.309	0.295	0.296	0.325
90-3	90	0.236	0.312	0.298	0.298	0.328

Table B-4. BTEX sorption data from MSB-0.2 batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg) Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.251	0.254	0.268	0.259	0.286
0.5-2	0.58	0.257	0.267	0.275	0.265	0.295
0.5-3	0.5	0.232	0.225	0.228	0.218	0.236
1-1	1	0.295	0.321	0.340	0.213	0.365
1-3	1	0.283	0.310	0.325	0.186	0.351
2-1	2	0.325	0.415	0.442	0.422	0.481
2-2	2	0.335	0.426	0.460	0.441	0.499
2-3	2	0.317	0.409	0.445	0.427	0.484
4-1	4	0.395	0.457	0.512	0.498	0.555
4-2	4	0.374	0.460	0.504	0.489	0.547
4-3	4	0.385	0.444	0.498	0.483	0.541
6-1	6	0.453	0.509	0.550	0.530	0.595
6-2	6	0.447	0.495	0.543	0.523	0.589
6-3	6	0.451	0.498	0.545	0.525	0.591
9-1	9	0.459	0.507	0.558	0.540	0.605
9-2	9	0.461	0.508	0.558	0.541	0.607
9-3	9	0.457	0.507	0.559	0.543	0.607
12-1	12	0.469	0.519	0.568	0.552	0.618
12-2	12	0.465	0.529	0.572	0.556	0.623
12-3	12	0.461	0.533	0.575	0.558	0.625
15-2	15	0.484	0.528	0.575	0.555	0.625
15-3	15	0.478	0.526	0.574	0.554	0.625
20-1	20	0.484	0.537	0.580	0.562	0.630
20-2	20	0.478	0.536	0.581	0.564	0.632
20-3	20	0.480	0.537	0.581	0.564	0.633
25-1	25	0.485	0.533	0.578	0.562	0.631
25-2	25	0.482	0.533	0.579	0.563	0.631
25-3	25	0.471	0.525	0.574	0.558	0.626
30-1	30.3	0.481	0.529	0.572	0.552	0.621
30-2	30	0.490	0.535	0.579	0.559	0.630
30-3	30	0.501	0.542	0.584	0.565	0.636
40-1	40	0.470	0.531	0.579	0.568	0.630
40-2	40	0.493	0.539	0.583	0.566	0.635
40-3	40	0.481	0.535	0.583	0.566	0.635
60-1	60	0.480	0.529	0.573	0.557	0.626
60-2	60	0.490	0.539	0.583	0.566	0.636
60-3	60	0.485	0.539	0.585	0.568	0.638
90-1	90	0.486	0.535	0.578	0.561	0.631
90-3	90	0.500	0.546	0.589	0.572	0.642

Table B-5. BTEX sorption data from MSB-0.3 batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg) Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.277	0.353	0.417	0.402	0.403
0.5-2	0.5	0.218	0.285	0.361	0.350	0.346
0.5-3	0.5	0.179	0.300	0.435	0.423	0.419
1-1	1	0.444	0.497	0.505	0.466	0.490
1-3	1	0.411	0.488	0.512	0.472	0.500
2-1	2	0.467	0.585	0.588	0.566	0.580
2-2	2	0.453	0.580	0.589	0.568	0.583
2-3	2	0.464	0.589	0.582	0.562	0.577
4-1	4	0.543	0.707	0.740	0.712	0.733
4-2	4	0.542	0.694	0.705	0.678	0.701
4-3	4.1	0.564	0.717	0.741	0.711	0.734
6-1	6	0.607	0.752	0.781	0.752	0.772
6-2	6	0.607	0.749	0.777	0.747	0.768
6-3	6	0.609	0.751	0.781	0.752	0.771
9-1	9	0.628	0.774	0.807	0.775	0.795
9-2	9	0.623	0.777	0.813	0.782	0.802
9-3	9	0.610	0.765	0.805	0.775	0.796
12-2	12	0.636	0.788	0.822	0.790	0.813
12-3	12	0.639	0.790	0.824	0.792	0.813
15-1	15	0.658	0.806	0.834	0.801	0.823
15-2	14.8	0.661	0.821	0.840	0.807	0.829
15-3	15	0.655	0.799	0.829	0.797	0.819
20-1	20	0.667	0.807	0.832	0.799	0.821
20-3	20	0.677	0.821	0.845	0.811	0.836
25-1	20	0.671	0.808	0.838	0.808	0.831
25-2	25	0.676	0.812	0.842	0.812	0.835
25-3	25	0.677	0.810	0.839	0.809	0.833
30-1	30.2	0.687	0.828	0.847	0.813	0.836
30-2	30	0.688	0.832	0.853	0.819	0.843
30-3	30	0.680	0.826	0.849	0.815	0.839
40-1	40	0.689	0.833	0.853	0.819	0.843
40-2	40	0.653	0.816	0.847	0.814	0.838
40-3	40	0.670	0.827	0.853	0.820	0.845
60-1	60	0.657	0.813	0.839	0.807	0.831
60-2	60	0.674	0.828	0.852	0.819	0.845
60-3	60	0.675	0.831	0.855	0.822	0.847
90-2	90	0.663	0.822	0.841	0.809	0.834
90-3	90	0.683	0.835	0.855	0.821	0.847

Table B-6. BTEX sorption data from MSB-0.5T batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.196	0.575	0.272	0.261	0.259
0.5-2	0.5	0.189	0.524	0.190	0.180	0.183
1-1	1	0.282	0.788	0.308	0.234	0.300
1-2	1	0.281	0.784	0.315	0.239	0.302
1-3	1	0.273	0.807	0.311	0.233	0.301
2-1	2	0.348	0.994	0.390	0.368	0.374
2-2	2	0.332	0.928	0.365	0.345	0.353
2-3	2	0.347	0.998	0.393	0.373	0.383
4-1	4	0.377	1.122	0.482	0.459	0.467
4-2	4	0.384	1.130	0.477	0.454	0.464
4-3	4.2	0.380	1.133	0.488	0.465	0.474
6-1	6	0.423	1.228	0.521	0.495	0.504
6-2	6	0.435	1.243	0.535	0.507	0.516
6-3	6	0.439	1.249	0.533	0.506	0.515
9-1	9	0.448	1.272	0.544	0.516	0.526
9-2	2.8	0.363	1.067	0.447	0.425	0.431
9-3	9	0.443	1.266	0.541	0.514	0.524
12-1	12	0.449	1.283	0.555	0.527	0.537
12-3	12	0.442	1.275	0.549	0.522	0.532
15-1	15	0.454	1.294	0.554	0.526	0.536
15-2	15	0.455	1.294	0.554	0.526	0.536
15-3	15	0.460	1.311	0.559	0.530	0.540
20-1	20	0.457	1.317	0.557	0.528	0.538
20-2	20	0.458	1.307	0.566	0.537	0.548
20-3	20	0.455	1.324	0.574	0.545	0.555
25-1	25	0.462	1.283	0.555	0.524	0.534
25-2	25	0.454	1.312	0.565	0.534	0.544
25-3	25	0.464	1.318	0.565	0.534	0.545
30-1	30	0.468	1.324	0.559	0.531	0.540
30-2	30.2	0.462	1.318	0.562	0.534	0.544
40-1	40	0.462	1.326	0.564	0.534	0.545
40-2	40	0.466	1.329	0.566	0.538	0.549
40-3	40	0.463	1.329	0.567	0.538	0.549
60-1	60	0.462	1.317	0.559	0.532	0.543
60-2	60	0.466	1.330	0.566	0.538	0.549
60-3	60	0.467	1.336	0.569	0.540	0.552
90-1	90	0.456	1.318	0.564	0.536	0.547
90-3	90	0.458	1.327	0.569	0.540	0.552

Table B-7. BTEX sorption data from MSB-0.5E batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.176	0.223	0.684	0.269	0.266
0.5-2	0.5	0.161	0.220	0.744	0.294	0.292
0.5-3	0.63	0.172	0.240	0.746	0.294	0.296
1-1	1	0.272	0.331	0.935	0.339	0.374
1-2	1	0.278	0.330	0.836	0.294	0.337
1-3	1.1	0.189	0.269	0.804	0.282	0.324
2-1	2	0.321	0.406	1.046	0.415	0.434
2-2	2	0.326	0.419	1.087	0.433	0.452
2-3	2	0.324	0.417	1.103	0.439	0.458
4-1	4	0.335	0.454	1.240	0.493	0.514
4-2	4	0.349	0.462	1.245	0.497	0.520
6-1	6	0.385	0.496	1.336	0.534	0.558
6-2	6	0.393	0.499	1.331	0.533	0.556
6-3	6	0.378	0.496	1.347	0.539	0.563
9-1	9	0.401	0.510	1.364	0.546	0.571
9-2	9	0.411	0.519	1.382	0.554	0.579
9-3	9	0.415	0.523	1.389	0.556	0.583
12-1	12	0.427	0.533	1.411	0.563	0.592
12-2	12	0.416	0.527	1.405	0.563	0.590
12-3	12	0.414	0.524	1.396	0.559	0.585
15-1	15	0.417	0.527	1.407	0.563	0.591
15-2	15	0.413	0.524	1.405	0.563	0.589
15-3	15	0.414	0.525	1.408	0.564	0.590
20-1	20	0.429	0.536	1.414	0.566	0.593
20-2	20	0.419	0.533	1.418	0.568	0.595
20-3	20	0.431	0.540	1.425	0.571	0.599
25-1	25	0.418	0.532	1.411	0.567	0.595
25-2	25	0.422	0.538	1.422	0.572	0.600
30-1	30	0.419	0.533	1.421	0.567	0.593
30-2	29.3	0.422	0.537	1.431	0.573	0.601
30-3	30	0.424	0.536	1.425	0.571	0.599
40-1	40	0.419	0.540	1.437	0.573	0.601
40-2	40	0.416	0.538	1.434	0.574	0.603
40-3	40	0.427	0.544	1.441	0.577	0.606
60-1	60	0.425	0.539	1.420	0.568	0.597
60-2	60	0.427	0.549	1.444	0.578	0.608
60-3	60	0.433	0.554	1.455	0.582	0.613
90-1	90	0.420	0.537	1.413	0.566	0.595
90-2	90	0.423	0.544	1.437	0.575	0.605
90-3	90	0.429	0.549	1.446	0.579	0.609

Table B-8. BTEX sorption data from MSB-0.5M batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg) Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.202	0.223	0.295	0.695	0.274
0.5-2	0.5	0.194	0.203	0.258	0.604	0.235
0.5-3	0.5	0.212	0.224	0.269	0.633	0.252
1-1	1	0.266	0.289	0.344	0.713	0.323
1-2	1	0.237	0.287	0.374	0.793	0.357
2-1	2	0.292	0.358	0.415	0.968	0.394
2-2	2	0.315	0.382	0.436	1.015	0.418
2-3	2	0.307	0.373	0.421	0.983	0.403
4-1	4	0.355	0.448	0.523	1.220	0.501
4-2	4	0.344	0.442	0.526	1.226	0.506
4-3	4	0.328	0.424	0.501	1.167	0.483
6-1	6	0.356	0.455	0.545	1.272	0.525
6-2	6	0.367	0.487	0.570	1.324	0.546
6-3	6	0.381	0.474	0.558	1.297	0.536
9-1	9	0.408	0.497	0.583	1.352	0.557
9-2	9	0.412	0.504	0.590	1.367	0.565
9-3	9	0.420	0.507	0.592	1.371	0.567
12-1	12	0.420	0.502	0.594	1.378	0.570
12-2	12	0.422	0.513	0.599	1.388	0.575
15-1	15	0.431	0.535	0.612	1.415	0.586
15-2	15	0.422	0.534	0.614	1.421	0.589
20-1	20	0.431	0.523	0.606	1.403	0.581
20-3	20	0.435	0.528	0.613	1.418	0.588
25-1	25	0.431	0.526	0.613	1.416	0.586
25-2	25	0.423	0.522	0.611	1.412	0.585
25-3	25	0.428	0.525	0.613	1.416	0.587
30-1	30	0.434	0.534	0.614	1.425	0.587
30-2	30	0.419	0.529	0.614	1.424	0.589
30-3	30	0.428	0.531	0.612	1.418	0.588
40-1	40	0.434	0.532	0.615	1.428	0.589
40-2	40	0.429	0.532	0.618	1.432	0.593
40-3	40	0.434	0.534	0.618	1.431	0.594
60-1	60	0.422	0.520	0.605	1.402	0.582
60-2	60	0.426	0.529	0.615	1.423	0.591
60-3	60	0.432	0.534	0.619	1.434	0.596
90-1	90	0.422	0.528	0.617	1.429	0.593
90-2	90	0.426	0.531	0.620	1.435	0.596
90-3	90	0.432	0.542	0.625	1.446	0.601

Table B-9. BTEX sorption data from MSB-0.5O batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.186	0.224	0.251	0.254	0.656
0.5-2	0.5	0.207	0.238	0.267	0.270	0.691
1-2	1	0.265	0.360	0.353	0.294	0.931
1-3	1	0.250	0.339	0.351	0.293	0.920
2-1	2	0.308	0.390	0.397	0.403	1.051
2-2	2	0.337	0.417	0.431	0.438	1.139
2-3	2.1	0.322	0.410	0.419	0.426	1.115
4-1	4	0.392	0.494	0.520	0.529	1.378
4-2	4	0.380	0.485	0.510	0.528	1.351
4-3	4	0.369	0.469	0.492	0.502	1.301
6-1	6	0.408	0.511	0.537	0.547	1.416
6-3	6	0.422	0.519	0.542	0.552	1.429
9-1	9	0.447	0.534	0.554	0.563	1.459
9-2	9	0.429	0.520	0.546	0.556	1.441
12-1	12	0.442	0.535	0.559	0.569	1.473
12-2	12.3	0.433	0.536	0.562	0.572	1.485
12-3	12	0.447	0.542	0.565	0.575	1.490
15-1	15	0.458	0.558	0.575	0.585	1.517
15-2	15	0.458	0.555	0.573	0.583	1.510
15-3	15	0.442	0.543	0.568	0.578	1.497
20-1	20	0.456	0.551	0.570	0.580	1.502
20-2	20	0.473	0.560	0.576	0.586	1.519
20-3	20	0.476	0.567	0.579	0.589	1.528
25-1	25	0.458	0.553	0.568	0.583	1.515
25-2	25.3	0.463	0.556	0.571	0.585	1.518
25-3	25	0.463	0.556	0.572	0.587	1.522
30-1	30	0.463	0.557	0.574	0.584	1.520
30-2	30	0.469	0.562	0.580	0.590	1.533
30-3	30	0.447	0.553	0.577	0.587	1.524
40-1	40	0.471	0.563	0.579	0.589	1.534
40-2	40	0.468	0.565	0.582	0.592	1.539
40-3	40	0.468	0.565	0.583	0.593	1.541
60-1	60	0.449	0.551	0.571	0.581	1.511
60-2	60	0.476	0.584	0.590	0.600	1.560
60-3	60	0.459	0.563	0.582	0.593	1.540
90-1	90	0.456	0.558	0.575	0.586	1.523
90-2	90	0.468	0.568	0.585	0.595	1.547
90-3	90	0.464	0.567	0.585	0.595	1.547

Table B-10. BTEX sorption data from MSB-0.35T batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.173	0.356	0.253	0.262	0.253
0.5-2	0.5	0.150	0.322	0.251	0.258	0.246
0.5-3	4	0.396	0.812	0.511	0.523	0.513
1-1	1	0.250	0.502	0.314	0.271	0.314
1-2	1	0.259	0.507	0.313	0.268	0.312
1-3	1	0.256	0.521	0.326	0.284	0.325
2-1	2	0.345	0.680	0.402	0.412	0.408
2-2	2	0.333	0.674	0.394	0.403	0.401
2-3	2	0.337	0.672	0.398	0.408	0.404
4-1	4	0.382	0.800	0.501	0.513	0.504
4-2	4	0.378	0.786	0.488	0.500	0.491
4-3	4	0.372	0.788	0.494	0.506	0.497
6-1	6	0.433	0.861	0.538	0.550	0.538
6-2	6	0.434	0.838	0.528	0.541	0.530
6-3	5.9	0.438	0.877	0.544	0.556	0.544
9-1	9	0.448	0.891	0.558	0.571	0.559
9-2	2.8	0.370	0.755	0.449	0.459	0.453
9-3	9	0.460	0.905	0.565	0.578	0.565
12-1	12	0.462	0.886	0.558	0.571	0.560
12-2	12	0.477	0.903	0.565	0.578	0.567
15-1	15.1	0.471	0.923	0.573	0.586	0.574
15-2	15	0.490	0.936	0.576	0.589	0.577
15-3	15	0.484	0.936	0.578	0.591	0.580
20-1	20	0.486	0.940	0.579	0.592	0.579
20-2	20	0.491	0.947	0.583	0.596	0.584
20-3	20	0.475	0.934	0.579	0.593	0.581
25-1	25	0.480	0.931	0.577	0.592	0.581
25-2	25	0.480	0.930	0.577	0.591	0.580
25-3	25	0.478	0.934	0.580	0.594	0.583
30-1	30	0.477	0.941	0.579	0.592	0.580
30-2	30	0.475	0.940	0.583	0.596	0.585
40-1	40	0.487	0.953	0.585	0.598	0.586
40-2	40	0.470	0.941	0.585	0.598	0.586
40-3	40	0.483	0.952	0.588	0.601	0.590
60-1	60	0.494	0.965	0.594	0.607	0.596
60-2	60	0.485	0.956	0.590	0.603	0.592
60-3	60	0.483	0.950	0.586	0.599	0.588
90-1	90	0.490	0.956	0.587	0.600	0.589
90-2	90	0.490	0.965	0.595	0.608	0.598
90-3	90	0.489	0.964	0.594	0.608	0.597

Table B-11. BTEX sorption data from MSB-0.35E batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.162	0.202	0.486	0.261	0.271
0.5-2	0.5	0.195	0.227	0.480	0.256	0.267
0.5-3	0.5	0.158	0.186	0.363	0.189	0.203
1-1	1	0.274	0.320	0.608	0.281	0.352
1-2	1	0.231	0.281	0.550	0.244	0.319
2-1	2	0.328	0.395	0.753	0.409	0.433
2-2	2	0.316	0.398	0.724	0.391	0.420
2-3	2	0.328	0.397	0.708	0.384	0.412
4-1	4	0.381	0.489	0.945	0.515	0.547
4-2	4	0.382	0.485	0.917	0.499	0.534
4-3	4	0.374	0.483	0.925	0.505	0.540
6-1	6	0.413	0.513	0.973	0.539	0.567
6-2	6	0.425	0.516	0.966	0.528	0.563
6-3	6	0.420	0.518	0.976	0.534	0.570
9-1	9	0.438	0.533	1.000	0.546	0.582
9-2	9	0.446	0.541	1.015	0.555	0.591
9-3	9	0.425	0.528	1.002	0.548	0.583
12-1	12	0.454	0.549	1.022	0.558	0.595
12-2	12	0.432	0.547	1.036	0.567	0.603
12-3	12	0.430	0.530	1.011	0.554	0.590
15-1	15	0.452	0.550	1.028	0.562	0.600
15-2	15	0.443	0.545	1.027	0.562	0.600
15-3	15	0.441	0.540	1.024	0.560	0.597
20-1	20	0.464	0.559	1.038	0.567	0.604
20-2	20	0.467	0.567	1.045	0.571	0.610
20-3	20	0.452	0.553	1.035	0.566	0.604
25-1	25	0.461	0.558	1.036	0.568	0.606
25-2	25	0.460	0.560	1.041	0.571	0.610
30-1	30	0.466	0.562	1.044	0.569	0.606
30-2	30	0.464	0.564	1.050	0.574	0.612
30-3	30	0.457	0.559	1.043	0.570	0.609
40-1	40	0.451	0.559	1.047	0.571	0.609
40-2	40	0.471	0.569	1.057	0.577	0.617
40-3	40	0.469	0.569	1.056	0.577	0.617
60-1	60	0.463	0.565	1.050	0.574	0.614
60-2	60	0.472	0.573	1.063	0.581	0.622
60-3	60	0.469	0.571	1.059	0.579	0.620
90-1	90	0.462	0.567	1.055	0.577	0.617
90-2	90	0.468	0.572	1.064	0.582	0.622
90-3	90	0.468	0.572	1.062	0.581	0.622

Table B-12. BTEX sorption data from MSB-0.35M batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.139	0.185	0.238	0.423	0.231
0.5-2	0.5	0.113	0.159	0.206	0.367	0.199
0.5-3	0.5	0.161	0.214	0.252	0.447	0.245
1-1	1	0.263	0.333	0.359	0.622	0.351
1-2	1	0.216	0.284	0.301	0.513	0.289
1-3	1	0.275	0.346	0.350	0.595	0.335
2-2	2	0.318	0.397	0.410	0.715	0.400
2-3	2	0.305	0.380	0.409	0.716	0.395
4-1	4	0.379	0.463	0.505	0.883	0.488
4-2	4	0.340	0.443	0.497	0.867	0.482
4-3	4	0.360	0.466	0.526	0.917	0.510
6-1	6	0.408	0.506	0.558	0.970	0.538
6-2	6	0.419	0.510	0.559	0.972	0.539
6-3	6	0.418	0.512	0.564	0.981	0.545
9-2	9	0.435	0.525	0.579	1.005	0.559
9-3	9	0.435	0.527	0.582	1.011	0.562
12-1	12	0.443	0.511	0.571	0.995	0.553
12-2	12	0.428	0.520	0.579	1.007	0.560
12-3	12	0.448	0.545	0.590	1.025	0.570
15-1	15	0.448	0.534	0.587	1.020	0.567
15-3	15	0.455	0.538	0.590	1.024	0.570
20-1	20	0.459	0.548	0.595	1.032	0.574
20-2	20	0.467	0.555	0.602	1.044	0.582
25-1	25	0.462	0.543	0.598	1.039	0.578
25-2	25	0.458	0.540	0.596	1.036	0.577
25-3	25	0.461	0.540	0.595	1.035	0.576
30-1	30	0.478	0.560	0.602	1.046	0.580
30-2	30	0.471	0.556	0.603	1.047	0.583
30-3	30	0.457	0.550	0.602	1.045	0.582
40-1	40	0.465	0.556	0.604	1.050	0.583
40-2	40	0.449	0.550	0.603	1.049	0.584
40-3	40	0.454	0.552	0.605	1.050	0.585
60-1	60	0.468	0.555	0.601	1.043	0.582
60-2	60	0.460	0.557	0.607	1.053	0.588
60-3	60	0.459	0.556	0.607	1.054	0.588
90-1	90	0.458	0.553	0.602	1.046	0.583
90-2	90	0.462	0.559	0.609	1.057	0.590
90-3	90	0.464	0.560	0.609	1.058	0.590

Table B-13. BTEX sorption data from MSB-0.35O batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg)				
		Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.168	0.223	0.270	0.268	0.473
0.5-2	0.5	0.154	0.208	0.237	0.235	0.420
0.5-3	0.5	0.118	0.177	0.231	0.230	0.403
1-1	1	0.187	0.259	0.312	0.291	0.547
1-2	1	0.244	0.304	0.311	0.288	0.543
1-3	1	0.260	0.337	0.351	0.329	0.617
2-1	2	0.337	0.434	0.434	0.427	0.767
2-2	2	0.351	0.440	0.431	0.424	0.765
2-3	2	0.308	0.408	0.415	0.409	0.737
4-1	4	0.350	0.477	0.500	0.493	0.888
4-2	4	0.344	0.468	0.493	0.486	0.873
4-3	4	0.358	0.479	0.506	0.499	0.893
6-1	6	0.401	0.519	0.539	0.531	0.951
6-3	6	0.403	0.519	0.537	0.529	0.948
9-1	9	0.412	0.530	0.551	0.543	0.971
9-2	9	0.420	0.538	0.559	0.550	0.986
9-3	9	0.425	0.541	0.560	0.551	0.987
12-2	12	0.422	0.538	0.562	0.554	0.991
12-3	12	0.426	0.553	0.569	0.561	1.004
15-1	15	0.435	0.555	0.573	0.564	1.011
15-2	15	0.443	0.562	0.574	0.565	1.012
15-3	15	0.441	0.555	0.572	0.563	1.009
20-1	20	0.432	0.552	0.570	0.562	1.005
20-2	20	0.442	0.560	0.578	0.569	1.021
20-3	20	0.437	0.557	0.575	0.567	1.017
25-1	25.3	0.434	0.559	0.576	0.569	1.023
25-2	25	0.440	0.560	0.576	0.570	1.023
25-3	25	0.424	0.552	0.572	0.566	1.016
30-1	30	0.449	0.564	0.577	0.568	1.020
30-2	30.2	0.445	0.565	0.581	0.573	1.028
30-3	30	0.441	0.563	0.581	0.572	1.026
40-1	40	0.434	0.562	0.580	0.572	1.029
40-2	40	0.439	0.565	0.583	0.574	1.032
40-3	40	0.443	0.567	0.584	0.575	1.034
60-1	60	0.451	0.568	0.581	0.573	1.029
60-2	60	0.434	0.564	0.583	0.575	1.032
60-3	60	0.434	0.566	0.585	0.577	1.036
90-2	90	0.444	0.572	0.589	0.581	1.043
90-3	90	0.439	0.570	0.589	0.581	1.043

Table B-14. Overall results from MSB-0.0.5 batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.76	9.27	0.20	0.957	0.047	9.81	3.002	2.13	1850
Toluene	18.22	4.73	0.11	0.890	0.049	9.81	3.002	2.69	470
Ethylbenzene	36.25	3.59	0.07	0.931	0.05	9.81	3.002	3.15	140
M-Xylene	38.33	3.55	0.06	0.924	0.049	9.81	3.002	3.20	173
O-Xylene	34.39	3.45	0.07	0.912	0.05	9.81	3.002	3.15	204

Table B-15. Overall results from MSB-0.1 batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.27	8.52	0.16	0.96	0.103	9.77	3.002	2.13	1850
Toluene	17.53	4.96	0.09	0.939	0.112	9.77	3.002	2.69	470
Ethylbenzene	34.73	3.40	0.04	0.921	0.098	9.77	3.002	3.15	140
M-Xylene	37.25	2.95	0.03	0.947	0.098	9.77	3.002	3.2	173
O-Xylene	34.41	3.19	0.04	0.923	0.108	9.77	3.002	3.15	204

Table B-16. Overall results from MSB-0.2 batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.31	7.61	0.2	0.984	0.214	9.85	2.998	2.13	1850
Toluene	17.68	4.45	0.08	0.945	0.194	9.85	2.998	2.69	470
Ethylbenzene	35.37	2.63	0.03	0.944	0.193	9.85	2.998	3.15	140
M-Xylene	37.51	2.14	0.01	0.9	0.187	9.85	2.998	3.2	173
O-Xylene	34.71	2.54	0.03	0.938	0.211	9.85	2.998	3.15	204

Table B-17. Overall results from MSB-0.3 batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.67	6.5	0.11	0.925	0.293	9.84	3	2.13	1850
Toluene	17.96	3.84	0.06	0.923	0.296	9.84	3	2.69	470
Ethylbenzene	35.44	2.41	0.04	0.96	0.282	9.84	3	3.15	140
M-Xylene	37.9	1.94	0.04	0.943	0.27	9.84	3	3.2	173
O-Xylene	34.91	2.35	0.04	0.962	0.28	9.84	3	3.15	204

Table B-18. Overall results from MSB-0.35T batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.85	7.07	0.14	0.954	0.2	9.78	3.003	2.13	1850
Toluene	18.6	3.63	0.07	0.908	0.476	9.78	3.003	2.69	470
Ethylbenzene	35.09	2.05	0.03	0.926	0.189	9.78	3.003	3.15	140
M-Xylene	36.58	1.87	0.02	0.922	0.179	9.78	3.003	3.2	173
O-Xylene	33.94	2.03	0.03	0.913	0.184	9.78	3.003	3.15	204

Table B-19. Overall results from MSB-0.35E batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.13	7.75	0.12	0.924	0.188	9.89	3.004	2.13	1850
Toluene	17.25	4.35	0.06	0.939	0.195	9.89	3.004	2.69	470
Ethylbenzene	35.42	2.34	0.05	0.95	0.475	9.89	3.004	3.15	140
M-Xylene	36.39	2.07	0.03	0.895	0.19	9.89	3.004	3.2	173
O-Xylene	33.14	2.26	0.04	0.925	0.201	9.89	3.004	3.15	204

Table B-20. Overall results from MSB-0.35M batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.55	7.08	0.18	0.975	0.188	9.84	3.008	2.13	1850
Toluene	17.3	3.52	0.07	0.957	0.192	9.84	3.008	2.69	470
Ethylbenzene	34.86	2.16	0.04	0.965	0.205	9.84	3.008	3.15	140
M-Xylene	37.98	1.92	0.03	0.947	0.472	9.84	3.008	3.2	173
O-Xylene	33.9	2.1	0.04	0.931	0.197	9.84	3.008	3.15	204

Table B-21. Overall results from MSB-0.35O batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.21	6.94	0.15	0.971	0.205	9.87	2.998	2.13	1850
Toluene	17.68	3.33	0.08	0.902	0.202	9.87	2.998	2.69	470
Ethylbenzene	34.77	2.08	0.04	0.908	0.192	9.87	2.998	3.15	140
M-Xylene	37.4	2.16	0.03	0.941	0.192	9.87	2.998	3.2	173
O-Xylene	35.24	1.93	0.04	0.894	0.509	9.87	2.998	3.15	204

Table B-22. Overall results from MSB-0.5T batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.27	7.11	0.11	0.966	0.214	9.80	3.005	2.13	1850
Toluene	17.75	3.54	0.05	0.92	0.344	9.80	3.005	2.69	470
Ethylbenzene	35.01	2.21	0.03	0.961	0.196	9.80	3.005	3.15	140
M-Xylene	37.36	2.05	0.02	0.955	0.199	9.80	3.005	3.2	173
O-Xylene	34.72	2.18	0.03	0.954	0.197	9.80	3.005	3.15	204

Table B-23. Overall results from MSB-0.5E batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.64	6.81	0.11	0.961	0.202	9.84	3.003	2.13	1850
Toluene	17.66	3.87	0.05	0.945	0.204	9.84	3.003	2.69	470
Ethylbenzene	36.09	2.35	0.03	0.93	0.349	9.84	3.003	3.15	140
M-Xylene	37.7	2.22	0.02	0.964	0.19	9.84	3.003	3.2	173
O-Xylene	34.8	2.33	0.03	0.961	0.205	9.84	3.003	3.15	204

Table B-24. Overall results from MSB-0.5M batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.43	7.1	0.08	0.971	0.203	9.81	2.999	2.13	1850
Toluene	17.31	4.11	0.05	0.941	0.201	9.81	2.999	2.69	470
Ethylbenzene	34.52	2.35	0.02	0.946	0.202	9.81	2.999	3.15	140
M-Xylene	37.49	2.23	0.02	0.954	0.348	9.81	2.999	3.2	173
O-Xylene	34.14	2.38	0.02	0.944	0.195	9.81	2.999	3.15	204

Table B-25. Overall results from MSB-0.5O batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	7.53	7.4	0.08	0.932	0.192	9.84	3.001	2.13	1850
Toluene	17.63	3.91	0.04	0.924	0.204	9.84	3.001	2.69	470
Ethylbenzene	34.91	2.46	0.03	0.96	0.194	9.84	3.001	3.15	140
M-Xylene	37.4	2.23	0.02	0.938	0.19	9.84	3.001	3.2	173
O-Xylene	34.98	2.4	0.03	0.957	0.343	9.84	3.001	3.15	204

APPENDIX C. MONOLAYER SMZ BATCH EXPERIMENT DATA

The monolayer batch experiment data is contained in this appendix. Tables C-1 through C-3 contain the BTEX sorption data from each experiment. The overall results from each experiment are displayed in Tables C-4 through C-6. Three replicate batch experiments with the same initial conditions were run, and are referred to as M1, M2, and M3 batch experiments.

Table C-1. BTEX sorption data from M1 monolayer batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg) Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.176	0.240	0.271	0.326	0.279
0.5-2	0.5	0.154	0.228	0.264	0.318	0.272
0.5-3	0.5	0.140	0.233	0.274	0.331	0.284
1-1	1	0.132	0.195	0.253	0.307	0.264
1-2	1	0.140	0.200	0.255	0.310	0.267
1-3	1	0.152	0.206	0.260	0.316	0.271
2-1	2	0.180	0.248	0.286	0.344	0.298
2-2	2	0.173	0.233	0.271	0.327	0.282
2-3	2	0.158	0.230	0.273	0.330	0.285
4-1	4	0.170	0.236	0.276	0.334	0.289
4-2	4	0.148	0.224	0.271	0.329	0.285
4-3	4	0.170	0.242	0.283	0.342	0.297
6-1	6.67	0.197	0.262	0.295	0.355	0.309
6-2	6	0.198	0.262	0.295	0.355	0.308
6-3	6	0.185	0.247	0.288	0.347	0.301
9-1	9	0.210	0.266	0.296	0.355	0.309
9-2	9	0.188	0.259	0.294	0.355	0.308
9-3	9	0.214	0.279	0.304	0.365	0.317
12-1	12	0.177	0.252	0.292	0.352	0.306
12-2	12	0.178	0.252	0.291	0.351	0.306
12-3	12	0.187	0.258	0.295	0.356	0.310
15-2	15	0.215	0.277	0.305	0.367	0.319
15-3	15	0.229	0.285	0.309	0.371	0.324
20-1	20	0.205	0.272	0.302	0.364	0.317
20-2	20	0.223	0.284	0.310	0.372	0.325
25-1	25	0.219	0.281	0.309	0.371	0.323
25-2	25	0.215	0.281	0.309	0.372	0.324
25-3	25	0.215	0.281	0.310	0.372	0.325
30-1	30	0.242	0.295	0.313	0.375	0.325
30-2	30	0.215	0.280	0.308	0.370	0.322
30-3	30	0.238	0.289	0.312	0.374	0.326
40-1	40	0.211	0.278	0.306	0.368	0.319
40-2	40	0.206	0.276	0.306	0.368	0.321
40-3	40	0.219	0.284	0.310	0.373	0.326
60-1	60	0.228	0.286	0.309	0.372	0.324
60-2	60	0.224	0.286	0.311	0.374	0.327
60-3	60	0.217	0.284	0.311	0.374	0.327
90-1	90	0.208	0.280	0.309	0.372	0.325
90-2	90	0.222	0.288	0.314	0.378	0.330
90-3	90	0.219	0.287	0.315	0.379	0.331

Table C-2. BTEX sorption data from M2 monolayer batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg) Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.187	0.237	0.272	0.281	0.291
0.5-2	0.5	0.176	0.231	0.272	0.281	0.290
0.5-3	0.5	0.165	0.224	0.265	0.274	0.284
1-1	1	0.154	0.230	0.279	0.287	0.301
1-2	1	0.166	0.240	0.287	0.295	0.310
1-3	1	0.157	0.235	0.284	0.293	0.306
2-1	2	0.193	0.258	0.292	0.301	0.314
2-2	2	0.206	0.265	0.296	0.305	0.318
2-3	2	0.220	0.276	0.303	0.312	0.326
4-1	4	0.213	0.280	0.309	0.318	0.332
4-2	4	0.209	0.274	0.305	0.313	0.327
4-3	4	0.216	0.282	0.311	0.320	0.335
6-1	6	0.201	0.265	0.303	0.313	0.328
6-2	6	0.207	0.268	0.303	0.312	0.326
6-3	6	0.211	0.284	0.316	0.325	0.341
9-1	9	0.220	0.297	0.320	0.329	0.345
9-2	9	0.239	0.308	0.326	0.334	0.351
9-3	9	0.228	0.301	0.322	0.330	0.346
12-1	12	0.221	0.288	0.317	0.325	0.341
12-2	12	0.228	0.294	0.320	0.329	0.346
12-3	12	0.225	0.292	0.319	0.328	0.345
15-1	15	0.212	0.283	0.316	0.325	0.341
15-2	15	0.215	0.285	0.316	0.326	0.342
15-3	15	0.237	0.301	0.324	0.333	0.350
20-1	20	0.246	0.307	0.328	0.336	0.354
20-2	20	0.231	0.295	0.320	0.328	0.345
20-3	20	0.256	0.313	0.329	0.337	0.354
25-1	25	0.239	0.303	0.326	0.335	0.352
25-2	25	0.241	0.303	0.325	0.333	0.350
25-3	25	0.235	0.302	0.327	0.335	0.352
30-1	30	0.246	0.307	0.327	0.335	0.351
30-2	30	0.235	0.300	0.324	0.333	0.349
30-3	30	0.250	0.310	0.329	0.338	0.355
40-1	40	0.246	0.306	0.325	0.333	0.349
40-2	40	0.238	0.305	0.328	0.336	0.353
40-3	40	0.233	0.302	0.327	0.336	0.353
60-1	60	0.236	0.297	0.322	0.331	0.349
60-2	60	0.227	0.294	0.323	0.332	0.350
90-1	90	0.233	0.300	0.326	0.335	0.353
90-2	90	0.238	0.305	0.330	0.339	0.357
90-3	90	0.240	0.307	0.331	0.339	0.358

Table C-3. BTEX sorption data from M3 monolayer batch experiment.

Sample	Experiment Time (min)	Amount Sorbed (mmol/kg) Benzene	Toluene	Ethylbenzene	M-Xylene	O-Xylene
0.5-1	0.5	0.149	0.221	0.278	0.277	0.291
0.5-2	0.5	0.156	0.220	0.274	0.273	0.286
0.5-3	0.5	0.123	0.190	0.246	0.247	0.260
1-1	1	0.131	0.212	0.273	0.271	0.288
1-2	1	0.119	0.199	0.263	0.261	0.277
1-3	1	0.127	0.207	0.268	0.267	0.283
2-1	2	0.180	0.247	0.290	0.288	0.305
2-2	2	0.183	0.261	0.302	0.299	0.317
2-3	2	0.191	0.264	0.302	0.300	0.318
4-1	4	0.182	0.250	0.293	0.291	0.307
4-3	4	0.192	0.262	0.304	0.302	0.320
6-1	6	0.188	0.261	0.304	0.302	0.321
6-2	6	0.176	0.251	0.298	0.296	0.314
9-1	9	0.201	0.270	0.309	0.307	0.325
9-2	9	0.209	0.272	0.310	0.306	0.325
9-3	9	0.210	0.272	0.308	0.305	0.324
12-1	12	0.200	0.270	0.310	0.307	0.327
12-2	12	0.187	0.263	0.306	0.304	0.323
12-3	12	0.199	0.268	0.308	0.305	0.324
15-1	15	0.201	0.270	0.311	0.308	0.328
15-2	15	0.195	0.268	0.310	0.307	0.327
15-3	15	0.205	0.272	0.311	0.308	0.328
20-1	20	0.216	0.281	0.316	0.312	0.332
20-2	20	0.228	0.288	0.320	0.316	0.336
20-3	20	0.233	0.294	0.322	0.318	0.338
25-1	24.57	0.219	0.281	0.316	0.311	0.330
25-2	25	0.222	0.285	0.320	0.314	0.335
25-3	25	0.223	0.283	0.318	0.312	0.332
30-1	30	0.222	0.285	0.317	0.313	0.332
30-2	30	0.226	0.286	0.318	0.315	0.335
30-3	30	0.232	0.292	0.322	0.319	0.340
40-1	40	0.222	0.294	0.321	0.316	0.336
40-2	40	0.225	0.288	0.321	0.317	0.337
40-3	40	0.225	0.294	0.323	0.319	0.340
60-1	60	0.221	0.284	0.316	0.313	0.333
60-2	60	0.225	0.288	0.320	0.317	0.337
60-3	60	0.224	0.288	0.320	0.317	0.338
90-1	90	0.213	0.282	0.317	0.314	0.335
90-2	90	0.204	0.279	0.318	0.315	0.335
90-3	90	0.216	0.285	0.321	0.317	0.338

Table C-4. Overall results from M1 monolayer batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	5.25	4.97	0.43	0.784	0.108	9.94	2.997	2.13	1850
Toluene	12.86	4.08	0.39	0.811	0.107	9.94	2.997	2.69	470
Ethylbenzene	26.61	3.59	0.36	0.889	0.105	9.94	2.997	3.15	140
M-Xylene	28.26	3.8	0.36	0.895	0.125	9.94	2.997	3.2	173
O-Xylene	25.33	3.48	0.35	0.908	0.111	9.94	2.997	3.15	204

Table C-5. Overall results from M2 monolayer batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	6.22	5.91	0.44	0.781	0.11	9.97	2.996	2.13	1850
Toluene	13.53	5.18	0.36	0.864	0.114	9.97	2.996	2.69	470
Ethylbenzene	26.85	4.97	0.33	0.907	0.11	9.97	2.996	3.15	140
M-Xylene	28.52	4.26	0.32	0.897	0.113	9.97	2.996	3.2	173
O-Xylene	25.57	4.57	0.33	0.904	0.12	9.97	2.996	3.15	204

Table C-6. Overall results from M3 monolayer batch experiment.

