

**SORPTION AND REDUCTION OF PERCHLOROETHYLENE AND
CHROMATE BY A PELLETIZED ZERO VALENT
IRON/SURFACTANT-MODIFIED ZEOLITE**

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Abstract

A new method for sorption and reduction of perchloroethylene (PCE) and chromate was investigated. A series of pellets produced by Cercona of America, Inc. composed of 50% (by volume) iron and zeolite with an additional aluminosilicate binding material were subjected to a mechanical stability test. Pellets containing calcium as the primary exchangeable cation and that did not have aluminum metal added for additional foaming purposes were found to be the most stable. Batch sorption studies were performed on these most stable pellet forms in order to determine the surfactant loading capacity. The surfactant used was the solid bromide salt form of hexadecyltrimethyl ammonium. Results showed that the sorption behavior followed a consistent non-linear trend which could be well described by the Langmuir sorption model.

A series of iron types was characterized for their ability to chemically reduce PCE and chromate in batch kinetic studies; Fisher, US Metals, and Peerless iron. US Metals and Peerless gave very similar results and were more efficient at contaminant reduction than the Fisher iron. Pellets containing US Metals and Peerless iron treated to their maximum surfactant coverage were then used in a similar batch kinetic study to determine the efficiency of the pellets in PCE and chromate reduction. The pellets showed a dramatic increase in contaminant reduction, with the greatest amount of reduction seen in the surfactant modified pellets. In testing US Metals and Peerless pellet products in batch kinetic studies for the ability to remove and reduce chromate, it was found that the Fe powder and the non-surfactant-modified pellets each displayed a single process (reduction) which yielded decay constants of 0.0002 h^{-1} for the U0 pellets and

0.0069 h⁻¹ for the US Metals iron powder and 0.0008 h⁻¹ for the P0 pellets and 0.0231 h⁻¹ for the Peerless iron powder. The surfactant-modified pellets displayed a dual process region (anion exchange and reduction) for both iron types with a weighted average decay constant of 0.0208 h⁻¹ for the U1 pellets based on a k_{sorb} of 0.1336 h⁻¹ and a k_{red} of 0.0147 h⁻¹. The P1 pellets showed a weighted average decay constant of 0.0416 h⁻¹ based on a k_{sorb} of 0.2861 h⁻¹ and a k_{red} of 0.01 h⁻¹.

The Peerless iron pellets were then selected for use in the hydrodynamic column study which was performed at three different volumetric flow rates in order to generate more values for the decay coefficients for each system. The water used in the column study was a synthetically created groundwater similar to that used in a pilot-scale test at the Oregon Graduate Institute. Chromate-laden water was then used to test the dynamic efficiency of the material to remove and degrade chromate from solution. The results of the three column studies along with a tritium tracer study were then modeled using CXTFIT 2.0 in order to estimate retardation and decay. The material mean decay constant for the P1 pellets was estimated at 4.998 h⁻¹ and 4.487 h⁻¹ for the P0 pellets. These favorable results suggest that these pellets may be a beneficial material to be used in *in-situ* groundwater remediation.

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I.

Introduction

1.1 Scope of Work

In the expanding world of *in situ* permeable barrier remediation, a new approach is being investigated for the reduction of toxic aqueous oxyanions and dissolved chlorinated hydrocarbons. The project employs the use of a pellet product produced by Cercona of America that is a mixture of zero valent iron, zeolite (clinoptilolite), and an aluminosilicate binding material. The pellets are treated with the surfactant hexadecyltrimethylammonium (HDTMA) which imparts to them an affinity for dissolved organics and anions that the material would not otherwise possess. In this study, the removal of dissolved chlorinated hydrocarbons and toxic oxyanions from solution is investigated. It is hoped that this iron/surface-modified zeolite pellet (Fe/SMZ pellet) can then be utilized on a large scale as a permeable barrier material for passive groundwater remediation.

Permeable barriers have been used extensively in recent years in research, as well as industry, for *in situ* groundwater remediation. Figure 1.1.1 is a schematic diagram of an inplac barrier.

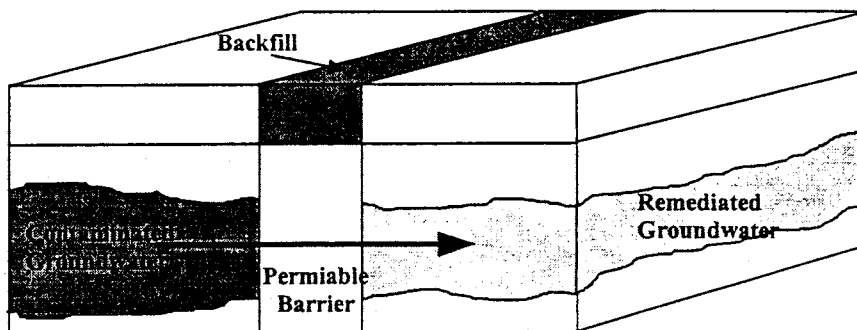


Figure 1.1.1 Schematic diagram of permeable barrier

Permeable barriers can be divided into two general categories. This division is based on the types of interactions between the barrier materials and the contaminants. The first type of barrier is a *sorption* or *retardation* type barrier. In this instance, the contaminant concentration is reduced by the removal of the contaminant from solution due to the sorption of the contaminant to the barrier material. In the majority of cases, the barrier will eventually reach some maximum sorption capacity, at which point the barrier begins to lose its function. In the case of sorption, the contaminant is not transformed by any means, it is merely retarded in its transport. An alternate type of barrier is a *degradation* or *reaction* type barrier and the contaminant concentration is reduced by chemical reactions between the contaminants and the barrier materials. In an ideal instance, the contaminant will be reduced to a nontoxic compound. The performance of these barrier types is dependent on several factors. Primarily, there must exist the specific reactions between the barrier material and contaminants for reduction. It can be difficult, as well as expensive, to find a barrier material that reacts with several different types of contaminants. In addition, for the reactions to effectively occur, the kinetics requires a minimum residence time of the contaminant to be within or in contact with the barrier itself. In some cases, these rates will be very slow and thick barriers have to be employed in order to provide the necessary residence times. This inevitably increases the remediation costs, and in some cases decreases efficiency.

By combining these two types of materials into one, it is hoped that both the advantages will still be achieved as well as compensating for each of their disadvantages. In this case, the Fe/SMZ pellets will be the testing medium of this concept of a sorption/degradation material. The HDMTA will provide the function of sorbing and

retaining the contaminants chromate (Cr^{6+}) and perchloroethylene, or PCE, from solution and subsequently providing the retention time, as well, for the reduction processes to occur by reaction with the zero valent iron in the pellets.

1.2 Relevant Chemical and Physical Theories

1.2.1 Fluid Dynamics and Solute Transport

Advective transport, or *convection*, is the transport of dissolved solids along with flowing ground water. The amount of solute that is actually being carried by the water is a function of its concentration within the groundwater as well as the quantity of ground water flowing. The actual velocity considered in this experiment is the *average linear velocity*, v_x , which is the rate at which the flux of water across the unit cross-sectional area of pore space occurs. During the course of advective fluid flow, solutes within the fluid will be subject to varying degrees of *molecular diffusion* and *mechanical dispersion* (hydrodynamic dispersion) which are functions of both the porous medium as well as the solute itself and its concentration.

Molecular diffusion, or simply diffusion, is the familiar process of a solute moving from an area of high concentration to an area of lower concentration. The diffusive process will occur in virtually any situation where there exists a concentration gradient, even in instances where there is no actual fluid flow; however, the diffusing species must maintain electrical neutrality while diffusing. If there exists a solution of KCl, the K^+ cannot diffuse faster than the Cl^- , unless there is also present some other negative ion in the region to which K^+ is diffusing. If a particular solute begins to sorb onto a mineral surface, it will have a net effect of slowing down the diffusive process. More exact, the term "diffusion" is reserved for the spreading of particles in stagnant fluid, whereas dispersion is used in the description of solute movement under hydrodynamic conditions.

Fick's First Law (Fetter, 1993), the basis for mathematical models that describe these phenomena, says that the mass of fluid diffusing is proportional to the concentration gradient. Fick's First law in its most simplistic form can be written as

$$F = -D_d \left(\frac{dC}{dx} \right) \quad 1.2.1$$

Where

F = mass flux of solute per unit area per unit time (M/TL^2)

D_d = diffusion coefficient (L^2/T)

C = concentration of solute (M/L^3)

dC/dx = concentration gradient ($M/L^3/L$)

The negative sign simply indicates that the movement is down gradient. The *diffusion coefficient*, D_d , is both concentration and temperature dependent. Robinson and Stokes (1965) have noted that at about 5°C the diffusion coefficients are roughly half of what they are at 25°C.

Under conditions where the concentration is changing with time, as will be seen in this experiment, *Fick's second law* will better describe the dynamics. The one dimension equation can be written as

$$\frac{\partial C}{\partial t} = D_d \frac{\partial^2 C}{\partial x^2} \quad 1.2.2$$

When advective flow is also moving the concentration gradient itself, the change in concentration then becomes (Appelo and Postma, 1993)

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} \quad 1.2.3$$

Generally, dispersion occurs in porous media because advective flow causes the water to be continuously forced to flow around sediment grains. This also has the effect of varying the fluid velocity at particular points in space within the system; however, the overall average linear velocity can remain constant. Water will move freely around particles carrying with it any solutes, thereby inducing two basic types of hydrodynamic dispersion (Domenico and Schwartz, 1990), those being longitudinal (D_L), and transverse (D_T). Longitudinal dispersion is a result of travel time differences along flowlines which is induced by flowline splitting at grain boundaries (changes in the x dimension). Transverse dispersion is caused by the intersection and blending of flowlines by diffusion (changes in the y dimension). The net result of these dispersion processes is the dilution of the solute at the advancing edge of flow due to induced mixing. These processes are illustrated in Figure 1.2.1.

