PERCHLOROETHYLENE AND CHROMATE SORPTION/REDUCTION USING A SURFACTANT-MODIFIED ZEOLITE/ZERO VALENT IRON PELLET

by

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Abstract

Due to the limitations of conventional pump and treat systems, *in-situ* methods have been sought for remediating groundwater. One such alternative is the permeable reactive barrier. Permeable reactive barriers are passive, low maintenance systems. A permeable reactive barrier is placed to intercept the contamination plume and remove it by physical, chemical or biological processes.

There are basically two types of reactive permeable barriers: sorption and transformation. A sorption barrier contains the contaminant within the barrier material so it essentially retards the contaminant in it's transport. However, sorption type barriers have a limited sorption capacity or a limited lifetime for remediation. One type of sorption barrier is surfactant-modified zeolite. Transformation type barriers transform the contaminant into another state. When designed properly, the new state of the contaminant is less toxic or less mobile.

To address the limitations of the two types of barriers, we developed and tested a surfactant-modified zeolite/zero valent iron (SMZ/ZVI) pellet to utilize both sorption and transformation processes. The SMZ/ZVI pellets were tested in both laboratory batch kinetic experiments and variable flow rate column studies to evaluate their ability to retard and transform chromate and perchloroethylene (PCE). The column study results were modeled with CXTFIT2 using the 1-D advection dispersion equation assuming linear sorption and first order transformation. The SMZ/ZVI pellets were compared to zeolite/zero valent iron pellets (Z/ZVI) to indicate whether or not surfactant treatment enhanced transformation of chromate or PCE.

The batch kinetic and variable flow rate column studies yielded similar results for chromate. The sorption was evaluated by determining the distribution coefficient (K_d) for both compounds. The average chromate distribution coefficient was determined to be 0.481 ± 0.46 L/kg for the SMZ/ZVI pellets, while no sorption of chromate was seen for the Z/ZVI pellets. The sorption of chromate onto the SMZ/ZVI pellets was low because a surfactant bilayer was not produced during pellet manufacture. Chromate sorbs to the cationic head of the surfactant bilayer by an ion exchange process. The Kd's measured for PCE were 2.28 ± 0.41 L/kg and 0.524 ± 0.07 L/kg for the SMZ/ZVI and Z/ZVI pellets from the batch kinetic and laboratory column studies.

The chromate batch kinetic first order transformation constants were determined to be 0.054 and 0.136 1/hr for the SMZ/ZVI and Z/ZVI pellets, respectively, while the PCE first order transformation constants were 0.136 and 0.054 1/hr for SMZ/ZVI and Z/ZVI, respectively. The results of the column study indicated chromate transformation constants were determined to increase with a decreasing velocity between 0.210 and 0.132 1/hr for the SMZ/ZVI pellets. Complete transformation of chromate was seen with the Z/ZVI pellets. An increase in the PCE transformation constant was also noticed for decreasing velocity in the column studies. The PCE transformation constants varied between 0.077 and 0.199 1/hr for the SMZ/ZVI pellets and between 0.037 and 0.144 1/hr for the Z/ZVI pellets. The transformation constants for chromate and PCE varied with linear velocity indicating that it is a mass transfer limited process. The first-order transformation constants determined from the batch and column studies were normalized to the surface area and the mass of pellet concentration. The normalized chromate transformation constants were determined to be 17.6 and 1160 mL/hr-m^2 for the

SMZ/ZVI and Z/ZVI pellets, respectively, and the normalized PCE transformation constants were 469 and 45.1 mL/hr-m^2 for the SMZ/ZVI and Z/ZVI pellets, respectively. The results of the first order transformation constants and the normalized transformation constants indicate an enhanced transformation of PCE is occurring with the SMZ/ZVI pellets. However, this enhanced transformation of PCE may be due to an larger surface area of the SMZ/ZVI pellets.

Acknowledgments

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I.

Introduction

In many cases, groundwater contamination plumes are managed by pump and treat remedial methods. The pump and treat methods are effective for preventing migration of plumes beyond extraction wells. However, pump and treat methods have many limitations (Mackay and Cherry, 1989). The pump and treat systems tend to capture and process a larger volume of water than is actually contaminated thus causing a low efficiency of the system. The reliability of pump and treat systems is controlled by intrinsic properties of the aquifer and the contaminant. The intrinsic properties include parameters such as contaminant solubility, density, wettability as well as heterogeneity of the porous media and tend to be limiting factors (Wilson, 1997). The limitations of conventional pump and treat systems have led to a search for *in-situ* methods for remediating groundwater contamination plumes.

One alternative to pump and treat systems is a reactive permeable barrier. A reactive permeable barrier is placed to intercept and remove the contamination plume. A reactive permeable barrier is a passive, low maintenance system in which physical, chemical or biological processes remove the contamination from the groundwater. There are basically two types of barrier materials: sorption and degradation. A sorption type barrier contains the contaminant on the surface of the barrier material. A surfactant-modified zeolite is one type of sorption material. Zeolite (clinoptilolite) has a high cation exchange capacity and naturally sorbs cations such as lead or strontium. This high cation exchange capacity can be used to alter the surface of the zeolite with a surfactant molecule. A surfactant molecule is characterized by a hydrophilic cationic head group with a hydrophobic carbon tail. When surfactant molecules are exposed to the zeolite surface, the hydrophilic head sorbs to surface of the zeolite by ion exchange. Due to a

limited sorption capacity, the zeolite surface will become saturated with surfactant molecules at which point a surfactant monolayer has formed. With an excess of surfactant molecules, interactions between the hydrophobic tail groups will also occur. The surfactant molecules in solution will attach to the hydrophobic tail groups of the surfactant monolayer on the zeolite surface. This second layer of surfactant molecules on the zeolite surface is referred to as the surfactant bilayer. A cationic head group is exposed at the surface of a surfactant bilayer formation. Organic contaminants, such as perchloroethylene (PCE), are able to sorb within the hydrophobic tail region of the surfactant layer by organic partitioning, while many oxyanions, such as chromate, sorb onto the head group of the surfactant bilayer by an ion exchange process. The main limitation of sorption barrier is that it is capable of sorbing only a limited amount of contaminant, or essentially the barrier material has a limited lifetime.

The second type of barrier material is a degradation barrier. A degradation barrier transforms the contaminant into another state. When designed correctly, the transformed states is less toxic or less mobile than the contaminant of concern. One type of degradation barrier is zero valent iron. Zero valent iron has shown the ability to degrade contaminants such as chromate and PCE. The removal efficiency of zero valent iron is dependent upon the residence time of the contaminant within the barrier material.

Cercona of America, Inc. has developed a process to manufacture a pellet composed of both surfactant-modified zeolite and zero valent iron materials. This surfactant modified zeolite/zero valent iron pellet (SMZ/ZVI) should be able to combine the advantages of both types of barrier materials while still being permeable enough to allow ease of ground water flow.

The surfactant modified zeolite/zero valent iron pellet was tested under batch kinetic, column and pilot scale conditions for the contaminants of chromate and PCE. This report presents the results of chromate and PCE batch kinetic studies and variable-flow-rate column studies. The experiments performed on the SMZ/ZVI were to determine:

1. First order transformation constants and distribution coefficients for chromate and PCE for both surfactant modified zeolite/zero valent iron pellets and for zeolite/zero valent iron pellets.
2. If an enhanced transformation is occurring with the surfactant modified zeolite/zero valent iron pellet.
3. If sorption of the contaminant onto the zeolite surface is the most likely cause for an enhanced transformation.

II.

Theoretical Background

2.1 Chromium Chemistry

Chromium (Cr) is an industrial metal commonly used in diverse products and processes (Nriagu, 1988). Cr is found in primarily two oxidation states: Cr (VI) and Cr (III). Cr (VI) is relatively mobile in the environment and acutely toxic, mutagenic and carcinogenic (Bianchi et al.; 1984; Beyersmann et al., 1984; Yassi and Nieboer, 1988; Ono, 1988). However, Cr (III) is immobile in alkaline to slightly acidic conditions, and of relatively low toxicity (van Weerelt et al., 1984).

Cr (VI) is a strong oxidant and is reduced to the Cr (III) in the presence of electron donors, such as zero valent iron (Palmer and Puls, 1994; Blowes et al., 1997). For this report transformation will be used when discussing chemical reduction or decay processes. As shown in Figure 1, Cr (III) often forms a precipitate as an insoluble hydroxide in alkaline to slightly acidic conditions. The hatched zone in Figure 1 represents the domain of stability of $Cr(OH)_3$ (s) for 10^{-6} M of total dissolved Cr, which

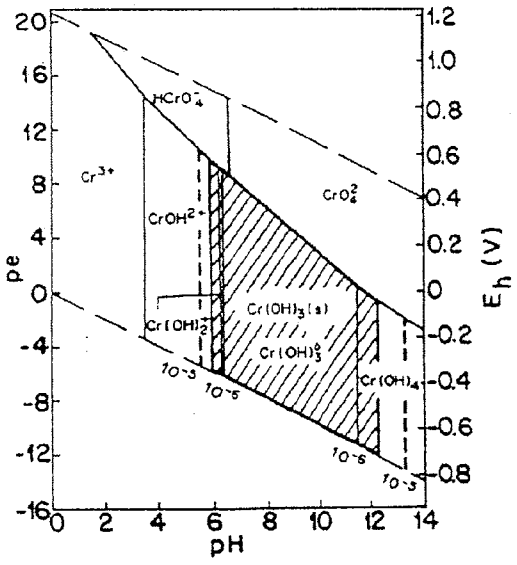

Figure 1. pe-pH Relationship for Aqueous Chromium

can be extended to the dashed lines for 10^{-5} M of total dissolved Cr. Figure 1 shows that under the conditions of the laboratory experiments, pH 9.5 and E_h of –0.4 V, the most stable form of Cr is the chromium hydroxide ($Cr(OH)_3$) precipitate. Equation 1 describes the reaction of chromate with ZVI (Powell et al, 1995). The reaction rate for

$$Fe^0 + CrO_4^{2-} + 4H_2O \Leftrightarrow Fe(OH)_3 + Cr(OH)_3 + 2OH^- \qquad (1)$$

the transformation of Cr (VI) is dependent on both pH and E_h conditions. The reaction rate decreases with increasing pH, while the reaction rate increases with increasing E_h condition (Stollenwerk and Grove, 1985).

The corrosion mechanism to explain the reduction of Cr (VI) by ZVI requires an electrochemical corrosion cell and the onset of aqueous corrosion (Powell et al, 1995). An electrochemical corrosion mechanism occurs when ZVI is exposed to an aqueous salt solution. Electrons are released from the anodic region of the metal and taken up by oxidized species at the cathodic region of the metal surface to avoid the accumulation of charge (Powell et al, 1995). The electrochemical cell can form in two ways: when dissimilar metals are connected (one becoming the cathode and the other the anode), or when anodic and cathodic regions develop on the same metal surface (Snoeyink and Jenkins, 1980). The electrochemical corrosion mechanism provides electron transfer from the anode to the cathode where they can react other oxidized species such as Cr (VI) to form Cr (III).

2.2 Perchloroethylene Chemistry

Tetrachloroethylene, commonly referred to as perchloroethylene or PCE, is a common solvent used in the dry cleaning industry. PCE is a volatile organic compound with a relatively low water solubility (200 mg/L) and is toxic (Maimone, 1997). PCE

belongs to a class of pollutants referred to as dense non-aqueous phase liquids (DNAPLS) because they do not dissolve into water easily and are denser than water (Maimone, 1997). When released to the environment, DNAPLs tend to sink through the unsaturated zone and are trapped by capillary forces in the soil pores (Schwille, 1988).

PCE can be reduced to other organic compound forms by a process referred to as reductive dehalogenation. Reductive dehalogenation is the replacement of a halogen, chloride in the case of PCE, on an organic molecule by a hydrogen atom (Sims et al., 1991). Figure 2 shows the reductive dehalogenation process of PCE. As Figure 2 shows, the reduction of PCE results in the formation of a series of daughter products, such as trichloroethylene (TCE), three isomers of dichloroethylene (DCE), vinyl chloride and eventually ethylene. In the transformation process, 1,2-DCE is the predominant species formed (Jackson, 1985). Some of the PCE daughter products are also of concern as drinking water contaminants, especially vinyl chloride (Pontius, 1995). Ethylene is the least toxic compound in the transformation sequence of PCE.

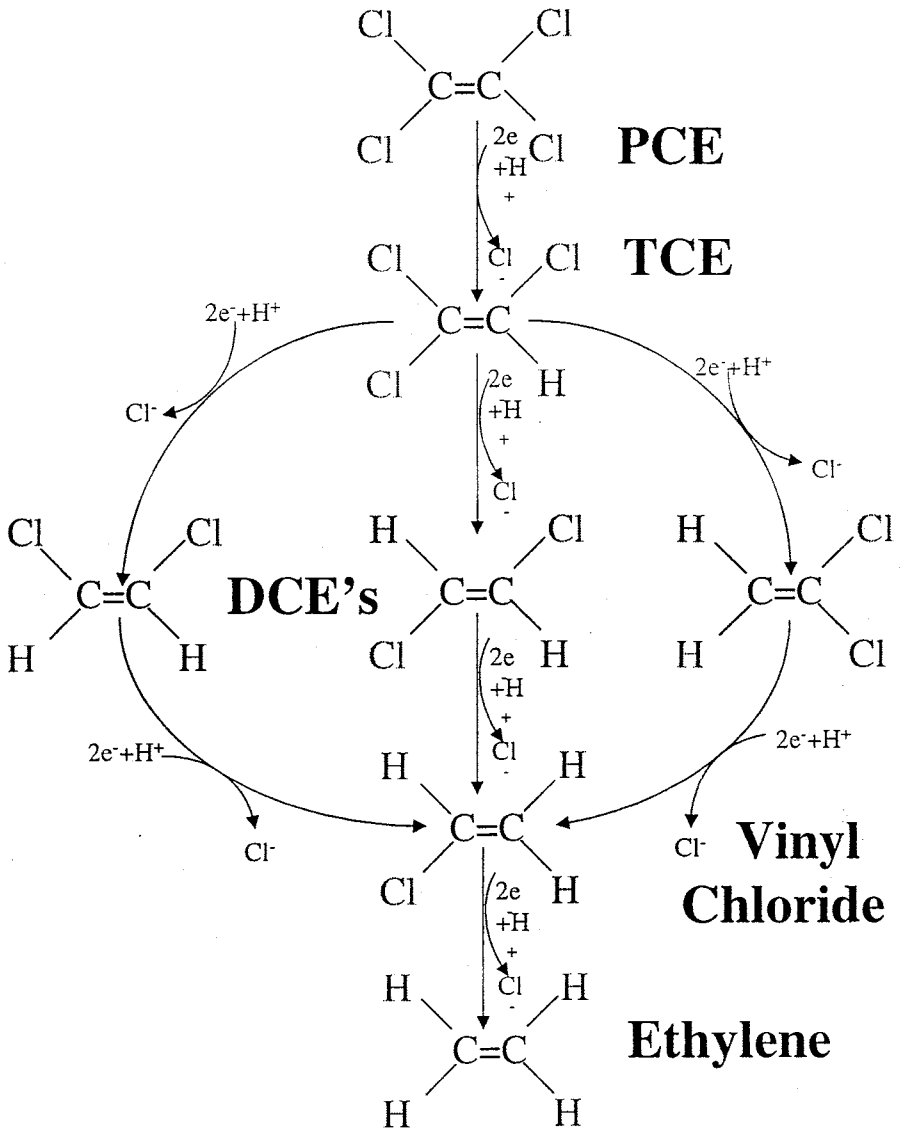

Figure 2. Reductive Dehalogenation of Perchloroethylene

2.3 Reactive Solute Transport

The advection dispersion equation for one-dimensional equilibrium transport for a reactive solute undergoing instantaneous linear reversible sorption and first order transformation in a homogenous soil under steady-state flow conditions is shown in Equation 2.

$$R\frac{\partial C_F}{\partial t} = D\frac{\partial^2 C_F}{\partial x^2} - v\frac{\partial C_F}{\partial x} - \mu C_F \qquad (2)$$

Where:

R = retardation factor = $1 + \frac{\rho_b K_d}{\theta}$ (--)

C_F = flux averaged concentration (mg/L)

D = dispersion coefficient (cm^2/min)

v = average linear velocity (cm/min)

μ = lumped first order transformation coefficient (min^{-1}) and

$\mu = \mu_L + \frac{\rho_b K_d \mu_S}{\theta}$

μ_L = liquid phase first order transformation coefficient (min^{-1})

μ_S = sorbed phase first order transformation coefficient (min^{-1})

ρ_b = bulk density of material (g/cm^3)

K_d = distribution coefficient (L/kg)

θ = porosity (--)

t = time (min)

x = distance (cm)

The mathematical model stated in Equation 2 is appropriate for the conditions of the column study experiments. The dispersion coefficient can be determined from the transport of a non-reactive tracer study. For the reactive chemicals such as PCE and chromate, the parameters of concern are the retardation factor and the first-order transformation rates, in this case chemical transformation rates.

The dispersion coefficient can be approximated by Equation 3. Equation 3 indicates the dispersion coefficient is linearly related to the velocity.

$$D = \alpha v + D_d^* \qquad (3)$$

Where:

α = dispersivity (cm)

D_d^* = effective molecular diffusion coefficient (cm^2/min)

III.

Materials and Methods

3.1 Manufacturing and Composition of the Pellet

The pellet materials tested in the laboratory and in the pilot scale at Oregon Graduate Institute (OGI) were made by Zhaohui Li and Richard Helferich at Cercona of America, Inc., Dayton, OH. Twenty 55-gallon drums were needed for the pilot project at OGI. The materials tested at New Mexico Institute of Mining and Technology were grab samples from randomly selected drums. The zeolite (minus 40 mesh) was obtained from St. Cloud Mine located in Winston, New Mexico. Zeolites have a cage like structure composed of SiO_4 and AlO_4. Zeolites have a high cation exchange capacity, which allows them to naturally sorb many cationic species, such as Sr^{2+}. The zero valent iron, from U.S. Metals (Houston, Texas), was less than 100 mesh. Zeolite pellets without zero valent iron were also manufactured for laboratory testing only. The zeolite pellets were manufactured at an earlier time than the pellets produced for the pilot scale project at OGI. However, the manufacturing process for the zeolite pellets was similar to the pilot scale pellets except zero valent iron or surfactant were not added to these pellets.

During the manufacturing process, the zeolite was manually mixed and blended with zero valent iron at a 1:1 volume ratio to yield a gray mixture for the zeolite/ zero valent iron pellets. The mixture was transferred to a pelletizing machine to mix with the binder. The binder consisted of 1:1 mass ratio of sodium silicate and sodium aluminate in liquid form. The binder quickly solidified the zeolite and the iron together. The solidification process occurs by the chemical reaction shown in Equation 4.

$$Na_2O{:}2SiO_{2(aq)} + Na_2O{:}Al_2O_{3(aq)} + H_2O \Rightarrow Na_2O{:}Al_2O_3{:}2SiO_{2(gel)} + 2NaOH \quad (4)$$

The solidification process occurs in a rotating dish. The spinning of the dish allows the pellets to grow larger. After the pellets were the necessary size, they were sun-dried. Once dry, the pellets were transferred into the 55-gallon drums. Each drum contained a circulation well at the bottom screened by 40-mesh nylon. When 5/6 full of pellets, the drums were leached with tap water. The leaching began at the top of the drum and was siphoned from the bottom through the circulation well for 8-10 cycles until the effluent Na^+ concentration was less than 400 mg/L. The Na^+ concentration was monitored with a Na^+ electrode. After the leaching, the pelletization process was complete. Pellet samples were taken for the laboratory experiments. These pellets are referred to as the zeolite/ iron pellets or Z/ZVI.

The next step was to treat the Z/ZVI pellets with surfactant. The surfactant used for this process is hexadecyltrimethylammonium chloride (HDTMA-Cl). The pellets were treated by adding sufficient 5% HDTMA-Cl in water to each drum to be equivalent to 40 mmol HDTMA/kg pellets if all of the surfactant was sorbed on the surface of pellet. The method for the HDTMA sorption analysis is described in section 3.2.1. Forty-mmol HDTMA/kg pellets refers to a surfactant loading above the sorption maximum of the Z/ZVI pellets. The sorption maximum for the Z/ZVI pellets was determined to be 23.6 mmol HDTMA/kg pellets (see section 4.1.). The surfactant solution was allowed to circulate from the bottom to the top of the drum for a period of 8-hr. At the end of the surfactant circulation period, each drum was flushed with five portions of tap water and allowed to drain. The surfactant modified zeolite/zero valent iron pellets will be referred to as SMZ/ZVI.

3.2 Synthetic Water

To simulate the conditions at OGI, a water sample was analyzed for the major compounds in solution. The results of the OGI water analysis are shown in Table 1. The synthetic water was made by vacuum filtering de-ionized water from a MILLI-Q_{PLUS} system (Millipore Corp., Bedford, Massachusetts) through a 0.45-μm filter to remove any particulates and dissolved gases. The appropriate mass of each compound was added to the degassed water to match the composition of the analysis of Table 1. The synthetic water was stored in a 20-L plastic reservoir and stirred for a 24-hr period prior to use. For the purpose of this report the synthetic water will be referred to as synthetic OGI water.

Table 1. Analysis of Water Sample from Oregon Graduate Institute

Compound	meq	Molecular Weight	mg/L
$NaHCO_3$	0.52	84.00	43.68
$MgSO_4$	0.08	120.36	9.03
$CaCl_2$	0.09	110.99	9.43
KNO_3	0.01	101.09	1.01
$CaCO_3$	0.12	100.09	12.01
$Mg(NO_3)_2$	0.02	148.32	2.97

3.2 Initial Characterization for Manufacturing and Evaluation

3.2.1 Batch HDTMA Sorption Isotherm

A batch sorption isotherm was performed to evaluate the HDTMA surfactant loading capacity on the Z/ZVI and retreated SMZ/ZVI (section 3.2.3). This batch HDTMA sorption isotherm was necessary for the manufacturing of the pellets. Duplicate samples were prepared by placing 2-g of Z/ ZVI pellets in a 40-mL HPDE Nalgene® HDPE centrifuge tubes and 1-mL of HDTMA-Cl solution was added. For this batch sorption isotherm, the mass of pellets to volume of solution ratio was kept high to simulate the conditions of the manufacturing process. The HDTMA-Cl solution concentration was prepared by diluting a 200-mM stock solution of HDTMA-Cl with de-ionized water from the Milli-Q_{PLUS} system. The initial HDTMA-Cl concentrations were 10, 20, 30, 40, 50, 60, 70, 80 and 90 mM. The samples were shaken for a 24-hr period at 25°C and 25 rpm in an Innova 4335 Refrigerated Incubator Shaker (New Brunswick Scientific, Edison, New Jersey). At the end of the 24-hr period, the samples were centrifuged at 1500 rpm for 10 min in a Beckman J2-MI(Fullerton, California) and then analyzed for the HDTMA concentration as described in section 3.5.1.

3.2.2 Chromate and Perchloroethylene Batch Sorption/Reduction Studies

Initial characterization of the SMZ/ZVI pellets was performed by 24-hr batch sorption/reduction studies. The initial characterization of the pellets indicated to what extent the surfactant layer had formed on the surface of the pellet. The sorption/reduction studies are similar to the HDTMA batch study except the mass of pellets to solution ratio was 1:4.

For the chromate batch study, duplicate samples were prepared with 2.5-g of SMZ/ZVI pellets in 40-mL Nalgene® HDPE centrifuge tubes. The duplicate samples

were spiked with 10 mL of chromate solution. The chromate solution was diluted from a 400-mg/L stock solution prepared by dissolving K_2CrO_4 in de-ionized water from the Milli-Q_{PLUS} system. The initial chromate concentrations of the duplicate samples were 40, 80, 120, 160, 240, 320 and 400 mg/L. The samples were then shaken at 25 rpm and 25°C in an Innova 4335 Refrigerated Incubator Shaker. Once shaken for 24-hr, the samples were centrifuged at 1500 rpm for 10 min to yield a clear supernatant. The chromate concentrations were then analyzed as described in section 3.5.2.

The PCE sorption/reduction batch study was performed in the same manner as chromate. However, triplicate samples were prepared for each concentration and the samples were placed in 10-mL Wheaton® glass headspace vials. The aqueous PCE solution was made by diluting a saturated PCE solution with de-ionized water from the Milli-Q_{PLUS} system. To limit volatiliztion of PCE, the samples were immediately capped with Supelco® Teflon Faced Butyl Septum and aluminum seal. The saturated PCE solution was prepared by placing free phase PCE into a 250-mL amber glass vial filled with de-ionized water. The saturated solution was stirred for a 24-hr period and allowed to settle for 1hr prior to use. It was assumed that the saturated PCE solution concentration was at the maximum water solubility for PCE of 200 mg/L. The initial PCE concentrations were 10, 20, 30, 40 and 50 mg/L. The samples were shaken and centrifuged just like the chromate samples. The samples were analyzed by the method described in section 3.5.3.

3.2.2 Re-treatment of SMZ/ZVI

Due to an insufficient surfactant bilayer formation during the manufacturing process, it was necessary to retreat 200 g of SMZ/ZVI pellets to evaluate the extent of the

surfactant loading on the SMZ/ZVI pellets. The retreatment of pellets was performed by placing 50 g of SMZ/ZVI pellets into a 250-mL HDPE® Nalgene Centrifuge bottle with 150-mL of 200-mM HDTMA-Cl solution. The samples were allowed to shake in an Innova 4335 Refrigerated Incubator Shaker at 25 rpm and 25° C for 24 hr. The samples were then centrifuged in a Beckan J2-MI at 1500 rpm for 20-min. The supernatant was removed from each bottle and the retreated SMZ/ZVI pellets were removed and rinsed with 100-mL of de-ionized water. The retreated pellets were then placed into a dish and allowed to air dry prior to use. Chromate and PCE batch sorption/reduction studies were performed on the retreated pellets to characterize the surfactant loading of the manufactured pellets. The retreated pellets were not used for any other experiments other than to characterize the surfactant loading of the manufactured SMZ/ZVI pellets.

3.3 Batch Kinetic Studies

Chromate and PCE batch kinetic studies were performed for comparison to the column studies. The batch studies consisted of 5-g of either the SMZ/ZVI or Z/ZVI pellets with 10 mL of solution.

For the chromate batch study, an initial concentration of 25-mg/L CrO_4^{2-} was used. The chromate solution was made by diluting a 400-mg/L CrO_4^{2-} solution prepared from K_2CrO_4 salt with synthetic OGI water. Samples were placed in 40-mL Nalgene® HDPE centrifuge tubes and shaken at 25°C and 50 rpm. Duplicate samples were sacrificed at certain time intervals. The samples were centrifuged for 15 minutes at 2000 rpm to yield a clear supernatant. One milliliter of supernatant was then placed into an amber glass vial for the Waters 717 autosampler. Samples were analyzed for the

chromate concentration as described in section 3.5.1. Samples were sacrificed at time intervals of 1.5, 2.5, 4, 6, 8, 13, 20, 26, 27 and 45 hr.

For the PCE batch study, an initial concentration of 20 mg/L was used. The solution was made by diluting a saturated aqueous solution of PCE with the synthetic OGI water. Samples were prepared in 10-mL Wheaton® headspace vials with 5-g of pellets and sacrificed at a certain time interval. Nine milliliters of the synthetic OGI water was then added to each vial and the sample was spiked with 1-mL of the saturated solution of PCE using a 1-mL glass syringe to yield an initial PCE concentration of 20 mg/L. The sample was immediately capped with a Supleco® Teflon Faced Butyl Septum and aluminum seal to limit mass loss due to volatilization. Blank samples were prepared with no pellets and analyzed at various time intervals to observe any mass losses due to volatilization of PCE. The samples were then shaken and triplicate samples were periodically sacrificed for PCE analysis. Once the centrifugation process was complete, the supernatants were analyzed for PCE and daughter products as described in section 3.5.2. The sample time intervals were 0.25, 0.5, 0.75, 1.0, 1.75, 2, 3, 6, 8 and 11 hr.

3.4 Column Study

The column studies were designed to limit the losses of PCE due to volatilization and accurately quantify the mass of chromate or PCE in the column influent and effluent. The following sections describe the setup of the column study and the steps taken prior to the tracer studies.

3.4.1 Column Apparatus

The column study consisted of six 32-cm long by 5.0-cm ID glass columns, manufactured by Adjust-a-chrom (Vineland, New Jersey) (Figure 3), which had end caps

constructed of Teflon. Glass and Teflon were chosen because of their limited sorption capacity for PCE as compared to plexiglass. The input solution was contained in a 35-L, 0.01-cm Tedlar bag with a on/off valve (Lab Safety Supply, Janesville, Wisconsin). The Tedlar Bag was contained in a 75-cm wide by 75-cm long by 26.41-cm high box constructed of 1.91-cm (3/4-inch) plywood. The Tedlar bag was placed on a piece of plywood 10.5-cm in height from the bottom of the box. A 2.54-cm (1-inch) hole was drilled in the center of this plywood board so that the on/off valve would be accessible from the bottom of the box. Nineteen centimeter in length legs, constructed of 5.08-cm by 5.08-cm (2 inch by 2 inch) pine, were attached to the four inner corners of the plywood box below the piece holding the Tedlar bag. A schematic of the plywood box is shown in Figure 4. The pine legs allowed the box to be elevated from the table surface to allow for Teflon tubing connections to the Tedlar bag. A 15.24-cm piece of 0.3175-cm ID Teflon tubing was attached to the on/off valve. A three-way stainless steel valve was attached to the end of this 15.24-cm Teflon tubing to allow for ease of connections either to the Harvard pump for the column studies or the Chemfeed pump when pumping in the solution for the column studies.

The solution was pumped with a Harvard Apparatus, PHD 2000 Programmable multi-channel syringe pump. Ten milliliter Hamilton gastight syringes were used with the Harvard pump. Teflon tubing was used to connect the Tedlar bag to the Harvard Pump and the Harvard pump to the columns. An inlet and outlet sampling point was located on each of the six columns. The PCE sample point was made from a Swagelok® stainless steel union tee where a 1-cm diameter, 0.0127-cm thick PTFE lined 0.0889-cm thick silicone septum (Van Waters and Rogers, Albuquerque, New Mexico) was placed

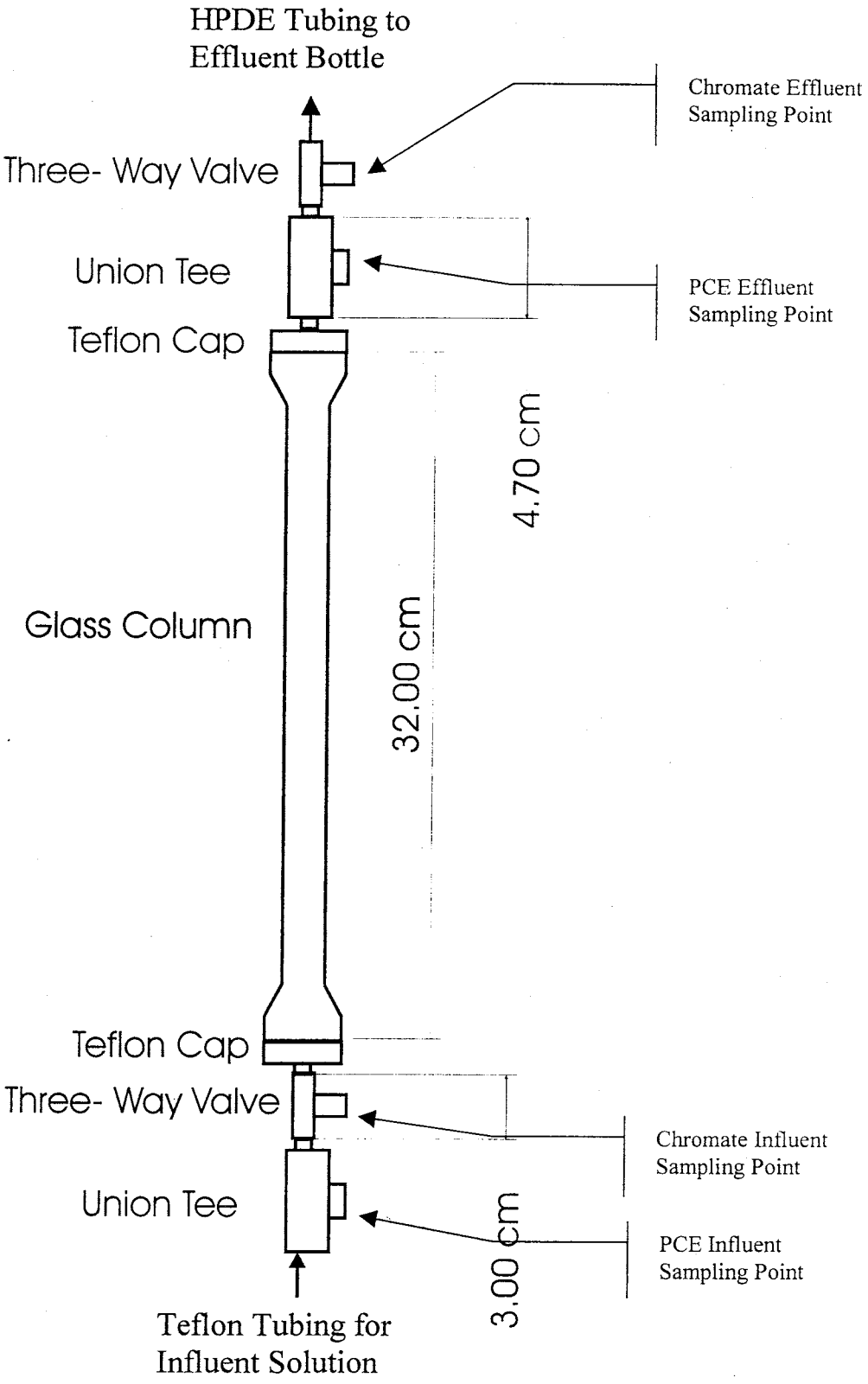

Figure 3. Column Design

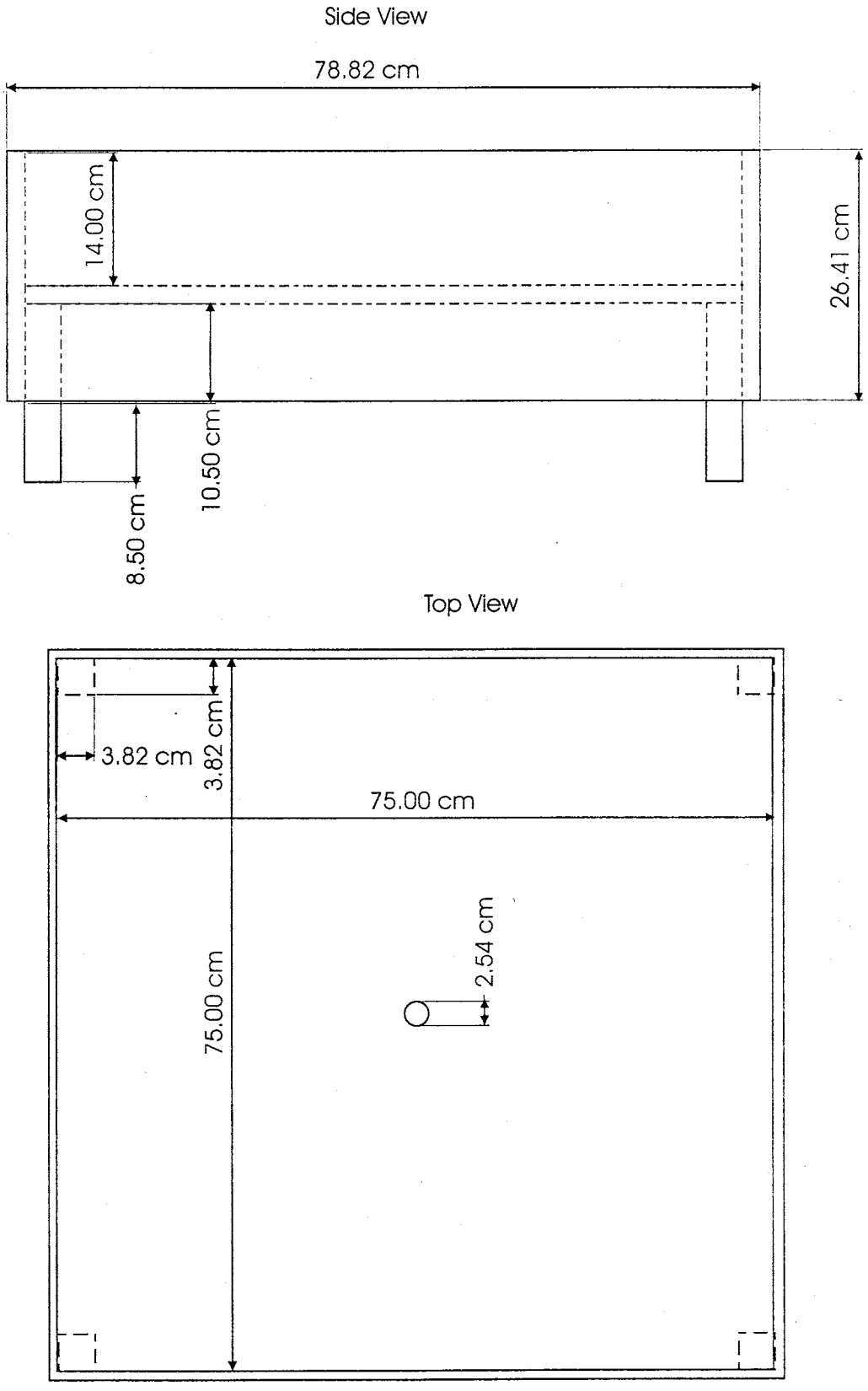

Figure 4. Schematic of Plywood Box

in the center port and used for sampling. The sample was taken with a 100-μL Hamilton Gastight syringe. A schematic of the sampling point is shown in

Figure 5. This sampling method allowed removing solution from the system accurately with limited losses due to volatilization of PCE.

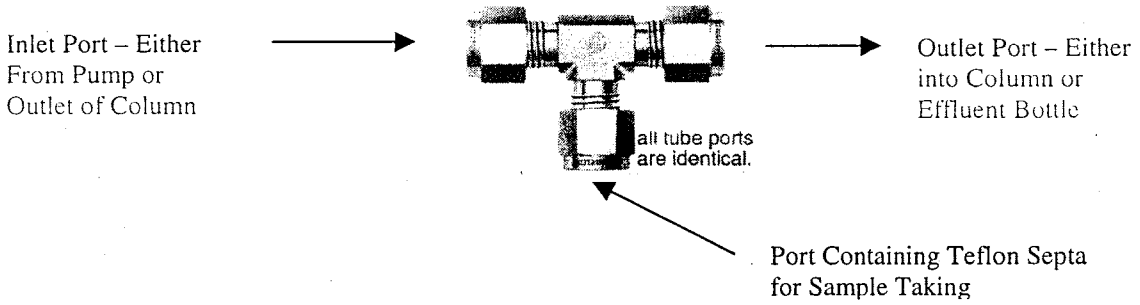

Figure 5. Union Tee used as PCE Sample Measuring Point for Column Studies

Just above the union tee, a three-way stainless steel valve was used to collect the chromate samples. The three-way valve allowed for the diversion of the flow into a 1-mL plastic syringe to collect the sample. Short pieces of the 0.375-cm ID Teflon tubing were used to connect the union tee and the three way valve together at the influent and effluent ends of the column. The effluent HDPE tube led to a plastic bottle to determine the effluent mass that had gone through the column. A schematic of the column study set up is shown in Figure 6. Figure 6 only shows the setup for one column and not all six.

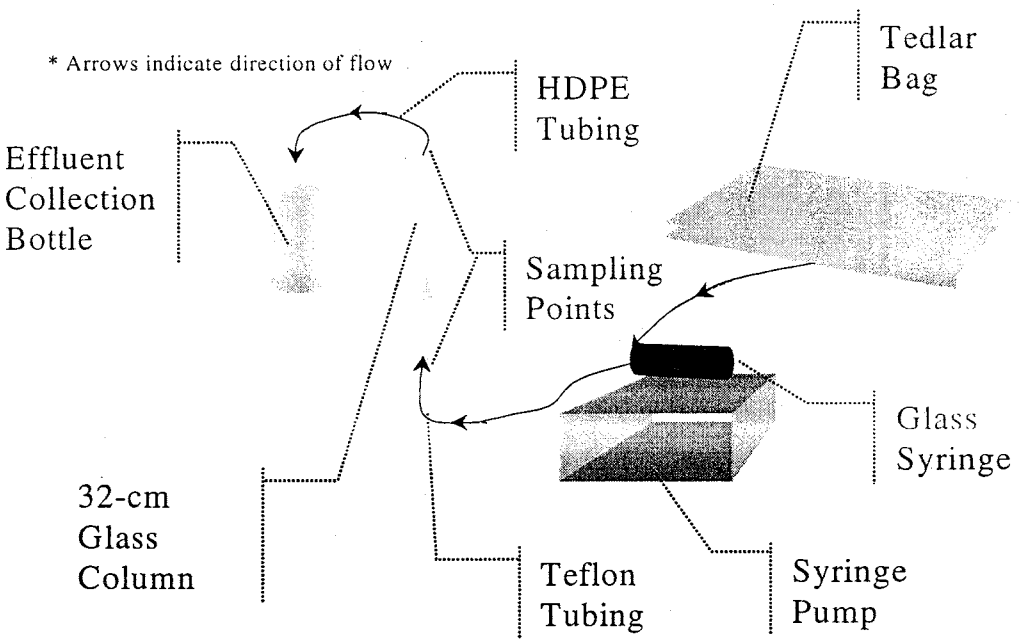

Figure 6. Schematic of Column Setup

3.4.2 Column Preparation

The three materials tested in the column studies were the SMZ/ZVI pellets, Z/ZVI pellets and zeolite pellets. Each material was tested in two separate columns (duplicates). It was expected that of the three materials, sorption and reduction should occur in the SMZ/ZVI pellets while the main process in the Z/ZVI pellets would be reduction of chromate or PCE. No sorption or reduction of chromate or PCE was expected for the zeolite pellets. The 32-cm by 2.5-cm glass columns were packed with approximately 130 to 275 g of the appropriate pellet and capped. All columns were then flooded with CO_2 gas for 2 hr. The columns were then saturated from the bottom with synthetic OGI water until their weights changed by no more than 1% of the preceding weight for three consecutive trials. The porosity of the columns was determined by the difference between the saturated column weight and the packed dry column weight. The packed dry

column weight adjusted the mass of the pellets to the dry mass using the gravimetric water content as described in section 3.5.5. A column pore volume was determined by the difference in the saturated mass of each column from the packed mass of each column and then adjusted for the mass of water retained within the pellets using the gravimetric water content. Details on the gravimetric water content and mass of pellets can be found in Appendix A. Table 2 indicates the porosity and column pore volume values obtained. The columns were then flushed with approximately 40 pore volumes of

Table 2. Column Porosity and Pore Volume Values

Material	Column	Porosity (g H_2O/ g dry pellet)	Column Pore Volume (mL)
SMZ/ ZVI	A	0.156	96.38
	B	0.167	103.19
Z/ZVI	C	0.173	106.65
	D	0.164	101.09
Zeolite	E	0.220	145.90
	F	0.220	143.06

synthetic OGI water at a flowrate of 10-mL/m min to reduce the high Na^+ concentration associated with the pellets.

3.4.3 Input Solution Preparation

The input solution for the column studies was prepared by using synthetic OGI water to dilute saturated PCE solution (200 mg/L) and a 875 mg/L chromate solution to the desired concentration of 25 mg/L chromate and 20 mg/L PCE. A Chemfeed

diaphragm pump rated at 4.5 GPH was used to fill the Tedlar bag. The saturated PCE solution was prepared as described in section 3.4 for the batch PCE kinetic study but instead a 4-L amber glass bottle was used. First, 4-L of the saturated PCE solution was pumped into the Tedlar Bag. The next step was to pump in 1-L of the 875-mg/L chromate solution and approximately 10-L of the synthetic OGI water. The pump allowed enough circulation of the mixtures for the solution to become well mixed. It was necessary to periodically remove a solution sample from the Tedlar bag and analyze the PCE concentration because the saturation point of PCE in 4-L of solution was hard to maintain. The analysis of the aqueous solution in the Tedlar bag allowed for additional saturated PCE solution to be added to the Tedlar Bag, if necessary, prior to the Tedlar bag being full at which point solution would have to be removed from the Tedlar bag to raise the PCE concentration. The desired chromate concentration was easier to maintain since there are no concerns regarding the solubility or volatilization of chromate. So, after the initial 10-L of synthetic OGI water was added, PCE and synthetic OGI water were added to gain an initial concentration of 20-mg/L and approximately 30 L of solution.

3.4.4 Column Operation

For the column studies, one non-reactive tracer study of tritium and three chromate/PCE studies were performed. The non-reactive tracer study was performed to evaluate the hydrodynamic characteristics of each column. This column study was performed at a flow rate of 1-mL/min and the average linear velocity was determined by calculating the actual flow rate of each column from the effluent mass and dividing by the cross sectional area and the porosity of each column. The cumulative pore volume was determined from the cumulative effluent mass and the mass removed for sampling

(1-mL for each sampling period) divided by the column pore volume. The non-reactive tracer study was performed as a tritium slug input with an activity of approximately 100,000 counts/min-mL.