Constituent	K_d (L/kg)	k_2 (1/hr)	F	Bicontinuum Fit (r^2)	Starting Conc. (mmol/L)	Water Added (mL)	Zeolite Added (g)	Log K_{ow}	Solubility (mg/L)
Benzene	5.99	6.35	0.38	0.766	0.105	9.97	3.004	2.13	1850
Toluene	13.83	4.25	0.36	0.772	0.107	9.97	3.004	2.69	470
Ethylbenzene	28.3	4.49	0.35	0.817	0.107	9.97	3.004	3.15	140
M-Xylene	30.09	4.71	0.35	0.816	0.105	9.97	3.004	3.2	173
O-Xylene	27	4.85	0.36	0.831	0.113	9.97	3.004	3.15	204

APPENDIX D. BTEX ISOTHERMS FROM BATCH EXPERIMENT'S EQUILIBRIUM DATA.

Overall, nineteen batch experiments were run for the current research project. Because each vial was essentially an independent batch experiment, hundreds of equilibrium data points (vials allowed to shake for greater than twenty minutes) for each constituent were gathered. Batch equilibrium isotherms for individual constituents were constructed using the equilibrium data from each test. The equilibrium batch experiment data can be seen in Tables D-1 through D-5, and the overall isotherm results can be seen in Table D-6. Figures D-1 through D-5 represent the isotherm results from the equilibrium batch experiment data. Prior to this analysis, complete equilibrium was assumed to occur after twenty minutes. However, inspection of Figures D-1 through D-5 reveals that only a "quasi" equilibrium was reached over the entire batch experiment time period. Minimal changes (3-5.5%) in total sorption are observed; however, a 10-30% change in "equilibrium" aqueous concentration is observed for all five constituents at maximum concentrations (see Table D-7). As expected, a closer inspection of the data revealed a decreasing trend in aqueous concentration over the entire "equilibrium" period. The data from twenty minutes and ninety minutes (batch experiment completion) can be seen in Tables D-8 through D-12, with the overall data trends in Table D-7. Figures D-6 through D-10 display the "equilibrium" conditions for the twenty and ninety minute samples. These results indicate an increase in K_d from the ninety-minute samples, representing a decrease in aqueous concentration.

Table D-1. Benzene equilibrium data from kinetic batch experiments

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.081	0.596	0.015	0.107	0.064	0.490
0.081	0.586	0.014	0.108	0.067	0.485
0.074	0.625	0.013	0.113	0.065	0.486
0.073	0.626	0.013	0.112	0.059	0.500
0.074	0.607	0.013	0.111	0.089	0.667
0.073	0.625	0.014	0.111	0.086	0.677
0.074	0.624	0.014	0.107	0.088	0.671
0.066	0.647	0.014	0.110	0.085	0.676
0.078	0.609	0.014	0.109	0.088	0.677
0.075	0.599	0.013	0.112	0.085	0.687
0.078	0.609	0.013	0.112	0.084	0.688
0.075	0.619	0.032	0.232	0.086	0.680
0.077	0.609	0.032	0.230	0.083	0.689
0.076	0.617	0.032	0.232	0.089	0.653
0.075	0.619	0.035	0.227	0.090	0.670
0.079	0.615	0.032	0.230	0.092	0.657
0.073	0.626	0.034	0.224	0.089	0.674
0.081	0.551	0.030	0.238	0.087	0.675
0.084	0.539	0.031	0.234	0.092	0.652
0.085	0.541	0.030	0.237	0.092	0.663
0.083	0.552	0.033	0.226	0.085	0.683
0.078	0.560	0.031	0.232	0.061	0.457
0.083	0.539	0.031	0.233	0.059	0.458
0.076	0.562	0.033	0.230	0.060	0.455
0.077	0.564	0.032	0.232	0.059	0.462
0.076	0.561	0.030	0.236	0.062	0.454
0.078	0.562	0.032	0.233	0.058	0.464
0.072	0.582	0.031	0.231	0.057	0.468
0.074	0.579	0.032	0.236	0.058	0.462
0.076	0.574	0.067	0.484	0.058	0.462
0.079	0.568	0.068	0.478	0.057	0.466
0.077	0.569	0.067	0.480	0.057	0.463
0.077	0.562	0.066	0.485	0.059	0.462
0.075	0.576	0.067	0.482	0.056	0.466
0.076	0.565	0.071	0.471	0.057	0.467
0.013	0.109	0.067	0.481	0.061	0.456
0.013	0.115	0.065	0.490	0.060	0.458
0.014	0.110	0.063	0.501	0.058	0.429
0.014	0.110	0.071	0.470	0.060	0.419
0.015	0.107	0.064	0.493	0.057	0.431
0.014	0.111	0.066	0.481	0.062	0.418
0.015	0.107	0.068	0.480	0.060	0.422

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.062	0.419	0.066	0.459	0.061	0.461
0.060	0.422	0.067	0.456	0.057	0.478
0.059	0.424	0.063	0.468	0.058	0.471
0.060	0.419	0.063	0.464	0.063	0.457
0.061	0.416	0.066	0.486	0.061	0.465
0.058	0.427	0.064	0.491	0.067	0.449
0.059	0.425	0.068	0.475	0.064	0.454
0.058	0.427	0.066	0.480	0.062	0.468
0.057	0.433	0.066	0.480	0.063	0.460
0.060	0.420	0.068	0.478	0.062	0.459
0.058	0.423	0.068	0.477	0.063	0.458
0.059	0.429	0.069	0.475	0.062	0.462
0.056	0.431	0.066	0.487	0.062	0.464
0.057	0.435	0.070	0.470	0.060	0.432
0.056	0.431	0.066	0.483	0.057	0.442
0.059	0.423	0.064	0.494	0.059	0.437
0.057	0.428	0.067	0.485	0.059	0.434
0.056	0.434	0.067	0.483	0.058	0.440
0.059	0.419	0.064	0.490	0.063	0.424
0.057	0.428	0.066	0.490	0.056	0.449
0.055	0.434	0.065	0.489	0.055	0.445
0.056	0.429	0.061	0.464	0.057	0.441
0.056	0.434	0.058	0.467	0.059	0.434
0.059	0.422	0.063	0.452	0.059	0.439
0.057	0.426	0.063	0.461	0.056	0.443
0.055	0.432	0.062	0.460	0.057	0.451
0.058	0.422	0.060	0.466	0.059	0.434
0.056	0.426	0.060	0.464	0.060	0.434
0.055	0.432	0.062	0.457	0.058	0.444
0.066	0.456	0.062	0.451	0.057	0.439
0.062	0.473	0.060	0.471		
0.063	0.458	0.058	0.469		
0.064	0.463	0.061	0.463		
0.065	0.463	0.060	0.472		
0.064	0.463	0.060	0.469		
0.063	0.469	0.061	0.462		
0.068	0.447	0.060	0.468		
0.062	0.471	0.059	0.468		
0.063	0.468	0.064	0.459		
0.062	0.468	0.062	0.467		
0.068	0.449	0.061	0.462		
0.061	0.476	0.062	0.458		

Table D-2. Toluene equilibrium data from kinetic batch experiments

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.033	0.492	0.008	0.133	0.029	0.539
0.032	0.496	0.008	0.134	0.030	0.539
0.031	0.500	0.007	0.138	0.031	0.535
0.029	0.508	0.007	0.137	0.024	0.558
0.028	0.508	0.007	0.136	0.026	0.546
0.029	0.506	0.007	0.135	0.050	0.807
0.030	0.503	0.008	0.135	0.046	0.821
0.028	0.511	0.007	0.136	0.050	0.808
0.027	0.511	0.007	0.135	0.048	0.812
0.027	0.513	0.007	0.138	0.050	0.810
0.024	0.521	0.007	0.138	0.044	0.828
0.026	0.517	0.019	0.303	0.043	0.832
0.028	0.510	0.018	0.302	0.045	0.826
0.024	0.523	0.018	0.303	0.043	0.833
0.025	0.522	0.019	0.302	0.045	0.816
0.029	0.508	0.018	0.303	0.045	0.827
0.024	0.523	0.019	0.301	0.048	0.813
0.024	0.520	0.017	0.308	0.044	0.828
0.040	0.615	0.017	0.307	0.043	0.831
0.041	0.609	0.017	0.308	0.046	0.822
0.042	0.610	0.018	0.304	0.042	0.835
0.041	0.615	0.017	0.307	0.073	1.317
0.038	0.621	0.017	0.308	0.075	1.307
0.041	0.609	0.018	0.305	0.070	1.324
0.037	0.622	0.017	0.309	0.084	1.283
0.037	0.625	0.016	0.312	0.075	1.312
0.037	0.621	0.017	0.307	0.072	1.318
0.036	0.626	0.016	0.309	0.071	1.324
0.033	0.638	0.016	0.312	0.071	1.318
0.034	0.635	0.030	0.537	0.065	1.335
0.037	0.626	0.031	0.536	0.069	1.326
0.037	0.628	0.030	0.537	0.068	1.329
0.035	0.630	0.031	0.533	0.067	1.329
0.037	0.623	0.032	0.533	0.072	1.317
0.034	0.635	0.034	0.525	0.067	1.330
0.034	0.632	0.032	0.529	0.066	1.336
0.007	0.137	0.031	0.535	0.073	1.318
0.008	0.134	0.029	0.542	0.069	1.327
0.008	0.134	0.032	0.531	0.033	0.536
0.008	0.133	0.030	0.539	0.033	0.533
0.007	0.135	0.030	0.535	0.032	0.540
0.008	0.132	0.033	0.529	0.034	0.532

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.032	0.538	0.030	0.565	0.029	0.572
0.034	0.533	0.035	0.551	0.033	0.548
0.032	0.537	0.025	0.584	0.031	0.555
0.032	0.536	0.031	0.563	0.037	0.536
0.031	0.540	0.033	0.558	0.034	0.543
0.031	0.538	0.030	0.568	0.035	0.540
0.030	0.544	0.029	0.567	0.035	0.540
0.031	0.539	0.056	0.940	0.030	0.560
0.029	0.549	0.054	0.947	0.030	0.556
0.027	0.554	0.057	0.934	0.032	0.550
0.032	0.537	0.058	0.931	0.030	0.556
0.029	0.544	0.058	0.930	0.033	0.550
0.029	0.549	0.058	0.934	0.031	0.552
0.033	0.523	0.055	0.941	0.031	0.555
0.028	0.536	0.056	0.940	0.030	0.557
0.032	0.528	0.048	0.964	0.030	0.556
0.032	0.526	0.053	0.953	0.031	0.553
0.033	0.522	0.055	0.941	0.029	0.559
0.032	0.525	0.051	0.952	0.030	0.560
0.030	0.534	0.049	0.965	0.035	0.552
0.031	0.529	0.052	0.956	0.032	0.560
0.030	0.531	0.053	0.950	0.034	0.557
0.030	0.532	0.051	0.956	0.032	0.559
0.030	0.532	0.050	0.965	0.033	0.560
0.030	0.534	0.049	0.964	0.035	0.552
0.034	0.520	0.034	0.559	0.032	0.564
0.031	0.529	0.030	0.567	0.030	0.565
0.029	0.534	0.035	0.553	0.031	0.563
0.031	0.528	0.035	0.558	0.032	0.562
0.029	0.531	0.033	0.560	0.031	0.565
0.027	0.542	0.036	0.548	0.030	0.567
0.035	0.551	0.032	0.562	0.031	0.568
0.032	0.560	0.032	0.564	0.031	0.564
0.030	0.567	0.033	0.559	0.031	0.566
0.033	0.553	0.032	0.559	0.034	0.558
0.033	0.556	0.031	0.569	0.030	0.572
0.033	0.556	0.030	0.569	0.029	0.570
0.033	0.557	0.031	0.565		
0.032	0.562	0.030	0.573		
0.034	0.553	0.030	0.571		
0.031	0.563	0.031	0.567		
0.031	0.565	0.030	0.572		

Table D-3. Ethylbenzene equilibrium data from kinetic batch experiments

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.017	0.628	0.005	0.145	0.019	0.573
0.018	0.627	0.004	0.148	0.015	0.583
0.027	0.598	0.004	0.149	0.015	0.585
0.020	0.621	0.004	0.151	0.017	0.578
0.020	0.620	0.004	0.151	0.012	0.597
0.019	0.623	0.004	0.151	0.014	0.589
0.020	0.622	0.004	0.149	0.028	0.832
0.019	0.622	0.004	0.150	0.022	0.857
0.018	0.625	0.004	0.151	0.024	0.845
0.021	0.616	0.004	0.148	0.026	0.838
0.018	0.626	0.004	0.152	0.025	0.842
0.018	0.628	0.003	0.152	0.026	0.839
0.016	0.631	0.009	0.289	0.024	0.847
0.016	0.633	0.009	0.290	0.022	0.853
0.016	0.635	0.009	0.290	0.024	0.849
0.019	0.622	0.011	0.284	0.022	0.853
0.017	0.630	0.010	0.285	0.023	0.847
0.015	0.638	0.011	0.284	0.022	0.853
0.021	0.563	0.008	0.292	0.026	0.839
0.021	0.561	0.008	0.293	0.023	0.852
0.021	0.561	0.008	0.294	0.021	0.855
0.021	0.562	0.009	0.290	0.026	0.841
0.019	0.567	0.007	0.294	0.021	0.855
0.021	0.559	0.007	0.295	0.019	0.557
0.019	0.568	0.009	0.292	0.016	0.566
0.018	0.570	0.007	0.295	0.013	0.574
0.018	0.568	0.007	0.297	0.020	0.555
0.018	0.572	0.008	0.292	0.016	0.565
0.016	0.578	0.007	0.295	0.016	0.565
0.017	0.577	0.007	0.298	0.018	0.559
0.021	0.563	0.017	0.580	0.017	0.562
0.019	0.571	0.017	0.581	0.016	0.564
0.017	0.573	0.016	0.581	0.016	0.564
0.019	0.566	0.017	0.578	0.016	0.566
0.017	0.576	0.017	0.579	0.015	0.567
0.016	0.577	0.019	0.574	0.018	0.559
0.004	0.148	0.019	0.572	0.015	0.566
0.004	0.150	0.017	0.579	0.015	0.569
0.004	0.149	0.016	0.584	0.017	0.564
0.005	0.148	0.017	0.579	0.012	0.576
0.004	0.148	0.016	0.583	0.015	0.569
0.004	0.149	0.015	0.583	0.045	1.414

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.043	1.418	0.017	0.577	0.026	1.059
0.042	1.425	0.016	0.579	0.027	1.055
0.047	1.411	0.015	0.582	0.025	1.064
0.043	1.422	0.015	0.583	0.024	1.062
0.043	1.421	0.019	0.571	0.020	0.595
0.040	1.431	0.013	0.590	0.018	0.602
0.041	1.425	0.015	0.582	0.020	0.593
0.038	1.437	0.018	0.575	0.019	0.598
0.038	1.434	0.015	0.585	0.019	0.596
0.036	1.441	0.014	0.585	0.019	0.595
0.042	1.420	0.019	0.579	0.018	0.602
0.036	1.444	0.017	0.583	0.017	0.603
0.033	1.455	0.018	0.579	0.017	0.602
0.045	1.413	0.019	0.577	0.017	0.604
0.037	1.437	0.019	0.577	0.017	0.603
0.036	1.446	0.018	0.580	0.017	0.605
0.020	0.606	0.018	0.579	0.018	0.601
0.017	0.616	0.018	0.583	0.016	0.607
0.019	0.613	0.015	0.589	0.015	0.607
0.019	0.613	0.017	0.585	0.017	0.602
0.019	0.611	0.017	0.585	0.015	0.609
0.018	0.613	0.016	0.588	0.015	0.609
0.018	0.614	0.014	0.594	0.020	0.570
0.018	0.614	0.015	0.590	0.017	0.578
0.018	0.612	0.016	0.586	0.018	0.575
0.018	0.615	0.016	0.587	0.017	0.576
0.017	0.618	0.014	0.595	0.018	0.576
0.017	0.618	0.014	0.594	0.019	0.572
0.020	0.605	0.033	1.038	0.018	0.577
0.017	0.615	0.030	1.045	0.016	0.581
0.016	0.619	0.033	1.035	0.016	0.581
0.017	0.617	0.034	1.036	0.017	0.580
0.016	0.620	0.032	1.041	0.016	0.583
0.014	0.625	0.034	1.032	0.015	0.584
0.019	0.570	0.030	1.044	0.017	0.581
0.017	0.576	0.029	1.050	0.015	0.583
0.016	0.579	0.031	1.043	0.015	0.585
0.019	0.568	0.029	1.047	0.017	0.579
0.019	0.571	0.028	1.057	0.014	0.589
0.019	0.572	0.026	1.056	0.014	0.589
0.018	0.574	0.028	1.050		
0.016	0.580	0.026	1.063		

Table D-4. *m*-Xylene equilibrium data from kinetic batch experiments

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.018	0.620	0.004	0.148	0.017	0.636
0.018	0.620	0.004	0.148	0.017	0.638
0.017	0.620	0.003	0.150	0.019	0.631
0.017	0.623	0.004	0.150	0.013	0.649
0.017	0.623	0.003	0.150	0.015	0.642
0.018	0.619	0.004	0.148	0.026	0.799
0.017	0.620	0.004	0.149	0.020	0.822
0.017	0.620	0.003	0.150	0.022	0.811
0.018	0.619	0.004	0.148	0.023	0.808
0.015	0.630	0.003	0.151	0.022	0.812
0.015	0.629	0.003	0.151	0.023	0.809
0.016	0.628	0.009	0.290	0.022	0.813
0.018	0.619	0.009	0.291	0.020	0.819
0.015	0.627	0.008	0.291	0.021	0.815
0.014	0.632	0.009	0.291	0.020	0.819
0.017	0.624	0.008	0.291	0.020	0.814
0.014	0.633	0.009	0.291	0.020	0.820
0.014	0.630	0.008	0.292	0.024	0.807
0.019	0.553	0.008	0.294	0.020	0.819
0.019	0.553	0.008	0.294	0.019	0.822
0.019	0.554	0.009	0.291	0.023	0.809
0.019	0.555	0.007	0.295	0.019	0.821
0.017	0.559	0.007	0.296	0.017	0.528
0.019	0.552	0.008	0.292	0.014	0.537
0.016	0.560	0.007	0.296	0.012	0.545
0.016	0.562	0.006	0.298	0.019	0.524
0.016	0.560	0.008	0.293	0.015	0.534
0.015	0.564	0.007	0.296	0.015	0.534
0.014	0.569	0.007	0.298	0.016	0.531
0.014	0.568	0.020	0.630	0.015	0.534
0.018	0.556	0.019	0.632	0.015	0.535
0.016	0.563	0.018	0.633	0.015	0.534
0.015	0.565	0.019	0.631	0.014	0.538
0.017	0.558	0.019	0.631	0.013	0.538
0.014	0.567	0.021	0.626	0.016	0.532
0.014	0.568	0.021	0.621	0.014	0.538
0.004	0.149	0.019	0.630	0.013	0.540
0.004	0.148	0.018	0.636	0.015	0.536
0.004	0.147	0.020	0.630	0.011	0.547
0.004	0.148	0.017	0.635	0.013	0.540
0.004	0.149	0.017	0.635	0.018	0.566
0.005	0.144	0.021	0.626	0.017	0.568

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.016	0.571	0.016	0.589	0.014	0.577
0.017	0.567	0.015	0.592	0.013	0.582
0.016	0.572	0.014	0.593	0.013	0.581
0.018	0.567	0.018	0.581	0.032	1.032
0.016	0.573	0.013	0.600	0.029	1.044
0.016	0.571	0.014	0.593	0.033	1.030
0.015	0.573	0.017	0.586	0.030	1.039
0.015	0.574	0.014	0.595	0.030	1.036
0.014	0.577	0.013	0.595	0.031	1.035
0.017	0.568	0.018	0.592	0.028	1.046
0.014	0.578	0.017	0.596	0.027	1.047
0.013	0.582	0.017	0.593	0.028	1.045
0.018	0.566	0.018	0.592	0.026	1.050
0.015	0.575	0.018	0.591	0.027	1.049
0.014	0.579	0.017	0.594	0.026	1.050
0.043	1.403	0.018	0.592	0.029	1.043
0.037	1.426	0.017	0.596	0.026	1.053
0.040	1.418	0.015	0.602	0.025	1.054
0.041	1.416	0.016	0.598	0.027	1.046
0.041	1.412	0.016	0.598	0.024	1.057
0.039	1.416	0.015	0.601	0.024	1.058
0.038	1.425	0.014	0.607	0.018	0.562
0.037	1.424	0.015	0.603	0.016	0.569
0.039	1.418	0.016	0.599	0.017	0.567
0.036	1.428	0.015	0.600	0.016	0.569
0.035	1.432	0.013	0.608	0.016	0.570
0.035	1.431	0.013	0.608	0.017	0.566
0.044	1.402	0.017	0.567	0.016	0.568
0.037	1.423	0.016	0.571	0.015	0.573
0.034	1.434	0.017	0.566	0.015	0.572
0.036	1.429	0.017	0.568	0.015	0.572
0.033	1.435	0.016	0.571	0.014	0.574
0.030	1.446	0.017	0.566	0.014	0.575
0.018	0.580	0.016	0.569	0.015	0.573
0.017	0.586	0.015	0.574	0.014	0.575
0.016	0.589	0.016	0.570	0.014	0.577
0.017	0.583	0.016	0.571	0.016	0.570
0.017	0.585	0.015	0.577	0.013	0.581
0.016	0.587	0.014	0.577	0.013	0.581
0.017	0.584	0.015	0.574		
0.015	0.590	0.013	0.581		
0.016	0.587	0.013	0.579		

Table D-5. o-Xylene equilibrium data from kinetic batch experiments

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.015	0.560	0.005	0.149	0.017	0.636
0.013	0.565	0.005	0.149	0.017	0.638
0.013	0.564	0.004	0.152	0.019	0.631
0.015	0.561	0.004	0.151	0.013	0.649
0.015	0.558	0.004	0.151	0.015	0.642
0.015	0.558	0.004	0.150	0.029	0.821
0.016	0.558	0.004	0.151	0.022	0.846
0.015	0.556	0.004	0.151	0.025	0.836
0.017	0.553	0.004	0.149	0.026	0.831
0.014	0.563	0.004	0.152	0.025	0.835
0.013	0.564	0.004	0.153	0.026	0.833
0.012	0.569	0.011	0.317	0.025	0.836
0.017	0.554	0.010	0.318	0.023	0.843
0.014	0.562	0.010	0.319	0.024	0.839
0.013	0.564	0.011	0.318	0.023	0.843
0.016	0.555	0.010	0.319	0.023	0.838
0.014	0.564	0.010	0.319	0.022	0.845
0.013	0.566	0.010	0.319	0.026	0.831
0.017	0.548	0.009	0.321	0.022	0.845
0.017	0.546	0.009	0.322	0.021	0.847
0.018	0.546	0.010	0.318	0.025	0.834
0.018	0.546	0.009	0.323	0.021	0.847
0.016	0.550	0.008	0.324	0.019	0.538
0.018	0.543	0.010	0.321	0.016	0.548
0.016	0.550	0.008	0.325	0.014	0.555
0.015	0.552	0.008	0.327	0.020	0.534
0.015	0.551	0.009	0.322	0.017	0.544
0.014	0.556	0.008	0.325	0.017	0.545
0.013	0.559	0.008	0.328	0.018	0.540
0.014	0.558	0.020	0.630	0.017	0.544
0.017	0.548	0.019	0.632	0.016	0.545
0.015	0.555	0.018	0.633	0.017	0.545
0.014	0.557	0.019	0.631	0.015	0.549
0.017	0.548	0.019	0.631	0.015	0.549
0.014	0.558	0.021	0.626	0.017	0.543
0.013	0.559	0.021	0.621	0.015	0.549
0.004	0.151	0.019	0.630	0.014	0.552
0.004	0.149	0.018	0.636	0.016	0.547
0.005	0.149	0.020	0.630	0.012	0.558
0.005	0.149	0.017	0.635	0.014	0.552
0.004	0.150	0.017	0.635	0.021	0.593
0.006	0.144	0.021	0.626	0.019	0.595

Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mg/kg)
0.019	0.599	0.042	1.534	0.016	0.617
0.020	0.595	0.040	1.539	0.015	0.622
0.018	0.600	0.039	1.541	0.014	0.622
0.021	0.593	0.049	1.511	0.020	0.574
0.018	0.601	0.035	1.560	0.017	0.582
0.019	0.599	0.040	1.540	0.020	0.574
0.018	0.601	0.047	1.523	0.018	0.578
0.017	0.603	0.039	1.547	0.018	0.577
0.016	0.606	0.037	1.547	0.019	0.576
0.019	0.597	0.019	0.579	0.018	0.580
0.016	0.608	0.018	0.584	0.017	0.583
0.015	0.613	0.018	0.581	0.017	0.582
0.020	0.595	0.018	0.581	0.017	0.583
0.017	0.605	0.019	0.580	0.017	0.584
0.016	0.609	0.018	0.583	0.016	0.585
0.020	0.581	0.019	0.580	0.017	0.582
0.017	0.591	0.018	0.585	0.015	0.588
0.019	0.588	0.016	0.591	0.015	0.588
0.019	0.586	0.018	0.586	0.017	0.583
0.019	0.585	0.017	0.586	0.015	0.590
0.018	0.587	0.016	0.590	0.015	0.590
0.019	0.587	0.014	0.596	0.036	1.005
0.018	0.589	0.016	0.592	0.031	1.021
0.018	0.588	0.017	0.588	0.033	1.017
0.018	0.589	0.016	0.589	0.030	1.023
0.016	0.593	0.014	0.598	0.031	1.023
0.016	0.594	0.014	0.597	0.033	1.016
0.020	0.582	0.020	0.604	0.031	1.020
0.017	0.591	0.018	0.610	0.028	1.028
0.015	0.596	0.020	0.604	0.029	1.026
0.016	0.593	0.020	0.606	0.029	1.029
0.015	0.596	0.019	0.610	0.028	1.032
0.014	0.601	0.020	0.604	0.027	1.034
0.051	1.502	0.019	0.606	0.030	1.029
0.047	1.519	0.018	0.612	0.027	1.032
0.044	1.528	0.019	0.609	0.027	1.036
0.046	1.515	0.018	0.609	0.031	1.024
0.047	1.518	0.017	0.617	0.025	1.043
0.046	1.522	0.016	0.617	0.024	1.043
0.046	1.520	0.017	0.614		
0.043	1.533	0.015	0.622		
0.044	1.524	0.015	0.620		

Table D-6. Overall isotherm results from equilibrium data of batch experiments

Constituent	Number of Samples	Average K_d (L/kg)	Linear Isotherm r^2
Benzene	240	7.50	0.951
Toluene	247	17.77	0.959
Ethylbenzene	250	34.54	0.922
M-Xylene	249	36.87	0.933
O-Xylene	249	34.57	0.935

Table D-7. Overall "quasi" equilibrium results from batch experiment data

	20-Minute		**90-Minute**		Aqueous Concentration	Amount Sorbed
Constituent	K_d (L/kg)	r^2	K_d (L/kg)	r^2	difference (%)	difference (%)
Benzene	7.32	0.944	7.57	0.964	9.9	5.5
Toluene	16.91	0.971	18.77	0.971	21.9	3.9
Ethylbenzene	32.1	0.936	37.54	0.913	29.0	3.1
M-Xylene	34.09	0.958	41.21	0.931	31.3	3.0
O-Xylene	31.88	0.953	37.93	0.928	31.6	3.7

Table D-8. Twenty and ninety-minute data from benzene batch experiments

20 Minute Data		90 Minute Data	
Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)
0.081	0.596	0.075	0.619
0.081	0.586	0.079	0.615
0.074	0.625	0.073	0.626
0.081	0.551	0.077	0.562
0.084	0.539	0.075	0.576
0.085	0.541	0.076	0.565
0.014	0.109	0.014	0.111
0.015	0.108	0.014	0.112
0.032	0.232	0.032	0.233
0.032	0.230	0.031	0.231
0.032	0.232	0.032	0.236
0.067	0.484	0.065	0.486
0.068	0.478	0.059	0.500
0.067	0.480	0.092	0.652
0.089	0.667	0.092	0.663
0.086	0.677	0.085	0.683
0.061	0.457	0.061	0.456
0.059	0.458	0.060	0.458
0.060	0.455	0.060	0.420
0.058	0.429	0.058	0.423
0.060	0.419	0.059	0.429
0.057	0.431	0.058	0.422
0.056	0.431	0.056	0.426
0.057	0.435	0.055	0.432
0.066	0.456	0.067	0.456
0.062	0.473	0.063	0.468
0.066	0.486	0.063	0.464
0.064	0.491	0.064	0.490
0.068	0.475	0.066	0.490
0.061	0.464	0.065	0.489
0.058	0.467	0.061	0.462
0.063	0.452	0.060	0.468
0.064	0.459	0.059	0.468
0.062	0.467	0.063	0.458
0.060	0.432	0.062	0.462
0.057	0.442	0.062	0.464
0.059	0.437	0.058	0.444
		0.057	0.439

Table D-9. Twenty and ninety-minute data from toluene batch experiments

20 Minute Data		90 Minute Data	
Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)
0.033	0.492	0.029	0.508
0.032	0.496	0.024	0.523
0.031	0.500	0.024	0.520
0.040	0.615	0.037	0.623
0.041	0.609	0.034	0.635
0.042	0.610	0.034	0.632
0.007	0.137	0.007	0.138
0.008	0.134	0.007	0.138
0.008	0.134	0.017	0.307
0.019	0.303	0.016	0.309
0.018	0.302	0.016	0.312
0.018	0.303	0.031	0.535
0.030	0.537	0.024	0.558
0.031	0.536	0.026	0.546
0.030	0.537	0.046	0.822
0.050	0.807	0.042	0.835
0.046	0.821	0.073	1.318
0.050	0.808	0.069	1.327
0.073	1.317	0.032	0.537
0.075	1.307	0.029	0.544
0.070	1.324	0.029	0.549
0.033	0.536	0.031	0.528
0.033	0.533	0.029	0.531
0.032	0.540	0.027	0.542
0.033	0.523	0.033	0.558
0.028	0.536	0.030	0.568
0.032	0.528	0.029	0.567
0.035	0.551	0.051	0.956
0.032	0.560	0.050	0.965
0.030	0.567	0.049	0.964
0.056	0.940	0.031	0.567
0.054	0.947	0.030	0.572
0.057	0.934	0.029	0.572
0.034	0.559	0.031	0.553
0.030	0.567	0.029	0.559
0.035	0.553	0.030	0.560
0.033	0.548	0.034	0.558
0.031	0.555	0.030	0.572
0.037	0.536	0.029	0.570
0.035	0.552		
0.032	0.560		
0.034	0.557		

Table D-10. Twenty and ninety-minute data from ethylbenzene batch experiments

20 Minute Data		90 Minute Data	
Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)
0.017	0.628	0.019	0.622
0.018	0.627	0.017	0.630
0.027	0.598	0.015	0.638
0.021	0.563	0.019	0.566
0.021	0.561	0.017	0.576
0.021	0.561	0.016	0.577
0.004	0.148	0.004	0.152
0.004	0.150	0.003	0.152
0.004	0.149	0.008	0.292
0.009	0.289	0.007	0.295
0.009	0.290	0.007	0.298
0.009	0.290	0.017	0.578
0.017	0.580	0.012	0.597
0.017	0.581	0.014	0.589
0.016	0.581	0.026	0.841
0.028	0.832	0.021	0.855
0.022	0.857	0.017	0.564
0.024	0.845	0.012	0.576
0.019	0.557	0.015	0.569
0.016	0.566	0.045	1.413
0.013	0.574	0.037	1.437
0.045	1.414	0.036	1.446
0.043	1.418	0.017	0.617
0.042	1.425	0.016	0.620
0.020	0.606	0.014	0.625
0.017	0.616	0.018	0.575
0.019	0.613	0.015	0.585
0.019	0.570	0.014	0.585
0.017	0.576	0.016	0.587
0.016	0.579	0.014	0.595
0.019	0.579	0.014	0.594
0.017	0.583	0.027	1.055
0.018	0.579	0.025	1.064
0.033	1.038	0.024	1.062
0.030	1.045	0.017	0.602
0.033	1.035	0.015	0.609
0.020	0.595	0.015	0.609
0.018	0.602	0.017	0.579
0.020	0.593	0.014	0.589
0.020	0.570	0.014	0.589
0.017	0.578		
0.018	0.575		

Table D-11. Twenty and ninety-minute data from *m*-xylene batch experiments

20 Minute Data		90 Minute Data	
Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)
0.018	0.620	0.017	0.624
0.018	0.620	0.014	0.633
0.017	0.620	0.014	0.630
0.019	0.553	0.017	0.558
0.019	0.553	0.014	0.567
0.019	0.554	0.014	0.568
0.004	0.149	0.003	0.151
0.004	0.148	0.003	0.151
0.004	0.147	0.008	0.293
0.009	0.290	0.007	0.296
0.009	0.291	0.007	0.298
0.008	0.291	0.019	0.631
0.020	0.630	0.013	0.649
0.019	0.632	0.015	0.642
0.018	0.633	0.023	0.809
0.026	0.799	0.019	0.821
0.020	0.822	0.015	0.536
0.022	0.811	0.011	0.547
0.017	0.528	0.013	0.540
0.014	0.537	0.018	0.566
0.012	0.545	0.015	0.575
0.018	0.566	0.014	0.579
0.017	0.568	0.036	1.429
0.016	0.571	0.033	1.435
0.043	1.403	0.030	1.446
0.037	1.426	0.017	0.586
0.040	1.418	0.014	0.595
0.018	0.580	0.013	0.595
0.017	0.586	0.015	0.600
0.016	0.589	0.013	0.608
0.018	0.592	0.013	0.608
0.017	0.596	0.014	0.577
0.017	0.593	0.013	0.582
0.017	0.567	0.013	0.581
0.016	0.571	0.027	1.046
0.017	0.566	0.024	1.057
0.032	1.032	0.024	1.058
0.029	1.044	0.016	0.570
0.033	1.030	0.013	0.581
0.018	0.562	0.013	0.581
0.016	0.569		
0.017	0.567		

Table D-12. Twenty and ninety-minute data from *o*-xylene batch experiments

20 Minute Data		90 Minute Data	
Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)	Aqueous Concentration (mmol/L)	Amount Sorbed (mmol/kg)
0.015	0.560	0.016	0.555
0.013	0.565	0.014	0.564
0.013	0.564	0.013	0.566
0.017	0.548	0.017	0.548
0.017	0.546	0.014	0.558
0.018	0.546	0.013	0.559
0.004	0.151	0.004	0.152
0.004	0.149	0.004	0.153
0.005	0.149	0.009	0.322
0.011	0.317	0.008	0.325
0.010	0.318	0.008	0.328
0.010	0.319	0.019	0.631
0.020	0.630	0.013	0.649
0.019	0.632	0.015	0.642
0.018	0.633	0.025	0.834
0.029	0.821	0.021	0.847
0.022	0.846	0.016	0.547
0.025	0.836	0.012	0.558
0.019	0.538	0.014	0.552
0.016	0.548	0.020	0.595
0.014	0.555	0.017	0.605
0.021	0.593	0.016	0.609
0.019	0.595	0.016	0.593
0.019	0.599	0.015	0.596
0.020	0.581	0.014	0.601
0.017	0.591	0.047	1.523
0.019	0.588	0.039	1.547
0.051	1.502	0.037	1.547
0.047	1.519	0.016	0.589
0.044	1.528	0.014	0.598
0.019	0.579	0.014	0.597
0.018	0.584	0.016	0.617
0.018	0.581	0.015	0.622
0.020	0.604	0.014	0.622
0.018	0.610	0.017	0.583
0.020	0.604	0.015	0.590
0.020	0.574	0.015	0.590
0.017	0.582	0.031	1.024
0.020	0.574	0.025	1.043
0.036	1.005	0.024	1.043
0.031	1.021		
0.033	1.017		

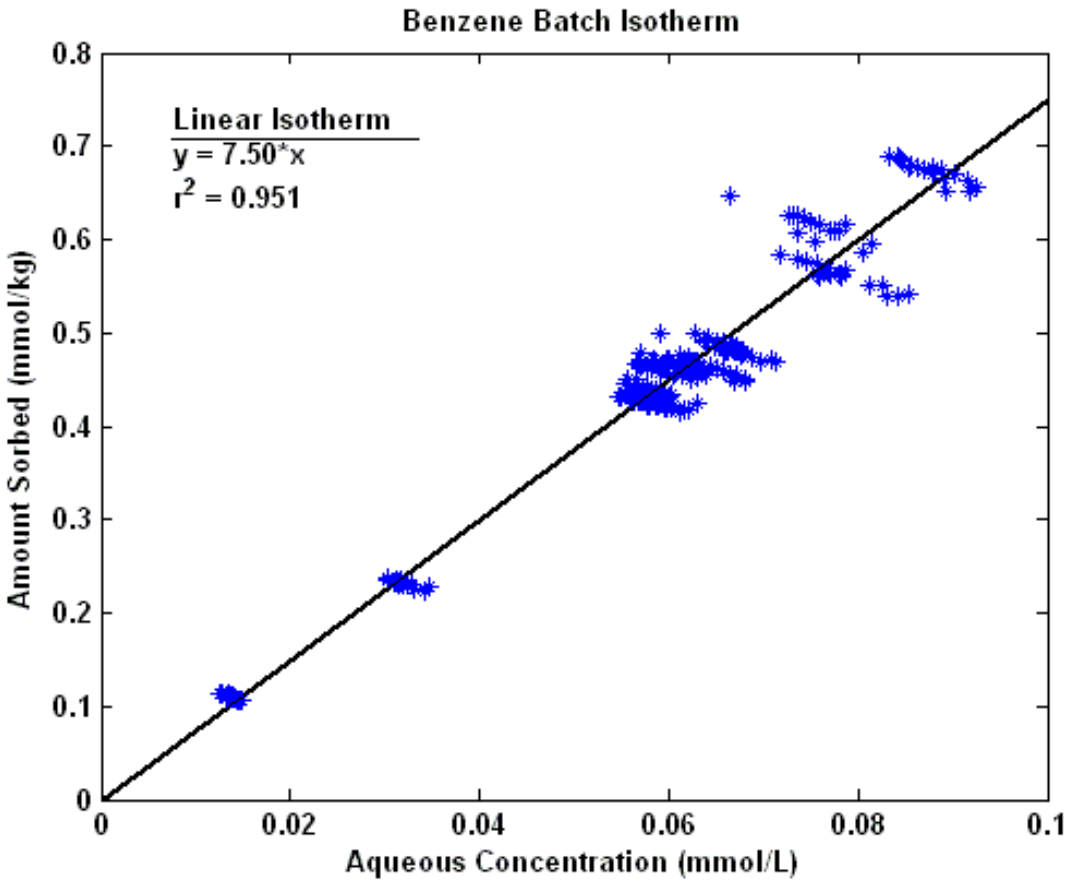

Figure D-1. Isotherm results for benzene equilibrium batch experiment data.