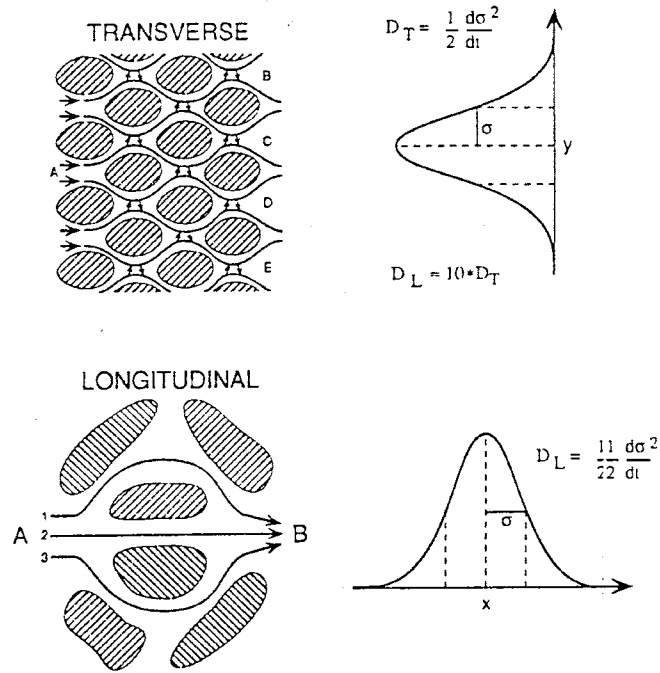


Figure 1.2.1 Illustration of longitudinal and transversal dispersion
(reprinted from Appelo and Postma 1993)

When considering transport processes in a porous medium, additional consideration needs to be given to the fact that there is some hindrance involved from the porous media itself. The path of transport becomes more tortuous, thus the term *tortuosity* is used to describe this effect (Bear, 1972) and basically becomes a coefficient of modification to the original diffusion coefficient yielding a new *effective diffusion coefficient*, D^* . This can be written as

$$D^* = \omega D_d$$

1.2.4

Where ω is the tortuosity.

An additional parameter that needs consideration is the *effective porosity*, n_e , of the medium (Fetter, 1993). This is the pore space through which advective flow actually occurs. Dead-end and noninterconnected pores are not included in the effective porosity.

In transport processes, mechanical dispersion and molecular diffusion must be treated together. These two concepts can be combined to define a parameter called the *hydrodynamic dispersion coefficient*, $D_{(L \text{ or } T)}$, (Fetter, 1993) which can be represented by the following

$$\begin{aligned} D_L &= \alpha_L v_i + D^* \\ D_T &= \alpha_T v_i + D^* \end{aligned} \quad 1.2.5$$

Where

D_L = longitudinal hydrodynamic dispersion coefficient (L^2/T)

D_T = transversal hydrodynamic dispersion coefficient (L^2/T)

α_L = longitudinal dispersivity (L)

α_T = transversal dispersivity (L)

v_i = velocity in the relative direction (L/T)

1.2.2 Column Breakthrough Curves

When a tracer is supplied at some concentration $C=C_0$ in a column which was initially free of the tracer, the tracer will move at the average water flow velocity through the column. At the same time the above discussed hydrodynamic and chemical effects begin to occur as shown below in Figure 1.2.2.

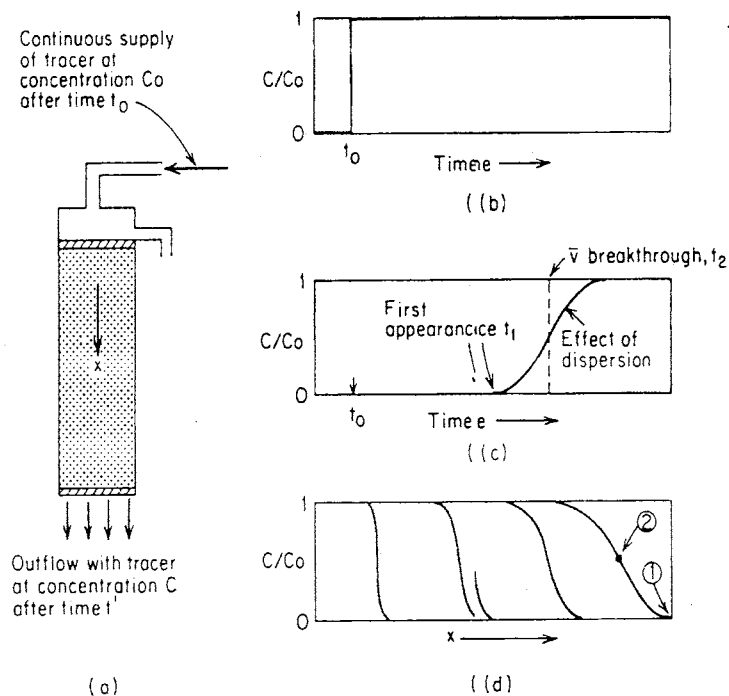


Figure 1.2.2. Column of porous media displaying longitudinal dispersion. (a) steady state flow and continuous supply of tracer after $t=t_0$; (b) relation of step-function tracer input; (c) relative tracer concentration in effluent from column (solid line represents the effects of molecular diffusion and mechanical dispersion and dashed line indicates the tracer front); (d) concentration profile in column at various times. (reprinted from Freeze and Cherry, 1979)

The concentrations in this figure are normalized to the initial concentration (that is C/C_0).

If the tracer is relatively inert in the system (nonreactive), then the condition of the input can be represented mathematically as (Appelo and Postma, 1993)

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad 1.2.6$$

which is subject to the initial and boundary conditions

$$C(x, 0) = C_i$$

$$C(\infty, t) = \text{finite}$$

$$C(0, t) = C_0 \quad 0 < t < t_0$$

$$C(0, t) = 0 \quad t > t_0$$

The solution to this equation bound by the given conditions can be obtained from the following

$$C(x, t) = C_i + \frac{1}{2}(C_0 - C_i) \operatorname{erfc}\left(\frac{x - vt}{\sqrt{4D_L t}}\right) \quad 1.2.7$$

where $\operatorname{erfc}(z)$ is the complementary error function. The equation is symmetric around $x_{0.5} = vt$ due to the fact that $\operatorname{erfc}(-z) = 1 + \operatorname{erf}(z)$ (Appelo and Postma, 1993). The complementary error function (erfc) is a mathematical function related to the Gaussian distribution which relates a standard error to the mean and standard deviation which is a basic statistical analysis that can also be applied to the effects of diffusion (Strobel and Heineman, 1989). This means that the solution to equation 1.2.7 is normally distributed.

We can also see that at one pore volume for an ideal tracer that does not chemically react with the porous medium, the concentration should be 0.5. The overall effects from the advective transport of solute and the resulting dispersion on a tracer slug is illustrated below in Figure 1.2.3.

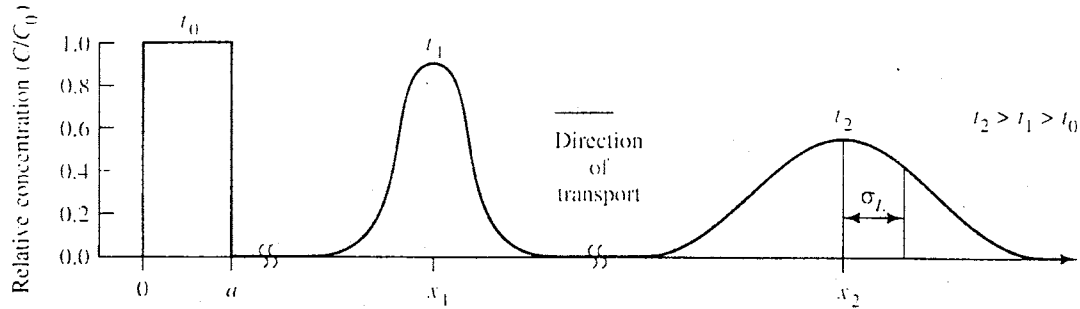


Figure 1.2.3 Effects of advection and dispersion on solute transport with time (reprinted from Appelo and Postma, 1993)

When the contribution to the dispersion coefficient from molecular diffusion is relatively small, the solutions to the advection dispersion equation are the same in all locations of the system, due to the fact that mechanical dispersion is the prime contributor to the dispersion coefficient. It is also possible to evaluate the relative contribution of mechanical dispersion and diffusion to solute transport by the determination of a dimensionless parameter called the *Peclet number*. This parameter relates the effectiveness of mass transport by advection to the effectiveness of transport by either molecular diffusion or dispersion (Fetter 1993). It is essentially a transport rate ratio which can be defined mathematically as

$$P = \frac{v_x L}{D_L}$$

where

$P =$ Peclet number

$L =$ length of flow

At higher Peclet numbers, advection is the controlling process of solute transport, while at lower Peclet numbers, dispersion is more important. The solutions for flux concentration of stable solute species (e.g. nondecaying) that experience retarding effects with linear sorption is given (Parker and van Genuchten 1984) as

$$C(x,t) = C_i + (C_0 - C_i)A(x,t) \quad 1.2.9$$

for $0 < t < t_0$

and

$$C(x,t) = C_i + (C_0 - C_i)A(x,t) - C_0A(x,t - t_0) \quad 1.2.10$$

for $t > t_0$

where

$$A(x,t) = \frac{1}{2} \operatorname{erfc} \left[\frac{Rx - vt}{2(DRt)^{1/2}} \right] + \frac{1}{2} \exp \left(\frac{vx}{D} \right) \operatorname{erfc} \left[\frac{(Rx + vt)^2}{2(DRt)^{1/2}} \right] \quad 1.2.11$$

The retarded species generally show the same amount of spreading at all points in the system as would a conservative tracer, only it would arrive later depending on the retardation factor. The effects of retardation on a species as compared to an inert species are illustrated in Figure 1.2.4.