Table 3 indicates the tritium slug volume for each column. Prior to starting the column study, all of the solution was removed from the Teflon tubes at the influent end of each column. The influent Teflon tubes were completely filled with tritium solution to ensure that tracer was at the closest influent point of the column. At the end of the slug period, all of the tritium solution was removed from the influent lines. The influent Teflon lines were then completely filled with synthetic OGI water. Samples for tritium analysis were collected from the three-way valve used for the chromate sampling point approximately every 0.2 pore volumes until the effluent tritium counts were near the background level of synthetic OGI water.

Table 3. Tritium Slug Intervals

Material	Column	Slug (Pore Volumes)
SMZ/ ZVI	A	2.33
	B	2.26
Z/ZVI	C	2.17
	D	2.28
Zeolite	E	1.61
	F	1.56

The chromate and PCE reactive tracer studies were step input column studies. As in the non-reactive tritium study, the influent lines were filled with air and refilled with

the input solution to ensure that the solution was at the closest influent point of the columns. The chromate and PCE studies were performed at three different flow rates of 1, 0.5 and 0.25-mL/min. The column study flow rates were chosen to be near the flow conditions at OGI and also would give an indication of the mass transfer limitations of the sorption or reduction processes. However, due to inconsistencies with the pump, the average linear velocity is not a 1:2:4 ratio. The average linear velocity was calculated in the same manner as the non-reactive study while corrections to the cumulative pore volume were made from the 1-mL chromate sample removed from the three-way tee. No corrections were made for the 50-μL sample removed for PCE. The columns were sampled for PCE and chromate approximately every pore volume and the column studies were continued until steady-state conditions were achieved. In between the chromate and PCE reactive tracer studies, the columns were flushed with 20 pore volumes of synthetic OGI water at 10-mL/min.

3.4.5 Post- Column Analyses

3.4.5.1 Particle Size Distribution

After all column experiments had been performed and the columns had been flushed with synthetic OGI water, the column material was unpacked and placed into 500-mL glass beakers to dry in an oven at 105° C for 72 hr. The particle size distribution of each column was then determined.

The particle size distribution for each column was performed according to ASTM methods. The SMZ/ZVI materials were shaken through ASTM sieve nos. 30-mm, 4, 6, 8, 10, 14, 16, 20, 30, 40, 50, 70, 100, 120, 140, 170 and 200 for 2-min. The Z/ZVI materials were shaken through ASTM sieve nos. 30-mm, 4, 6, 8 and 10 for 2-min. Prior

to sieving, each sample was weighed to determine the total mass. The mass of each sieve interval was determined by weight of the sample in the particular sieve. The individual weights were then normalized to the total mass of the sample to show the particle size distribution of each column. The particle size distribution was also used to estimate the surface area of the pellet material in analyzing the results.

3.4.5.2 Dry Bulk Density

The dry bulk density was determined for the SMZ/ZVI and Z/ZVI pellets. The materials from each column were placed into 250-mL glass beakers and allowed to dry in an oven at 105° C for 72 hr. The initial weight of a 125-mL Erlenmeyer flask was determined. For each column, 125 mL of the dried pellets was placed into the Erlenmeyer flask and the flask was weighed to determine the mass of pellets. The dry bulk density was calculated from the mass of pellets in the Erlenmeyer flask and the volume of pellets.

3.5 Analytical Methods

3.5.1 HDTMA Analysis

HDTMA analysis was performed with a high performance liquid chromatography system. The mobile phase was 5 mM p-toluenesulphonic acid in water mixed with methanol in a 55:45 by volume ratio. The flow rate of the mobile phase was 0.7-mL/min and was maintained by a Waters 510 pump (Milford, MA). HDTMA detection was with a Waters 486 UV-VIS detector at a wavelength of 254-nanometers. A Nucleosil-CN column with dimensions of 150-mm by 4.6-mm and packed with 5 μm particles was used. The injection volume of 25 μL was provided by a Waters 717 autosampler. A

four-point calibration curve was established using concentrations of 10, 20, 40 and 60 mM. The retention time of HDTMA was approximately 7.4 min.

3.5.2 Chromate Analysis

The chromate concentration analysis was performed using high performance liquid chromatography. Each sample was placed into a 1-mL amber glass vial for the Waters 717 Plus autosampler and analyzed by either a Waters 486 or 481 UV-VIS detector at a wavelength of 365 nanometers. The mobile phase was 5-mM tetrabutyl ammonim hydrogen sulfate mobile phase pumped at 1.5-mL/min using a Waters 510 HPLC pump. Prior to use, the mobile phase was vacuum filtered through a 0.22-micron filter to remove any particles and dissolved gases present in the mobile phase. The column used was a 2-mm by 150-mm Waters – NOVA – Pak C_{18} with 5-μm particles. The injection volume was 25 μL. A four-point calibration curve was established using concentrations of 1, 5, 10 and 20 mg/L CrO_4^{2-}. Chromate had a retention time of 2.4 min and a detection limit of 0.5-mg/L.

3.5.3 Perchloroethylene and Daughter Products Analysis

PCE and the daughter products of PCE were also analyzed by high performance liquid chromatography. For the PCE analysis, a 50-μL manual injection was performed with a 100-μL Hamilton gastight syringe into a Waters U6K injector. The PCE was analyzed with a Waters 486 UV detector at wavelength of 195 nanometers. The mobile phase consisted of a solution of 70% acetonitrile and 30% de-ionized water, from the MILLI-Q_{PLUS} system, by volume. The mobile phase solution was filtered and degassed through a 0.22-μm filter prior to use. The solution was pumped with a Waters 510 pump at a flow rate of 2.0-mL/min. The column used was a 4.6-mm by 150-mm Regis –

Rexchrom –ODS, with 5-μm particles. A four-point calibration curve was prepared using PCE concentrations of 1, 5, 10 and 20 mg/L. The daughter products of PCE, such as trichloroethylene (TCE), were not calibrated for unless other peaks besides the PCE peak were present on the chromatogram. If it was necessary to calibrate for TCE, a four-point calibration curve was also established from concentration levels of 0.5, 1, 2 and 5 mg/L. The retention times for PCE and TCE were 5.1 and 3.3 min, respectively, while the detection limits were 0.2 and 0.2 mg/L, respectively.

3.5.4 Tritium Analysis

Tritium was used for the non-reactive tracer column studies. During the tracer study, a 1-mL sample was taken from the effluent bottle and put into a 20-mL glass vial with 9-mL of ICN Biomedical, Ecolite (ICN, Costa Mesa California) liquid scintillation cocktail. The scintillation counting was then done on a Packard TRI-CARB 460C liquid scintillation system.

3.5.5 Gravimetric Water Content

The gravimetric water content was determined by placing 5 g of material in an oven dish. The 5-g sample was then placed in an oven at 105°C for 24-hr. At the end of this time, the samples were placed in a dessicator to cool for 15-min and then the final mass was determined. The mass of water was considered to be the difference between the initial mass and the final dry mass. The gravimetric water content was calculated as the mass of water divided by the dry mass of material present. An average gravimetric water content was determined from 5 samples for each pellet material.

IV.

Results and Discussion

4.1 Characterization of SMZ/ZVI Pellets

During the manufacturing process, it was necessary to perform a HDTMA batch sorption isotherm on the zeolite/zero valent iron (Z/ZVI) pellets to determine the HDTMA loading capacity of the manufactured pellets. Figure 7 shows the linear and Langmuir curves for the HDTMA sorption isotherm. Figure 7 indicates that the Z/ZVI pellets were able to sorb 23.6 mmol HDTMA/kg pellets.

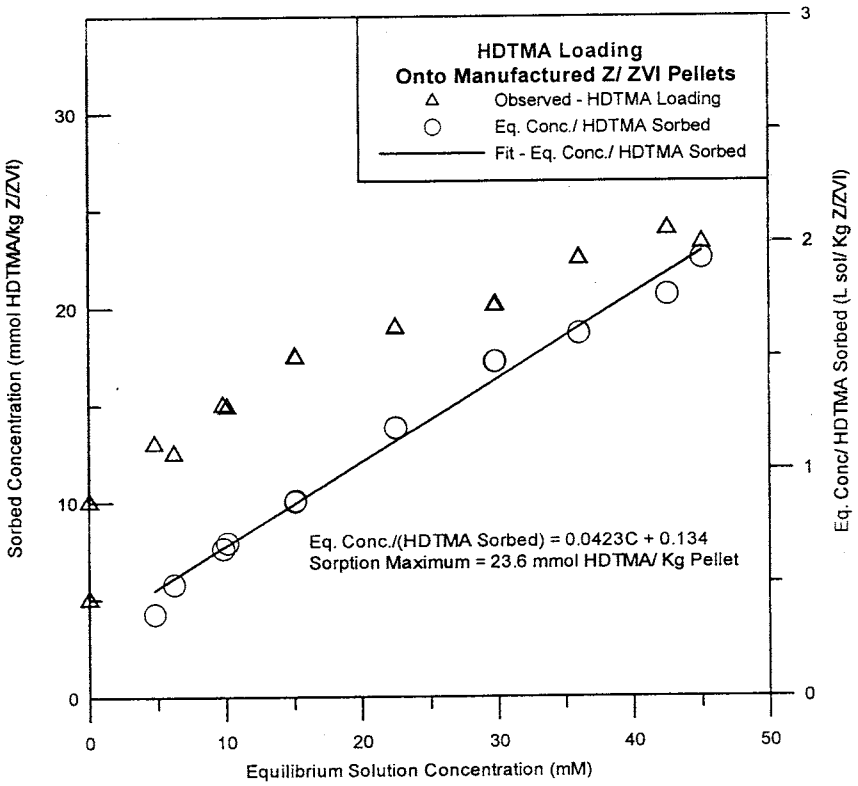

Figure 7. HDTMA Sorption onto Z/ZVI Pellets

Chromate sorption occurs by an ion exchange process with the cation on the bilayer of the surfactant head group (Li and Bowman, 1997). In the case of the SMZ/ZVI pellets, chromate would exchange with the chloride ion on the surfactant. However, this process will not occur unless a surfactant bilayer is formed, while sorption of perchloroethylene (PCE) occurs within the hydrophobic tail of the surfactant molecule by

organic partitioning (Li and Bowman, 1998). Initial chromate batch studies indicated that chromate was not being sorbed by the manufactured SMZ/ZVI pellets so an HDTMA batch study was performed on the manufactured SMZ/ZVI pellets. The results of the HDTMA batch isotherm are shown in Figure 8.

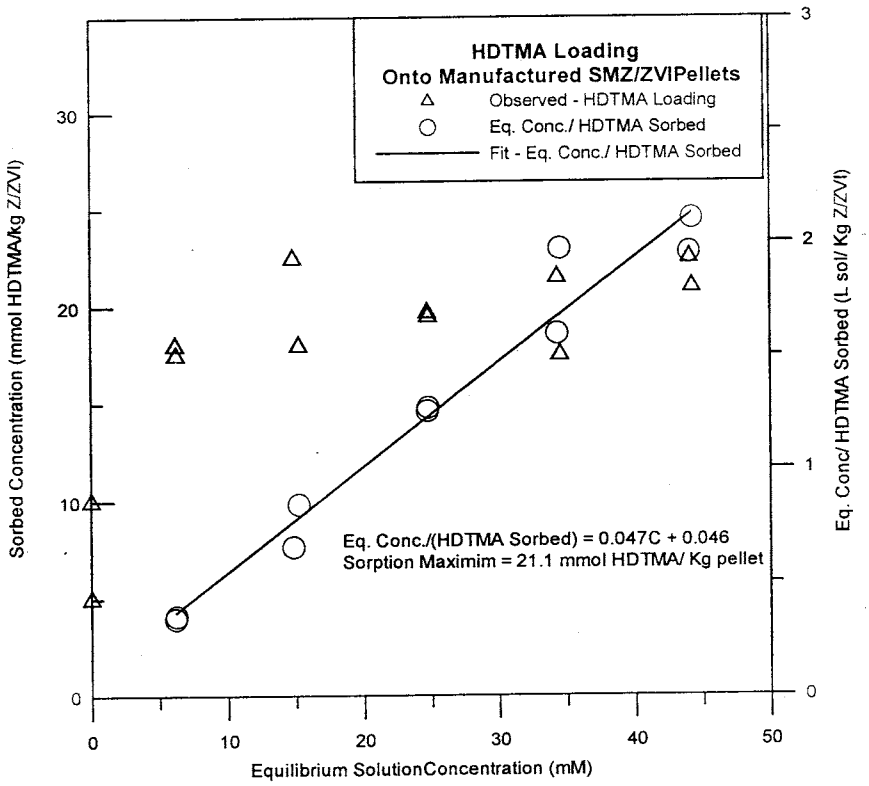

Figure 8. HDTMA Loading onto SMZ/ZVI Pellets

Figure 8 indicates that the SMZ/ZVI pellets were able to sorb 21.1 mmol HDTMA per kg pellet. In comparing Figure 7 to Figure 8, it appears that the manufactured SMZ/ZVI pellets only sorbed 3 mmol HDTMA/kg pellet. (This HDTMA sorption was considerably low for the manufacturing process. The sorption of HDTMA onto the manufactured SMZ/ZVI pellets due to either the high pH conditions or Na^+ concentration.) The initial HDTMA batch sorption onto the Z/ZVI pellets was under neutral pH conditions and no Na^+ in solution. The high ionic strength and pH of the

solution during the manufacturing process may have inhibited the sorption of HDTMA onto the surface of the Z/ZVI pellets. The conditions may have been more favorable for HDTMA sorption with the de-ionized water used in the laboratory studies.

The SMZ/ZVI material were further evaluated by retreating the manufactured material as described in section 3.2.3 and performing 24-hr PCE and chromate batch studies (section 3.2.2). The results for the chromate batch study are shown in Figure 9. Figure 9 indicates, chromate sorption occurred with the retreated SMZ/ZVI material.

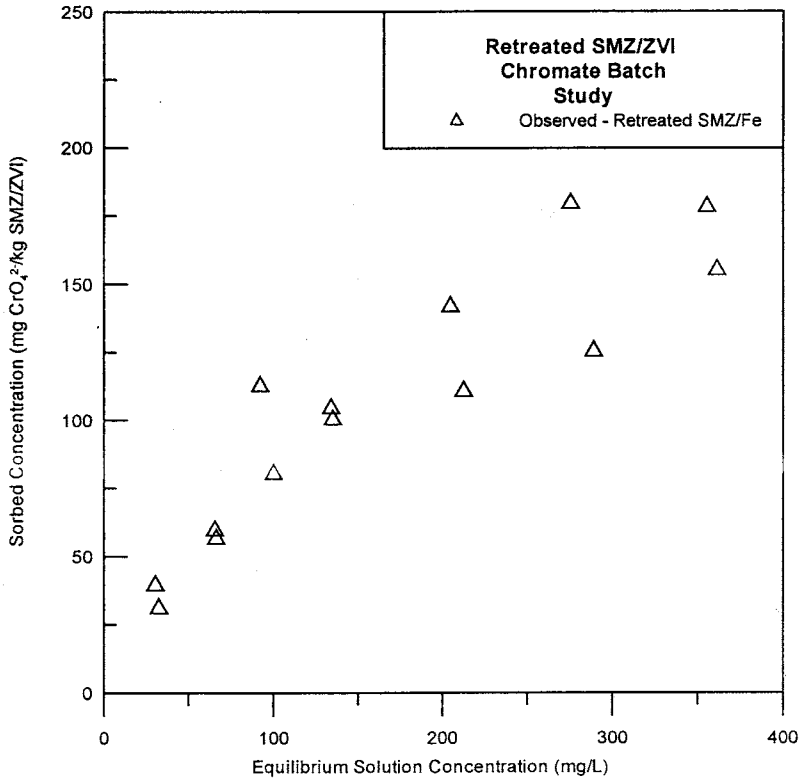

Figure 9. Chromate Sorption/Reduction Isotherm after Further HDTMA Loading

The results for the 24-hr PCE batch study are shown in Figure 10. Figure 10 indicates linear isotherm relationships for PCE sorption onto the SMZ/ZVI material. The distribution coefficients, K_d, for the manufactured SMZ/ZVI pellets and the retreated

pellets were similar, 5.46 and 5.71 L/kg, respectively. Due to the mechanism of sorption for PCE, monolayer formation of the surfactant layer is sufficient for sorption of PCE. For the PCE bath sorption/reduction studies, a lower K_d would have been expected for the manufactured SMZ/ZVI pellets compared to the retreated pellets. The sorption of PCE is highly dependent upon the fraction of organic carbon content and the configuration of the surfactant on the surface of the pellet (Li and Bowman, 1998). Li and Bowman noticed that as the surfactant coverage increases, a proportional increase is seen in K_d until a complete monolayer has been formed. The presence of a surfactant bilayer does not increase K_d for PCE (Li and Bowman, 1998). The PCE batch sorption/reduction results are contradictory to these conclusions. A possible explanation for the PCE results is the initial HDTMA sorption isotherm performed on the Z/ZVI pellets was not a representative sample of the manufactured pellets. Jones et al (1998) indicated prior studies on surfactant-modified zeolite/zero valent iron pellets manufactured by Cercona of America could sorb up to 80-mmol HDTMA/kg pellet. The manufactured SMZ/ZVI pellets could have had a surfactant coverage of approximately 20 mmol HDTMA/kg pellet which would have formed a complete surfactant monolayer on the surface of the SMZ/ZVI pellet.

Since Figure 9 indicates the pellets are sorbing chromate after further HDTMA loading, the manufactured pellets lack the presence of a bilayer. However, the retreated pellets were only used to determine the presence of the bilayer. The retreated pellets were not used for any other experiments.

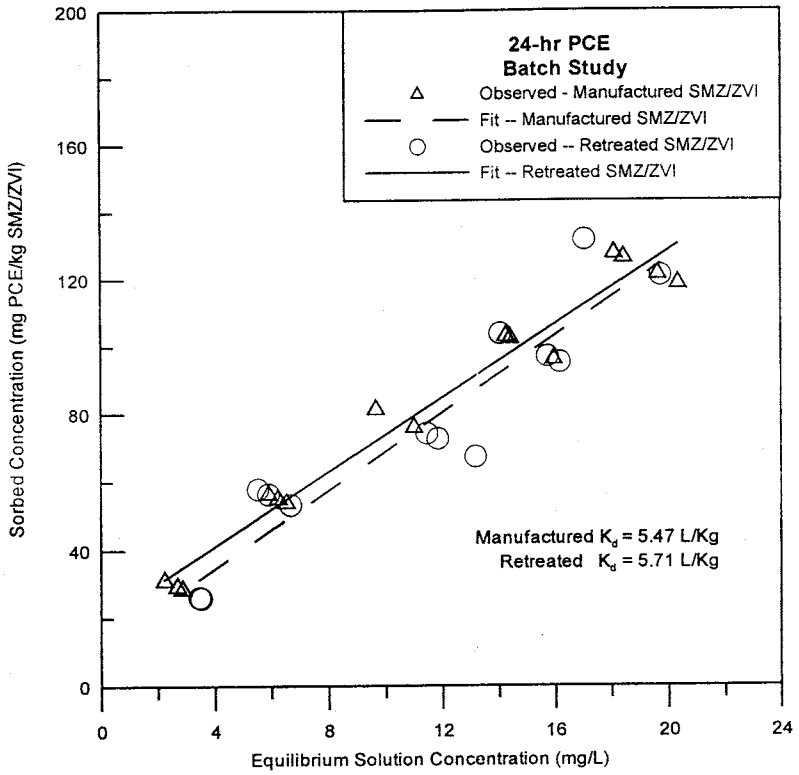

Figure 10. 24-Hour Perchloroethylene Batch Study

To determine particle size distribution of the SMZ/ZVI and Z/ZVI pellet material, sieve analyses were performed as described in section 3.4.5.1. The results of the sieve analyses are shown in Figure 11. The SMZ/ZVI pellets had a non-uniform particle size distribution and contained a significant amount, approximately 25%, of finer grain sized pellets (< 600 μm). The Z/ZVI pellets indicated a much more uniform particle size distribution and did not contain any fines.

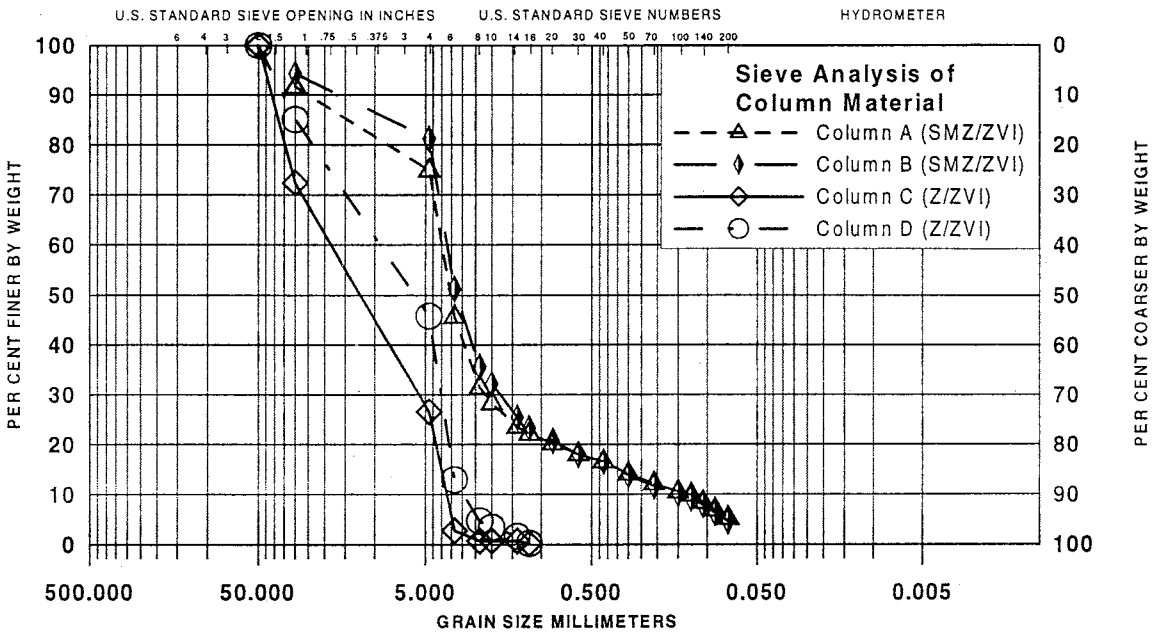

Figure 11. Particle Size Distribution of SMZ/ZVI and Z/ZVI Pellets

4.2 Batch Kinetic Studies

4.2.1 Chromate Batch Kinetic Studies

The results of the batch kinetic study for chromate are shown in Figure 12 and Figure 13. The relative concentration was the aqueous concentration at that time normalized to the initial solution concentration. Figure 13 indicates the transformation is occurring by a first-order process. The batch kinetic study results indicate a greater amount of chromate transformation is occurring in the Z/ZVI pellets compared to the SMZ/ZVI pellets while very little sorption of chromate is occurring with either of the pellets. The lack of chromate sorption with the SMZ/ZVI pellets indicates an incomplete formation of the bilayer during the manufacturing process as evaluated in the previous section.

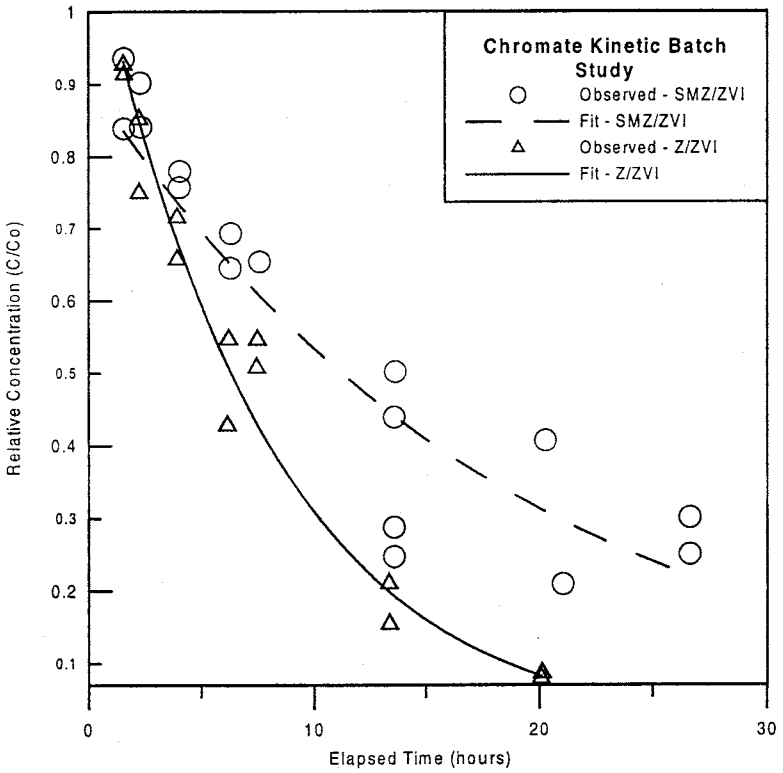

Figure 12. Chromate Batch Kinetic Study

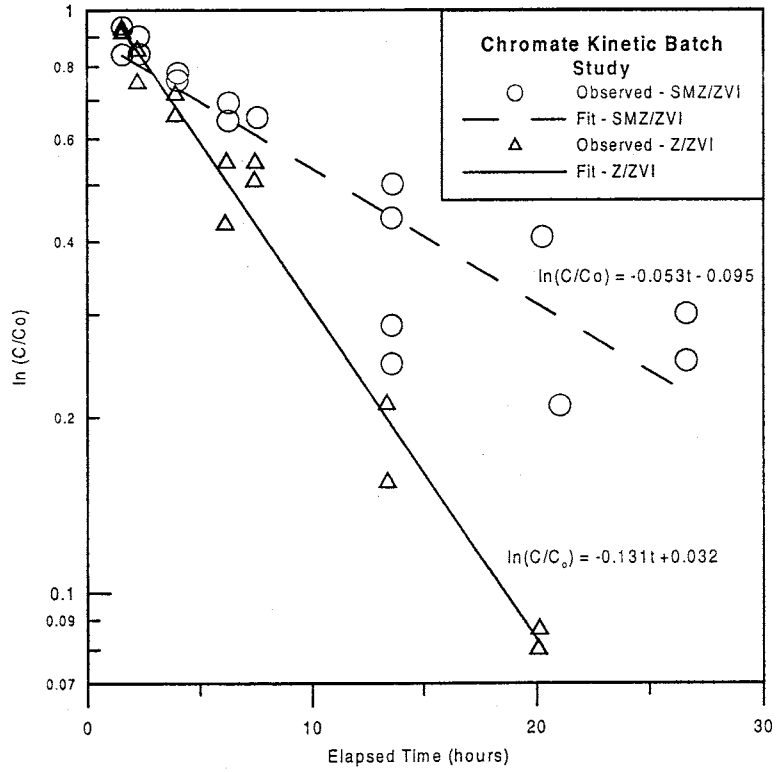

Figure 13. Semi-Log Plot of Chromate Batch Kinetic Study

4.2.2 Perchloroethylene Batch Kinetic Studies

The results of the PCE batch kinetic studies are shown in Figure 14 and Figure 15. Figure 14 indicates that sorption and degradation of PCE is occurring with the SMZ/ZVI pellets while Figure 15 indicates that the transformation is a first-order process. Transformation is the dominant process occurring in the Z/ZVI pellets. However, some sorption may be occurring with the Z/ZVI due to non-reactive carbon sites, such as graphite, imbedded within the iron material (Burris et al. 1998).

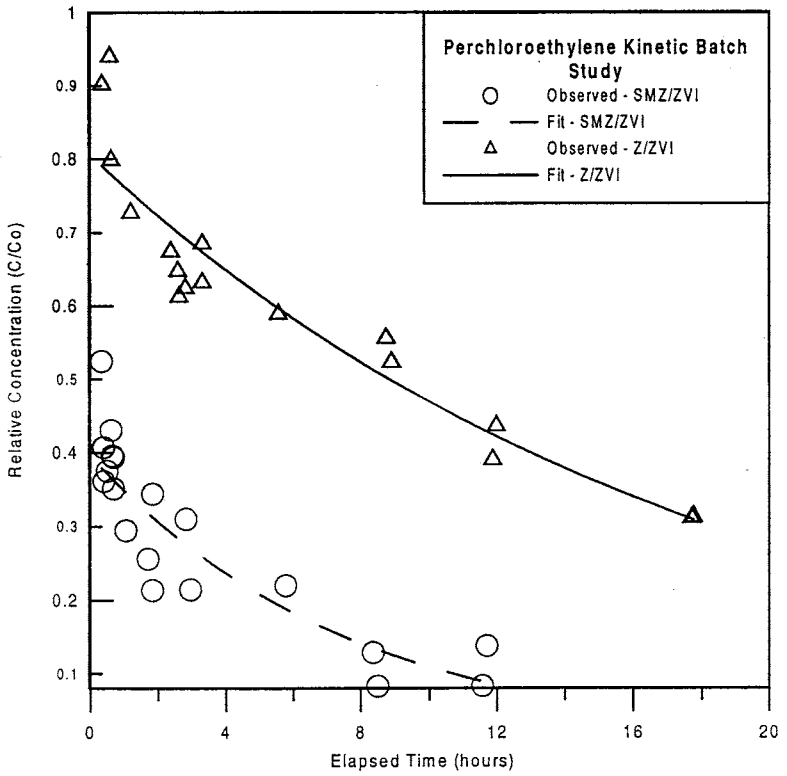

Figure 14. Perchloroethylene Batch Kinetic Study Results

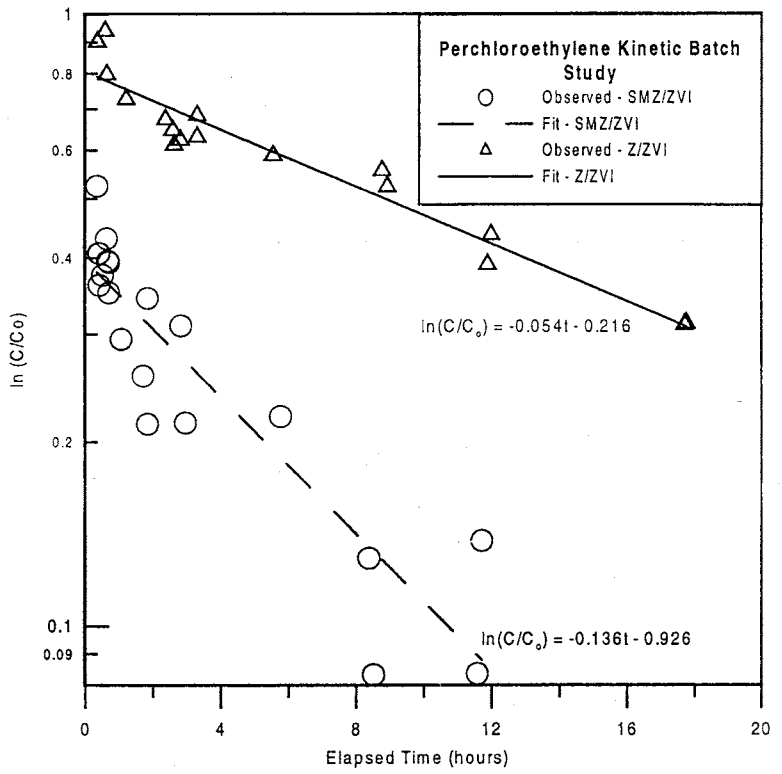

Figure 15. Semi-Log plot of Perchloroethylene Batch Kinetic Study

4.2.3 Evaluation of Batch Kinetic Data

Batch kinetic studies were performed to determine the first order transformation constant, μ_{obs}, and the distribution coefficient, K_d, for chromate and PCE. The sorption/ transformation process shows essentially two trends on the semi-log plot, the initial mass loss due to sorption and the straight line due to transformation. This two-step process has also been noted by Li and Jones (1998). The differential equation describing first order transformation is shown in Equation 5.

$$\frac{dC}{dt} = -\mu_{obs} C \qquad (5)$$

Where: C = aqueous concentration (mg/L)
t = elapsed time (hr)
μ_{obs} = first order transformation constant (hr^{-1})

Equation 5 can be solved for by integrating both sides of the equation and knowing the initial concentration (time zero). The solution for equation 5 is shown in equation 6. The first order transformation constant is the slope of

$$\ln(\frac{C}{C_o}) = -\mu_{obs} t \tag{6}$$

the straight line indicated on the semi-log plots for the batch kinetic studies. By assuming sorption of PCE or chromate is instantaneous relative to the transformation process, the distribution coefficient can be determined from the y-intercept of the straight line on the semi-log plot. Since the plot is the natural log of the relative concentration, the y-intercept must be raised to the power *e*. The following equations can be used to determine the distribution coefficient from the semi-log plots determined in the batch kinetic studies.

$$\frac{C}{C_o} = e^b$$

$$C^* = \frac{\left[1 - \left(\frac{C}{C_o}\right)\right] * V}{M} \tag{7}$$

$$K_d = \frac{C^*}{C/C_o}$$

Where:

b	=	y-intercept determined from semi-log plot
V	=	volume of solution (mL)
M	=	mass of pellets (g)
K_d	=	distribution coefficient (L/kg)
C_o	=	Initial Aqueous Concentration (mg/L)

This method for assumes a two-point linear isotherm, which goes through the origin. The initial aqueous concentration for chromate and PCE were 25.9 and 19.8 mg/L,

respectively. Table 4 indicates the observed results from the chromate and PCE batch kinetic studies.

Table 4. Observed Results of Batch Kinetic Studies

Material	Compound	μ_{obs} (hr^{-1})	K_d (L/kg)
SMZ/ ZVI	Chromate	0.053	0.198
	PCE	0.136	3.05
Z/ ZVI	Chromate	0.131	0.00
	PCE	0.054	0.481

4.3 Column Study

4.3.1 Non-Reactive Tracer Study

The purpose of the non-reactive tracer study was to determine the hydrodynamic properties of a solute as it moves through the pellets. The physical parameters of interest are the hydrodynamic dispersion and the percentage of mobile/immobile water.

The non-reactive tracer study was performed by injecting a pulse input of tritium solution into the columns at a flow rate of approximately 1-mL/min as described in section 3.4.4. The actual discharge rate of each column was determined by measuring the mass of effluent water, assuming a solution density of 1-g/cm^3, with time. Thus, the average linear velocity was determined by dividing the actual volumetric flowrate by the cross sectional area of the column and the porosity. Figures 16, 17 and 18 are the tritium breakthrough curves for the three materials tested.

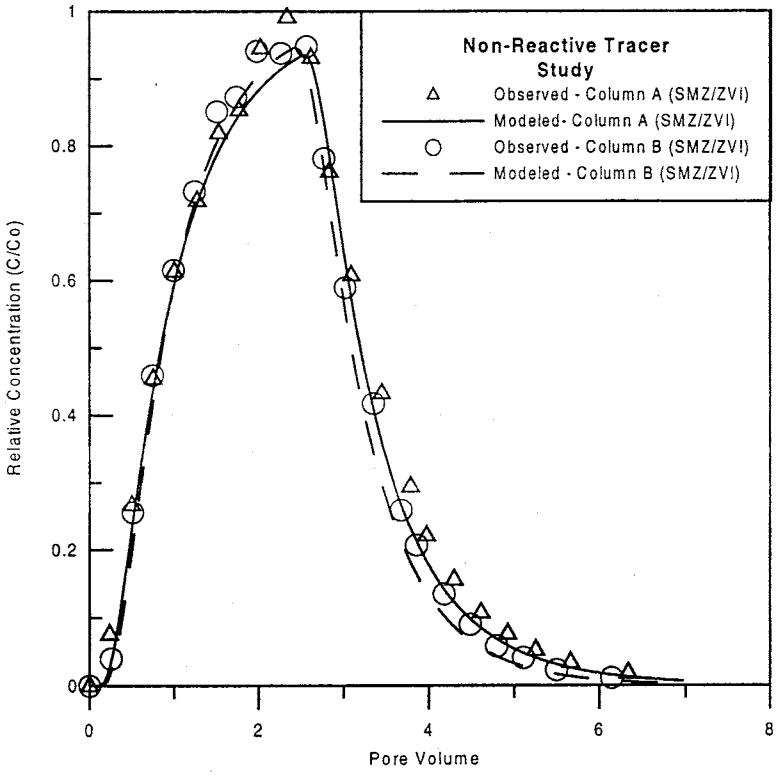

Figure 16. Tritium Breakthrough Curve for SMZ/ZVI Pellets

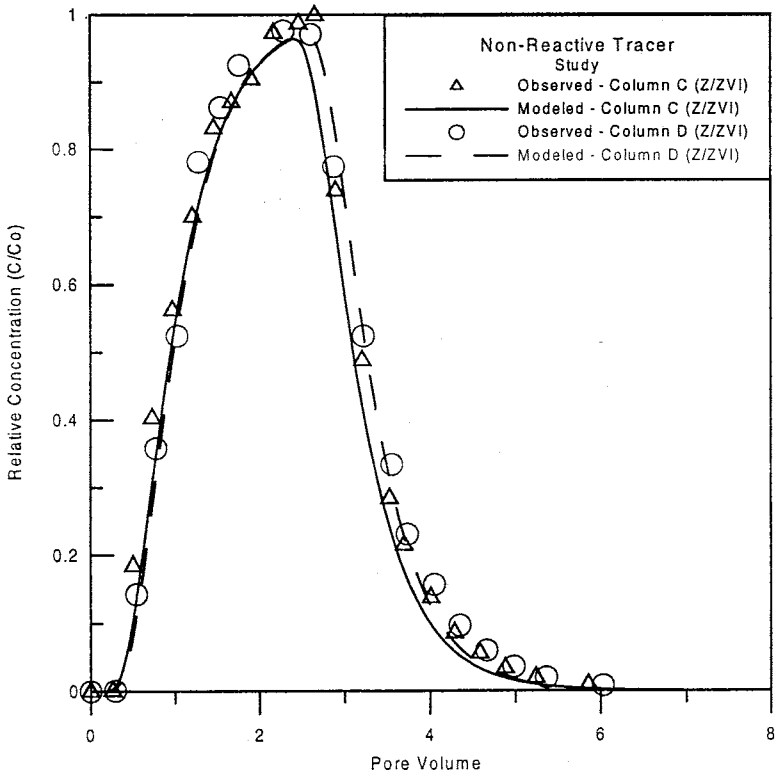

Figure 17. Tritium Breakthrough Curve for Z/ZVI Pellets

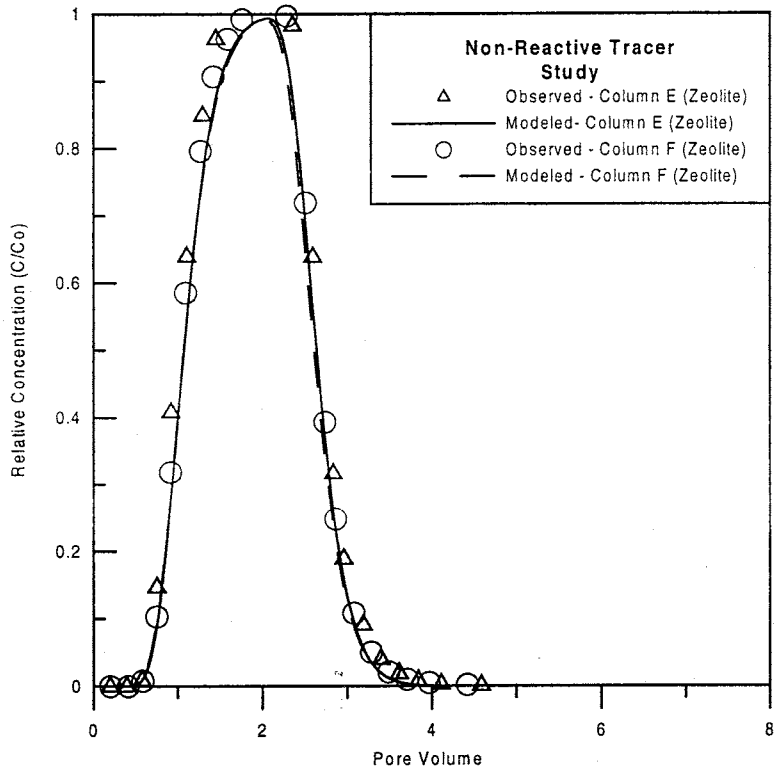

Figure 18. Tritium Breakthrough Curve for Zeolite Pellets

The greatest amount of tailing was seen in the SMZ/ZVI pellets while the least in the zeolite pellets. The tailing associated with the materials is probably due to the uniformity of the grain sizes. Prior to packing, the zeolite pellets were seized to a uniform particle size distribution where as the Z/ZVI and SMZ/ZVI pellets were not. Figure 11 indicates the grain size distribution for the Z/ZVI and SMZ/ZVI pellets. Figure 11 shows that the Z/ZVI pellets have a more uniform grain size distribution than the SMZ/ZVI pellets. Modeling of the breakthrough curves with a physical equilibrium model fit the observed data well. The good model fits suggest that the immobile water fraction was negligible for all materials. The small retardation factors (section 4.3.3.2) determined for this tracer study are most likely due to analytical error but not to sorption of tritium. Appendix B contains the raw data for the non-reactive tracer study.

4.3.2 Variable Flow Rate Reactive Solute Study

The reactive tracer study was performed by injecting a step input solution of PCE and chromate as described in section 3.4.4. These two species should not compete for sorption sites or interfere with chemical reactions due to their different chemical properties. Anion exchange sites on the surfactant bilayer would retard chromate, an oxyanion, whereas PCE, a nonpolar organic molecule, would preferentially sorb into the hydrophobic carbon chain of the monolayer (Li et al, 1998).

The average linear velocity for each column was determined by calculating the volumetric flow rate through each column, based on elapsed time and effluent mass, and then dividing the volumetric flow rate by the cross sectional area of the column and the porosity. The column study velocities were not the 1:2:4 ratio as hoped due to greater resistance of the 10-mL glass syringes used in the Harvard Pump for the 1-mL/min study. The normalized time or pore volume was determined by dividing the cumulative effluent mass by the mass of water in one column pore volume. Appendix A contains information regarding the pore volume of each column. PCE, chromate and the by-products of PCE were analyzed by the methods described in sections 3.3.1 and 3.3.2.

4.3.2.1 Chromate Breakthrough Curves

The breakthrough curves for the SMZ/ZVI pellets are shown in Figure 19 and Figure 20. The results of the SMZ/ZVI chromate column study, indicate that little sorption of chromate is occurring while transformation of chromate is continuing to occur. The chromate breakthrough curves also indicate an increase in the amount of transformation with a decreasing velocity. This increase in transformation is due to an increase in the residence time of chromate within the column.