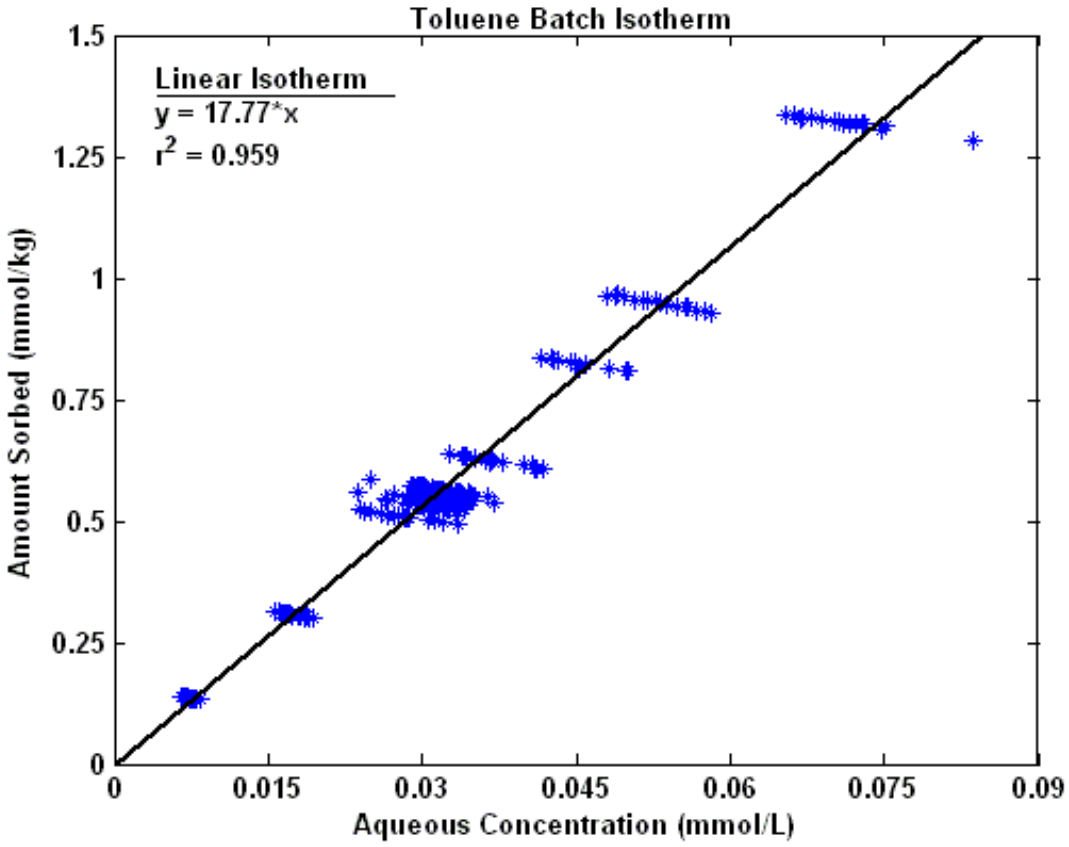

Figure D-2. Isotherm results for toluene equilibrium batch experiment data.

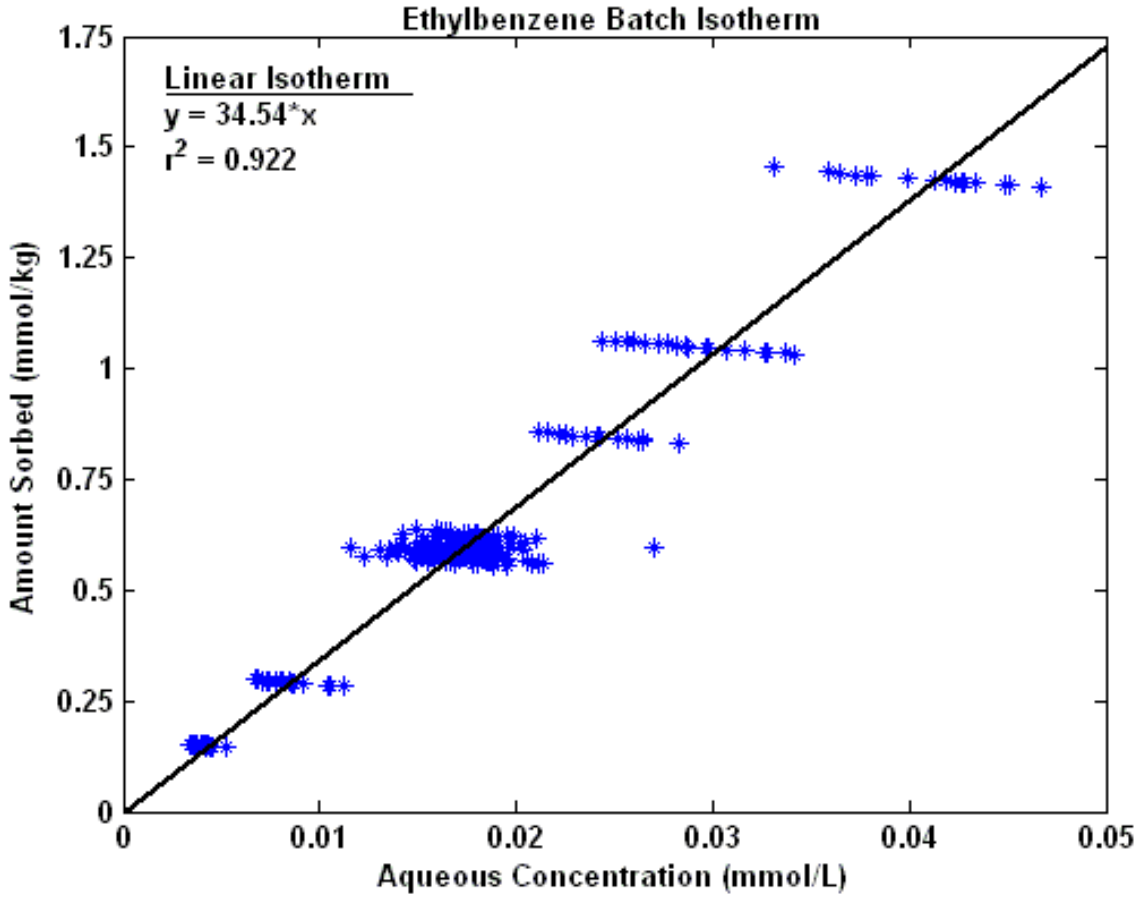

Figure D-3. Isotherm results for ethylbenzene equilibrium batch experiment data.

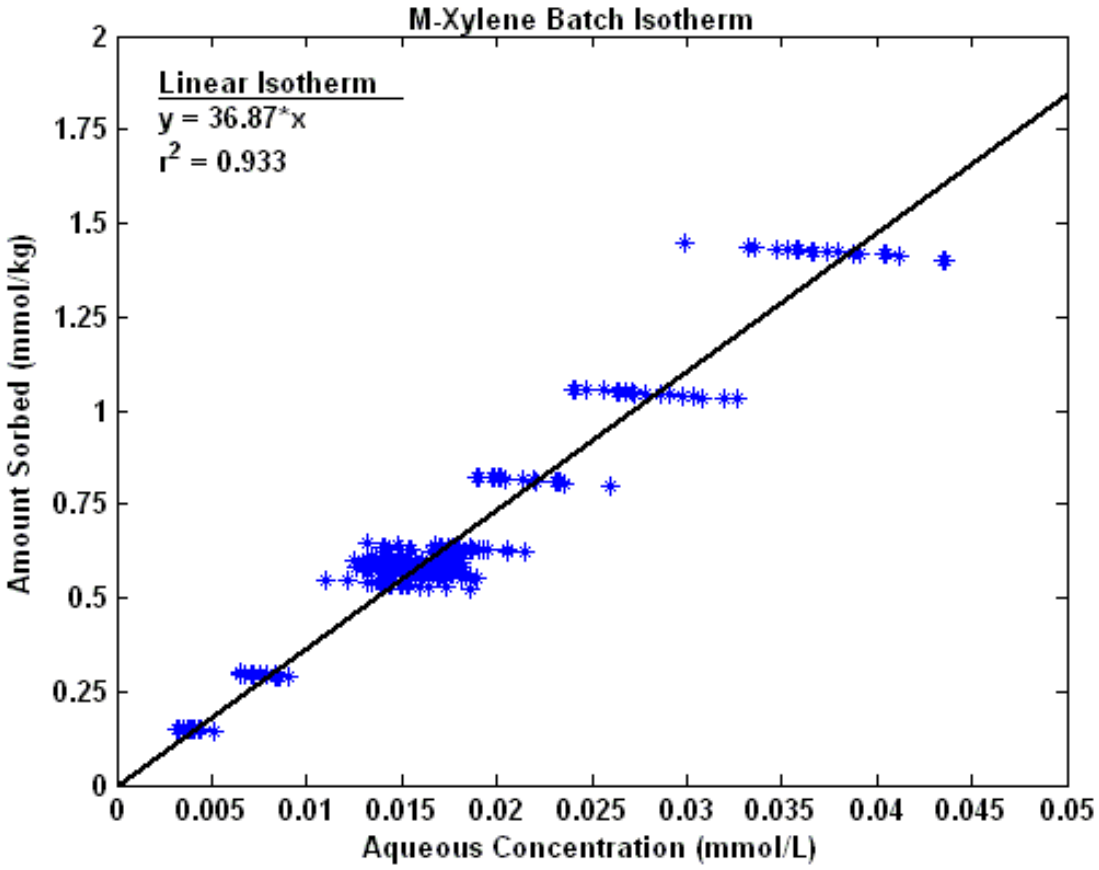

Figure D-4. Isotherm results for *m*-xylene equilibrium batch experiment data.

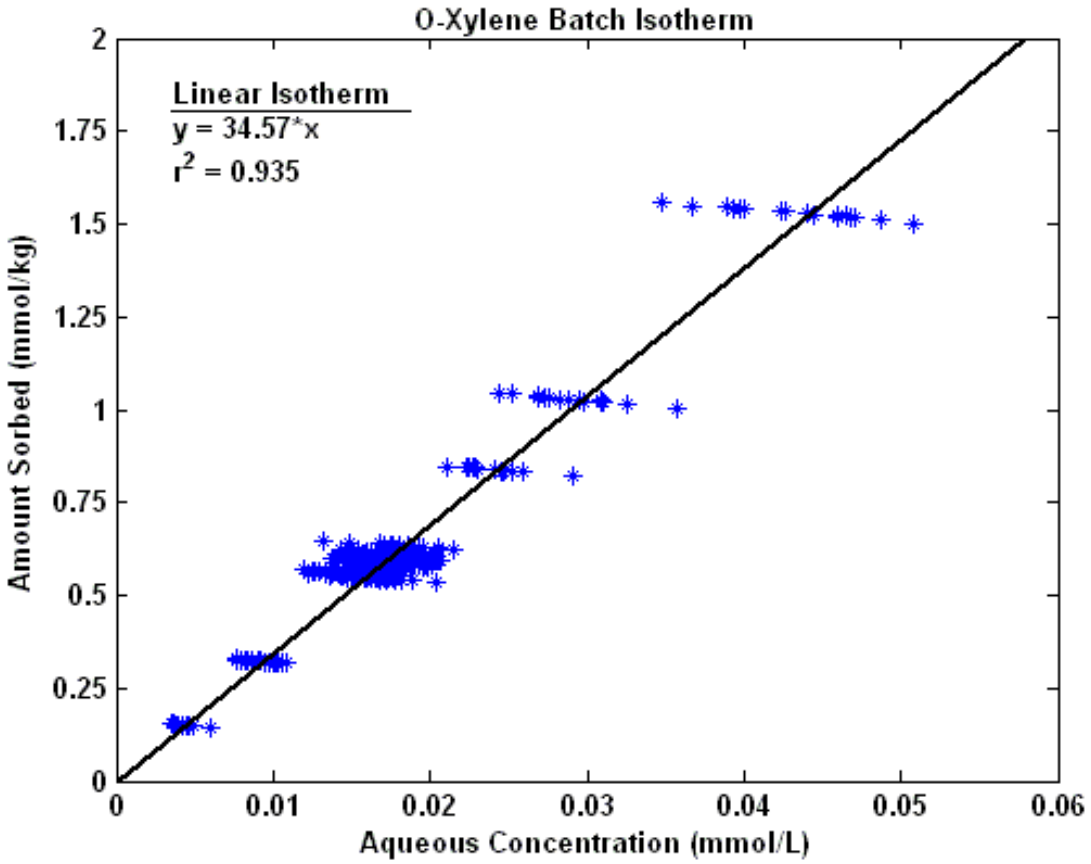

Figure D-5. Isotherm results for *o*-xylene equilibrium batch experiment data.

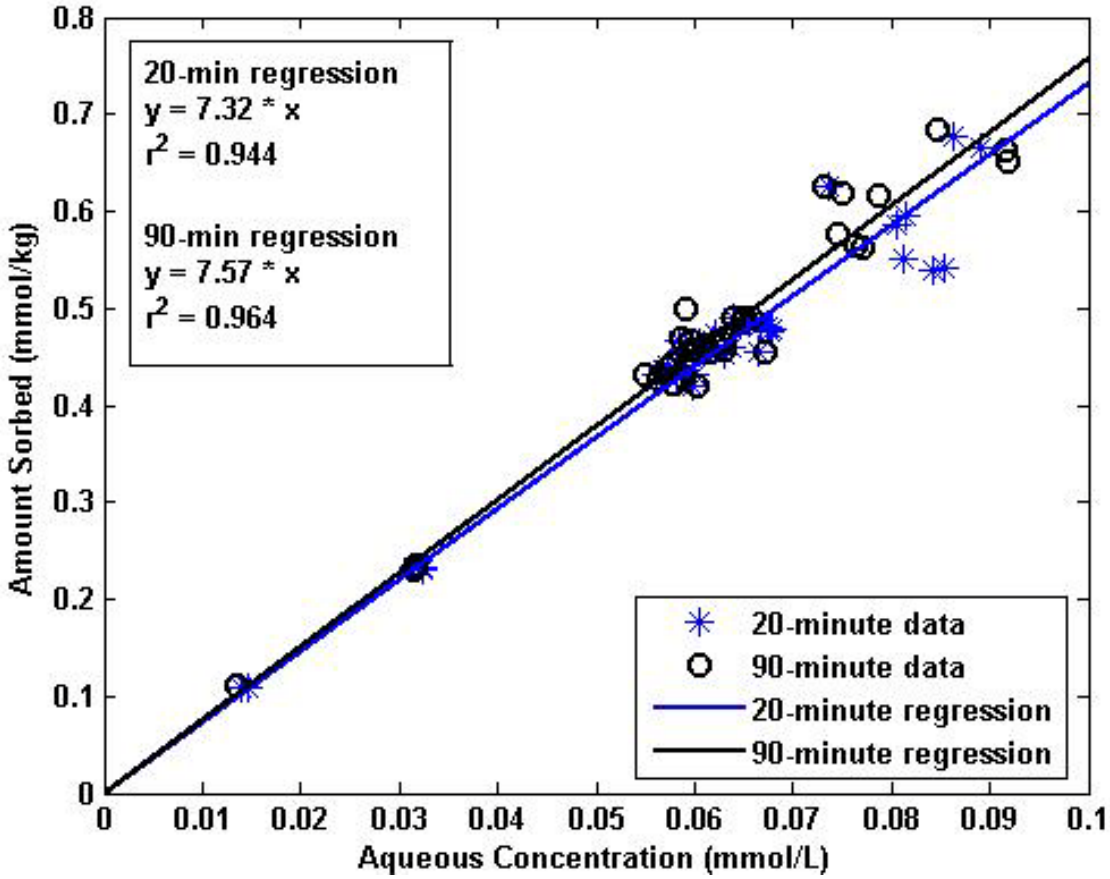

Figure D-6. Twenty and ninety-minute data from the benzene batch experiments fitted with linear isotherms.

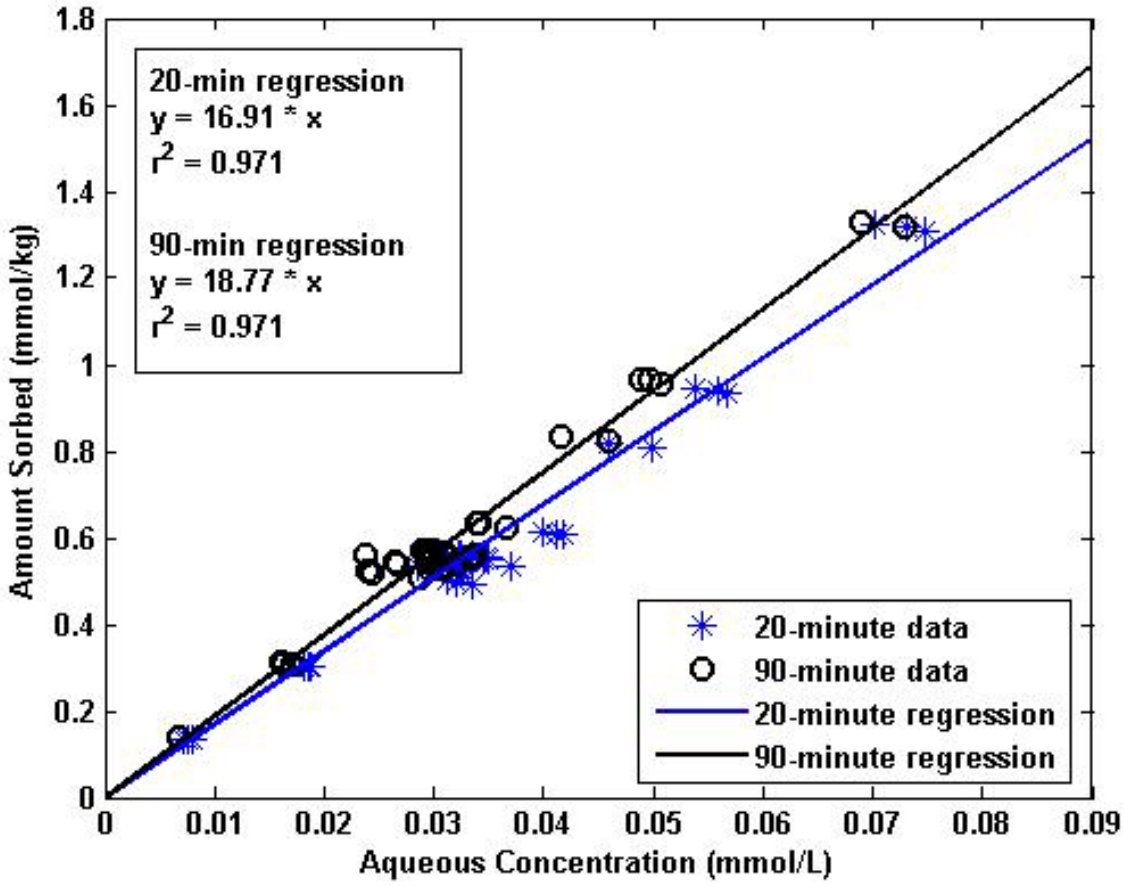

Figure D-7. Twenty and ninety-minute data from the toluene batch experiments fitted with linear isotherms.

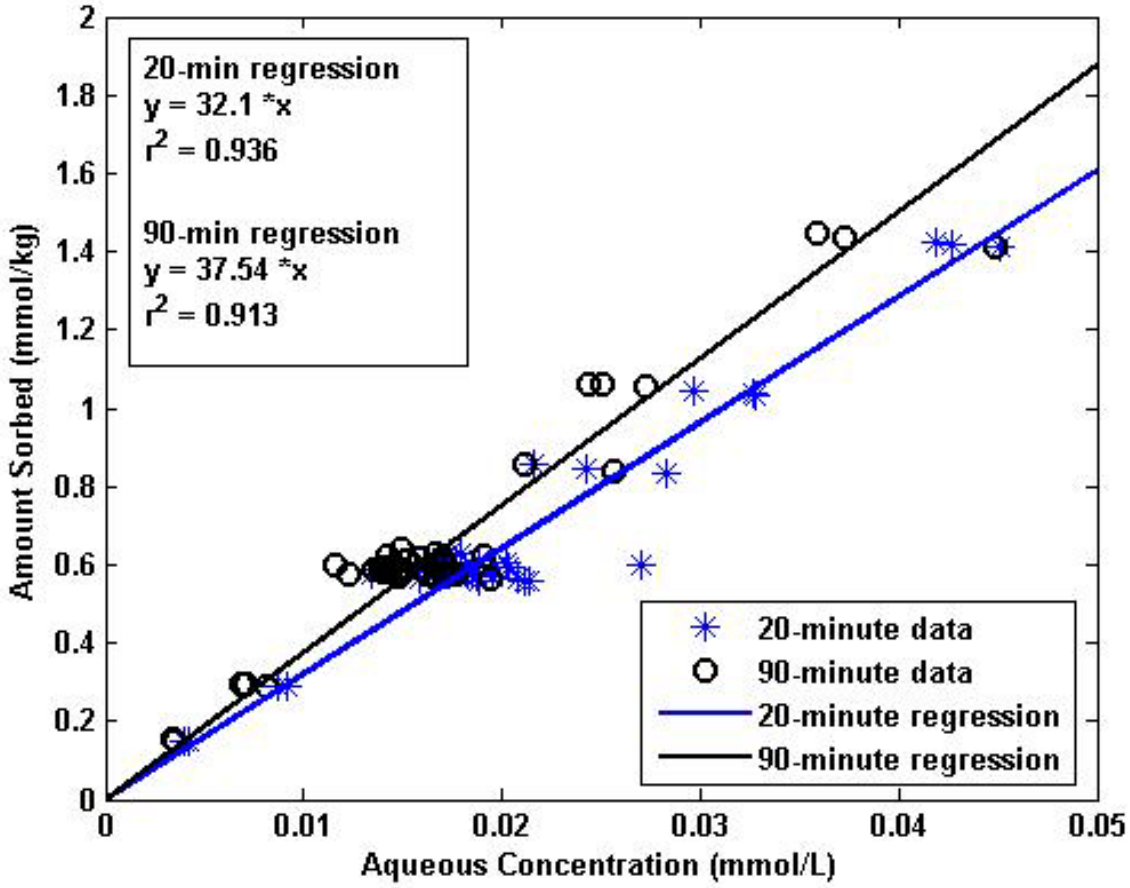

Figure D-8. Twenty and ninety-minute data from the ethylbenzene batch experiments fitted with linear isotherms.

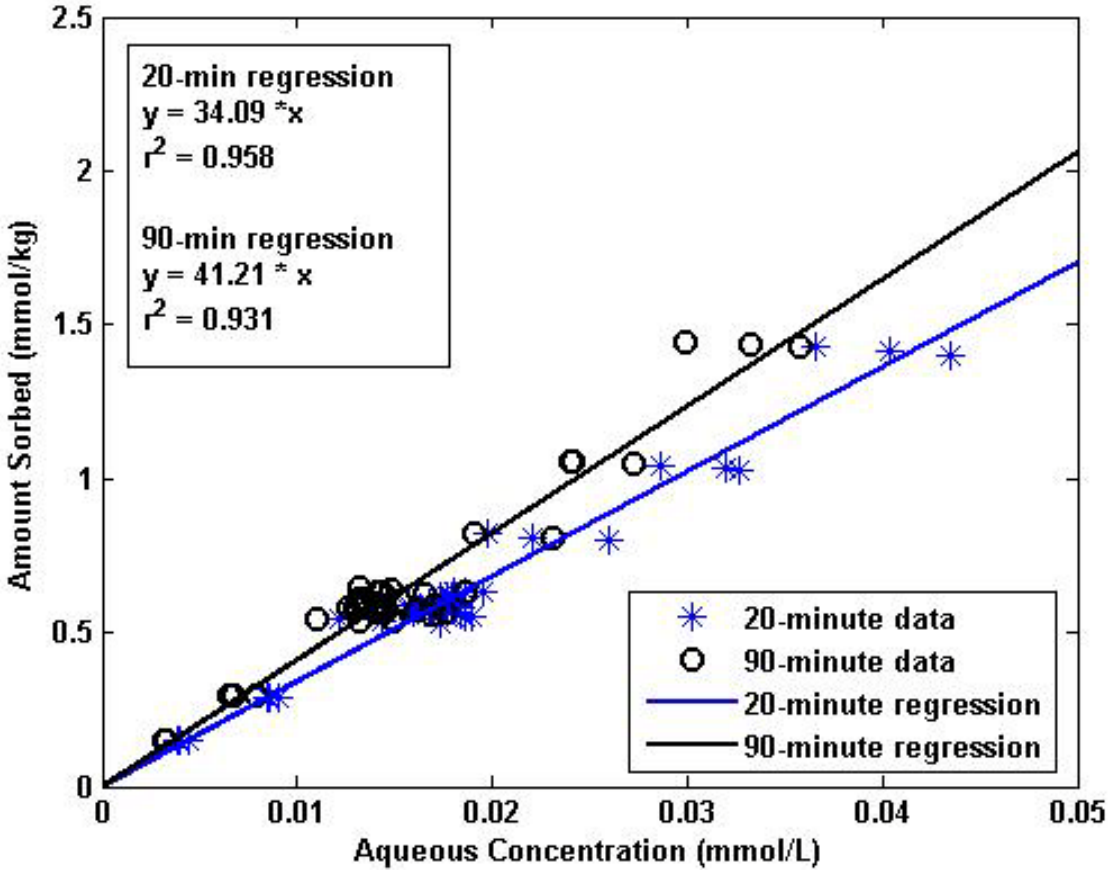

Figure D-9. Twenty and ninety-minute data from the *m*-xylene batch experiments fitted linear isotherms.

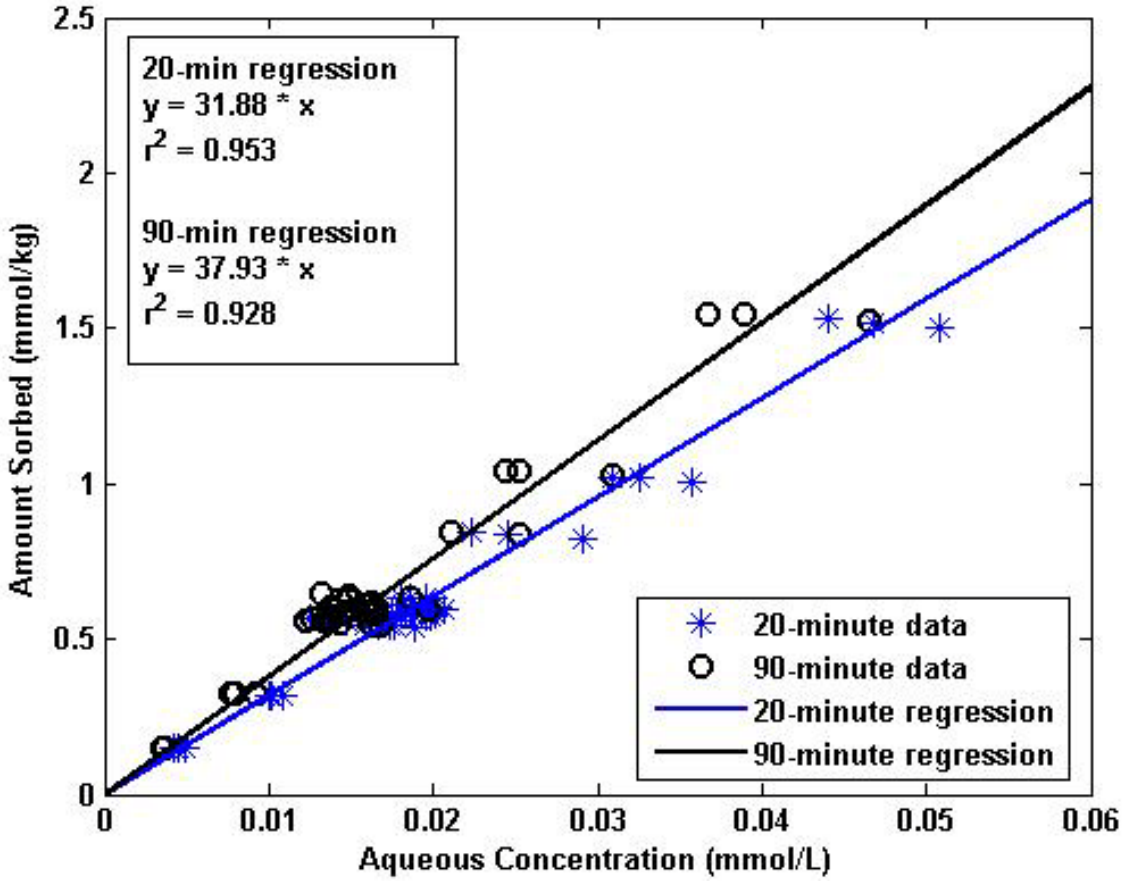

Figure D-10. Twenty and ninety-minute data from the *o*-xylene batch experiments fitted with linear isotherms.

APPENDIX E. TRITIUM BTC DATA.

The data from the tritium transport experiments can be seen in Tables E-1 through E-6. These data are represented in relative concentration as a function of pore volumes. A single tritium experiment was run prior to each BTEX transport experiment in order to obtain column parameters. These results are seen in Table V of the manuscript. Figures E-1 through E-6 show the chemical equilibrium model (CXTFIT version 2.1 (Toride et al., 1999)) inversely fit to the experimental data.

Table E-1. Tritium BTC data from column 1A.

Sample	Pore Volumes	Observed C/C_o	Fit C/C_o	Sample	Pore Volumes	Observed C/C_o	Fit C/C_o
1	0.060	0.000	0.000	**28**	3.307	0.272	0.319
2	0.180	0.000	0.000	**29**	3.427	0.211	0.247
3	0.301	0.000	0.000	**30**	3.548	0.159	0.189
4	0.421	0.003	0.008	**31**	3.668	0.117	0.143
5	0.541	0.022	0.042	**32**	3.788	0.090	0.108
6	0.661	0.077	0.112	**33**	3.908	0.068	0.081
7	0.782	0.168	0.214	**34**	4.029	0.051	0.060
8	0.902	0.280	0.330	**35**	4.149	0.041	0.045
9	1.022	0.391	0.447	**36**	4.269	0.031	0.033
10	1.142	0.532	0.554	**37**	4.389	0.025	0.025
11	1.263	0.613	0.649	**38**	4.510	0.019	0.018
12	1.383	0.708	0.727	**39**	4.630	0.016	0.013
13	1.503	0.781	0.790	**40**	4.750	0.012	0.010
14	1.623	0.829	0.840	**41**	4.870	0.010	0.007
15	1.744	0.856	0.879	**42**	4.991	0.008	0.005
16	1.864	0.905	0.909	**43**	5.111	0.007	0.004
17	1.984	0.917	0.932	**44**	5.231	0.006	0.003
18	2.104	0.933	0.950	**45**	5.351	0.005	0.002
19	2.225	0.952	0.963	**46**	5.472	0.004	0.002
20	2.345	0.955	0.971	**47**	5.592	0.003	0.001
21	2.465	0.937	0.963	**48**	5.712	0.003	0.001
22	2.585	0.890	0.922	**49**	5.832	0.002	0.001
23	2.706	0.811	0.842	**50**	5.953	0.002	0.000
24	2.826	0.703	0.736	**51**	6.073	0.002	0.000
25	2.946	0.585	0.621	**52**	6.193	0.001	0.000
26	3.067	0.472	0.507	**53**	6.313	0.001	0.000
27	3.187	0.369	0.406	**54**	6.434	0.001	0.000

Table E-2. Tritium BTC data from column 1B.

Sample	Pore Volumes	Observed C/C_o	Fit C/C_o	Sample	Pore Volumes	Observed C/C_o	Fit C/C_o
1	0.117	0.000	0.000	**28**	3.285	0.250	0.313
2	0.235	0.000	0.000	**29**	3.402	0.202	0.245
3	0.352	0.000	0.003	**30**	3.519	0.157	0.190
4	0.469	0.000	0.026	**31**	3.637	0.122	0.146
5	0.587	0.014	0.083	**32**	3.754	0.098	0.111
6	0.704	0.074	0.174	**33**	3.871	0.077	0.085
7	0.821	0.197	0.284	**34**	3.989	0.060	0.064
8	0.939	0.306	0.400	**35**	4.106	0.047	0.049
9	1.056	0.460	0.509	**36**	4.223	0.038	0.037
10	1.173	0.569	0.605	**37**	4.341	0.029	0.028
11	1.290	0.660	0.688	**38**	4.458	0.023	0.021
12	1.408	0.737	0.757	**39**	4.575	0.019	0.016
13	1.525	0.786	0.812	**40**	4.693	0.015	0.012
14	1.642	0.826	0.855	**41**	4.810	0.012	0.009
15	1.760	0.872	0.889	**42**	4.927	0.010	0.007
16	1.877	0.896	0.916	**43**	5.044	0.008	0.005
17	1.994	0.917	0.936	**44**	5.162	0.006	0.004
18	2.112	0.934	0.952	**45**	5.279	0.005	0.003
19	2.229	0.949	0.964	**46**	5.396	0.004	0.002
20	2.346	0.956	0.970	**47**	5.514	0.003	0.002
21	2.464	0.945	0.956	**48**	5.631	0.003	0.001
22	2.581	0.881	0.905	**49**	5.748	0.002	0.001
23	2.698	0.769	0.820	**50**	5.866	0.002	0.001
24	2.816	0.639	0.713	**51**	5.983	0.002	0.001
25	2.933	0.507	0.600	**52**	6.100	0.001	0.000
26	3.050	0.415	0.492	**53**	6.218	0.001	0.000
27	3.167	0.322	0.396	**54**	6.335	0.001	0.000

Table E-3. Tritium BTC data from column 2A.

Sample	Pore Volumes	Observed C/C_o	Fit C/C_o	Sample	Pore Volumes	Observed C/C_o	Fit C/C_o
1	0.119	0.000	0.000	**28**	3.334	0.184	0.245
2	0.238	0.000	0.000	**29**	3.453	0.142	0.180
3	0.357	0.000	0.002	**30**	3.573	0.106	0.130
4	0.476	0.002	0.019	**31**	3.692	0.079	0.093
5	0.595	0.019	0.073	**32**	3.811	0.060	0.066
6	0.715	0.073	0.169	**33**	3.930	0.046	0.047
7	0.834	0.187	0.293	**34**	4.049	0.034	0.033
8	0.953	0.327	0.423	**35**	4.168	0.027	0.023
9	1.072	0.478	0.546	**36**	4.287	0.021	0.016
10	1.191	0.610	0.652	**37**	4.406	0.016	0.011
11	1.310	0.705	0.740	**38**	4.525	0.013	0.008
12	1.429	0.778	0.808	**39**	4.644	0.010	0.005
13	1.548	0.834	0.861	**40**	4.763	0.008	0.004
14	1.667	0.869	0.900	**41**	4.882	0.006	0.003
15	1.786	0.904	0.929	**42**	5.002	0.005	0.002
16	1.905	0.930	0.949	**43**	5.121	0.003	0.001
17	2.024	0.945	0.964	**44**	5.240	0.002	0.001
18	2.144	0.964	0.975	**45**	5.359	0.002	0.001
19	2.263	0.973	0.983	**46**	5.478	0.001	0.000
20	2.382	0.967	0.985	**47**	5.597	0.001	0.000
21	2.501	0.947	0.965	**48**	5.716	0.001	0.000
22	2.620	0.862	0.905	**49**	5.835	0.001	0.000
23	2.739	0.739	0.803	**50**	5.954	0.001	0.000
24	2.858	0.591	0.678	**51**	6.073	0.001	0.000
25	2.977	0.447	0.549	**52**	6.192	0.001	0.000
26	3.096	0.341	0.430	**53**	6.311	0.000	0.000
27	3.215	0.259	0.328	**54**	6.431	0.000	0.000

Table E-4. Tritium BTC data from column 2B.

Sample	Pore Volumes	Observed C/C_o	Fit C/C_o	Sample	Pore Volumes	Observed C/C_o	Fit C/C_o
1	0.126	0.000	0.000	**28**	3.525	0.172	0.181
2	0.252	0.000	0.000	**29**	3.651	0.128	0.133
3	0.378	0.000	0.003	**30**	3.777	0.100	0.097
4	0.504	0.007	0.028	**31**	3.903	0.074	0.070
5	0.629	0.053	0.093	**32**	4.029	0.057	0.051
6	0.755	0.166	0.197	**33**	4.154	0.043	0.037
7	0.881	0.320	0.323	**34**	4.280	0.032	0.026
8	1.007	0.446	0.450	**35**	4.406	0.024	0.019
9	1.133	0.556	0.567	**36**	4.532	0.019	0.013
10	1.259	0.660	0.667	**37**	4.658	0.015	0.010
11	1.385	0.743	0.748	**38**	4.784	0.011	0.007
12	1.511	0.801	0.812	**39**	4.910	0.009	0.005
13	1.637	0.855	0.862	**40**	5.036	0.007	0.003
14	1.763	0.885	0.899	**41**	5.162	0.006	0.002
15	1.888	0.902	0.927	**42**	5.288	0.004	0.002
16	2.014	0.933	0.947	**43**	5.413	0.003	0.001
17	2.140	0.948	0.962	**44**	5.539	0.003	0.001
18	2.266	0.967	0.973	**45**	5.665	0.002	0.001
19	2.392	0.971	0.976	**46**	5.791	0.002	0.000
20	2.518	0.961	0.953	**47**	5.917	0.002	0.000
21	2.644	0.898	0.886	**48**	6.043	0.001	0.000
22	2.770	0.772	0.781	**49**	6.169	0.001	0.000
23	2.896	0.640	0.657	**50**	6.295	0.001	0.000
24	3.021	0.502	0.533	**51**	6.421	0.001	0.000
25	3.147	0.386	0.419	**52**	6.546	0.001	0.000
26	3.273	0.300	0.322	**53**	6.672	0.001	0.000
27	3.399	0.230	0.243	**54**	6.798	0.001	0.000

Table E-5. Tritium BTC data from column 3A.