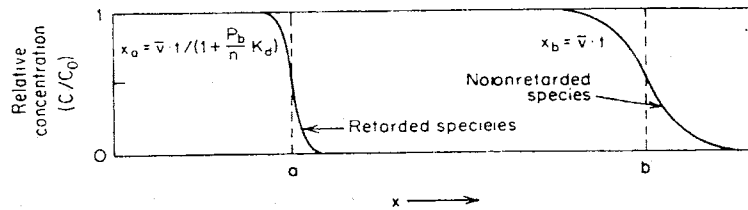


Figure 1.2.4. Effects of arrival time on a retarded solute (reprinted from Appelo and Postma, 1993)

Using the above equations and ideas, it is possible to deduce the transport processes in a system.

1.2.3 Sorption Processes

Equation 1.2.6 is the one-dimensional advection/dispersion equation which can be modified to include such things as sorption (retardation) and decay. In the presence of sorption processes, equation 1.2.6 becomes

$$R \frac{\partial C}{\partial t} = D_L \left(\frac{\partial^2 C}{\partial x^2} \right) - v \left(\frac{\partial C}{\partial x} \right) \quad 1.2.12$$

Where

$S =$ amount of solute sorbed per unit weight of solid

$R =$ retardation coefficient $= 1 + \rho K_d / \theta$

When the solute of interest is subject to sorption in the medium some adjustments need to be made to the advection dispersion equation 1.2.6 which will give account for the retarding of the solute transport. This is done by adding a factor that contains a distribution coefficient, in which case equation 1.2.6 becomes

$$\left(1 + \frac{\rho K_d}{\theta}\right) \frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2} \quad 1.2.13$$

where

$K_d =$ empirical distribution coefficient (L^3/M)

$\rho =$ ~~density of water~~ ^{Soil bulk density} (M/L^3)

$\theta =$ water content (%)

which can also be written as

$$R \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad 1.2.14$$

The usefulness of sorption studies has many applications. Sorption studies are generally used in transport studies and in the determination of migration velocities and are a very useful tool when attempting to quantify the partitioning of a solute between the

sorbed phase and the solution phase. If a substance is in contact with two other phases then, in general, it will have a different affinity for each phase. Part of the substance will be adsorbed or dissolved by one and part by the other, the relative amounts would, of course, depend on the relative affinities.

The actual sorption is determined experimentally by measuring how much of a solute can be sorbed by a particular substrate. Aliquots of the solute in varying concentrations are well-mixed with the solid, and the amount of solute that is removed from solution is then determined. The capacity of a solid to remove a solute is a function of the solute concentration. The results of an experiment are plotted on a graph that shows the solute concentration versus the amount of solute sorbed onto the solid. In the case of a rapid sorptive process in comparison to the flow velocity, the solute will reach an equilibrium condition with the sorbed phase. When the equilibrium conditions have been established, the process can be described by an equilibrium sorption isotherm. If on the other hand, the sorptive process is slow compared to the flow velocity, the solute may not actually come to an equilibrium with the sorbed phase in which case a kinetic sorption model would be needed to describe the process (Fetter, 1993).

In equilibrium surface reaction, we can define three basic types of equilibrium sorption isotherms: 1) linear, 2) Freundlich, and 3) Langmuir isotherms. This, of course, is not an exhaustive list of isotherms. If there is a direct, linear relationship to the amount of solute sorbed onto solid, S , and the solute concentration, C , the sorption isotherm will plot as a straight line. The *linear sorption isotherm* can be described by the equation

$$S = K_D C$$

The coefficient K_D is known as the *distribution coefficient*. Graphically, it is equal to the slope of the linear sorption isotherm.

There are two major limitations to the linear isotherm model. The first is that there is no upper boundary condition for the amount of solute that can be sorbed onto the solid. Secondly, the sorption isotherm may not be properly interpreted if only a few data points exist. A curvilinear plot may appear to be linear with only a few data points (Fetter, 1993).

The *Freundlich sorption isotherm* is a more general isotherm that is defined by a nonlinear relationship. The Freundlich isotherm can be described by the equation

$$S = K_F C^N \quad 1.2.16$$

Where K_F and N are both constants. If N is greater than 1, then there is a spreading front, whereas if N is less than 1, the front will be self sharpening. If N is equal to 1, the Freundlich sorption isotherm becomes equivalent to the linear sorption isotherm, that is, $K_F = K_D$.

The Freundlich sorption isotherm has the same problem that the linear isotherm does, in that there is no upper boundary condition for solute sorption. The equation should not be extrapolated beyond the limits of the experimental data.

The Freundlich isotherm will yield a curvilinear graph which can be linearized by the following algebraic relationship

$$\log S = \log K_F + N \log C \quad 1.2.17$$

In which case $\log S$ is plotted against $\log C$, resulting in a linear graph with slope N and a y intercept of $\log K_F$.

The *Langmuir sorption isotherm* was developed with the basic concept that a solid has a finite sorption capacity which the previous two models have ignored (Fetter, 1993). It is based on the assumptions that every adsorption site is equivalent and that the ability of a particle to bind there is independent of whether or not nearby sites are occupied (Atkins, 1990). When the surface has become effectively saturated, the surface will no longer sorb solute from solution. The Langmuir isotherm can be represented by the equation

$$S = \frac{MK_L C}{1 + K_L C} \quad 1.2.18$$

Where

$M =$ an absorption constant related to the binding energy (L/mg)

$K_L =$ the maximum amount of solute that can be absorbed by the solid (mg/kg)

The Langmuir isotherm ignores the possibility that the initial monolayer may act as a substrate for further physisorption. Multilayer sorption can be dealt with by using the BET sorption isotherm (Atkins, 1990), but will not be discussed here.

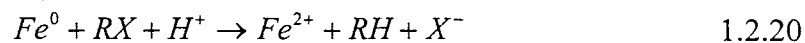
If the sorption curve of S vs. C is plotted for a solute and it follows a Langmuir sorption isotherm, it will have a curved shape that reaches a maximum value. If C/S is

plotted vs. C , the data will follow a straight line. The value for K_L , maximum ion sorption, is the reciprocal of the slope of the line and the binding energy constant, M , is the slope of the line divided by the intercept (Fetter, 1993). This can be seen by the rearrangement of equation 1.2.19 to

$$\frac{C}{S} = \frac{1}{MK_L} + \frac{S}{M} \quad 1.2.19$$

1.2.4 Reduction Chemistry

Several studies within the past few years have shown that metallic iron is a strong reducing agent in the reduction of chlorinated hydrocarbons; however, the actual processes that occur during these reactions are still the subject of debate. However, it has been established that the degradation occurs through a reductive dechlorination process (Senzaki and Kumagai, 1988). Matheson and Tratnyek (1994) described what is the generally accepted process by which this phenomenon occurs. The idea is based on a mechanism of simple corrosion with contaminants substituting for oxygen as the dominant oxidant. Dechlorination occurs in the process described by equation 1.2.21.



Where

$R =$ a hydrocarbon

$X =$ halogen

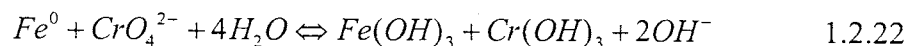
Iron is simply oxidized by



Other processes of reductive dechlorination have been suggested (Tratnyek et al, 1995) that involve the reduction of chlorinated hydrocarbons by ferrous iron which precipitates ferric (oxy)hydroxides and also by hydrogen with a catalyst.

It has been determined that iron is a significant reducing agent for chromate as well. Studies in the reduction of CrO_4^{2-} by iron have focused on ferrous ions present in solution as well as ferrous iron-bearing minerals (Powell et al, 1995). In these sorts of situations, a redox couple forms where Cr^{6+} is reduced to Cr^{3+} and Fe^{2+} is oxidized to Fe^{3+} .

The net reaction for the reduction of Cr^{6+} to Cr^{3+} by zero valent iron is as follows:



As can be seen by equation 1.2.23, the production of OH^- increases the pH of the system. The zero valent thermodynamically unstable form of iron is a strong driving force in this reaction (Sculley, 1975) without any external energy input. This reaction was illustrated by Blowes and Ptacek (1992) as well by reduction chromate with iron filings.