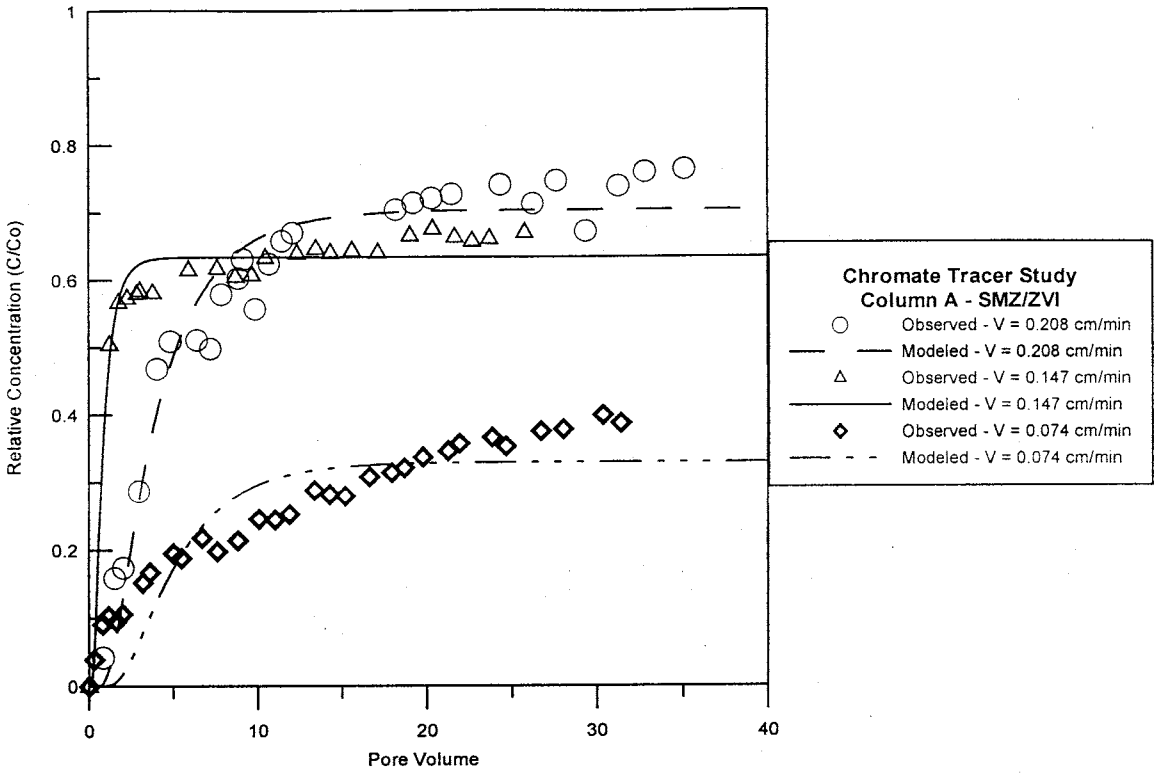

Figure 19. Chromate Breakthrough Curves - Column A (SMZ/ZVI)

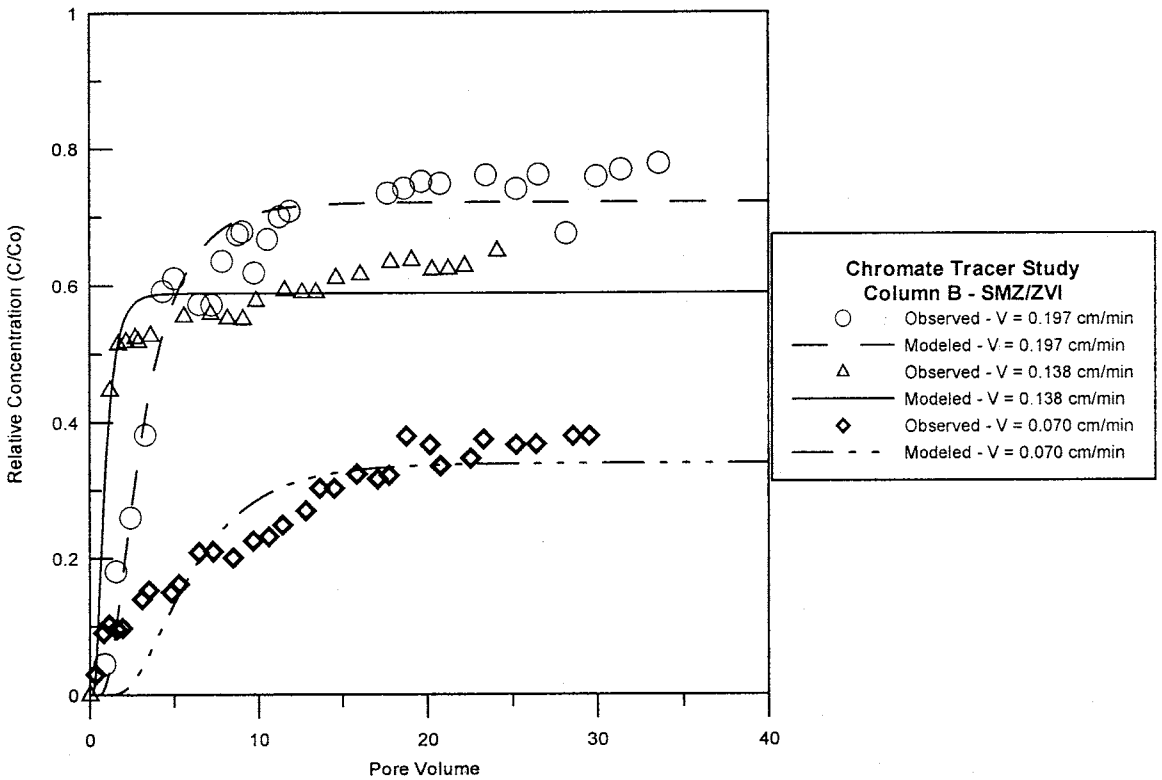

Figure 20. Chromate Breakthrough Curves - Column B (SMZ/ZVI)

For the Z/ZVI pellets (Figure 21 and Figure 22), complete transformation of chromate was seen in all of the column studies performed. The exact reason for this phenomenon is uncertain. These results may indicate that the HDTMA monolayer of the SMZ/ZVI inhibited the transformation of chromate. The surfactant monolayer may reduce the reduction potential of the iron surface or limit the number of available reactive sites for chromate to react with; however, these conclusions are speculative.

In general, chromate acted as an ideal tracer for the zeolite pellets. No significant amount of retardation or transformation was seen in any of the column studies performed. The breakthrough curves for the zeolite pellets are shown in Figure 23 and Figure 24. The apparent transformation shown in the breakthrough curves is due to fluctuations in the input concentration, 25.91 ± 1.94 and 27.7 ± 2.94 mg/L for velocities of 0.134 and

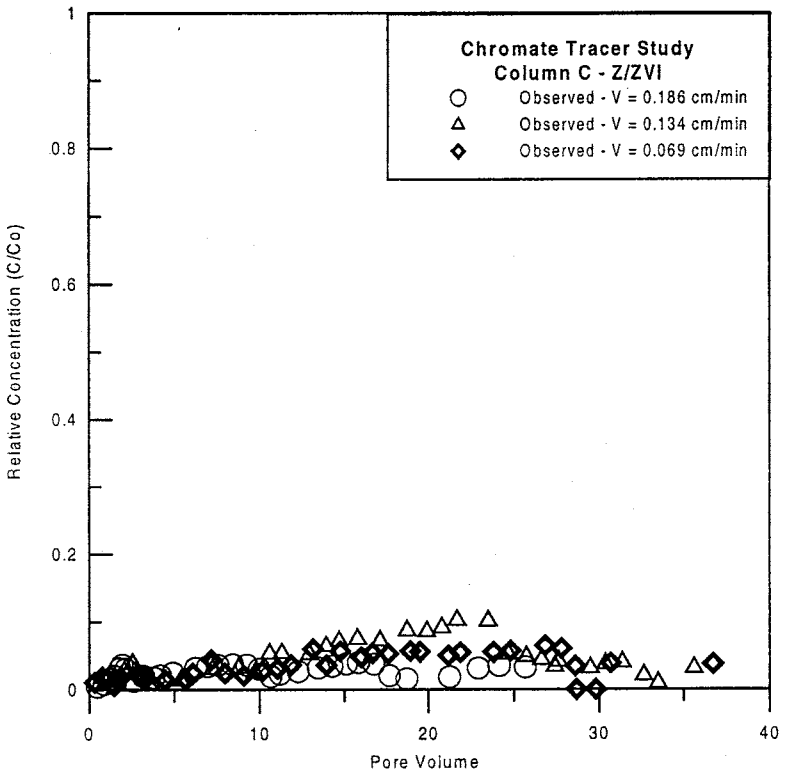

Figure 21. Chromate Breakthrough Curves – Column C (Z/ZVI)

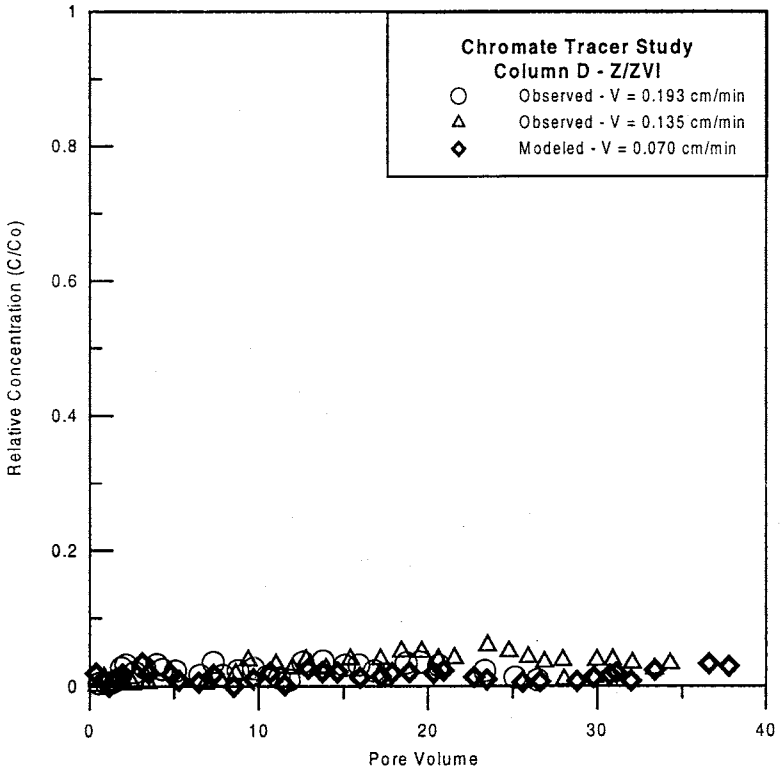

Figure 22. Chromate Breakthrough Curves - Column D (Z/ZVI)

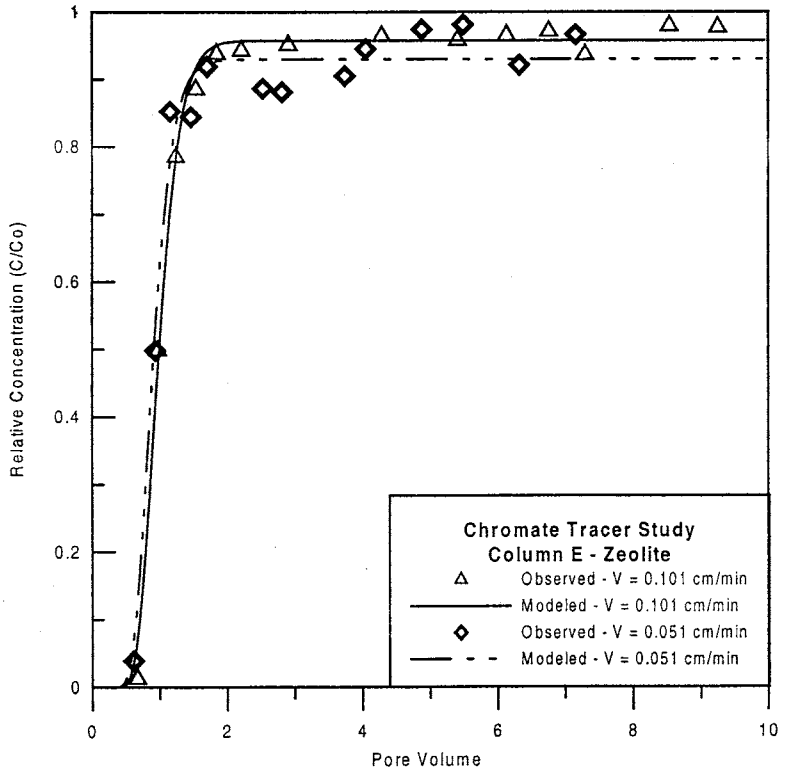

Figure 23. Chromate Breakthrough Curves - Column E (Zeolite)

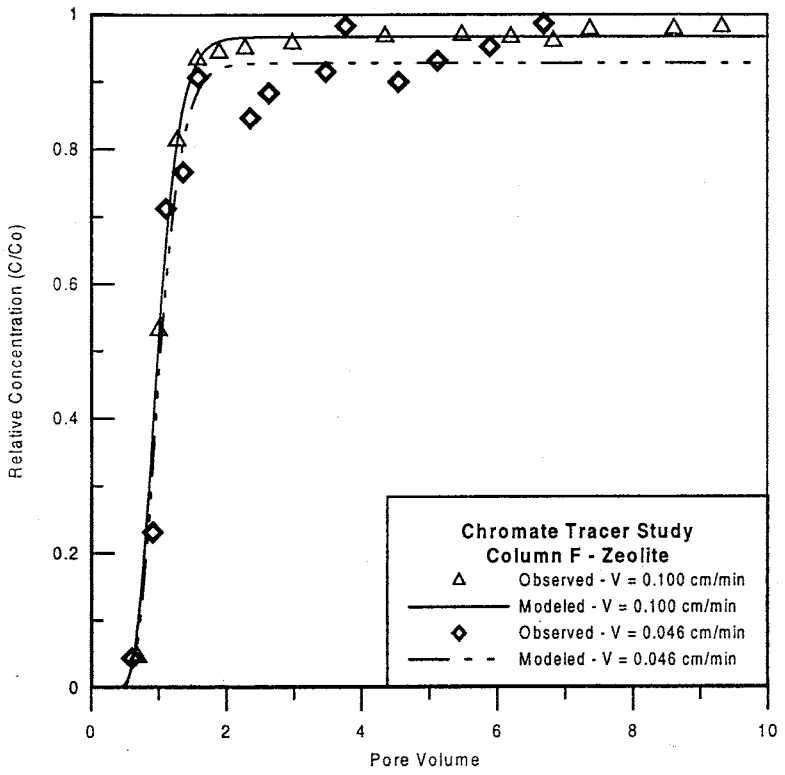

Figure 24. Chromate Breakthrough Curves - Column F (Zeolite)

0.069 cm/min, respectively. The steady-state effluent concentration plateaued at 24.8 ± 0.41 and 25.8 ± 1.04 mg/L for velocities of 0.134 and 0.069 cm/min, respectively. In considering the deviations from the average, the steady-state concentrations are within 1 standard deviation of the input concentrations.

Appendix C contains the raw data for the column studies. Due to pump error, a chromate breakthrough curve was not determined for the 1-mL/min flowrate for the zeolite pellets. At the 1-mL/min flowrate, the pump was unable to handle the backpressure of all six 10-mL Hamilton Glass Syringes. The problem was fixed in the remaining column studies by greasing the moving parts of the Harvard Pump.

4.3.2.2 Perchloroethylene Breakthrough Curves

The results for the SMZ/ZVI-PCE column studies are shown in Figure 25 and Figure 26. The PCE breakthrough curves show the transformation and retardation of

PCE expected for the SMZ/ZVI pellets. Trichloroethylene (TCE) was also seen in the effluent solution of the columns. Figure 27 and Figure 28 represent the formation of TCE for the SMZ/ZVI pellets. The greatest amount of transformation of PCE, 65% reduction, or largest production of TCE, 3 mg/L, was seen at the slowest flow rate. This is due to the longer residence time of PCE within the column or the time available for PCE to interact with the iron surface. However, little difference was seen in the PCE transformation, 35% transformed, or TCE formation, 1.5 mg/L, between the 1 and 0.5 mL/min flowrate.

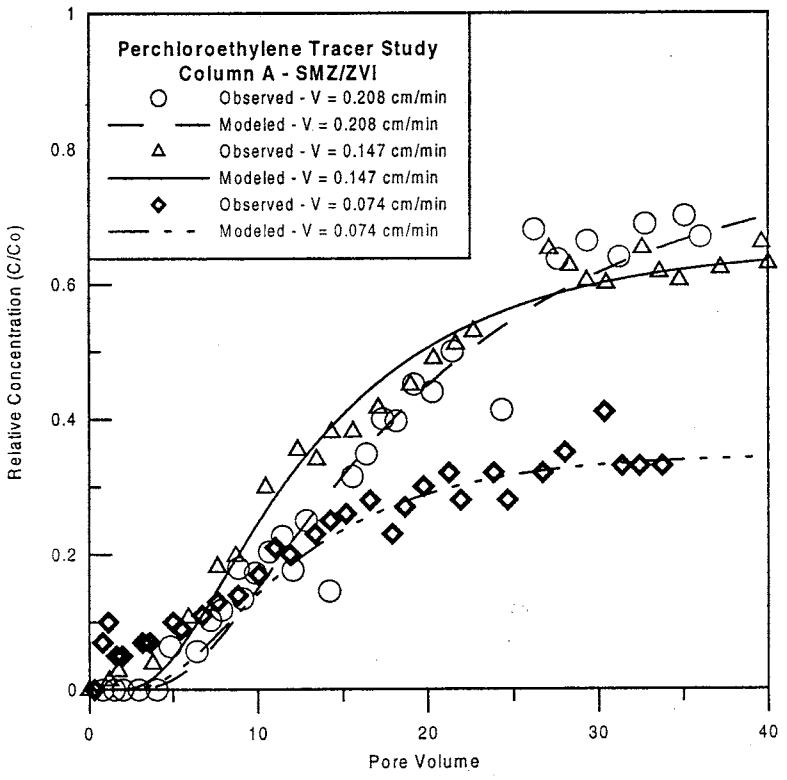

Figure 25. Perchloroethylene Breakthrough Curve - Column A (SMZ/ZVI)

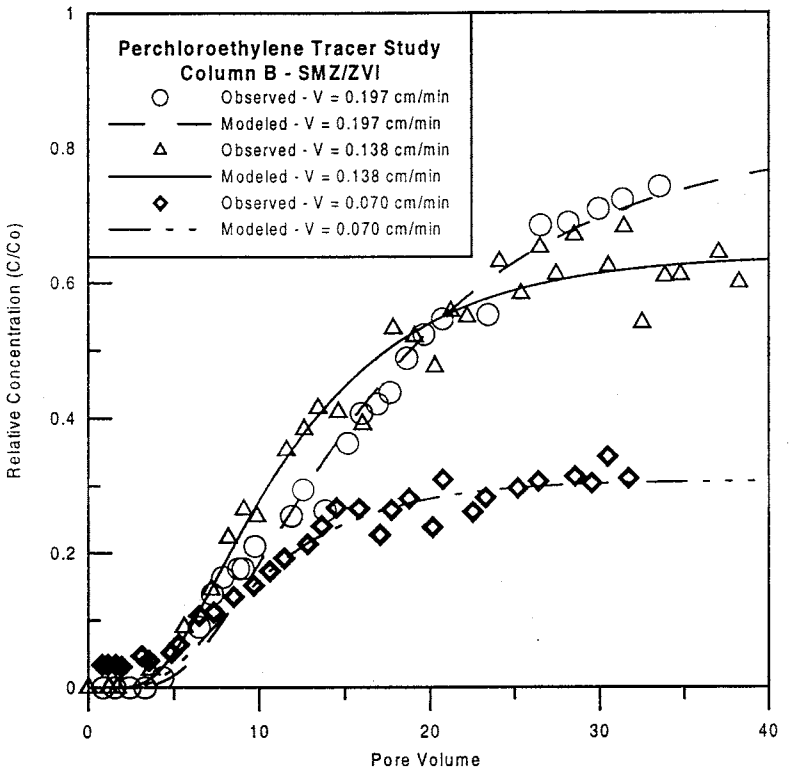

Figure 26. Perchloroethylene Breakthrough Curve - Column B (SMZ/ZVI)

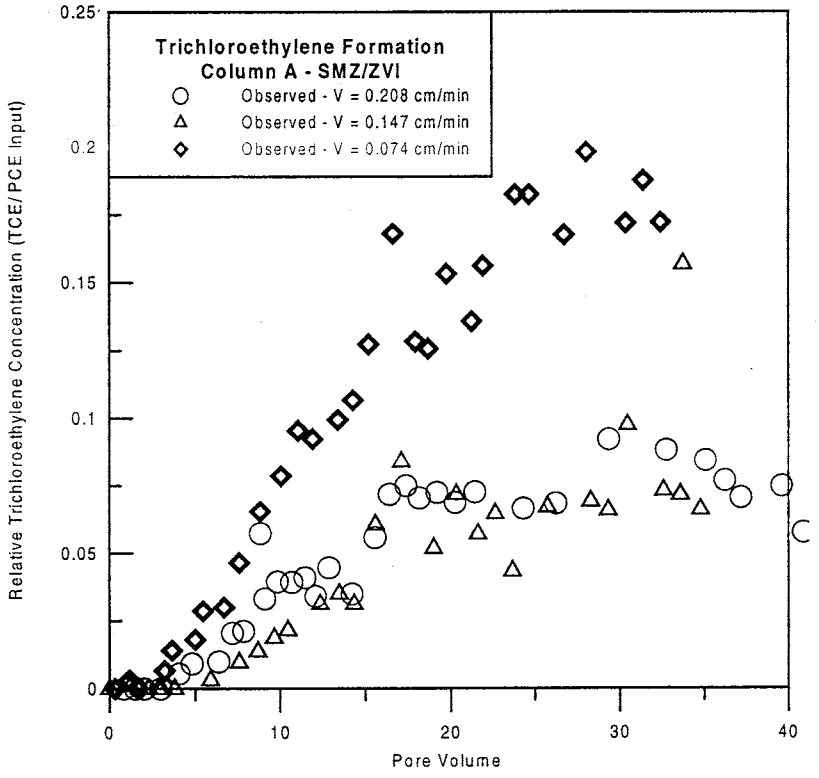

Figure 27. Relative Trichloroethylene Formation - Column A (SMZ/ZVI)

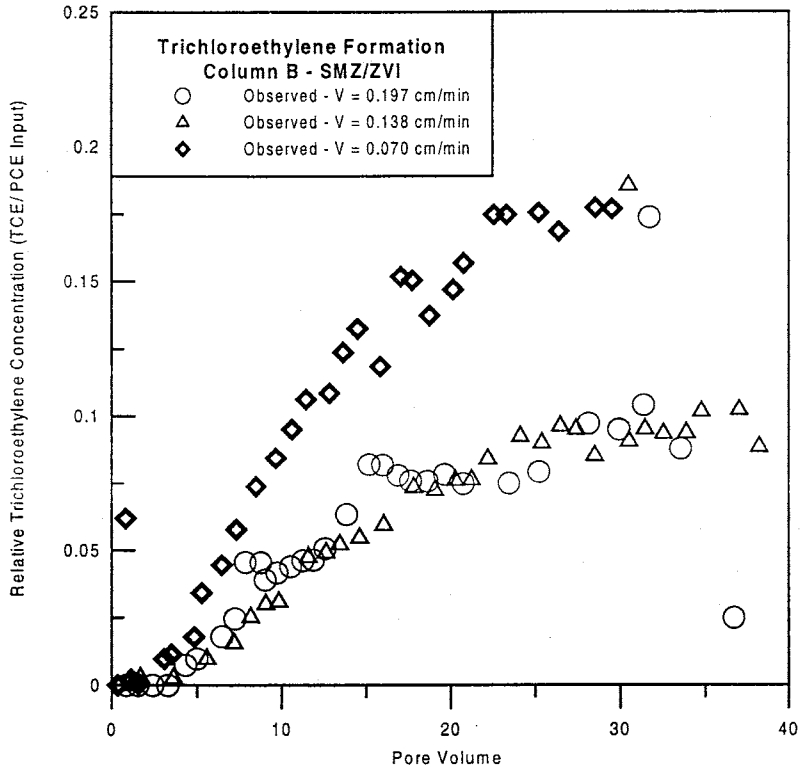

Figure 28. Relative Trichloroethylene Formation - Column B (SMZ/ZVI)

The results for the Z/ZVI pellets are shown in Figure 29 and Figure 30. The transformation of PCE with the change in velocity is well seen in Figure 29 and Figure 30. Each breakthrough curve indicates some retardation of PCE by the time lag of the breakthrough curve. The retardation of PCE is more than likely due to sorption onto non-reducing carbon sites, such as graphite, contained within the iron (Burris et al, 1998). Transformation of PCE was seen in the 0.5 and 0.25-mL/min column studies, 32% and 62% transformation of PCE, respectively. No apparent transformation of PCE or formation of TCE was seen in the 1-mL/min column study. The formation of TCE for the Z/ZVI pellets is shown in Figure 31 and Figure 32. The formation of TCE for the Z/ZVI pellets between the 0.25-mL/min and 0.5-mL/min column studies showed a relatively small difference.

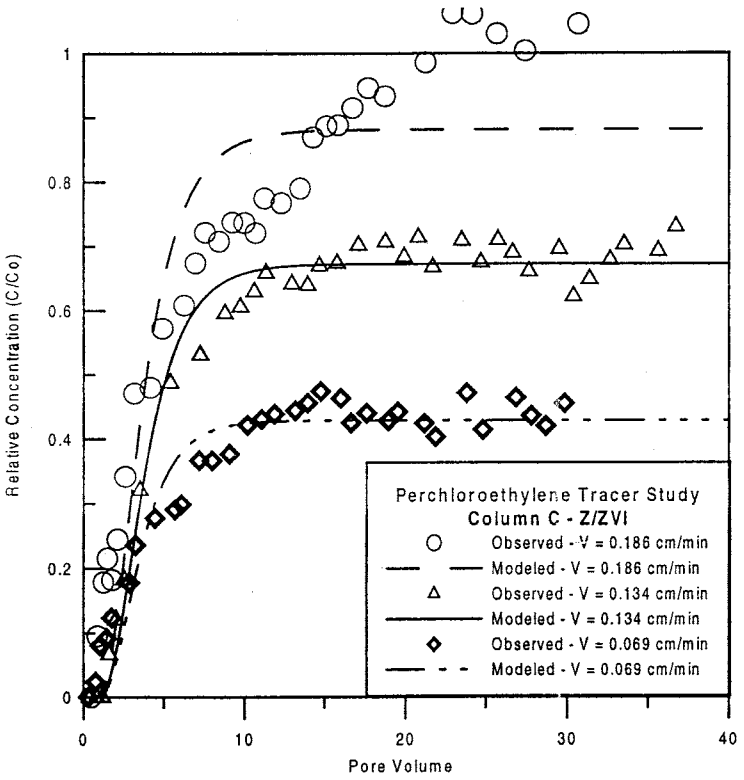

Figure 29. Perchloroethylene Breakthrough Curve - Column C (Z/ZVI)

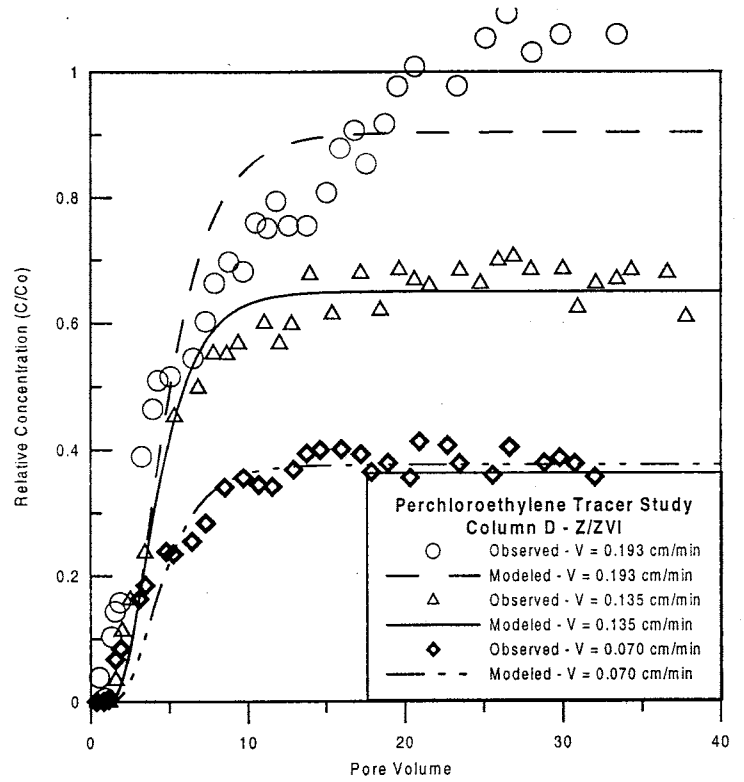

Figure 30. Perchloroethylene Breakthrough Curve - Column D (Z/ZVI)

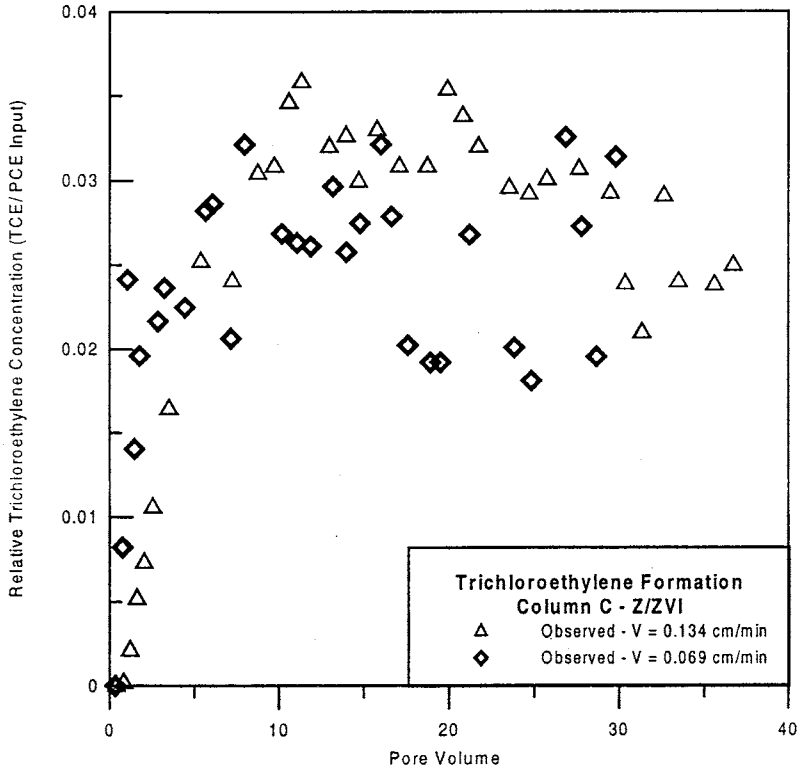

Figure 31. Relative Trichloroethylene Formation - Column C (Z/ZVI)

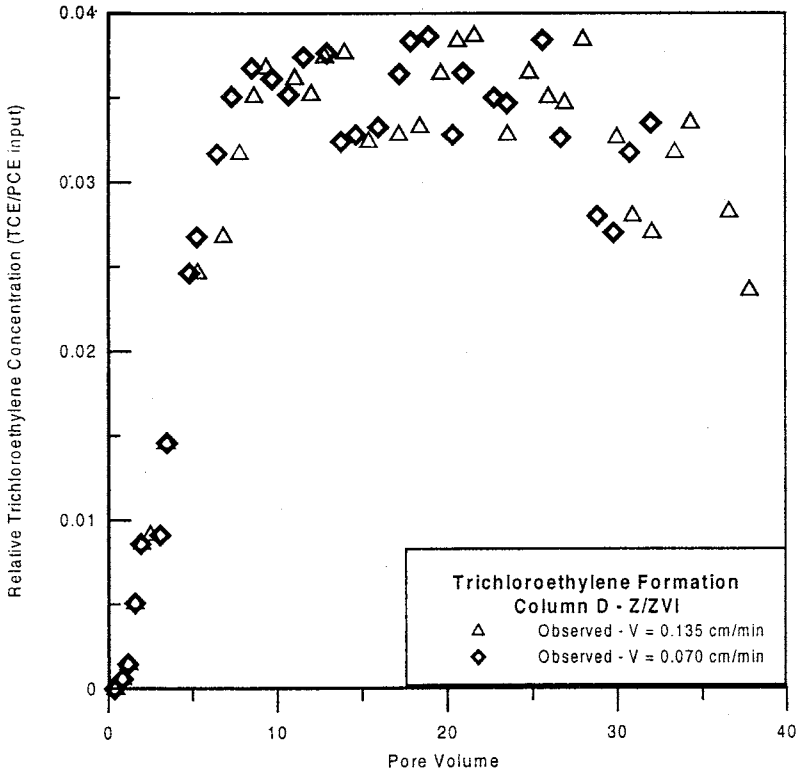

Figure 32. Relative Trichloroethylene Formation - Column D (Z/ZVI)

The PCE breakthrough curves for the SMZ/ZVI and Z/ZVI indicate an enhanced transformation for the SMZ/ZVI. However, the enhanced transformation can be attributed to either the surfactant modification of the pellets or the increased surface area of the SMZ/ZVI pellets. These observations will be discussed in more detail in section 4.3.3.2.

The steady-state PCE concentrations in the Z/ZVI pellets were greater than the average input concentration due to fluctuations in the input PCE concentration, 18.24 ± 2.73 mg/L. The highest effluent PCE concentrations analyzed were 19.36 and 19.93 for column C and column D, respectively, and are within a standard deviation from the average input concentration. At the two lowest flow rates, effluent PCE concentrations were transformed to nearly the same value, however, TCE formation in the Z/ZVI pellets was lower. The smaller formation of TCE in the Z/ZVI pellets may indicate that TCE is being transformed into less chlorinated ethylenes such as DCE or vinyl chloride or to the final product of ethylene. Roberts et al. (1996) has performed research investigating the possibility that PCE can be transformed to DCE bypassing the TCE formation. The mechanism for this reaction is referred to as reductive-β-elimination. The reductive-β-elimination process accounts for two halide ions (chloride) being released from PCE as compared to the one halide of reductive dehalogenation. Roberts et al. (1996) indicates that the reductive-β-elimination process is energetically similar to the reductive dehalogentaion process at neutral pH. However, analysis of the effluent concentration did not indicate detectable levels of DCE or vinyl chloride.

The PCE breakthrough curves for the zeolite pellets indicate essentially no retardation or transformation of PCE. Figure 33 and Figure 34 are the breakthrough

curves for the zeolite pellets. The 1-mL/min column study for the zeolite pellets was not performed due to the pump problems as stated earlier (section 4.3.2.1). For the zeolite pellets, the steady-state concentration does not approach the average input concentration due to variations in the input PCE concentration. The input PCE concentrations for the 0.5 and 0.25-mL/min column studies were 17.23 ± 3.47 and 14.60 ± 1.31 mg/L, respectively. The steady-state effluent concentrations for column E and column F were 16.3 ± 0.47 and 17.3 ± 0.45 mg/L, respectively, for the 0.5-mL/min flow rate column study and 12.71 ± 0.59 and 13.27 ± 0.53 mg/L, respectively, for the flow rate of 0.25 mL/min. The average steady-state effluent PCE concentrations were within a standard deviation of the average input PCE concentration except for the 0.25-mL/min-column study of column E. PCE analysis error may be attributed to the larger deviation from a standard deviation for 0.25-mL/min column study results for column E.

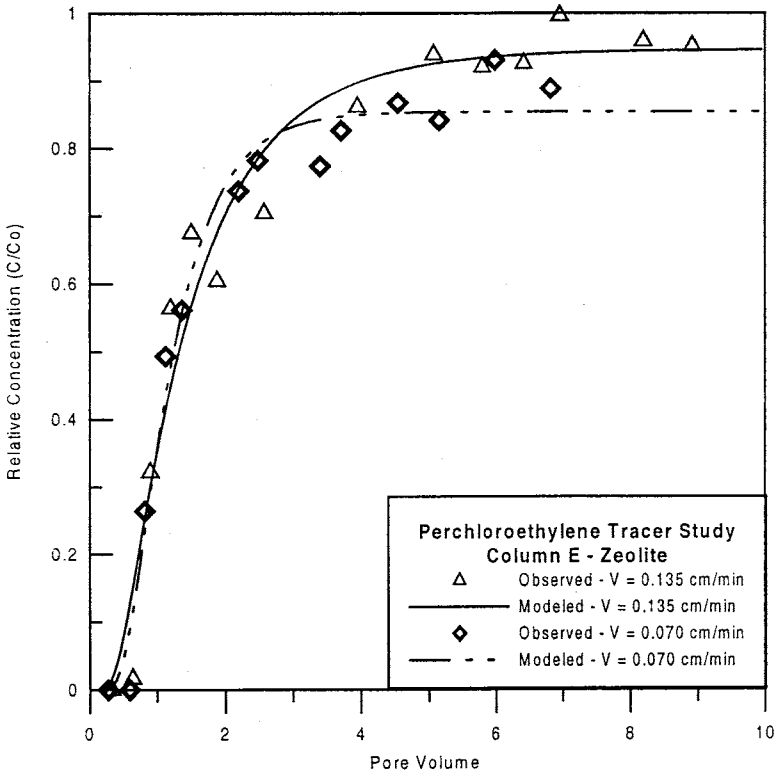

Figure 33. Perchloroethylene Breakthrough Curves - Column E (Zeolite)

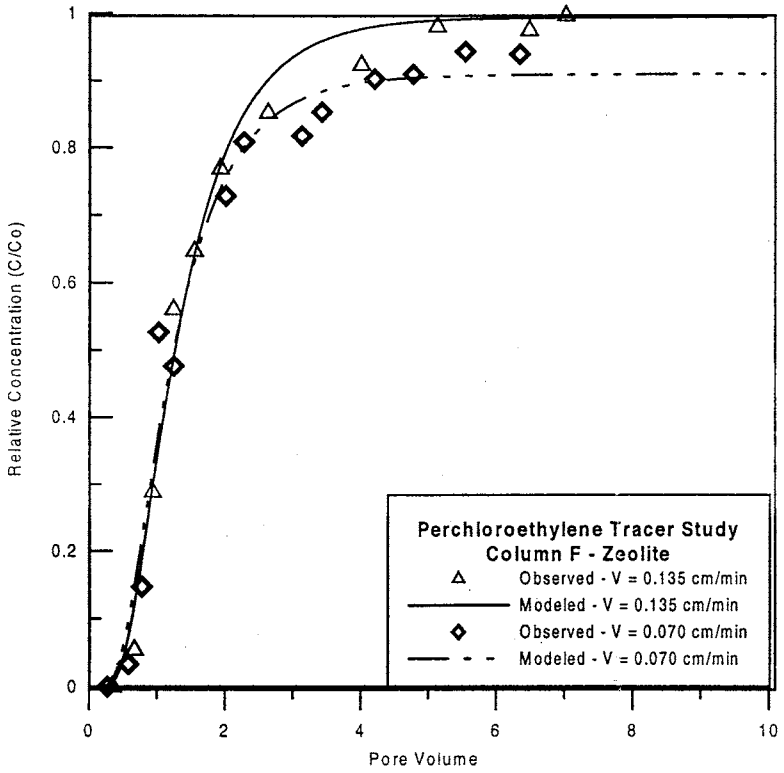

Figure 34. Perchloroethylene Breakthrough Curves - Column F (Zeolite)

4.3.3 Breakthrough Curve Modeling with CXTFIT2

4.3.3.1 Modeling Assumptions

CXTFIT2 is computer program that estimates solute transport parameters from observed concentration data using the advection-dispersion equation as the transport model. CXTFIT2 uses a non-linear least squares parameter optimization method developed by the U.S. Salinity Laboratory (Toride et al, 1995). In order to limit the number of parameters being estimated by CXTFIT2, assumptions had to be made regarding the physical and chemical characteristics of the interaction between the pellet material and reactions occurring. The first assumption was the dispersion coefficient is a linear function of the velocity and the dispersivity is a constant. The effective molecular diffusion coefficient is assumed to be negligible for the velocity range of the column

study experiments (Bear, 1972). The dispersivity value obtained from the non-reactive tracer study will be assumed to be valid for the reactive.

For the chemical reactions, a first order transformation was seen in the batch kinetic studies for PCE and chromate. Transformation of PCE by zero valent iron has been reported as a first order process by Burris et al (1997) and Johnson et al (1996), while Powell et al (1995) has noted first order chromate transformation. The sorption of PCE and chromate is assumed to be described by linear isotherms. Li et al (1998) noted that sorption of PCE was linear on surfactant-modified zeolite. However, Li et al (1997) noted Langmuir type sorption for chromate (1998). It was assumed for this analysis that the chromate concentration in the aqueous phase was small enough to be in the linear sorption region of the Langmuir isotherm.

4.3.3.2 Determination of Solute Transport Parameters

4.3.3.2.1 Non-Reactive Tracer Study

CXTFIT2 was used to determine the dispersion coefficient and retardation factor from the non-reactive tracer study using the velocity as a fixed value. The dispersion coefficient estimates from the non-reactive tracer studies are listed inTable 5. The CXTFIT2 files for the non-reactive tracer modeling are found in Appendix D. Also listed in the tables for the results of CXTFIT2 are the R^2 value and the 95% confidence interval limits of the unknown parameters. The R^2 value gives an indication of how well the best-fit values for the unknown parameters fit to the observed data while knowing the 95% confidence interval limits indicates the accuracy of the best-fit values.

Table 5. CXTFIT2 Parameter Estimates for the Non-Reactive Tracer Study

Material	Column	v (cm/min)	D (cm^2/min) and 95% Confidence Interval	R	R^2
SMZ/ ZVI	A	0.273	**2.60** (2.51 – 2.69)	1.09	0.989
	B	0.263	**1.95** (1.87 – 2.03)	1.06	0.991
Z/ZVI	C	0.250	**1.12** (1.01 – 1.23)	1.08	0.984
	D	0.254	**1.05** (0.95 – 1.15)	1.09	0.987
Zeolite	E	0.196	**0.226** (0.114 – 0.337)	1.11	0.986
	F	0.184	**0.222** (0.193 – 0.252)	1.10	0.999

The ratio of transport by advection to transport by dispersion is referred to as the Peclet number, Equation 8. Table 6 indicates the calculated dispersivity values (D/v) and the Peclet number for each column.

$$P = \frac{v * L}{D} \tag{8}$$

Where: L = length of packed material in column
P = peclet number

Table 6. Dispersivity and Peclet Numbers

Material	Column	α (cm)	P
SMZ/ ZVI	A	9.52	3.29
	B	7.41	4.26
Z/ZVI	C	4.48	6.92
	D	4.14	7.76
Zeolite	E	1.15	27.8
	F	1.21	26.5

Table 6 indicates that hydrodynamic dispersion contributes to the solute transport the most in the SMZ/ZVI columns while the least in the zeolite columns. The apparent differences in the dispersivity values are more than likely due to the difference in grain size distributions among the materials. The SMZ/ZVI material has a relatively wide grain size distribution (Figure 11) compared to either the Z/ZVI or the zeolite pellets. The Peclet numbers also indicate the SMZ/ZVI pellets have a larger dispersive flux compared to the advective flux. The dispersive flux in the zeolite pellets is not as significant. The estimated retardation factors indicate a time lag in the non-reactive breakthrough curve. However, small retardation factors greater than 1 are common for tritium breakthrough curves.

4.3.3.2.2 Reactive Tracer Study

For the chromate and PCE modeling, the retardation factor and the lumped first order transformation constant were determined while dispersion coefficient and velocity were fixed. The parameters of concern for the reactive tracer study were the retardation coefficient and the observed first order decay constant. These parameters were estimated using CXTFIT2 by calculating the hydrodynamic dispersion from the dispersivity values (Table 6) determined from the non-reactive tracer study and the linear velocity using Equation 3, assuming molecular diffusion was negligible. The transformation constant value determined by CXTFIT2 is a dimensionless first order transformation constant, β, that includes transformations occurring in both the liquid and sorbed phases. This dimensionless first order transformation constant will be further evaluated when comparing the batch kinetic study results to the column study results in section 4.3.

Table 4 lists the CXTFIT2 results for the chromate column studies. The chromate results for the Z/ZVI material were not modeled since a breakthrough curve was not produced. Complete degradation of chromate was seen in the Z/ZVI material. As

Table 4 indicates, retardation factors varying between 1 and 10 for SMZ/ZVI material while no sorption was seen in the zeolite pellets. The decrease in sorption from the 1-mL/min to the 0.5-mL/min-column study may be due to desorption of the manufactured surfactant bilayer, if any surfactant bilayer was present. The retardation factor for the 0.25-mL/min-column study did not represent the early time data for the breakthrough curve well. By visual inspection of the 0.25-mL/min chromate breakthrough, an estimated retardation factor of 4.7 and 4.8 for the column A and column B, respectively, were determined by matching the pore volume at which the data was equivalent to half of the steady-state chromate concentration. An increase in β is seen with a decrease in velocity as expressed in Equation 9. In section 4.4, β will be further evaluated for comparison to the batch

$$\beta = \frac{L(\theta\mu_L + \rho_b K_d \mu_S)}{\theta v} \qquad (9)$$

kinetic studies. However, β for the zeolite material varies significantly as seen by the 95% confidence interval limits. The apparent transformation of chromate is more than likely due to analytical error and fluctuations of the input chromate concentration, as

described in section 4.3.2.2, since no mechanism is available for chromate transformation (Figure 23 and Figure 24).

Table 7. CXTFIT2 Parameter Estimates for Chromate Column Studies

Column	v (cm/min)	R and 95% Confidence Intervals	β and 95% Confidence Intervals	R^2
A	0.208	**5.41** (5.29 – 5.52)	**0.389** (0.274 – 0.505)	0.937
	0.147	**1.21** (1.15 – 1.27)	**0.519** (0.459 – 0.579)	0.961
	0.074	**9.48** (9.36 – 9.60)	**1.480** (1.36 – 1.60)	0.769
B	0.197	**4.13** (4.01 – 4.23)	**0.352** (0.244 – 0.460)	0.937
	0.138	**1.26** (1.18 – 1.35)	**0.514** (0.596 – 0.679)	0.918
	0.070	**10.0** (9.92 – 10.2)	**1.356** (1.231 – 1.480)	0.748
E	0.101	**1.02** (0.96 – 1.07)	**0.044** (-0.011 – 0.097)	0.993
	0.051	**0.93** (0.83 – 1.03)	**0.072** (-0.031 - 1.752)	0.973
F	0.110	**1.02** (0.98 – 1.05)	**0.035** (0.000 – 0.0702)	0.996
	0.046	**1.05** (0.91 – 1.19)	**0.076** (-0.065 – 0.218)	0.961

From the PCE parameters, the data were well fitted by the model.