Sample	Pore Volumes	Observed C/C_o	Fit C/C_o	Sample	Pore Volumes	Observed C/C_o	Fit C/C_o
1	0.124	0.000	0.000	**28**	3.475	0.206	0.289
2	0.248	0.000	0.001	**29**	3.599	0.164	0.237
3	0.372	0.001	0.018	**30**	3.724	0.152	0.194
4	0.496	0.023	0.069	**31**	3.848	0.127	0.159
5	0.621	0.088	0.151	**32**	3.972	0.103	0.130
6	0.745	0.185	0.250	**33**	4.096	0.082	0.105
7	0.869	0.296	0.355	**34**	4.220	0.063	0.086
8	0.993	0.387	0.453	**35**	4.344	0.052	0.070
9	1.117	0.475	0.542	**36**	4.468	0.041	0.057
10	1.241	0.563	0.620	**37**	4.592	0.032	0.046
11	1.365	0.636	0.686	**38**	4.717	0.027	0.038
12	1.489	0.702	0.743	**39**	4.841	0.022	0.031
13	1.614	0.770	0.789	**40**	4.965	0.018	0.025
14	1.738	0.811	0.827	**41**	5.089	0.015	0.020
15	1.862	0.846	0.859	**42**	5.213	0.012	0.017
16	1.986	0.874	0.885	**43**	5.337	0.010	0.014
17	2.110	0.895	0.907	**44**	5.461	0.009	0.011
18	2.234	0.922	0.924	**45**	5.585	0.008	0.009
19	2.358	0.936	0.935	**46**	5.710	0.006	0.007
20	2.482	0.910	0.923	**47**	5.834	0.006	0.006
21	2.607	0.812	0.873	**48**	5.958	0.005	0.005
22	2.731	0.733	0.792	**49**	6.082	0.004	0.004
23	2.855	0.660	0.696	**50**	6.206	0.004	0.003
24	2.979	0.553	0.599	**51**	6.330	0.003	0.003
25	3.103	0.464	0.506	**52**	6.454	0.003	0.002
26	3.227	0.391	0.423	**53**	6.578	0.002	0.002
27	3.351	0.246	0.351	**54**	6.702	0.002	0.002

Table E-6. Tritium BTC data from column 3B.

Sample	Pore Volumes	Observed C/C_o	Fit C/C_o	Sample	Pore Volumes	Observed C/C_o	Fit C/C_o
1	0.121	0.000	0.000	**28**	3.392	0.246	0.289
2	0.242	0.000	0.000	**29**	3.513	0.202	0.233
3	0.363	0.000	0.008	**30**	3.635	0.163	0.186
4	0.485	0.001	0.041	**31**	3.756	0.133	0.149
5	0.606	0.022	0.109	**32**	3.877	0.109	0.119
6	0.727	0.105	0.203	**33**	3.998	0.087	0.094
7	0.848	0.244	0.308	**34**	4.119	0.067	0.075
8	0.969	0.366	0.413	**35**	4.240	0.054	0.059
9	1.090	0.478	0.511	**36**	4.362	0.042	0.047
10	1.212	0.578	0.598	**37**	4.483	0.033	0.037
11	1.333	0.650	0.673	**38**	4.604	0.026	0.029
12	1.454	0.719	0.736	**39**	4.725	0.020	0.023
13	1.575	0.760	0.787	**40**	4.846	0.016	0.018
14	1.696	0.806	0.830	**41**	4.967	0.013	0.015
15	1.817	0.841	0.864	**42**	5.088	0.010	0.012
16	1.938	0.870	0.892	**43**	5.210	0.008	0.009
17	2.060	0.890	0.914	**44**	5.331	0.006	0.007
18	2.181	0.914	0.932	**45**	5.452	0.005	0.006
19	2.302	0.927	0.944	**46**	5.573	0.004	0.005
20	2.423	0.941	0.937	**47**	5.694	0.003	0.004
21	2.544	0.896	0.896	**48**	5.815	0.003	0.003
22	2.665	0.791	0.821	**49**	5.937	0.002	0.002
23	2.787	0.671	0.725	**50**	6.058	0.002	0.002
24	2.908	0.553	0.623	**51**	6.179	0.002	0.001
25	3.029	0.447	0.524	**52**	6.300	0.001	0.001
26	3.150	0.362	0.434	**53**	6.421	0.001	0.001
27	3.271	0.298	0.356	**54**	6.542	0.001	0.001

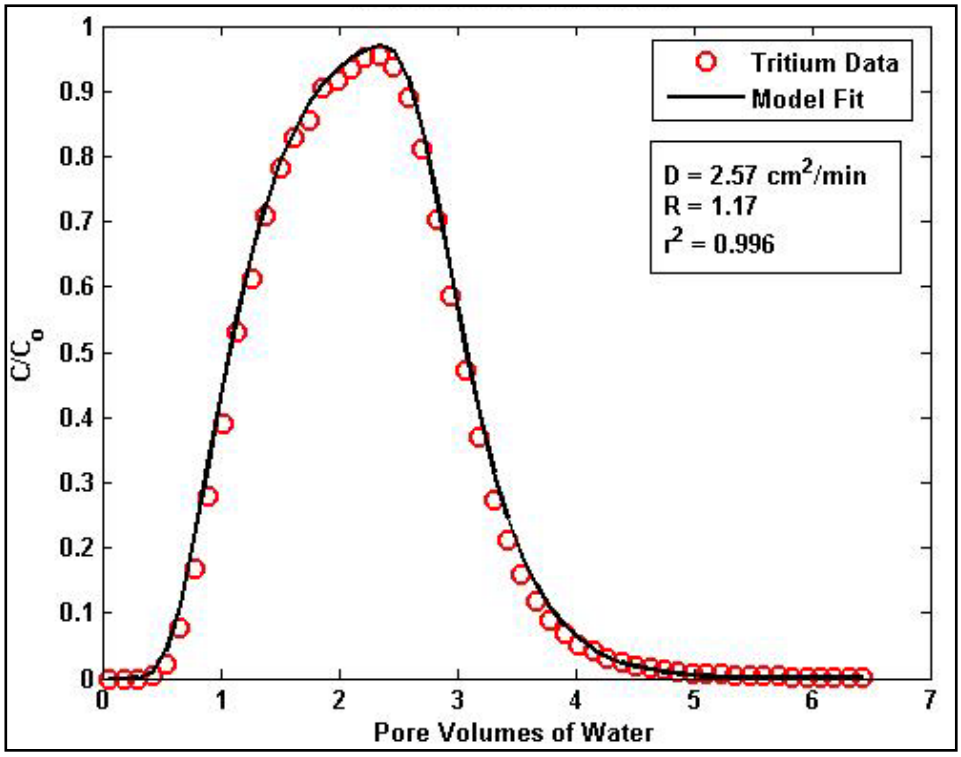

Figure E-1. Tritium BTC data from column 1A. The solid line represents the physical equilibrium model inversely fit to the data.

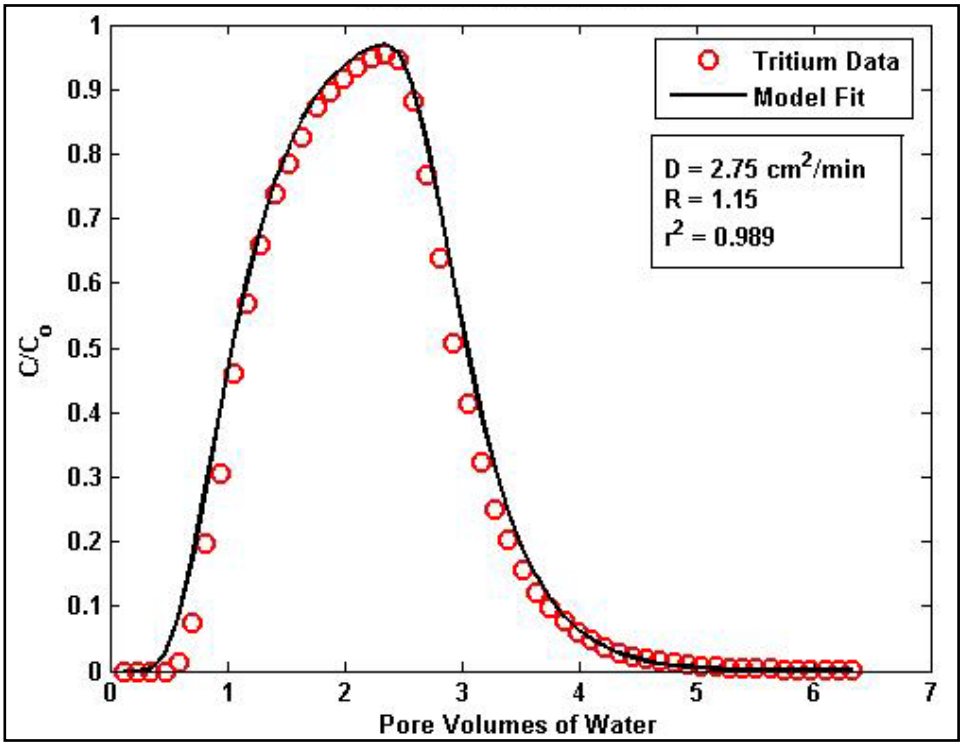

Figure E-2. Tritium BTC data from column 1B. The solid line represents the physical equilibrium model inversely fit to the data.

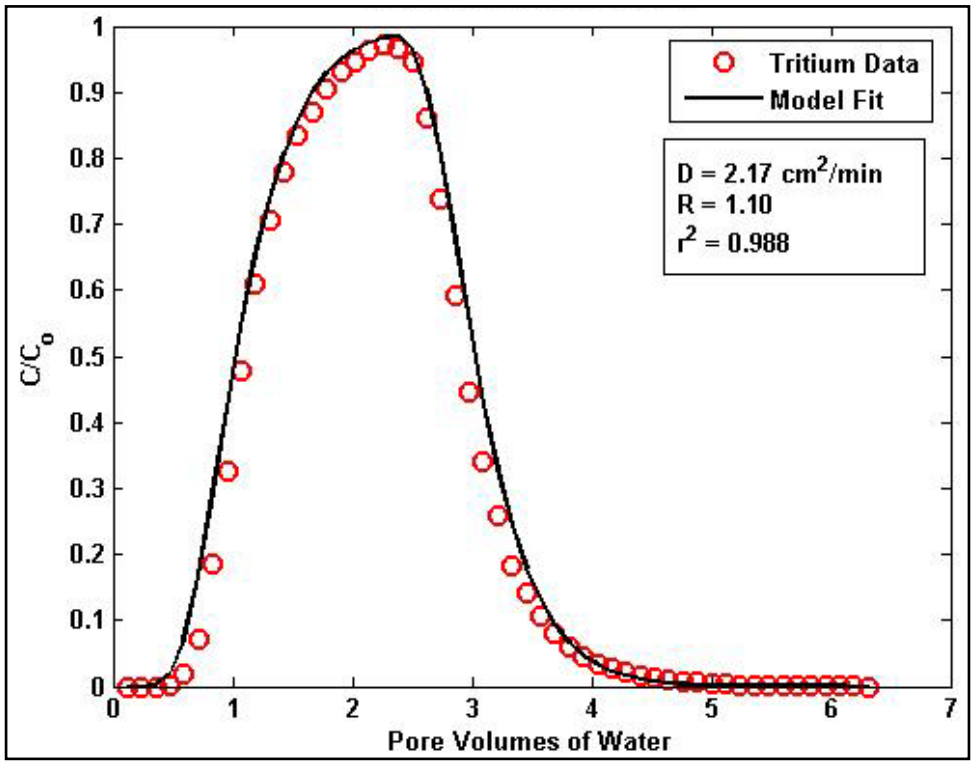

Figure E-3. Tritium BTC data from column 2A. The solid line represents the physical equilibrium model inversely fit to the data.

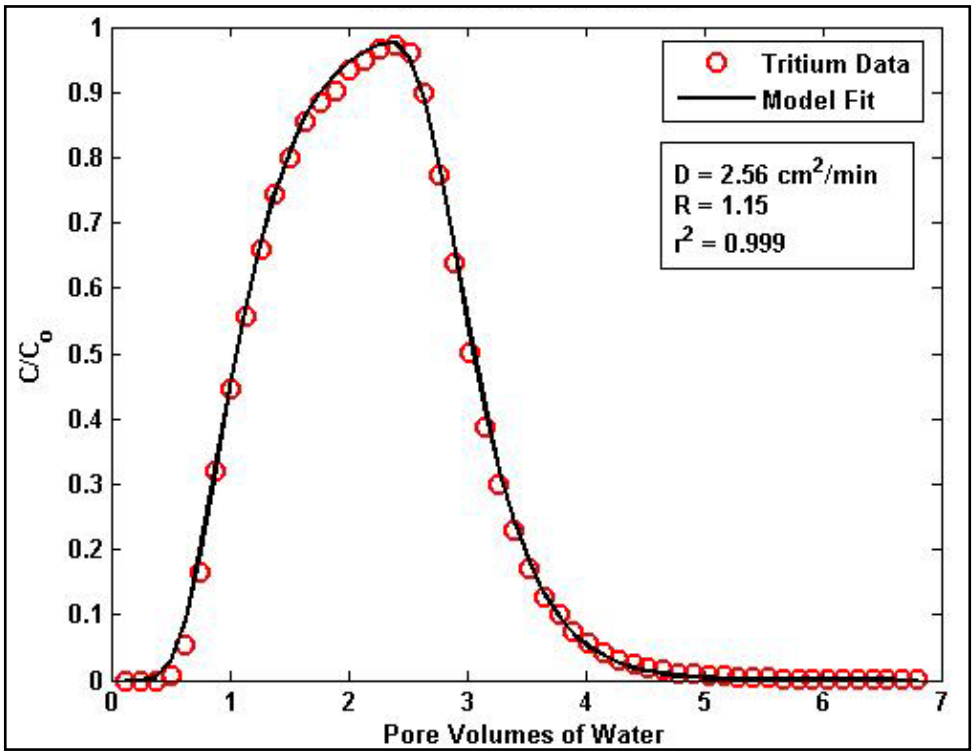

Figure E-4. Tritium BTC data from column 2B. The solid line represents the physical equilibrium model inversely fit to the data.

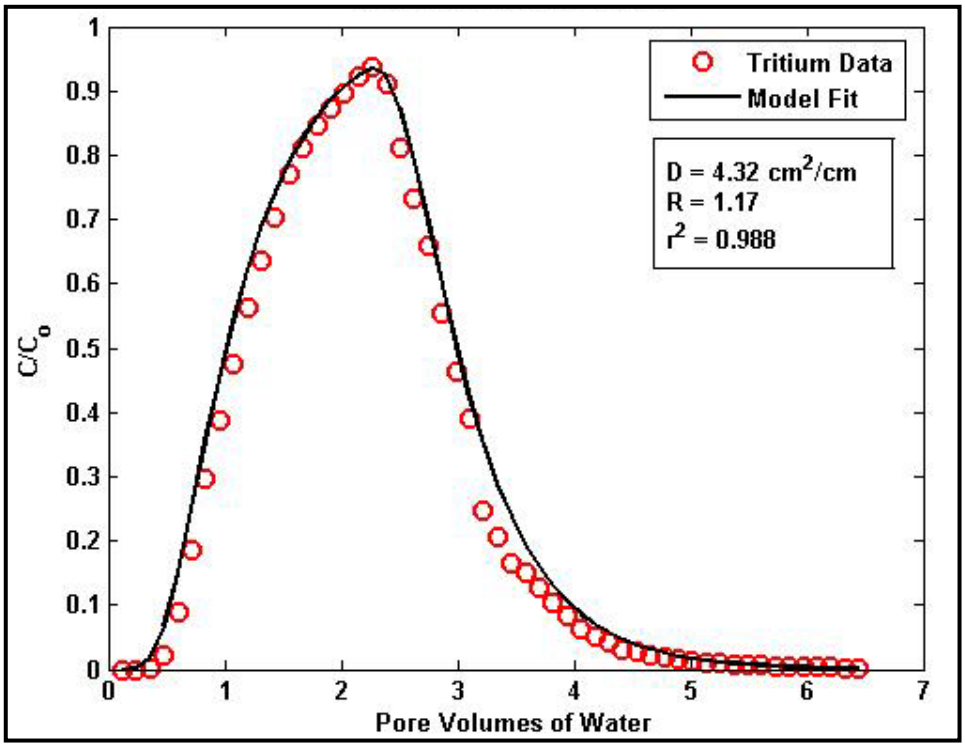

Figure E-5. Tritium BTC data from column 3A. The solid line represents the physical equilibrium model inversely fit to the data.

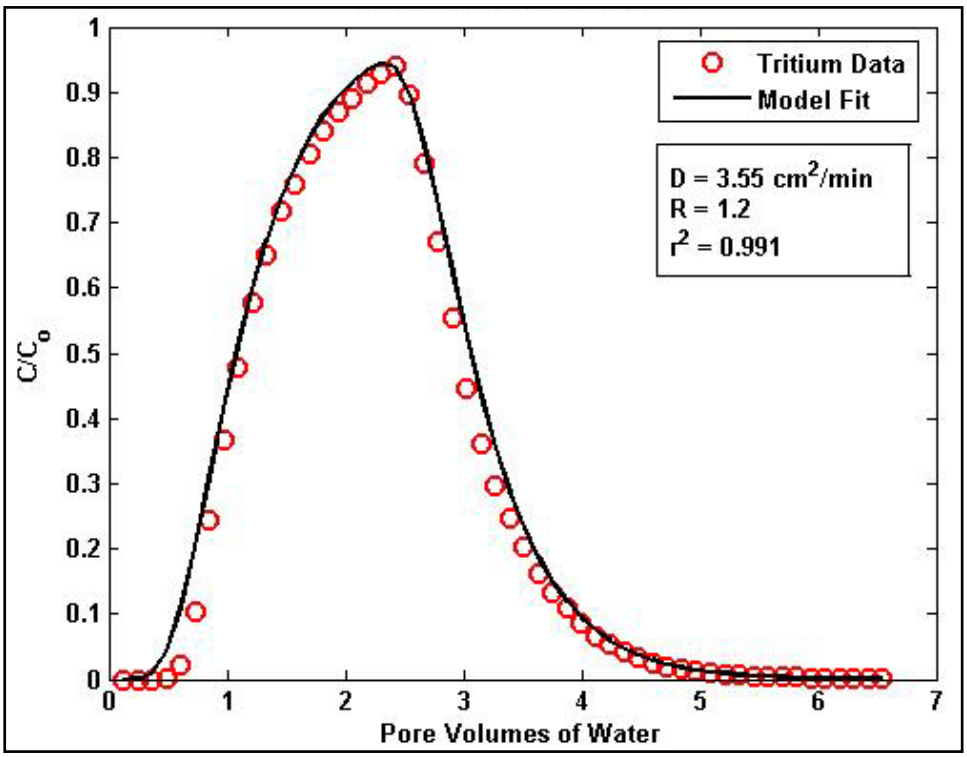

Figure E-6. Tritium BTC data from column 3B. The solid line represents the physical equilibrium model inversely fit to the data.

APPENDIX F. LABORATORY COLUMN BTEX BTC AND MODEL PREDICTION DATA.

This appendix contains the BTEX BTC data and modeling results from each laboratory transport experiment. Tables F-1 through F-6 contain the BTEX BTC data. The nonequilibrium prediction results are seen in Tables F-7 through F-12. Tables F-13 through F-18 present the equilibrium model data inversely fit to the BTEX BTC data, while the inverse nonequilibrium fit is presented in Tables F-19 through F-24. The data is presented as relative effluent concentrations as a function of effluent pore volumes. The parameters obtained from the equilibrium model fits are presented in Table F-25, while the parameters obtained from the nonequilibrium model fits are presented in Table F-26.

Table F-1. BTEX BTC data from column 1A transport experiment.

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**1.2**	0.004	0.002	0.003	0.002	0.003
2	**2.8**	0.040	0.006	0.002	0.002	0.002
3	**5.2**	0.147	0.025	0.004	0.004	0.005
4	**7.5**	0.267	0.053	0.008	0.007	0.010
5	**9.8**	0.368	0.081	0.013	0.011	0.016
6	**12.3**	0.446	0.112	0.019	0.016	0.022
7	**14.9**	0.501	0.144	0.025	0.021	0.029
8	**17.2**	0.610	0.213	0.038	0.032	0.043
9	**19.6**	0.623	0.219	0.041	0.035	0.047
10	**24.5**	0.724	0.302	0.061	0.051	0.068
11	**29.6**	0.784	0.378	0.083	0.071	0.094
12	**34.3**	0.842	0.486	0.109	0.092	0.117
13	**39.6**	0.924	0.469	0.117	0.099	0.127
14	**44.2**	0.917	0.579	0.147	0.124	0.157
15	**49.5**	1.010	0.681	0.186	0.156	0.195
16	**53.1**	0.964	0.677	0.193	0.164	0.204
17	**57.7**	0.987	0.716	0.214	0.181	0.225
18	**62.9**	1.032	0.780	0.220	0.211	0.258
19	**68.3**	1.056	0.814	0.244	0.255	0.282
20	**73.3**	1.060	0.836	0.257	0.282	0.287
21	**78.1**	0.959	0.850	0.247	0.281	0.295
22	**83.1**	0.988	0.888	0.267	0.316	0.324
23	**88.1**	0.971	0.887	0.274	0.340	0.340
24	**92.6**	0.975	0.899	0.281	0.363	0.359
25	**97.4**	0.949	0.877	0.270	0.360	0.353
26	**102.3**	1.133	0.964	0.329	0.440	0.419
27	**107.2**	1.070	0.920	0.325	0.437	0.416
28	**112.0**	1.067	0.927	0.339	0.457	0.433
29	**117.3**	1.064	0.934	0.354	0.481	0.452
30	**122.0**	0.937	0.956	0.325	0.445	0.421
31	**127.0**	0.847	0.949	0.358	0.499	0.472
32	**133.7**	0.891	0.919	0.393	0.522	0.501
33	**136.3**	0.989	1.006	0.442	0.554	0.543
34	**141.3**	0.911	0.956	0.442	0.532	0.535
35	**146.0**	1.023	0.921	0.455	0.538	0.547
36	**151.1**	0.948	1.007	0.444	0.548	0.575
37	**156.0**	0.927	1.004	0.466	0.559	0.587
38	**161.8**	0.977	0.888	0.509	0.573	0.610
39	**165.7**	1.031	0.936	0.551	0.588	0.640
40	**170.5**	0.888	0.828	0.511	0.557	0.606
41	**175.6**	0.996	0.922	0.571	0.597	0.663
42	**180.3**	1.092	1.099	0.583	0.614	0.683
43	**185.2**	0.977	0.921	0.605	0.554	0.694

Table F-1 (continued).

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**190.4**	1.127	1.080	0.622	0.657	0.720
45	**195.0**	1.171	1.113	0.662	0.686	0.763
46	**200.0**	1.133	1.082	0.650	0.679	0.754
47	**205.2**	1.047	1.002	0.705	0.640	0.709
48	**215.0**	1.078	1.095	0.734	0.669	0.751
49	**219.6**	1.061	0.971	0.734	0.673	0.753
50	**224.9**	1.028	0.956	0.740	0.683	0.767
51	**231.1**	1.082	0.986	0.751	0.691	0.797

Table F-2. BTEX BTC data from column 1B transport experiment.

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.5**	0.011	0.015	0.008	0.009	0.009
2	**2.7**	0.029	0.005	0.003	0.004	0.004
3	**5.0**	0.126	0.010	0.002	0.003	0.002
4	**7.4**	0.266	0.028	0.003	0.003	0.003
5	**10.0**	0.400	0.058	0.004	0.003	0.005
6	**12.4**	0.420	0.076	0.006	0.005	0.007
7	**14.7**	0.557	0.116	0.009	0.007	0.011
8	**17.1**	0.628	0.153	0.012	0.010	0.015
9	**19.4**	0.704	0.193	0.017	0.013	0.020
10	**24.5**	0.825	0.279	0.029	0.022	0.034
11	**29.2**	0.900	0.355	0.046	0.037	0.055
12	**34.3**	0.930	0.381	0.054	0.042	0.062
13	**38.8**	0.976	0.498	0.077	0.060	0.087
14	**43.5**	0.984	0.537	0.094	0.073	0.105
15	**48.4**	1.033	0.610	0.118	0.092	0.129
16	**53.4**	1.007	0.639	0.137	0.108	0.152
17	**58.1**	1.047	0.764	0.174	0.138	0.189
18	**62.9**	1.026	0.714	0.181	0.146	0.198
19	**67.3**	1.032	0.818	0.216	0.173	0.229
20	**72.1**	1.025	0.838	0.239	0.192	0.253
21	**76.9**	0.987	0.759	0.236	0.193	0.252
22	**82.2**	1.070	0.843	0.277	0.229	0.294
23	**86.2**	1.036	0.831	0.287	0.238	0.306
24	**91.2**	0.955	0.788	0.291	0.242	0.308
25	**95.8**	0.937	0.783	0.309	0.258	0.325
26	**100.6**	1.017	0.902	0.337	0.289	0.363
27	**105.6**	0.993	0.892	0.364	0.310	0.387
28	**110.1**	1.104	0.982	0.410	0.348	0.428
29	**114.9**	0.990	0.908	0.401	0.345	0.421
30	**119.5**	1.024	0.945	0.432	0.373	0.454
31	**124.8**	0.991	0.922	0.437	0.380	0.457
32	**143.5**	0.954	0.949	0.491	0.435	0.513
33	**148.1**	0.856	0.903	0.476	0.424	0.501
34	**152.9**	1.001	0.829	0.545	0.484	0.569
35	**158.0**	0.981	0.952	0.555	0.496	0.576
36	**162.6**	0.935	0.938	0.552	0.498	0.578
37	**167.5**	0.950	0.906	0.565	0.512	0.594
38	**172.4**	0.987	0.925	0.596	0.544	0.620
39	**177.6**	1.041	0.975	0.628	0.573	0.656
40	**182.1**	0.915	0.862	0.574	0.528	0.603
41	**186.5**	1.063	0.994	0.658	0.605	0.695
42	**191.6**	0.984	0.933	0.640	0.591	0.674
43	**196.3**	1.014	1.015	0.699	0.644	0.727

Table F-2 (continued).

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**201.1**	1.066	1.057	0.732	0.672	0.755
45	**205.9**	0.968	0.972	0.690	0.635	0.725
46	**210.4**	1.016	1.008	0.730	0.671	0.767
47	**215.5**	0.957	0.957	0.712	0.660	0.746
48	**219.7**	1.014	1.006	0.755	0.698	0.792
49	**224.9**	0.990	0.905	0.648	0.605	0.703
50	**225.1**	1.028	0.953	0.696	0.652	0.746
51	**225.3**	1.112	1.032	0.753	0.707	0.795

Table F-3. BTEX BTC data from column 2A transport experiment.

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.008	0.006	0.006	0.006	0.006
2	**2.5**	0.011	0.002	0.002	0.003	0.002
3	**5.0**	0.079	0.005	0.002	0.002	0.002
4	**7.5**	0.214	0.014	0.002	0.002	0.002
5	**9.7**	0.325	0.027	0.002	0.002	0.002
6	**12.4**	0.460	0.050	0.003	0.003	0.004
7	**14.7**	0.443	0.062	0.004	0.003	0.004
8	**17.3**	0.578	0.100	0.006	0.004	0.007
9	**21.8**	0.665	0.157	0.010	0.007	0.012
10	**24.4**	0.741	0.236	0.015	0.011	0.018
11	**29.4**	0.836	0.284	0.025	0.020	0.031
12	**34.7**	0.936	0.380	0.033	0.025	0.038
13	**39.9**	0.944	0.435	0.043	0.032	0.049
14	**44.2**	0.962	0.489	0.054	0.040	0.062
15	**49.1**	1.024	0.562	0.070	0.052	0.079
16	**54.1**	0.967	0.573	0.080	0.060	0.090
17	**58.8**	0.955	0.597	0.090	0.068	0.102
18	**64.9**	0.965	0.644	0.113	0.085	0.123
19	**68.6**	0.955	0.656	0.134	0.106	0.148
20	**73.2**	1.065	0.748	0.147	0.113	0.161
21	**78.3**	0.977	0.716	0.155	0.120	0.169
22	**83.0**	0.953	0.716	0.165	0.129	0.181
23	**88.2**	0.976	0.750	0.184	0.145	0.201
24	**92.6**	0.895	0.761	0.185	0.146	0.204
25	**97.2**	0.905	0.779	0.201	0.162	0.221
26	**102.3**	0.985	0.784	0.246	0.197	0.261
27	**107.0**	1.023	0.793	0.266	0.214	0.282
28	**111.8**	1.069	0.828	0.298	0.239	0.312
29	**116.8**	0.926	0.781	0.266	0.217	0.285
30	**121.9**	1.071	0.900	0.310	0.253	0.325
31	**126.7**	0.988	0.846	0.312	0.258	0.333
32	**131.5**	0.940	0.812	0.311	0.258	0.332
33	**136.4**	0.918	0.801	0.318	0.266	0.338
34	**141.1**	0.965	0.847	0.345	0.290	0.367
35	**145.9**	1.026	0.896	0.372	0.312	0.391
36	**150.9**	0.966	0.855	0.371	0.315	0.393
37	**155.8**	0.843	0.757	0.342	0.291	0.364
38	**160.5**	0.953	0.858	0.396	0.338	0.419
39	**165.6**	0.953	0.860	0.407	0.351	0.429
40	**165.8**	0.977	0.879	0.424	0.366	0.438
41	**176.0**	0.912	0.835	0.419	0.367	0.435
42	**179.9**	0.921	0.844	0.438	0.397	0.468
43	**184.6**	1.050	0.901	0.499	0.458	0.492

Table F-3 (continued).

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**189.7**	0.970	0.841	0.486	0.450	0.478
45	**194.4**	1.084	0.942	0.550	0.507	0.529
46	**199.2**	1.111	0.961	0.563	0.521	0.551
47	**204.3**	1.074	0.937	0.561	0.521	0.561
48	**209.7**	1.065	0.927	0.566	0.526	0.581
49	**213.9**	1.015	0.885	0.557	0.517	0.586
50	**219.1**	0.933	0.902	0.568	0.532	0.555
51	**223.5**	0.979	0.944	0.582	0.559	0.589
52	**228.7**	1.000	0.968	0.577	0.566	0.608

Table F-4. BTEX BTC data from column 2B transport experiment.

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.7**	0.006	0.000	0.000	0.000	0.000
2	**2.7**	0.015	0.005	0.005	0.004	0.005
3	**5.2**	0.092	0.007	0.003	0.003	0.003
4	**7.8**	0.208	0.018	0.003	0.003	0.003
5	**11.1**	0.314	0.040	0.004	0.003	0.004
6	**12.9**	0.394	0.059	0.004	0.003	0.005
7	**15.5**	0.435	0.082	0.006	0.005	0.007
8	**18.1**	0.486	0.111	0.008	0.006	0.010
9	**21.5**	0.576	0.161	0.013	0.010	0.016
10	**26.1**	0.709	0.245	0.024	0.019	0.029
11	**31.2**	0.837	0.335	0.043	0.034	0.051
12	**36.6**	0.880	0.415	0.063	0.050	0.072
13	**41.6**	0.916	0.477	0.087	0.069	0.097
14	**47.6**	0.944	0.560	0.121	0.097	0.133
15	**49.2**	0.974	0.583	0.130	0.105	0.143
16	**57.2**	0.981	0.650	0.177	0.146	0.190
17	**62.4**	0.969	0.671	0.202	0.169	0.217
18	**67.8**	0.939	0.737	0.211	0.179	0.229
19	**72.8**	0.966	0.776	0.239	0.201	0.255
20	**77.9**	1.005	0.814	0.258	0.219	0.274
21	**83.3**	0.960	0.877	0.270	0.230	0.286
22	**88.5**	0.998	0.872	0.291	0.239	0.294
23	**93.4**	0.897	0.891	0.299	0.235	0.290
24	**98.7**	0.998	0.903	0.325	0.261	0.322
25	**103.9**	0.938	0.883	0.355	0.270	0.331
26	**108.8**	1.055	0.910	0.361	0.312	0.358
27	**113.8**	1.036	0.905	0.369	0.322	0.368
28	**119.5**	1.066	0.927	0.387	0.340	0.392
29	**124.4**	1.091	0.956	0.410	0.362	0.421
30	**129.6**	0.986	0.880	0.398	0.356	0.414
31	**134.9**	1.058	0.939	0.435	0.392	0.462
32	**146.2**	0.988	0.944	0.440	0.415	0.478
33	**148.3**	0.966	0.944	0.460	0.413	0.476
34	**155.3**	0.967	0.909	0.467	0.437	0.488
35	**160.8**	0.962	0.888	0.482	0.444	0.481
36	**165.7**	0.965	0.901	0.495	0.456	0.511
37	**170.6**	1.010	0.932	0.502	0.464	0.511
38	**175.9**	1.088	0.970	0.541	0.488	0.559
39	**185.9**	0.958	0.956	0.557	0.497	0.530
40	**191.3**	0.962	0.962	0.565	0.505	0.534
41	**197.0**	0.953	0.953	0.576	0.513	0.549
42	**202.4**	0.923	0.947	0.576	0.522	0.563
43	**207.3**	0.981	0.977	0.584	0.539	0.609

Table F-4 (continued).