When chemical decay enters into the system, once again, our advection/dispersion equation needs to be modified in order to properly model the dynamics occurring. The equation would then read

$$R \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \mu C \quad 1.2.23$$

In this case, μ , is the 1st order decay constant with units of inverse time (T^{-1}). This decay constant is actually a lumped parameter that is a function of two separate decay processes given by:

$$\mu = \mu_l + \frac{\rho K_d \mu_s}{\theta} \quad 1.2.24$$

where

μ_l = first order decay coefficient for degradation of the solute in the liquid (T^{-1})

μ_s = first order decay coefficient for degradation of the solute in the
absorbed phase (T^{-1})

II.

Materials and Methods

2.1 Zeolite

2.1.1 Structure and Properties

Silicates contain tetrahedral SiO_4 units, which may be linked together by the sharing of corners, but never by the sharing of entire edges or sides (Douglas et al, 1994). When other cations are present in the coordinated structure, it is quite common for the SiO_4 to share oxygens. When this occurs it gives an octahedral configuration around the silicon. It also possible, and common, for aluminum to replace the silicon in the silicate tetrahedral. This of course requires the addition of another cation or the replacement of one by another of higher charge to maintain the charge balance. It is also possible for aluminum to occupy octahedral sites.

Zeolites, which have been investigated now for over 200 years, are hydrated aluminosilicate minerals belonging to the framework silicate family. Their fundamental building units are tetrahedral SiO_4 as well as AlO_4 . Zeolites have a highly open structure which is formed by the joining of silicate chains or cages, such as the truncated octahedron, to yield a three-dimensional anionic network in which each oxygen of a given tetrahedron is shared between this tetrahedron and one of four others. This would imply then that there are no unshared oxygens in the frameworks and we would have a ratio for $(\text{Si} + \text{Al}) : \text{O}$ of 1:2 (Barrer, 1978).

Because of their highly open structure, water molecules can move easily within the crystals as well as cations. These cations are therefore able to readily undergo cation exchange with inherent surface cations of the zeolite. The water molecules can be removed and replaced in a continuous manner and often reversibly (Barrer, 1978).

2.1.2 General Occurrence and Deposition

Natural zeolites are often found lining the cracks and cavities within basalts. One theory of zeolitic origin and crystallization is that the cavities are formed in the parent magma by bubbles in the fluid. The zeolite crystals then form as a result of the chemical action in the magma of these fluids or of the fluids that have displaced them (Barrer, 1978). Of course, the formed zeolite's composition tends to be strongly correlated with that of the parent rock. More aluminous zeolites are associated with rocks that are silica deficient, while the more siliceous zeolites are associated with silica enriched rocks. It is also not uncommon to find more than one zeolite species present and evidence shows that this probably due to slow replacement of one zeolite species for another rather than co-crystallization (Barrer, 1978). More massive deposition of zeolite generally occur as small crystalline grains in metamorphic rocks and particular sediments. Zeolitization of this type may be accounted for by the acting of aqueous and normally alkaline solutions upon volcanic ash that has been deposited into large surface water bodies.

Strictly in terms of volume and frequency of occurrence, anaclime, laumontite, and heulandite-clinoptilolite are the most common naturally occurring zeolites. The lowest temperatures -- around 4°C -- at which zeolites form are in deep sea sediments (Kallo, 1988) as is the case for phillipsite and clinoptilolite forming from volcanic debris. Phillipsite will tend to form directly at the sediment-water interface and then continues to grow in the sediment column. The formation of phillipsite tends to be most common in Miocene and younger sediments. We tend to see clinoptilolite dominating in the early tertiary and Cretaceous sediments (Barrer, 1978). Glass composition is probably the main factor involved in the distribution of phillipsite vs. clinoptilolite. Phillipsite is believed to

be associated with basaltic glass, while clinoptilolite is associated with silicic glass (Kastner, 1976) or with the conversion of phillipsite to clinoptilolite (Boles, 1976).

2.1.3 Cuchillo Negro Clinoptilolite Deposit, Sierra County, New Mexico

The zeolite used in this experiment was mined by the St. Cloud Mining company at the southern end of the Winston graben in south-central New Mexico. In this area primary zeolitization occurs in the tertiary tuff of Little Mineral Creek, a lithic-rich rhyolitic ash flow crystal tuff with a thickness of approximately 600 ft, as well as in a tuffaceous sedimentary sequence from 50 to 200 ft thick that overlays the material of Little Mineral Creek. These sediments consist primarily of immature arenite interbedded with tuffaceous conglomerates (White et al, 1996). Zeolite alteration has been noted also in the Santa Fe Formation, another tuffaceous sedimentary unit that directly overlays the previously mentioned clinoptilolite rich sediments, as well as the volcanic units that underlie the Little Mineral Creek Formation (White et al, 1996).

The zeolite from the St. Cloud Mining company was subjected to x-ray diffraction analysis at Los Alamos National Laboratory that employed an internal standard analysis method using an internal standard of 20% corundum (Al_2O_3) (Sullivan, 1997). The results of this analysis showed that the St. Cloud sample consisted of 74($\pm$ 4)% clinoptilolite, 5($\pm$ 2)% smectite, 10($\pm$ 1)% quartz, 2($\pm$ 1)% cristobolite, 12($\pm$ 2)% feldspar, and 1($\pm$ 1)% mica (Sullivan, 1997).

2.2 Water and Reagent Chemistry

2.2.1 Water chemistry

The water used in this series of experiments in this report is a synthetic water made to chemically emulate a water sample obtained from the Oregon Graduate Institute (OGI) where a later phase of this work is expected to take place. 500 mL of the water was analyzed by the New Mexico Bureau of Mines and the results are shown below in table 2.2.1.

Table 2.2.1 Analytic results of actual OGI water (a) anions (b) cations

Anions				
	MW	ppm	mmol	meq
HCO ₃	61.02	50.00	0.82	0.82
Cl	35.45	6.00	0.17	0.17
SO ₄	96.06	7.00	0.07	0.15
NO ₃	62.00	2.10	0.03	0.03

Total meq = 1.17

(a)

Cations				
	MW	ppm	mmol	meq
Na	22.99	12.00	0.52	0.52
K	39.10	0.47	0.01	0.01
Mg	24.31	2.50	0.10	0.21
Ca	40.08	8.00	0.20	0.40

Total meq = 1.13

(b)

The water had a pH equal to 7.62 and an ionic strength of $I = 0.0015$ mol/kg.

The next task involved the synthesis of this water in order to use it in the transport studies. A simple spreadsheet was formulated in order to balance the species used with the individual ions needed and then converged to an output that described a "recipe" for the synthetic groundwater. The converged output used in this synthesis is shown in table 2.2.2. The water was prepared in 20 L batches in polyethylene carboys.

Table 2.2.2 Quantitative values for OGI groundwater synthesis

Species	meq	MW	mg/L	mg/20L
NaHCO ₃	0.52	84.00	43.68	873.60
MgSO ₄	0.08	120.36	9.03	180.54
CaCl ₂	0.09	110.99	9.43	188.68
KNO ₃	0.01	101.09	1.01	20.22
CaCO ₃	0.12	100.09	12.01	240.22
Mg(NO ₃)	0.02	148.32	2.97	59.33

2.2.2 Surfactant

The surfactant, a term that refers to a “surface-active-agent”, used in this study was hexadecyltrimethylammonium (HDTMA) in the bromide salt form. HDTMA is a quaternary ammonium salt that is commercially available and can be purchased from any major scientific chemical supply company. It is a component that is commonly found in household products such as toothpastes, mouthwashes, and detergents.

The ammonium head group of HDTMA is positively charged which makes it subject to cation exchange process. Haggerty and Bowman (1994) described this as the primary process in which HDTMA arranges itself on the mineral surface of zeolite. The HDTMA molecules themselves are too large to enter into the internal zeolitic portion of the mineral and thus all addition is to the external cation exchange sites. It is thought that the molecules actually form a series of hemimicelles and admicelles on the zeolite surface which was further described as a patchy bilayer by Sullivan (1997) as illustrated in figure 2.2.1 below.