Table 8 indicates the results for the best-fit values of CXTFIT2. The retardation coefficients did not vary much due to changes in the linear velocity of the column study, which indicates

Table 8. CXTFIT2 Parameter Estimation for Perchloroethylene Column Studies

Material	Column	v (cm/min)	R	β	R^2
Synthetic	A	0.208	**25.43** (25.57 - 25.25)	**0.2480** (0.1032 – 0.3930)	0.967
		0.147	**19.10** (19.03 – 19.26)	**0.4740** (0.4060 – 0.5420)	0.986
		0.074	**22.17** (22.09 – 22.24)	**1.398** (1.322 – 1.473)	0.948
Synthetic	B	0.197	**20.92** (20.81 – 21.02)	**0.2068** (0.1007 – 0.3182)	0.984
		0.138	**15.81** (15.78 – 15.97)	**0.4889** (0.3963 – 0.5816)	0.976
		0.070	**17.37** (17.32 – 17.42)	**1.507** (1.460 – 1.554)	0.973
Natural	C	0.186	**4.24** (3.98 – 4.50)	**0.1287** (-0.1283 – 0.3857)	0.859
		0.134	**4.70** (4.63 – 4.77)	**0.4190** (0.3480 – 0.4900)	0.981
		0.070	**4.81** (4.72 – 4.90)	**0.9510** (0.8616 – 1.040)	0.917
Natural	D	0.193	**5.47** (5.21 – 5.73)	**0.1028** (-0.1609 – 0.3664)	0.866
		0.135	**5.23** (5.14 – 5.31)	**0.4554** (0.3698 – 0.5418)	0.972
		0.070	**6.25** (6.18 – 6.32)	**1.100** (1.031 – 1.169)	0.943
Zeolite	E	0.101	**1.66** (1.33 – 1.96)	**0.0559** (-0.1525 – 0.2643)	0.959
		0.051	**1.33** (1.13 – 1.53)	**0.1608** (0.0246 – 0.2970)	0.979
Zeolite	F	0.1100	**1.47** (1.34 – 1.60)	**0.0065** (-0.0980 – 0.111)	0.988
		0.0460	**1.41** (1.16 – 1.66)	**0.0978** (-0.0815 – 0.277)	0.974

the sorption of PCE is not mass transfer limited. The values determined for the dimensionless modeled first transformation decay constant increased with the decreasing velocity. The transformation constant, μ, in the advection-dispersion equation (equation 3) is treated as a lumped parameter by CXTFIT2.

Equation 9 defines CXTFIT2's dimensionless transformation constant. According to Equation 9, an increase in β is expected for a decrease in the velocity. The actual first order transformation constant will be evaluated in section 4.4 when comparing the column study results to the kinetic batch study.

The zeolite material indicated some retardation of PCE while a small amount of transformation may have been occurring. The apparent transformation may be due to small volatilization losses and fluctuations in the input concentration. The retardation factor may be due to sorption onto grease used to seal the caps of the columns. However, no mechanisms are available for sorption or decay of PCE by the zeolite material.

4.4 Comparison of Kinetic Batch Study and Column Study Results

The results for the column studies and the batch kinetic studies cannot be directly related to each other based on the observed values. This section describes the adjustments needed to compare the results of the two studies.

4.4.1 Distribution Coefficient Evaluation

For the batch kinetic studies the distribution coefficient was determined from the linear portion of the semi-log plots as described in section 4.2.3. The K_d is related to retardation by equation 4 for linear type sorption. The bulk density of the Z/ZVI and the SMZ/ZVI material is 1.3 g/cm^3 (section 3.4.5.2) while the porosity values are located in section 3.4.2. The best-fit values for the chromate and PCE retardation factor are listed in

Table 7 and Table 8. Table 7 and Table 8 were used to estimate K_d for chromate and PCE for the SMZ/ZVI and Z/ZVI materials are listed in

Table 9 No sorption of PCE or chromate was apparent for the zeolite pellets, so no K_ds were calculated for this material.

The average chromate K_d value was determined to be 0.197 ± 0.46 for the SMZ/ZVI material while no sorption of chromate was seen with the Z/ZVI material. The chromate column study results indicated high variability in chromate sorption. The high variability of chromate sorption may be due to changes in the amount of surfactant bilayer on the manufactured pellets from desorption during previous column studies. The 0.25-mL/min chromate column study data was not modeled well with CXTFIT2 and may have over predicted the retardation factor for this column study. Since complete transformation of chromate occurred in the Z/ZVI column studies, a K_d could not be calculated.

Table 9 indicates the batch kinetic and column studies compare well to each other for PCE. The average PCE K_d values were determined to be 2.28 ± 0.41 L/Kg and 0.524 ± 0.07 L/Kg for the SMZ/ZVI and Z/ZVI pellets, respectively.

Table 9. Distribution Coefficients

Study		Material	v (cm/min)	K_d Chromate (L/Kg)	K_d PCE (L/Kg)
Batch		SMZ/ZVI	---	0.197	2.01
Kinetic		Z/ZVI	---	0	0.481
Column Studies	A	SMZ/ZVI	2.93	0.208	0.529
			2.17	0.147	0.025
			2.54	0.074	1.02
	B	SMZ/ZVI	2.55	0.197	0.402
			1.77	0.138	0.033
			1.96	0.070	1.16
Column Studies	C	Z/ZVI	0.431	0.186	---
			0.492	0.134	---
			0.507	0.070	---
	D	Z/ZVI	0.564	0.193	---
			0.534	0.135	---
			0.662	0.070	---

4.4.2 First Order Transformation Evaluation

The observed first order transformation constants were determined in the batch kinetic studies from the slope of the line on the semi-log plots. The dimensional lumped first order transformation constant from the column studies was determined by multiplying the best-fit value of β by the linear velocity and dividing by the length of pellet material in the column (Appendix A). Table 10 indicates the results for the lumped first order transformation constants for transformation of chromate and PCE with the SMZ/ZVI and Z/ZVI pellets. Lumped first order transformation constants for chromate with the Z/ZVI pellets were not determined since break through curves were not produced in the column studies. Table 10 indicates the SMZ/ZVI pellets have a lower chromate transformation rate than the Z/ZVI pellets, 0.053 and 0.131 hr^{-1}. The PCE results in Table 10 indicate that the SMZ/ZVI material transformed PCE faster than the Z/ZVI pellets. Table 10 also indicates an increase in the transformation rate with the decreasing linear velocity which indicates that transformation is a mass transfer limited process.

The batch kinetic studies and the column studies suggest first-order transformation constants for chromate and PCE. The observed constant is a lumped parameter for transformation occurring in the liquid phase and in the sorbed phase (definition for μ in Equation 2). However, the relationship between transformation in the two regions is unknown. Two approaches have been proposed as to where the transformation is occurring: transformation is only occurring in the liquid phase, or transformation is occurring at equal rates in both the liquid and sorbed phases (Backhus et al, 1997). Equation 3 describes the observed lumped transformation constant (Toride

et al, 1995). Due to the uncertainty of where the decay is occurring, the decay constants will be calculated for both of the cases described above.

Table 10. Lumped First Order Transformation Constants

Study		Material	v (cm/min)	μ Chromate (1/hr)	μ PCE (1/hr)
Batch Kinetic		SMZ/ZVI	---	**0.053**	**0.136**
		Z/ZVI	---	**0.131**	**0.054**
Column Studies	A	SMZ/ZVI	0.208	**0.155**	**0.099**
			0.147	**0.147**	**0.134**
			0.074	**0.210**	**0.197**
	B	SMZ/ZVI	0.197	**0.132**	**0.077**
			0.138	**0.156**	**0.128**
			0.070	**0.179**	**0.199**
Column Studies	C	Z/ZVI	0.186		**0.046**
			0.134		**0.108**
			0.070		**0.126**
	D	Z/ZVI	0.193		**0.037**
			0.135		**0.115**
			0.070		**0.144**

Johnson et al (1996) and Powell et al (1995) have noted that the solid to solution ratio and the surface area affect the rate of transformation for chromate or PCE in batch ZVI studies. The first order transformation constant thus must be normalized to the surface area of the material and the concentration of iron within the system. Equation 10 describes the normalized transformation rate constant (Johnson, 1995).

$$\mu_{SA} = \frac{\mu_{L\,or\,S}}{\rho_m S_a} \tag{10}$$

Where:
- μ_{SA} = normalized decay constant (mL/hr-cm^2)
- $\mu_{L\,or\,S}$ = first order transformation constant (liquid or sorbed phase) (1/hr)
- ρ_m = mass concentration of Fe^0 (g/mL)
- S_A = specific surface area (cm^2/g)

The surface area of the pellets was estimated from the sieve analysis (Figure 11) assuming spherically shaped particles and that the iron surface area is similar to that of the spherically shaped particle. From the sieve analysis, the mass of pellets in between two sieve mesh was determined. The diameter of the particles was taken as the average of the sieve diameter the pellets were retained on and the last sieve the pellets passed through. The volume of a single particle could be calculated from $4/3\pi\ r^3$, where r is the effective radius or half of the diameter. The number of pellets retained on each sieve was estimated by the following equation, using a pellet bulk density 1.3 g/cm^3:

$$np = \frac{M_{ret}}{V_{particle} * \rho_{bulk}} \tag{11}$$

Where:
- np = number of pellets
- $V_{particle}$ = volume of a single pellet = $\frac{4}{3}\pi r^3$ (cm^3)
- M_{ret} = mass of pellets retained on the sieve (g)

The surface area for a single pellet was assumed to be equal to $2\pi r^2$ refleting the assumption that iron represented only half of the pellet surface. By multiplying the surface area of a single pellet by the number of pellets retained on the sieve, the total surface area for each sieve fraction could be determined. The specific surface area for each sieve fraction could then be determined by dividing by the mass retained on the sieve. The specific surface area for the entire sample was determined by summing the percentage of pellets, based on number of pellets, by the specific surface area for each sieve interval. The specific surface areas were determined to be 60.3 and 2.4 cm^2/g for the SMZ/ZVI and Z/ZVI materials, respectively (The specific surface areas were not adjusted to the iron ratio for the normalization of the transformation constant). Table 11 lists the results for the normalized first order transformation constants determined from the batch kinetic and column studies for both cases listed above. The porosity values are listed in Appendix A and it was assumed that the porosity of the batch kinetic studies was similar to that of the column studies.

Table 11 indicates that the rate of decay increases as the velocity decreases. The highest rate of transformation is apparent from the batch kinetic studies. These results imply transformation of PCE and chromate with the SMZ/ZVI and Z/ZVI material is a mass transferred limited process. Burris et al (1998) speculated that the rate limiting step in the transformation of chlorinated ethylenes was the desorption of the solute off of the reactive iron site. Figure 35 shows how the solution velocity affects the normalized transformation constant ($\mu_S = 0$) for chromate by the SMZ/ZVI pellets and for PCE by

the Z/ZVI and SMZ/ZVI pellets. Two axes are shown in Figure 35 to combine the SMZ/ZVI and Z/ZVI values.

Table 11. Normalized First Order Decay Constants

Study		Material	V (cm/min)	μ_{SA} Chromate (mL/hr-m^2)		μ_{SA} Perchloroethylene (mL/hr-m^2)	
				$\mu_S=0$	$\mu_L=\mu_S$	$\mu_S=0$	$\mu_L=\mu_S$
Kinetic Batch		SMZ/ZVI	---	**17.6**	**6.65**	**45.1**	**2.54**
		Z/ZVI	---	**1160**	**1160**	**469**	**99.0**
Column Studies	A	SMZ/ZVI	0.208	**11.2**	**2.08**	**7.16**	**0.281**
			0.147	**10.3**	**8.78**	**9.68**	**0.507**
			0.074	**15.2**	**1.60**	**14.3**	**0.646**
	B	SMZ/ZVI	0.197	**10.8**	**2.62**	**6.35**	**0.305**
			0.138	**12.8**	**10.2**	**10.5**	**0.711**
			0.070	**14.7**	**1.46**	**16.3**	**1.00**
Column Studies	C	Z/ZVI	0.186	--	--	**103**	**24.4**
			0.134	--	--	**243**	**51.6**
			0.070	--	--	**284**	**59.0**
	D	Z/ZVI	0.193	--	--	**71.9**	**13.1**
			0.135	--	--	**222**	**42.4**
			0.070	--	--	**279**	**44.6**

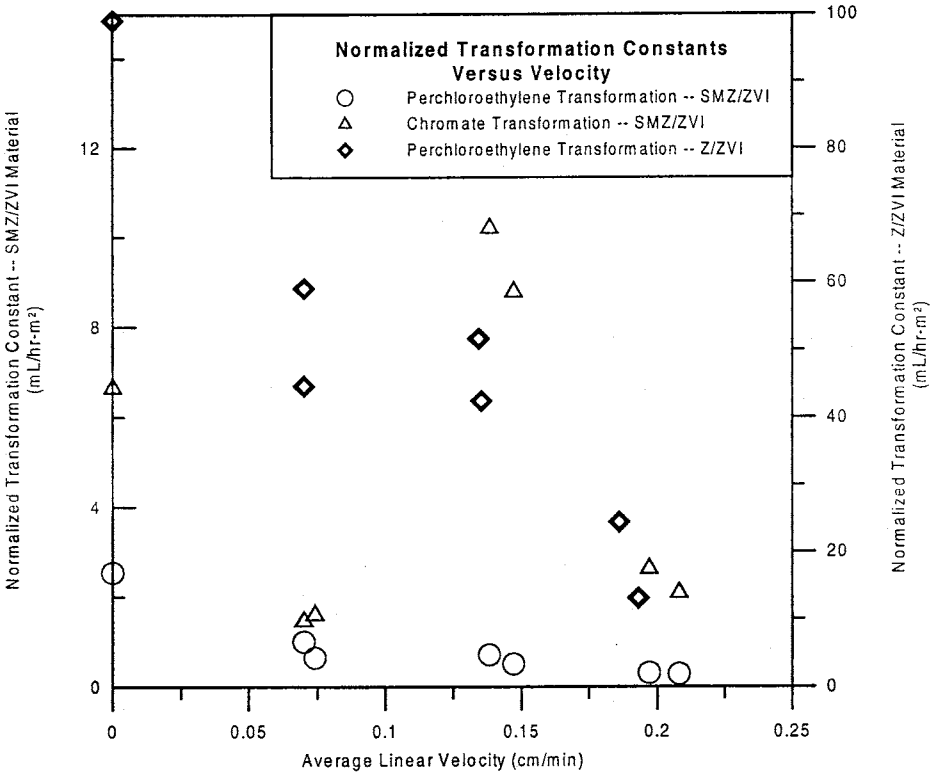

Figure 35. Normalized Decay Constants ($\mu_S = 0$) versus Velocity

Figure 35 indicates that the normalized transformation constant increases towards the value determined from the batch kinetic study results. The batch kinetic study results should indicate the maximum transformation constant for the material since no mass transfer limitations are present during this experiment (plotted at a velocity of zero). Figure 36 shows how the results for the normalized transformation constant ($\mu_S = \mu_L$) varies with velocity for chromate and PCE transformation with the SMZ/ZVI pellet and PCE for the Z/ZVI pellet.

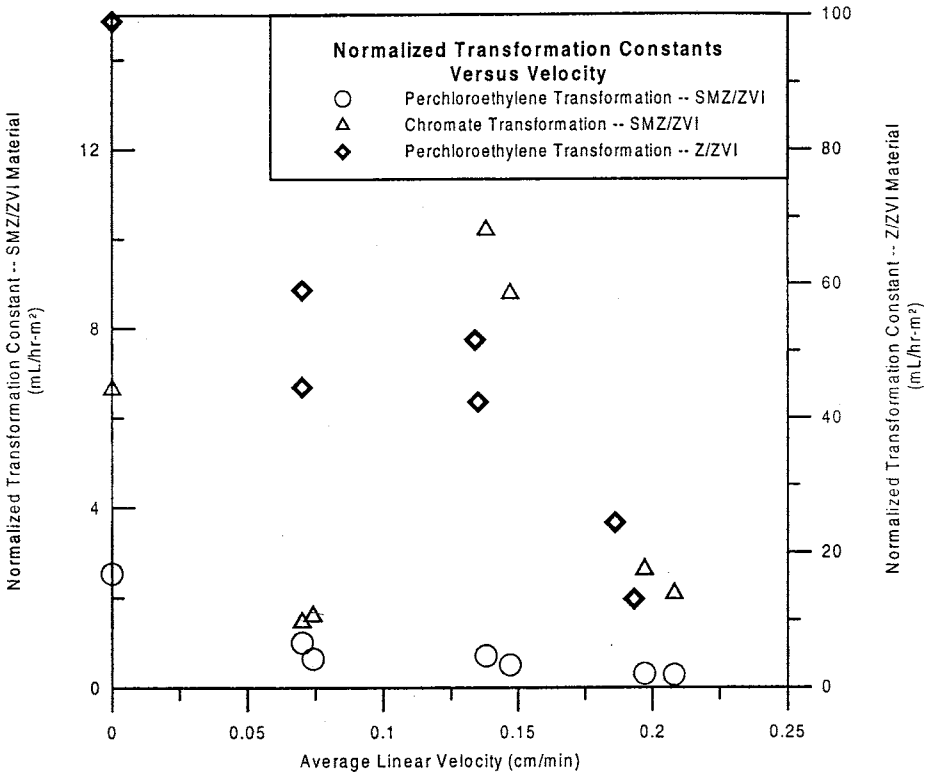

Figure 36. Normalized Transformation Constants ($\mu_S = \mu_L$) versus Velocity

The results of the normalized transformation constant show a larger normalized transformation rate if PCE or chromate can be transformed within the sorbed phase. Figure 36 indicates that as the velocity decreased the normalized transformation constant increases. These results indicate mass transfer limitations during the transformation process of PCE and chromate. The results for chromate transformation by the SMZ/ZVI pellet do not indicate the trend as well as the PCE data shows. The error in measuring the retardation of chromate by SMZ/ZVI has a strong affect on the normalized transformation constant when transformation in the sorbed phase is considered.

V.

Summary and Conclusions

The results from the batch kinetic studies and the variable flow rate column studies indicate transformation of chromate is occurring in both the SMZ/ZVI and Z/ZVI pellets, while sorption and degradation of perchloroethylene (PCE) is occurring with the SMZ/ZVI and Z/ZVI pellets. The sorption of PCE onto the Z/ZVI pellets is smaller than the SMZ/ZVI pellets and is more than likely due to non-reductive carbon sites within the iron material. The lack of sorption of chromate is due to incomplete surfactant bilayer formation on the SMZ/ZVI pellets. The incomplete bilayer formation was evident from the SMZ/ZVI pellets ability to sorb an additional 21.1 mmol HDTMA /kg pellet and from the observation that SMZ/ZVI pellets retreated with HDTMA were able to sorb chromate. The presence of a monolayer was seen by sorption of PCE with the SMZ/ZVI and retreated pellets with little change in the distribution coefficient, 5.46 versus 5.71 L/kg.

The Z/ZVI and SMZ/ZVI pellets had different particle size distributions. The SMZ/ZVI pellets had a broader particle size distribution with approximately 25% of the pellets less than 600 μm in diameter. The variation in the particle size distribution caused a difference in the hydrodynamic properties of each column. Due to the finer-grain-sized particles, more dispersion was seen in the SMZ/ZVI columns, (dispersivities of 9.52 and 7.41 cm), than in Z/ZVI columns, (dispersivities of 4.48 and 4.14 cm), or the zeolite columns, (dispersivities of 1.15 and 1.21 cm)..

The chromate batch kinetic and column study results compared well to each other. The average chromate distribution coefficient was determined to be 0.481 ±0.46 L/kg for the SMZ/ZVI pellets; no sorption of chromate was seen for the Z/ZVI pellets. The first order transformation constant increased with a decreasing velocity indicating a mass-

transfer-limited process. For the chromate column studies, the first order transformation constant ranged from 0.037 to 0.144 hr^{-1} for the SMZ/ZVI pellets, while the results of the chromate batch kinetic study indicated a first order transformation constant of 0.136 and 0.054 hr^{-1} for the SMZ/ZVI and Z/ZVI pellets, respectively. First order transformation constants were not determined for the Z/ZVI column studies since complete transformation of chromate occurred. The batch kinetic and column study results indicated that the Z/ZVI pellets transform chromate faster than SMZ/ZVI pellets. However, without sorption of chromate no conclusions can be inferred about the enhanced transformation process for chromate. The complete transformation of chromate seen for the Z/ZVI pellets may indicate the surfactant monolayer formed on the surface of the pellets may inhibit the reduction potential of the pellet material. The exact reason for the greater transformation seen in the Z/ZVI pellets is uncertain.

The results for the batch kinetic and column studies for PCE were similar. The average PCE distribution coefficient was determined to be 2.28 ±0.41 L/kg and 0.524 ± 0.07 L/kg for the SMZ/ZVI and Z/ZVI pellets, respectively. The sorption of PCE onto the SMZ/ZVI or Z/ZVI pellets was not a mass-transfer-limited process. The transformation of PCE also varied with the linear velocity. The lumped first order transformation constant varied from 0.077 to 0.199 hr^{-1} and 0.037 to 0.144 hr^{-1} for the SMZ/ZVI and Z/ZVI pellets, respectively. The batch kinetic studies indicated first order transformation constants of 0.136 and 0.054 hr^{-1} for the SMZ/ZVI and Z/ZVI pellets. The observed results for the batch kinetic and column studies indicate that the SMZ/ZVI pellets transform PCE more readily than the Z/ZVI pellets. There was an apparent enhanced transformation.

The lumped first order transformation constants were normalized to the specific surface area and the mass concentration of pellets to better compare the first order lumped transformation constants. The observed first order transformation constant is a lumped parameter of the transformation occurring in the sorbed phase and the liquid phase. Two possible cases were considered: transformation is only occurring in the liquid, or and transformation is occurring at equal rates in both the liquid and sorbed phases. The normalized PCE transformation constants for only transformation in the liquid phase ranged from 6.35 to 45.1 mL/hr-m^2 and 71.9 to 469 mL/hr-m^2 for the SMZ/ZVI and Z/ZVI pellets, while the normalized chromate transformation constants ranged from 10.8 to 17.6 mL/hr-m^2 for the SMZ/ZVI pellets. The Z/ZVI chromate batch kinetic study indicated a normalized transformation constant of 1160 hr/mL-m^2. In the case of transformation occurring equally in both sorbed and liquid phases, the normalized PCE transformation constants ranged from 0.281 to 2.54 mL/hr-m^2 for the SMZ/ZVI pellets, while the Z/ZVI pellets ranged from 13.1 to 99.0 hr/mL-m^2. The chromate batch kinetic studies produced a normalized transformation constant of 6.65 mL/hr-m^2 for the SMZ/ZVI pellets. The results of the normalized transformation constant indicate the greater transformation seen in the batch kinetic studies and column studies for PCE may not have been due to sorption of PCE onto the surface of the pellet. The apparent enhanced transformation seems to be due primarily to an increased surface area with the finer grain sized particles.

If research continues on the SMZ/ZVI pellets, I recommend the following work to be performed:

1) To study the effects of the dual sorption/reduction process in better detail, the ration of zeolite/iron in the pellet material should be altered. When more zeolite material is present, the extent of the surfactant layer will also increase while so will the ability for the pellet to sorb chromate or PCE. Increased sorption of chromate or PCE may also allow for a more enhanced transformation than was seen in these studies.
2) The pH conditions of the pellet material should be lowered. Lowering the pH conditions would increase the transformation rate of chromate. However, a new binder solution may be needed that does not produce the large amount of NaOH.
3) Studies should also be performed to determine the transformation rate constants for the daughter products of PCE. Ethylene is the least toxic compound in the PCE transformation process. The individual rate constants would allow for someone to design the permeable reactive barrier if the SMZ/ZVI material were to be used at an actual site.

VI.

References

VI.

References

Backhus, D.A., Picardal, F.W., Johnson, S., Knowles, T., Collins, R., Radue, A., and Kim, S., (1997) "Soil- and Surfactant-Enhanced Reductive Dechlorination of Carbon Tetrechlride in the Presence of *Shewanella Putrefaciens 300.*" *Journal of Contaminant Hydrology*, 28, 337-361.

Bear, J., Dynamics of Fluids in Porous Media. New York, Dover Publications, Inc, 1972.

Beyersmann, D., Koester, A., Buttner, B., Flessel, P., (1984) "Model reactions of Chromium Compounds with Mammalian and Bacterial Cells." *Environmental Toxicology and Chemistry*, 8, 279-286.

Bianchi,V., Zantedeschi, A., Montaldi, A., and Majone, F., (1984) "Trivalent Chromium is Neither Cytotoxic nor Mutagenic in Permealized Hamster Fibroblasts." *Toxicological Letters*, 23, 51-59.

Blowes, D.W., Ptacek, C.J., Jambor, .L. (1997). "*In-Situ* of Cr (VI)- Contaminated Groundwater Using Permeable Reactive Walls: Laboratory Studies." *Environmental Science and Technology*, 31(12), 3348-3357.

Burris, D.R., Allen-King, M.A., Manoranjan, V.S., Campbell, T.J.m Loraine, G.A., and Deng, B., (1998). "Chlorinated Ethene Reduction By Cast Iron: Sorption and Mass Transfer." *Journal of Environmental Engineering*, 124(10), 1012- 1019.

Jackson, D.E., (1985). "Anaerobic Degradation of Trichloroethylene in Soil." *Environmental Science and Technology*, 19(3), 277-279.

Johnson, T.L., Scherer, M.M., and Tratnyek, P.G., (1996). "Kinetics of Halogenated Organic Compound Degradation by Iron Metal." *Environmental Science and Technology*, 30, 2634-2640.

Li, Z., and Bowman, R.S., (1997). "Counterion Effects on the Sorption of Cationic Surfactant and Chromate on Natural Clinoptilolite." *Environmental Science and Technology*, 31(8), 3407-2412.

Li, Z., and Bowman, R.S., (1998). "Sorption of Chromate and PCE By Surfactant-Modified Clay Minerals." *Environmental Engineering Science*, 15(3), 237-245.

Mackay, D.M. and Cherry, J.A., (1989). "Groundwater Contamination: Pump-and-treat remediation." *Environmental Science and Technology*, 23(6) 630-636.

Jones, H., Li, Z, and Bowman, R.S., (1998). "Reduction of Dissolved Perchloroethylene by Pelletized Zero Valent Iron/Surfacatnt-Modified Zeolite." In Proceedings of WERC/ WRHSRC/ NMHWMS Joint Conference on the Environment, Albuquerque, NM, March 31- April 1, 1998.

Maimone, M. (1997). "Coping with Groundwater Contamination," *Chemical Engineering*, October, p. 195-202.

Nriagu, J.O., (1988). "Production and Uses of Chromium." Chromium in the Natural and Human Environments, Vol. 20, 1-2; New York: John Wiley & Sons.

Ono,B., (1988). "Genetic Approaches in the Study of Chromium Toxicity and Resistance in Yeast and Bacteria." Chromium in the Natural and Human Environments, Vol. 20, pg. 351-368; New York: John Wiley and Sons.

Palmer, C.D. and Puls, R.W. (1994). "Natural Attenuation of Hexavalent Chromium in Ground Water and Soils." *Ground Water Issue*, EPA/540/S-94/505, October.

Pontius, F.W., (1995). "An Update of the Federal Drinking-Water Regs," *Journal American Water Works Association*, 87(2), 48-58

Powell, R.M., Puls, R.W., Hightower, S.K., and Sabatini, D.A., (1995). "Coupled Iron Corrosion and Chromate Reduction: Mechanisms for Subsurface Remediation." *Environmental Science and Technology*, 29(8), 1913- 1922.

Roberts, L.A., Totten, L.A., Arnold, W.A., Burris, D.R., and Campbell, T.J., (1996). "Reductive Elimination of Chlorinated Ethylenes by Zero-Valent Iron Metals," *Environmental Science and Technology*, 30(8), 2654-2659.

Schwille, F., (1988). "Dense Chlorinated Solvents in Porous and Fractured Media," Lewis Publishers, Chelsea, Mich., p.146.

Sims, J.L., Suflita, J.M., Russell, H.H., (1991). "Reductive Dehalogenation of Organic Contaminants in Soils and Ground Water," *Ground Water Issue*, January, EPA/540/4-90/054.

Snoeyink, V.L., and Jenkins, D., (1980). Water Chemistry, pg. 463, New York: John Wiley & Sons.

Stollenwerk, K.G., and Grove, D.B., (1985). "Reduction of Hexavalent Chromium in Water Sampled Acidified for Preservation," *Journal of Environmental Quality*, 14, 396-399.

Toride, N., Leij, F.J., and Van Genuchten, M. Th. The CXTFIT Code for Estimating Transport Parameters from Laboratort or Field Tracer Experiments version 2.0. U.S. Salinity Laboratory, August 1995.

van Weerelt, M., Pfeiffer, W.C., and Fiszman, M., (1984). "Uptake and Release of $^{51}Cr(VI)$ and $^{51}Cr(III)$ by Barnacles." *Marine Environmental Research*, 11, 201-211.

Wilson, J.L. (1997). "Removal of Aqueous Phase Dissolved Contamination: Non-chemcially enhanced pump-and-treat." Subsurface Restoration, Ward, C.H., Cherry, J.A., Scalf, M.R., Ann Arbor Press, Chelsea, Mich.

Yassi, A., and Nieboer, E., (1988). "Carcinogenicity of Chromium Compounds." Chromium in the Natural and Human Environments, pg 443-496; New York: John Wiley & Sons.

Appendix A

General Column Information

Column A -- SMZ/ZVI

Unpacked Weight	491.30	g
Packed Weight	755.32	g
Saturated Mass of Column	810.00	g
Mass of Pellets(not dry)	264.02	g
Mass of Pellets (Dry)	220.32	g
Mass of Water in Fittings	2.00	g
Mass of Water in Column	96.38	g
Gravimetric Water Content	16.55%	
Mass to Volume	2.286	
Cross Sectional Area	19.6	cm^2
Length	31.5	cm
Porosity	**0.156**	
Pore Volume	**96.38**	**ml**

Column B -- SMZ/ZVI

Unpacked Weight	544.13	g
Packed Weight	794.20	g
Saturated Mass of Column	858.00	g
Mass of Pellets(not dry)	250.07	g
Mass of Pellets (Dry)	208.68	g
Mass of Water in Fittings	2.00	g
Mass of Water in Column	103.19	g
Gravimetric Water Content	16.55%	
Mass to Volume	2.022	
Cross Sectional Area	19.6	cm^2
Length	31.5	cm
Porosity	**0.167**	
Pore Volume	**103.19**	**ml**

Column C -- Z/ZVI

Unpacked Weight	527.23	g
Packed Weight	746.80	g
Saturated Mass of Column	823.00	g
Mass of Pellets(not dry)	219.57	g
Mass of Pellets (Dry)	189.12	g
Mass of Water in Fittings	2.00	g
Mass of Water in Column	106.65	g
Gravimetric Water Content	13.87%	
Mass to Volume	1.773	
Cross Sectional Area	19.6	cm^2
Length	31.5	cm
Porosity	**0.173**	
Pore Volume	**106.65**	**ml**

Column D -- Z/ZVI

Unpacked Weight	508.30	g
Packed Weight	744.70	g
Saturated Mass of Column	815.00	g
Mass of Pellets(not dry)	236.40	g
Mass of Pellets (Dry)	203.61	g
Mass of Water in Fittings	2.00	g
Mass of Water in Column	101.09	g
Gravimetric Water Content	13.87%	
Mass to Volume	2.014	
Cross Sectional Area	19.6	cm^2
Length	31.5	cm
Porosity	**0.164**	
Pore Volume	**101.09**	**ml**

Column E -- Zeolite

Unpacked Weight	452.24	g
Packed Weight	586.34	g
Saturated Mass of Column	732.24	g
Mass of Pellets(not dry)	--	g
Mass of Pellets (Dry)	134.10	g
Mass of Water in Fittings	--	g
Mass of Water in Column	145.90	g
Gravimetric Water Content	---	
Mass to Volume	0.919	
Cross Sectional Area	19.6	cm^2
Length	32	cm
Porosity	**0.220**	
Pore Volume	**145.90**	**ml**

Column F -- Zeolite

Unpacked Weight	466.47	g
Packed Weight	601.51	g
Saturated Mass of Column	744.57	g
Mass of Pellets(not dry)	--	g
Mass of Pellets (Dry)	135.04	g
Mass of Water in Fittings	--	g
Mass of Water in Column	143.06	g
Gravimetric Water Content	---	
Mass to Volume	0.944	
Cross Sectional Area	19.6	cm^2
Length	32.8	cm
Porosity	**0.220**	
Pore Volume	**143.06**	**ml**

Appendix B

Raw Data for Non- Reactive Tracer Study

Column A - SMZ/ZVI Pellets

Bottle Weight 76.78 g

Pore Volume 96.38 ml

Sample	Time	Elapsed time(min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Tritium	C/Co
Aout-0	10:18:00 AM	0.00	0	0	0.000	0.000	22	0.000
Aout-1	10:49	31.00	99.63	22.85	0.237	0.237	22441	0.076
Aout-2	11:18	29.00	102.33	25.55	0.265	0.502	78547	0.267
Aout-3	11:46	28.00	100.77	23.99	0.249	0.751	133255	0.454
Aout-4	12:15	29.00	100.88	24.1	0.250	1.001	180123	0.613
Aout-5	12:45	30.00	103	26.22	0.272	1.273	211062	0.718
Aout-6	13:15	30.00	101.2	24.42	0.253	1.527	240643	0.819
Aout-7	13:42	27.00	100.03	23.25	0.241	1.768	250489	0.853
Aout-8	14:02	20.00	101.41	24.63	0.256	2.023	277708	0.945
Aout-9	14:48	46.00	106.63	29.85	0.310	**2.333**	291095	0.991
Aout-10	15:31	43.00	103.82	27.04	0.281	2.614	273626	0.931
Aout-11	16:01	30.00	97.83	21.05	0.218	2.832	223551	0.761
Aout-12	16:31	30.00	101.84	25.06	0.260	3.092	178228	0.607
Aout-13	17:14	43.00	110.67	33.89	0.352	3.444	126968	0.432
Aout-14	17:55	41.00	109.42	32.64	0.339	3.782	86293	0.294
Aout-15	18:14	19.00	94.57	17.79	0.185	3.967	65063	0.221
Aout-16	18:51	37.00	108.41	31.63	0.328	4.295	45752	0.156
Aout-17	19:26	35.00	107.08	30.3	0.314	4.609	31532	0.107
Aout-18	20:01	35.00	106.6	29.82	0.309	4.919	22372	0.076
Aout-19	20:39	38.00	108.74	31.96	0.332	5.250	15344	0.052
Aout-20	21:24	45.00	116.35	39.57	0.411	5.661	9979	0.034
Aout-21	22:42	78.00	141.9	65.12	0.676	6.337	5212	0.018

BOLD - End of Tritium Slug

Column B - SMZ/ZVI Pellets

Bottle Weight 70.39 g

Pore Volume 103.19 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Tritium (counts)	C/Co
Bout-0	10:18:00 AM		0	0	0.000	0.000	17	0.000
Bout-1	10:50	32.00	96.72	26.33	0.255	0.255	11823	0.040
Bout-2	11:19	29.00	96.85	26.46	0.256	0.512	75193	0.256
Bout-3	11:47	28.00	94.43	24.04	0.233	0.745	134824	0.459
Bout-4	12:16	29.00	95.98	25.59	0.248	0.993	180585	0.615
Bout-5	12:46	30.00	96.16	25.77	0.250	1.242	215013	0.732
Bout-6	13:16	30.00	97.56	27.17	0.263	1.506	250050	0.851
Bout-7	13:43	27.00	93.85	23.46	0.227	1.733	256320	0.873
Bout-8	14:13	30.00	95.82	25.43	0.246	1.979	276421	0.941
Bout-9	14:49	36.00	99.7	29.31	0.284	**2.263**	275577	0.938
Bout-10	15:39	50.00	101.19	30.8	0.298	2.562	278553	0.948
Bout-11	16:02	23.00	91.62	21.23	0.206	2.768	229562	0.781
Bout-12	16:33	31.00	96.38	25.99	0.252	3.019	173005	0.589
Bout-13	17:15	42.00	104.46	34.07	0.330	3.350	122389	0.417
Bout-14	17:56	41.00	103.74	33.35	0.323	3.673	76178	0.259
Bout-15	18:15	19.00	88.91	18.52	0.179	3.852	60945	0.207
Bout-16	18:53	38.00	103.89	33.5	0.325	4.177	39523	0.135
Bout-17	19:28	35.00	102.05	31.66	0.307	4.484	26423	0.090
Bout-18	20:04	36.00	102.18	31.79	0.308	4.792	17115	0.058
Bout-19	20:40	36.00	102.68	32.29	0.313	5.105	12115	0.041
Bout-20	21:25	45.00	110.54	40.15	0.389	5.494	6834	0.023
Bout-21	22:43	78.00	137.58	67.19	0.651	6.145	3232	0.011

BOLD - End of Tritium Slug

Column C - Z/ZVI Pellets

Bottle Weight 70.8 g

Pore Volume 106.65 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Tritium (counts)	C/Co
Cout-0	10:18:00 AM		0	0	0.000	0.000	21	0.000
Cout-1	10:52	34.00	98.63	27.83	0.261	0.261	426	0.001
Cout-2	11:21	29.00	96.4	25.6	0.240	0.501	54211	0.185
Cout-3	11:48	27.00	95.08	24.28	0.228	0.729	118510	0.403
Cout-4	12:17	29.00	96.5	25.7	0.241	0.970	165086	0.562
Cout-5	12:47	30.00	96.23	25.43	0.238	1.208	205715	0.700
Cout-6	13:17	30.00	97.45	26.65	0.250	1.458	244187	
Cout-7	13:44	27.00	93.55	22.75	0.213	1.671	255556	0.870
Cout-8	14:14	30.00	95.73	24.93	0.234	1.905	265595	0.904
Cout-9	14:51	37.00	98.91	28.11	0.264	**2.168**	285860	0.973
Cout-10	15:41	50.00	101.89	31.09	0.292	2.460	289855	0.987
Cout-11	16:04	23.00	91.35	20.55	0.193	2.653	293591	0.999
Cout-12	16:34	30.00	96.53	25.73	0.241	2.894	216832	0.738
Cout-13	17:16	42.00	104.5	33.7	0.316	3.210	143299	0.488
Cout-14	17:57	41.00	104.39	33.59	0.315	3.525	83490	0.284
Cout-15	18:16	19.00	89.1	18.3	0.172	3.696	63184	0.215
Cout-16	18:55	39.00	103.96	33.16	0.311	4.007	40539	0.138
Cout-17	19:29	34.00	100.64	29.84	0.280	4.287	25292	0.086
Cout-18	20:05	36.00	102.26	31.46	0.295	4.582	16391	0.056
Cout-19	20:42	37.00	102.28	31.48	0.295	4.877	10008	0.034
Cout-20	21:27	45.00	109.19	38.39	0.360	5.237	5974	0.020
Cout-21	22:45	78.00	137.08	66.28	0.621	5.859	2679	0.009

BOLD - End of Tritium Slug

Column D - Z/ZVI Pellets

Bottle Weight 70.8

Pore Volume 101.09

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Tritium Counts	C/Co
Dout-0	10:18:00 AM		0	0	0.000	0.000	0	0.000
Dout-1	10:53	35.00	100.06	29.26	0.289	0.289	293.774	0.001
Dout-2	11:22	29.00	96.35	25.55	0.253	0.542	42009.682	0.143
Dout-3	11:50	28.00	94.34	23.54	0.233	0.775	105171.092	0.358
Dout-4	12:19	29.00	96.15	25.35	0.251	1.026	153937.576	0.524
Dout-5	12:48	29.00	96.33	25.53	0.253	1.278	229437.494	0.781
Dout-6	13:19	31.00	96.8	26	0.257	1.536	253233.188	0.862
Dout-7	13:45	26.00	93.41	22.61	0.224	1.759	271740.95	0.925
Dout-8	14:15	30.00	96.93	26.13	0.258	2.018		
Dout-9	14:52	37.00	97.65	26.85	0.266	**2.283**	286723.424	0.976
Dout-10	15:41	49.00	103.29	32.49	0.321	2.605	285254.554	0.971
Dout-11	16:05	24.00	91.26	20.46	0.202	2.807	295242.87	1.005
Dout-12	16:35	30.00	78.01	7.21	0.071	2.878	227381.076	0.774
Dout-13	17:17	42.00	105.72	34.92	0.345	3.224	153937.576	0.524
Dout-14	17:58	41.00	104.22	33.42	0.331	3.554	98414.29	0.335
Dout-15	18:17	19.00	88.8	18	0.178	3.733	67861.794	0.231
Dout-16	18:56	39.00	102.8	32	0.317	4.049	46122.518	0.157
Dout-17	19:30	34.00	101.09	30.29	0.300	4.349	28496.078	0.097
Dout-18	20:06	36.00	102.45	31.65	0.313	4.662	17626.44	0.060
Dout-19	20:43	37.00	103.07	32.27	0.319	4.981	10575.864	0.036
Dout-20	21:28	45.00	109.13	38.33	0.379	5.360	5875.48	0.020
Dout-21	22:46	78.00	138.62	67.82	0.671	6.031	2350.192	0.008

BOLD - End of Tritium Slug

Column E - Zeolite Pellets

Bottle Weight	64.08	g
Pore Volume	145.90	ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Tritium (counts)	C/Co
Eout-0	10:18:00 AM					0.000	12	0.000
Eout-1	10:54	36.00	93.15	29.07	0.399	0.399	14	0.000
Eout-2	11:24	30.00	90.54	26.46	0.181	0.580	2656	0.009
Eout-3	11:52	28.00	89.48	25.4	0.174	0.754	43188	0.147
Eout-4	12:20	28.00	88.08	24	0.164	0.919	119936	0.408
Eout-5	12:49	29.00	90.96	26.88	0.184	1.103	187733	0.639
Eout-6	13:20	31.00	90.85	26.77	0.183	1.287	249427	
Eout-7	13:46	26.00	87.18	23.1	0.158	1.445	282782	0.963
Eout-8	14:17	31.00	90.3	26.22	0.180	1.625	299125	1.018
Eout-9	14:53	36.00	90.72	26.64	0.183	**1.807**	298451	1.016
Eout-10	15:43	50.00	97.74	33.66	0.231	2.038	298848	1.017
Eout-11	16:07	24.00	86.04	21.96	0.151	2.189	316773	1.078
Eout-12	16:37	30.00	89.05	24.97	0.171	2.360	288835	0.983
Eout-13	17:18	41.00	98.48	34.4	0.236	2.595	187382	0.638
Eout-14	17:59	41.00	98.79	34.71	0.238	2.833	92822	0.316
Eout-15	18:19	20.00	82.55	18.47	0.127	2.960	55463	0.189
Eout-16	18:57	38.00	97.09	33.01	0.226	3.186	26590	0.091
Eout-17	19:32	35.00	94.92	30.84	0.211	3.398	11677	0.040
Eout-18	20:07	35.00	95.44	31.36	0.215	3.613	5505	0.019
Eout-19	20:44	37.00	96.86	32.78	0.225	3.837	2452	0.008
Eout-20	21:28	44.00	103.68	39.6	0.271	4.109	1021	0.003
Eout-21	22:48	80.00	133.07	68.99	0.473	4.581	398	0.001

BOLD - End of Tritium Slug

Column F - Zeolite Pellets

Bottle Weight 69.82 g

Pore Volume 143.06 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Tritium (counts)	C/Co
Fout-0	10:18:00 AM		0	0	0.000	0.000	22	0.000
Fout-1	10:56	38.00	131.5	61.5	0.415	0.415	17	0.000
Fout-2	11:25	29.00	94.74	24.92	0.174	0.589	2361	0.008
Fout-3	11:54	29.00	93.35	23.53	0.164	0.754	30185	0.103
Fout-4	12:21	27.00	92.68	22.86	0.160	0.913	93563	0.318
Fout-5	12:50	29.00	94.97	25.15	0.176	1.089	171821	0.585
Fout-6	13:21	31.00	94.71	24.89	0.174	1.263	233900	
Fout-7	13:47	26.00	91.23	21.41	0.150	1.413	266529	0.907
Fout-8	14:18	31.00	93.95	24.13	0.169	1.582	282887	0.963
Fout-9	14:54	36.00	94.62	24.8	0.173	**1.755**	291358	0.992
Fout-10	15:44	50.00	102.03	32.21	0.225	1.980	312343	1.063
Fout-11	16:08	24.00	90.84	21.02	0.147	2.127	308720	1.051
Fout-12	16:38	30.00	92.81	22.99	0.161	2.288	292795	0.997
Fout-13	17:19	41.00	101.64	31.82	0.222	2.510	211263	0.719
Fout-14	18:00	41.00	102.34	32.52	0.227	2.737	115543	0.393
Fout-15	18:20	20.00	87.83	18.01	0.126	2.863	72736	0.248
Fout-16	18:58	38.00	100.57	30.75	0.215	3.078	31634	0.108
Fout-17	19:32	34.00	99.06	29.24	0.204	3.283	14776	0.050
Fout-18	20:08	36.00	99.29	29.47	0.206	3.489	6248	0.021
Fout-19	20:45	37.00	100.9	31.08	0.217	3.706	2877	0.010
Fout-20	21:29	44.00	106.96	37.14	0.260	3.966	1510	0.005
Fout-21	22:49	80.00	134.37	64.55	0.451	4.417	595	0.002

BOLD - End of Tritium Slug

Appendix C

Raw Data for Reactive Tracer Studies

Column A - SMZ/ZVI Pellets (1 mL/min)