Sample	Pore Volumes	C/C$_o$ Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.8**	0.968	0.970	0.591	0.546	0.618
45	**217.0**	0.943	0.948	0.583	0.539	0.617
46	**222.1**	1.001	0.994	0.610	0.569	0.641
47	**226.8**	1.047	1.045	0.652	0.608	0.691
48	**233.0**	0.938	0.936	0.626	0.586	0.663
49	**237.9**	0.970	0.879	0.567	0.529	0.600
50	**241.7**	0.954	0.939	0.653	0.611	0.692

Table F-5. BTEX BTC data from column 3A transport experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.007	0.005	0.009	0.006	0.009
2	**3.4**	0.109	0.019	0.007	0.005	0.007
3	**5.1**	0.169	0.033	0.008	0.006	0.008
4	**7.7**	0.302	0.070	0.013	0.011	0.015
5	**10.1**	0.351	0.091	0.017	0.014	0.020
6	**13.4**	0.388	0.114	0.022	0.019	0.026
7	**15.6**	0.554	0.185	0.035	0.029	0.039
8	**18.5**	0.574	0.191	0.039	0.033	0.043
9	**20.9**	0.720	0.251	0.052	0.043	0.056
10	**26.5**	0.806	0.318	0.068	0.057	0.075
11	**31.3**	0.781	0.346	0.081	0.070	0.090
12	**36.5**	0.874	0.424	0.100	0.085	0.110
13	**41.4**	0.995	0.519	0.126	0.107	0.135
14	**46.7**	0.872	0.499	0.128	0.110	0.139
15	**51.9**	0.930	0.562	0.148	0.126	0.159
16	**58.4**	1.007	0.651	0.182	0.154	0.192
17	**60.9**	0.924	0.616	0.174	0.149	0.186
18	**69.7**	0.905	0.644	0.184	0.156	0.198
19	**72.3**	0.901	0.655	0.195	0.165	0.208
20	**77.4**	0.959	0.717	0.218	0.184	0.232
21	**82.6**	0.991	0.702	0.227	0.192	0.242
22	**87.9**	1.017	0.736	0.236	0.204	0.248
23	**93.7**	1.094	0.764	0.279	0.242	0.294
24	**98.2**	0.990	0.787	0.279	0.243	0.297
25	**103.9**	0.972	0.808	0.326	0.288	0.349
26	**109.9**	1.037	0.877	0.372	0.320	0.382
27	**112.7**	1.053	0.902	0.384	0.334	0.395
28	**118.4**	1.021	0.901	0.407	0.360	0.417
29	**126.6**	0.992	0.889	0.415	0.370	0.425
30	**129.0**	0.931	0.881	0.385	0.348	0.402
31	**133.0**	0.921	0.881	0.392	0.359	0.413
32	**139.1**	0.946	0.911	0.421	0.385	0.437
33	**143.8**	0.940	0.907	0.439	0.398	0.455
34	**153.8**	0.911	1.077	0.464	0.423	0.483
35	**159.7**	1.037	0.956	0.523	0.472	0.539
36	**164.7**	1.081	0.982	0.546	0.492	0.556
37	**169.2**	0.914	0.887	0.500	0.455	0.522
38	**179.7**	0.916	0.901	0.533	0.488	0.558
39	**184.2**	1.027	1.004	0.596	0.548	0.621
40	**190.0**	0.924	0.911	0.549	0.507	0.576
41	**196.2**	0.989	0.857	0.555	0.514	0.579
42	**200.5**	1.107	1.060	0.591	0.550	0.604
43	**205.3**	1.019	0.979	0.552	0.517	0.569

Table F-5 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.4**	1.062	1.021	0.588	0.555	0.613
45	**215.3**	1.064	1.027	0.613	0.580	0.636
46	**221.0**	0.938	0.899	0.560	0.532	0.593
47	**226.0**	1.048	0.998	0.634	0.597	0.665
48	**230.8**	1.010	0.958	0.610	0.583	0.650
49	**235.7**	0.945	0.895	0.577	0.553	0.620
50	**238.3**	1.038	0.975	0.637	0.609	0.669

Table F-6. BTEX BTC data from column 3B transport experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.3**	0.009	0.011	0.011	0.009	0.011
2	**2.7**	0.052	0.006	0.005	0.004	0.004
3	**5.2**	0.215	0.026	0.005	0.004	0.005
4	**7.6**	0.321	0.053	0.006	0.005	0.007
5	**9.8**	0.370	0.074	0.008	0.007	0.010
6	**12.8**	0.505	0.124	0.014	0.011	0.017
7	**15.4**	0.558	0.155	0.019	0.015	0.022
8	**18.7**	0.662	0.224	0.030	0.024	0.034
9	**20.3**	0.703	0.237	0.033	0.027	0.038
10	**24.8**	0.751	0.278	0.044	0.036	0.051
11	**30.4**	0.809	0.324	0.062	0.051	0.071
12	**35.9**	0.874	0.421	0.085	0.069	0.095
13	**39.8**	0.943	0.483	0.102	0.083	0.114
14	**45.1**	0.908	0.505	0.117	0.096	0.129
15	**49.8**	0.918	0.541	0.134	0.111	0.146
16	**54.6**	0.947	0.588	0.155	0.128	0.168
17	**59.9**	0.960	0.626	0.175	0.146	0.188
18	**64.8**	0.910	0.661	0.184	0.154	0.198
19	**73.1**	1.019	0.732	0.235	0.197	0.249
20	**74.8**	1.000	0.732	0.241	0.206	0.259
21	**79.5**	1.010	0.757	0.258	0.220	0.275
22	**84.5**	1.074	0.823	0.292	0.249	0.308
23	**89.8**	0.966	0.791	0.307	0.259	0.311
24	**95.2**	1.011	0.808	0.312	0.269	0.331
25	**99.5**	1.004	0.855	0.340	0.296	0.357
26	**104.5**	1.009	0.865	0.359	0.323	0.373
27	**109.5**	1.069	0.899	0.388	0.339	0.404
28	**113.3**	1.074	0.910	0.404	0.353	0.421
29	**119.0**	1.040	0.892	0.410	0.361	0.425
30	**125.7**	1.020	0.885	0.423	0.374	0.441
31	**131.7**	1.077	0.944	0.470	0.417	0.486
32	**134.3**	0.965	0.895	0.459	0.415	0.480
33	**139.4**	1.047	0.963	0.497	0.445	0.507
34	**144.2**	0.975	0.914	0.490	0.442	0.509
35	**148.6**	0.994	0.944	0.519	0.470	0.535
36	**154.4**	0.911	0.915	0.549	0.499	0.564
37	**164.0**	0.996	0.912	0.533	0.482	0.549
38	**168.7**	1.035	0.946	0.563	0.511	0.580
39	**175.1**	0.984	0.914	0.565	0.516	0.587
40	**179.3**	1.109	1.025	0.633	0.577	0.646
41	**184.1**	0.969	0.903	0.597	0.544	0.622
42	**188.6**	1.027	0.966	0.636	0.585	0.658
43	**193.1**	1.014	0.956	0.634	0.586	0.651

Table F-6 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	197.2	0.922	0.879	0.601	0.557	0.621
45	202.8	1.000	0.943	0.640	0.595	0.665
46	207.1	0.931	0.891	0.648	0.573	0.638
47	212.3	1.013	0.978	0.659	0.624	0.692
48	217.2	1.043	0.993	0.666	0.631	0.699
49	222.3	1.041	0.999	0.682	0.651	0.722
50	227.5	0.988	0.946	0.696	0.652	0.735
51	232.6	0.961	0.920	0.680	0.641	0.720

Table F-7. Nonequilibrium prediction model results for column 1A experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**1.2**	0.012	0.001	0.001	0.001	0.001
2	**2.8**	0.080	0.014	0.004	0.004	0.005
3	**5.2**	0.215	0.042	0.010	0.010	0.012
4	**7.5**	0.358	0.082	0.019	0.019	0.023
5	**9.8**	0.493	0.131	0.032	0.030	0.037
6	**12.3**	0.617	0.192	0.048	0.045	0.055
7	**14.9**	0.723	0.263	0.070	0.065	0.079
8	**17.2**	0.795	0.328	0.093	0.085	0.103
9	**19.6**	0.852	0.396	0.119	0.109	0.130
10	**24.5**	0.927	0.530	0.182	0.166	0.196
11	**29.6**	0.965	0.648	0.253	0.231	0.269
12	**34.3**	0.983	0.739	0.325	0.297	0.341
13	**39.6**	0.992	0.817	0.405	0.372	0.422
14	**44.2**	0.996	0.867	0.473	0.436	0.489
15	**49.5**	0.998	0.910	0.547	0.508	0.562
16	**53.1**	0.999	0.932	0.594	0.554	0.608
17	**57.7**	1.000	0.952	0.649	0.609	0.663
18	**62.9**	1.000	0.969	0.706	0.666	0.718
19	**68.3**	1.000	0.980	0.756	0.719	0.767
20	**73.3**	1.000	0.986	0.796	0.761	0.805
21	**78.1**	1.000	0.991	0.830	0.797	0.838
22	**83.1**	1.000	0.994	0.859	0.829	0.866
23	**88.1**	1.000	0.996	0.885	0.858	0.891
24	**92.6**	1.000	0.997	0.904	0.879	0.909
25	**97.4**	1.000	0.998	0.921	0.899	0.925
26	**102.3**	1.000	0.999	0.935	0.916	0.939
27	**107.2**	1.000	0.999	0.947	0.931	0.950
28	**112.0**	1.000	1.000	0.957	0.942	0.959
29	**117.3**	1.000	1.000	0.966	0.953	0.968
30	**122.0**	1.000	1.000	0.972	0.961	0.974
31	**127.0**	1.000	1.000	0.978	0.968	0.979
32	**133.7**	1.000	1.000	0.983	0.976	0.984
33	**136.3**	1.000	1.000	0.985	0.978	0.986
34	**141.3**	1.000	1.000	0.988	0.982	0.989
35	**146.0**	1.000	1.000	0.990	0.985	0.991
36	**151.1**	1.000	1.000	0.992	0.988	0.993
37	**156.0**	1.000	1.000	0.994	0.990	0.994
38	**161.8**	1.000	1.000	0.995	0.993	0.996
39	**165.7**	1.000	1.000	0.996	0.994	0.996
40	**170.5**	1.000	1.000	0.997	0.995	0.997
41	**175.6**	1.000	1.000	0.998	0.996	0.998
42	**180.3**	1.000	1.000	0.998	0.997	0.998
43	**185.2**	1.000	1.000	0.998	0.997	0.999

Table F-7 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**190.4**	1.000	1.000	0.999	0.998	0.999
45	**195.0**	1.000	1.000	0.999	0.998	0.999
46	**200.0**	1.000	1.000	0.999	0.999	0.999
47	**205.2**	1.000	1.000	0.999	0.999	0.999
48	**215.0**	1.000	1.000	1.000	0.999	1.000
49	**219.6**	1.000	1.000	1.000	0.999	1.000
50	**224.9**	1.000	1.000	1.000	1.000	1.000
51	**231.1**	1.000	1.000	1.000	1.000	1.000

Table F-8. Nonequilibrium prediction model results for column 1B experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.5**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.050	0.011	0.003	0.003	0.003
3	**5.0**	0.160	0.033	0.007	0.008	0.009
4	**7.4**	0.303	0.069	0.015	0.015	0.018
5	**10.0**	0.458	0.119	0.027	0.026	0.031
6	**12.4**	0.587	0.175	0.042	0.039	0.048
7	**14.7**	0.688	0.233	0.058	0.054	0.066
8	**17.1**	0.776	0.299	0.080	0.073	0.088
9	**19.4**	0.839	0.363	0.103	0.094	0.113
10	**24.5**	0.926	0.498	0.162	0.147	0.174
11	**29.2**	0.965	0.610	0.224	0.203	0.239
12	**34.3**	0.985	0.710	0.297	0.270	0.312
13	**38.8**	0.993	0.782	0.362	0.331	0.379
14	**43.5**	0.997	0.840	0.431	0.396	0.447
15	**48.4**	0.999	0.886	0.500	0.461	0.515
16	**53.4**	0.999	0.920	0.565	0.525	0.580
17	**58.1**	1.000	0.943	0.622	0.582	0.636
18	**62.9**	1.000	0.960	0.675	0.634	0.687
19	**67.3**	1.000	0.972	0.718	0.679	0.730
20	**72.1**	1.000	0.980	0.760	0.722	0.770
21	**76.9**	1.000	0.986	0.797	0.761	0.806
22	**82.2**	1.000	0.991	0.832	0.799	0.840
23	**86.2**	1.000	0.994	0.855	0.824	0.862
24	**91.2**	1.000	0.996	0.879	0.852	0.886
25	**95.8**	1.000	0.997	0.899	0.874	0.904
26	**100.6**	1.000	0.998	0.916	0.893	0.920
27	**105.6**	1.000	0.999	0.931	0.911	0.935
28	**110.1**	1.000	0.999	0.942	0.924	0.945
29	**114.9**	1.000	0.999	0.952	0.937	0.955
30	**119.5**	1.000	1.000	0.960	0.946	0.963
31	**124.8**	1.000	1.000	0.968	0.956	0.970
32	**143.5**	1.000	1.000	0.985	0.979	0.986
33	**148.1**	1.000	1.000	0.988	0.982	0.989
34	**152.9**	1.000	1.000	0.990	0.985	0.991
35	**158.0**	1.000	1.000	0.992	0.988	0.993
36	**162.6**	1.000	1.000	0.993	0.990	0.994
37	**167.5**	1.000	1.000	0.995	0.992	0.995
38	**172.4**	1.000	1.000	0.996	0.993	0.996
39	**177.6**	1.000	1.000	0.997	0.994	0.997
40	**182.1**	1.000	1.000	0.997	0.995	0.997
41	**186.5**	1.000	1.000	0.998	0.996	0.998
42	**191.6**	1.000	1.000	0.998	0.997	0.998
43	**196.3**	1.000	1.000	0.998	0.997	0.999

Table F-8 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**201.1**	1.000	1.000	0.999	0.998	0.999
45	**205.9**	1.000	1.000	0.999	0.998	0.999
46	**210.4**	1.000	1.000	0.999	0.999	0.999
47	**215.5**	1.000	1.000	0.999	0.999	0.999
48	**219.7**	1.000	1.000	0.999	0.999	1.000
49	**224.9**	1.000	1.000	1.000	0.999	1.000
50	**225.1**	1.000	1.000	1.000	0.999	1.000
51	**225.3**	1.000	1.000	1.000	0.999	1.000

Table F-9. Nonequilibrium prediction model results for column 2A experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.000	0.000	0.000	0.000	0.000
2	**2.5**	0.042	0.010	0.003	0.004	0.004
3	**5.0**	0.153	0.033	0.009	0.009	0.010
4	**7.5**	0.298	0.070	0.017	0.017	0.020
5	**9.7**	0.428	0.110	0.027	0.027	0.031
6	**12.4**	0.571	0.168	0.042	0.041	0.048
7	**14.7**	0.680	0.226	0.059	0.057	0.067
8	**17.3**	0.774	0.294	0.081	0.076	0.090
9	**21.8**	0.882	0.414	0.126	0.117	0.137
10	**24.4**	0.922	0.481	0.156	0.144	0.168
11	**29.4**	0.965	0.598	0.218	0.200	0.232
12	**34.7**	0.986	0.705	0.291	0.267	0.307
13	**39.9**	0.994	0.787	0.365	0.335	0.381
14	**44.2**	0.997	0.840	0.426	0.392	0.442
15	**49.1**	0.999	0.886	0.492	0.455	0.508
16	**54.1**	1.000	0.920	0.556	0.517	0.571
17	**58.8**	1.000	0.944	0.613	0.573	0.628
18	**64.9**	1.000	0.965	0.680	0.639	0.692
19	**68.6**	1.000	0.974	0.715	0.675	0.727
20	**73.2**	1.000	0.982	0.756	0.717	0.767
21	**78.3**	1.000	0.988	0.796	0.759	0.805
22	**83.0**	1.000	0.992	0.827	0.792	0.835
23	**88.2**	1.000	0.995	0.857	0.825	0.864
24	**92.6**	1.000	0.996	0.879	0.849	0.885
25	**97.2**	1.000	0.998	0.899	0.872	0.904
26	**102.3**	1.000	0.998	0.917	0.893	0.922
27	**107.0**	1.000	0.999	0.931	0.910	0.935
28	**111.8**	1.000	0.999	0.943	0.924	0.947
29	**116.8**	1.000	1.000	0.954	0.937	0.957
30	**121.9**	1.000	1.000	0.963	0.948	0.965
31	**126.7**	1.000	1.000	0.970	0.957	0.971
32	**131.5**	1.000	1.000	0.975	0.964	0.977
33	**136.4**	1.000	1.000	0.980	0.971	0.981
34	**141.1**	1.000	1.000	0.984	0.976	0.985
35	**145.9**	1.000	1.000	0.987	0.980	0.988
36	**150.9**	1.000	1.000	0.989	0.984	0.990
37	**155.8**	1.000	1.000	0.991	0.987	0.992
38	**160.5**	1.000	1.000	0.993	0.989	0.994
39	**165.6**	1.000	1.000	0.994	0.991	0.995
40	**165.8**	1.000	1.000	0.995	0.991	0.995
41	**176.0**	1.000	1.000	0.997	0.994	0.997
42	**179.9**	1.000	1.000	0.997	0.995	0.997
43	**184.6**	1.000	1.000	0.998	0.996	0.998

Table F-9 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**189.7**	1.000	1.000	0.998	0.997	0.998
45	**194.4**	1.000	1.000	0.999	0.997	0.999
46	**199.2**	1.000	1.000	0.999	0.998	0.999
47	**204.3**	1.000	1.000	0.999	0.998	0.999
48	**209.7**	1.000	1.000	0.999	0.999	0.999
49	**213.9**	1.000	1.000	0.999	0.999	0.999
50	**219.1**	1.000	1.000	1.000	0.999	1.000
51	**223.5**	1.000	1.000	1.000	0.999	1.000
52	**228.7**	1.000	1.000	1.000	0.999	1.000

Table F-10. Nonequilibrium prediction model results for column 2B experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.7**	0.000	0.000	0.000	0.001	0.000
2	**2.7**	0.048	0.012	0.004	0.004	0.005
3	**5.2**	0.159	0.036	0.009	0.010	0.011
4	**7.8**	0.302	0.073	0.018	0.019	0.022
5	**11.1**	0.484	0.135	0.034	0.034	0.039
6	**12.9**	0.572	0.173	0.045	0.043	0.051
7	**15.5**	0.684	0.235	0.064	0.061	0.071
8	**18.1**	0.770	0.298	0.085	0.080	0.094
9	**21.5**	0.855	0.386	0.118	0.109	0.129
10	**26.1**	0.924	0.496	0.167	0.154	0.180
11	**31.2**	0.965	0.610	0.231	0.212	0.245
12	**36.6**	0.985	0.709	0.301	0.276	0.317
13	**41.6**	0.993	0.782	0.367	0.338	0.384
14	**47.6**	0.998	0.850	0.447	0.413	0.463
15	**49.2**	0.998	0.864	0.467	0.432	0.483
16	**57.2**	1.000	0.920	0.565	0.526	0.580
17	**62.4**	1.000	0.944	0.623	0.583	0.637
18	**67.8**	1.000	0.962	0.678	0.638	0.690
19	**72.8**	1.000	0.973	0.723	0.684	0.734
20	**77.9**	1.000	0.982	0.764	0.726	0.774
21	**83.3**	1.000	0.988	0.802	0.766	0.811
22	**88.5**	1.000	0.992	0.833	0.800	0.841
23	**93.4**	1.000	0.994	0.859	0.828	0.866
24	**98.7**	1.000	0.996	0.883	0.855	0.889
25	**103.9**	1.000	0.997	0.902	0.877	0.907
26	**108.8**	1.000	0.998	0.918	0.895	0.923
27	**113.8**	1.000	0.999	0.932	0.911	0.936
28	**119.5**	1.000	0.999	0.945	0.927	0.948
29	**124.4**	1.000	1.000	0.954	0.938	0.957
30	**129.6**	1.000	1.000	0.963	0.949	0.965
31	**134.9**	1.000	1.000	0.969	0.957	0.971
32	**146.2**	1.000	1.000	0.980	0.972	0.982
33	**148.3**	1.000	1.000	0.982	0.974	0.983
34	**155.3**	1.000	1.000	0.986	0.980	0.987
35	**160.8**	1.000	1.000	0.989	0.983	0.990
36	**165.7**	1.000	1.000	0.991	0.986	0.992
37	**170.6**	1.000	1.000	0.993	0.988	0.993
38	**175.9**	1.000	1.000	0.994	0.991	0.995
39	**185.9**	1.000	1.000	0.996	0.994	0.996
40	**191.3**	1.000	1.000	0.997	0.995	0.997
41	**197.0**	1.000	1.000	0.998	0.996	0.998
42	**202.4**	1.000	1.000	0.998	0.997	0.998
43	**207.3**	1.000	1.000	0.998	0.997	0.999

Table F-10 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.8**	1.000	1.000	0.999	0.998	0.999
45	**217.0**	1.000	1.000	0.999	0.998	0.999
46	**222.1**	1.000	1.000	0.999	0.998	0.999
47	**226.8**	1.000	1.000	0.999	0.999	0.999
48	**233.0**	1.000	1.000	0.999	0.999	1.000
49	**237.9**	1.000	1.000	1.000	0.999	1.000
50	**241.7**	1.000	1.000	1.000	0.999	1.000

Table F-11. Nonequilibrium prediction model results for column 3A experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.001	0.001	0.001	0.002	0.001
2	**3.4**	0.119	0.034	0.011	0.012	0.014
3	**5.1**	0.213	0.061	0.019	0.020	0.022
4	**7.7**	0.365	0.113	0.035	0.034	0.040
5	**10.1**	0.493	0.167	0.053	0.051	0.058
6	**13.4**	0.643	0.249	0.082	0.078	0.090
7	**15.6**	0.724	0.308	0.105	0.099	0.114
8	**18.5**	0.803	0.381	0.138	0.128	0.148
9	**20.9**	0.852	0.440	0.166	0.154	0.177
10	**26.5**	0.928	0.568	0.240	0.222	0.252
11	**31.3**	0.961	0.659	0.305	0.282	0.318
12	**36.5**	0.980	0.742	0.377	0.350	0.391
13	**41.4**	0.990	0.802	0.442	0.411	0.455
14	**46.7**	0.995	0.853	0.508	0.475	0.521
15	**51.9**	0.997	0.891	0.568	0.534	0.581
16	**58.4**	0.999	0.925	0.636	0.601	0.647
17	**60.9**	0.999	0.935	0.660	0.625	0.671
18	**69.7**	1.000	0.961	0.734	0.700	0.743
19	**72.3**	1.000	0.967	0.753	0.720	0.762
20	**77.4**	1.000	0.976	0.787	0.756	0.795
21	**82.6**	1.000	0.982	0.817	0.788	0.825
22	**87.9**	1.000	0.987	0.843	0.816	0.850
23	**93.7**	1.000	0.991	0.869	0.844	0.875
24	**98.2**	1.000	0.993	0.886	0.863	0.891
25	**103.9**	1.000	0.995	0.904	0.883	0.908
26	**109.9**	1.000	0.996	0.920	0.902	0.924
27	**112.7**	1.000	0.997	0.927	0.909	0.930
28	**118.4**	1.000	0.998	0.939	0.923	0.942
29	**126.6**	1.000	0.999	0.952	0.939	0.955
30	**129.0**	1.000	0.999	0.956	0.943	0.958
31	**133.0**	1.000	0.999	0.961	0.950	0.963
32	**139.1**	1.000	0.999	0.968	0.958	0.970
33	**143.8**	1.000	1.000	0.972	0.963	0.974
34	**153.8**	1.000	1.000	0.980	0.973	0.981
35	**159.7**	1.000	1.000	0.983	0.977	0.984
36	**164.7**	1.000	1.000	0.986	0.980	0.987
37	**169.2**	1.000	1.000	0.987	0.983	0.988
38	**179.7**	1.000	1.000	0.991	0.987	0.992
39	**184.2**	1.000	1.000	0.992	0.989	0.993
40	**190.0**	1.000	1.000	0.993	0.990	0.994
41	**196.2**	1.000	1.000	0.995	0.992	0.995
42	**200.5**	1.000	1.000	0.995	0.993	0.996
43	**205.3**	1.000	1.000	0.996	0.994	0.996

Table F-11 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.4**	1.000	1.000	0.997	0.995	0.997
45	**215.3**	1.000	1.000	0.997	0.995	0.997
46	**221.0**	1.000	1.000	0.998	0.996	0.998
47	**226.0**	1.000	1.000	0.998	0.997	0.998
48	**230.8**	1.000	1.000	0.998	0.997	0.998
49	**235.7**	1.000	1.000	0.998	0.998	0.999
50	**238.3**	1.000	1.000	0.999	0.998	0.999

Table F-12. Nonequilibrium prediction model results for column 3B experiment.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.3**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.076	0.021	0.007	0.007	0.008
3	**5.2**	0.207	0.055	0.016	0.016	0.019
4	**7.6**	0.353	0.101	0.029	0.029	0.033
5	**9.8**	0.474	0.149	0.043	0.042	0.049
6	**12.8**	0.624	0.225	0.068	0.064	0.076
7	**15.4**	0.724	0.293	0.093	0.087	0.102
8	**18.7**	0.818	0.380	0.129	0.120	0.140
9	**20.3**	0.854	0.423	0.149	0.138	0.160
10	**24.8**	0.921	0.532	0.206	0.190	0.219
11	**30.4**	0.964	0.651	0.284	0.262	0.298
12	**35.9**	0.984	0.743	0.362	0.334	0.376
13	**39.8**	0.991	0.795	0.415	0.384	0.430
14	**45.1**	0.996	0.851	0.486	0.452	0.500
15	**49.8**	0.998	0.889	0.545	0.509	0.558
16	**54.6**	0.999	0.918	0.601	0.564	0.614
17	**59.9**	1.000	0.942	0.657	0.620	0.669
18	**64.8**	1.000	0.958	0.703	0.667	0.714
19	**73.1**	1.000	0.976	0.769	0.736	0.779
20	**74.8**	1.000	0.978	0.782	0.749	0.791
21	**79.5**	1.000	0.984	0.812	0.781	0.820
22	**84.5**	1.000	0.989	0.840	0.811	0.847
23	**89.8**	1.000	0.992	0.866	0.839	0.872
24	**95.2**	1.000	0.994	0.888	0.864	0.893
25	**99.5**	1.000	0.996	0.903	0.881	0.908
26	**104.5**	1.000	0.997	0.918	0.898	0.922
27	**109.5**	1.000	0.998	0.931	0.913	0.935
28	**113.3**	1.000	0.998	0.940	0.923	0.943
29	**119.0**	1.000	0.999	0.951	0.936	0.953
30	**125.7**	1.000	0.999	0.961	0.949	0.963
31	**131.7**	1.000	1.000	0.968	0.958	0.970
32	**134.3**	1.000	1.000	0.971	0.961	0.973
33	**139.4**	1.000	1.000	0.976	0.967	0.977
34	**144.2**	1.000	1.000	0.980	0.972	0.981
35	**148.6**	1.000	1.000	0.983	0.976	0.984
36	**154.4**	1.000	1.000	0.986	0.980	0.987
37	**164.0**	1.000	1.000	0.990	0.985	0.991
38	**168.7**	1.000	1.000	0.992	0.988	0.992
39	**175.1**	1.000	1.000	0.993	0.990	0.994
40	**179.3**	1.000	1.000	0.994	0.991	0.995
41	**184.1**	1.000	1.000	0.995	0.993	0.996
42	**188.6**	1.000	1.000	0.996	0.994	0.996
43	**193.1**	1.000	1.000	0.996	0.995	0.997

Table F-12 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**197.2**	1.000	1.000	0.997	0.995	0.997
45	**202.8**	1.000	1.000	0.998	0.996	0.998
46	**207.1**	1.000	1.000	0.998	0.997	0.998
47	**212.3**	1.000	1.000	0.998	0.997	0.998
48	**217.2**	1.000	1.000	0.999	0.998	0.999
49	**222.3**	1.000	1.000	0.999	0.998	0.999
50	**227.5**	1.000	1.000	0.999	0.998	0.999
51	**232.6**	1.000	1.000	0.999	0.999	0.999

Table F-13. Equilibrium model inversely fit to column 1A data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**1.2**	0.000	0.000	0.000	0.000	0.000
2	**2.8**	0.000	0.000	0.000	0.000	0.000
3	**5.2**	0.004	0.000	0.000	0.000	0.000
4	**7.5**	0.048	0.000	0.000	0.000	0.000
5	**9.8**	0.163	0.000	0.000	0.000	0.000
6	**12.3**	0.332	0.001	0.000	0.000	0.000
7	**14.9**	0.515	0.006	0.000	0.000	0.000
8	**17.2**	0.650	0.017	0.000	0.000	0.000
9	**19.6**	0.758	0.037	0.000	0.000	0.000
10	**24.5**	0.895	0.115	0.000	0.000	0.000
11	**29.6**	0.957	0.231	0.000	0.000	0.000
12	**34.3**	0.982	0.357	0.000	0.000	0.000
13	**39.6**	0.993	0.493	0.000	0.001	0.001
14	**44.2**	0.997	0.598	0.001	0.002	0.002
15	**49.5**	0.999	0.700	0.002	0.004	0.006
16	**53.1**	1.000	0.756	0.003	0.007	0.010
17	**57.7**	1.000	0.816	0.007	0.013	0.018
18	**62.9**	1.000	0.867	0.013	0.024	0.032
19	**68.3**	1.000	0.906	0.022	0.039	0.050
20	**73.3**	1.000	0.932	0.033	0.057	0.072
21	**78.1**	1.000	0.951	0.048	0.078	0.097
22	**83.1**	1.000	0.965	0.066	0.104	0.127
23	**88.1**	1.000	0.975	0.088	0.134	0.160
24	**92.6**	1.000	0.982	0.110	0.163	0.193
25	**97.4**	1.000	0.987	0.136	0.195	0.229
26	**102.3**	1.000	0.991	0.165	0.231	0.267
27	**107.2**	1.000	0.993	0.195	0.268	0.306
28	**112.0**	1.000	0.995	0.226	0.304	0.345
29	**117.3**	1.000	0.997	0.263	0.345	0.388
30	**122.0**	1.000	0.998	0.295	0.381	0.425
31	**127.0**	1.000	0.998	0.329	0.419	0.463
32	**133.7**	1.000	0.999	0.377	0.469	0.513
33	**136.3**	1.000	0.999	0.394	0.487	0.531
34	**141.3**	1.000	0.999	0.429	0.522	0.566
35	**146.0**	1.000	1.000	0.461	0.554	0.598
36	**151.1**	1.000	1.000	0.494	0.587	0.630
37	**156.0**	1.000	1.000	0.525	0.617	0.658
38	**161.8**	1.000	1.000	0.560	0.650	0.690
39	**165.7**	1.000	1.000	0.583	0.671	0.710
40	**170.5**	1.000	1.000	0.610	0.696	0.734
41	**175.6**	1.000	1.000	0.637	0.721	0.757
42	**180.3**	1.000	1.000	0.660	0.742	0.777
43	**185.2**	1.000	1.000	0.684	0.762	0.796

Table F-13 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**190.4**	1.000	1.000	0.708	0.783	0.814
45	**195.0**	1.000	1.000	0.727	0.800	0.830
46	**200.0**	1.000	1.000	0.747	0.816	0.845
47	**205.2**	1.000	1.000	0.767	0.833	0.859
48	**215.0**	1.000	1.000	0.800	0.860	0.884
49	**219.6**	1.000	1.000	0.815	0.871	0.894
50	**224.9**	1.000	1.000	0.830	0.883	0.904
51	**231.1**	1.000	1.000	0.846	0.896	0.915

Table F-14. Equilibrium model inversely fit to column 1B data results.

Sample	Pore Volumes	C/Co				
		benzene	toluene	ethylbenzene	m-xylene	o-xylene
1	**0.5**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.000	0.000	0.000	0.000	0.000
3	**5.0**	0.007	0.000	0.000	0.000	0.000
4	**7.4**	0.073	0.000	0.000	0.000	0.000
5	**10.0**	0.234	0.000	0.000	0.000	0.000
6	**12.4**	0.417	0.001	0.000	0.000	0.000
7	**14.7**	0.573	0.004	0.000	0.000	0.000
8	**17.1**	0.709	0.012	0.000	0.000	0.000
9	**19.4**	0.803	0.028	0.000	0.000	0.000
10	**24.5**	0.920	0.092	0.000	0.000	0.000
11	**29.2**	0.967	0.184	0.000	0.000	0.000
12	**34.3**	0.987	0.304	0.000	0.000	0.000
13	**38.8**	0.995	0.413	0.000	0.000	0.001
14	**43.5**	0.998	0.521	0.001	0.000	0.002
15	**48.4**	0.999	0.619	0.003	0.001	0.004
16	**53.4**	1.000	0.704	0.006	0.003	0.009
17	**58.1**	1.000	0.769	0.012	0.006	0.016
18	**62.9**	1.000	0.822	0.020	0.011	0.027
19	**67.3**	1.000	0.861	0.030	0.017	0.040
20	**72.1**	1.000	0.894	0.044	0.026	0.057
21	**76.9**	1.000	0.920	0.061	0.038	0.078
22	**82.2**	1.000	0.941	0.084	0.054	0.105
23	**86.2**	1.000	0.954	0.105	0.069	0.128
24	**91.2**	1.000	0.966	0.132	0.090	0.159
25	**95.8**	1.000	0.974	0.160	0.111	0.191
26	**100.6**	1.000	0.981	0.190	0.136	0.224
27	**105.6**	1.000	0.986	0.223	0.163	0.260
28	**110.1**	1.000	0.989	0.255	0.190	0.294
29	**114.9**	1.000	0.992	0.289	0.219	0.330
30	**119.5**	1.000	0.994	0.321	0.248	0.364
31	**124.8**	1.000	0.996	0.359	0.282	0.404
32	**143.5**	1.000	0.999	0.488	0.403	0.535
33	**148.1**	1.000	0.999	0.518	0.433	0.564
34	**152.9**	1.000	0.999	0.548	0.462	0.594
35	**158.0**	1.000	0.999	0.578	0.493	0.623
36	**162.6**	1.000	1.000	0.605	0.520	0.649
37	**167.5**	1.000	1.000	0.631	0.548	0.675
38	**172.4**	1.000	1.000	0.657	0.575	0.699
39	**177.6**	1.000	1.000	0.682	0.602	0.723
40	**182.1**	1.000	1.000	0.703	0.625	0.742
41	**186.5**	1.000	1.000	0.722	0.646	0.760
42	**191.6**	1.000	1.000	0.743	0.669	0.779
43	**196.3**	1.000	1.000	0.761	0.690	0.796

Table F-14 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**201.1**	1.000	1.000	0.779	0.710	0.812
45	**205.9**	1.000	1.000	0.795	0.729	0.827
46	**210.4**	1.000	1.000	0.809	0.745	0.840
47	**215.5**	1.000	1.000	0.824	0.763	0.853
48	**219.7**	1.000	1.000	0.836	0.777	0.864
49	**224.9**	1.000	1.000	0.849	0.793	0.875
50	**225.1**	1.000	1.000	0.850	0.794	0.876
51	**225.3**	1.000	1.000	0.850	0.794	0.876

Table F-15. Equilibrium model inversely fit to column 2A data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.000	0.000	0.000	0.000	0.000
2	**2.5**	0.000	0.000	0.000	0.000	0.000
3	**5.0**	0.001	0.000	0.000	0.000	0.000
4	**7.5**	0.029	0.000	0.000	0.000	0.000
5	**9.7**	0.116	0.000	0.000	0.000	0.000
6	**12.4**	0.290	0.000	0.000	0.000	0.000
7	**14.7**	0.465	0.000	0.000	0.000	0.000
8	**17.3**	0.633	0.001	0.000	0.000	0.000
9	**21.8**	0.827	0.009	0.000	0.000	0.000
10	**24.4**	0.893	0.020	0.000	0.000	0.000
11	**29.4**	0.959	0.062	0.000	0.000	0.000
12	**34.7**	0.986	0.139	0.000	0.000	0.000
13	**39.9**	0.995	0.239	0.000	0.000	0.000
14	**44.2**	0.998	0.332	0.000	0.000	0.000
15	**49.1**	0.999	0.436	0.000	0.000	0.000
16	**54.1**	1.000	0.537	0.000	0.000	0.001
17	**58.8**	1.000	0.623	0.001	0.001	0.001
18	**64.9**	1.000	0.717	0.003	0.001	0.003
19	**68.6**	1.000	0.763	0.004	0.002	0.005
20	**73.2**	1.000	0.813	0.007	0.004	0.008
21	**78.3**	1.000	0.857	0.012	0.008	0.014
22	**83.0**	1.000	0.889	0.018	0.012	0.021
23	**88.2**	1.000	0.917	0.028	0.018	0.031
24	**92.6**	1.000	0.935	0.038	0.025	0.042
25	**97.2**	1.000	0.950	0.051	0.035	0.056
26	**102.3**	1.000	0.963	0.067	0.047	0.073
27	**107.0**	1.000	0.972	0.085	0.061	0.092
28	**111.8**	1.000	0.979	0.105	0.077	0.113
29	**116.8**	1.000	0.984	0.128	0.096	0.138
30	**121.9**	1.000	0.988	0.153	0.117	0.165
31	**126.7**	1.000	0.991	0.179	0.139	0.192
32	**131.5**	1.000	0.994	0.207	0.162	0.220
33	**136.4**	1.000	0.995	0.235	0.187	0.250
34	**141.1**	1.000	0.996	0.264	0.213	0.279
35	**145.9**	1.000	0.997	0.294	0.240	0.310
36	**150.9**	1.000	0.998	0.326	0.269	0.342
37	**155.8**	1.000	0.999	0.356	0.297	0.373
38	**160.5**	1.000	0.999	0.386	0.325	0.403
39	**165.6**	1.000	0.999	0.418	0.355	0.435
40	**165.8**	1.000	0.999	0.419	0.356	0.437
41	**176.0**	1.000	1.000	0.481	0.417	0.499
42	**179.9**	1.000	1.000	0.504	0.439	0.522
43	**184.6**	1.000	1.000	0.531	0.466	0.549

Table F-15 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**189.7**	1.000	1.000	0.559	0.494	0.577
45	**194.4**	1.000	1.000	0.585	0.520	0.602
46	**199.2**	1.000	1.000	0.609	0.546	0.627
47	**204.3**	1.000	1.000	0.635	0.572	0.651
48	**209.7**	1.000	1.000	0.660	0.599	0.677
49	**213.9**	1.000	1.000	0.679	0.618	0.695
50	**219.1**	1.000	1.000	0.701	0.642	0.716
51	**223.5**	1.000	1.000	0.719	0.662	0.734
52	**228.7**	1.000	1.000	0.739	0.683	0.754

Table F-16. Equilibrium model inversely fit to column 2B data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.7**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.000	0.000	0.000	0.000	0.000
3	**5.2**	0.001	0.000	0.000	0.000	0.000
4	**7.8**	0.019	0.000	0.000	0.000	0.000
5	**11.1**	0.128	0.000	0.000	0.000	0.000
6	**12.9**	0.224	0.000	0.000	0.000	0.000
7	**15.5**	0.386	0.002	0.000	0.000	0.000
8	**18.1**	0.535	0.008	0.000	0.000	0.000
9	**21.5**	0.700	0.027	0.000	0.000	0.000
10	**26.1**	0.842	0.077	0.000	0.000	0.000
11	**31.2**	0.928	0.170	0.000	0.000	0.000
12	**36.6**	0.969	0.290	0.000	0.000	0.000
13	**41.6**	0.986	0.408	0.000	0.000	0.000
14	**47.6**	0.995	0.542	0.000	0.000	0.001
15	**49.2**	0.996	0.573	0.001	0.000	0.001
16	**57.2**	0.999	0.712	0.003	0.001	0.003
17	**62.4**	1.000	0.782	0.006	0.003	0.007
18	**67.8**	1.000	0.838	0.011	0.006	0.012
19	**72.8**	1.000	0.878	0.018	0.010	0.020
20	**77.9**	1.000	0.909	0.027	0.016	0.031
21	**83.3**	1.000	0.934	0.041	0.026	0.046
22	**88.5**	1.000	0.952	0.057	0.037	0.063
23	**93.4**	1.000	0.964	0.075	0.050	0.082
24	**98.7**	1.000	0.974	0.098	0.067	0.107
25	**103.9**	1.000	0.981	0.123	0.086	0.133
26	**108.8**	1.000	0.986	0.148	0.107	0.160
27	**113.8**	1.000	0.990	0.177	0.130	0.189
28	**119.5**	1.000	0.993	0.211	0.158	0.225
29	**124.4**	1.000	0.995	0.242	0.184	0.257
30	**129.6**	1.000	0.996	0.275	0.213	0.291
31	**134.9**	1.000	0.997	0.310	0.244	0.326
32	**146.2**	1.000	0.999	0.384	0.312	0.402
33	**148.3**	1.000	0.999	0.398	0.325	0.416
34	**155.3**	1.000	0.999	0.443	0.367	0.461
35	**160.8**	1.000	1.000	0.477	0.400	0.496
36	**165.7**	1.000	1.000	0.507	0.430	0.526
37	**170.6**	1.000	1.000	0.536	0.459	0.555
38	**175.9**	1.000	1.000	0.566	0.489	0.584
39	**185.9**	1.000	1.000	0.620	0.544	0.637
40	**191.3**	1.000	1.000	0.646	0.572	0.663
41	**197.0**	1.000	1.000	0.673	0.600	0.690
42	**202.4**	1.000	1.000	0.697	0.626	0.713
43	**207.3**	1.000	1.000	0.717	0.648	0.733

Table F-16 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.8**	1.000	1.000	0.735	0.668	0.750
45	**217.0**	1.000	1.000	0.755	0.690	0.769
46	**222.1**	1.000	1.000	0.773	0.710	0.786
47	**226.8**	1.000	1.000	0.788	0.727	0.801
48	**233.0**	1.000	1.000	0.807	0.749	0.820
49	**237.9**	1.000	1.000	0.821	0.766	0.833
50	**241.7**	1.000	1.000	0.831	0.777	0.843

Table F-17. Equilibrium model inversely fit to column 3A data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.000	0.000	0.000	0.000	0.000
2	**3.4**	0.001	0.000	0.000	0.000	0.000
3	**5.1**	0.015	0.000	0.000	0.000	0.000
4	**7.7**	0.098	0.000	0.000	0.000	0.000
5	**10.1**	0.224	0.000	0.000	0.000	0.000
6	**13.4**	0.416	0.003	0.000	0.000	0.000
7	**15.6**	0.533	0.009	0.000	0.000	0.000
8	**18.5**	0.655	0.024	0.000	0.000	0.000
9	**20.9**	0.734	0.042	0.000	0.000	0.000
10	**26.5**	0.861	0.110	0.000	0.000	0.000
11	**31.3**	0.920	0.186	0.000	0.000	0.000
12	**36.5**	0.957	0.279	0.001	0.000	0.001
13	**41.4**	0.976	0.366	0.002	0.001	0.003
14	**46.7**	0.987	0.455	0.005	0.003	0.007
15	**51.9**	0.993	0.534	0.011	0.007	0.013
16	**58.4**	0.997	0.621	0.021	0.014	0.025
17	**60.9**	0.997	0.651	0.026	0.017	0.031
18	**69.7**	0.999	0.740	0.048	0.034	0.057
19	**72.3**	0.999	0.762	0.057	0.041	0.066
20	**77.4**	1.000	0.800	0.075	0.055	0.087
21	**82.6**	1.000	0.833	0.096	0.072	0.110
22	**87.9**	1.000	0.861	0.119	0.091	0.135
23	**93.7**	1.000	0.887	0.147	0.115	0.165
24	**98.2**	1.000	0.904	0.169	0.135	0.189
25	**103.9**	1.000	0.921	0.199	0.160	0.221
26	**109.9**	1.000	0.936	0.231	0.189	0.255
27	**112.7**	1.000	0.942	0.246	0.203	0.271
28	**118.4**	1.000	0.953	0.278	0.232	0.303
29	**126.6**	1.000	0.964	0.323	0.273	0.350
30	**129.0**	1.000	0.967	0.336	0.285	0.363
31	**133.0**	1.000	0.972	0.357	0.306	0.385
32	**139.1**	1.000	0.977	0.390	0.337	0.419
33	**143.8**	1.000	0.981	0.415	0.361	0.444
34	**153.8**	1.000	0.986	0.465	0.410	0.494
35	**159.7**	1.000	0.989	0.494	0.438	0.523
36	**164.7**	1.000	0.991	0.517	0.461	0.546
37	**169.2**	1.000	0.992	0.537	0.481	0.566
38	**179.7**	1.000	0.994	0.582	0.527	0.611
39	**184.2**	1.000	0.995	0.600	0.545	0.628
40	**190.0**	1.000	0.996	0.623	0.569	0.650
41	**196.2**	1.000	0.997	0.646	0.593	0.673
42	**200.5**	1.000	0.997	0.661	0.608	0.687
43	**205.3**	1.000	0.998	0.677	0.626	0.703