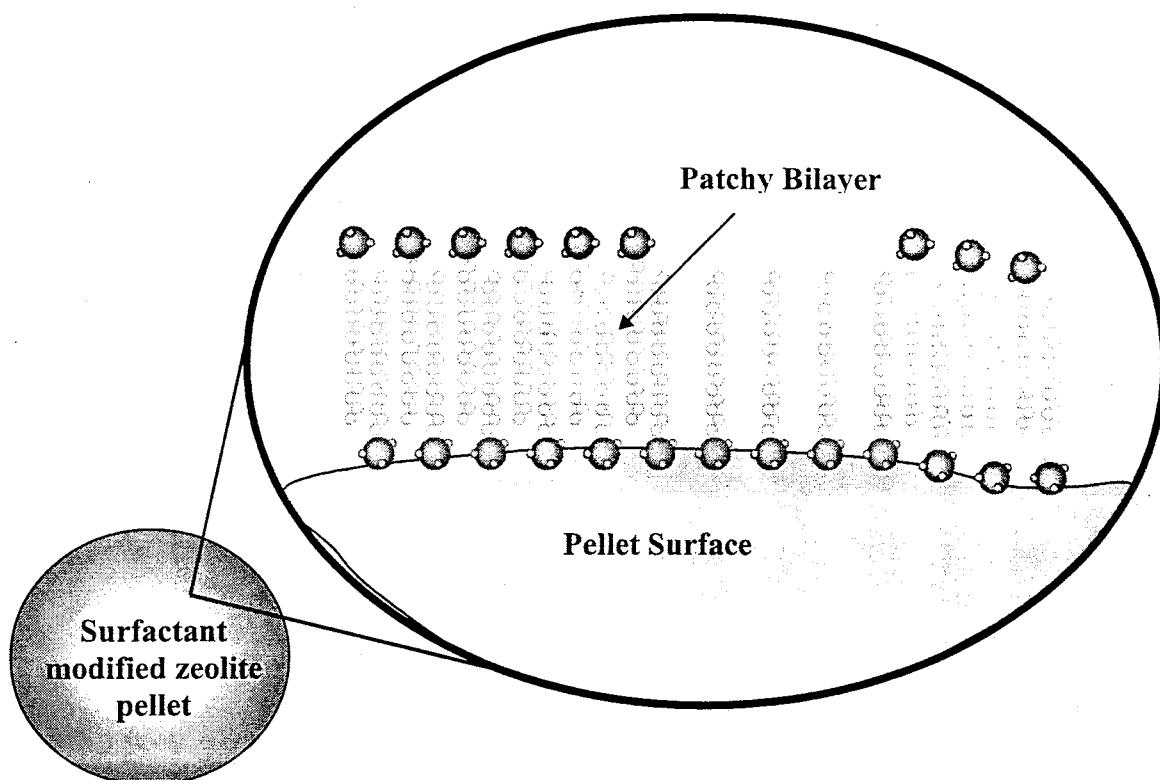


Figure 2.2.1 Enlarged section of surfactant modified zeolite pellet showing patchy bilayer formation

2.2.3 PCE and its daughter products

Perchloroethylene, or PCE, continues to be a source of environmental concern in the biosphere affecting many surface water bodies, groundwater systems, and soils linked with industrial exposure. It is a common component in degreasers, solvents, dry-cleaning agents, and heat transfer media and has the simple structure of CCl_2CCl_2 .

When placed in a reducing (reductive dechlorination) environment, PCE undergoes transformation to a series of daughter products which are environmentally toxic species as well. The reduction series proceeds as illustrated in figure 2.2.2 which theoretically displays the stepwise reduction of PCE to ethylene.

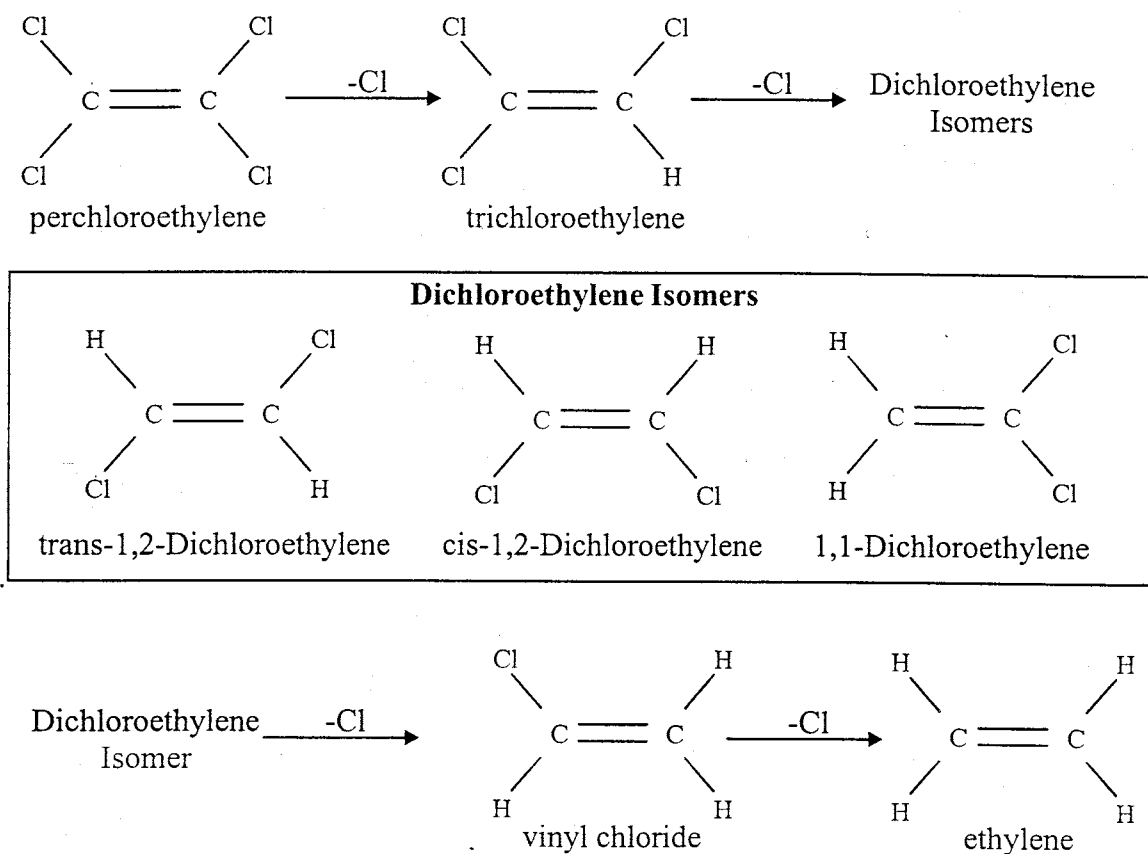


Figure 2.2.2 Progressive dechlorination series of perchloroethylene

Studies have shown (Chiou, 1989) that PCE is sorbed into an organic phase through a simple organic partitioning mechanism driven primarily by van der Waals forces. Both Chiou (1989) and Whitworth (1997) showed that this sort of PCE uptake follows a linear isotherm trend. Chiou concluded that this linear trend is expected because the partitioning coefficient and the solute concentration in the system are independent of one another. This would mean that the ratio of the sorbed species to the species in solution would not vary with changing solute concentration (i.e. it is constant for a given set of conditions). This type of sorption is the type of process that will be taken advantage

of in order to provide the residence time to effectively reduce PCE by dechlorination using iron components.

Several studies and field demonstrations in the past few years have used various forms of iron at varying valence states for the remediation of contaminant species. However, recent work has also shown that trichloroethylene (TCE) and PCE have a potential for sorbing onto non-reactive iron sites (Burris et al, 1995). The complex reaction mechanisms exhibited nonlinear sorption behavior which could generally be described by the Langmuir isotherm model and the reaction rates were found to be first order.

A significant study performed by Johnson, Scherer, and Tratnyek (1996) examined the factors effect the actual degradation rates by iron reduction. This work was prompted by large variability and inconsistencies in reported values. The team of researchers considered the effect of the variability in iron surface area and then developed a series of area-normalized rate constants. By comparing these area-normalized rate constants, the variability of the resulting constants remained within one order of magnitude for individual halocarbons. They also in short determined that the above mentioned dehalogenation process occurs at faster rates at saturated carbon centers than at unsaturated carbon centers and also that greater amounts of halogenation favor greater rates of dehalogenation.

2.2.4 Chromate

The element chromium exists in a range of oxidation states, as do most transition metals, varying most commonly between 2+ and 6+. The principle valence distribution is shown below in figure 2.2.3.

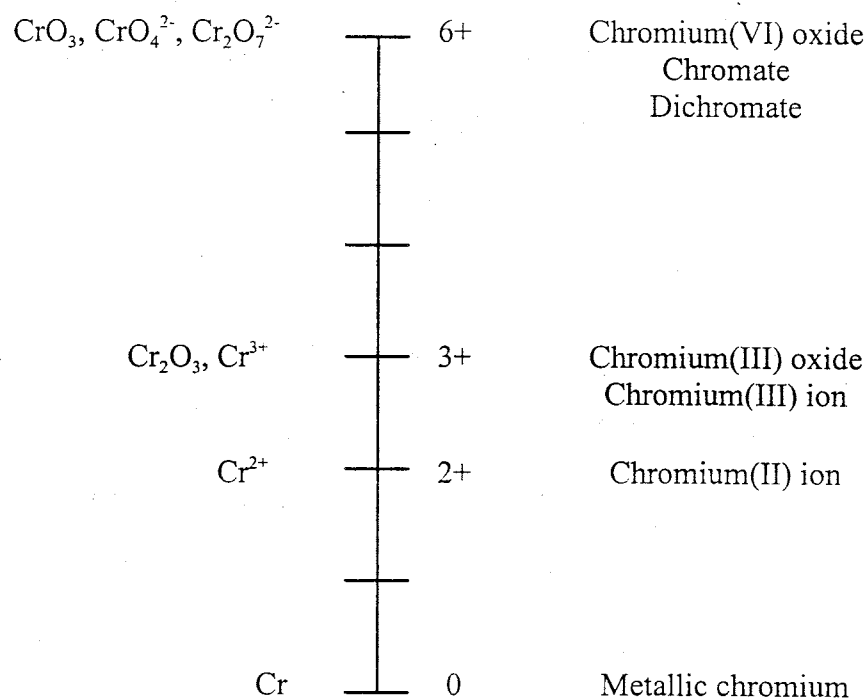


Figure 2.2.3 Principle valence distribution of the element chromium

Chromium in its hexavalent form is the most toxic oxidation state (Pauling, 1970). The work in this investigation deals with the chromate ion, CrO_4^{2-} . A study was performed in 1965 by Zhang and Li (1987) outside of Jinzhou, China on 155 human subjects who had been exposed to chromate through drinking water. The exposed subjects exhibited diarrhea, stomachache, mouth sores, vomiting, elevated white blood

cell counts, and a higher per capita rate of cancers (primarily lung and stomach). The study also concluded that gastrointestinal effects are likely to occur in humans following exposures to hexavalent chromium in drinking water at concentrations greater than or equal to 20 mg/L.