Bottle Weight 76.78 g

Pore Volume 96.38 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Aout-1	7/27/98 11:13	0.00	156.14	79.36	0.823	0.823	1.159	0.042	0	0.000	0
Aout-2	7/27/98 13:13	120.00	142	65.22	0.677	1.500	4.401	0.159	0	0.000	0
Aout-3	7/27/98 17:31	258.00	126.02	49.24	0.511	2.011	4.818	0.174	0	0.000	0
Aout-4	7/27/98 19:33	122.00	168.6	91.82	0.953	2.964	7.959	0.287	0	0.000	0
Aout-5	7/27/98 21:56	143.00	180.36	103.58	1.075	4.038	12.992	0.468	0	0.000	0.102
Aout-6	7/28/98 1:53	237.00	151.9	75.12	0.779	4.818	14.119	0.509	1.163	0.064	0.169
Aout-7	7/28/98 7:00	307.00	226.98	150.2	1.558	6.376	14.184	0.511	1.0309	0.057	0.183
Aout-8	7/28/98 8:40	100.00	154.6	77.82	0.807	7.184	13.825	0.498	1.8789	0.103	0.375
Aout-9	7/28/98 10:05	85.00	140.19	63.41	0.658	7.841	16.06	0.579	2.147	0.118	0.388
Aout-10	7/28/98 12:15	130.00	172.32	95.54	0.991	8.833	16.716	0.603	3.2871	0.180	1.047
Aout-11	7/28/98 14:01	106.00	102.24	25.46	0.264	9.097	17.5	0.631	2.4596	0.135	0.607
Aout-12	7/28/98 15:33	92.00	148.16	71.38	0.741	9.837	15.447	0.557	3.151	0.173	0.721
Aout-13	7/28/98 17:23	110.00	157.58	80.8	0.838	10.676	17.31	0.624	3.7225	0.204	0.718
Aout-14	7/28/98 19:05	102.00	151.31	74.53	0.773	11.449	18.257	0.658	4.137	0.227	0.749
Aout-15	7/28/98 21:38	153.00	137.42	60.64	0.629	12.078	18.589	0.670	3.22	0.177	0.623
Aout-16	7/28/98 23:30	112.00	152.37	75.59	0.784	12.863			4.568	0.250	0.816
Aout-17	7/29/98 8:30	540.00	206.31	129.53	1.344	14.207			2.655	0.146	0.638
Aout-18	7/29/98 11:08	158.00	206.86	130.08	1.350	15.556			5.748	0.315	1.019
Aout-19	7/29/98 13:00	112.00	157	80.22	0.832	16.388			6.34	0.348	1.31
Aout-20	7/29/98 15:12	132.00	169.72	92.94	0.964	17.353			7.305	0.400	1.368
Aout-21	7/29/98 16:54	102.00	152.43	75.65	0.785	18.138	19.537	0.704	7.246	0.397	1.285
Aout-22	7/29/98 19:09	135.00	176.88	100.1	1.039	19.176	19.808	0.714	8.223	0.451	1.323
Aout-23	7/29/98 21:32	143.00	181.28	104.5	1.084	20.260	20.008	0.721	8.032	0.440	1.255
Aout-24	7/30/98 0:06	154.00	190.51	113.73	1.180	21.440	20.156	0.727	9.127	0.500	1.326
Aout-25	7/30/98 7:04	418.00	352.99	276.21	2.866	24.306	20.559	0.741	7.531	0.413	1.215
Aout-26	7/30/98 11:08	244.00	261.25	184.47	1.914	26.220	19.762	0.713	12.419	0.681	1.249
Aout-27	7/30/98 14:08	180.00	210.08	133.3	1.383	27.603	20.718	0.747	11.628	0.637	
Aout-28	7/30/98 20:02	354.00	244.21	167.43	1.737	29.340	18.633	0.672	12.105	0.664	1.681
Aout-29	7/31/98 0:10	248.00	259.69	182.91	1.898	31.238	20.49	0.739	11.682	0.640	
Aout-30	7/31/98 3:27	197.00	223.67	146.89	1.524	32.762	21.088	0.760	12.563	0.689	1.609
Aout-31	7/31/98 8:29	302.00	298.45	221.67	2.300	35.062	21.198	0.764	12.796	0.701	1.539

Column A - SMZ/ZVI Pellets (0.5 mL/min)

Bottle Weight 76.78 g

Pore Volume 96.38 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Aout-0	8/5/98 10:25	0.00	0	0	0	0	0		0	0.00	0.233
Aout-1	8/5/98 14:54	269.00	192.91	116.13	1.205	1.205	13.047	0.504	0.235	0.01	0.252
Aout-2	8/5/98 16:46	112.00	128.37	51.59	0.535	1.740	14.689	0.567	0.49	0.03	
Aout-3	8/5/98 18:37	111.00	127.67	50.89	0.528	2.268	14.855	0.573			
Aout-4	8/5/98 20:38	121.00	131.58	54.8	0.569	2.837	15.028	0.580			
Aout-5	8/5/98 21:11	33.00	93.82	17.04	0.177	3.014	15.127	0.584			
Aout-6	8/5/98 23:58	167.00	151.91	75.13	0.780	3.793	15.052	0.581	0.678	0.04	0.221
Aout-7	8/6/98 7:36	458.00	279.31	202.53	2.101	5.894	15.925	0.615	1.847	0.11	0.288
Aout-8	8/6/98 13:45	369.00	239.73	162.95	1.691	7.585	15.997	0.617	3.139	0.18	0.401
Aout-9	8/6/98 17:40	235.00	182.09	105.31	1.093	8.678	15.666	0.605	3.405	0.20	0.471
Aout-10	8/6/98 21:08	208.00	169.99	93.21	0.967	9.645	15.718	0.607	6.128	0.36	0.557
Aout-11	8/7/98 0:00	172.00	154.91	78.13	0.811	10.455	16.392	0.633	5.149	0.30	0.605
Aout-12	8/7/98 6:50	410.00	259.06	182.28	1.891	12.347	16.557	0.639	6.102	0.35	0.773
Aout-13	8/7/98 10:50	240.00	184.03	107.25	1.113	13.459	16.747	0.646	5.867	0.34	0.838
Aout-14	8/7/98 14:02	192.00	160.67	83.89	0.870	14.330	16.578	0.640	6.556	0.38	0.773
Aout-15	8/7/98 18:31	269.00	197.96	121.18	1.257	15.587	16.656	0.643	6.558	0.38	1.278
Aout-16	8/7/98 23:56	325.00	221.36	144.58	1.500	17.087	16.592	0.640	7.176	0.42	1.679
Aout-17	8/8/98 6:46	410.00	259.4	182.62	1.895	18.982	17.236	0.665	7.751	0.45	1.128
Aout-18	8/8/98 11:31	285.00	206.25	129.47	1.343	20.325	17.496	0.675	8.421	0.49	1.471
Aout-19	8/8/98 15:11	220.00	201.47	124.69	1.294	21.619	17.17	0.663	8.78	0.51	1.219
Aout-20	8/8/98 19:54	283.00	175.47	98.69	1.024	22.643	17.024	0.657	9.118	0.53	1.348
Aout-21	8/8/98 23:37	223.00	176.23	99.45	1.032	23.675	17.119	0.661	6.103	0.35	0.982
Aout-22	8/9/98 7:04	447.00	275.35	198.57	2.060	25.735	17.353	0.670	13.061	0.76	1.389
Aout-23	8/9/98 11:56	292.00	208.12	131.34	1.363	27.098			11.239	0.65	0
Aout-24	8/9/98 16:15	259.00	192.08	115.3	1.196	28.294			10.806	0.63	1.426
Aout-25	8/9/98 19:54	219.00	175.09	98.31	1.020	29.314			10.414	0.60	1.369
Aout-26	8/10/98 0:01	247.00	186.8	110.02	1.142	30.456			10.332	0.60	1.914
Aout-27	8/10/98 7:45	464.00	282.99	206.21	2.140	32.595			11.257	0.65	1.495
Aout-28	8/10/98 11:17	212.00	172.75	95.97	0.996	33.591			10.637	0.62	1.468
Aout-29	8/10/98 15:23	246.00	189.49	112.71	1.169	34.760			10.428	0.61	1.374
Aout-30	8/10/98 20:35	312.00	216.54	139.76	1.450	36.210			12.942	0.75	1.559
Aout-31	8/11/98 0:01	206.00	169.3	92.52	0.960	37.170			10.74	0.62	1.45
Aout-32	8/11/98 8:44	523.00	310.77	233.99	2.428	39.598			11.39	0.66	1.524
Aout-33	8/11/98 13:20	276.00	200.78	124	1.287	40.885			8.33	0.48	1.229

Column A - SMZ/ZVI Pellets (0.25 mL/min)

Bottle Weight 76.78 g

Pore Volume 96.38 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Aout-0				0	0.000	0.000				0.00	
Aout-1	8/18/98 10:49	0.00	106.61	29.83	0.310	0.310	1.068	0.039	0	0.00	0.341
Aout-2	8/18/98 14:25	216.00	124.30	47.52	0.493	0.803	2.51	0.091	1.029	0.07	0.338
Aout-3	8/18/98 16:54	149.00	110.06	33.28	0.345	1.148	2.84	0.103	1.468	0.10	0.386
Aout-4	8/18/98 20:13	199.00	121.56	44.78	0.465	1.612	2.631	0.095	0.671	0.05	0.346
Aout-5	8/18/98 22:46	153.00	111.64	34.86	0.362	1.974	2.941	0.106	0.773	0.05	0.245
Aout-6	8/19/98 7:47	541.00	195.07	118.29	1.227	3.201	4.199	0.152	0.956	0.07	0.438
Aout-7	8/19/98 10:48	181.00	118.07	41.29	0.428	3.630	4.638	0.167	0.989	0.07	0.547
Aout-8	8/19/98 20:54	606.00	208.70	131.92	1.369	4.999	5.405	0.195	1.397	0.10	0.607
Aout-9	8/20/98 0:14	200.00	121.42	44.64	0.463	5.462	5.201	0.188	1.376	0.09	0.76
Aout-10	8/20/98 9:16	542.00	195.08	118.30	1.227	6.689	6.04	0.218	1.64	0.11	0.78
Aout-11	8/20/98 15:50	394.00	163.15	86.37	0.896	7.585	5.49	0.198	1.839	0.13	1.02
Aout-12	8/21/98 0:52	542.00	195.00	118.22	1.227	8.812	5.922	0.214	2.052	0.14	1.30
Aout-13	8/21/98 9:58	546.00	196.00	119.22	1.237	10.049	6.813	0.246	2.511	0.17	1.49
Aout-14	8/21/98 17:13	435.00	171.51	94.73	0.983	11.032	6.795	0.245	3.048	0.21	1.73
Aout-15	8/21/98 23:33	380.00	160.07	83.29	0.864	11.896	7.013	0.253	2.978	0.20	1.69
Aout-16	8/22/98 10:01	628.00	220.08	143.30	1.487	13.383	7.987	0.288	3.416	0.23	1.79
Aout-17	8/22/98 16:23	382.00	161.44	84.66	0.878	14.261	7.814	0.282	3.685	0.25	1.90
Aout-18	8/22/98 22:45	382.00	164.66	87.88	0.912	15.173	7.748	0.280	3.801	0.26	2.20
Aout-19	8/23/98 8:49	604.00	213.59	136.81	1.419	16.592	8.538	0.308	4.037	0.28	2.79
Aout-20	8/23/98 17:57	548.00	202.74	125.96	1.307	17.899	8.706	0.314	3.381	0.23	2.21
Aout-21	8/23/98 22:49	292.00	148.08	71.30	0.740	18.639	8.885	0.321	4.006	0.27	2.18
Aout-22	8/24/98 6:41	472.00	182.71	105.93	1.099	19.738	9.329	0.337	4.312	0.30	2.58
Aout-23	8/24/98 17:17	636.00	220.69	143.91	1.493	21.231	9.573	0.346	4.63	0.32	2.32
Aout-24	8/24/98 21:53	276.00	141.94	65.16	0.676	21.907	9.888	0.357	4.116	0.28	2.62
Aout-25	8/25/98 11:24	811.00	261.84	185.06	1.920	23.827	10.133	0.366	4.742	0.32	3.00
Aout-26	8/25/98 16:59	335.00	155.24	78.46	0.814	24.641	9.774	0.353	4.13	0.28	3.004
Aout-27	8/26/98 7:28	869.00	275.84	199.06	2.065	26.707	10.399	0.375	4.613	0.32	2.786
Aout-28	8/26/98 16:35	547.00	203.26	126.48	1.312	28.019	10.458	0.378	5.118	0.35	3.232
Aout-29	8/27/98 8:57	982.00	301.13	224.35	2.328	30.347	11.057	0.399	5.951	0.41	2.849
Aout-30	8/27/98 16:11	434.00	177.02	100.24	1.040	31.387	10.719	0.387	4.801	0.33	3.079
Aout-31	8/27/98 23:23	432.00	176.08	99.30	1.030	32.417			4.848	0.33	2.853
Aout-32	8/28/98 8:35	552.00	204.38	127.60	1.324	33.741			4.829	0.33	2.629

Column B - SMZ/ZVI Pellets (1 mL/min)

Bottle Weight 70.39 g

Pore Volume 103.19 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Bout-1	7/27/98 11:17	0.00	159.05	88.66	0.859	0.859	1.255	0.045	0	0	0
Bout-2	7/27/98 13:17	120.00	139.62	69.23	0.671	1.530	5.025	0.181	0	0	0
Bout-3	7/27/98 17:37	260.00	160.26	89.87	0.871	2.401	7.206	0.260	0	0	0
Bout-4	7/27/98 19:41	124.00	162.29	91.9	0.891	3.292	10.601	0.382	0	0	0
Bout-5	7/27/98 22:03	142.00	177.29	106.9	1.036	4.327	16.432	0.592	0.271	0.01485623	0.136
Bout-6	7/28/98 1:58	235.00	138.29	67.9	0.658	4.985	16.942	0.611	1.365	0.07482937	0.179
Bout-7	7/28/98 7:07	309.00	222.2	151.81	1.471	6.457	15.905	0.573	1.6392	0.08986103	0.33
Bout-8	7/28/98 8:48	101.00	149.61	79.22	0.768	7.224	15.877	0.572	2.5431	0.13941288	0.45
Bout-9	7/28/98 10:11	83.00	133.94	63.55	0.616	7.840	17.653	0.636	2.9969	0.16429022	0.832
Bout-10	7/28/98 12:22	131.00	166.55	96.16	0.932	8.772	18.715	0.675	3.2201	0.17652605	0.83
Bout-11	7/28/98 14:06	104.00	97.34	26.95	0.261	9.033	18.822	0.679	3.2333	0.17724968	0.713
Bout-12	7/28/98 15:40	94.00	142.29	71.9	0.697	9.730	17.158	0.619	3.828	0.20985116	0.761
Bout-13	7/28/98 17:30	110.00	153.34	82.95	0.804	10.534	18.525	0.668	4.7689	0.26143135	0.803
Bout-14	7/28/98 19:11	101.00	145.21	74.82	0.725	11.259	19.438	0.701	5.232	0.28681852	0.843
Bout-15	7/28/98 21:46	155.00	133.32	62.93	0.610	11.869	19.654	0.709	4.65	0.25491325	0.847
Bout-16	7/28/98 23:57	131.00	141.7	71.31	0.691	12.560			5.359	0.29378066	0.924
Bout-17	7/29/98 8:23	506.00	202.74	132.35	1.283	13.842			4.794	0.26280733	1.155
Bout-18	7/29/98 11:22	179.00	206.73	136.34	1.321	15.163			6.626	0.36323767	1.494
Bout-19	7/29/98 13:00	98.00	152.93	82.54	0.800	15.963			7.423	0.40692925	1.49
Bout-20	7/29/98 15:15	135.00	164.25	93.86	0.910	16.873			7.678	0.42090837	1.42
Bout-21	7/29/98 17:01	106.00	147.06	76.67	0.743	17.616	20.375	0.735	7.986	0.43779294	1.382
Bout-22	7/29/98 19:15	134.00	171.61	101.22	0.981	18.597	20.59	0.742	8.897	0.48773401	1.38
Bout-23	7/29/98 21:38	143.00	175.6	105.21	1.020	19.616	20.855	0.752	9.549	0.52347669	1.426
Bout-24	7/30/98 0:12	154.00	184.43	114.04	1.105	20.721	20.787	0.749	9.957	0.54584327	1.363
Bout-25	7/30/98 7:13	421.00	349.01	278.62	2.700	23.421	21.111	0.761	10.075	0.55231204	1.365
Bout-26	7/30/98 11:15	242.00	254.37	183.98	1.783	25.204	20.545	0.741	13.386	0.73382123	1.442
Bout-27	7/30/98 14:14	179.00	205.51	135.12	1.309	26.514	21.143	0.762	12.494	0.68492174	
Bout-28	7/30/98 20:09	355.00	238.78	168.39	1.632	28.146	18.757	0.676	12.576	0.68941699	1.771
Bout-29	7/31/98 0:17	248.00	253.26	182.87	1.772	29.918	21.056	0.759	12.925	0.70854919	1.73
Bout-30	7/31/98 3:32	195.00	218.32	147.93	1.434	31.351	21.321	0.769	13.185	0.7228024	1.897
Bout-31	7/31/98 8:36	304.00	295.77	225.38	2.184	33.535	21.571	0.778	13.531	0.74177014	1.6

Column B - SMZ/ZVI Pellets (0.5 mL/min)

Bottle Weight 70.39 g

Pore Volume 103.19 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Bout-0	8/5/98 10:35	0.00	0	0	0	0	0	0	0	0.000	
Bout-1	8/5/98 15:00	265.00	191.27	120.88	1.171	1.171	11.592	0.447	0	0.000	0.133
Bout-2	8/5/98 16:52	112.00	122.03	51.64	0.500	1.672	13.351	0.515	0	0.000	0.182
Bout-3	8/5/98 18:39	107.00	119.36	48.97	0.475	2.146	13.419	0.518			
Bout-4	8/5/98 20:39	120.00	127.65	57.26	0.555	2.701	13.575	0.524			
Bout-5	8/5/98 21:17	38.00	89.51	19.12	0.185	2.887	13.424	0.518			
Bout-6	8/6/98 0:04	167.00	146.05	75.66	0.733	3.620	13.649	0.527	0.471	0.027	0.179
Bout-7	8/6/98 7:42	458.00	272.22	201.83	1.956	5.576	14.38	0.555	1.559	0.090	0.302
Bout-8	8/6/98 13:51	369.00	233.82	163.43	1.584	7.159	14.479	0.559	2.513	0.146	0.403
Bout-9	8/6/98 17:46	235.00	174.57	104.18	1.010	8.169	14.312	0.552	3.839	0.223	0.569
Bout-10	8/6/98 21:15	209.00	163.47	93.08	0.902	9.071	14.28	0.551	4.565	0.265	0.652
Bout-11	8/7/98 0:11	176.00	150.11	79.72	0.773	9.843	14.976	0.578	4.393	0.255	0.667
Bout-12	8/7/98 6:56	405.00	249.03	178.64	1.731	11.575	15.36	0.593	6.081	0.353	0.952
Bout-13	8/7/98 10:56	240.00	178.6	108.21	1.049	12.623	15.284	0.590	6.624	0.384	0.981
Bout-14	8/7/98 14:08	192.00	154.23	83.84	0.812	13.436	15.286	0.590	7.147	0.415	1.033
Bout-15	8/7/98 18:37	269.00	191.45	121.06	1.173	14.609	15.834	0.611	7.049	0.409	1.075
Bout-16	8/8/98 0:04	327.00	216.32	145.93	1.414	16.023	15.967	0.616	6.735	0.391	1.158
Bout-17	8/8/98 6:52	408.00	253.67	183.28	1.776	17.799	16.419	0.634	9.175	0.532	1.397
Bout-18	8/8/98 11:38	286.00	198.94	128.55	1.246	19.045	16.514	0.637	8.96	0.520	1.379
Bout-19	8/8/98 15:18	220.00	195.04	124.65	1.208	20.253	16.153	0.623	8.207	0.476	1.442
Bout-20	8/8/98 20:01	283.00	169.34	98.95	0.959	21.212	16.174	0.624	9.597	0.557	1.446
Bout-21	8/8/98 23:43	222.00	169.39	99	0.959	22.171	16.284	0.628	9.466	0.549	1.579
Bout-22	8/9/98 7:08	445.00	268.79	198.4	1.923	24.094	16.842	0.650	10.865	0.631	1.724
Bout-23	8/9/98 12:03	295.00	201.74	131.35	1.273	25.367			10.054	0.583	1.681
Bout-24	8/9/98 16:19	256.00	185.19	114.8	1.112	26.479			11.226	0.652	1.789
Bout-25	8/9/98 19:58	219.00	168.06	97.67	0.946	27.426			10.537	0.612	1.769
Bout-26	8/10/98 0:07	249.00	181.43	111.04	1.076	28.502			11.546	0.670	1.6
Bout-27	8/10/98 7:51	464.00	276.75	206.36	2.000	30.501			10.748	0.624	1.691
Bout-28	8/10/98 11:24	213.00	166.2	95.81	0.928	31.430			11.743	0.682	1.77
Bout-29	8/10/98 15:30	246.00	181.92	111.53	1.081	32.511			9.3	0.540	1.741
Bout-30	8/10/98 20:42	312.00	209.99	139.6	1.353	33.863			10.494	0.609	1.746
Bout-31	8/11/98 0:05	203.00	162.37	91.98	0.891	34.755			10.529	0.611	1.884
Bout-32	8/11/98 8:50	525.00	305	234.61	2.274	37.028			11.094	0.644	1.894
Bout-33	8/11/98 13:26	276.00	194.78	124.39	1.205	38.234			10.336	0.600	1.657

Column B - SMZ/ZVI Pellets (0.25 mL/min)

Bottle Weight 70.39 g

Pore Volume 103.19 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Bout-0				0	0.000	0.000				0.000	
Bout-1	8/18/98 10:59	0.00	104.87	34.48	0.334	0.334	0.84	0.030	0	0.000	0.347
Bout-2	8/18/98 14:33	214.00	119.07	48.68	0.472	0.806	2.53	0.091	0.5	0.034	1.25
Bout-3	8/18/98 17:00	147.00	104.06	33.67	0.326	1.132	2.853	0.103	0.5	0.034	0.378
Bout-4	8/18/98 20:21	201.00	115.99	45.6	0.442	1.574	2.653	0.096	0.5	0.034	0.355
Bout-5	8/18/98 22:54	153.00	106.45	36.06	0.349	1.923	2.717	0.098	0.455	0.031	0.333
Bout-6	8/19/98 7:54	540.00	191.42	121.03	1.173	3.096	3.867	0.140	0.683	0.047	0.489
Bout-7	8/19/98 10:58	184.00	112.73	42.34	0.410	3.507	4.244	0.153	0.591	0.040	0.514
Bout-8	8/19/98 21:02	604.00	206.3	135.91	1.317	4.824	4.165	0.150	0.757	0.052	0.609
Bout-9	8/20/98 0:21	199.00	116.32	45.93	0.445	5.269	4.475	0.162	0.929	0.064	0.848
Bout-10	8/20/98 9:24	543.00	192.51	122.12	1.183	6.452	5.794	0.209	1.566	0.107	0.998
Bout-11	8/20/98 15:59	395.00	158.85	88.46	0.857	7.309	5.817	0.210	1.634	0.112	1.19
Bout-12	8/21/98 0:58	539.00	191.42	121.03	1.173	8.482	5.571	0.201	1.97	0.135	1.423
Bout-13	8/21/98 10:05	547.00	192.38	121.99	1.182	9.664	6.258	0.226	2.225	0.152	1.577
Bout-14	8/21/98 17:21	436.00	167.75	97.36	0.943	10.608	6.417	0.232	2.532	0.173	1.733
Bout-15	8/21/98 23:40	379.00	156.24	85.85	0.832	11.440	6.908	0.249	2.795	0.192	1.897
Bout-16	8/22/98 10:09	629.00	212.63	142.24	1.378	12.818	7.475	0.270	3.114	0.213	1.93
Bout-17	8/22/98 16:31	382.00	155.38	84.99	0.824	13.642	8.406	0.303	3.505	0.240	2.152
Bout-18	8/22/98 22:54	383.00	158.07	87.68	0.850	14.492	8.386	0.303	3.891	0.267	2.279
Bout-19	8/23/98 8:56	602.00	206.63	136.24	1.320	15.812	8.975	0.324	3.876	0.266	2.076
Bout-20	8/23/98 18:05	549.00	195.57	125.18	1.213	17.025	8.78	0.317	3.309	0.227	2.561
Bout-21	8/23/98 23:06	301.00	140.12	69.73	0.676	17.701	8.922	0.322	3.848	0.264	2.543
Bout-22	8/24/98 6:48	462.00	175.67	105.28	1.020	18.721	10.534	0.380	4.108	0.281	2.351
Bout-23	8/24/98 17:24	636.00	214.58	144.19	1.397	20.118	10.154	0.367	3.47	0.238	2.491
Bout-24	8/24/98 21:59	275.00	134.24	63.85	0.619	20.737	9.304	0.336	4.512	0.309	2.635
Bout-25	8/25/98 11:30	811.00	254.47	184.08	1.784	22.521	9.623	0.347	3.808	0.261	2.897
Bout-26	8/25/98 17:06	336.00	147.5	77.11	0.747	23.268	10.397	0.375	4.113	0.282	2.897
Bout-27	8/26/98 7:35	869.00	267.68	197.29	1.912	25.180	10.164	0.367	4.325	0.296	2.908
Bout-28	8/26/98 16:39	544.00	195.02	124.63	1.208	26.388	10.2	0.368	4.462	0.306	2.807
Bout-29	8/27/98 9:06	987.00	292.21	221.82	2.150	28.537	10.516	0.380	4.563	0.313	2.934
Bout-30	8/27/98 16:18	432.00	170.95	100.56	0.974	29.512	10.537	0.380	4.418	0.303	2.928
Bout-31	8/27/98 23:31	433.00	169.21	98.82	0.958	30.469			5.008	0.343	3.055
Bout-32	8/28/98 8:43	552.00	196.86	126.47	1.226	31.695			4.53	0.310	2.883

Column C - Z/ZVI Pellets (1 mL/min)

Bottle Weight 70.8 g

Pore Volume 106.65 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Cout-1	7/27/98 10:20	0.00	120.16	49.36	0.463	0.463	0.115	0.004	0	0.000	
Cout-2	7/27/98 11:23	63.00	113.05	42.25	0.396	0.859	0.238	0.009	1.7447	0.096	
Cout-3	7/27/98 12:30	67.00	112.31	41.51	0.389	1.248	0.457	0.016	3.263	0.179	
Cout-4	7/27/98 13:22	52.00	97.18	26.38	0.247	1.495	0.566	0.020	3.936	0.216	
Cout-5	7/27/98 14:54	92.00	101.71	30.91	0.290	1.785	0.874	0.032	3.3287	0.182	
Cout-6	7/27/98 17:09	135.00	85.69	14.89	0.140	1.925	1.02	0.037			
Cout-6b	7/27/98 17:42	33.00	92.27								
Cout-7	7/27/98 18:25	43.00	121.51	21.47	0.201	2.126	0.857	0.031	4.4696	0.245	
Cout-8	7/27/98 19:46	81.00	129.46	50.71	0.475	2.602	0.359	0.013	6.24	0.342	
Cout-9	7/27/98 21:16	90.00	137.55	58.66	0.550	3.152	0.568	0.020	8.591	0.471	
Cout-10	7/27/98 22:09	53.00	111.27	66.75	0.626	3.778	0.498	0.018			
Cout-11	7/28/98 2:12	243.00	149.21	40.47	0.379	4.157	0.587	0.021	8.7566	0.480	
Cout-12	7/28/98 7:15	303.00	213.23	78.41	0.735	4.892	0.698	0.025	10.4379	0.572	
Cout-13	7/28/98 8:55	100.00	145.99	142.43	1.335	6.228	0.893	0.032	11.1015	0.609	
Cout-14	7/28/98 10:25	90.00	134.74	75.19	0.705	6.933	0.962	0.035	12.3013	0.674	
Cout-15	7/28/98 12:35	130.00	163.11	63.94	0.600	7.532	1.015	0.037	13.1697	0.722	
Cout-16	7/28/98 15:47	192.00	159.33	92.31	0.866	8.398	1.035	0.037	12.9164	0.708	
Cout-17	7/28/98 17:37	110.00	149.84	88.53	0.830	9.228	1.02	0.037	13.4584	0.738	
Cout-18	7/28/98 19:21	104.00	144.54	79.04	0.741	9.969	0.85	0.031	13.4484	0.737	
Cout-19	7/28/98 21:53	152.00	128.58	73.74	0.691	10.660	0.548	0.020	13.157	0.721	
Cout-20	7/28/98 23:52	119.00	155.05	57.78	0.542	11.202	0.65	0.023	14.141	0.775	
Cout-21	7/29/98 8:30	518.00	185.41	114.61	1.075	12.276	0.75	0.027	14.004	0.768	
Cout-22	7/29/98 11:23	173.00	197.7	126.9	1.190	13.466	0.896	0.032	14.418	0.790	
Cout-23	7/29/98 13:19	116.00	155.7	84.9	0.796	14.262	0.968	0.035	15.859	0.869	
Cout-24	7/29/98 15:26	127.00	161.1	90.3	0.847	15.109	1.062	0.038	16.174	0.887	
Cout-25	7/29/98 17:12	106.00	146.54	75.74	0.710	15.819	1.12	0.040	16.203	0.888	
Cout-26	7/29/98 19:23	131.00	167.1	96.3	0.903	16.722	1.05	0.038	16.694	0.915	
Cout-27	7/29/98 21:45	142.00	171.88	101.08	0.948	17.670	0.58	0.021	17.264	0.946	
Cout-28	7/30/98 0:19	154.00	181.15	110.35	1.035	18.704	0.446	0.016	17.026	0.933	
Cout-29	7/30/98 7:19	420.00	341.86	271.06	2.541	21.246	0.523	0.019	17.985	0.986	
Cout-30	7/30/98 11:23	244.00	249.79	178.99	1.678	22.924	0.879	0.032	19.374	1.062	
Cout-31	7/30/98 14:21	178.00	199.92	129.12	1.211	24.135	0.987	0.036	19.358	1.061	
Cout-32	7/30/98 20:16	355.00	233.83	163.03	1.529	25.663	0.921	0.033	18.8	1.031	
Cout-33	7/31/98 0:27	251.00	254.56	183.76	1.723	27.386	0.954	0.034	18.315	1.004	
	7/31/98 3:27	180.00	199.82	129.02	1.210	28.596	0.963	0.035		0.000	
Cout-34	7/31/98 8:43	316.00	292.88	222.08	2.082	30.678	1.087	0.039	19.072	1.046	

Column C - Z/ZVI Pellets (0.5 mL/min)

Bottle Weight	70.8	g
Pore Volume	106.65	ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Cout-1	8/5/98 12:00	0.00	112.22	41.42	0.388	0.388			0	0.000	0
Cout-2	8/5/98 13:40	100.00	116.84	46.04	0.432	0.820	0.467	0.018	0	0.000	0.003
Cout-3	8/5/98 15:06	86.00	111.41	40.61	0.381	1.201	0.593	0.023	0	0.000	0.036
Cout-4	8/5/98 16:43	97.00	115.1	44.3	0.415	1.616	0.376	0.015	1.158	0.067	0.089
Cout-5	8/5/98 18:23	100.00	116.4	45.6	0.428	2.044	0.723	0.028	2.09	0.121	0.126
Cout-6	8/5/98 20:23	120.00	125.3	54.5	0.511	2.555	1.006	0.039	3.158	0.183	0.182
Cout-7	8/6/98 0:11	228.00	172.91	102.11	0.957	3.512	0.212	0.008	5.528	0.321	0.283
Cout-8	8/6/98 7:48	457.00	269.24	198.44	1.861	5.373	0.37	0.014	8.398	0.487	0.434
Cout-9	8/6/98 13:57	369.00	233.26	198.44	1.861	7.233	0.805	0.031	9.147	0.531	0.414
Cout-10	8/6/98 17:53	236.00	174.22	162.46	1.523	8.756	0.842	0.032	10.278	0.596	0.524
Cout-11	8/6/98 21:21	208.00	161.75	103.42	0.970	9.726	0.667	0.026	10.445	0.606	0.531
Cout-12	8/7/98 0:17	176.00	148.67	90.95	0.853	10.579	1.392	0.054	10.858	0.630	0.596
Cout-13	8/7/98 7:01	404.00	245.45	77.87	0.730	11.309	1.41	0.054	11.355	0.659	0.617
Cout-14	8/7/98 11:05	244.00	176.33	174.65	1.638	12.947	1.371	0.053	11.065	0.642	0.551
Cout-15	8/7/98 14:14	189.00	150.24	105.53	0.989	13.936	1.673	0.065	11.035	0.640	0.562
Cout-16	8/7/98 18:44	270.00	187.45	79.44	0.745	14.681	1.875	0.072	11.536	0.670	0.516
Cout-17	8/8/98 0:09	325.00	210.93	116.65	1.094	15.775	1.953	0.075	11.612	0.674	0.568
Cout-18	8/8/98 6:59	410.00	245.84	140.13	1.314	17.088	1.887	0.073	12.094	0.702	0.531
Cout-19	8/8/98 11:44	285.00	194.58	175.04	1.641	18.730	2.274	0.088	12.182	0.707	0.531
Cout-20	8/8/98 16:23	279.00	190.42	123.78	1.161	19.890	2.241	0.086	11.778	0.684	0.609
Cout-21	8/8/98 20:08	225.00	166.83	96.03	0.900	20.791	2.382	0.092	12.301	0.714	0.582
Cout-22	8/8/98 23:47	219.00	166.44	95.64	0.897	21.687	2.667	0.103	11.511	0.668	0.551
Cout-23	8/9/98 7:20	453.00	264.07	193.27	1.812	23.499	2.624	0.101	12.215	0.709	0.509
Cout-24	8/9/98 12:09	289.00	195.83	125.03	1.172	24.672	1.36	0.052	11.63	0.675	0.503
Cout-25	8/9/98 16:27	258.00	182.84	112.04	1.050	25.722	1.27	0.049	12.226	0.710	0.518
Cout-26	8/9/98 20:04	217.00	166.22	95.42	0.895	26.617	1.15	0.044	11.881	0.690	
Cout-27	8/10/98 0:13	249.00	177.75	106.95	1.003	27.620	1.08	0.042	11.398	0.661	0.528
Cout-28	8/10/98 7:57	464.00	269.29	198.49	1.861	29.481	0.83	0.032	11.999	0.696	0.504
Cout-29	8/10/98 11:34	217.00	165.91	95.11	0.892	30.372	0.98	0.038	10.724	0.622	0.411
Cout-30	8/10/98 15:38	244.00	177.12	106.32	0.997	31.369	1.05	0.041	11.177	0.649	0.361
Cout-31	8/10/98 20:49	311.00	206.35	135.55	1.271	32.640	0.54	0.021	11.706	0.679	0.501
Cout-32	8/11/98 0:17	208.00	161.85	91.05	0.854	33.494	0.25	0.010	12.119	0.703	0.413
Cout-33	8/11/98 8:59	522.00	295.17	224.37	2.104	35.598	0.83	0.032	11.938	0.693	0.41
Cout-34	8/11/98 13:33	274.00	189.72	118.92	1.115	36.713	0.98	0.038	12.603	0.731	0.43

Column C - Z/ZVI Pellets (0.25 mL/min)

Bottle Weight	70.8	g
Pore Volume	106.65	ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Cout-1	8/18/98 11:07	0.00	103.7	32.9	0.308	0.308	0.308	0.011		0.000	
Cout-2	8/18/98 14:59	232.00	117.25	46.45	0.436	0.744	0.519	0.019	0.352	0.024	0.12
Cout-3	8/18/98 18:07	188.00	101.85	31.05	0.291	1.035	0.466	0.017	1.182	0.081	0.352
Cout-4	8/18/98 20:29	142.00	114.37	43.57	0.409	1.444	0.172	0.006	1.338	0.092	0.205
Cout-5	8/18/98 23:02	153.00	105.65	34.85	0.327	1.770	0.459	0.017	1.806	0.124	0.286
Cout-6	8/19/98 8:02	540.00	186.69	115.89	1.087	2.857	0.62	0.022	2.603	0.178	0.316
Cout-7	8/19/98 11:05	183.00	111.05	40.25	0.377	3.234	0.53	0.019	3.451	0.236	0.345
Cout-8	8/19/98 21:09	604.00	199.46	128.66	1.206	4.441	0.403	0.015	4.057	0.278	0.328
Cout-9	8/20/98 0:28	199.00	114.97	128.66	1.206	5.647	0.414	0.015	4.252	0.291	0.412
Cout-10	8/20/98 9:31	543.00	187.93	44.17	0.414	6.061	0.671	0.024	4.361	0.299	0.418
Cout-11	8/20/98 16:07	396.00	155.94	117.13	1.098	7.159	1.223	0.044	5.35	0.367	0.301
Cout-12	8/21/98 1:07	540.00	187.15	85.14	0.798	7.958	0.677	0.024	5.353	0.367	0.469
Cout-13	8/21/98 10:13	546.00	189.39	116.35	1.091	9.049	0.588	0.021	5.507	0.377	1.063
Cout-14	8/21/98 17:23	430.00	164.89	118.59	1.112	10.160	0.767	0.028	6.164	0.422	0.392
Cout-15	8/21/98 23:56	393.00	157.36	94.09	0.882	11.043	0.863	0.031	6.285	0.431	0.384
Cout-16	8/22/98 10:23	627.00	209.34	86.56	0.812	11.854	1.019	0.037	6.401	0.439	0.381
Cout-17	8/22/98 16:39	376.00	155.38	138.54	1.299	13.153	1.669	0.060	6.476	0.444	0.433
Cout-18	8/22/98 23:02	383.00	156.52	84.58	0.793	13.946	1.005	0.036	6.661	0.456	0.376
Cout-19	8/23/98 9:04	602.00	204.36	85.72	0.804	14.750	1.577	0.057	6.912	0.474	0.401
Cout-20	8/23/98 18:12	548.00	192.9	133.56	1.252	16.002	1.334	0.048	6.759	0.463	0.469
Cout-21	8/23/98 22:14	242.00	138.26	67.46	0.633	16.635	1.504	0.054	6.196	0.425	0.407
Cout-22	8/24/98 6:54	520.00	172.9	102.1	0.957	17.592	1.472	0.053	6.418	0.440	0.295
Cout-23	8/24/98 17:32	638.00	211.62	140.82	1.320	18.912	1.578	0.057	6.244	0.428	0.28
Cout-24	8/24/98 22:05	273.00	131.94	61.14	0.573	19.486	1.562	0.056	6.453	0.442	0.28
Cout-25	8/25/98 11:40	815.00	250.2	179.4	1.682	21.168	1.395	0.050	6.193	0.424	0.391
Cout-26	8/25/98 17:12	332.00	145.17	74.37	0.697	21.865	1.526	0.055	5.876	0.403	0.321
Cout-27	8/26/98 8:54	942.00	277.34	206.54	1.937	23.801	1.537	0.055	6.871	0.471	0.293
Cout-28	8/26/98 16:49	475.00	176.75	105.95	0.993	24.795	1.598	0.058	6.044	0.414	0.264
Cout-29	8/27/98 9:13	984.00	287.12	216.32	2.028	26.823	1.801	0.065	6.777	0.464	0.475
Cout-30	8/27/98 16:27	434.00	170.52	99.72	0.935	27.758	1.691	0.061	6.364	0.436	0.398
Cout-31	8/27/98 23:38	431.00	166.75	95.95	0.900	28.658		0.000	6.127	0.420	0.285
Cout-32	8/28/98 8:50	552.00	193.11	122.31	1.147	29.804		0.000	6.644	0.455	0.458

Column D - Z/ZVI Pellets (1 mL/min)

Bottle Weight	70.8	g
Pore Volume	101.09	ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Dout-1	7/27/98 10:26	0.00	125.98	55.18	0.546	0.546	0.122	0.0044	0.7067	0.0387	
Dout-2	7/27/98 11:28	62.00	110.80	40	0.396	0.942	0.154	0.0056	0.106	0.0058	
Dout-3	7/27/98 12:35	67.00	110.24	39.44	0.390	1.332	0.165	0.0059	1.883	0.1032	
Dout-4	7/27/98 13:27	52.00	95.74	24.94	0.247	1.578	0.256	0.0092	2.6145	0.1433	
Dout-5	7/27/98 14:59	92.00	100.81	30.01	0.297	1.875	0.754	0.0272	2.8744	0.1576	
Dout-6	7/27/98 17:13	134.00	96.41	25.61	0.253	2.129	0.875	0.0315	5.5241	0.3028	
Dout-6b	7/27/98 17:47	34.00	94.40								
Dout-7	7/27/98 18:30	43.00	124.25	53.45	0.529	2.657	0.568	0.0205			
Dout-8	7/27/98 19:53	83.00	130.72	59.92	0.593	3.250	0.758	0.0273	7.11	0.3898	
Dout-9	7/27/98 21:16	83.00	142.67	71.87	0.711	3.961	0.896	0.0323	8.48	0.4649	
Dout-10	7/27/98 22:16	60.00	103.55	32.75	0.324	4.285	0.695	0.0251	9.3	0.5098	
Dout-11	7/28/98 2:18	242.00	149.45	78.65	0.778	5.063	0.632	0.0228	9.4107	0.5159	
Dout-12	7/28/98 7:20	302.00	216.55	145.75	1.442	6.505	0.456	0.0164	9.9421	0.5450	
Dout-13	7/28/98 9:10	110.00	150.23	79.43	0.786	7.291	0.982	0.0354	10.9929	0.6026	
Dout-14	7/28/98 10:30	80.00	128.32	57.52	0.569	7.860	0.458	0.0165	12.105	0.6636	
Dout-15	7/28/98 12:37	127.00	162.39	91.59	0.906	8.766	0.654	0.0236	12.7189	0.6973	
Dout-16	7/28/98 15:54	197.00	163.63	92.83	0.918	9.684	0.741	0.0267	12.4391	0.6819	
Dout-17	7/28/98 17:44	110.00	151.34	80.54	0.797	10.481	0.41	0.0148	13.8607	0.7598	
Dout-18	7/28/98 19:29	105.00	145.65	74.85	0.740	11.221	0.354	0.0128	13.697	0.7509	
Dout-19	7/28/98 22:00	151.00	128.00	57.2	0.566	11.787	0.258	0.0093	14.49	0.7943	
Dout-20	7/28/98 23:57	117.00	152.44	81.64	0.808	12.595	0.987	0.0356	13.773	0.7550	
Dout-21	7/29/98 8:37	520.00	190.84	120.04	1.187	13.782	1.032	0.0372	13.773	0.7550	
Dout-22	7/29/98 11:29	172.00	198.09	127.29	1.259	15.041	0.857	0.0309	14.739	0.8080	
Dout-23	7/29/98 13:27	118.00	157.30	86.5	0.856	15.897	0.874	0.0315	16.025	0.8785	
Dout-24	7/29/98 15:33	126.00	162.80	92	0.910	16.807	0.634	0.0229	16.544	0.9069	
Dout-25	7/29/98 17:14	101.00	144.21	73.41	0.726	17.533	0.521	0.0188	15.575	0.8538	
Dout-26	7/29/98 19:57	163.00	188.88	118.08	1.168	18.701	0.951	0.0343	16.732	0.9172	
Dout-27	7/29/98 21:51	114.00	152.91	82.11	0.812	19.513	0.982	0.0354	17.825	0.9772	
Dout-28	7/30/98 0:25	154.00	182.18	111.38	1.102	20.615	0.851	0.0307	18.392	1.0083	
Dout-29	7/30/98 7:24	419.00	345.78	274.98	2.720	23.335	0.634	0.0229	17.83	0.9774	
Dout-30	7/30/98 11:30	246.00	252.3	181.5	1.795	25.131	0.357	0.0129	19.215	1.0534	
Dout-31	7/30/98 14:26	176.00	205.34	134.54	1.331	26.462	0.254	0.0092	19.93	1.0926	
Dout-32	7/30/98 20:23	357.00	230.58	159.78	1.581	28.042	0.264	0.0095	18.8	1.0306	
Dout-33	7/31/98 0:34	251.00	253.02	182.22	1.803	29.845	0.354	0.0128	19.321	1.0592	
	7/31/98 3:27	173.00	199.65	128.85	1.275	31.120	0.541	0.0195		0.0000	
Dout-34	7/31/98 8:46	319.00	302.2	231.4	2.289	33.409	0.654	0.0236	19.321	1.0592	

Column D - Z/ZVI Pellets (0.5 mL/min)