Table F-17 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.4**	1.000	0.998	0.697	0.646	0.722
45	**215.3**	1.000	0.998	0.709	0.659	0.733
46	**221.0**	1.000	0.999	0.725	0.677	0.749
47	**226.0**	1.000	0.999	0.739	0.692	0.763
48	**230.8**	1.000	0.999	0.752	0.706	0.775
49	**235.7**	1.000	0.999	0.765	0.720	0.787
50	**238.3**	1.000	0.999	0.771	0.727	0.793

Table F-18. Equilibrium model inversely fit to column 3B data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.3**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.000	0.000	0.000	0.000	0.000
3	**5.2**	0.016	0.000	0.000	0.000	0.000
4	**7.6**	0.106	0.000	0.000	0.000	0.000
5	**9.8**	0.237	0.000	0.000	0.000	0.000
6	**12.8**	0.443	0.001	0.000	0.000	0.000
7	**15.4**	0.594	0.006	0.000	0.000	0.000
8	**18.7**	0.739	0.020	0.000	0.000	0.000
9	**20.3**	0.793	0.032	0.000	0.000	0.000
10	**24.8**	0.891	0.081	0.000	0.000	0.000
11	**30.4**	0.953	0.171	0.000	0.000	0.000
12	**35.9**	0.979	0.276	0.001	0.000	0.001
13	**39.8**	0.988	0.352	0.002	0.001	0.002
14	**45.1**	0.995	0.453	0.004	0.002	0.006
15	**49.8**	0.997	0.535	0.009	0.005	0.011
16	**54.6**	0.999	0.610	0.016	0.009	0.019
17	**59.9**	0.999	0.681	0.027	0.016	0.032
18	**64.8**	1.000	0.737	0.040	0.026	0.047
19	**73.1**	1.000	0.812	0.069	0.047	0.080
20	**74.8**	1.000	0.825	0.077	0.053	0.088
21	**79.5**	1.000	0.856	0.098	0.069	0.112
22	**84.5**	1.000	0.883	0.123	0.089	0.140
23	**89.8**	1.000	0.906	0.152	0.113	0.171
24	**95.2**	1.000	0.926	0.184	0.139	0.204
25	**99.5**	1.000	0.938	0.211	0.162	0.233
26	**104.5**	1.000	0.950	0.242	0.189	0.265
27	**109.5**	1.000	0.960	0.274	0.217	0.299
28	**113.3**	1.000	0.966	0.299	0.240	0.325
29	**119.0**	1.000	0.973	0.336	0.273	0.363
30	**125.7**	1.000	0.980	0.378	0.313	0.406
31	**131.7**	1.000	0.985	0.416	0.349	0.444
32	**134.3**	1.000	0.986	0.432	0.364	0.460
33	**139.4**	1.000	0.989	0.462	0.393	0.491
34	**144.2**	1.000	0.991	0.491	0.421	0.519
35	**148.6**	1.000	0.993	0.515	0.445	0.544
36	**154.4**	1.000	0.994	0.547	0.477	0.575
37	**164.0**	1.000	0.996	0.596	0.527	0.624
38	**168.7**	1.000	0.997	0.619	0.551	0.646
39	**175.1**	1.000	0.998	0.648	0.581	0.674
40	**179.3**	1.000	0.998	0.666	0.600	0.691
41	**184.1**	1.000	0.998	0.685	0.621	0.710
42	**188.6**	1.000	0.999	0.703	0.640	0.727
43	**193.1**	1.000	0.999	0.720	0.658	0.743

Table F-18 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**197.2**	1.000	0.999	0.734	0.674	0.757
45	**202.8**	1.000	0.999	0.753	0.694	0.775
46	**207.1**	1.000	0.999	0.767	0.710	0.788
47	**212.3**	1.000	1.000	0.782	0.727	0.803
48	**217.2**	1.000	1.000	0.796	0.742	0.816
49	**222.3**	1.000	1.000	0.809	0.758	0.828
50	**227.5**	1.000	1.000	0.822	0.773	0.840
51	**232.6**	1.000	1.000	0.834	0.786	0.852

Table F-19. Nonequilibrium model inversely fit to column 1A data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**1.2**	0.000	0.000	0.000	0.000	0.000
2	**2.8**	0.030	0.000	0.000	0.000	0.000
3	**5.2**	0.161	0.006	0.009	0.000	0.000
4	**7.5**	0.266	0.034	0.021	0.000	0.001
5	**9.8**	0.353	0.076	0.028	0.000	0.007
6	**12.3**	0.436	0.121	0.034	0.000	0.018
7	**14.9**	0.516	0.165	0.040	0.000	0.033
8	**17.2**	0.579	0.202	0.046	0.001	0.045
9	**19.6**	0.638	0.239	0.052	0.002	0.057
10	**24.5**	0.738	0.315	0.064	0.009	0.079
11	**29.6**	0.814	0.388	0.078	0.026	0.098
12	**34.3**	0.867	0.454	0.091	0.051	0.117
13	**39.6**	0.909	0.523	0.107	0.085	0.138
14	**44.2**	0.935	0.577	0.121	0.117	0.156
15	**49.5**	0.956	0.635	0.138	0.155	0.178
16	**53.1**	0.967	0.670	0.150	0.179	0.193
17	**57.7**	0.977	0.711	0.165	0.209	0.212
18	**62.9**	0.984	0.753	0.183	0.239	0.234
19	**68.3**	0.990	0.790	0.202	0.268	0.257
20	**73.3**	0.993	0.820	0.219	0.292	0.278
21	**78.1**	0.995	0.846	0.236	0.313	0.298
22	**83.1**	0.997	0.869	0.254	0.333	0.319
23	**88.1**	0.998	0.889	0.273	0.353	0.341
24	**92.6**	0.999	0.904	0.289	0.369	0.359
25	**97.4**	0.999	0.919	0.306	0.386	0.379
26	**102.3**	0.999	0.931	0.324	0.403	0.399
27	**107.2**	1.000	0.942	0.342	0.418	0.419
28	**112.0**	1.000	0.951	0.359	0.433	0.438
29	**117.3**	1.000	0.959	0.378	0.450	0.458
30	**122.0**	1.000	0.965	0.395	0.463	0.476
31	**127.0**	1.000	0.971	0.413	0.478	0.495
32	**133.7**	1.000	0.977	0.436	0.497	0.520
33	**136.3**	1.000	0.979	0.445	0.504	0.529
34	**141.3**	1.000	0.983	0.462	0.517	0.546
35	**146.0**	1.000	0.986	0.478	0.530	0.563
36	**151.1**	1.000	0.988	0.495	0.543	0.580
37	**156.0**	1.000	0.990	0.511	0.555	0.596
38	**161.8**	1.000	0.992	0.529	0.570	0.614
39	**165.7**	1.000	0.993	0.541	0.579	0.626
40	**170.5**	1.000	0.994	0.556	0.590	0.640
41	**175.6**	1.000	0.995	0.572	0.602	0.655
42	**180.3**	1.000	0.996	0.585	0.613	0.668
43	**185.2**	1.000	0.997	0.600	0.623	0.682

Table F-19 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**190.4**	1.000	0.997	0.614	0.634	0.696
45	**195.0**	1.000	0.998	0.627	0.644	0.707
46	**200.0**	1.000	0.998	0.640	0.654	0.720
47	**205.2**	1.000	0.998	0.654	0.665	0.732
48	**215.0**	1.000	0.999	0.678	0.683	0.755
49	**219.6**	1.000	0.999	0.689	0.692	0.764
50	**224.9**	1.000	0.999	0.702	0.701	0.775
51	**231.1**	1.000	0.999	0.716	0.712	0.788

Table F-20. Nonequilibrium model inversely fit to column 1B data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.5**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.035	0.000	0.000	0.000	0.000
3	**5.0**	0.134	0.000	0.000	0.000	0.000
4	**7.4**	0.244	0.001	0.000	0.000	0.000
5	**10.0**	0.362	0.012	0.000	0.000	0.000
6	**12.4**	0.467	0.040	0.000	0.000	0.001
7	**14.7**	0.555	0.080	0.001	0.001	0.003
8	**17.1**	0.641	0.135	0.003	0.002	0.008
9	**19.4**	0.710	0.190	0.006	0.005	0.014
10	**24.5**	0.823	0.302	0.020	0.016	0.033
11	**29.2**	0.892	0.387	0.038	0.031	0.053
12	**34.3**	0.938	0.460	0.061	0.048	0.075
13	**38.8**	0.963	0.513	0.082	0.064	0.094
14	**43.5**	0.978	0.561	0.103	0.081	0.114
15	**48.4**	0.988	0.605	0.125	0.098	0.135
16	**53.4**	0.993	0.644	0.146	0.115	0.156
17	**58.1**	0.996	0.678	0.167	0.132	0.176
18	**62.9**	0.998	0.709	0.187	0.149	0.197
19	**67.3**	0.999	0.735	0.205	0.165	0.216
20	**72.1**	0.999	0.760	0.225	0.183	0.237
21	**76.9**	1.000	0.784	0.245	0.200	0.258
22	**82.2**	1.000	0.807	0.267	0.220	0.281
23	**86.2**	1.000	0.823	0.284	0.235	0.299
24	**91.2**	1.000	0.842	0.304	0.254	0.320
25	**95.8**	1.000	0.857	0.323	0.271	0.340
26	**100.6**	1.000	0.871	0.342	0.289	0.361
27	**105.6**	1.000	0.885	0.362	0.308	0.382
28	**110.1**	1.000	0.896	0.379	0.325	0.401
29	**114.9**	1.000	0.907	0.398	0.343	0.420
30	**119.5**	1.000	0.916	0.416	0.359	0.439
31	**124.8**	1.000	0.925	0.435	0.379	0.460
32	**143.5**	1.000	0.951	0.503	0.445	0.531
33	**148.1**	1.000	0.956	0.519	0.461	0.548
34	**152.9**	1.000	0.961	0.535	0.477	0.565
35	**158.0**	1.000	0.965	0.551	0.494	0.582
36	**162.6**	1.000	0.969	0.566	0.509	0.597
37	**167.5**	1.000	0.972	0.582	0.525	0.613
38	**172.4**	1.000	0.975	0.596	0.540	0.629
39	**177.6**	1.000	0.978	0.612	0.556	0.644
40	**182.1**	1.000	0.980	0.625	0.570	0.658
41	**186.5**	1.000	0.982	0.637	0.583	0.670
42	**191.6**	1.000	0.984	0.651	0.597	0.684
43	**196.3**	1.000	0.986	0.664	0.611	0.697

Table F-20 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**201.1**	1.000	0.987	0.676	0.624	0.710
45	**205.9**	1.000	0.989	0.688	0.637	0.722
46	**210.4**	1.000	0.990	0.699	0.648	0.733
47	**215.5**	1.000	0.991	0.711	0.661	0.745
48	**219.7**	1.000	0.992	0.721	0.672	0.754
49	**224.9**	1.000	0.993	0.732	0.684	0.766
50	**225.1**	1.000	0.993	0.733	0.685	0.766
51	**225.3**	1.000	0.993	0.733	0.685	0.766

Table F-21. Nonequilibrium model inversely fit to column 2A data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.000	0.000	0.000	0.000	0.000
2	**2.5**	0.002	0.000	0.000	0.000	0.000
3	**5.0**	0.088	0.000	0.000	0.000	0.000
4	**7.5**	0.214	0.000	0.000	0.001	0.000
5	**9.7**	0.308	0.001	0.000	0.003	0.000
6	**12.4**	0.411	0.006	0.000	0.006	0.000
7	**14.7**	0.496	0.020	0.000	0.008	0.000
8	**17.3**	0.578	0.050	0.001	0.010	0.001
9	**21.8**	0.696	0.135	0.005	0.014	0.005
10	**24.4**	0.752	0.195	0.010	0.017	0.009
11	**29.4**	0.833	0.306	0.021	0.022	0.020
12	**34.7**	0.893	0.407	0.034	0.029	0.037
13	**39.9**	0.932	0.481	0.048	0.037	0.054
14	**44.2**	0.954	0.527	0.060	0.043	0.068
15	**49.1**	0.971	0.566	0.073	0.052	0.083
16	**54.1**	0.982	0.597	0.086	0.061	0.098
17	**58.8**	0.988	0.622	0.099	0.070	0.112
18	**64.9**	0.994	0.648	0.116	0.083	0.131
19	**68.6**	0.995	0.662	0.126	0.091	0.142
20	**73.2**	0.997	0.679	0.139	0.102	0.156
21	**78.3**	0.998	0.696	0.154	0.114	0.171
22	**83.0**	0.999	0.711	0.168	0.126	0.185
23	**88.2**	0.999	0.726	0.184	0.139	0.201
24	**92.6**	1.000	0.739	0.197	0.151	0.215
25	**97.2**	1.000	0.751	0.211	0.164	0.229
26	**102.3**	1.000	0.764	0.227	0.178	0.245
27	**107.0**	1.000	0.776	0.242	0.192	0.260
28	**111.8**	1.000	0.787	0.257	0.206	0.275
29	**116.8**	1.000	0.798	0.273	0.221	0.290
30	**121.9**	1.000	0.808	0.289	0.237	0.306
31	**126.7**	1.000	0.818	0.304	0.252	0.321
32	**131.5**	1.000	0.827	0.319	0.267	0.336
33	**136.4**	1.000	0.836	0.334	0.282	0.351
34	**141.1**	1.000	0.844	0.349	0.297	0.365
35	**145.9**	1.000	0.851	0.364	0.313	0.379
36	**150.9**	1.000	0.859	0.380	0.329	0.395
37	**155.8**	1.000	0.866	0.395	0.344	0.409
38	**160.5**	1.000	0.873	0.409	0.359	0.423
39	**165.6**	1.000	0.880	0.424	0.376	0.438
40	**165.8**	1.000	0.880	0.425	0.377	0.438
41	**176.0**	1.000	0.893	0.455	0.409	0.467
42	**179.9**	1.000	0.897	0.467	0.421	0.478
43	**184.6**	1.000	0.902	0.480	0.436	0.491

Table F-21 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**189.7**	1.000	0.907	0.495	0.452	0.505
45	**194.4**	1.000	0.912	0.508	0.466	0.518
46	**199.2**	1.000	0.916	0.521	0.481	0.530
47	**204.3**	1.000	0.921	0.535	0.496	0.543
48	**209.7**	1.000	0.925	0.550	0.512	0.557
49	**213.9**	1.000	0.929	0.560	0.524	0.568
50	**219.1**	1.000	0.933	0.574	0.539	0.580
51	**223.5**	1.000	0.936	0.585	0.552	0.591
52	**228.7**	1.000	0.939	0.598	0.566	0.603

Table F-22. Nonequilibrium model inversely fit to column 2B data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.7**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.015	0.000	0.000	0.000	0.000
3	**5.2**	0.104	0.000	0.000	0.000	0.000
4	**7.8**	0.192	0.000	0.000	0.000	0.000
5	**11.1**	0.304	0.006	0.000	0.000	0.000
6	**12.9**	0.363	0.016	0.000	0.000	0.000
7	**15.5**	0.447	0.045	0.000	0.000	0.000
8	**18.1**	0.521	0.087	0.001	0.001	0.002
9	**21.5**	0.612	0.158	0.003	0.003	0.006
10	**26.1**	0.712	0.256	0.012	0.009	0.019
11	**31.2**	0.799	0.356	0.030	0.024	0.044
12	**36.6**	0.865	0.441	0.058	0.047	0.075
13	**41.6**	0.908	0.506	0.087	0.071	0.105
14	**47.6**	0.943	0.572	0.124	0.100	0.140
15	**49.2**	0.949	0.587	0.133	0.108	0.148
16	**57.2**	0.974	0.655	0.176	0.143	0.187
17	**62.4**	0.983	0.693	0.201	0.164	0.209
18	**67.8**	0.990	0.728	0.224	0.184	0.230
19	**72.8**	0.993	0.757	0.244	0.201	0.248
20	**77.9**	0.996	0.783	0.262	0.218	0.265
21	**83.3**	0.997	0.808	0.280	0.234	0.283
22	**88.5**	0.998	0.830	0.296	0.249	0.299
23	**93.4**	0.999	0.848	0.311	0.263	0.314
24	**98.7**	0.999	0.866	0.327	0.278	0.330
25	**103.9**	1.000	0.881	0.341	0.292	0.345
26	**108.8**	1.000	0.894	0.355	0.305	0.359
27	**113.8**	1.000	0.906	0.368	0.319	0.373
28	**119.5**	1.000	0.918	0.383	0.334	0.389
29	**124.4**	1.000	0.927	0.396	0.346	0.403
30	**129.6**	1.000	0.935	0.409	0.360	0.417
31	**134.9**	1.000	0.943	0.423	0.373	0.431
32	**146.2**	1.000	0.957	0.450	0.401	0.460
33	**148.3**	1.000	0.959	0.455	0.406	0.465
34	**155.3**	1.000	0.965	0.472	0.423	0.483
35	**160.8**	1.000	0.970	0.484	0.436	0.496
36	**165.7**	1.000	0.973	0.496	0.447	0.508
37	**170.6**	1.000	0.976	0.507	0.459	0.520
38	**175.9**	1.000	0.979	0.518	0.471	0.532
39	**185.9**	1.000	0.984	0.540	0.493	0.555
40	**191.3**	1.000	0.986	0.551	0.505	0.567
41	**197.0**	1.000	0.988	0.562	0.517	0.579
42	**202.4**	1.000	0.989	0.573	0.528	0.590
43	**207.3**	1.000	0.991	0.583	0.538	0.600

Table F-22 (continued).

Sample	Pore Volumes	C/Co Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.8**	1.000	0.992	0.592	0.547	0.609
45	**217.0**	1.000	0.993	0.602	0.558	0.620
46	**222.1**	1.000	0.994	0.611	0.568	0.629
47	**226.8**	1.000	0.994	0.620	0.577	0.638
48	**233.0**	1.000	0.995	0.631	0.588	0.650
49	**237.9**	1.000	0.996	0.639	0.598	0.659
50	**241.7**	1.000	0.996	0.646	0.605	0.665

Table F-23. Nonequilibrium model inversely fit to column 3A data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.6**	0.000	0.000	0.000	0.000	0.000
2	**3.4**	0.103	0.000	0.000	0.000	0.000
3	**5.1**	0.180	0.005	0.000	0.000	0.000
4	**7.7**	0.277	0.036	0.001	0.001	0.001
5	**10.1**	0.358	0.080	0.003	0.004	0.007
6	**13.4**	0.463	0.143	0.013	0.013	0.020
7	**15.6**	0.527	0.180	0.023	0.021	0.031
8	**18.5**	0.600	0.222	0.037	0.032	0.046
9	**20.9**	0.653	0.252	0.048	0.041	0.057
10	**26.5**	0.758	0.317	0.073	0.061	0.080
11	**31.3**	0.823	0.367	0.091	0.075	0.097
12	**36.5**	0.876	0.418	0.109	0.089	0.115
13	**41.4**	0.912	0.462	0.125	0.103	0.131
14	**46.7**	0.939	0.508	0.141	0.117	0.148
15	**51.9**	0.958	0.549	0.157	0.131	0.164
16	**58.4**	0.974	0.597	0.177	0.149	0.185
17	**60.9**	0.978	0.614	0.185	0.156	0.193
18	**69.7**	0.988	0.670	0.212	0.181	0.222
19	**72.3**	0.990	0.685	0.220	0.188	0.230
20	**77.4**	0.993	0.713	0.236	0.203	0.247
21	**82.6**	0.995	0.739	0.252	0.218	0.264
22	**87.9**	0.997	0.763	0.268	0.233	0.281
23	**93.7**	0.998	0.788	0.286	0.250	0.300
24	**98.2**	0.999	0.805	0.299	0.263	0.314
25	**103.9**	0.999	0.825	0.316	0.279	0.332
26	**109.9**	0.999	0.844	0.334	0.296	0.351
27	**112.7**	1.000	0.852	0.343	0.304	0.359
28	**118.4**	1.000	0.868	0.359	0.321	0.377
29	**126.6**	1.000	0.888	0.383	0.344	0.402
30	**129.0**	1.000	0.893	0.390	0.350	0.409
31	**133.0**	1.000	0.901	0.401	0.362	0.421
32	**139.1**	1.000	0.912	0.418	0.378	0.439
33	**143.8**	1.000	0.920	0.432	0.391	0.453
34	**153.8**	1.000	0.935	0.459	0.418	0.481
35	**159.7**	1.000	0.942	0.474	0.434	0.497
36	**164.7**	1.000	0.948	0.487	0.447	0.510
37	**169.2**	1.000	0.952	0.499	0.458	0.522
38	**179.7**	1.000	0.961	0.525	0.485	0.549
39	**184.2**	1.000	0.965	0.536	0.496	0.560
40	**190.0**	1.000	0.969	0.550	0.510	0.574
41	**196.2**	1.000	0.972	0.564	0.525	0.589
42	**200.5**	1.000	0.975	0.574	0.535	0.599
43	**205.3**	1.000	0.977	0.585	0.546	0.610

Table F-23 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**211.4**	1.000	0.980	0.598	0.560	0.624
45	**215.3**	1.000	0.981	0.607	0.568	0.632
46	**221.0**	1.000	0.984	0.619	0.581	0.644
47	**226.0**	1.000	0.985	0.629	0.591	0.655
48	**230.8**	1.000	0.987	0.639	0.602	0.665
49	**235.7**	1.000	0.988	0.648	0.612	0.674
50	**238.3**	1.000	0.989	0.653	0.617	0.679

Table F-24. Nonequilibrium model inversely fit to column 3B data results.

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
1	**0.3**	0.000	0.000	0.000	0.000	0.000
2	**2.7**	0.048	0.000	0.000	0.000	0.000
3	**5.2**	0.212	0.004	0.000	0.000	0.000
4	**7.6**	0.326	0.028	0.000	0.000	0.000
5	**9.8**	0.401	0.065	0.000	0.000	0.001
6	**12.8**	0.494	0.125	0.001	0.001	0.004
7	**15.4**	0.563	0.171	0.003	0.002	0.010
8	**18.7**	0.639	0.221	0.010	0.007	0.023
9	**20.3**	0.673	0.244	0.014	0.011	0.030
10	**24.8**	0.751	0.299	0.032	0.025	0.051
11	**30.4**	0.826	0.363	0.058	0.047	0.078
12	**35.9**	0.878	0.420	0.085	0.069	0.103
13	**39.8**	0.905	0.458	0.104	0.084	0.119
14	**45.1**	0.934	0.508	0.128	0.105	0.140
15	**49.8**	0.952	0.548	0.148	0.122	0.159
16	**54.6**	0.965	0.587	0.168	0.139	0.178
17	**59.9**	0.976	0.627	0.190	0.158	0.198
18	**64.8**	0.983	0.661	0.209	0.175	0.218
19	**73.1**	0.991	0.712	0.240	0.204	0.250
20	**74.8**	0.992	0.722	0.247	0.210	0.257
21	**79.5**	0.994	0.747	0.265	0.226	0.275
22	**84.5**	0.996	0.772	0.283	0.243	0.294
23	**89.8**	0.997	0.795	0.303	0.261	0.314
24	**95.2**	0.998	0.817	0.323	0.280	0.335
25	**99.5**	0.999	0.833	0.338	0.294	0.351
26	**104.5**	0.999	0.850	0.356	0.311	0.370
27	**109.5**	0.999	0.865	0.373	0.328	0.388
28	**113.3**	1.000	0.876	0.387	0.341	0.402
29	**119.0**	1.000	0.891	0.407	0.359	0.423
30	**125.7**	1.000	0.906	0.429	0.381	0.446
31	**131.7**	1.000	0.917	0.449	0.400	0.467
32	**134.3**	1.000	0.922	0.457	0.409	0.476
33	**139.4**	1.000	0.930	0.473	0.424	0.492
34	**144.2**	1.000	0.938	0.488	0.439	0.508
35	**148.6**	1.000	0.943	0.502	0.452	0.522
36	**154.4**	1.000	0.950	0.519	0.470	0.540
37	**164.0**	1.000	0.960	0.547	0.498	0.569
38	**168.7**	1.000	0.964	0.561	0.511	0.583
39	**175.1**	1.000	0.969	0.578	0.529	0.601
40	**179.3**	1.000	0.972	0.589	0.540	0.612
41	**184.1**	1.000	0.975	0.602	0.553	0.625
42	**188.6**	1.000	0.977	0.614	0.565	0.637
43	**193.1**	1.000	0.980	0.625	0.576	0.649

Table F-24 (continued).

Sample	Pore Volumes	C/Co				
		Benzene	Toluene	Ethylbenzene	M-xylene	O-xylene
44	**197.2**	1.000	0.982	0.635	0.587	0.659
45	**202.8**	1.000	0.984	0.648	0.601	0.672
46	**207.1**	1.000	0.985	0.658	0.611	0.683
47	**212.3**	1.000	0.987	0.670	0.623	0.694
48	**217.2**	1.000	0.989	0.681	0.634	0.705
49	**222.3**	1.000	0.990	0.692	0.646	0.716
50	**227.5**	1.000	0.991	0.703	0.657	0.727
51	**232.6**	1.000	0.992	0.713	0.668	0.737

Table F-25. Parameters obtained from equilibrium fit model.

Column	Constituent	P	R	r^2
1A	Benzene	11.32	15.96	0.889
	Toluene	11.32	43.36	0.931
	Ethylbenzene	11.32	165.3	0.768
	M-xylene	11.32	150.1	0.684
	O-xylene	11.32	143.4	0.788
1B	Benzene	10.69	14.81	0.944
	Toluene	10.69	46.51	0.928
	Ethylbenzene	10.69	158.8	0.832
	M-xylene	10.69	173.9	0.842
	O-xylene	10.69	151.1	0.852
2A	Benzene	13.29	16.37	0.916
	Toluene	13.29	56.07	0.815
	Ethylbenzene	13.29	192.6	0.761
	M-xylene	13.29	204.9	0.817
	O-xylene	13.29	189.3	0.729
2B	Benzene	11.90	18.88	0.938
	Toluene	11.90	49.45	0.949
	Ethylbenzene	11.90	178.2	0.603
	M-xylene	11.90	192.7	0.622
	O-xylene	11.90	174.9	0.624
3A	Benzene	6.69	17.18	0.922
	Toluene	6.69	56.9	0.91
	Ethylbenzene	6.69	184.7	0.782
	M-xylene	6.69	198.8	0.799
	O-xylene	6.69	177.7	0.803
3B	Benzene	8.11	15.38	0.92
	Toluene	8.11	53.51	0.919
	Ethylbenzene	8.11	163.5	0.828
	M-xylene	8.11	178	0.828
	O-xylene	8.11	158	0.839

Table F-26. Parameters obtained from nonequilibrium fit model.

Column	Constituent	P	R	B	w	r^2
1A	Benzene	11.32	18.39	0.346	2.12	0.946
	Toluene	11.32	45.86	0.296	2.74	0.979
	Ethylbenzene	11.32	179.10	0.057	5.04	0.983
	M-xylene	11.32	184.60	0.341	1.54	0.989
	O-xylene	11.32	153.90	0.150	3.72	0.995
1B	Benzene	10.69	15.58	0.292	3.54	0.973
	Toluene	10.69	52.99	0.486	1.05	0.98
	Ethylbenzene	10.69	171.60	0.297	2.98	0.993
	M-xylene	10.69	188.70	0.267	3.62	0.994
	O-xylene	10.69	160.40	0.260	3.51	0.995
2A	Benzene	13.29	18.10	0.379	2.19	0.961
	Toluene	13.29	76.60	0.424	0.68	0.987
	Ethylbenzene	13.29	223.00	0.220	3.95	0.993
	M-xylene	13.29	230.70	0.078	7.46	0.992
	O-xylene	13.29	222.30	0.235	3.38	0.995
2B	Benzene	11.90	20.66	0.264	3.17	0.979
	Toluene	11.90	55.20	0.548	1.00	0.988
	Ethylbenzene	11.90	223.80	0.274	1.83	0.996
	M-xylene	11.90	242.30	0.258	2.18	0.995
	O-xylene	11.90	211.90	0.261	2.01	0.994
3A	Benzene	6.69	18.78	0.263	2.74	0.957
	Toluene	6.69	61.13	0.308	2.06	0.982
	Ethylbenzene	6.69	212.70	0.178	3.57	0.986
	M-xylene	6.69	229.00	0.158	4.21	0.989
	O-xylene	6.69	200.80	0.165	3.76	0.99
3B	Benzene	8.11	17.79	0.320	1.72	0.976
	Toluene	8.11	57.82	0.310	2.07	0.989
	Ethylbenzene	8.11	183.80	0.288	2.80	0.996
	M-xylene	8.11	201.70	0.270	3.20	0.996
	O-xylene	8.11	173.90	0.240	3.30	0.997

APPENDIX G. BICONTINUUM MODEL MODIFICATIONS AND CODE.

During the course of this research, it was noted that the bicontinuum model derived by Selim et al, 1976 was most sensitive to early time data (one to four minute data). Because of the lower sensitivity to late time data, the model was under predicting the amount of time required to reach sorption equilibrium. Consequently, the kinetic rate coefficient was skewed higher than the true data suggested (Figures G-1 and G-2). In order to provide a more accurate estimation of the kinetic rate coefficient, a weighted version of the bicontinuum model was developed. The weighted model included the following two-step process:

1) Inversely fit the non-weighted bicontinuum model to the batch experiment data. K_d was calculated from equilibrium data of the batch experiments and allowed to vary by 0.01 L/kg; F and k_2 were inversely fit to the data based on a least sum of squared errors method. Obtain the fraction of instantaneous sorption from this fit.
2) Run the weighted bicontinuum model with values for K_d and F determined in part 1. Inversely fit k_2 to the "approaching equilibrium" batch experiment data (six through twenty-minute data) based on a least sum of squared errors method.

Once these two models were sequentially run, the three desired nonequilibrium parameters were obtained. The final MATLAB code used to fit the model can be seen after figure G-1.

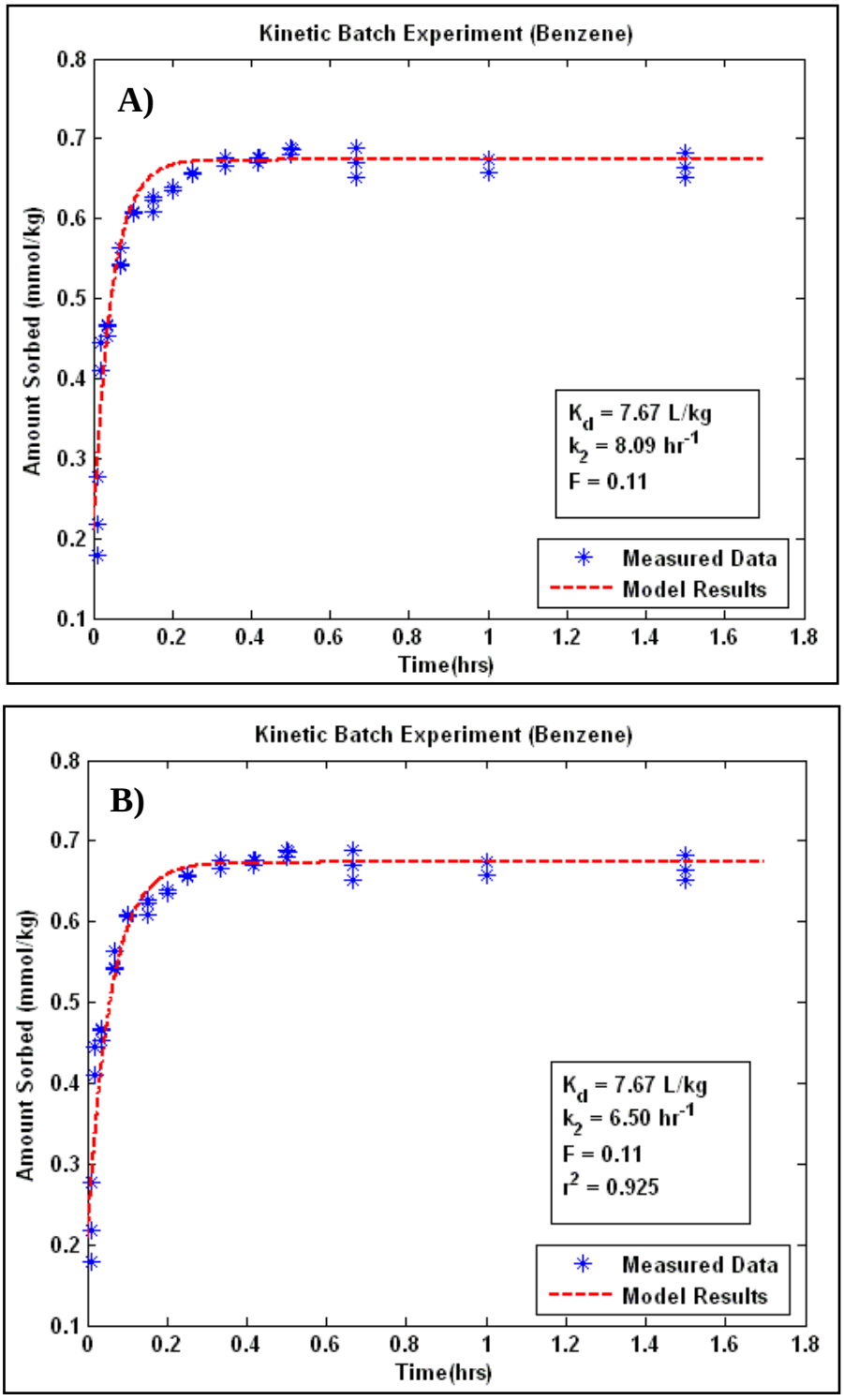

Figure G-1. A) Unmodified model fit to benzene batch data. B) Modified model fit to same benzene dataset.

```
% Josh Simpson

clear;

load SorbedB.txt;

sorb = SorbedB(:, 1);              % sorption data from a batch experiment
timed = SorbedB(:, 2);             % time into experiment that sorption data was taken
ConcAq = SorbedB(:, 3);
meanvalue = mean(sorb);

plot(timed,sorb,'b*')
hold on

Cstart = input('Enter the starting aqueous concentration (mmol/L).  ');
WatVol = input('Enter the amount of water added (mL).  ');
SoilMass = input('Enter the amount of soil added (g).  ');
Kdval = input('Enter the constituents Kd (L/kg).  ');

Ctot = Cstart;

[numsamples, columntime] = size(sorb);

S = 0;                             % total amount sorbed
S2new = 0;                         % amount sorbed by rate-limited sites
S1 = 0;                            % amount sorbed by instantaneous sites
deltaS2 = 0;
timestep = 0.001;                  % timestep in hrs
Sorbed = ones(1,1700);             % variable to store the model's sorption over time to find Kd and F
Sorbed2 = ones(1,1700);            % variable to store the model's sorption over time to find k2
bestfitline = ones(1,1700);        % will only write to this when the sum of square errors is minimized
bestfitline2 = ones(1,1700);       % will only write to this when the sum of square errors is minimized
bestfit = 100000;                  % arbitrary, original sum of square errors value
bestfit2 = 100000;                 % arbitrary, original sum of square errors value
big = 0;                           % counting variable for the sorption variable
finaltime = 1.7;

Fkeep = 0;                         % F value for the best-fit line
```

```
Kdkeep = 0;                          % Kd value for the best-fit line
k2keep = 0;                          % k2 value for the best-fit line
k2keep2 = 0;                         % k2 value for the best-fit line

% this loop determines the correct F and Kd

for F = 0.00:0.01:0.35

    for Kd = Kdval-0.01:0.01:Kdval+0.01

        for k2 = 1:0.01:13.5

            big = 0;
            Ctot = Cstart;
            S = 0;
            S2new = 0;

           for time = 0.001:timestep:finaltime

                big = big+1;

                S1 = ((Kd*F*(Ctot-S2new*(SoilMass/WatVol)))/(1+(F*Kd*(SoilMass/WatVol))));
                deltaS2 = (k2*((1-F)*Kd*(Ctot-((S1+S2new)*(SoilMass/WatVol)))-S2new))*(timestep);
% k2 units are 1/hr
                S2old = S2new;
                S2new = deltaS2 + S2old;

                S = S1 + S2new;
                Sorbed(big)=S;
                Caq(big) = Cstart - S*(SoilMass/WatVol);

           end

           sumsquare = 0;

           for i=1:numsamples

                square = (Sorbed(round(timed(i)*1000))-sorb(i))^2;
```

```
                sumsquare = sumsquare + square;

            end

             if sumsquare < bestfit

                bestfitline = Sorbed;
                bestfit = sumsquare;
                Fkeep = F;
                Kdkeep = Kd;
                k2keep = k2;

             end

        end

    end

end

% time to determine the best-fit k2

for k2 = 1:0.01:16

    F = Fkeep;
    Kd = Kdkeep;

             big = 0;
             Ctot = Cstart;
             S = 0;
             S2new = 0;

            for time = 0.001:timestep:finaltime

                big = big+1;

                S1 = ((Kd*F*(Ctot-2new*(SoilMass/WatVol)))/(1+(F*Kd*(SoilMass/WatVol))));
```

```
                deltaS2 = (k2*((1-F)*Kd*(Ctot-((S1+S2new)*(SoilMass/WatVol)))-S2new))*(timestep);
% k2 units are 1/hr
                S2old = S2new;
                S2new = deltaS2 + S2old;

                S = S1 + S2new;
                Sorbed2(big)=S;
                Caq(big) = Cstart - S*(SoilMass/WatVol);
            end

            % need conditional statement to find best fit along “approaching equilibrium” curve

            sumsquare2 = 0;
            sumsquare3 = 0;

            for i=1:numsamples

                timevalue = timed(i);

                if (timevalue >=0.0999) & (timevalue <=0.34)
                 square2 = (Sorbed2(round(timed(i)*1000))-sorb(i))^2;
                 sumsquare2 = sumsquare2 + square2;    % finding best fit of specified points only
                end

            end

            if sumsquare2 < bestfit2

                for i=1:numsample     % determining total sum of squared error for new line

                 square3 = (Sorbed2(round(timed(i)*1000))-sorb(i))^2;
                 sumsquare3 = sumsquare3 + square3;

                end

                 bestfitline2 = Sorbed2;
               bestfit2 = sumsquare2;
```

```
      bestfit3 = sumsquare3;
                Fkeep = F;
                Kdkeep = Kd;
                k2keep2 = k2;

            end

end


  title('Kinetic Batch Experiment (Benzene)');
  xlabel('Time(hrs)');
  ylabel('Amount Sorbed (mmol/kg)');

  t = 0.001:timestep:1.7;

  plot(t, bestfitline2, '--r')

  legend('Measured Data', 'Model Fit',4)

% Coefficient of determination

ssyy = 0;

for k = 1:numsamples
    syy = (sorb(k) - meanvalue)^2;
    ssyy = ssyy + syy;

end

r2 = 1 - (bestfit3/ssyy);
```

APPENDIX H. PARTICLE SIZE ANALYSIS OF SURFACTANT MODIFIED ZEOLITE FROM THE 2005 FARMINGTON, NM PILOT TEST.