In industrial countries, chromium is the most common contact sensitizer in males and is very often associated with occupational exposures from numerous materials and processes. These would include, but not be limited to, textiles and furs, cleaning materials, lubricating greases and oils, welding fumes, anticorrosive agents, tanning agents, wood preservatives, chrome colors in dyes and cements, and chrome plating baths (Burrows and Adams, 1990).

A study presented in 1994 by Haggerty and Bowman revealed that chromate is also sorbed by surfactant modified zeolite. Again, this is the process that is used in this study to provide longer residence times for a subsequent reduction process that reduces Cr^{6+} to Cr^{3+} which is considered to be a relatively non-toxic or more benign form of chromium. Chromate is thought to bind on the HDTMA bilayer surface through a simple anion exchange reaction which exchanges bromide from the HDTMA headgroup for chromate ion. The study determined that this process followed a non-linear sorption type behavior that could be well described by the Langmuir sorption isotherm model. This is due most likely to the finite number of exchange sites on the outermost portion of the organic bilayer. Figure 2.2.4 below is a simple schematic of PCE partitioning into the organic region of the bilayer and of the cation exchange process involving bromide and chromate.

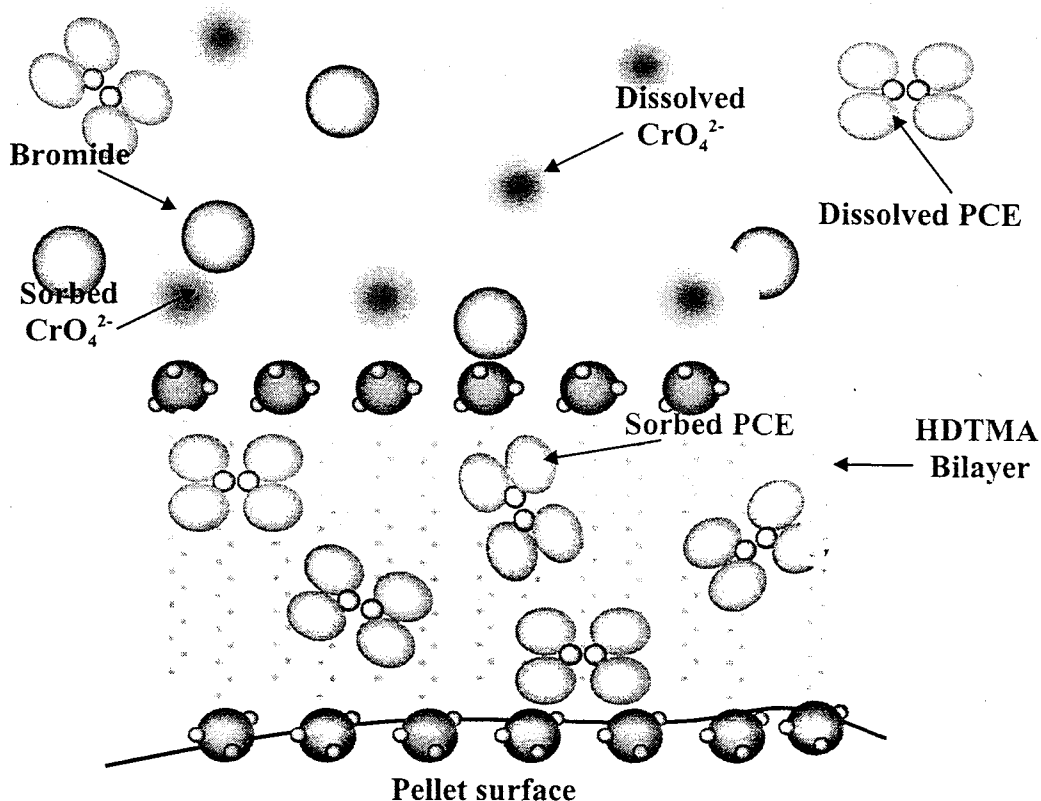


Figure 2.2.4 HDTMA bilayer sorption processes

Recent work has been done that illustrates the effectiveness of iron as a reducing agent for chromate reduction (Powell et al, 1995). This research examined a series of varying metal types and oxidation levels and determined that impure, slightly oxidized iron was the most effective reducing agent in the batch. Since this is a corrosion mechanism, the researchers also concluded that it was important for there to be present an effective electron acceptor.

This work was further supported by research performed at the University of Waterloo (Blowes et al, 1997). Here it was determined that by using zero valent iron,

chromate could be dramatically reduced under hydrodynamic conditions, suggesting that the use of reactive iron walls may be a good alternative to in-situ chromate remediation.

2.3 Pelletization Process

In order to effectively combine the zeolite and the iron into a relatively homogeneous material, a pelletized material has been designed. The pelletization of the material yields a solid combination of the two materials due to the simple fact that it is eliminating any separation that would arise due to differences in bulk density, thus maintaining favorable hydraulic properties in the overall medium. The formation of the pellets is a process performed by Richard Helferich at Cercona of America, Inc. of Dayton, Ohio. The basis of the process is the aqueous combination of the zeolite with an aluminosilicate binder material as well as the iron powder. The St. Cloud zeolite used in this research is from the same batch that was used in two previous studies done in order to quantify the sorption of hexadecyltrimethylammonium (HDTMA) on to the surface of the zeolite, and the subsequent removal of perchloroethylene (Whitworth, 1997) and chromate (Anghel, 1997) from a synthetic groundwater solution.

Initially, sodium silicate and sodium aluminate are combined with the required amount of zeolite and iron. Most batches were a 50:50 (iron:zeolite) by volume combination consisting of 7% amorphous binding material, 20% zeolite, and 73% iron (by mass). The zeolite from St. Cloud used was 40 mesh and below. Two iron types were tested in this research. Initially iron powder supplied by US Metals, which was a labeled as a dust size material, was investigated. In general, it measured -50 mesh (less than 300 μm) with the majority of the material falling the -100 mesh (less than 150 μm) range. The second iron type used was supplied by Peerless Metal Powders and Abrasives Co., Inc. The iron type is classified as fines, type T, size 76D.

When the required materials are mixed, the silicate and aluminate form permutite, a gel-like substance. The resulting gel-like material is of a high pH (12-13) that then binds the materials together. This product is then leached with water primarily to reduce the material pH leaving the final product with sodium as the primary cation. This material is then basically "snowballed" with air to form the pellets and then dried at 177°C (350°F), which then yields the desirable ion-exchangeable, porous, iron/zeolite pellet.

There are some alternative pellet types that may be formed with additional or varying treatment. One variation is a pellet that contains calcium as the primary cation rather than sodium. Instead of leaching the pellets with water, they are leached with a CaCl_2 solution. Essentially, the sodium present in the material is exchanged for calcium. The leaching process is monitored and continued until the aqueous sodium concentration has become stabilized or equilibrated.

Another variation on the pellet theme is the application of "foaming" agent which acts to essentially increase the effective surface area of the pellets. The two aforementioned pellets were of the non-foamed type. Foaming in the pellets may be induced by the addition of aluminum metal to the permutite before the leaching and drying processes. Through redox reactions between the aluminum metal and the high pH material, hydrogen gas is evolved. As the gas escapes, it leaves behind channels and pores which upon drying, increase the available surface for the process of ion exchange.

2.4 Pellet Formulation and Testing

2.4.1 Mechanical Stability Study

We received and/or requested over twenty different types of pellets from Cercona of America, Inc., with varying formulations with respect to the pellet size, iron to zeolite ratio, type of iron powder and iron particle size, primary cation present, and the presence of an aluminum foaming agent. Several of these batches contained no iron and served as blank pellets. In performing an initial HDTMA surface sorption study onto the pellet surface, I noted that the mechanical stability of the pellets varied with the chemical and physical composition of the pellets. I treated the pellets with HDTMA solution concentrations that varied from 50 to 100 mM and equilibrated them for 8 hours in an orbital shaker at 25°C and 150 rpm. At the end of the equilibration period, many of the pellets had mechanically decomposed by at least 80%, while others remained fully intact or only slightly decomposed. In light of this information, I began a mechanical stability study of seventeen different pellet types in order to find the most favorable combination of pellet characteristics that yielded the most stable pellet. Table 2.4.1 shows the pellets that were selected for the study.

The mechanical stability study was a simple test in which I varied the solution surfactant concentration as well as the rate at which the pellets were being shaken. I tested 23 different representative Cercona pellets by placing 2 g each into two 50 mL polyallomer centrifuge tubes. In one of the tubes I then added 6 mL of Millipore Milli-Q water and in the second tube I added 6 mL of a 100 mM HDTMABr (Aldrich) solution. I then subjected the samples to shaking at 75 rpm for 8 hours at 25°C. After the 8 hour

period, I increased the rate to 100 rpm for the pellets that had not broken down. Upon the completion of this test, I then further increased the rate to 150 rpm which is our normal operating rate for chemical equilibration, still maintaining a constant temperature of 25°C. It should be noted that all pellets containing iron described in Table 2.4.1, were formed using the US Metals type iron powder as described in section 2.3.

Table 2.4.1. Description of Cercona pellets inspected in a mechanical stability study.