Bottle Weight 70.8 g

Pore Volume 101.09 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Dout-1	8/5/98 12:06	0.00	112.15	41.35	0.409	0.409	0.023	0.001	0.000	0.000	0
Dout-2	8/5/98 13:47	101.00	113.90	43.1	0.426	0.835	0.336	0.013	0.000	0.000	0.01
Dout-3	8/5/98 15:13	86.00	106.86	36.06	0.357	1.192	0.044	0.002	0.000	0.000	0.025
Dout-4	8/5/98 16:48	95.00	111.74	40.94	0.405	1.597	0.24	0.009	0.580	0.034	0.087
Dout-5	8/5/98 18:29	101.00	112.59	41.79	0.413	2.011	0.114	0.004	1.930	0.112	0.148
Dout-6	8/5/98 20:29	120.00	122.35	51.55	0.510	2.520	0.087	0.003	2.793	0.162	0.157
Dout-7	8/6/98 0:18	229.00	164.95	94.15	0.931	3.452	0.133	0.005	4.087	0.237	0.251
Dout-8	8/6/98 7:54	456.00	259.11	188.3118	1.863	5.315	0.219	0.008	7.803	0.453	0.424
Dout-9	8/6/98 14:02	368.00	223.11	152.31	1.507	6.821	0.118	0.005	8.581	0.498	0.461
Dout-10	8/6/98 18:00	238.00	168.38	97.58	0.965	7.787	0.175	0.007	9.510	0.552	0.546
Dout-11	8/6/98 21:27	207.00	156.38	85.58	0.847	8.633	0.486	0.019	9.497	0.551	0.604
Dout-12	8/7/98 0:23	176.00	144.71	73.91	0.731	9.364	0.995	0.038	9.783	0.568	0.633
Dout-13	8/7/98 7:12	409.00	239.13	168.33	1.665	11.029	0.843	0.033	10.345	0.600	0.622
Dout-14	8/7/98 11:11	239.00	168.34	97.54	0.965	11.994	0.691	0.027	9.791	0.568	0.606
Dout-15	8/7/98 14:20	189.00	150.82	80.02	0.792	12.786	1.016	0.039	10.301	0.598	0.644
Dout-16	8/7/98 18:49	269.00	189.80	119	1.177	13.963	0.674	0.026	11.658	0.677	0.648
Dout-17	8/8/98 0:16	327.00	215.29	144.49	1.429	15.392	1.037	0.040	10.573	0.614	0.558
Dout-18	8/8/98 7:05	409.00	251.47	180.67	1.787	17.180	1.035	0.040	11.695	0.679	0.565
Dout-19	8/8/98 11:50	285.00	196.64	125.84	1.245	18.425	1.327	0.051	10.683	0.620	0.573
Dout-20	8/8/98 16:29	279.00	191.07	120.27	1.190	19.614	1.317	0.051	11.778	0.684	0.627
Dout-21	8/8/98 20:16	227.00	169.95	99.15	0.981	20.595	1.018	0.039	11.505	0.668	0.66
Dout-22	8/8/98 23:52	216.00	167.71	96.91	0.959	21.554	1.066	0.041	11.348	0.659	0.665
Dout-23	8/9/98 7:26	454.00	268.20	197.4	1.953	23.506	1.545	0.060	11.769	0.683	0.565
Dout-24	8/9/98 12:15	289.00	199.22	128.42	1.270	24.777	1.321	0.051	11.402	0.662	0.628
Dout-25	8/9/98 16:33	258.00	185.12	114.32	1.131	25.908	1.1	0.042	12.044	0.699	0.603
Dout-26	8/9/98 20:10	217.00	168.24	97.44	0.964	26.872	0.917	0.035	12.154	0.705	0.597
Dout-27	8/10/98 0:19	249.00	180.53	109.73	1.085	27.957	0.987	0.038	11.790	0.684	0.661
Dout-28	8/10/98 8:04	465.00	274.97	204.17	2.020	29.977	0.988	0.038	11.807	0.685	0.562
Dout-29	8/10/98 11:36	212.00	166.18	95.38	0.944	30.920	0.994	0.038	10.757	0.624	0.482
Dout-30	8/10/98 15:42	246.00	186.76	115.96	1.147	32.067	0.875	0.034	11.401	0.662	0.465
Dout-31	8/10/98 20:55	313.00	203.95	133.15	1.317	33.385	0.654	0.025	11.522	0.669	0.547
Dout-32	8/11/98 0:23	208.00	163.18	92.38	0.914	34.298	0.856	0.033	11.761	0.683	0.577
Dout-33	8/11/98 8:44	501.00	301.3	230.5	2.280	36.579	0.852	0.033	11.701	0.679	0.486
Dout-34	8/11/98 13:38	294.00	192.65	121.85	1.205	37.784	0.752	0.029	10.485	0.609	0.406

Column D - Z/ZVI Pellets (0.25 mL/min)

Bottle Weight 70.8 g

Pore Volume 101.09 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co	TCE (ppm)
Dout-1	8/18/98 11:14	0.00	106.89	36.09	0.357	0.357	0.525	0.019		0.000	
Dout-2	8/18/98 14:47	213.00	117.96	47.16	0.467	0.824	0.227	0.008	0	0.000	0
Dout-3	8/18/98 17:15	148.00	103.94	33.14	0.328	1.151	0	0.000	0.059	0.004	0.255
Dout-4	8/18/98 20:36	201.00	115.00	44.2	0.437	1.589	0.33	0.012	0.983	0.067	1.14
Dout-5	8/18/98 23:09	153.00	105.44	34.64	0.343	1.931	0.493	0.018	1.23	0.084	0.651
Dout-6	8/19/98 8:09	540.00	188.76	117.96	1.167	3.098	0.949	0.034	2.384	0.163	0.32
Dout-7	8/19/98 11:12	183.00	110.69	39.89	0.395	3.493	0.536	0.019	2.7	0.185	0.399
Dout-8	8/19/98 21:17	605.00	204.28	133.48	1.320	4.813	0.487	0.018	3.485	0.239	0.417
Dout-9	8/20/98 0:36	199.00	115.07	44.27	0.438	5.251	0.239	0.009	3.429	0.235	0.423
Dout-10	8/20/98 9:40	544.00	190.90	120.1	1.188	6.439	0.162	0.006	3.726	0.255	0.422
Dout-11	8/20/98 16:14	394.00	159.09	88.29	0.873	7.313	0.486	0.018	4.148	0.284	0.416
Dout-12	8/21/98 1:07	533.00	191.86	121.06	1.198	8.510	0	0.000	4.97	0.341	0.475
Dout-13	8/21/98 10:21	554.00	190.61	119.81	1.185	9.695	0.299	0.011	5.196	0.356	0.499
Dout-14	8/21/98 17:39	438.00	169.07	98.27	0.972	10.667	0.553	0.020	5.029	0.345	0.416
Dout-15	8/22/98 0:09	390.00	158.96	88.16	0.872	11.540	0.058	0.002	4.987	0.342	0.328
Dout-16	8/22/98 10:30	621.00	209.90	139.1	1.376	12.916	0.72	0.026	5.382	0.369	0.77
Dout-17	8/22/98 16:46	376.00	156.31	85.51	0.846	13.761	0.592	0.021	5.75	0.394	0.7
Dout-18	8/22/98 23:10	384.00	157.52	86.72	0.858	14.619	0.579	0.021	5.839	0.400	0.371
Dout-19	8/23/98 9:14	604.00	207.04	136.24	1.348	15.967	0.363	0.013	5.858	0.401	0.362
Dout-20	8/23/98 18:24	550.00	195.34	124.54	1.232	17.199	0.397	0.014	5.735	0.393	0.409
Dout-21	8/24/98 1:20	416.00	138.07	67.27	0.665	17.864	0.535	0.019	5.333	0.365	0.311
Dout-22	8/24/98 7:03	343.00	175.53	104.73	1.036	18.900	0.568	0.021	5.528	0.379	0.335
Dout-23	8/24/98 17:39	636.00	213.32	142.52	1.410	20.310	0.538	0.019	5.192	0.356	0.469
Dout-24	8/24/98 22:12	273.00	131.21	60.41	0.598	20.908	0.643	0.023	6.035	0.413	0.312
Dout-25	8/25/98 11:48	816.00	253.16	182.36	1.804	22.712	0.374	0.014	5.935	0.407	0.349
Dout-26	8/25/98 17:19	331.00	147.41	76.61	0.758	23.470	0.277	0.010	5.521	0.378	0.461
Dout-27	8/26/98 9:06	947.00	282.75	211.95	2.097	25.566	0.164	0.006	5.248	0.360	0.385
Dout-28	8/26/98 16:55	469.00	177.27	106.47	1.053	26.620	0.195	0.007	5.903	0.404	0.314
Dout-29	8/27/98 9:21	986.00	291.79	220.99	2.186	28.806	0.205	0.007	5.527	0.379	0.314
Dout-30	8/27/98 16:37	436.00	170.22	99.42	0.983	29.789	0.354	0.013	5.555	0.387	0.315
Dout-31	8/27/98 23:45	428.00	167.11	96.31	0.953	30.742	0.451	0.016	5.516	0.378	0.36
Dout-32	8/28/98 9:00	555.00	197.08	126.28	1.249	31.991	0.212	0.008	5.205	0.357	0.295

Column E - Zeolite Pellets (0.5 mL/min)

Bottle Weight 64.08 g
Pore Volume 145.90 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co
										0
Eout-1	8/5/98 12:12	0.00	112.15	48.07	0.329	0.329	0.335	0.013	0	0
Eout-2	8/5/98 13:53	101.00	108.81	44.73	0.307	0.636	12.912	0.498	0.288	0.0167143
Eout-3	8/5/98 15:17	84.00	102.55	38.47	0.264	0.900	20.341	0.785	5.546	0.32186643
Eout-4	8/5/98 16:55	98.00	107.54	43.46	0.298	1.198	22.924	0.885	9.714	0.56375956
Eout-5	8/5/98 18:35	100.00	108.93	44.85	0.307	1.505	24.295	0.938	11.626	0.67472397
Eout-6	8/5/98 20:34	119.00	117.80	53.72	0.368	1.873	24.432	0.943	10.416	0.60450067
Eout-7	8/6/98 0:24	230.00	165.33	101.25	0.694	2.567	24.649	0.951	12.136	0.70432221
Eout-8	8/6/98 8:00	456.00	265.32	201.24	1.379	3.946	24.982	0.964	14.854	0.86206346
Eout-9	8/6/98 14:09	369.00	227.26	163.18	1.118	5.065	24.831	0.958	16.18	0.93901891
Eout-10	8/6/98 18:08	239.00	169.92	105.84	0.725	5.790	25.017	0.965	15.861	0.92050549
Eout-11	8/6/98 21:33	205.00	155.52	91.44	0.627	6.417	25.156	0.971	15.954	0.92590282
Eout-12	8/7/98 0:29	176.00	142.37	78.29	0.537	6.954	24.251	0.936	17.165	0.99618415
Eout-13	8/7/98 7:18	409.00	244.64	180.56	1.238	8.191	25.364	0.979	16.521	0.95880911
Eout-14	8/7/98 11:17	239.00	169.82	105.74	0.725	8.916	25.319	0.977	16.393	0.95138053

Column E - Zeolite Pellets (0.25 mL/min)

Bottle Weight 64.08 g
Pore Volume 145.90 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co
										0
Eout-1	8/18/98 11:21	0.00	103.99	39.91	0.274	0.274	1.082	0.039		0
Eout-2	8/18/98 14:54	213.00	110.93	46.85	0.321	0.595	13.8	0.498	0	0.263926
Eout-3	8/18/98 17:23	149.00	96.40	32.32	0.222	0.816	23.601	0.852	3.852	0.49345666
Eout-4	8/18/98 20:44	201.00	109.01	44.93	0.308	1.124	23.38	0.844	7.202	0.56142515
Eout-5	8/18/98 23:13	149.00	98.57	34.49	0.236	1.361	25.457	0.919	8.194	0.73696471
Eout-6	8/19/98 8:17	544.00	185.12	121.04	0.830	2.190	24.543	0.886	10.756	0.78239123
Eout-7	8/19/98 11:20	183.00	105.43	41.35	0.283	2.474	24.413	0.881	11.419	0.7736211
Eout-8	8/19/98 21:24	604.00	198.79	134.71	0.923	3.397	25.077	0.905	11.291	0.82665296
Eout-9	8/20/98 0:44	200.00	108.98	44.9	0.308	3.705	26.181	0.945	12.065	0.86776293
Eout-10	8/20/98 9:47	543.00	185.85	121.77	0.835	4.539	26.991	0.974	12.665	0.8416581
Eout-11	8/20/98 16:23	396.00	152.80	88.72	0.608	5.147	27.172	0.981	12.284	0.93086674
Eout-12	8/21/98 1:22	539.00	185.24	121.16	0.830	5.978	25.504	0.921	13.586	0.88872902
Eout-13	8/21/98 10:29	547.00	186.34	122.26	0.838	6.816	26.752	0.966	12.971	0

Column F - Zeolite Pellets (0.5 mL/min)

Bottle Weight 69.82 g
Pore Volume 143.06 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co
										0
Fout-1	8/5/98 12:20	0.00	119.11	49.29	0.345	0.345	1.192	0.046	0	0
Fout-2	8/5/98 13:59	99.00	115.57	45.75	0.320	0.664	13.754	0.531	0.937	0.05437952
Fout-3	8/5/98 15:26	87.00	108.82	39	0.273	0.937	21.075	0.813	4.97	0.28843782
Fout-4	8/5/98 16:59	93.00	112.82	43	0.301	1.238	24.175	0.933	9.653	0.56021938
Fout-5	8/5/98 18:40	101.00	114.53	44.71	0.313	1.550	24.434	0.943	11.138	0.64640251
Fout-6	8/5/98 20:42	122.00	124.68	54.86	0.383	1.934	24.589	0.949	13.242	0.76850979
Fout-7	8/6/98 0:30	228.00	169.78	99.96	0.699	2.632	24.785	0.956	14.681	0.85202327
Fout-8	8/6/98 8:06	456.00	266.42	196.6	1.374	4.007	25.03	0.966	15.909	0.92329121
Fout-9	8/6/98 14:17	371.00	230.82	161	1.125	5.132	25.078	0.968	16.885	0.97993413
Fout-10	8/6/98 18:15	238.00	173.89	104.07	0.727	5.859	25.009	0.965	17.966	1.04267081
Fout-11	8/6/98 21:39	204.00	158.82	89	0.622	6.481	24.862	0.959	16.787	0.97424662
Fout-12	8/7/98 0:34	175.00	147.19	77.37	0.541	7.022	25.28	0.976	17.158	0.9957779
Fout-13	8/7/98 7:27	413.00	247.19	177.37	1.240	8.262	25.306	0.977	17.579	1.02021096
Fout-14	8/7/98 11:23	236.00	172.36	102.54	0.717	8.979	25.385	0.980	17.501	1.01568417

Column F - Zeolite Pellets (0.25 mL/min)

Bottle Weight 69.82 g
Pore Volume 143.06 ml

Sample	Time	Elapsed Time (min)	Bottle Weight (g)	Water Weight (g)	Pore Volume	Cumulative Pore Volume	Chrom (ppm)	C/Co	PCE (ppm)	C/Co
Fout-1	8/18/98 11:29	0.00	107.88	38.06	0.266	0.266	1.226	0.044		
Fout-2	8/18/98 15:01	212.00	113.78	43.96	0.307	0.573	6.394	0.231	0.487	0.0334
Fout-3	8/18/98 17:30	149.00	98.83	29.01	0.203	0.776	19.708	0.712	2.151	0.1474
Fout-4	8/18/98 20:52	202.00	105.15	35.33	0.247	1.023	21.208	0.766	7.679	0.5261
Fout-5	8/18/98 23:24	152.00	101.47	31.65	0.221	1.244	25.104	0.906	6.942	0.4756
Fout-6	8/19/98 8:25	541.00	179.47	109.65	0.766	2.011	23.429	0.846	10.625	0.7280
Fout-7	8/19/98 11:34	189.00	108.91	39.09	0.273	2.284	24.465	0.883	11.798	0.8084
Fout-8	8/19/98 21:27	593.00	191.01	121.19	0.847	3.131	25.314	0.914	11.932	0.8175
Fout-9	8/20/98 0:52	205.00	111.70	41.88	0.293	3.424	27.203	0.982	12.447	0.8528
Fout-10	8/20/98 9:56	544.00	181.12	111.3	0.778	4.202	24.891	0.899	13.168	0.9022
Fout-11	8/20/98 16:30	394.00	151.65	81.83	0.572	4.774	25.764	0.930	13.268	0.9091
Fout-12	8/21/98 1:29	539.00	180.49	110.67	0.774	5.547	26.334	0.951	13.76	0.9428
Fout-13	8/21/98 10:36	547.00	183.28	113.46	0.793	6.341	27.284	0.985	13.702	0.9388

Appendix D

CXTFIT2 Files for Non-Reactive Tracer Studies

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Tritium Tracer (8/16/98) - SMZ/ZVI Pellets (Column A)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.3
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .273      1.0        1.0      0.0
     0        1          1        0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   3
   1   2.333
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
  1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.000  0.000
       0.237  0.076
       0.502  0.267
       0.751  0.454
       1.001  0.613
       1.273  0.718
       1.527  0.819
       1.768  0.853
       2.023  0.945
       2.333  0.991
       2.614  0.931
       2.832  0.761
       3.092  0.607
       3.444  0.432
       3.782  0.294
       3.967  0.221
       4.295  0.156
       4.609  0.107
       4.919  0.076
       5.250  0.052
       5.661  0.034
       6.337  0.018
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Tritium Tracer (8/16/98) - SMZ/ZVI Pellets (Column B)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.6
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .263       1.0        1.0      0.0
     0         1          1        0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   3
   1   2.263
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
  1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.000  0.000
       0.255  0.040
       0.512  0.256
       0.745  0.459
       0.993  0.615
       1.242  0.732
       1.506  0.851
       1.733  0.873
       1.979  0.941
       2.263  0.938
       2.562  0.948
       2.768  0.781
       3.019  0.589
       3.350  0.417
       3.673  0.259
       3.852  0.207
       4.177  0.135
       4.484  0.090
       4.792  0.058
       5.105  0.041
       5.494  0.023
       6.145  0.011
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Tritium Tracer (8/16/98) - Z/ZVI Pellets (Column C)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE       NREDU
   1         1          2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.1
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT        ILMT     MASS
  300        0          0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .250       1.0        1.0       0.0
     0         1          1         0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                  =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   3
   1   2.168
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
  1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0.000  0.000
       0.261  0.001
       0.501  0.185
       0.729  0.403
       0.970  0.562
       1.208  0.700
       1.458  0.831
       1.671  0.870
       1.905  0.904
       2.168  0.973
       2.460  0.987
       2.653  0.999
       2.894  0.738
       3.210  0.488
       3.525  0.284
       3.696  0.215
       4.007  0.138
       4.287  0.086
       4.582  0.056
       4.877  0.034
       5.237  0.020
       5.859  0.009
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Tritium Tracer (8/16/98) - Z/ZVI Pellets (Column D)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D         R       Mu
    .254      1.0       1.0      0.0
     0        1         1        0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   3
   1   2.283
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
  1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.000  0.000
       0.289  0.001
       0.542  0.143
       0.775  0.358
       1.026  0.524
       1.278  0.781
       1.536  0.862
       1.759  0.925
       2.283  0.976
       2.605  0.971
       2.807  1.005
       2.878  0.774
       3.224  0.524
       3.554  0.334
       3.733  0.231
       4.049  0.157
       4.349  0.097
       4.662  0.060
       4.981  0.036
       5.360  0.020
       6.031  0.008
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Tritium Tracer (8/16/98) - Zeolite Pellets (Column E)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D         R      Mu
    .196      1.0       1.0     0.0
     0        1         1       0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB               =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   3
   1.0 1.808
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ***********************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
      0.200  0.000
      0.399  0.000
      0.581  0.009
      0.755  0.147
      0.919  0.408
      1.103  0.639
      1.287  0.849
      1.445  0.963
      1.625  1.018
      1.808  1.016
      2.038  1.017
      2.189  1.078
      2.360  0.983
      2.596  0.638
      2.834  0.316
      2.960  0.189
      3.186  0.091
      3.398  0.040
      3.613  0.019
      3.837  0.008
      4.109  0.003
      4.582  0.001
      0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Tritium Tracer (8/16/98) - Zeolite Pellets (Column F)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32.8
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D         R       Mu
    .184       1.0       1.0      0.0
     0         1         1        0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   3
   1.0    1.755
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ***********************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
      0.2002 0.000
      0.415   0.000
      0.589  0.008
      0.754  0.103
      0.913  0.318
      1.089  0.585
      1.263   0.796
      1.413  0.907
      1.582  0.963
      1.755  0.992
      1.980  1.063
      2.127  1.051
      2.288  0.997
      2.510  0.719
      2.737  0.393
      2.863   0.248
      3.078  0.108
      3.283  0.050
      3.489  0.021
      3.706  0.010
      3.965  0.005
      4.417  0.002
    0    0    0
```

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     Tritium Tracer (8/16/98) - SMZ/ZVI Pellets (Column A)         *
*        (1 ml/min) (M in mg, L in cm, Time in min)                 *
*                                                                   *
*     DATA INPUT FILE:  tritcola.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.3000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .2730E+00       N
 D........      .1000E+01       Y
 R........      .1000E+01       Y
 mu.......      .0000E+00       N


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  SINGLE PULSE OF CONC. =    1.0000 & DURATION =    2.333
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ          D....      R....
 0     .1530E+00   .100E+01   .100E+01
 1     .3628E-01   .206E+01   .106E+01
 2     .2778E-01   .258E+01   .110E+01
 3     .2775E-01   .260E+01   .109E+01
 4     .2775E-01   .260E+01   .109E+01


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
            D....  R....
    D....  1.000
    R....   .525  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98929397
```

(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.2602E+01	.4376E-01	.5945E+02	.2510E+01	.2693E+01
R....	.1093E+01	.4376E-01	.2498E+02	.1002E+01	.1184E+01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.0000	.0000	.0000	.0000
	2	1.0000	.2370	.0760	.0264	.0496
	3	1.0000	.5020	.2670	.2305	.0365
	4	1.0000	.7510	.4540	.4357	.0183
	5	1.0000	1.0010	.6130	.5926	.0204
	6	1.0000	1.2730	.7180	.7130	.0050
	7	1.0000	1.5270	.8190	.7914	.0276
	8	1.0000	1.7680	.8530	.8446	.0084
	9	1.0000	2.0230	.9450	.8852	.0598
	10	1.0000	2.3330	.9910	.9198	.0712
	11	1.0000	2.6140	.9310	.9245	.0065
	12	1.0000	2.8320	.7610	.7858	-.0248
	13	1.0000	3.0920	.6070	.5743	.0327
	14	1.0000	3.4440	.4320	.3615	.0705
	15	1.0000	3.7820	.2940	.2333	.0607
	16	1.0000	3.9670	.2210	.1847	.0363
	17	1.0000	4.2950	.1560	.1236	.0324
	18	1.0000	4.6090	.1070	.0852	.0218
	19	1.0000	4.9190	.0760	.0596	.0164
	20	1.0000	5.2500	.0520	.0412	.0108
	21	1.0000	5.6610	.0340	.0263	.0077
	22	1.0000	6.3370	.0180	.0129	.0051

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     Tritium Tracer (8/16/98) - SMZ/ZVI Pellets (Column B)         *
*        (1 ml/min) (M in mg, L in cm, Time in min)                 *
*                                                                   *
*     DATA INPUT FILE:  tritcolb.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.6000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .2630E+00       N
 D........      .1000E+01       Y
 R........      .1000E+01       Y
 mu.......      .0000E+00       N


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  SINGLE PULSE OF CONC. =   1.0000 & DURATION =    2.2630
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         D....      R....
 0     .8955E-01   .100E+01   .100E+01
 1     .2536E-01   .176E+01   .104E+01
 2     .2358E-01   .196E+01   .106E+01
 3     .2357E-01   .195E+01   .105E+01
 4     .2357E-01   .195E+01   .105E+01
 5     .2357E-01   .195E+01   .105E+01


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           D....  R....
    D....  1.000
    R....   .472  1.000
```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99131407
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.1952E+01	.3895E-01	.5012E+02	.1871E+01	.2034E+01
R....	.1055E+01	.3895E-01	.2708E+02	.9734E+00	.1136E+01

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESIDUAL
1	1.0000	.0000	.0000	.0000	.0000
2	1.0000	.2550	.0400	.0203	.0197
3	1.0000	.5120	.2560	.2066	.0494
4	1.0000	.7450	.4590	.4130	.0460
5	1.0000	.9930	.6150	.5889	.0261
6	1.0000	1.2420	.7320	.7150	.0170
7	1.0000	1.5060	.8510	.8064	.0446
8	1.0000	1.7330	.8730	.8607	.0123
9	1.0000	1.9790	.9410	.9019	.0391
10	1.0000	2.2630	.9380	.9342	.0038
11	1.0000	2.5620	.9480	.9162	.0318
12	1.0000	2.7680	.7810	.7668	.0142
13	1.0000	3.0190	.5890	.5545	.0345
14	1.0000	3.3500	.4170	.3429	.0741
15	1.0000	3.6730	.2590	.2127	.0463
16	1.0000	3.8520	.2070	.1636	.0434
17	1.0000	4.1770	.1350	.1023	.0327
18	1.0000	4.4840	.0900	.0663	.0237
19	1.0000	4.7920	.0580	.0432	.0148
20	1.0000	5.1050	.0410	.0282	.0128
21	1.0000	5.4940	.0230	.0168	.0062
22	1.0000	6.1450	.0110	.0072	.0038

```
**********************************************************************

*                                                                    *

*     CXTFIT VERSION 2.0 (1/2/95)                                    *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                   *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                              *
*                                                                    *
*     Tritium Tracer (8/16/98) - Z/ZVI Pellets (Column C)            *
*        (1 ml/min) (M in mg, L in cm, Time in min)                  *
*                                                                    *
*     DATA INPUT FILE:  tritcolc.txt                                 *
*                                                                    *
**********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.1000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .2500E+00       N
 D........      .1000E+01       Y
 R........      .1000E+01       Y
 mu.......      .0000E+00       N


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  SINGLE PULSE OF CONC. =    1.0000 & DURATION =    2.1680
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         D....      R....
 0     .7145E-01   .100E+01   .100E+01
 1     .4836E-01   .116E+01   .108E+01
 2     .4807E-01   .112E+01   .108E+01
 3     .4807E-01   .112E+01   .108E+01
 4     .4807E-01   .112E+01   .108E+01


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
            D....  R....
```

```
      D....  1.000
      R....   .356  1.000

   RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98418524
      (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.1123E+01	.5246E-01	.2141E+02	.1014E+01	.1233E+01
R....	.1083E+01	.5246E-01	.2065E+02	.9738E+00	.1193E+01

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.0000	.0000	.0000	.0000
2	1.0000	.2610	.0010	.0033	-.0023
3	1.0000	.5010	.1850	.1028	.0822
4	1.0000	.7290	.4030	.3044	.0986
5	1.0000	.9700	.5620	.5171	.0449
6	1.0000	1.2080	.7000	.6790	.0210
7	1.0000	1.4580	.8310	.7961	.0349
8	1.0000	1.6710	.8700	.8628	.0072
9	1.0000	1.9050	.9040	.9116	-.0076
10	1.0000	2.1680	.9730	.9462	.0268
11	1.0000	2.4600	.9870	.9619	.0251
12	1.0000	2.6530	.9990	.8873	.1117
13	1.0000	2.8940	.7380	.6848	.0532
14	1.0000	3.2100	.4880	.4207	.0673
15	1.0000	3.5250	.2840	.2412	.0428
16	1.0000	3.6960	.2150	.1761	.0389
17	1.0000	4.0070	.1380	.0983	.0397
18	1.0000	4.2870	.0860	.0579	.0281
19	1.0000	4.5820	.0560	.0332	.0228
20	1.0000	4.8770	.0340	.0190	.0150
21	1.0000	5.2370	.0200	.0097	.0103
22	1.0000	5.8590	.0090	.0030	.0060

```
**********************************************************************
*                                                                    *
*     CXTFIT VERSION 2.0 (1/2/95)                                    *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                   *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                              *
*                                                                    *
*     Tritium Tracer (8/16/98) - Z/ZVI Pellets (Column D)            *
*        (1 ml/min) (M in mg, L in cm, Time in min)                  *
*                                                                    *
*     DATA INPUT FILE:  tritcold.txt                                 *
*                                                                    *
**********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.0000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .2540E+00       N
 D........      .1000E+01       Y
 R........      .1000E+01       Y
 mu.......      .0000E+00       N


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  SINGLE PULSE OF CONC. =     1.0000 & DURATION =     2.2830
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ          D....      R....
 0     .6405E-01   .100E+01   .100E+01
 1     .3548E-01   .107E+01   .109E+01
 2     .3535E-01   .105E+01   .109E+01
 3     .3535E-01   .105E+01   .109E+01
 4     .3535E-01   .105E+01   .109E+01


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           D....  R....
    D....  1.000
    R....   .373  1.000
```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98797074
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.1048E+01	.4648E-01	.2254E+02	.9504E+00	.1145E+01
R....	.1090E+01	.4648E-01	.2344E+02	.9925E+00	.1187E+01

ORDERED BY COMPUTER INPUT

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESIDUAL
1	1.0000	.0000	.0000	.0000	.0000
2	1.0000	.2890	.0010	.0040	-.0030
3	1.0000	.5420	.1430	.1141	.0289
4	1.0000	.7750	.3580	.3253	.0327
5	1.0000	1.0260	.5240	.5478	-.0238
6	1.0000	1.2780	.7810	.7142	.0668
7	1.0000	1.5360	.8620	.8266	.0354
8	1.0000	1.7590	.9250	.8888	.0362
9	1.0000	2.2830	.9760	.9616	.0144
10	1.0000	2.6050	.9710	.9716	-.0006
11	1.0000	2.8070	1.0050	.8862	.1188
12	1.0000	2.8780	.7740	.8313	-.0573
13	1.0000	3.2240	.5240	.5166	.0074
14	1.0000	3.5540	.3340	.2867	.0473
15	1.0000	3.7330	.2310	.2033	.0277
16	1.0000	4.0490	.1570	.1086	.0484
17	1.0000	4.3490	.0970	.0592	.0378
18	1.0000	4.6620	.0600	.0313	.0287
19	1.0000	4.9810	.0360	.0163	.0197
20	1.0000	5.3600	.0200	.0075	.0125
21	1.0000	6.0310	.0080	.0019	.0061

```
$
**********************************************************************
*                                                                    *
*     CXTFIT VERSION 2.0 (1/2/95)                                    *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                   *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                              *
*                                                                    *
*     Tritium Tracer (8/16/98) - Zeolite Pellets (Column E)          *
*        (1 ml/min) (M in mg, L in cm, Time in min)                  *
*                                                                    *
*     DATA INPUT FILE:  tritcole.txt                                 *
*                                                                    *
**********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.0000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .1960E+00       N
 D........      .1000E+01       Y
 R........      .1000E+01       Y
 mu.......      .0000E+00       N


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  SINGLE PULSE OF CONC. =     1.0000 & DURATION =     1.808
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         D....      R....
 0     .6629E+00   .100E+01   .100E+01
 1     .2057E+00   .500E+00   .106E+01
 2     .7941E-01   .145E+00   .111E+01
 3     .5622E-01   .216E+00   .111E+01
 4     .5597E-01   .226E+00   .111E+01
 5     .5597E-01   .226E+00   .111E+01
 6     .5597E-01   .226E+00   .111E+01


COVARIANCE MATRIX FOR FITTED PARAMETERS
```

```
==========================================
           D....  R....
     D....  1.000
     R....   .135  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98595542
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
==================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.2257E+00	.5339E-01	.4228E+01	.1143E+00	.3371E+00
R....	.1107E+01	.5339E-01	.2074E+02	.9959E+00	.1219E+01

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.2000	.0000	.0000	.0000
2	1.0000	.3990	.0000	.0001	-.0001
3	1.0000	.5810	.0090	.0102	-.0012
4	1.0000	.7550	.1470	.0986	.0484
5	1.0000	.9190	.4080	.2987	.1093
6	1.0000	1.1030	.6390	.5742	.0648
7	1.0000	1.2870	.8490	.7954	.0536
8	1.0000	1.4450	.9630	.9156	.0474
9	1.0000	1.6250	1.0180	.9904	.0276
10	1.0000	1.8080	1.0160	1.0000	-.0160
11	1.0000	2.0380	1.0170	1.0000	-.0170
12	1.0000	2.1890	1.0780	1.0000	.0780
13	1.0000	2.3600	.9830	.8826	.1004
14	1.0000	2.5960	.6380	.5439	.0941
15	1.0000	2.8340	.3160	.2479	.0681
16	1.0000	2.9600	.1890	.1494	.0396
17	1.0000	3.1860	.0910	.0539	.0371
18	1.0000	3.3980	.0400	.0188	.0212
19	1.0000	3.6130	.0190	.0061	.0129
20	1.0000	3.8370	.0080	.0018	.0062
21	1.0000	4.1090	.0030	.0004	.0026
22	1.0000	4.5820	.0010	.0000	.0010

```
$
□

□

□
      ************************************************************************

□
      *                                                                      *

□
      *     CXTFIT VERSION 2.0 (1/2/95)                                      *
      *     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                     *
      *     NON-LINEAR LEAST-SQUARES ANALYSIS                                *
      *                                                                      *
      *     Tritium Tracer (8/16/98) - Zeolite Pellets (Column F)            *
      *        (1 ml/min) (M in mg, L in cm, Time in min)                    *
      *                                                                      *
      *     DATA INPUT FILE:  tritcolf.txt                                   *
      *                                                                      *
      ************************************************************************


      MODEL DESCRIPTION
      =================
         DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
         FLUX-AVERAGED CONCENTRATION
         REDUCED TIME (T), POSITION(Z)
           (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
         CHARACTERISTIC LENGTH =   32.8000
           FOR DIMENSIONLESS PARAMETERS


      INITIAL VALUES OF COEFFICIENTS
      ==============================
      NAME         INITIAL VALUE    FITTING
       V........      .1840E+00       N
       D........      .1000E+01       Y
       R........      .1000E+01       Y
       mu.......      .0000E+00       N


      BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
      ============================================
        SINGLE PULSE OF CONC. =    1.000 & DURATION =    1.7550
        SOLUTE FREE INITIAL CONDITION
        NO PRODUCTION TERM


      PARAMETER ESTIMATION MODE
      =========================
        MAXIMUM NUMBER OF ITERATIONS =  300


      ITER      SSQ         D....      R....
       0     .6038E+00   .100E+01   .100E+01
       1     .1457E+00   .500E+00   .106E+01
       2     .2296E-01   .148E+00   .110E+01
       3     .4233E-02   .211E+00   .110E+01
       4     .3926E-02   .222E+00   .110E+01
       5     .3926E-02   .222E+00   .110E+01
       6     .3926E-02   .222E+00   .110E+01


      COVARIANCE MATRIX FOR FITTED PARAMETERS
```

```
=======================================
          D....  R....
    D....  1.000
    R....   .133  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99897591
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.2222E+00	.1414E-01	.1572E+02	.1927E+00	.2517E+00
R....	.1100E+01	.1414E-01	.7782E+02	.1071E+01	.1130E+01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.2002	.0000	.0000	.0000
	2	1.0000	.4150	.0000	.0001	-.0001
	3	1.0000	.5890	.0080	.0136	-.0056
	4	1.0000	.7540	.1030	.1054	-.0024
	5	1.0000	.9130	.3180	.3020	.0160
	6	1.0000	1.0890	.5850	.5652	.0198
	7	1.0000	1.2630	.7960	.7784	.0176
	8	1.0000	1.4130	.9070	.8998	.0072
	9	1.0000	1.5820	.9630	.9786	-.0156
	10	1.0000	1.7550	.9920	1.0000	-.0080
	11	1.0000	1.9800	1.0630	1.0000	.0630
	12	1.0000	2.1270	1.0510	1.0000	.0510
	13	1.0000	2.2880	.9970	.9731	.0239
	14	1.0000	2.5100	.7190	.7074	.0116
	15	1.0000	2.7370	.3930	.3799	.0131
	16	1.0000	2.8630	.2480	.2426	.0054
	17	1.0000	3.0780	.1080	.0997	.0083
	18	1.0000	3.2830	.0500	.0384	.0116
	19	1.0000	3.4890	.0210	.0136	.0074
	20	1.0000	3.7060	.0100	.0043	.0057
	21	1.0000	3.9650	.0050	.0010	.0040
	22	1.0000	4.4170	.0020	.0001	.0019

Appendix E

CXTFIT2 Files for Reactive Tracer Studies

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Chromate Step - SMZ/ZVI Pellets (Column A)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.5
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .208       1.982      1.0      0.0
     0         0          1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.823  0.042
       1.500  0.159
       2.011  0.174
       2.964  0.287
       4.038  0.468
       4.818  0.509
       6.376  0.511
       7.184  0.498
       7.841  0.579
       8.833  0.603
       9.097  0.631
       9.837  0.557
       10.676 0.624
       11.449 0.658
       12.078 0.670
       18.138 0.704
       19.176 0.714
       20.260 0.721
       21.440 0.727
       24.306 0.741
       26.220 0.713
       27.603 0.747
       29.340 0.672
       31.238 0.739
       32.762 0.760
       35.062 0.764
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Chromate Step - SMZ/ZVI Pellets (Column A)
   (0.5 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.5
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .147       1.400      1.0       0.0
     0         0         1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0      0
       1.205  0.504
       1.740  0.567
       2.268  0.573
       2.837  0.580
       3.014  0.584
       3.793  0.581
       5.894  0.615
       7.585  0.617
       8.678  0.605
       9.645  0.607
       10.455 0.633
       12.347 0.639
       13.459 0.646
       14.330 0.640
       15.587 0.643
       17.087 0.640
       18.982 0.665
       20.325 0.675
       21.619 0.663
       22.643 0.657
       23.675 0.661
       25.735 0.670
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Chromate Step - SMZ/ZVI Pellets (Column A)
   (0.25 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.5
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .074       0.705      1.0      0.0
     0         0          1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
   0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.000  0
       0.310  0.039
       0.803  0.091
       1.148  0.103
       1.612  0.095
       1.974  0.106
       3.201  0.152
       3.630  0.167
       4.999  0.195
       5.462  0.188
       6.689  0.218
       7.585  0.198
       8.812  0.214
       10.049 0.246
       11.032 0.245
       11.896 0.253
       13.383 0.288
       14.261 0.282
       15.173 0.280
       16.592 0.308
       17.899 0.314
       18.639 0.321
       19.738 0.337
       21.231 0.346
       21.907 0.357
       23.827 0.366
       24.641 0.353
       26.707 0.375
       28.019 0.378
       30.347 0.399
       31.387 0.387
              0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION ***********************************************
"
Chromate Step - SMZ/ZVI Pellets (Column B)
"
   (1 ml/min) (M in mg, L in cm, Time in min)
"
INVERSE    MODE      NREDU
"
   1         1        2
"
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.6
*** BLOCK B: INVERSE PROBLEM ***********************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ******************************************
    V(cm/min)  D          R      Mu
    .197      1.462      1      0.0
     0         0         1       1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0.859  0.045
       1.530  0.181
       2.401  0.260
       3.292  0.382
       4.327  0.592
       4.985  0.611
       6.457  0.573
       7.224  0.572
       7.840  0.636
       8.772  0.675
       9.033  0.679
       9.730  0.619
       10.534 0.668
       11.259 0.701
       11.869 0.709
       17.616 0.735
       18.597 0.742
       19.616 0.752
       20.721 0.749
       23.421 0.761
       25.204 0.741
       26.514 0.762
       28.146 0.676
       29.918 0.759
       31.351 0.769
       33.535  0.778
       0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION ***********************************************
"
Chromate Step - SMZ/ZVI Pellets (Column B)
"
   (0.5 ml/min) (M in mg, L in cm, Time in min)
"
INVERSE    MODE      NREDU
"
   1         1         2
"
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.6
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT        ILMT    MASS
  300         0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .138       1.023       1.0      0.0
     0         0         1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0      0
       1.171  0.447
       1.672  0.515
       2.146  0.518
       2.701  0.524
       2.887  0.518
       3.620  0.527
       5.576  0.555
       7.159  0.559
       8.169  0.552
       9.071  0.551
       9.843  0.578
       11.575 0.593
       12.623 0.590
       13.436 0.590
       14.609 0.611
       16.023 0.616
       17.799 0.634
       19.045 0.637
       20.253 0.623
       21.212 0.624
       22.171 0.628
       24.094 0.650
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
Chromate Step - SMZ/ZVI Pellets (Column B)
   (0.25 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.6
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .069       0.515       1.0      0.0
     0         0         1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.334  0.030
       0.806  0.091
       1.132  0.103
       1.574  0.096
       1.923  0.098
       3.096  0.140
       3.507  0.153
       4.824  0.150
       5.269  0.162
       6.452  0.209
       7.309  0.210
       8.482  0.201
       9.664  0.226
       10.608 0.232
       11.440 0.249
       12.818 0.270
       13.642 0.303
       14.492 0.303
       15.812 0.324
       17.025 0.317
       17.701 0.322
       18.721 0.380
       20.118 0.367
       20.737 0.336
       22.521 0.347
       23.268 0.375
       25.180 0.367
       26.388 0.368
       28.537 0.380
       29.512 0.380
       0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION ***********************************************
"
PCE Step - Zeolite Pellets (Column E)
"
   (1 ml/min) (M in mg, L in cm, Time in min)
"
INVERSE    MODE      NREDU
"
   1         1         2
"
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32
*** BLOCK B: INVERSE PROBLEM ***********************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ******************************************
    V(cm/min)  D          R       Mu
    .101       .1162       1.0      0.0
     0         0         1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
  1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0.6674 0.013
       0.9740 0.498
       1.2377 0.785
       1.5356 0.885
       1.8430 0.938
       2.2112 0.943
       2.9051 0.951
       4.2844 0.964
       5.4029 0.958
       6.1283 0.965
       6.7550 0.971
       7.2916 0.936
       8.5292 0.979
       9.2539 0.977
       0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION ***********************************************
"
PCE Step - Zeolite Pellets (Column E)
"
   (0.25 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32
*** BLOCK B: INVERSE PROBLEM ***********************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ******************************************
    V(cm/min)  D          R       Mu
     0.051   0.0587    1.0       0.0
     0        0         1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ************
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
   0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
   0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.6115 0.039
       0.9326 0.498
       1.1541 0.852
       1.4621 0.844
       1.6985 0.919
       2.5281 0.886
       2.8115 0.881
       3.7348 0.905
       4.0425 0.945
       4.8772 0.974
       5.4852 0.981
       6.3157 0.921
       7.1536 0.966
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - Zeolite Pellets (Column F)
   (0.5 ml/min) (M in mg, L in cm, Time in min)
INVERSE     MODE       NREDU
   1          1          2
 MODC        ZL(BLANK IF MODE=NREDU=1)
   1          32.8
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT         ILMT     MASS
  300         0          0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .100       0.121      1.0       0.0
     0         0          1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
   0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
   0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.6825 0.046
       1.0023 0.531
       1.2749 0.813
       1.5755 0.933
       1.8880 0.943
       2.2715 0.949
       2.9702 0.956
       4.3445 0.966
       5.4699 0.968
       6.1973 0.965
       6.8194 0.959
       7.3602 0.976
       8.6001 0.977
       9.3168 0.980
       0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION ***********************************************
"
PCE Step - Zeolite Pellets (Column F)
"
   (0.25 ml/min) (M in mg, L in cm, Time in min)
"
INVERSE    MODE      NREDU
"
   1         1        2
"
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32.8
*** BLOCK B: INVERSE PROBLEM ***********************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ***************************************
    V(cm/min)  D         R      Mu
    .046     0.0557      1.0      0.0
     0        0         1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ***********************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.6040 0.044
       0.9113 0.231
       1.1141 0.712
       1.3610 0.766
       1.5823 0.906
       2.3487 0.846
       2.6220 0.883
       3.4691 0.914
       3.7618 0.982
       4.5398 0.899
       5.1118 0.930
       5.8854 0.951
       6.6785 0.985
       0      0      0
```

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     Chromate Step - SMZ/ZVI Pellets (Column A)                    *
*        (1 ml/min) (M in mg, L in cm, Time in min)                 *
*                                                                   *
*     DATA INPUT FILE:  onechrma.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.5000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V........      .2080E+00       N
 D........      .1982E+01       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .4542E+01   .100E+01   .000E+00
 1     .5652E+00   .206E+01   .359E+00
 2     .1479E+00   .350E+01   .461E+00
 3     .7454E-01   .466E+01   .424E+00
 4     .6389E-01   .517E+01   .399E+00
 5     .6293E-01   .534E+01   .392E+00
 6     .6286E-01   .539E+01   .390E+00
 7     .6286E-01   .540E+01   .389E+00
 8     .6286E-01   .540E+01   .389E+00


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           R....  mu...
```

```
R....  1.000
mu...  -.405  1.000

 RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .93788875
    (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.5405E+01	.5597E-01	.9656E+02	.5289E+01	.5520E+01
mu...	.3890E+00	.5597E-01	.6950E+01	.2735E+00	.5045E+00

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.8230	.0420	.0044	.0376
2	1.0000	1.5000	.1590	.0586	.1004
3	1.0000	2.0110	.1740	.1301	.0439
4	1.0000	2.9640	.2870	.2718	.0152
5	1.0000	4.0380	.4680	.4015	.0665
6	1.0000	4.8180	.5090	.4719	.0371
7	1.0000	6.3760	.5110	.5667	-.0557
8	1.0000	7.1840	.4980	.5989	-.1009
9	1.0000	7.8410	.5790	.6192	-.0402
10	1.0000	8.8330	.6030	.6423	-.0393
11	1.0000	9.0970	.6310	.6473	-.0163
12	1.0000	9.8370	.5570	.6590	-.1020
13	1.0000	10.6760	.6240	.6693	-.0453
14	1.0000	11.4490	.6580	.6766	-.0186
15	1.0000	12.0780	.6700	.6813	-.0113
16	1.0000	18.1380	.7040	.6998	.0042
17	1.0000	19.1760	.7140	.7008	.0132
18	1.0000	20.2600	.7210	.7015	.0195
19	1.0000	21.4400	.7270	.7021	.0249
20	1.0000	24.3060	.7410	.7029	.0381
21	1.0000	26.2200	.7130	.7032	.0098
22	1.0000	27.6030	.7470	.7033	.0437
23	1.0000	29.3400	.6720	.7034	-.0314
24	1.0000	31.2380	.7390	.7034	.0356
25	1.0000	32.7620	.7600	.7035	.0565
26	1.0000	35.0620	.7640	.7035	.0605