This appendix describes particle size analyses that were conducted on spent SMZ from a field test in 2005. The supporting data are also presented in this appendix.

INTRODUCTION

A pilot test designed to remove organic hydrocarbons from produced water was conducted during the summer of 2005. New Mexico Tech (NMT) and the University of Texas at Austin (UT Austin) carried out the pilot test near Farmington, NM. Two surfactant-modified zeolite (SMZ) columns, A and B, were constructed in order to remove the volatile hydrocarbons—benzene, toluene, ethyl benzene, and xylenes (BTEX)—from the produced water. After the pilot test was completed, SMZ samples were taken from both columns. Duplicate samples were acquired from the top portion and bottom portion of column A; the same procedure was conducted on column B.

Because SMZ breakdown during produced water treatment was previously reported (Ranck et al., 2005), the spent SMZ was analyzed to determine how the produced water had affected the zeolite's particle size distribution. Samples were compared to the particle size distribution results of one virgin SMZ sample. Hydrometer tests were conducted to analyze the particle distribution of fine particles (anything passing the 200 sieve), while sieve analyses measured the distribution of particles retained on and above the 200 sieve. The combination of the two tests produced the particle size distribution data of the spent and virgin SMZ samples.

METHODS AND MATERIALS

Each sample was initially run through a number 10 sieve in order to separate the coarse grained particles from the remaining sample. Both the retained mass and the passing mass were recorded. Since the virgin SMZ did not contain a significant amount of particles larger than the number 10 sieve (<1%), it was unnecessary to perform a particle distribution analysis of the coarse particles. Once the sample was separated, 100 grams of the particles passing the number 10 sieve were measured for the remaining analyses.

The hydrometer test followed ASTM standards (ASTM International, 2002). A dispersing solution (125 mL) containing sodium hexametaphosphate (40 g/L) was mixed with the 100-gram sample in a mixing bowl and allowed to sit for 16 hours in order to minimize sediment flocculation during the hydrometer test. The mixture was then stirred with an electric mixer and poured into a 1,000 mL graduated cylinder. Distilled water was added to the cylinder until the solution reached 1,000 mL. The graduated cylinder was covered and shook by hand for approximately 40 seconds. Once the shaking was completed, hydrometer (152H hydrometer) and temperature readings were recorded according to ASTM standards (after 1, 2, 4, 8, 15, 30, 60, 120, 240, 960, and 1440 minutes). Once the hydrometer readings were complete, the sample was shook on a number 200 sieve. Because particles finer than the 200 sieve were analyzed by the hydrometer test, particles passing the 200 sieve were disregarded. The particles retained on the number 200 sieve were placed on a tin plate and baked in an oven for three days.

The sieve analysis was performed with ASTM number 16, 30, 40, 50, 70, 100, and 200 sieves. Samples were shaken with an electric sieve shaker for approximately 25

minutes. Once the samples had been shaken, the mass retained on each sieve was weighed and recorded. The percentage of mass retained on the sieve was calculated after the sieves were weighed. The results from the sieve test and the hydrometer test provided a particle size distribution for each sample.

The effective grain size is a common parameter used to compare soil samples. 10% of a sample's particles are finer than the effective grain size (d_{10}). The effective grain size is important because flow through a sample is controlled by the fine particles in a sample. Therefore, the smallest 10% of the soil's particles will greatly influence the permeability of a sample. The effective grain size also is important because the finer particles can control the mechanical behavior of a soil (Budhu, 2000). Coarser particles tend to "float" on the smaller particles, so the small particles dictate the movement of the soil. The second influence is not as important in this study because the particles are bound in columns. However, the flow regime is a great concern of the research group. Long-term stability would enhance the effectiveness of the SMZ sorption system.

The d_{60} (60% finer than this particle size) and d_{30} (30% finer than this particle size) values were also recorded. The percentage of gravel, sand, silt, and clay were also calculated from the particle size distribution data. Gravel was defined as anything retained on the ASTM number 4 sieve and larger (4.75 mm and larger). Sand was defined as particles retained between the number 10 sieve and the number 200 sieve (2 mm – 0.075 mm). Silt and clay were combined into a "fines" category, which represented any particle smaller than the 200 sieve. Particle sizes ranging between 0.075 mm and 0.005 mm were defined as silts, while particles smaller than 0.005 mm were defined as a clay particle.

Another parameter used to classify and compare soil samples is the uniformity coefficient. The uniformity coefficient (C_u) is typically calculated for medium to coarse-grained samples and represents the d_{60} value divided by the d_{10} value. For a sample of uniformly sized particles, the uniformity coefficient will equal one (Hillel, 1998). As the sample becomes more poorly sorted, the uniformity coefficient will increase. The C_u is typically less than four for well-sorted soils (Budhu, 2000); but in poorly sorted sands, the uniformity coefficient can reach 1,000 (Hillel, 1998). Therefore, as the grains become more non-uniform, the uniformity coefficient increases.

The coefficient of gradation (C_c) is another parameter that is commonly used to classify soil samples. The C_c is often used to determine if a soil sample is gap graded. For typical well-sorted and poorly-sorted samples, the C_c usually equals between one and three (Budhu, 2000). A gap-graded soil will produce a C_c outside of this range. The sudden change of slope produces the deviations from the normal values. Equation H-1 is used to calculate the coefficient of gradation.

$$C_c = \frac{(d_{30})^2}{d_{10} * d_{60}} \qquad \text{(H-1)}$$

The primary concern of particle breakdown is the influence on the column's permeability; therefore, the permeability of each sample was calculated. Initially, the Hazen method was used to approximate the hydraulic conductivity of each sample. This method is applicable for sands with a d_{10} value between 0.1 mm and 3.0 mm (Fetter, 2001). The SMZ samples have d_{10} values approximately equaling 0.1 mm; so this method is a valid approximation for the hydraulic conductivity of the SMZ samples. The

Hazen method uses Equation H-2 to approximate the hydraulic conductivity of sandy sediments.

$$K = C(d_{10})^2 \quad \text{(H-2)}$$

Where K is the hydraulic conductivity (cm/sec), C is a coefficient based on the properties of the sample, and d_{10} is in cm. Because the majority of the samples were medium to fine grained sands, the constant, C, was set as 80 (Fetter, 2001). Once the hydraulic conductivity was approximated, each sample's permeability was calculated with Equation H-3.

$$K = \frac{k * \rho_w * g}{\mu} \quad \text{(H-3)}$$

Where k is permeability (cm^2), g is gravity (m/s^2), ρ_w is the density of water (kg/m^3), and μ is dynamic viscosity (kg/(m*sec)). These parameters were calculated and compared in order to determine the extent of the particle breakdown that occurred during the pilot test. The permeability and d_{10} values are of particular importance because the flow characteristics through the columns are directly related to these two parameters. When both the permeability and the d_{10} decrease, produced water treatment efficiency decreases. Clogging issues, immobile sections, and backpressure buildups could also be of concern when these parameters decrease.

RESULTS AND DISCUSSION

Tables H-1 through H-9 present the hydrometer and sieve test data. The overall results from the hydrometer and sieve tests are presented in Tables H-10 and H-11. Samples were defined as top or bottom (T or B), column A or B (A or B), and sample 1

or 2 (-1 or -2). For example, sample BA-2 represents the second sample for the bottom of column B. The percentage of finer particles was calculated for each sieve and for the hydrometer test data. From this data, particle size distribution histograms and graphs were created. Figures H-1 through H-9 show the histograms of each sample's particle size distribution compared to the virgin SMZ. The particle size distribution graphs of each sample are seen in Figures H-10 through H-16. The spent SMZ histograms show similar particle distribution results. The percentages of particles ranging from 0.6 mm – 0.3 mm decreased in the spent SMZ compared to the virgin SMZ. The most consistent and significant loss in percentage occurred on the ASTM number 40 sieve (0.425 mm). This particle size recorded a drop from 27% retained to only approximately 20% retained. Since the medium grained particles all saw a decrease in percentage retained, the fine particles saw the increase in percentage retained. The results show that particles ranging from 0.212 mm – 0.0361 mm consistently had higher percentages retained in the spent SMZ than the virgin SMZ. The increase in percentage retained on these sieves was not significant, but the results show that a definite increase occurred for the majority of the samples. Even though the fines from 0.212 mm – 0.0361 mm showed an increase in percentage retained, the fines below 0.031 mm did not show consistent increases in percentages retained. Both of the samples from the top of column B show and increase in particles between 0.0180 mm – 0.0094 mm; however, no other samples have similar results. Therefore, the medium grained particles were broken down into semi-fine grained particles during the pilot test. However, a consistent increase in extremely fine grained particles was not observed in the results.

The particle size distribution graphs indicate that the percentage of coarse grained particles (2 mm – 0.5 mm) was not significantly affected during the pilot test. A slight increase in the particles retained on the number 10 sieve is seen in some of the samples; however, these results are explained by particles bonding together during the test. Therefore, the increase in percentage is not due to single large particles but to the cementing of multiple particles together. These particle groups were not crushed prior to the hydrometer and sieve analysis because the individual particles could be affected / crushed when attempting to split the group. This process could lead to an increase in fine particles and skew the results. Even though no significant change in the coarse particles was seen from the graphs, the graphs do indicate that the pilot test did alter the percentage of fine grained particles in the majority of the samples. The percentage of particles 0.5 mm and smaller increased for all of the spent SMZ samples compared to the virgin SMZ. Therefore, as expected, an increase in fines occurred during the pilot test due to particle break down. The extent of particle breakdown was examined using the parameters discussed in the methods section. The effective grain size (d_{10}), d_{30}, and d_{60} values were obtained from the particle size distribution graphs. As stated previously, these parameters were used to calculate the uniformity coefficient and the coefficient of gradation. Also, the effective grain size was used to approximate the hydraulic conductivity of each sample using the Hazen Method. The results from these calculations can be seen in Table H-10. Top A 1 and Top A 2 represent the two samples taken from the top of column A. Bot A 1 and Bot A 2 are samples taken from the bottom of column A. The same naming procedure applies to column B. Raw SMZ 1 represents the virgin SMZ sample that underwent both the hydrometer and sieve analyses.

As stated previously, the data in Table H-10 indicates that no change in the d_{60} value is seen between the virgin SMZ and the spent SMZ. The d_{60} value for the virgin SMZ is 0.68 mm, and the average value of the spent SMZ is 0.70 mm. The slight increase in the d_{60} value is caused by the grouping of particles discussed previously. Table H-10 shows that some of the samples had large increases in the d_{60} value (Top B 2), while other samples had significant breakdown of the coarse grained particles and the d_{60} value was substantially smaller (Top A 1). The d_{30} value for the virgin SMZ is 0.44 mm, while the average value from the spent SMZ is 0.41 mm. So, on average the d_{30} particle size decreased during the pilot test by only 7%. Again, the d_{30} value increased for the Top B 2 sample, while it was significantly smaller for the Top A 1 and Bot A 1 samples. These two samples show a decrease of 20% from the original d_{30} value. The data shows that, on average, only a slight decrease of the d_{30} occurred. A significant decrease in the effective grain size for the majority of the samples compared to the virgin SMZ is seen in Table H-10. On average, the d_{10} value for the spent SMZ was 0.12 mm and it was 0.29 mm for the virgin SMZ sample. These values indicate that the effective grain size decreased by 58% during the pilot test.

The uniformity coefficient is used to determine the sorting of a sample. As stated previously, it can range from one (uniform grain size) to around 1000 (poorly sorted). Since the virgin SMZ's C_u equals 2.3, it lies within the typical range of a well-sorted sample. However, the average C_u of 6.1 from the spent SMZ is not in the typical range of a well-sorted soil. Therefore, the pilot test started with well-sorted SMZ and particle break down caused the spent SMZ to be classified as a poorly sorted sample. The maximum change in the uniformity coefficient occurred in the samples from the bottom

of column A. The C_u for these samples ranged from 3 to 4 times the virgin SMZ's uniformity coefficient. Both samples from the top of column B show the least amount of change in the uniformity coefficient as they doubled the original value. If the coefficient of gradation (C_c) is larger than 3, a soil is defined as gap graded. As expected, the results show that none of the SMZ samples are gap graded. All of the samples lie in the range for typical poorly and well sorted soils. The C_c increased for all of the samples because the d_{30} and d_{60} remained constant while the d_{10} decreased. Since you divide the squared d_{30} value by the d_{60} and d_{10} values, a decrease in the d_{10} value will naturally produce a larger coefficient of gradation.

Because the Hazen method is only an approximation of hydraulic conductivity, the results from the virgin SMZ were compared to lab measurements on virgin SMZ. Column measurements in the lab resulted in a hydraulic conductivity range of 31.5 – 35.8 m/day for virgin SMZ (Altare, 2006). The results from the Hazen method indicate that the virgin SMZ has a hydraulic conductivity of 58 m/day. So, the Hazen method slightly overestimates the hydraulic conductivity value; but it provides a good approximation for the virgin and spent SMZ. The average hydraulic conductivity of the spent SMZ is approximately 12 m/day. Therefore, the hydraulic conductivity of the spent SMZ is 1/5 of the virgin SMZ's hydraulic conductivity. Two of the spent SMZ samples are even one order of magnitude less than the virgin SMZ. In order to calculate the permeability, a density of 998.2 kg/m^3, and a viscosity of 1.002 * 10^{-3} kg/(m*sec) were used. Therefore, only a conversion factor of 1.023 * 10^{-7} (m*sec) was needed to convert the hydraulic conductivity to permeability (m^2) (Schwartz and Zhang, 2003). These values assume 20^{o}C and water as the fluid. Since the same conversion factor was used to calculate the

permeabilities, the results for the permeability data matched the results from the hydraulic conductivity data. Both the hydraulic conductivity and permeability lie within the typical range for a medium grained, clean sand (Freeze and Cherry, 1979 and Schwartz and Zhang, 2003). Both the particle size analysis in Table H-11 and the particle size distribution graphs (Figures H-9 through H-16) indicate that the majority of the SMZ samples are medium grained sand particles.

The particle classification results are seen in Table H-11. The same sample-naming scheme is used in Table H-11 as was used in Table H-10. The results from this analysis also indicate that the percentage of fines (silt and clay combined) increased during the pilot test because of particles breaking down. Prior to the pilot test, the virgin SMZ contained 98% sand and 2% fines. The average values for the spent SMZ are: 93% sand and 7% fines. Therefore, the spent SMZ has approximately 3.7 times the amount of fines in the virgin SMZ. The same trends within the columns are seen with the particle size analysis. On average, the top sample has a lower amount of fines than the bottom sample in each column. Also, column A was usually the first column in series during the pilot test. The data shows that a greater amount of particle breakdown occurred in this column than column B.

The results from the two virgin SMZ samples that only underwent the sieve analysis show an even greater amount of particle breakdown. The percentage of fines in these two samples was four times smaller than the virgin SMZ that underwent both the hydrometer and sieve analyses. Similar results are seen for the effective grain size, the d_{30}, and the hydraulic conductivity of these two samples. The uniformity constant for these two samples also indicate that the virgin SMZ is a well sorted sample.

CONCLUSIONS

Particles in a media naturally break down when water flows through it, so some particle breakdown was expected. The results from the particle size distribution test confirm that particle break down did occur during the pilot test. Both of the columns show a higher percentage of fines in the lower sample than the upper sample. Since flow occurred from the top of the columns to the bottom of the columns, some fine particles were probably carried downward in the column during the pilot test. The samples were also taken approximately 6 months after the pilot test was completed, so particle settling could have occurred during that period of time. The effective grain size and amount of fines were important parameters because the small grain sizes control the ability for produced water to flow through the columns. The results from these parameters indicate that the fines did increase significantly in some of the samples; for example, in the bottom of column A. Even though the percentage of fines did increase, the histograms show that an increase in the extremely fine grained particles did not occur. Since these particles would greatly influence the flow regime, no consistent increase in these particles is promising. One major effect of particle breakdown is the back pressure will build up when produced water is forced through the columns. No back pressure build up was observed during the field test, which also indicates that the overall particle breakdown did not greatly influence the flow regime. Although particle breakdown is seen in the results, the results do not provide any significant reason for doubting the long term stability of the SMZ particles.

Table H-1. Combined sieve and hydrometer data for sample TA-1.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percent Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	99.70	0.30
1.18	**16**	98.40	1.30
0.60	**30**	57.03	41.37
0.43	**40**	37.54	19.49
0.30	**50**	24.67	12.87
0.21	**70**	19.41	5.26
0.15	**100**	14.56	4.85
0.08	**200**	8.93	5.63
0.0498	Hydrometer	8.33	0.60
0.0357		5.72	2.61
0.0255		3.63	2.09
0.0180		3.63	0.00
0.0133		3.11	0.52
0.0094		2.59	0.52
0.0066		2.59	0.00
0.0047		2.59	0.00
0.0033		2.59	0.00
0.0017		2.59	0.00
0.0014		2.59	0.00

Table H-2. Combined sieve and hydrometer data for sample TA-2.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	99.69	0.31
1.18	**16**	97.49	2.20
0.60	**30**	50.85	46.64
0.43	**40**	30.07	20.78
0.30	**50**	17.41	12.66
0.21	**70**	13.31	4.10
0.15	**100**	10.69	2.62
0.08	**200**	5.63	5.06
0.0507	Hydrometer	4.68	0.96
0.0361		4.15	0.52
0.0257		3.11	1.04
0.0182		3.11	0.00
0.0133		2.59	0.52
0.0094		2.59	0.00
0.0066		2.59	0.00
0.0047		2.59	0.00
0.0033		2.59	0.00
0.0017		2.59	0.00
0.0014		2.59	0.00

Table H-3. Combined sieve and hydrometer data for sample BA-1.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	96.02	3.98
1.18	**16**	93.79	2.23
0.60	**30**	52.84	40.95
0.43	**40**	35.95	16.89
0.30	**50**	24.41	11.54
0.21	**70**	20.32	4.10
0.15	**100**	17.24	3.08
0.08	**200**	10.03	7.21
0.0501	Hydrometer	7.31	2.72
0.0361		3.78	3.53
0.0257		2.98	0.80
0.0182		2.98	0.00
0.0133		2.48	0.50
0.0094		2.48	0.00
0.0066		2.48	0.00
0.0047		2.48	0.00
0.0033		1.98	0.50
0.0017		2.48	-0.50
0.0014		2.48	0.00

Table H-4. Combined sieve and hydrometer data for sample BA-2.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	98.92	1.08
1.18	**16**	97.04	1.88
0.60	**30**	48.28	48.76
0.43	**40**	29.70	18.58
0.30	**50**	18.71	10.99
0.21	**70**	15.38	3.33
0.15	**100**	12.39	2.98
0.08	**200**	7.18	5.21
0.0505	Hydrometer	5.90	1.28
0.0361		3.58	2.32
0.0257		3.07	0.51
0.0182		3.07	0.00
0.0133		3.07	0.00
0.0094		3.07	0.00
0.0066		2.56	0.51
0.0047		2.56	0.00
0.0033		2.56	0.00
0.0017		2.56	0.00
0.0014		2.56	0.00

Table H-5. Combined sieve and hydrometer data for sample TB-1.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	98.65	1.35
1.18	**16**	97.02	1.63
0.60	**30**	46.41	50.61
0.43	**40**	25.92	20.49
0.30	**50**	14.43	11.49
0.21	**70**	11.39	3.04
0.15	**100**	8.72	2.68
0.08	**200**	8.40	0.29
0.0501	Hydrometer	7.26	1.03
0.0357		5.83	1.44
0.0252		5.62	0.21
0.0179		4.60	1.03
0.0132		4.09	0.51
0.0093		3.57	0.51
0.0066		3.06	0.51
0.0047		3.06	0.00
0.0033		2.55	0.51
0.0017		2.55	0.00
0.0014		2.55	0.00

Table H-6. Combined sieve and hydrometer data for sample TB-2.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	92.79	7.21
1.18	**16**	89.95	2.85
0.60	**30**	41.12	48.83
0.43	**40**	23.50	17.62
0.30	**50**	12.98	10.52
0.21	**70**	10.24	2.75
0.15	**100**	8.97	1.26
0.08	**200**	5.00	3.97
0.0505	Hydrometer	5.53	-0.53
0.0358		4.33	1.21
0.0253		4.33	0.00
0.0180		3.84	0.48
0.0132		3.36	0.48
0.0094		2.88	0.48
0.0066		2.40	0.48
0.0047		2.40	0.00
0.0033		2.40	0.00
0.0017		2.40	0.00
0.0014		2.40	0.00

Table H-7. Combined sieve and hydrometer data for sample BB-1.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	99.85	0.15
1.18	**16**	97.03	2.82
0.60	**30**	50.13	46.90
0.43	**40**	29.70	20.43
0.30	**50**	17.13	12.57
0.21	**70**	13.54	3.59
0.15	**100**	10.78	2.76
0.08	**200**	6.09	4.68
0.0507	Hydrometer	5.48	0.61
0.0363		2.79	2.70
0.0257		2.58	0.21
0.0182		2.06	0.52
0.0133		2.06	0.00
0.0094		1.54	0.52
0.0067		1.54	0.00
0.0047		1.54	0.00
0.0033		1.54	0.00
0.0017		2.06	-0.52
0.0014		2.06	0.00

Table H-8. Combined sieve and hydrometer data for sample BB-2.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	99.86	0.14
1.18	**16**	98.18	1.68
0.60	**30**	55.32	42.86
0.43	**40**	33.85	21.47
0.30	**50**	20.20	13.65
0.21	**70**	16.01	4.19
0.15	**100**	12.26	3.74
0.08	**200**	6.47	5.79
0.0505	Hydrometer	5.69	0.78
0.0361		4.39	1.30
0.0255		3.61	0.78
0.0180		3.61	0.00
0.0133		3.09	0.52
0.0094		3.09	0.00
0.0066		3.09	0.00
0.0047		3.09	0.00
0.0033		3.09	0.00
0.0017		3.09	0.00
0.0014		2.58	0.52

Table H-9. Combined sieve and hydrometer data for sample Virgin SMZ.

Grain size (mm)	U.S. Standard Sieve No.	Percent Finer by weight	Percentage Retained
75.00	**3 in.**	100.00	0.00
50.00	**2 in.**	100.00	0.00
37.50	**1-1/2 in.**	100.00	0.00
25.00	**1 in.**	100.00	0.00
19.00	**3/4 in.**	100.00	0.00
9.50	**3/8 in.**	100.00	0.00
4.75	**4**	100.00	0.00
2.00	**10**	99.91	0.09
1.18	**16**	98.63	1.28
0.60	**30**	52.80	45.83
0.43	**40**	26.00	26.80
0.30	**50**	10.45	15.56
0.21	**70**	7.71	2.74
0.15	**100**	5.47	2.24
0.08	**200**	1.83	3.64
0.0513	Hydrometer	2.63	-0.80
0.0364		2.10	0.53
0.0258		1.57	0.53
0.0182		1.57	0.00
0.0133		1.57	0.00
0.0094		1.57	0.00
0.0067		1.04	0.53
0.0047		1.04	0.00
0.0033		1.04	0.00
0.0017		0.51	0.53
0.0014		0.51	0.00

Table H-10. Overall parameter results from the particle size distribution data.

Sample	d_{10} (mm)	d_{30} (mm)	d_{60} (mm)	C_u	C_c	Hydraulic Conductivity (m/sec)	Permeability (cm^2)
Top A 1	0.08	0.34	0.62	7.5	2.25	5.51E-05	5.64E-08
Top A 2	0.13	0.42	0.70	5.4	1.94	1.35E-04	1.38E-07
Bot A 1	0.08	0.36	0.69	9.2	2.50	4.50E-05	4.60E-08
Bot A 2	0.10	0.43	0.71	7.1	2.60	8.00E-05	8.18E-08
Top B 1	0.17	0.46	0.71	4.2	1.75	2.31E-04	2.37E-07
Top B 2	0.20	0.49	0.79	4.0	1.52	3.20E-04	3.27E-07
Bot B 1	0.13	0.43	0.70	5.4	2.03	1.35E-04	1.38E-07
Bot B 2	0.11	0.38	0.66	6.0	1.99	9.68E-05	9.90E-08
Raw Zeolite	0.29	0.44	0.68	2.3	0.98	6.73E-04	6.88E-07
VIR SMZ 1	0.40	0.61	0.82	2.1	1.13	1.28E-03	1.31E-06
VIR SMZ 2	0.43	0.61	0.82	1.9	1.06	1.48E-03	1.51E-06

Table H-11. Particle size breakdown results from particle size distribution data.

Sample	% Gravel	% Sand	% Fines	% Silt	% Clay
Top A 1	0	91.07	8.93	6.34	2.59
Top A 2	0	94.37	5.63	3.04	2.59
Bot A 1	0	89.97	10.03	7.55	2.48
Bot A 2	0	92.82	7.18	4.63	2.56
Top B 1	0	95.60	4.40	1.34	3.06
Top B 2	0	95.00	5.00	2.60	2.40
Bot B 1	0	93.91	6.09	4.55	1.54
Bot B 2	0	93.53	6.47	3.38	3.09
Raw Zeolite	0	98.17	1.83	0.79	1.04
VIR SMZ 1	0	99.32	0.68	0.68	0.00
VIR SMZ 2	0	99.77	0.23	0.22	0.01

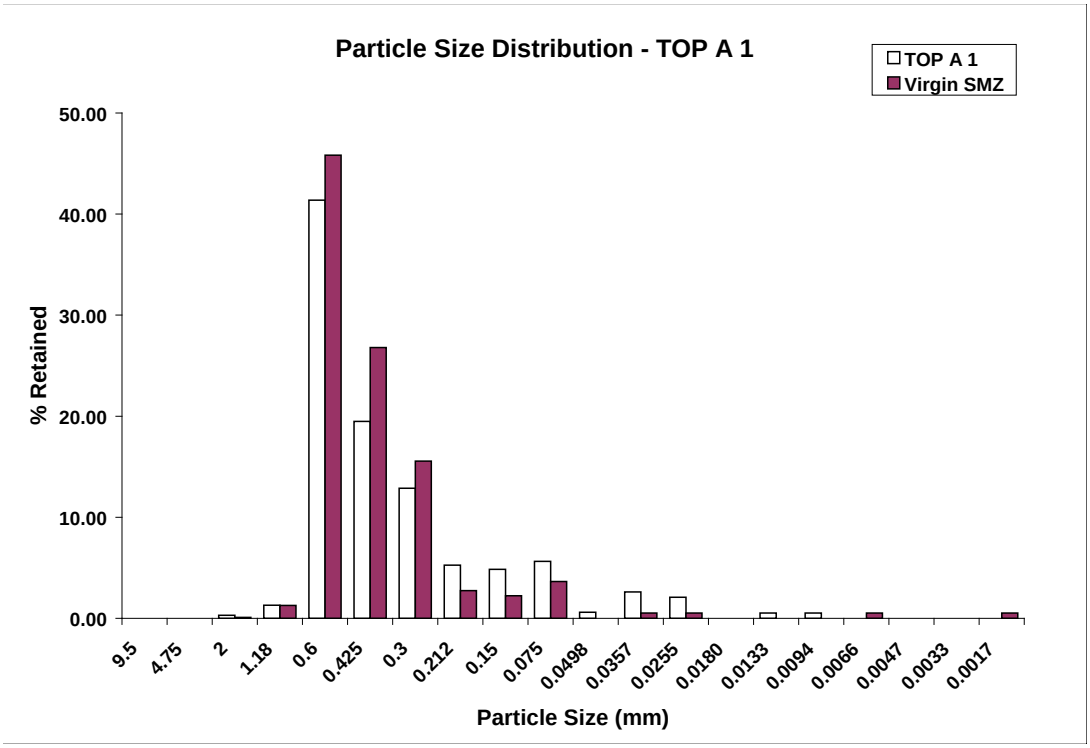

Figure H-1. Bar graph representation of particle size distribution of sample TA-1. Virgin SMZ represents unspent particle size distribution.

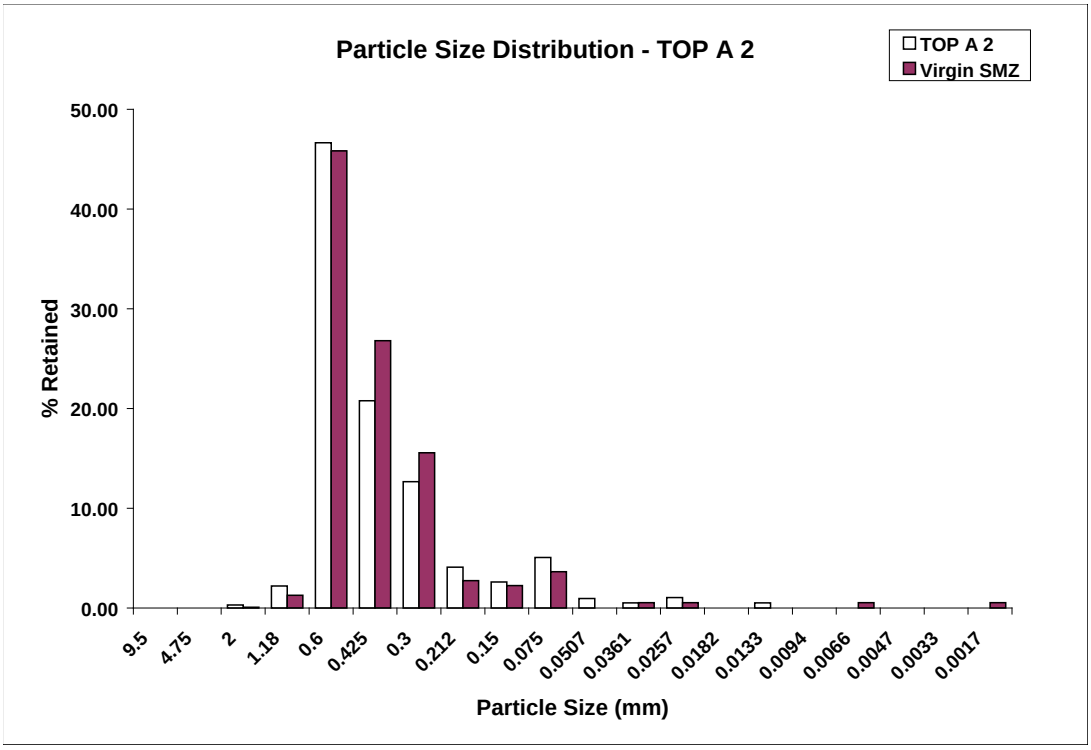

Figure H-2. Bar graph representation of particle size distribution of sample TA-2. Virgin SMZ represents unspent particle size distribution.

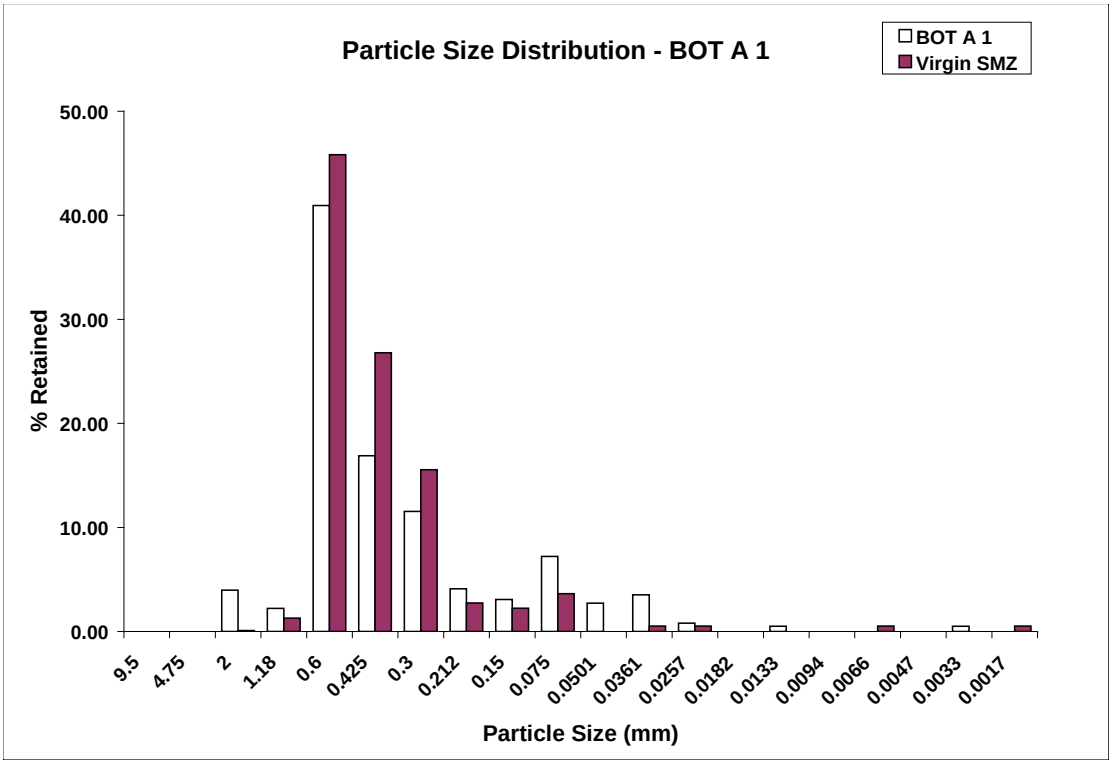

Figure H-3. Bar graph representation of particle size distribution of sample BA-1. Virgin SMZ represents unspent particle size distribution.

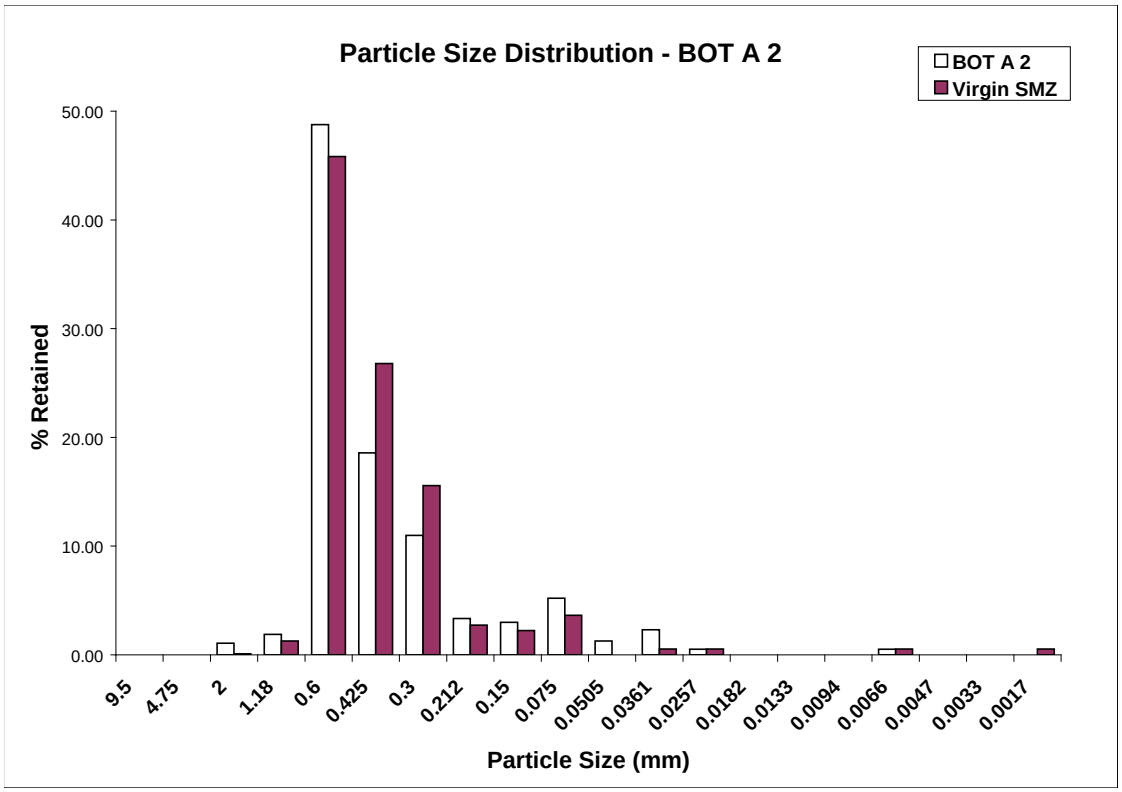

Figure H-4. Bar graph representation of particle size distribution of sample BA-2. Virgin SMZ represents unspent particle size distribution.

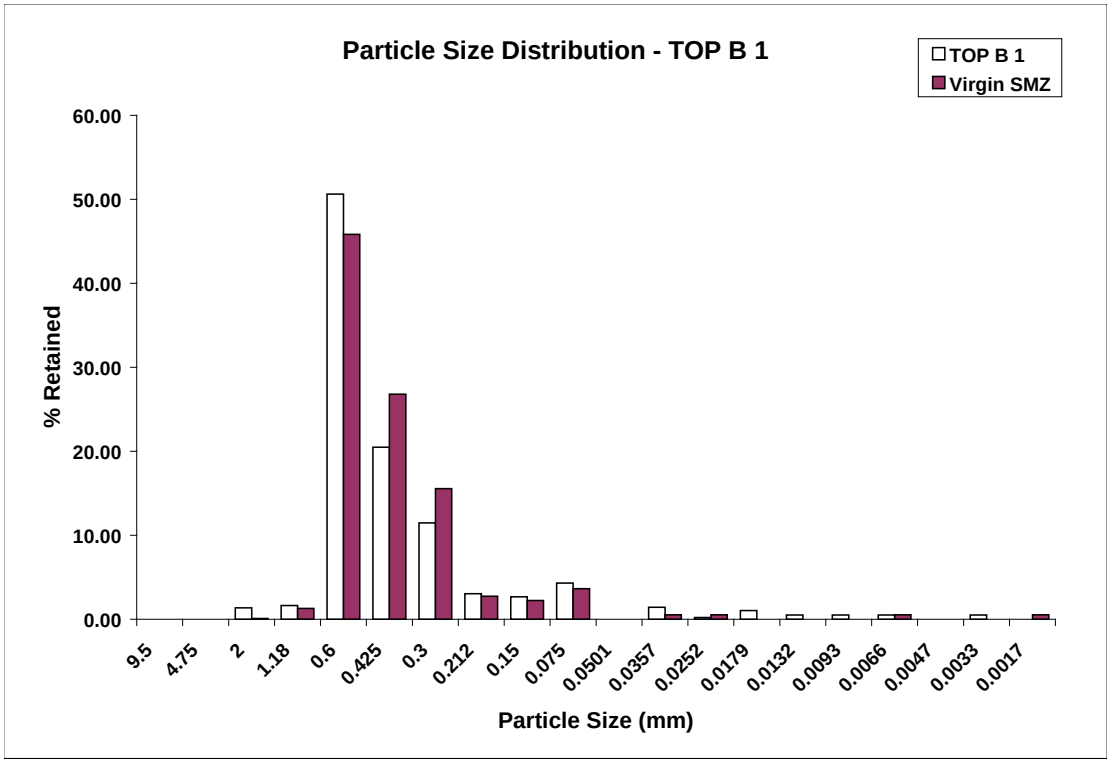

Figure H-5. Bar graph representation of particle size distribution of sample TB-1. Virgin SMZ represents unspent particle size distribution.