Description	Pellet Size	Cercona Workbook Reference
foamed/calcium form	-3 +8 mesh	C960510A p54
foamed/calcium form	-12 +20 mesh	C960510A p54
nonfoamed, porous/NH ₃ form/baked at 220°C	-3 +8 mesh	C960205A p2
nonfoamed, porous/NH ₃ form/baked at 220°C	-12 +20 mesh	C960205A p3
foamed/sodium form	-3 +8 mesh	C960708A p38
foamed/sodium form	-8 +12 mesh	C960708A p38
nonfoamed/sodium form	-12 +20 mesh	C960708A p39
nonfoamed/sodium form	-3 +8 mesh	C960708A p39
foamed/calcium form	-3 +8 mesh	C960708A p35
nonfoamed/calcium form	-12 +20 mesh	C960708A p35
nonfoamed/calcium form	-3 +8 mesh	C960708A p36
* higher density, nonfoamed/bimetallic iron media	-3 +8 mesh	C960708A p48
higher density, nonfoamed/iron media	-3 +8 mesh	C960708A p50
Type Z _{Na-1:10}	-3 +8 mesh	C960205A p18
Type Z _{Na-1:2}	-3 +8 mesh	C960205A p29
Type ZP _{NUSMC-1:2} /10 vol% iron	-3 +8 mesh	C960205A p5
Type Z _{USMC-1:2} /50 vol% iron	-3 +8 mesh	C960205A p36

* *bimetallic* refers to an iron mixture made up of 13.5% high silicon iron and 54% regular US Metals iron by volume

2.4.2 Final Pellet Formulation

Based on the results of the mechanical stability test (presented in section 3.1), a pellet formulation was decided upon and all subsequent pellet production schemes were based upon this. All pellets used henceforth (batch and column studies) were of a nonfoamed nature with calcium as the primary exchangeable cation with either the Peerless or US Metals iron incorporated for the metallic pellet types. Table 2.4.2 below lists the pellet types that were formulated for the experimentation with a brief description and the nomenclature that will be used in the remainder of this report to refer to each of them.

Table 2.4.2 Finalized Pellet Formulation

Pellet Type	Composition	Sizing	Cercona Workbook Reference	Reporting Nomenclature
Cercona clinoptilolite nonfoamed, porous pellets, calcium form	11.5% calcium aluminosilicate 88.5% clinoptilolite	-3 +8 mesh	C960708A p36	B0
Cercona US Metals iron/c clinoptilolite porous pellets	50/50 volume % iron/c clinoptilolite iron from US Metals May 1997 - zeolite and Cercona binder in calcium form	-3 +20 mesh	C9760723 p2	U0
Surfactant-modified Cercona US Metals iron/c clinoptilolite porous pellets	50/50 volume % iron/c clinoptilolite iron from US Metals May 1997 - zeolite and Cercona binder in calcium form with HDTMA treatment	-3 +20 mesh	C9760723 p2	U1
Cercona Peerless 76D iron/c clinoptilolite porous pellets	50/50 volume % iron/c clinoptilolite iron from Peerless, 76D, Type T - zeolite and Cercona binder in calcium form	-3 +20 mesh	C9760723 p4	P0
Surfactant-modified Cercona Peerless 76D iron/c clinoptilolite porous pellets	50/50 volume % iron/c clinoptilolite iron from Peerless, 76D, Type T - zeolite and Cercona binder in calcium form with HDTMA treatment	-3 +20 mesh	C9760723 p4	P1

The reporting nomenclature set forth in the last column of Table 2.4.2 is a simple indicator of iron type present and whether or not the pellet has been modified with the surfactant HDTMA. The initial letter is the iron type indicator; U = US Metals iron, P = Peerless iron, B = no iron or blank. The binary digit in the second place is a simple "yes or no" indicator of the presence of HDTMA; 0 = unmodified, 1 = modified. This nomenclature will be used throughout the remainder of the text.

2.5 Surface Modifications

2.5.1 HDTMA Sorption Study

From the iron characterization study as well as the pellet batch studies looking at the sorption and reduction of chromate and PCE (sections 3.4 and 3.5), the US Metals and Peerless 76D products emulated each other very closely. Initially, US Metals products were chosen because of logistic ease -- it is the iron type that Cercona works with normally and had on site. I tested the maximum surfactant loading of the US Metals pellets (pellet U0 to pellet U1) in a standard isothermal evaluation using HDTMA aqueous solutions with concentrations varying between 1 and 24 mM and a solid to liquid ratio of 1:5. The U0 pellets were -3 + 20 mesh size with calcium as the primary exchangeable cation and no foaming agent, based on the results of the mechanical stability study (section 3.1). Each sample type contained 2.00 g (± 0.05 g) of the U0 pellets which were placed in 50-mL polyallomer centrifuge tubes and to each tube was then added 10 mL of the respective HDTMA solutions in varying concentrations. Each sample was prepared in duplicate. The mixtures were shaken for 18 hours at 60 rpm and 25°C. The solutions were then removed and filtered using PTFE Iso-disc syringe-tip filters (Supelco) in order to remove any large, undesirable particulate matter which might be maleficent for the analytic apparatus. The acquired equilibration HDTMA and bromide solution concentrations were then analyzed by HPLC as described herein in section 2.11.

After experimentation had continued up through the column studies described in this report, additional material was needed to complete the work. Since the Peerless 76D

products emulated the US Metals so well, as described in sections 3.4 and 3.5, additional work was done in this project using the Peerless 76D material. It was handled in the exact same manner as far as isothermal experimentation with some minor exceptions. Each Peerless 76D sample contained 1.5 g (± 0.05 g) of the P0 pellets and 20 mL of the same HDTMA solutions for a solid to liquid ratio of 1:13.3. This was done in order to allow for any unexpected increased sorption capacity of the Peerless product.

2.5.2 Pellet Surface Modification

Based on the results as discussed in sections 3.2 and 3.3 herein, a 2.0-kg batch of the Cercona U0 pellets containing calcium as the primary cation and the iron powder obtained from US Metals was treated with HDTMA to its maximum sorption capacity of about 12 mmol/kg. A 6.0-L batch of a 75-mM solution of HDTMA was prepared and placed in several 500 mL polyallomer bottles. These were then placed on an orbital shaker and allowed to equilibrate for 24 hours at a rate of 75 rpm and 30°C. The slightly higher temperature was used in order insure that the HDTMA would not form liquid crystals which seems to happen generally above concentrations of 20 mM at 25°C.

Once the pellet/surfactant equilibration period was complete, the, now, U1 pellets were removed from the shaker and the solution discarded. In each bottle, an equivalent amount of Type I water was added in replacement of the surfactant solution and then shaken for 0.5 hours at the same rate and temperature in order to wash away any residual, non-sorbed surfactant. This washing process was repeated twice and equilibrium concentrations analyzed in order to quantify the actual surfactant loading in the treatment

process. The same procedure was used on the P0 pellets in order to obtain the P1 product pellets.

2.6 Hydraulic Characterizations

2.6.1 Gravimetric Water Content Analysis

In order to determine the amount of non-coordinated water in the pellets, a gravimetric water content analysis was performed on the material. The samples were prepared in duplicate and ranged between 4.6 g and 10.7 g. The range in mass was due to differences in bulk density as the pellet volumes were approximated rather than the masses. The analysis was performed on the B0, U0, U1, P0, and P1 pellets.

Each sample was weighed out into an aluminum drying dish, which had been previously tared, and placed in a drying oven for 48 hours at a constant temperature of 105°C. After the drying period, the mass was immediately determined again and the loss of water due to evaporation was quantified.

2.6.2 Saturated Hydraulic Conductivity

The saturated hydraulic conductivity of the material actually within the columns used in the hydrodynamic studies was determined by a constant head method. Each column was individually monitored for its volumetric output with respect to time while applying some greater and constant hydraulic head across the system. Figure 2.6.1 depicts the system apparatus used in this method.