```
$
"
"
      ************************************************************************
"
      *                                                                      *
"
      *     CXTFIT VERSION 2.0 (1/2/95)                                      *
      *     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                     *
      *     NON-LINEAR LEAST-SQUARES ANALYSIS                                *
      *                                                                      *
      *     Chromate Step - SMZ/ZVI Pellets (Column A)                           *
      *        (0.5 ml/min) (M in mg, L in cm, Time in min)                  *
      *                                                                      *
      *     DATA INPUT FILE:  hlfchrma.txt                                   *
      *                                                                      *
      ************************************************************************


      MODEL DESCRIPTION
      =================
         DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
         FLUX-AVERAGED CONCENTRATION
         REDUCED TIME (T), POSITION(Z)
           (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
         CHARACTERISTIC LENGTH =   31.5000
           FOR DIMENSIONLESS PARAMETERS


      INITIAL VALUES OF COEFFICIENTS
      ==============================
      NAME         INITIAL VALUE    FITTING
       V........      .1470E+00       N
       D........      .1400E+01       N
       R........      .1000E+01       Y
       mu.......      .0000E+00       Y


      BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
      ============================================
        STEP INPUT OF CONC. =    1.0000
        SOLUTE FREE INITIAL CONDITION
        NO PRODUCTION TERM


      PARAMETER ESTIMATION MODE
      =========================
        MAXIMUM NUMBER OF ITERATIONS =  300


      ITER      SSQ         R....      mu...
       0     .2790E+01   .100E+01   .000E+00
       1     .1647E+00   .120E+01   .362E+00
       2     .1726E-01   .123E+01   .503E+00
       3     .1608E-01   .121E+01   .519E+00
       4     .1607E-01   .121E+01   .519E+00
       5     .1607E-01   .121E+01   .519E+00
       6     .1607E-01   .121E+01   .519E+00


      COVARIANCE MATRIX FOR FITTED PARAMETERS
```

```
=======================================
           R....  mu...
    R....  1.000
    mu...  -.288  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .96053895
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1208E+01	.2889E-01	.4182E+02	.1148E+01	.1268E+01
mu...	.5192E+00	.2889E-01	.1797E+02	.4591E+00	.5792E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.0000	.0000	.0000	.0000
	2	1.0000	1.2050	.5040	.4777	.0263
	3	1.0000	1.7400	.5670	.5675	-.0005
	4	1.0000	2.2680	.5730	.6044	-.0314
	5	1.0000	2.8370	.5800	.6211	-.0411
	6	1.0000	3.0140	.5840	.6240	-.0400
	7	1.0000	3.7930	.5810	.6305	-.0495
	8	1.0000	5.8940	.6150	.6335	-.0185
	9	1.0000	7.5850	.6170	.6337	-.0167
	10	1.0000	8.6780	.6050	.6337	-.0287
	11	1.0000	9.6450	.6070	.6337	-.0267
	12	1.0000	10.4550	.6330	.6337	-.0007
	13	1.0000	12.3470	.6390	.6337	.0053
	14	1.0000	13.4590	.6460	.6337	.0123
	15	1.0000	14.3300	.6400	.6337	.0063
	16	1.0000	15.5870	.6430	.6337	.0093
	17	1.0000	17.0870	.6400	.6337	.0063
	18	1.0000	18.9820	.6650	.6337	.0313
	19	1.0000	20.3250	.6750	.6337	.0413
	20	1.0000	21.6190	.6630	.6337	.0293
	21	1.0000	22.6430	.6570	.6337	.0233
	22	1.0000	23.6750	.6610	.6337	.0273
	23	1.0000	25.7350	.6700	.6337	.0363

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*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     Chromate Step - SMZ/ZVI Pellets (Column A)                    *
*        (0.25 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*     DATA INPUT FILE:  qrtchrma.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.5000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V........      .7400E-01       N
 D........      .7050E+00       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .1453E+02   .100E+01   .000E+00
 1     .2149E+01   .161E+01   .709E+00
 2     .2962E+00   .241E+01   .136E+01
 3     .1363E+00   .334E+01   .166E+01
 4     .1174E+00   .432E+01   .167E+01
 5     .1052E+00   .530E+01   .163E+01
 6     .9642E-01   .627E+01   .160E+01
 7     .9069E-01   .715E+01   .157E+01
 8     .8744E-01   .788E+01   .154E+01
 9     .8583E-01   .842E+01   .152E+01
10     .8510E-01   .881E+01   .151E+01
```

11	.8480E-01	.907E+01	.150E+01
12	.8468E-01	.924E+01	.149E+01
13	.8464E-01	.935E+01	.149E+01
14	.8463E-01	.942E+01	.149E+01
15	.8462E-01	.946E+01	.148E+01
16	.8462E-01	.948E+01	.148E+01
17	.8462E-01	.948E+01	.148E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.393	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .76975656
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

				95% CONFIDENCE LIMITS	
NAME	VALUE	S.E.COEFF.	T-VALUE	LOWER	UPPER
R....	.9477E+01	.5874E-01	.1613E+03	.9357E+01	.9598E+01
mu...	.1484E+01	.5874E-01	.2527E+02	.1364E+01	.1604E+01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	CONCENTRATION FITTED	RESI-DUAL
	1	1.0000	.0000	.0000	.0000	.0000
	2	1.0000	.3100	.0390	.0000	.0390
	3	1.0000	.8030	.0910	.0000	.0910
	4	1.0000	1.1480	.1030	.0009	.1021
	5	1.0000	1.6120	.0950	.0068	.0882
	6	1.0000	1.9740	.1060	.0170	.0890
	7	1.0000	3.2010	.1520	.0775	.0745
	8	1.0000	3.6300	.1670	.1020	.0650
	9	1.0000	4.9990	.1950	.1731	.0219
	10	1.0000	5.4620	.1880	.1931	-.0051
	11	1.0000	6.6890	.2180	.2355	-.0175
	12	1.0000	7.5850	.1980	.2583	-.0603
	13	1.0000	8.8120	.2140	.2809	-.0669
	14	1.0000	10.0490	.2460	.2964	-.0504
	15	1.0000	11.0320	.2450	.3050	-.0600
	16	1.0000	11.8960	.2530	.3107	-.0577
	17	1.0000	13.3830	.2880	.3175	-.0295
	18	1.0000	14.2610	.2820	.3203	-.0383
	19	1.0000	15.1730	.2800	.3224	-.0424
	20	1.0000	16.5920	.3080	.3248	-.0168
	21	1.0000	17.8990	.3140	.3262	-.0122
	22	1.0000	18.6390	.3210	.3268	-.0058
	23	1.0000	19.7380	.3370	.3275	.0095
	24	1.0000	21.2310	.3460	.3281	.0179
	25	1.0000	21.9070	.3570	.3283	.0287
	26	1.0000	23.8270	.3660	.3287	.0373
	27	1.0000	24.6410	.3530	.3288	.0242
	28	1.0000	26.7070	.3750	.3290	.0460
	29	1.0000	28.0190	.3780	.3291	.0489
	30	1.0000	30.3470	.3990	.3292	.0698
	31	1.0000	31.3870	.3870	.3292	.0578

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*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     Chromate Step - OGI Pellets (Column B)                        *
*        (1 ml/min) (M in mg, L in cm, Time in min)                 *
*                                                                   *
*     DATA INPUT FILE:  onechrmb.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.6000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V........      .1970E+00       N
 D........      .1462E+01       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .3672E+01   .100E+01   .000E+00
 1     .4104E+00   .189E+01   .323E+00
 2     .1074E+00   .304E+01   .395E+00
 3     .6129E-01   .382E+01   .367E+00
 4     .5786E-01   .406E+01   .355E+00
 5     .5770E-01   .411E+01   .353E+00
 6     .5770E-01   .413E+01   .352E+00
 7     .5770E-01   .413E+01   .352E+00


COVARIANCE MATRIX FOR FITTED PARAMETERS
```

```
=======================================
           R....  mu...
    R....  1.000
    mu...  -.353  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .93762100
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.4125E+01	.5241E-01	.7872E+02	.4017E+01	.4234E+01
mu...	.3522E+00	.5241E-01	.6721E+01	.2440E+00	.4604E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.8590	.0450	.0090	.0360
	2	1.0000	1.5300	.1810	.0920	.0890
	3	1.0000	2.4010	.2600	.2591	.0009
	4	1.0000	3.2920	.3820	.4069	-.0249
	5	1.0000	4.3270	.5920	.5257	.0663
	6	1.0000	4.9850	.6110	.5771	.0339
	7	1.0000	6.4570	.5730	.6481	-.0751
	8	1.0000	7.2240	.5720	.6696	-.0976
	9	1.0000	7.8400	.6360	.6821	-.0461
	10	1.0000	8.7720	.6750	.6954	-.0204
	11	1.0000	9.0330	.6790	.6982	-.0192
	12	1.0000	9.7300	.6190	.7042	-.0852
	13	1.0000	10.5340	.6680	.7092	-.0412
	14	1.0000	11.2590	.7010	.7124	-.0114
	15	1.0000	11.8690	.7090	.7144	-.0054
	16	1.0000	17.6160	.7350	.7204	.0146
	17	1.0000	18.5970	.7420	.7206	.0214
	18	1.0000	19.6160	.7520	.7207	.0313
	19	1.0000	20.7210	.7490	.7208	.0282
	20	1.0000	23.4210	.7610	.7210	.0400
	21	1.0000	25.2040	.7410	.7210	.0200
	22	1.0000	26.5140	.7620	.7210	.0410
	23	1.0000	28.1460	.6760	.7210	-.0450
	24	1.0000	29.9180	.7590	.7210	.0380
	25	1.0000	31.3510	.7690	.7210	.0480
	26	1.0000	33.5350	.7780	.7210	.0570

```
$
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"
*********************************************************************
"
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     Chromate Step - SMZ/ZVI Pellets (Column B)                    *
*        (0.5 ml/min) (M in mg, L in cm, Time in min)               *
*                                                                   *
*     DATA INPUT FILE:  h1fchrmb.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.6000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V........      .1380E+00       N
 D........      .1023E+01       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER     SSQ         R....      mu...
 0    .3576E+01   .100E+01   .000E+00
 1    .2353E+00   .121E+01   .407E+00
 2    .3257E-01   .127E+01   .575E+00
 3    .3057E-01   .127E+01   .596E+00
 4    .3057E-01   .126E+01   .596E+00
 5    .3057E-01   .126E+01   .596E+00


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           R....  mu...
```

```
R....  1.000
mu...  -.279  1.000

 RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .91806355
    (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1263E+01	.3974E-01	.3179E+02	.1180E+01	.1346E+01
mu...	.5964E+00	.3974E-01	.1501E+02	.5138E+00	.6790E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.0000	.0000	.0000	.0000
	2	1.0000	1.1710	.4470	.4143	.0327
	3	1.0000	1.6720	.5150	.5145	.0005
	4	1.0000	2.1460	.5180	.5553	-.0373
	5	1.0000	2.7010	.5240	.5753	-.0513
	6	1.0000	2.8870	.5180	.5787	-.0607
	7	1.0000	3.6200	.5270	.5854	-.0584
	8	1.0000	5.5760	.5550	.5882	-.0332
	9	1.0000	7.1590	.5590	.5884	-.0294
	10	1.0000	8.1690	.5520	.5884	-.0364
	11	1.0000	9.0710	.5510	.5884	-.0374
	12	1.0000	9.8430	.5780	.5884	-.0104
	13	1.0000	11.5750	.5930	.5884	.0046
	14	1.0000	12.6230	.5900	.5884	.0016
	15	1.0000	13.4360	.5900	.5884	.0016
	16	1.0000	14.6090	.6110	.5884	.0226
	17	1.0000	16.0230	.6160	.5884	.0276
	18	1.0000	17.7990	.6340	.5884	.0456
	19	1.0000	19.0450	.6370	.5884	.0486
	20	1.0000	20.2530	.6230	.5884	.0346
	21	1.0000	21.2120	.6240	.5884	.0356
	22	1.0000	22.1710	.6280	.5884	.0396
	23	1.0000	24.0940	.6500	.5884	.0616

```
$
"
"
"
*********************************************************************

*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     Chromate Step - SMZ/ZVI Pellets (Column B)                    *
*        (0.25 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*     DATA INPUT FILE:  qrtchrmb.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.6000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .6900E-01       N
 D........      .5150E+00       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =     1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .1470E+02   .100E+01   .000E+00
 1     .2067E+01   .151E+01   .713E+00
 2     .3085E+00   .215E+01   .132E+01
 3     .1660E+00   .292E+01   .159E+01
 4     .1457E+00   .377E+01   .160E+01
 5     .1282E+00   .474E+01   .156E+01
 6     .1113E+00   .588E+01   .152E+01
 7     .9787E-01   .706E+01   .147E+01
 8     .8989E-01   .808E+01   .143E+01
 9     .8619E-01   .885E+01   .140E+01
10     .8475E-01   .935E+01   .138E+01
11     .8427E-01   .967E+01   .137E+01
```

12	.8412E-01	.985E+01	.136E+01
13	.8408E-01	.995E+01	.136E+01
14	.8407E-01	.100E+02	.136E+01
15	.8407E-01	.100E+02	.136E+01
16	.8407E-01	.100E+02	.136E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.438	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .74794787
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

				95% CONFIDENCE LIMITS	
NAME	VALUE	S.E.COEFF.	T-VALUE	LOWER	UPPER
R....	.1004E+02	.6097E-01	.1647E+03	.9918E+01	.1017E+02
mu...	.1355E+01	.6097E-01	.2223E+02	.1231E+01	.1480E+01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	CONCENTRATION FITTED	RESI-DUAL
	1	1.0000	.3340	.0300	.0000	.0300
	2	1.0000	.8060	.0910	.0000	.0910
	3	1.0000	1.1320	.1030	.0001	.1029
	4	1.0000	1.5740	.0960	.0014	.0946
	5	1.0000	1.9230	.0980	.0049	.0931
	6	1.0000	3.0960	.1400	.0399	.1001
	7	1.0000	3.5070	.1530	.0587	.0943
	8	1.0000	4.8240	.1500	.1255	.0245
	9	1.0000	5.2690	.1620	.1472	.0148
	10	1.0000	6.4520	.2090	.1979	.0111
	11	1.0000	7.3090	.2100	.2275	-.0175
	12	1.0000	8.4820	.2010	.2591	-.0581
	13	1.0000	9.6640	.2260	.2823	-.0563
	14	1.0000	10.6080	.2320	.2960	-.0640
	15	1.0000	11.4400	.2490	.3054	-.0564
	16	1.0000	12.8180	.2700	.3167	-.0467
	17	1.0000	13.6420	.3030	.3216	-.0186
	18	1.0000	14.4920	.3030	.3256	-.0226
	19	1.0000	15.8120	.3240	.3300	-.0060
	20	1.0000	17.0250	.3170	.3329	-.0159
	21	1.0000	17.7010	.3220	.3341	-.0121
	22	1.0000	18.7210	.3800	.3355	.0445
	23	1.0000	20.1180	.3670	.3368	.0302
	24	1.0000	20.7370	.3360	.3373	-.0013
	25	1.0000	22.5210	.3470	.3382	.0088
	26	1.0000	23.2680	.3750	.3385	.0365
	27	1.0000	25.1800	.3670	.3389	.0281
	28	1.0000	26.3880	.3680	.3391	.0289
	29	1.0000	28.5370	.3800	.3393	.0407
	30	1.0000	29.5120	.3800	.3394	.0406

```
$
"
"
 ******************************************************************
"
 *                                                                *
"
 *     CXTFIT VERSION 2.0 (1/2/95)                                *
 *     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                *
 *     NON-LINEAR LEAST-SQUARES ANALYSIS                          *
 *                                                                *
 *     PCE Step - SMZ/ZVI Pellets (Column E)                        *
 *        (1 ml/min) (M in mg, L in cm, Time in min)              *
 *                                                                *
 *     DATA INPUT FILE:  hlfcre.txt                               *
 *                                                                *
 ******************************************************************


 MODEL DESCRIPTION
 =================
    DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
    FLUX-AVERAGED CONCENTRATION
    REDUCED TIME (T), POSITION(Z)
      (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
    CHARACTERISTIC LENGTH =   32.0000
      FOR DIMENSIONLESS PARAMETERS


 INITIAL VALUES OF COEFFICIENTS
 ==============================
 NAME          INITIAL VALUE   FITTING
  V........       .1010E+00      N
  D........       .1162E+00      N
  R........       .1000E+01      Y
  mu.......       .0000E+00      Y


 BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
 ============================================
   STEP INPUT OF CONC. =     1.0000
   SOLUTE FREE INITIAL CONDITION
   NO PRODUCTION TERM


 PARAMETER ESTIMATION MODE
 =========================
   MAXIMUM NUMBER OF ITERATIONS =  300


 ITER      SSQ         R....      mu...
  0     .3096E-01  .100E+01  .000E+00
  1     .6880E-02  .102E+01  .421E-01
  2     .6852E-02  .102E+01  .437E-01
  3     .6852E-02  .102E+01  .437E-01


 COVARIANCE MATRIX FOR FITTED PARAMETERS
 =======================================
             R....   mu...
     R....   1.000
```

mu... -.275 1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99277098
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
==========

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1015E+01	.2486E-01	.4085E+02	.9612E+00	.1069E+01
mu...	.4366E-01	.2486E-01	.1757E+01	-.1049E-01	.9782E-01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.6675	.0130	.0706	-.0576
	2	1.0000	.9741	.4980	.4739	.0241
	3	1.0000	1.2377	.7850	.7789	.0061
	4	1.0000	1.5356	.8850	.9158	-.0308
	5	1.0000	1.8430	.9380	.9499	-.0119
	6	1.0000	2.2112	.9430	.9566	-.0136
	7	1.0000	2.9052	.9510	.9573	-.0063
	8	1.0000	4.2845	.9640	.9573	.0067
	9	1.0000	5.4029	.9580	.9573	.0007
	10	1.0000	6.1283	.9650	.9573	.0077
	11	1.0000	6.7551	.9710	.9573	.0137
	12	1.0000	7.2917	.9360	.9573	-.0213
	13	1.0000	8.5292	.9790	.9573	.0217
	14	1.0000	9.2540	.9770	.9573	.0197

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - SMZ/ZVI Pellets (Column E)                         *
*        (0.25 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*     DATA INPUT FILE:  qrtcre.txt                                  *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.0000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .5100E-01       N
 D........      .5870E-01       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ          R....       mu...
 0     .7444E-01   .100E+01   .000E+00
 1     .2204E-01   .931E+00   .708E-01
 2     .2202E-01   .930E+00   .723E-01
 3     .2202E-01   .930E+00   .723E-01


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           R....  mu...
    R....  1.000
```

mu... -.291 1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97369356
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.9298E+00	.4677E-01	.1988E+02	.8268E+00	.1033E+01
mu...	.7230E-01	.4677E-01	.1546E+01	-.3064E-01	.1752E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.6115	.0390	.0697	-.0307
	2	1.0000	.9327	.4980	.5255	-.0275
	3	1.0000	1.1542	.8520	.7755	.0765
	4	1.0000	1.4621	.8440	.9020	-.0580
	5	1.0000	1.6985	.9190	.9239	-.0049
	6	1.0000	2.5281	.8860	.9304	-.0444
	7	1.0000	2.8115	.8810	.9304	-.0494
	8	1.0000	3.7348	.9050	.9304	-.0254
	9	1.0000	4.0426	.9450	.9304	.0146
	10	1.0000	4.8772	.9740	.9304	.0436
	11	1.0000	5.4853	.9810	.9304	.0506
	12	1.0000	6.3157	.9210	.9304	-.0094
	13	1.0000	7.1537	.9660	.9304	.0356

$

```
*********************************************************************
*                                                                   *
*      CXTFIT VERSION 2.0 (1/2/95)                                  *
*      ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                 *
*      NON-LINEAR LEAST-SQUARES ANALYSIS                            *
*                                                                   *
*      PCE Step - OGI Pellets (Column F)                            *
*         (0.5 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*      DATA INPUT FILE:  hlfcrf.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
    DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
    FLUX-AVERAGED CONCENTRATION
    REDUCED TIME (T), POSITION(Z)
      (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
    CHARACTERISTIC LENGTH =    32.8000
      FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .1000E+00       N
 D........      .1210E+00       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =     1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .1959E-01   .100E+01   .000E+00
 1     .2893E-02   .102E+01   .339E-01
 2     .2880E-02   .102E+01   .350E-01
 3     .2880E-02   .102E+01   .350E-01


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
            R....  mu...
    R....  1.000
    mu...  -.276  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99675397
     (COEFFICIENT OF DETERMINATION)
```

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1017E+01	.1612E-01	.6309E+02	.9817E+00	.1052E+01
mu...	.3504E-01	.1612E-01	.2174E+01	-.7311E-04	.7016E-01

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.6825	.0460	.0855	-.0395
2	1.0000	1.0023	.5310	.5174	.0136
3	1.0000	1.2749	.8130	.8091	.0039
4	1.0000	1.5755	.9330	.9297	.0033
5	1.0000	1.8880	.9430	.9593	-.0163
6	1.0000	2.2715	.9490	.9650	-.0160
7	1.0000	2.9703	.9560	.9656	-.0096
8	1.0000	4.3445	.9660	.9656	.0004
9	1.0000	5.4699	.9680	.9656	.0024
10	1.0000	6.1974	.9650	.9656	-.0006
11	1.0000	6.8195	.9590	.9656	-.0066
12	1.0000	7.3603	.9760	.9656	.0104
13	1.0000	8.6001	.9770	.9656	.0114
14	1.0000	9.3169	.9800	.9656	.0144

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - OGI Pellets (Column F)                             *
*        (0.25 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*     DATA INPUT FILE:  qrtcrf.txt                                  *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.8000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V........      .4600E-01       N
 D........      .5570E-01       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER     SSQ         R....      mu...
 0    .1190E+00   .100E+01   .000E+00
 1    .4118E-01   .105E+01   .720E-01
 2    .4099E-01   .105E+01   .762E-01
 3    .4099E-01   .105E+01   .762E-01


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           R....  mu...
    R....  1.000
    mu...  -.313  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .96076561
     (COEFFICIENT OF DETERMINATION)
```

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1049E+01	.6428E-01	.1633E+02	.9080E+00	.1191E+01
mu...	.7624E-01	.6428E-01	.1186E+01	-.6523E-01	.2177E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.6040	.0440	.0249	.0191
	2	1.0000	.9113	.2310	.3291	-.0981
	3	1.0000	1.1141	.7120	.5996	.1124
	4	1.0000	1.3611	.7660	.8060	-.0400
	5	1.0000	1.5823	.9060	.8849	.0211
	6	1.0000	2.3488	.8460	.9262	-.0802
	7	1.0000	2.6220	.8830	.9267	-.0437
	8	1.0000	3.4691	.9140	.9268	-.0128
	9	1.0000	3.7619	.9820	.9268	.0552
	10	1.0000	4.5399	.8990	.9268	-.0278
	11	1.0000	5.1119	.9300	.9268	.0032
	12	1.0000	5.8855	.9510	.9268	.0242
	13	1.0000	6.6786	.9850	.9268	.0582

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - SMZ/ZVI Pellets (Column A)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.3
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D         R      Mu
    .208      1.982      1.0      0.0
     0        0         1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB               =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.823  0.000
       1.500  0.000
       2.011  0.000
       2.964  0.000
       4.038  0.000
       4.818  0.064
       6.376  0.057
       7.184  0.103
       7.841  0.118
       8.833  0.180
       9.097  0.135
       9.837  0.173
       10.676 0.204
       11.449 0.227
       12.078 0.177
       12.863 0.250
       14.207 0.146
       15.556 0.315
       16.388 0.348
       17.353 0.400
       18.138 0.397
       19.176 0.451
       20.260 0.440
       21.440 0.500
       24.306 0.413
       26.220 0.681
       27.603 0.637
       29.340 0.664
       31.238 0.640
       32.762 0.689
       35.062 0.701
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - SMZ/ZVI Pellets (Column A)
   (0.5 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.3
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D         R      Mu
    .147      1.40      1.0     0.0
     0        0          1       1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.000  0.000
       1.205  0.014
       1.740  0.028
       3.793  0.039
       5.894  0.107
       7.585  0.182
       8.678  0.198
       10.455 0.299
       12.347 0.354
       13.459 0.340
       14.330 0.380
       15.587 0.381
       17.087 0.416
       18.982 0.450
       20.325 0.489
       21.619 0.510
       22.643 0.529
       27.098 0.652
       28.294 0.627
       29.314 0.604
       30.456 0.600
       32.595 0.653
       33.591 0.617
       34.760 0.605
       37.170 0.623
       39.598 0.661
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***************************************
PCE Step - SMZ/ZVI Pellets (Column A)
   (0.25 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.3
*** BLOCK B: INVERSE PROBLEM *****************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS *************************************
    V(cm/min)  D         R      Mu
    .074     0.705     1.0     0.0
     0         0         1       1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
      1
      0.07
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM *********************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.310  0.00
       0.803  0.07
       1.148  0.10
       1.612  0.05
       1.974  0.05
       3.201  0.07
       3.630  0.07
       4.999  0.10
       5.462  0.09
       6.689  0.11
       7.585  0.13
       8.812  0.14
       10.049 0.17
       11.032 0.21
       11.896 0.20
       13.383 0.23
       14.261 0.25
       15.173 0.26
       16.592 0.28
       17.899 0.23
       18.639 0.27
       19.738 0.30
       21.231 0.32
       21.907 0.28
       23.827 0.32
       24.641 0.28
       26.707 0.32
       28.019 0.35
       30.347 0.41
       31.387 0.33
       32.417 0.33
       33.741 0.33
```

0 0 0

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - SMZ/ZVI Pellets (Column B)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE     MODE       NREDU
   1          1          2
 MODC        ZL(BLANK IF MODE=NREDU=1)
   1          31.6
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT        ILMT     MASS
  300         0         0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .197       1.462      1       0
     0         0          1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ***********************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0.859  0.000
       1.530  0.000
       2.401  0.000
       3.292  0.000
       4.327  0.015
       6.457  0.090
       7.224  0.139
       7.840  0.164
       8.772  0.177
       9.033  0.177
       9.730  0.210
       11.869 0.255
       12.560 0.294
       13.842 0.263
       15.163 0.363
       15.963 0.407
       16.873 0.421
       17.616 0.438
       18.597 0.488
       19.616 0.523
       20.721 0.546
       23.421 0.552
       26.514 0.685
       28.146 0.689
       29.918 0.709
       31.351 0.723
       33.535 0.742
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - SMZ/ZVI Pellets (Column B)
   (0.5 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.6
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)D(cm2/min) R(PV)     Mu(min-1)
    .138    1.023      20       0
     0        0         1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0       0.000
       1.171   0.000
       1.672   0.000
       3.620   0.027
       5.576   0.090
       7.159   0.146
       8.169   0.223
       9.071   0.265
       9.843   0.255
       11.575  0.353
       12.623  0.384
       13.436  0.415
       14.609  0.409
       16.023  0.391
       17.799  0.532
       19.045  0.520
       20.253  0.476
       21.212  0.557
       22.171  0.549
       24.094  0.631
       25.367  0.583
       26.479  0.652
       27.426  0.612
       28.502  0.670
       30.501  0.624
       31.430  0.682
       32.511  0.540
       33.863  0.609
       34.755  0.611
       37.028  0.644
       38.234  0.600
       0       0       0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - SMZ/ZVI Pellets (Column B)
   (0.25 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.6
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)D(cm2/min) R(PV)     Mu(min-1)
    .0695    0.515      1         0
     0        0         1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ************
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    1
    0.032
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.806  0.034
       1.132  0.034
       1.574  0.034
       1.923  0.031
       3.096  0.047
       3.507  0.040
       4.824  0.052
       5.269  0.064
       6.452  0.107
       7.309  0.112
       8.482  0.135
       9.664  0.152
       10.608 0.173
       11.440 0.192
       12.818 0.213
       13.642 0.240
       14.492 0.267
       15.812 0.266
       17.025 0.227
       17.701 0.264
       18.721 0.281
       20.118 0.238
       20.737 0.309
       22.521 0.261
       23.268 0.282
       25.180 0.296
       26.388 0.306
       28.537 0.313
       29.512 0.303
       30.469 0.343
       31.695 0.310
       0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - Z/ZVI Pellets (Column C)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.3
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R      Mu
    .186       0.8355      1.0      0.0
     0         0         1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ************
  MODB               =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.463  0
       0.859  0.095644547
       1.248  0.178877834
       1.495  0.215771729
       1.785  0.182479511
       2.126  0.24502371
       2.602  0.342077132
       3.152  0.470959077
       4.157  0.480037278
       4.892  0.572206233
       6.228  0.60858482
       6.933  0.67435792
       7.532  0.721963654
       8.398  0.708077735
       9.228  0.737790204
       9.969  0.737242003
       10.660 0.72126744
       11.202 0.775210372
       12.276 0.767700025
       13.466 0.790395527
       14.262 0.869391223
       15.109 0.88665954
       15.819 0.888249322
       16.722 0.915165968
       17.670 0.946413398
       18.704 0.933366225
       21.246 0.985938656
       22.924 1.06208371
       24.135 1.061206589
       25.663 1.030617
       27.386 1.004029274
       30.678 1.045528054
```

0 0 0

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - Z/ZVI Pellets (Column C)
   (0.5 ml/min) (M in mg, L in cm, Time in min)
INVERSE     MODE       NREDU
   1          1          2
 MODC        ZL(BLANK IF MODE=NREDU=1)
   1          31.1
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT        ILMT     MASS
  300         0         0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .134      0.600      1.0      0.0
     0         0          1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
  1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.388  0.000
       0.820  0.000
       1.201  0.000
       1.616  0.067
       2.044  0.121
       2.555  0.183
       3.512  0.321
       5.373  0.487
       7.233  0.531
       8.756  0.596
       9.726  0.606
       10.579 0.630
       11.309 0.659
       12.947 0.642
       13.936 0.640
       14.681 0.670
       15.775 0.674
       17.088 0.702
       18.730 0.707
       19.890 0.684
       20.791 0.714
       21.687 0.668
       23.499 0.709
       24.672 0.675
       25.722 0.710
       26.617 0.690
       27.620 0.661
       29.481 0.696
       30.372 0.622
       31.369 0.649
       32.640 0.679
       33.494 0.703
```

```
35.598 0.693
36.713 0.731
0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION ***********************************************
"
PCE Step - Z/ZVI Pellets (Column C)
"
   (0.25 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         31.1
*** BLOCK B: INVERSE PROBLEM ************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)   D          R       Mu
    .0693      0.3105      1.0      0.0
     0           0          1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.308  0.000
       0.744  0.024
       1.035  0.081
       1.444  0.092
       1.770  0.124
       2.857  0.178
       3.234  0.236
       4.441  0.278
       5.647  0.291
       6.061  0.299
       7.159  0.367
       7.958  0.367
       9.049  0.377
       10.160 0.422
       11.043 0.431
       11.854 0.439
       13.153 0.444
       13.946 0.456
       14.750 0.474
       16.002 0.463
       16.635 0.425
       17.592 0.440
       18.912 0.428
       19.486 0.442
       21.168 0.424
       21.865 0.403
       23.801 0.471
       24.795 0.414
       26.823 0.464
       27.758 0.436
```

```
28.658 0.420
29.804 0.455
0      0      0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - Z/ZVI Pellets (Column D)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32.0
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D         R      Mu
    .193       0.7963     1.0      0.0
     0         0        1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ************
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.546  0.038741332
       0.942  0.005810926
       1.332  0.10322616
       1.578  0.143327029
       1.875  0.157574761
       3.250  0.389770578
       3.961  0.464874051
       4.285  0.509826495
       5.063  0.515895074
       6.505  0.545026451
       7.291  0.602631363
       7.860  0.663596744
       8.766  0.697250774
       9.684  0.681912123
       10.481 0.759844311
       11.221 0.750870268
       11.787 0.794342571
       12.595 0.755036592
       13.782 0.755036592
       15.041 0.807992764
       15.897 0.878491352
       16.807 0.90694296
       17.533 0.853822328
       18.701 0.91724913
       19.513 0.977167448
       20.615 1.008250418
       23.335 0.977441548
       25.131 1.053367322
       26.462 1.09256366
       28.042 1.030617
       29.845 1.059178247
       33.409 1.059178247
```

0 0 0

```
 1
*** BLOCK A: MODEL DESCRIPTION ***********************************************
PCE Step - Z/ZVI Pellets (Column D)
   (0.5 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32.0
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D         R      Mu
    .135       0.558     1.0      0.0
     0         0         1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB               =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.409  0.000
       0.835  0.000
       1.192  0.000
       1.597  0.034
       2.011  0.112
       2.520  0.162
       3.452  0.237
       5.315  0.453
       6.821  0.498
       7.787  0.552
       8.633  0.551
       9.364  0.568
       11.029 0.600
       11.994 0.568
       12.786 0.598
       13.963 0.677
       15.392 0.614
       17.180 0.679
       18.425 0.620
       19.614 0.684
       20.595 0.668
       21.554 0.659
       23.506 0.683
       24.777 0.662
       25.908 0.699
       26.872 0.705
       27.957 0.684
       29.977 0.685
       30.920 0.624
       32.067 0.662
       33.385 0.669
       34.298 0.683
```

```
36.579 0.679
37.784 0.609
0       0       0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION *********************************************
"
PCE Step - Z/ZVI Pellets (Column D)
"
   (0.25 ml/min) (M in mg, L in cm, Time in min)
"
INVERSE     MODE       NREDU
   1          1          2
 MODC        ZL(BLANK IF MODE=NREDU=1)
   1          32.0
*** BLOCK B: INVERSE PROBLEM ***********************************************
  MIT         ILMT     MASS
  300         0          0
*** BLOCK C: TRANSPORT PARAMETERS ******************************************
    V(cm/min)  D          R       Mu
    .070       0.2891       1.0       0.0
     0         0          1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ************
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    1
   0.075
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM **************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0.357  0.000
       0.824  0.000
       1.151  0.004
       1.589  0.067
       1.931  0.084
       3.098  0.163
       3.493  0.185
       4.813  0.239
       5.251  0.235
       6.439  0.255
       7.313  0.284
       8.510  0.341
       9.695  0.356
       10.667 0.345
       11.540 0.342
       12.916 0.369
       13.761 0.394
       14.619 0.400
       15.967 0.401
       17.199 0.393
       17.864 0.365
       18.900 0.379
       20.310 0.356
       20.908 0.413
       22.712 0.407
       23.470 0.378
       25.566 0.360
       26.620 0.404
```

```
28.806 0.379
29.789 0.387
30.742 0.378
31.991 0.357
0       0       0
```

```
 1
*** BLOCK A: MODEL DESCRIPTION ***************************************
PCE Step - Zeolite Pellets (Column E)
   (1 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32
*** BLOCK B: INVERSE PROBLEM *****************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ************************************
    V(cm/min)  D          R      Mu
    .101       .1162       1.0      0.0
     0         1          1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM *********************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
  1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.329  0
       0.636  0.016714304
       0.900  0.321866431
       1.198  0.563759558
       1.505  0.674723967
       1.873  0.604500675
       2.567  0.704322215
       3.946  0.862063462
       5.065  0.939018905
       5.790  0.920505492
       6.417  0.925902819
       6.954  0.996184148
       8.191  0.958809106
       8.916  0.951380526
       0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION ***********************************************
"
PCE Step - Zeolite Pellets (Column E)
"
   (0.25 ml/min) (M in mg, L in cm, Time in min)
"
INVERSE    MODE      NREDU
"
   1         1        2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
     0.051   0.0587     1.0      0.0
     0        1         1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0.274  0
       0.595  0
       0.816  0.263926002
       1.124  0.493456663
       1.361  0.561425146
       2.190  0.736964714
       2.474  0.78239123
       3.397  0.773621103
       3.705  0.826652963
       4.539  0.867762933
       5.147  0.841658102
       5.978  0.930866735
       6.816  0.888729017
       0      0      0
```

```
 1
"
*** BLOCK A: MODEL DESCRIPTION *********************************************
"
PCE Step - Zeolite Pellets (Column F)
   (0.5 ml/min) (M in mg, L in cm, Time in min)
INVERSE     MODE       NREDU
   1          1          2
 MODC         ZL(BLANK IF MODE=NREDU=1)
   1          32.8
*** BLOCK B: INVERSE PROBLEM ***********************************************
  MIT         ILMT     MASS
  300         0          0
*** BLOCK C: TRANSPORT PARAMETERS ******************************************
    V(cm/min)  D          R       Mu
    .100       0.121      1.0       0.0
     0         1          1         1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ************
  MODB                 =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM **************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)      C/Co      (Give "0 0 0" after last data set.)
       0.345  0
       0.664  0.054379525
       0.937  0.288437822
       1.238  0.560219375
       1.550  0.646402507
       1.934  0.768509786
       2.632  0.852023272
       4.007  0.923291209
       5.132  0.979934129
       5.859  1.042670807
       6.481  0.974246623
       7.022  0.995777897
       8.262  1.02021096
       8.979  1.015684169
       0      0      0
```

```
 1
'
*** BLOCK A: MODEL DESCRIPTION ***********************************************
'
PCE Step - Zeolite Pellets (Column F)
   (0.25 ml/min) (M in mg, L in cm, Time in min)
INVERSE    MODE      NREDU
   1         1         2
 MODC       ZL(BLANK IF MODE=NREDU=1)
   1         32.8
*** BLOCK B: INVERSE PROBLEM *************************************************
  MIT       ILMT    MASS
  300        0        0
*** BLOCK C: TRANSPORT PARAMETERS ********************************************
    V(cm/min)  D          R       Mu
    .046      0.0557      1.0      0.0
     0         1          1        1
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE  ***********
  MODB                =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
   2
   1
*** BLOCK E: IVP; MODI=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
  MODI
    0
*** BLOCK F: PVP; MODP=0 ZERO; =1 CONSTANT; =2 STEPWISE; =3 EXPONENTIAL **
   MODP
    0
*** BLOCK G: DATA FOR INVERSE PROBLEM ************************************
INPUTM =0; Z,T,C  =1; T,C FOR SAME Z  =2; Z,C FOR SAME T
   1
   1
  TIME(PV)     C/Co     (Give "0 0 0" after last data set.)
       0.266  0
       0.573  0.033367592
       0.776  0.147379239
       1.023  0.526139089
       1.244  0.475642343
       2.011  0.727989037
       2.284  0.808359027
       3.131  0.817540254
       3.424  0.85282631
       4.202  0.90222679
       4.774  0.909078452
       5.547  0.942788626
       6.341  0.938814663
       0      0      0
```

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - SMZ/ZVI Pellets (Column A)                         *
*        (1 ml/min) (M in mg, L in cm, Time in min)                 *
*                                                                   *
*     DATA INPUT FILE:  onepcea.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.3000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .2080E+00       N
 D........      .1982E+01       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .1649E+02   .100E+01   .000E+00
 1     .3675E+01   .209E+01   .605E+00
 2     .1852E+01   .433E+01   .103E+01
 3     .1149E+01   .973E+01   .103E+01
 4     .2342E+00   .207E+02   .606E+00
 5     .7874E-01   .254E+02   .264E+00
 6     .7820E-01   .254E+02   .248E+00
 7     .7820E-01   .254E+02   .248E+00


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           R....  mu...
    R....  1.000
```

mu... -.749 1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .96736798
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
==========

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.2543E+02	.7132E-01	.3566E+03	.2528E+02	.2557E+02
mu...	.2480E+00	.7132E-01	.3477E+01	.1032E+00	.3928E+00

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.8230	.0000	.0000	.0000
2	1.0000	1.5000	.0000	.0000	.0000
3	1.0000	2.0110	.0000	.0000	.0000
4	1.0000	2.9640	.0000	.0008	-.0008
5	1.0000	4.0380	.0000	.0058	-.0058
6	1.0000	4.8180	.0640	.0141	.0499
7	1.0000	6.3760	.0570	.0436	.0134
8	1.0000	7.1840	.1030	.0646	.0384
9	1.0000	7.8410	.1180	.0839	.0341
10	1.0000	8.8330	.1800	.1154	.0646
11	1.0000	9.0970	.1350	.1241	.0109
12	1.0000	9.8370	.1730	.1492	.0238
13	1.0000	10.6760	.2040	.1780	.0260
14	1.0000	11.4490	.2270	.2046	.0224
15	1.0000	12.0780	.1770	.2261	-.0491
16	1.0000	12.8630	.2500	.2524	-.0024
17	1.0000	14.2070	.1460	.2959	-.1499
18	1.0000	15.5560	.3150	.3370	-.0220
19	1.0000	16.3880	.3480	.3610	-.0130
20	1.0000	17.3530	.4000	.3875	.0125
21	1.0000	18.1380	.3970	.4080	-.0110
22	1.0000	19.1760	.4510	.4335	.0175
23	1.0000	20.2600	.4400	.4585	-.0185
24	1.0000	21.4400	.5000	.4838	.0162
25	1.0000	24.3060	.4130	.5374	-.1244
26	1.0000	26.2200	.6810	.5678	.1132
27	1.0000	27.6030	.6370	.5874	.0496
28	1.0000	29.3400	.6640	.6095	.0545
29	1.0000	31.2380	.6400	.6308	.0092
30	1.0000	32.7620	.6890	.6460	.0430
31	1.0000	35.0620	.7010	.6662	.0348

```
$
~
~
      ************************************************************************
~
      *                                                                      *
      *      CXTFIT VERSION 2.0 (1/2/95)                                     *
      *      ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                    *
      *      NON-LINEAR LEAST-SQUARES ANALYSIS                               *
      *                                                                      *
      *      PCE Step - SMZ/ZVI Pellets (Column A)
*
~
      *         (0.5 ml/min) (M in mg, L in cm, Time in min)                 *
~
      *                                                                      *
      *      DATA INPUT FILE:  hlfpcea.txt                                   *
      *                                                                      *
      ************************************************************************


      MODEL DESCRIPTION
      =================
         DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
         FLUX-AVERAGED CONCENTRATION
         REDUCED TIME (T), POSITION(Z)
           (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
         CHARACTERISTIC LENGTH =    31.3000
           FOR DIMENSIONLESS PARAMETERS


      INITIAL VALUES OF COEFFICIENTS
      ==============================
      NAME         INITIAL VALUE    FITTING
       V........      .1470E+00       N
       D........      .1400E+01       N
       R........      .1000E+01       Y
       mu.......      .0000E+00       Y


      BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
      ============================================
        STEP INPUT OF CONC. =     1.0000
        SOLUTE FREE INITIAL CONDITION
        NO PRODUCTION TERM


      PARAMETER ESTIMATION MODE
      =========================
        MAXIMUM NUMBER OF ITERATIONS =  300


      ITER      SSQ          R....      mu...
       0     .9781E+01   .100E+01   .000E+00
       1     .1733E+01   .231E+01   .506E+00
       2     .7951E+00   .440E+01   .787E+00
       3     .3804E+00   .932E+01   .774E+00
       4     .5102E-01   .168E+02   .590E+00
       5     .2095E-01   .190E+02   .481E+00
       6     .2086E-01   .191E+02   .474E+00
       7     .2086E-01   .191E+02   .474E+00
```

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.611	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98643039
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1910E+02	.3331E-01	.5733E+03	.1903E+02	.1916E+02
mu...	.4740E+00	.3331E-01	.1423E+02	.4060E+00	.5421E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.0000	.0000	.0000	.0000
	2	1.0000	1.2050	.0140	.0000	.0140
	3	1.0000	1.7400	.0280	.0001	.0279
	4	1.0000	3.7930	.0390	.0168	.0222
	5	1.0000	5.8940	.1070	.0796	.0274
	6	1.0000	7.5850	.1820	.1480	.0340
	7	1.0000	8.6780	.1980	.1935	.0045
	8	1.0000	10.4550	.2990	.2637	.0353
	9	1.0000	12.3470	.3540	.3298	.0242
	10	1.0000	13.4590	.3400	.3641	-.0241
	11	1.0000	14.3300	.3800	.3886	-.0086
	12	1.0000	15.5870	.3810	.4205	-.0395
	13	1.0000	17.0870	.4160	.4537	-.0377
	14	1.0000	18.9820	.4500	.4890	-.0390
	15	1.0000	20.3250	.4890	.5101	-.0211
	16	1.0000	21.6190	.5100	.5279	-.0179
	17	1.0000	22.6430	.5290	.5404	-.0114
	18	1.0000	27.0980	.6520	.5816	.0704
	19	1.0000	28.2940	.6270	.5898	.0372
	20	1.0000	29.3140	.6040	.5961	.0079
	21	1.0000	30.4560	.6000	.6024	-.0024
	22	1.0000	32.5950	.6530	.6124	.0406
	23	1.0000	33.5910	.6170	.6164	.0006
	24	1.0000	34.7600	.6050	.6206	-.0156
	25	1.0000	37.1700	.6230	.6279	-.0049
	26	1.0000	39.5980	.6610	.6337	.0273