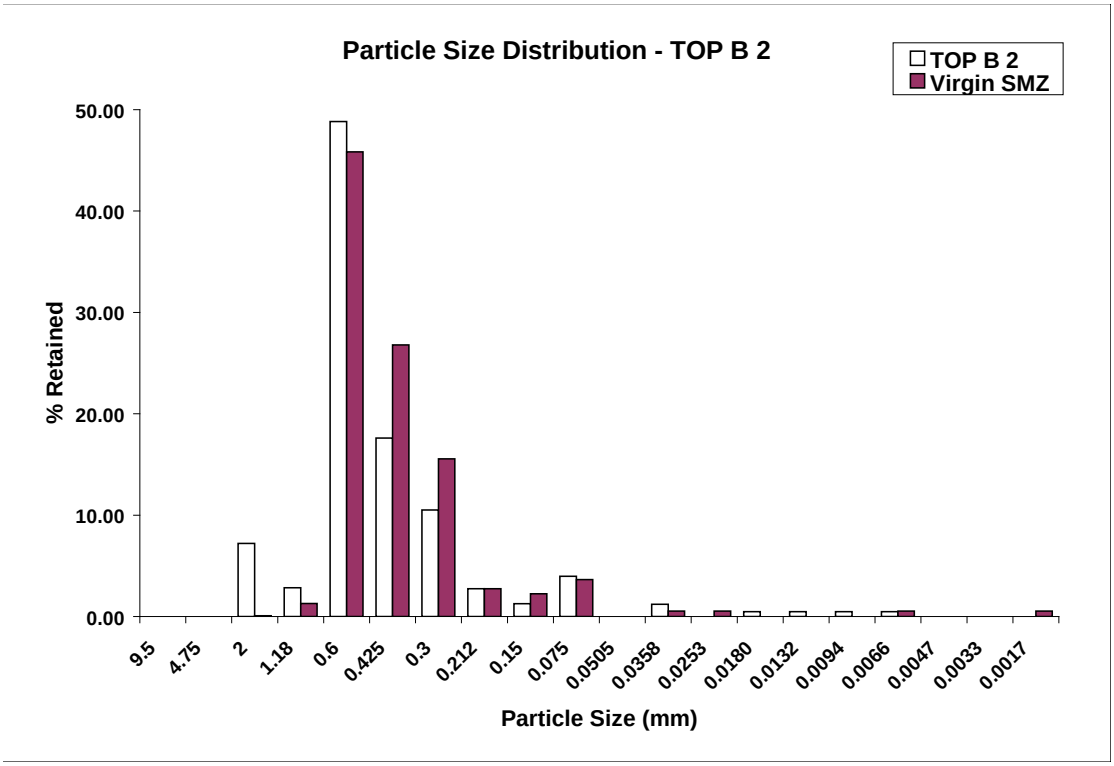

Figure H-6. Bar graph representation of particle size distribution of sample TB-2. Virgin SMZ represents unspent particle size distribution.

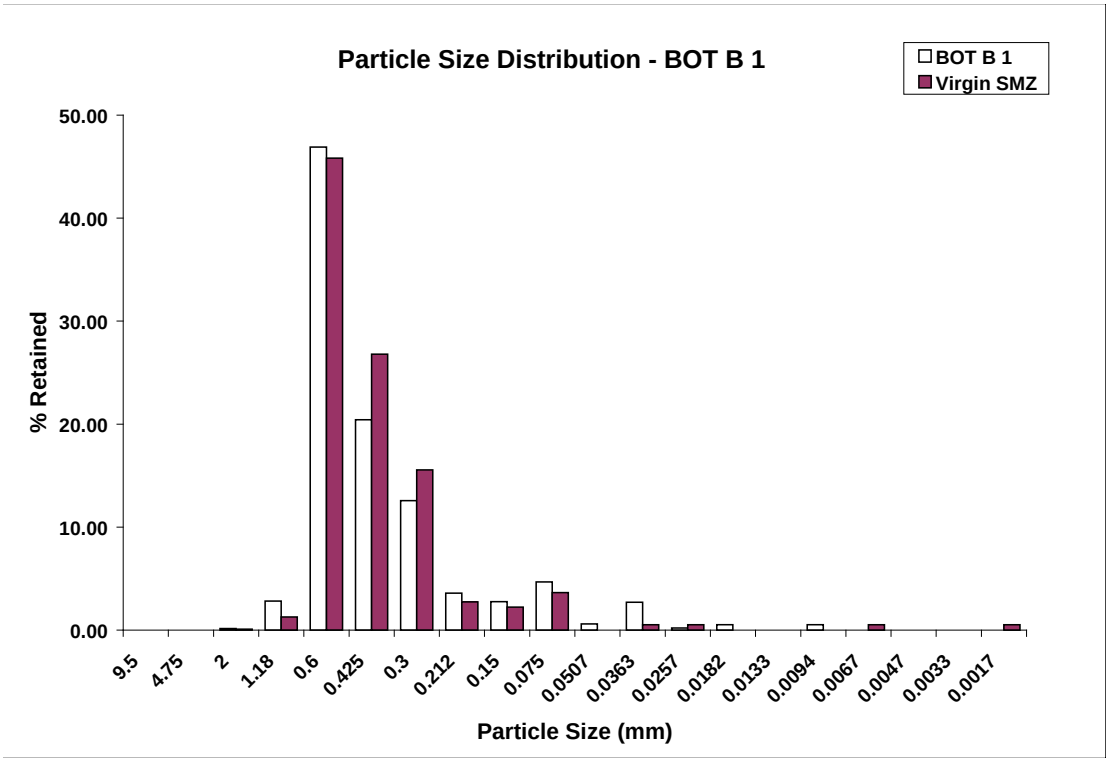

Figure H-7. Bar graph representation of particle size distribution of sample BB-1. Virgin SMZ represents unspent particle size distribution.

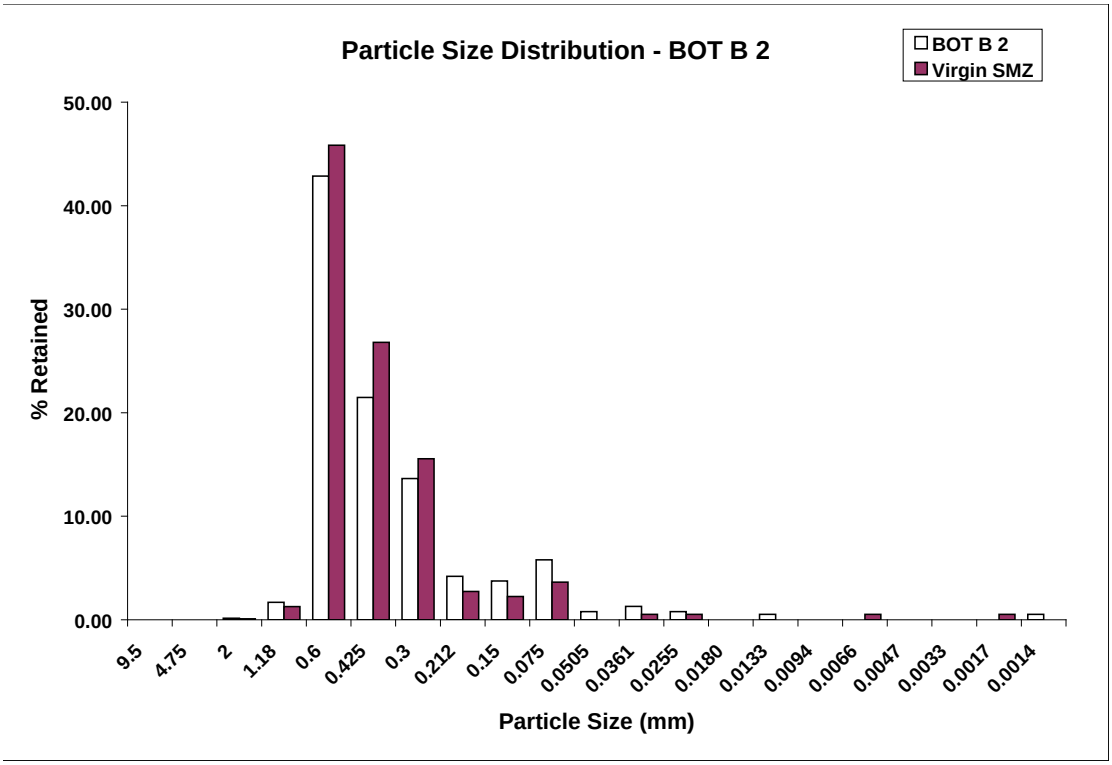

Figure H-8. Bar graph representation of particle size distribution of sample BB-2. Virgin SMZ represents unspent particle size distribution.

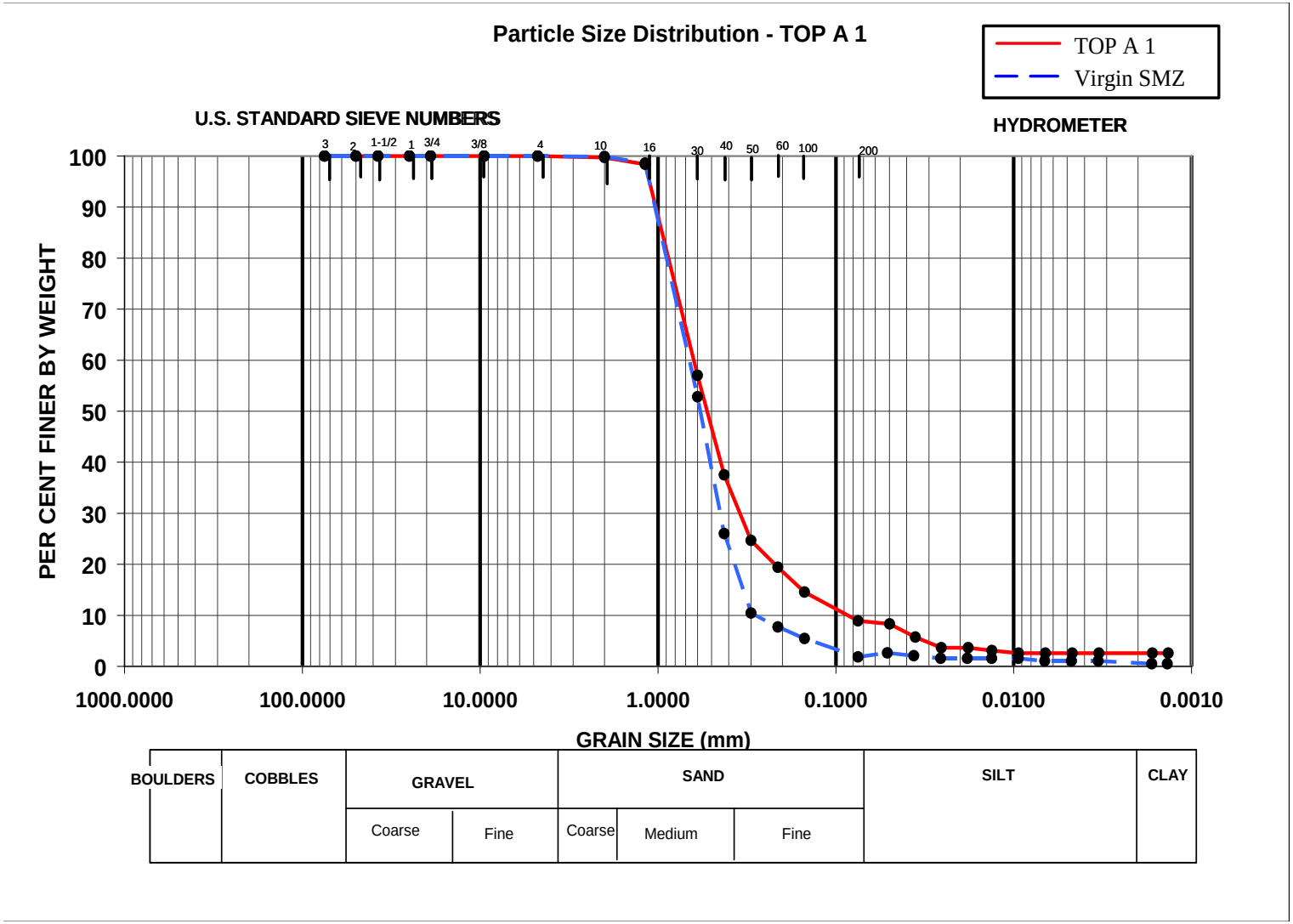

Figure H-9. Particle size distribution results for sample TA-1.

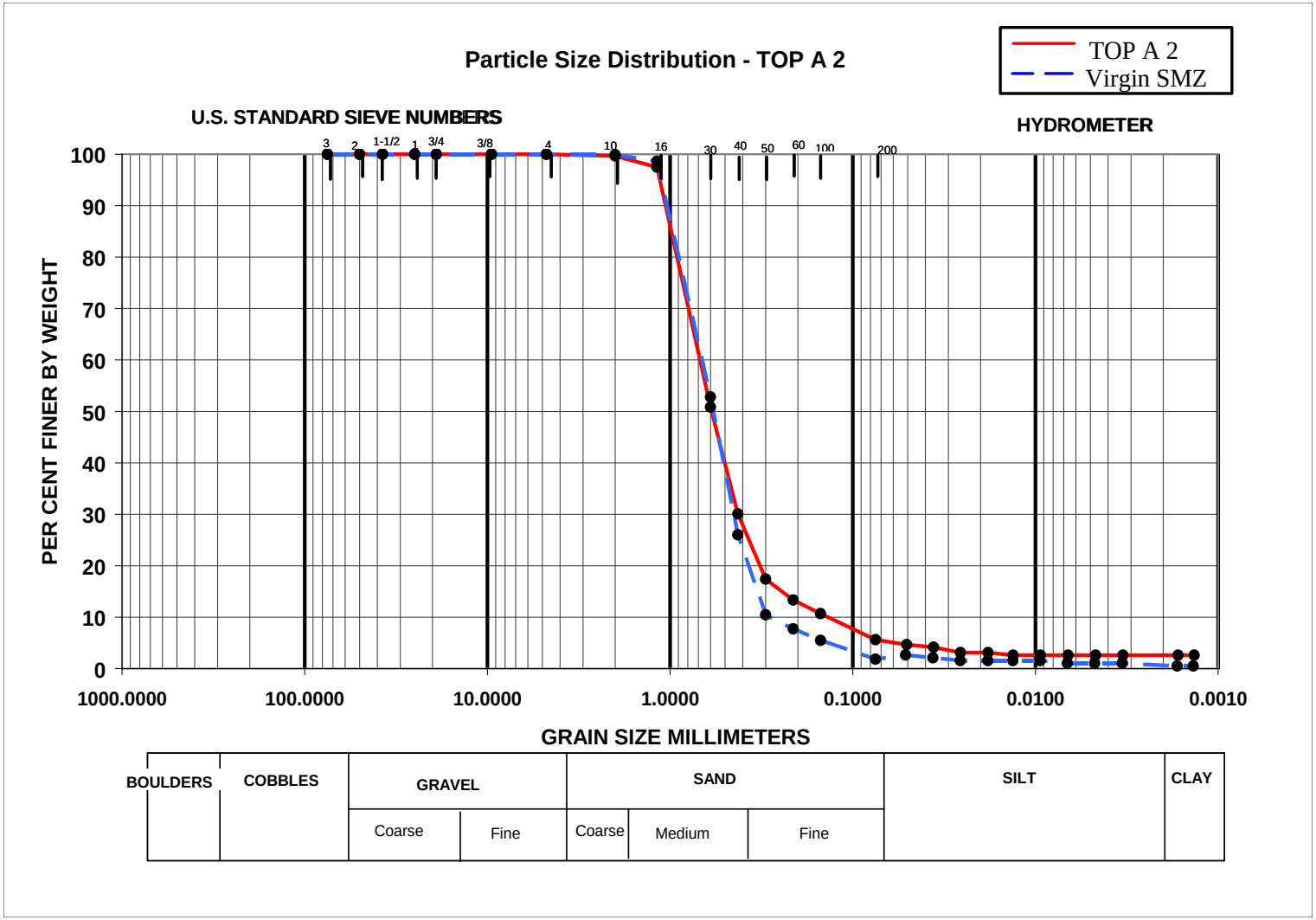

Figure H-10. Particle size distribution results for sample TA-2.

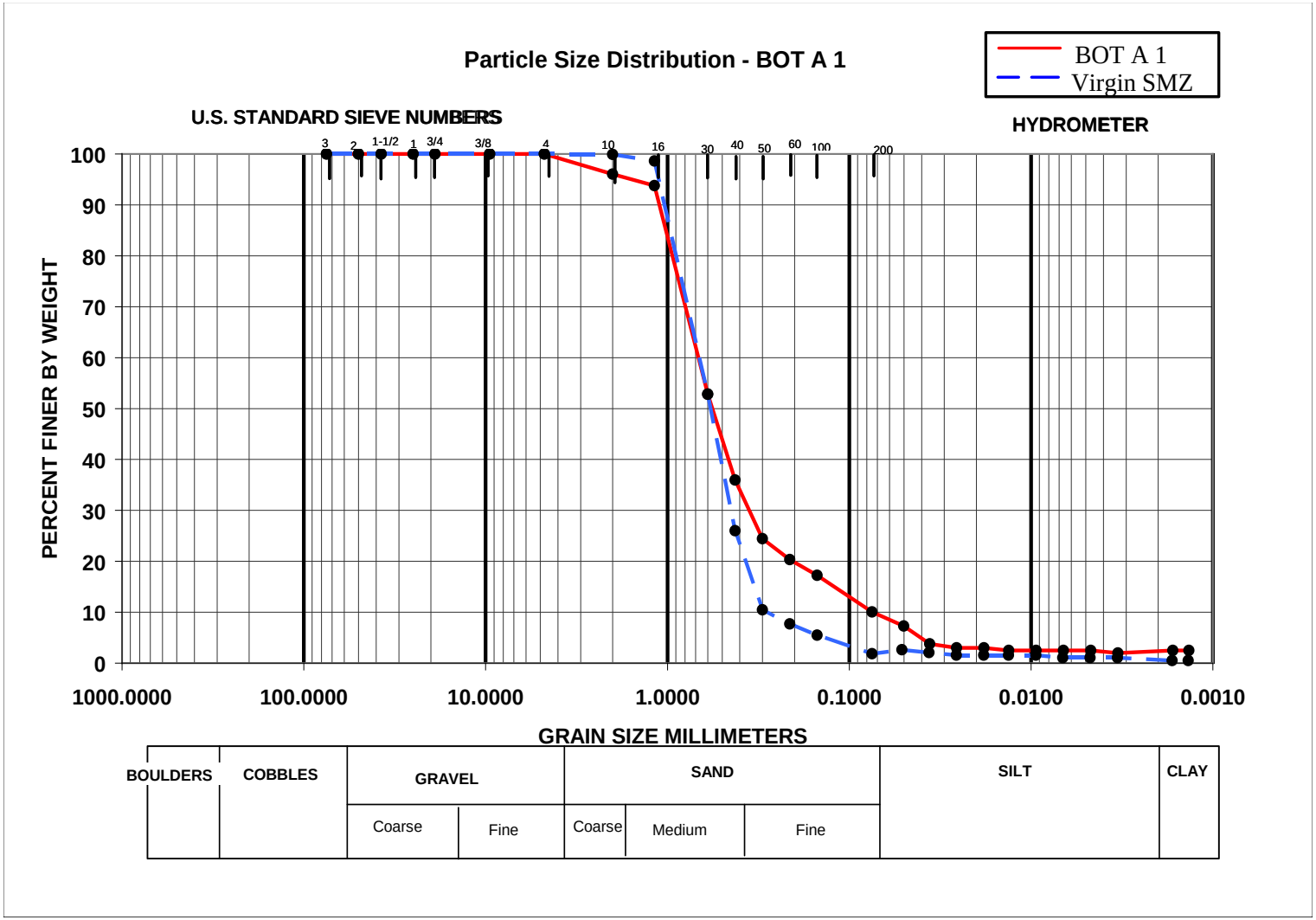

Figure H-11. Particle size distribution results for sample BA-1.

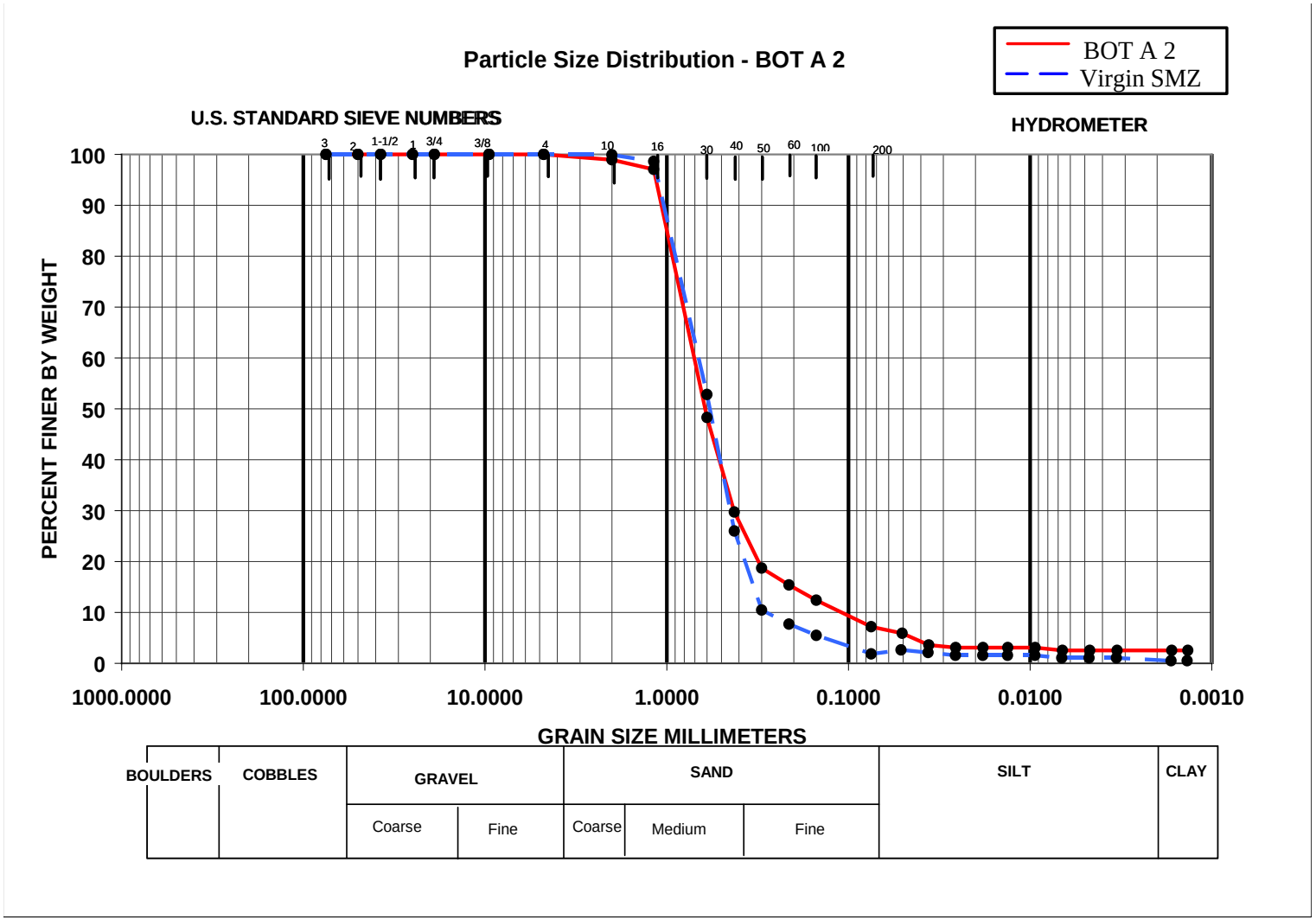

Figure H-12. Particle size distribution results for sample BA-2.

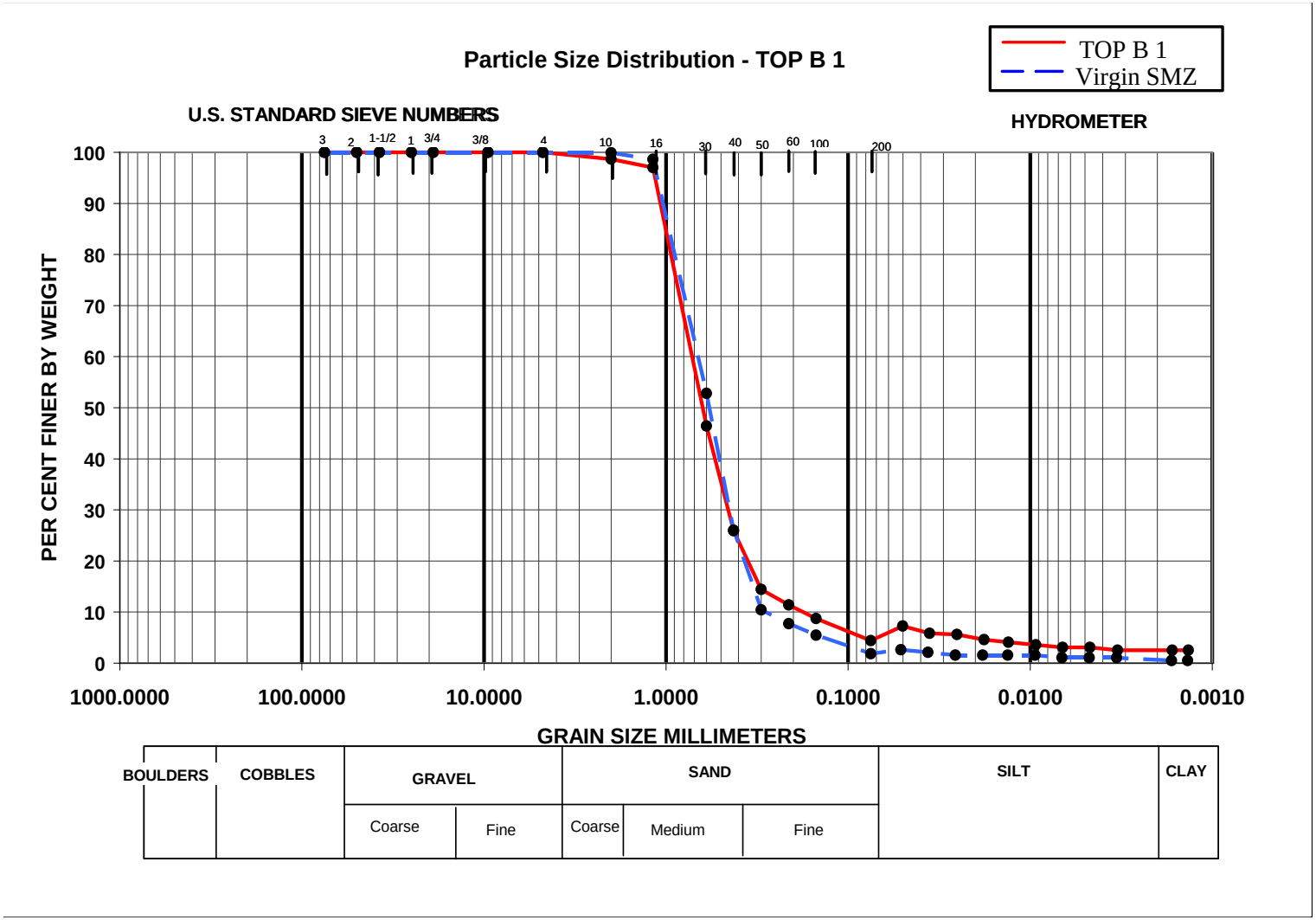

Figure H-13. Particle size distribution results for sample TB-1.

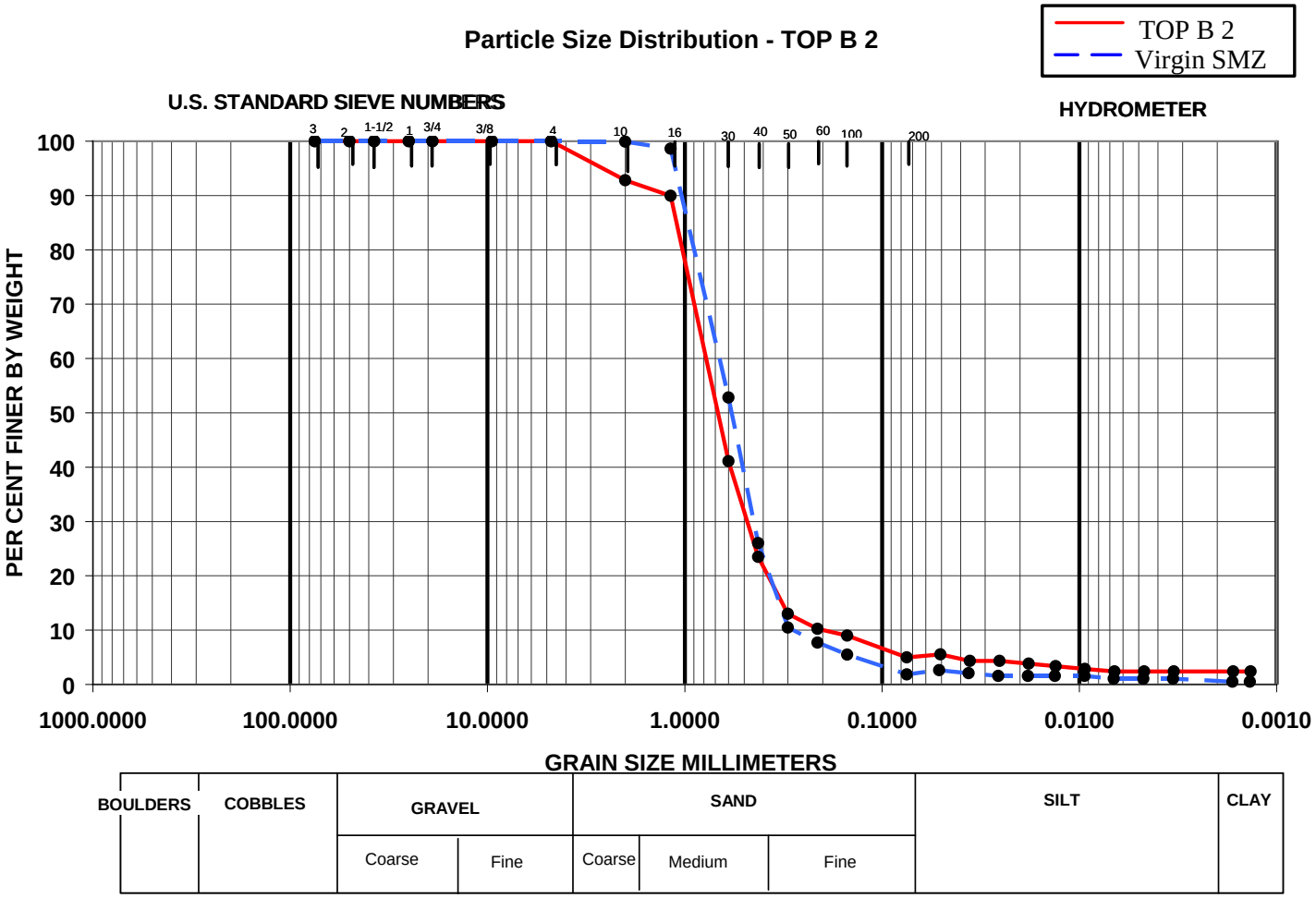

Figure H-14. Particle size distribution results for sample TB-2.

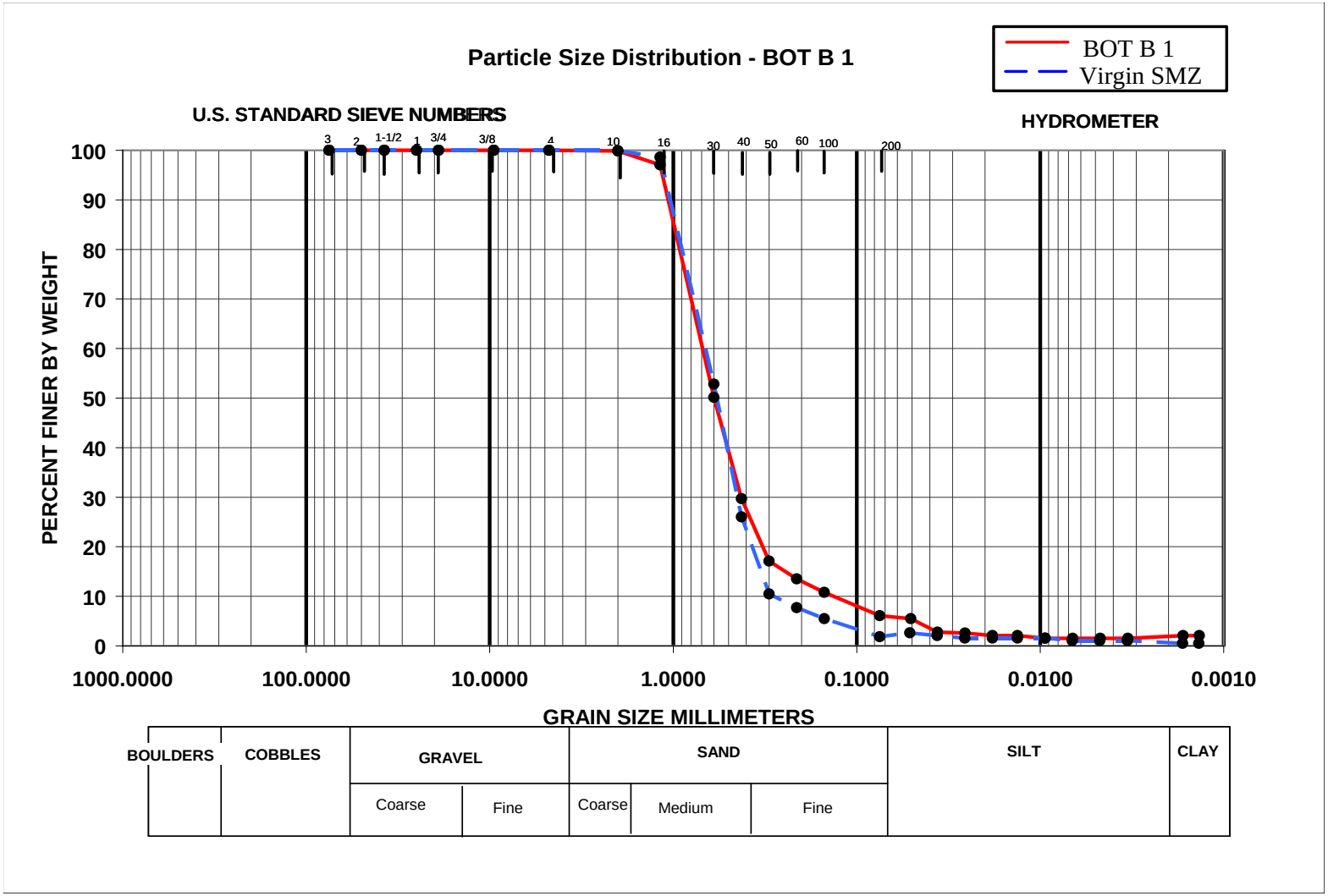

Figure H-15. Particle size distribution results for sample BB-1.

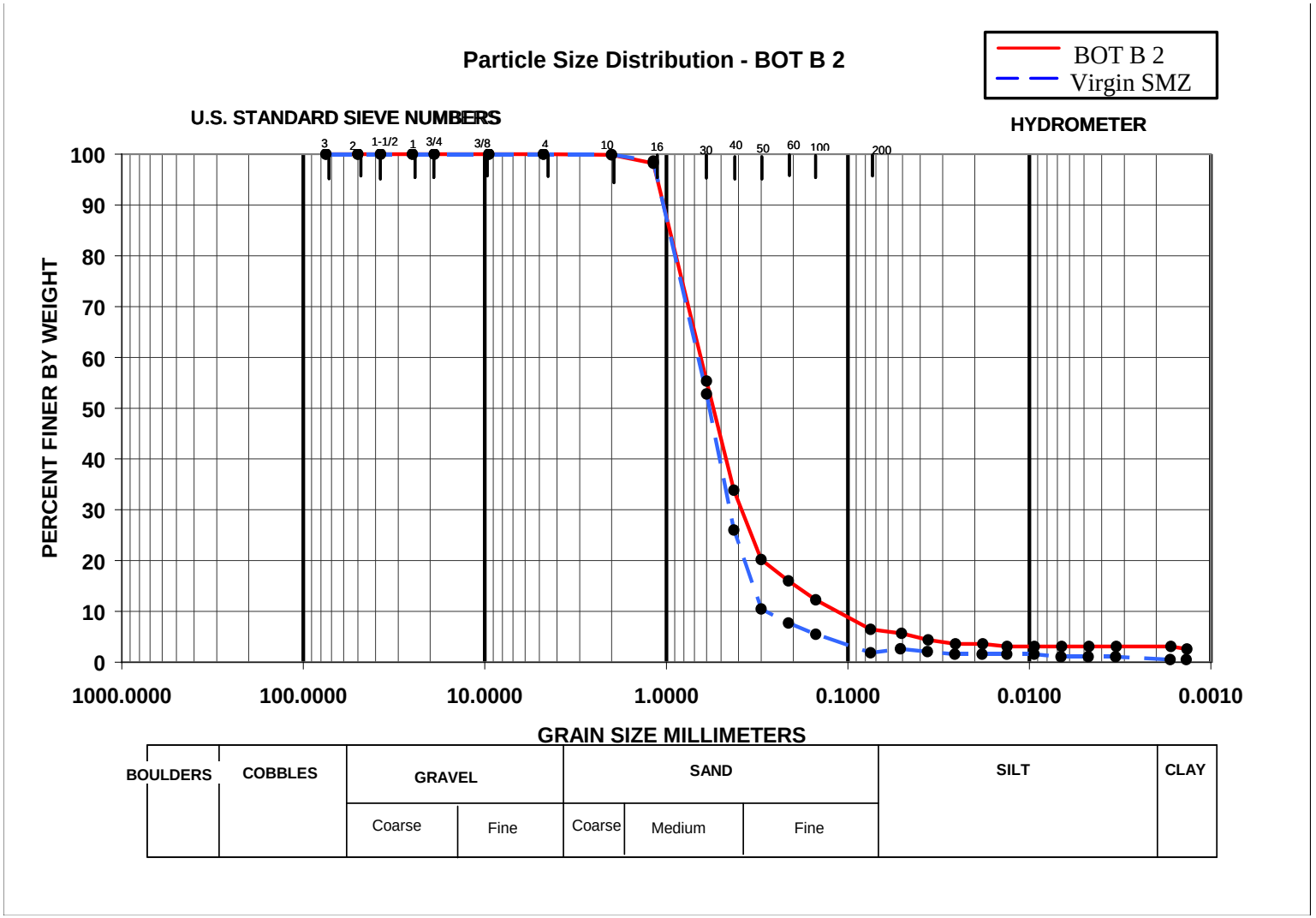

Figure H-16. Particle size distribution results for sample BB-2.

APPENDIX I. APPENDICES REFERENCES.

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