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*********************************************************************

*                                                                   *
*      CXTFIT VERSION 2.0 (1/2/95)                                  *
*      ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                 *
*      NON-LINEAR LEAST-SQUARES ANALYSIS                            *
*                                                                   *
*      PCE Step - SMZ/ZVI Pellets (Column A)                        *
*         (0.25 ml/min) (M in mg, L in cm, Time in min)             *
*                                                                   *
*      DATA INPUT FILE:  qrtpcea.txt                                *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
    DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
    FLUX-AVERAGED CONCENTRATION
    REDUCED TIME (T), POSITION(Z)
      (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
    CHARACTERISTIC LENGTH =    31.3000
      FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME          INITIAL VALUE    FITTING
 V.........      .7400E-01        N
 D.........      .7050E+00        N
 R.........      .1000E+01        Y
 mu........      .0000E+00        Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =     1.0000
  CONSTANT INITIAL CONC. =      .0700
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ          R....       mu...
 0     .1795E+02   .100E+01   .000E+00
 1     .2931E+01   .172E+01   .757E+00
 2     .4930E+00   .283E+01   .152E+01
 3     .2225E+00   .478E+01   .193E+01
 4     .1268E+00   .919E+01   .191E+01
 5     .4017E-01   .164E+02   .167E+01
 6     .2077E-01   .211E+02   .146E+01
 7     .2005E-01   .221E+02   .140E+01
 8     .2005E-01   .222E+02   .140E+01
 9     .2005E-01   .222E+02   .140E+01
```

COVARIANCE MATRIX FOR FITTED PARAMETERS
==========

	R....	mu...
R....	1.000	
mu...	-.714	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .94806001
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
==========

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.2217E+02	.3694E-01	.6001E+03	.2209E+02	.2224E+02
mu...	.1398E+01	.3694E-01	.3783E+02	.1322E+01	.1473E+01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.3100	.0000	.0686	-.0686
	2	1.0000	.8030	.0700	.0665	.0035
	3	1.0000	1.1480	.1000	.0651	.0349
	4	1.0000	1.6120	.0500	.0632	-.0132
	5	1.0000	1.9740	.0500	.0619	-.0119
	6	1.0000	3.2010	.0700	.0599	.0101
	7	1.0000	3.6300	.0700	.0611	.0089
	8	1.0000	4.9990	.1000	.0733	.0267
	9	1.0000	5.4620	.0900	.0801	.0099
	10	1.0000	6.6890	.1100	.1022	.0078
	11	1.0000	7.5850	.1300	.1207	.0093
	12	1.0000	8.8120	.1400	.1467	-.0067
	13	1.0000	10.0490	.1700	.1722	-.0022
	14	1.0000	11.0320	.2100	.1911	.0189
	15	1.0000	11.8960	.2000	.2064	-.0064
	16	1.0000	13.3830	.2300	.2301	-.0001
	17	1.0000	14.2610	.2500	.2423	.0077
	18	1.0000	15.1730	.2600	.2539	.0061
	19	1.0000	16.5920	.2800	.2694	.0106
	20	1.0000	17.8990	.2300	.2816	-.0516
	21	1.0000	18.6390	.2700	.2876	-.0176
	22	1.0000	19.7380	.3000	.2955	.0045
	23	1.0000	21.2310	.3200	.3047	.0153
	24	1.0000	21.9070	.2800	.3083	-.0283
	25	1.0000	23.8270	.3200	.3169	.0031
	26	1.0000	24.6410	.2800	.3199	-.0399
	27	1.0000	26.7070	.3200	.3264	-.0064
	28	1.0000	28.0190	.3500	.3296	.0204
	29	1.0000	30.3470	.4100	.3342	.0758
	30	1.0000	31.3870	.3300	.3358	-.0058
	31	1.0000	32.4170	.3300	.3372	-.0072
	32	1.0000	33.7410	.3300	.3388	-.0088

```
$
"

"
      ********************************************************************
"
      *                                                                  *
      *     CXTFIT VERSION 2.0 (1/2/95)                                  *
      *     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                 *
      *     NON-LINEAR LEAST-SQUARES ANALYSIS                            *
      *                                                                  *
      *     PCE Step - SMZ/ZVI Pellets (Column B)
*
"
      *        (1 ml/min) (M in mg, L in cm, Time in min)                *
"
      *                                                                  *
      *     DATA INPUT FILE:  onepceb.txt                                *
      *                                                                  *
      ********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.6000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V.........     .1970E+00      N
 D.........     .1462E+01      N
 R.........     .1000E+01      Y
 mu........     .0000E+00      Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .1240E+02   .100E+01   .000E+00
 1     .2564E+01   .186E+01   .623E+00
 2     .1246E+01   .359E+01   .104E+01
 3     .8076E+00   .752E+01   .106E+01
 4     .2138E+00   .157E+02   .705E+00
 5     .2954E-01   .204E+02   .272E+00
 6     .2608E-01   .209E+02   .210E+00
 7     .2607E-01   .209E+02   .207E+00
 8     .2607E-01   .209E+02   .207E+00
```

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.779	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98406533
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.2092E+02	.5151E-01	.4061E+03	.2081E+02	.2102E+02
mu...	.2068E+00	.5151E-01	.4014E+01	.1007E+00	.3128E+00

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.8590	.0000	.0000	.0000
2	1.0000	1.5300	.0000	.0000	.0000
3	1.0000	2.4010	.0000	.0001	-.0001
4	1.0000	3.2920	.0000	.0017	-.0017
5	1.0000	4.3270	.0150	.0090	.0060
6	1.0000	6.4570	.0900	.0527	.0373
7	1.0000	7.2240	.1390	.0771	.0619
8	1.0000	7.8400	.1640	.0990	.0650
9	1.0000	8.7720	.1770	.1350	.0420
10	1.0000	9.0330	.1770	.1455	.0315
11	1.0000	9.7300	.2100	.1741	.0359
12	1.0000	11.8690	.2550	.2627	-.0077
13	1.0000	12.5600	.2940	.2906	.0034
14	1.0000	13.8420	.2630	.3402	-.0772
15	1.0000	15.1630	.3630	.3879	-.0249
16	1.0000	15.9630	.4070	.4150	-.0080
17	1.0000	16.8730	.4210	.4441	-.0231
18	1.0000	17.6160	.4380	.4665	-.0285
19	1.0000	18.5970	.4880	.4942	-.0062
20	1.0000	19.6160	.5230	.5209	.0021
21	1.0000	20.7210	.5460	.5475	-.0015
22	1.0000	23.4210	.5520	.6031	-.0511
23	1.0000	26.5140	.6850	.6531	.0319
24	1.0000	28.1460	.6890	.6746	.0144
25	1.0000	29.9180	.7090	.6948	.0142
26	1.0000	31.3510	.7230	.7090	.0140
27	1.0000	33.5350	.7420	.7276	.0144

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - SMZ/ZVI Pellets (Column B)
*
*        (0.5 ml/min) (M in mg, L in cm, Time in min)                *
*                                                                   *
*     DATA INPUT FILE:  hlfpceb.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.6000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .1380E+00       N
 D........      .1023E+01       N
 R........      .2000E+02       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =     1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .6708E+00   .200E+02   .000E+00
 1     .4360E-01   .169E+02   .435E+00
 2     .3702E-01   .159E+02   .489E+00
 3     .3701E-01   .159E+02   .489E+00
 4     .3701E-01   .159E+02   .489E+00
```

COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================

	R....	mu...
R....	1.000	
mu...	-.615	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97579677
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
==

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1587E+02	.4530E-01	.3504E+03	.1578E+02	.1597E+02
mu...	.4889E+00	.4530E-01	.1079E+02	.3963E+00	.5816E+00

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.0000	.0000	.0000	.0000
2	1.0000	1.1710	.0000	.0000	.0000
3	1.0000	1.6720	.0000	.0000	.0000
4	1.0000	3.6200	.0270	.0139	.0131
5	1.0000	5.5760	.0900	.0751	.0149
6	1.0000	7.1590	.1460	.1469	-.0009
7	1.0000	8.1690	.2230	.1951	.0279
8	1.0000	9.0710	.2650	.2372	.0278
9	1.0000	9.8430	.2550	.2715	-.0165
10	1.0000	11.5750	.3530	.3412	.0118
11	1.0000	12.6230	.3840	.3780	.0060
12	1.0000	13.4360	.4150	.4038	.0112
13	1.0000	14.6090	.4090	.4369	-.0279
14	1.0000	16.0230	.3910	.4711	-.0801
15	1.0000	17.7990	.5320	.5062	.0258
16	1.0000	19.0450	.5200	.5264	-.0064
17	1.0000	20.2530	.4760	.5432	-.0672
18	1.0000	21.2120	.5570	.5547	.0023
19	1.0000	22.1710	.5490	.5649	-.0159
20	1.0000	24.0940	.6310	.5818	.0492
21	1.0000	25.3670	.5830	.5909	-.0079
22	1.0000	26.4790	.6520	.5977	.0543
23	1.0000	27.4260	.6120	.6027	.0093
24	1.0000	28.5020	.6700	.6078	.0622
25	1.0000	30.5010	.6240	.6154	.0086
26	1.0000	31.4300	.6820	.6184	.0636
27	1.0000	32.5110	.5400	.6214	-.0814
28	1.0000	33.8630	.6090	.6246	-.0156
29	1.0000	34.7550	.6110	.6264	-.0154
30	1.0000	37.0280	.6440	.6303	.0137
31	1.0000	38.2340	.6000	.6319	-.0319

****

*

```
*      CXTFIT VERSION 2.0 (1/2/95)                                          *
*      ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                         *
*      NON-LINEAR LEAST-SQUARES ANALYSIS                                    *
*                                                                           *
*      PCE Step - OGI Pellets (Column B)
*
*         (0.25 ml/min) (M in mg, L in cm, Time in min)                     *
*                                                                           *
*      DATA INPUT FILE:  qrtpceb.txt                                        *
*                                                                           *
*****************************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.6000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........     .6950E-01        N
 D........     .5150E+00        N
 R........     .1000E+01        Y
 mu.......     .0000E+00        Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =     1.0000
  CONSTANT INITIAL CONC. =      .0320
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .1895E+02   .100E+01   .000E+00
 1     .2955E+01   .162E+01   .779E+00
 2     .4793E+00   .258E+01   .154E+01
 3     .2033E+00   .429E+01   .195E+01
 4     .1074E+00   .795E+01   .194E+01
 5     .2520E-01   .136E+02   .172E+01
 6     .9758E-02   .168E+02   .154E+01
 7     .9376E-02   .173E+02   .151E+01
 8     .9373E-02   .174E+02   .151E+01
 9     .9373E-02   .174E+02   .151E+01
```

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.623	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97275799
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.1737E+02	.2298E-01	.7558E+03	.1732E+02	.1742E+02
mu...	.1507E+01	.2298E-01	.6560E+02	.1460E+01	.1554E+01

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.8060	.0340	.0298	.0042
2	1.0000	1.1320	.0340	.0290	.0050
3	1.0000	1.5740	.0340	.0279	.0061
4	1.0000	1.9230	.0310	.0272	.0038
5	1.0000	3.0960	.0470	.0274	.0196
6	1.0000	3.5070	.0400	.0296	.0104
7	1.0000	4.8240	.0520	.0464	.0056
8	1.0000	5.2690	.0640	.0550	.0090
9	1.0000	6.4520	.1070	.0824	.0246
10	1.0000	7.3090	.1120	.1042	.0078
11	1.0000	8.4820	.1350	.1340	.0010
12	1.0000	9.6640	.1520	.1618	-.0098
13	1.0000	10.6080	.1730	.1818	-.0088
14	1.0000	11.4400	.1920	.1977	-.0057
15	1.0000	12.8180	.2130	.2202	-.0072
16	1.0000	13.6420	.2400	.2316	.0084
17	1.0000	14.4920	.2670	.2419	.0251
18	1.0000	15.8120	.2660	.2553	.0107
19	1.0000	17.0250	.2270	.2652	-.0382
20	1.0000	17.7010	.2640	.2700	-.0060
21	1.0000	18.7210	.2810	.2761	.0049
22	1.0000	20.1180	.2380	.2829	-.0449
23	1.0000	20.7370	.3090	.2854	.0236
24	1.0000	22.5210	.2610	.2913	-.0303
25	1.0000	23.2680	.2820	.2933	-.0113
26	1.0000	25.1800	.2960	.2972	-.0012
27	1.0000	26.3880	.3060	.2991	.0069
28	1.0000	28.5370	.3130	.3017	.0113
29	1.0000	29.5120	.3030	.3025	.0005
30	1.0000	30.4690	.3430	.3032	.0398
31	1.0000	31.6950	.3100	.3040	.0060

```
$
*
*
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - Z/ZVI Pellets (Column C)
*
*
*        (1 ml/min) (M in mg, L in cm, Time in min)                 *
*                                                                   *
*     DATA INPUT FILE:  onepcec.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.3000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V.........     .1860E+00      N
 D.........     .8355E+00      N
 R.........     .1000E+01      Y
 mu........     .0000E+00      Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .3933E+01   .100E+01   .000E+00
 1     .1160E+01   .175E+01   .218E+00
 2     .6386E+00   .262E+01   .204E+00
 3     .4853E+00   .326E+01   .169E+00
 4     .4437E+00   .366E+01   .151E+00
 5     .4314E+00   .391E+01   .141E+00
 6     .4276E+00   .405E+01   .136E+00
 7     .4264E+00   .414E+01   .133E+00
 8     .4260E+00   .419E+01   .131E+00
 9     .4259E+00   .422E+01   .129E+00
10     .4259E+00   .424E+01   .129E+00
```

```
11     .4259E+00  .424E+01  .129E+00


COVARIANCE MATRIX FOR FITTED PARAMETERS
=======================================
           R....  mu...
    R....  1.000
    mu...  -.322  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .85897627
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================

                                                  95% CONFIDENCE LIMITS
 NAME      VALUE      S.E.COEFF.  T-VALUE       LOWER          UPPER
 R....  .4239E+01   .1258E+00 .3369E+02   .3982E+01     .4496E+01
 mu...  .1287E+00   .1258E+00 .1023E+01  -.1283E+00     .3857E+00


------------------ORDERED BY COMPUTER INPUT-------------------
                                        CONCENTRATION          RESI-
$    NO    DISTANCE       TIME        OBS        FITTED        DUAL
      1      1.0000       .4630       .0000       .0000       .0000
      2      1.0000       .8590       .0956       .0008       .0949
      3      1.0000      1.2480       .1789       .0117       .1672
      4      1.0000      1.4950       .2158       .0310       .1848
      5      1.0000      1.7850       .1825       .0680       .1145
      6      1.0000      2.1260       .2450       .1279       .1171
      7      1.0000      2.6020       .3421       .2286       .1135
      8      1.0000      3.1520       .4710       .3494       .1216
      9      1.0000      4.1570       .4800       .5385      -.0584
     10      1.0000      4.8920       .5722       .6400      -.0678
     11      1.0000      6.2280       .6086       .7575      -.1490
     12      1.0000      6.9330       .6744       .7949      -.1206
     13      1.0000      7.5320       .7220       .8178      -.0958
     14      1.0000      8.3980       .7081       .8406      -.1326
     15      1.0000      9.2280       .7378       .8548      -.1170
     16      1.0000      9.9690       .7372       .8632      -.1259
     17      1.0000     10.6600       .7213       .8686      -.1473
     18      1.0000     11.2020       .7752       .8716      -.0964
     19      1.0000     12.2760       .7677       .8757      -.1080
     20      1.0000     13.4660       .7904       .8782      -.0878
     21      1.0000     14.2620       .8694       .8792      -.0098
     22      1.0000     15.1090       .8867       .8799       .0067
     23      1.0000     15.8190       .8882       .8803       .0079
     24      1.0000     16.7220       .9152       .8806       .0345
     25      1.0000     17.6700       .9464       .8809       .0655
     26      1.0000     18.7040       .9334       .8810       .0524
     27      1.0000     21.2460       .9859       .8812       .1048
     28      1.0000     22.9240      1.0621       .8812       .1809
     29      1.0000     24.1350      1.0612       .8812       .1800
     30      1.0000     25.6630      1.0306       .8812       .1494
     31      1.0000     27.3860      1.0040       .8812       .1228
     32      1.0000     30.6780      1.0455       .8812       .1643
```

```
**********************************************************************
*                                                                    *
*     CXTFIT VERSION 2.0 (1/2/95)                                    *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                   *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                              *
*                                                                    *
*     PCE Step - Z/ZVI Pellets (Column C)                              *
*        (0.5 ml/min) (M in mg, L in cm, Time in min)                  *
*                                                                    *
*     DATA INPUT FILE:  hlfpcec.txt                                  *
*                                                                    *
**********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   31.1000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V.........      .1340E+00      N
 D.........      .6000E+00      N
 R.........      .1000E+01      Y
 mu........      .0000E+00      Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .6381E+01   .100E+01   .000E+00
 1     .8107E+00   .177E+01   .375E+00
 2     .1722E+00   .297E+01   .458E+00
 3     .5253E-01   .400E+01   .434E+00
 4     .3831E-01   .448E+01   .423E+00
 5     .3713E-01   .464E+01   .420E+00
 6     .3705E-01   .469E+01   .419E+00
 7     .3705E-01   .470E+01   .419E+00
 8     .3705E-01   .470E+01   .419E+00
```

COVARIANCE MATRIX FOR FITTED PARAMETERS
==========

	R....	mu...
R....	1.000	
mu...	-.218	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98070038
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
==========

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.4702E+01	.3486E-01	.1349E+03	.4631E+01	.4773E+01
mu...	.4191E+00	.3486E-01	.1202E+02	.3481E+00	.4901E+00

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.3880	.0000	.0000	.0000
2	1.0000	.8200	.0000	.0002	-.0002
3	1.0000	1.2010	.0000	.0045	-.0045
4	1.0000	1.6160	.0670	.0253	.0417
5	1.0000	2.0440	.1210	.0698	.0512
6	1.0000	2.5550	.1830	.1453	.0377
7	1.0000	3.5120	.3210	.3015	.0195
8	1.0000	5.3730	.4870	.5167	-.0297
9	1.0000	7.2330	.5310	.6125	-.0815
10	1.0000	8.7560	.5960	.6456	-.0496
11	1.0000	9.7260	.6060	.6564	-.0504
12	1.0000	10.5790	.6300	.6623	-.0323
13	1.0000	11.3090	.6590	.6656	-.0066
14	1.0000	12.9470	.6420	.6697	-.0277
15	1.0000	13.9360	.6400	.6709	-.0309
16	1.0000	14.6810	.6700	.6715	-.0015
17	1.0000	15.7750	.6740	.6720	.0020
18	1.0000	17.0880	.7020	.6723	.0297
19	1.0000	18.7300	.7070	.6725	.0345
20	1.0000	19.8900	.6840	.6726	.0114
21	1.0000	20.7910	.7140	.6726	.0414
22	1.0000	21.6870	.6680	.6726	-.0046
23	1.0000	23.4990	.7090	.6727	.0363
24	1.0000	24.6720	.6750	.6727	.0023
25	1.0000	25.7220	.7100	.6727	.0373
26	1.0000	26.6170	.6900	.6727	.0173
27	1.0000	27.6200	.6610	.6727	-.0117
28	1.0000	29.4810	.6960	.6727	.0233
29	1.0000	30.3720	.6220	.6727	-.0507
30	1.0000	31.3690	.6490	.6727	-.0237
31	1.0000	32.6400	.6790	.6727	.0063
32	1.0000	33.4940	.7030	.6727	.0303
33	1.0000	35.5980	.6930	.6727	.0203
34	1.0000	36.7130	.7310	.6727	.0583

```
$
"
"
      ************************************************************************
"
      *                                                                      *
      *      CXTFIT VERSION 2.0 (1/2/95)                                     *
      *      ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                    *
      *      NON-LINEAR LEAST-SQUARES ANALYSIS                               *
      *                                                                      *
      *      PCE Step - Z/ZVI Pellets (Column C)
*
"
      *         (0.25 ml/min) (M in mg, L in cm, Time in min)                *
"
      *                                                                      *
      *      DATA INPUT FILE:  qrtpcec.txt                                   *
      *                                                                      *
      ************************************************************************


      MODEL DESCRIPTION
      =================
         DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
         FLUX-AVERAGED CONCENTRATION
         REDUCED TIME (T), POSITION(Z)
           (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
         CHARACTERISTIC LENGTH =    31.1000
           FOR DIMENSIONLESS PARAMETERS


      INITIAL VALUES OF COEFFICIENTS
      ==============================
      NAME         INITIAL VALUE    FITTING
       V........       .6930E-01       N
       D........       .3105E+00       N
       R........       .1000E+01       Y
       mu.......       .0000E+00       Y


      BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
      ============================================
        STEP INPUT OF CONC. =     1.0000
        SOLUTE FREE INITIAL CONDITION
        NO PRODUCTION TERM


      PARAMETER ESTIMATION MODE
      =========================
        MAXIMUM NUMBER OF ITERATIONS =  300


      ITER      SSQ          R....      mu...
       0     .1151E+02   .100E+01   .000E+00
       1     .1227E+01   .145E+01   .600E+00
       2     .1839E+00   .210E+01   .952E+00
       3     .1006E+00   .285E+01   .102E+01
       4     .7070E-01   .356E+01   .993E+00
       5     .5825E-01   .412E+01   .974E+00
       6     .5433E-01   .446E+01   .962E+00
       7     .5333E-01   .465E+01   .956E+00
       8     .5311E-01   .474E+01   .953E+00
```

9	.5307E-01	.479E+01	.952E+00
10	.5306E-01	.481E+01	.951E+00
11	.5306E-01	.481E+01	.951E+00

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.278	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .91615116
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

				95% CONFIDENCE LIMITS	
NAME	VALUE	S.E.COEFF.	T-VALUE	LOWER	UPPER
R....	.4812E+01	.4378E-01	.1099E+03	.4723E+01	.4902E+01
mu...	.9510E+00	.4378E-01	.2172E+02	.8616E+00	.1040E+01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.3080	.0000	.0000	.0000
	2	1.0000	.7440	.0240	.0000	.0240
	3	1.0000	1.0350	.0810	.0011	.0799
	4	1.0000	1.4440	.0920	.0107	.0813
	5	1.0000	1.7700	.1240	.0296	.0944
	6	1.0000	2.8570	.1780	.1447	.0333
	7	1.0000	3.2340	.2360	.1884	.0476
	8	1.0000	4.4410	.2780	.3001	-.0221
	9	1.0000	5.6470	.2910	.3647	-.0737
	10	1.0000	6.0610	.2990	.3787	-.0797
	11	1.0000	7.1590	.3670	.4031	-.0361
	12	1.0000	7.9580	.3670	.4130	-.0460
	13	1.0000	9.0490	.3770	.4206	-.0436
	14	1.0000	10.1600	.4220	.4245	-.0025
	15	1.0000	11.0430	.4310	.4262	.0048
	16	1.0000	11.8540	.4390	.4271	.0119
	17	1.0000	13.1530	.4440	.4279	.0161
	18	1.0000	13.9460	.4560	.4281	.0279
	19	1.0000	14.7500	.4740	.4282	.0458
	20	1.0000	16.0020	.4630	.4284	.0346
	21	1.0000	16.6350	.4250	.4284	-.0034
	22	1.0000	17.5920	.4400	.4284	.0116
	23	1.0000	18.9120	.4280	.4284	-.0004
	24	1.0000	19.4860	.4420	.4285	.0135
	25	1.0000	21.1680	.4240	.4285	-.0045
	26	1.0000	21.8650	.4030	.4285	-.0255
	27	1.0000	23.8010	.4710	.4285	.0425
	28	1.0000	24.7950	.4140	.4285	-.0145
	29	1.0000	26.8230	.4640	.4285	.0355
	30	1.0000	27.7580	.4360	.4285	.0075
	31	1.0000	28.6580	.4200	.4285	-.0085
	32	1.0000	29.8040	.4550	.4285	.0265

```
$
```

```
*************************************************************************
*                                                                       *
*     CXTFIT VERSION 2.0 (1/2/95)                                       *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                      *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                                 *
*                                                                       *
*     PCE Step - Z/ZVI Pellets (Column D)                                 *
*        (1 ml/min) (M in mg, L in cm, Time in min)                     *
*                                                                       *
*     DATA INPUT FILE:  onepced.txt                                     *
*                                                                       *
*************************************************************************

MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.0000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V.........     .1930E+00       N
 D.........     .7963E+00       N
 R.........     .1000E+01       Y
 mu........     .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .4128E+01   .100E+01   .000E+00
 1     .1338E+01   .177E+01   .219E+00
 2     .8560E+00   .268E+01   .218E+00
 3     .5994E+00   .365E+01   .179E+00
 4     .4772E+00   .448E+01   .144E+00
 5     .4426E+00   .495E+01   .123E+00
 6     .4338E+00   .521E+01   .113E+00
 7     .4316E+00   .534E+01   .108E+00
 8     .4311E+00   .541E+01   .105E+00
 9     .4310E+00   .545E+01   .103E+00
10     .4310E+00   .547E+01   .103E+00
11     .4310E+00   .547E+01   .103E+00
```

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.372	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .86546846
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.5468E+01	.1291E+00	.4235E+02	.5205E+01	.5732E+01
mu...	.1028E+00	.1291E+00	.7959E+00	-.1609E+00	.3664E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.5460	.0387	.0000	.0387
	2	1.0000	.9420	.0058	.0001	.0057
	3	1.0000	1.3320	.1032	.0020	.1012
	4	1.0000	1.5780	.1433	.0071	.1363
	5	1.0000	1.8750	.1576	.0203	.1373
	6	1.0000	3.2500	.3898	.1948	.1950
	7	1.0000	3.9610	.4649	.3206	.1442
	8	1.0000	4.2850	.5098	.3769	.1329
	9	1.0000	5.0630	.5159	.5001	.0158
	10	1.0000	6.5050	.5450	.6704	-.1253
	11	1.0000	7.2910	.6026	.7336	-.1309
	12	1.0000	7.8600	.6636	.7689	-.1053
	13	1.0000	8.7660	.6973	.8112	-.1140
	14	1.0000	9.6840	.6819	.8408	-.1589
	15	1.0000	10.4810	.7598	.8588	-.0989
	16	1.0000	11.2210	.7509	.8708	-.1199
	17	1.0000	11.7870	.7943	.8778	-.0835
	18	1.0000	12.5950	.7550	.8853	-.1303
	19	1.0000	13.7820	.7550	.8925	-.1375
	20	1.0000	15.0410	.8080	.8971	-.0891
	21	1.0000	15.8970	.8785	.8991	-.0206
	22	1.0000	16.8070	.9069	.9005	.0064
	23	1.0000	17.5330	.8538	.9013	-.0475
	24	1.0000	18.7010	.9172	.9022	.0151
	25	1.0000	19.5130	.9772	.9026	.0746
	26	1.0000	20.6150	1.0083	.9029	.1053
	27	1.0000	23.3350	.9774	.9034	.0741
	28	1.0000	25.1310	1.0534	.9035	.1499
	29	1.0000	26.4620	1.0926	.9035	.1891
	30	1.0000	28.0420	1.0306	.9035	.1271
	31	1.0000	29.8450	1.0592	.9035	.1556
	32	1.0000	33.4090	1.0592	.9035	.1556

```
$
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      ************************************************************************
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      *                                                                      *
~
      *     CXTFIT VERSION 2.0 (1/2/95)                                      *
      *     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                     *
      *     NON-LINEAR LEAST-SQUARES ANALYSIS                                *
      *                                                                      *
      *     PCE Step - Z/ZVI Pellets (Column D)                                *
      *        (0.5 ml/min) (M in mg, L in cm, Time in min)                  *
      *                                                                      *
      *     DATA INPUT FILE:  hlfpced.txt                                    *
      *                                                                      *
      ************************************************************************


      MODEL DESCRIPTION
      =================
         DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
         FLUX-AVERAGED CONCENTRATION
         REDUCED TIME (T), POSITION(Z)
           (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
         CHARACTERISTIC LENGTH =   32.0000
           FOR DIMENSIONLESS PARAMETERS


      INITIAL VALUES OF COEFFICIENTS
      ==============================
      NAME         INITIAL VALUE   FITTING
       V........      .1350E+00       N
       D........      .5580E+00       N
       R........      .1000E+01       Y
       mu.......      .0000E+00       Y


      BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
      ============================================
        STEP INPUT OF CONC. =    1.0000
        SOLUTE FREE INITIAL CONDITION
        NO PRODUCTION TERM


      PARAMETER ESTIMATION MODE
      =========================
        MAXIMUM NUMBER OF ITERATIONS =  300


      ITER      SSQ         R....      mu...
       0     .7209E+01   .100E+01   .000E+00
       1     .9470E+00   .171E+01   .406E+00
       2     .2452E+00   .286E+01   .511E+00
       3     .8849E-01   .399E+01   .485E+00
       4     .5785E-01   .470E+01   .468E+00
       5     .5298E-01   .503E+01   .460E+00
       6     .5233E-01   .516E+01   .457E+00
       7     .5226E-01   .521E+01   .456E+00
       8     .5225E-01   .522E+01   .455E+00
       9     .5225E-01   .522E+01   .455E+00
```

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.274	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97194940
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.5225E+01	.4202E-01	.1244E+03	.5139E+01	.5311E+01
mu...	.4554E+00	.4202E-01	.1084E+02	.3698E+00	.5410E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.4090	.0000	.0000	.0000
	2	1.0000	.8350	.0000	.0000	.0000
	3	1.0000	1.1920	.0000	.0011	-.0011
	4	1.0000	1.5970	.0340	.0094	.0246
	5	1.0000	2.0110	.1120	.0332	.0788
	6	1.0000	2.5200	.1620	.0852	.0768
	7	1.0000	3.4520	.2370	.2167	.0203
	8	1.0000	5.3150	.4530	.4475	.0055
	9	1.0000	6.8210	.4980	.5508	-.0528
	10	1.0000	7.7870	.5520	.5883	-.0363
	11	1.0000	8.6330	.5510	.6096	-.0586
	12	1.0000	9.3640	.5680	.6220	-.0540
	13	1.0000	11.0290	.6000	.6378	-.0378
	14	1.0000	11.9940	.5680	.6424	-.0744
	15	1.0000	12.7860	.5980	.6448	-.0468
	16	1.0000	13.9630	.6770	.6470	.0300
	17	1.0000	15.3920	.6140	.6483	-.0343
	18	1.0000	17.1800	.6790	.6491	.0299
	19	1.0000	18.4250	.6200	.6493	-.0293
	20	1.0000	19.6140	.6840	.6495	.0345
	21	1.0000	20.5950	.6680	.6495	.0185
	22	1.0000	21.5540	.6590	.6496	.0094
	23	1.0000	23.5060	.6830	.6496	.0334
	24	1.0000	24.7770	.6620	.6496	.0124
	25	1.0000	25.9080	.6990	.6496	.0494
	26	1.0000	26.8720	.7050	.6496	.0554
	27	1.0000	27.9570	.6840	.6496	.0344
	28	1.0000	29.9770	.6850	.6496	.0354
	29	1.0000	30.9200	.6240	.6496	-.0256
	30	1.0000	32.0670	.6620	.6496	.0124
	31	1.0000	33.3850	.6690	.6496	.0194
	32	1.0000	34.2980	.6830	.6496	.0334
	33	1.0000	36.5790	.6790	.6496	.0294
	34	1.0000	37.7840	.6090	.6496	-.0406

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*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - Z/ZVI Pellets (Column D)                             *
*        (0.25 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*     DATA INPUT FILE:  qrtpced.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.0000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V........      .7000E-01       N
 D........      .2891E+00       N
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  CONSTANT INITIAL CONC. =     .0750
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         R....      mu...
 0     .1395E+02   .100E+01   .000E+00
 1     .1580E+01   .154E+01   .656E+00
 2     .1944E+00   .247E+01   .108E+01
 3     .7174E-01   .385E+01   .117E+01
 4     .3775E-01   .522E+01   .114E+01
 5     .3164E-01   .589E+01   .111E+01
 6     .3092E-01   .614E+01   .110E+01
 7     .3086E-01   .622E+01   .110E+01
 8     .3085E-01   .625E+01   .110E+01
 9     .3085E-01   .625E+01   .110E+01
```

COVARIANCE MATRIX FOR FITTED PARAMETERS

	R....	mu...
R....	1.000	
mu...	-.325	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .94310610
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
R....	.6248E+01	.3392E-01	.1842E+03	.6179E+01	.6317E+01
mu...	.1100E+01	.3392E-01	.3243E+02	.1031E+01	.1169E+01

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESIDUAL
	1	1.0000	.3570	.0000	.0704	-.0704
	2	1.0000	.8240	.0000	.0649	-.0649
	3	1.0000	1.1510	.0040	.0614	-.0574
	4	1.0000	1.5890	.0670	.0588	.0082
	5	1.0000	1.9310	.0840	.0612	.0228
	6	1.0000	3.0980	.1630	.1111	.0519
	7	1.0000	3.4930	.1850	.1381	.0469
	8	1.0000	4.8130	.2390	.2285	.0105
	9	1.0000	5.2510	.2350	.2537	-.0187
	10	1.0000	6.4390	.2550	.3054	-.0504
	11	1.0000	7.3130	.2840	.3301	-.0461
	12	1.0000	8.5100	.3410	.3512	-.0102
	13	1.0000	9.6950	.3560	.3628	-.0068
	14	1.0000	10.6670	.3450	.3683	-.0233
	15	1.0000	11.5400	.3420	.3714	-.0294
	16	1.0000	12.9160	.3690	.3741	-.0051
	17	1.0000	13.7610	.3940	.3750	.0190
	18	1.0000	14.6190	.4000	.3755	.0245
	19	1.0000	15.9670	.4010	.3761	.0249
	20	1.0000	17.1990	.3930	.3763	.0167
	21	1.0000	17.8640	.3650	.3764	-.0114
	22	1.0000	18.9000	.3790	.3765	.0025
	23	1.0000	20.3100	.3560	.3765	-.0205
	24	1.0000	20.9080	.4130	.3765	.0365
	25	1.0000	22.7120	.4070	.3765	.0305
	26	1.0000	23.4700	.3780	.3765	.0015
	27	1.0000	25.5660	.3600	.3766	-.0166
	28	1.0000	26.6200	.4040	.3766	.0274
	29	1.0000	28.8060	.3790	.3766	.0024
	30	1.0000	29.7890	.3870	.3766	.0104
	31	1.0000	30.7420	.3780	.3766	.0014
	32	1.0000	31.9910	.3570	.3766	-.0196

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - Zeolite Pellets (Column E)                             *
*        (0.5 ml/min) (M in mg, L in cm, Time in min)                 *
*                                                                   *
*     DATA INPUT FILE:  hlfpcee.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =    32.0000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V........      .1010E+00       N
 D........      .1162E+00       Y
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =     1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         D....      R....      mu...
 0     .4147E+00   .116E+00   .100E+01   .000E+00
 1     .1327E+00   .215E+00   .110E+01   .125E+00
 2     .9359E-01   .370E+00   .124E+01   .113E+00
 3     .7185E-01   .587E+00   .139E+01   .905E-01
 4     .6379E-01   .793E+00   .152E+01   .733E-01
 5     .6196E-01   .924E+00   .161E+01   .625E-01
 6     .6172E-01   .978E+00   .164E+01   .578E-01
 7     .6169E-01   .995E+00   .165E+01   .564E-01
 8     .6169E-01   .999E+00   .166E+01   .560E-01
 9     .6169E-01   .100E+01   .166E+01   .559E-01
10     .6169E-01   .100E+01   .166E+01   .559E-01


COVARIANCE MATRIX FOR FITTED PARAMETERS
```

```
=======================================
          D....  R....  mu...
    D....  1.000
    R....   .839  1.000
    mu...  -.522  -.612  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .95941093
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.1000E+01	.1376E+00	.7269E+01	.6975E+00	.1303E+01
R....	.1658E+01	.1484E+00	.1118E+02	.1332E+01	.1985E+01
mu...	.5590E-01	.9468E-01	.5904E+00	-.1525E+00	.2643E+00

----------ORDERED BY COMPUTER INPUT----------

$ NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
1	1.0000	.3290	.0000	.0188	-.0188
2	1.0000	.6360	.0167	.1575	-.1408
3	1.0000	.9000	.3219	.3070	.0149
4	1.0000	1.1980	.5638	.4539	.1099
5	1.0000	1.5050	.6747	.5720	.1028
6	1.0000	1.8730	.6045	.6758	-.0713
7	1.0000	2.5670	.7043	.7967	-.0923
8	1.0000	3.9460	.8621	.8964	-.0344
9	1.0000	5.0650	.9390	.9247	.0143
10	1.0000	5.7900	.9205	.9335	-.0130
11	1.0000	6.4170	.9259	.9381	-.0122
12	1.0000	6.9540	.9962	.9407	.0555
13	1.0000	8.1910	.9588	.9440	.0148
14	1.0000	8.9160	.9514	.9450	.0064

$

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*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - Zeolite Pellets (Column E)                             *
*        (0.25 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*     DATA INPUT FILE:  qrtpcee.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.0000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE    FITTING
 V.........      .5100E-01       N
 D.........      .5870E-01       Y
 R.........      .1000E+01       Y
 mu........      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =     1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ          D....       R....       mu...
 0     .4241E+00   .587E-01   .100E+01   .000E+00
 1     .4926E-01   .109E+00   .108E+01   .170E+00
 2     .3151E-01   .162E+00   .119E+01   .182E+00
 3     .2824E-01   .203E+00   .125E+01   .172E+00
 4     .2747E-01   .229E+00   .129E+01   .166E+00
 5     .2729E-01   .243E+00   .131E+01   .163E+00
 6     .2726E-01   .249E+00   .132E+01   .162E+00
 7     .2725E-01   .252E+00   .133E+01   .161E+00
 8     .2725E-01   .254E+00   .133E+01   .161E+00
 9     .2725E-01   .254E+00   .133E+01   .161E+00
10     .2725E-01   .255E+00   .133E+01   .161E+00
11     .2725E-01   .255E+00   .133E+01   .161E+00
```

COVARIANCE MATRIX FOR FITTED PARAMETERS

	D....	R....	mu...
D....	1.000		
R....	.787	1.000	
mu...	-.412	-.520	1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97904331
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.2547E+00	.8453E-01	.3013E+01	.6634E-01	.4430E+00
R....	.1329E+01	.9016E-01	.1474E+02	.1128E+01	.1530E+01
mu...	.1608E+00	.6111E-01	.2631E+01	.2464E-01	.2970E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESIDUAL
	1	1.0000	.2740	.0000	.0014	-.0014
	2	1.0000	.5950	.0000	.0966	-.0966
	3	1.0000	.8160	.2639	.2392	.0247
	4	1.0000	1.1240	.4935	.4381	.0554
	5	1.0000	1.3610	.5614	.5584	.0030
	6	1.0000	2.1900	.7370	.7728	-.0358
	7	1.0000	2.4740	.7824	.8025	-.0201
	8	1.0000	3.3970	.7736	.8425	-.0689
	9	1.0000	3.7050	.8267	.8472	-.0206
	10	1.0000	4.5390	.8678	.8527	.0151
	11	1.0000	5.1470	.8417	.8539	-.0123
	12	1.0000	5.9780	.9309	.8545	.0764
	13	1.0000	6.8160	.8887	.8547	.0341

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - Zeolite Pellets (Column F)                             *
*        (0.5 ml/min) (M in mg, L in cm, Time in min)               *
*                                                                   *
*     DATA INPUT FILE:  hlfpcef.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.8000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V.........      .1000E+00       N
 D.........      .1210E+00       Y
 R.........      .1000E+01       Y
 mu........      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         D....      R....      mu...
 0     .2808E+00   .121E+00   .100E+01   .000E+00
 1     .6759E-01   .261E+00   .118E+01   .527E-01
 2     .2537E-01   .413E+00   .135E+01   .241E-01
 3     .1997E-01   .505E+00   .143E+01   .119E-01
 4     .1946E-01   .547E+00   .146E+01   .797E-02
 5     .1942E-01   .559E+00   .147E+01   .687E-02
 6     .1942E-01   .562E+00   .147E+01   .661E-02
 7     .1942E-01   .562E+00   .147E+01   .654E-02
 8     .1942E-01   .563E+00   .147E+01   .653E-02
 9     .1942E-01   .563E+00   .147E+01   .653E-02
10     .1942E-01   .563E+00   .147E+01   .653E-02


COVARIANCE MATRIX FOR FITTED PARAMETERS
```

```
=======================================
           D....  R....  mu...
    D....  1.000
    R....   .672  1.000
    mu...  -.350  -.463  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98877188
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.5626E+00	.5681E-01	.9904E+01	.4376E+00	.6877E+00
R....	.1468E+01	.6004E-01	.2444E+02	.1335E+01	.1600E+01
mu...	.6525E-02	.4749E-01	.1374E+00	-.9800E-01	.1111E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.3450	.0000	.0059	-.0059
	2	1.0000	.6640	.0544	.1207	-.0663
	3	1.0000	.9370	.2884	.2979	-.0095
	4	1.0000	1.2380	.5602	.4877	.0726
	5	1.0000	1.5500	.6464	.6426	.0038
	6	1.0000	1.9340	.7685	.7744	-.0059
	7	1.0000	2.6320	.8520	.9018	-.0498
	8	1.0000	4.0070	.9233	.9767	-.0534
	9	1.0000	5.1320	.9799	.9892	-.0092
	10	1.0000	5.8590	1.0427	.9917	.0510
	11	1.0000	6.4810	.9742	.9926	-.0184
	12	1.0000	7.0220	.9958	.9930	.0027
	13	1.0000	8.2620	1.0202	.9934	.0268
	14	1.0000	8.9790	1.0157	.9935	.0222

$

```
*********************************************************************
*                                                                   *
*     CXTFIT VERSION 2.0 (1/2/95)                                   *
*     ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE                  *
*     NON-LINEAR LEAST-SQUARES ANALYSIS                             *
*                                                                   *
*     PCE Step - Zeolite Pellets (Column F)                             *
*        (0.25 ml/min) (M in mg, L in cm, Time in min)              *
*                                                                   *
*     DATA INPUT FILE:  qrtpcef.txt                                 *
*                                                                   *
*********************************************************************


MODEL DESCRIPTION
=================
   DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
   FLUX-AVERAGED CONCENTRATION
   REDUCED TIME (T), POSITION(Z)
     (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
   CHARACTERISTIC LENGTH =   32.8000
     FOR DIMENSIONLESS PARAMETERS


INITIAL VALUES OF COEFFICIENTS
==============================
NAME         INITIAL VALUE   FITTING
 V........      .4600E-01       N
 D........      .5570E-01       Y
 R........      .1000E+01       Y
 mu.......      .0000E+00       Y


BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS
============================================
  STEP INPUT OF CONC. =    1.0000
  SOLUTE FREE INITIAL CONDITION
  NO PRODUCTION TERM


PARAMETER ESTIMATION MODE
=========================
  MAXIMUM NUMBER OF ITERATIONS =  300


ITER      SSQ         D....      R....      mu...
 0    .3204E+00   .557E-01   .100E+01   .000E+00
 1    .6823E-01   .971E-01   .108E+01   .137E+00
 2    .4817E-01   .156E+00   .119E+01   .137E+00
 3    .4072E-01   .217E+00   .130E+01   .119E+00
 4    .3887E-01   .256E+00   .136E+01   .107E+00
 5    .3857E-01   .275E+00   .139E+01   .101E+00
 6    .3853E-01   .281E+00   .140E+01   .988E-01
 7    .3853E-01   .284E+00   .141E+01   .981E-01
 8    .3853E-01   .284E+00   .141E+01   .979E-01
 9    .3853E-01   .284E+00   .141E+01   .979E-01
10    .3853E-01   .285E+00   .141E+01   .978E-01


COVARIANCE MATRIX FOR FITTED PARAMETERS
```

```
=======================================
           D....  R....  mu...
    D....  1.000
    R....   .801  1.000
    mu...  -.540  -.634  1.000

  RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97415813
     (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS
================================================
```

NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
D....	.2845E+00	.1040E+00	.2736E+01	.5281E-01	.5163E+00
R....	.1409E+01	.1132E+00	.1244E+02	.1156E+01	.1661E+01
mu...	.9784E-01	.8047E-01	.1216E+01	-.8146E-01	.2771E+00

----------ORDERED BY COMPUTER INPUT----------

$	NO	DISTANCE	TIME	CONCENTRATION OBS	FITTED	RESI-DUAL
	1	1.0000	.2660	.0000	.0020	-.0020
	2	1.0000	.5730	.0334	.0949	-.0615
	3	1.0000	.7760	.1474	.2202	-.0729
	4	1.0000	1.0230	.5261	.3788	.1473
	5	1.0000	1.2440	.4756	.5012	-.0256
	6	1.0000	2.0110	.7280	.7556	-.0276
	7	1.0000	2.2840	.8084	.8012	.0072
	8	1.0000	3.1310	.8175	.8723	-.0548
	9	1.0000	3.4240	.8528	.8835	-.0307
	10	1.0000	4.2020	.9022	.8990	.0033
	11	1.0000	4.7740	.9091	.9037	.0054
	12	1.0000	5.5470	.9428	.9065	.0362
	13	1.0000	6.3410	.9388	.9077	.0311