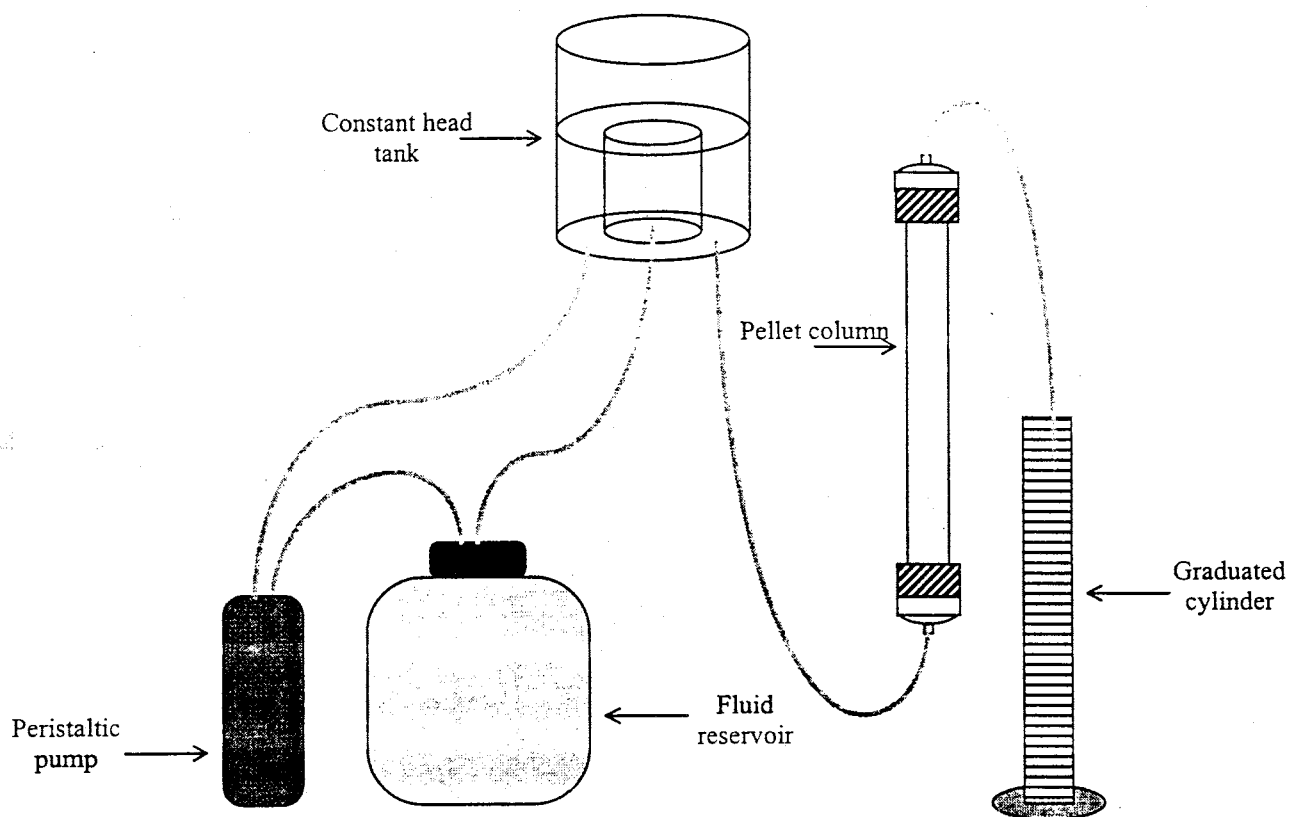


Figure 2.6.1 Constant head apparatus

A reservoir tank was connected to a peristaltic pump which circulated water through a constant head tank with a central overflow outlet which returned water to the reservoir tank. The outlet of the tank was connected to the column inlet. The column outlet and water flow path then terminated in a graduated cylinder. In this test, flow was engaged by releasing a hose clamp located at the base, or inlet, to the column. At this point in time, a stop watch was engaged and the time at which 100 mL of water was collected in the cylinder was indicated. Darcy's Law was then applied to these

measurements from which the values of K_s , saturated hydraulic conductivity, could be determined.

2.7 PCE Sorption/Degradation Batch Studies

2.7.1 Iron Characterization

Three different iron types (Fisher, Peerless 76D, and iron powder provided by US Metals) were evaluated in their performance of degrading dissolved PCE (in Millipore Milli-Q water) in order to select the best one for further use in this degradation study. All powders were on the order of a -50 mesh size. The study was done in triplicate in 10-mL glass head-space, crimp-top vials (Supleco) with a teflon septa with an additional blank set that employed glass beads to approximate the solid volume of the iron in order to monitor any PCE loss not attributed to degradation. Each vial contained 2.00 g (± 0.05 g) of the iron powder, and 11 mL of 20 mg/L PCE solution diluted from a saturated aqueous solution (200 mg/L) with no head space. The samples were then shaken at 150 rpm and 25°C, and sacrificed at timed intervals of 0.5, 1, 2, 4, 8, 16, and 32 hours and analyzed by gas chromatography for PCE as well as TCE (trichloroethylene).

2.7.2 US Metals Study

A batch of U1 pellets at maximum surfactant coverage (12 mmol/kg, based on HDTMA sorption isotherm results shown in section 3.2) was used in the assessment of their capability to reductively dechlorinate PCE. Three controls were used in the study; glass beads in order to monitor any PCE losses not attributed to sorption or reduction, US Metals iron powder, and U0 pellets. The experiment was performed in triplicate, once again using the 10-mL head space vials. 2.00 g (± 0.05 g) of each sample type was added to the vials. To this was added 11 mL of 20 mg/L PCE solution. The samples were

shaken at 75 rpm and 25°C, sacrificed at timed intervals of 0.5, 1, 2, 4, 8, 16, 32, and 78 hours, and equilibrium concentrations analyzed again by gas chromatography.

2.8 Chromate Sorption/Reduction Batch Study

A batch of U1 pellets at maximum surfactant coverage (12 mmol/kg, based on HDTMA sorption isotherm results shown in section 3.2) was again used in the assessment of their capability to reduce chromate (Cr^{6+} to Cr^{3+}). The three controls used in the study were; glass beads in order to monitor any adjuvant chromate losses not attributed to sorption or reduction, US Metals iron powder, and U0 pellets. The experiment was performed in triplicate once again using the 10 mL head space vials (Supelco). 2.00 g (± 0.05 g) of each sample type was added to the vials except the glass beads that were added to the same approximate volume as 2.0 g of U1 pellets. To this was added 11 mL of 105 mg/L CrO_4^{2-} solution. The samples were shaken at 75 rpm and 25°C, sacrificed at timed intervals of 0.5, 1, 2, 4, 8, 16, 32, and 78 hours, and equilibrium concentrations analyzed again by HPLC. From this data was then determined the reduction rate by plotting the natural log of the normalized concentration against the time in hours.

At a later time when it was determined that additional material was needed, the P1 pellets, treated to a surfactant modification level of 28 mmol/kg, were tested in the same manner with the same equipment and solutions. The only difference was the sample sacrifice times which have no bearing on the calculation of decay constant and P0 pellets of course replaced the U0 pellets as a control. The sacrifice times were 0.5, 1, 2, 4, 8, 28, 36, and 70 hours. This data was also plotted as the natural log of the normalized concentration as a function of time in hours.

2.9 Chromate Sorption/Reduction Column Study

2.9.1 Chromate Column Apparatus and Preparation

This experiment employed 3 different column material types in duplicate for a total of 6 columns. The columns were glass Adjusta-Chrom columns supplied by Ace Glass having a internal radius of 2.5 cm and a length (packed bed) ranging from 31.5 cm to 33.2 mm as shown in 2.9.1.

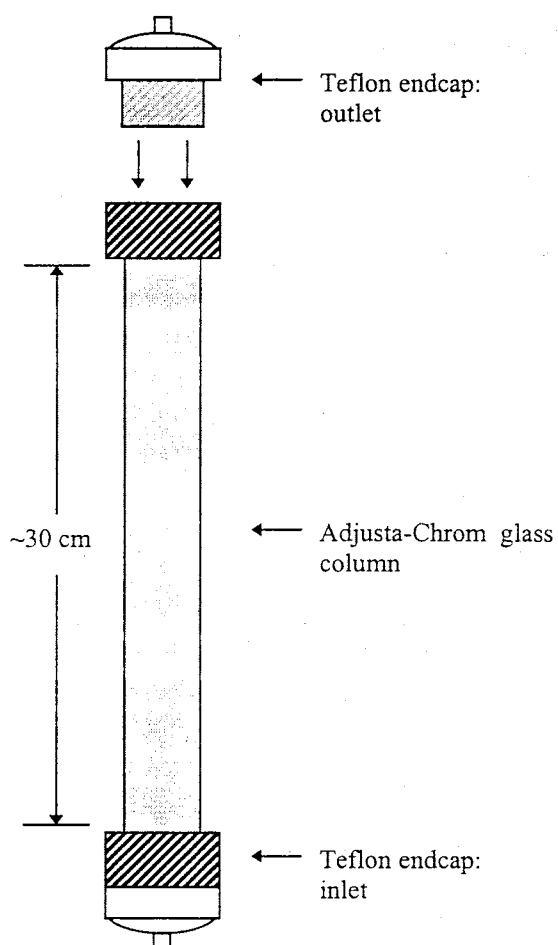


Figure 2.9.1. Adjusta-Chrom glass column used in column study

The inlet and outlet tips of the threaded Teflon endcaps were fitted with stainless steel three-way stopcocks (Fisher Scientific) in order to direct flow efficiently.

The tare weights of each of these six columns were recorded. The columns were then packed with each of the three pellets types; P1, P0, and B0. This combination of these materials yields three modes of comparison. Theoretically, the P1 column should display chromate sorption through simple cation exchange on the outer surface of the organic layer as well as reduction provided by the electric potential provided by the present zero valent iron. In the P0 columns, sorption is eliminated and the source of chromate removal is reduction by zero valent iron only. In the last column set, B0 pellets are the only material present, thus allowing for the monitoring of any losses of chromate due to other process outside of sorption and/or reduction. Once each of the columns was packed with its respective material, each was again weighed in order to determine the dry mass of the added material. The physical characteristics of each column are given in detail in table 2.9.1 below.

Table 2.9.1. Critical column characteristics for hydrodynamic study

Column	Pellet Type	Pellet Mass (g)	GWC Correction (g)	Packed Column Length (cm)	PV (mL)	Porosity (PV/AL)
A	P1	269.94	264.83	31.50	102.61	0.17
B	P1	267.83	262.76	31.50	109.07	0.18
C	P0	220.22	216.49	32.00	104.63	0.17
D	P0	231.33	227.41	32.80	108.72	0.17
E	B0	134.10	128.01	33.20	151.99	0.23
F	B0	135.04	128.90	33.20	146.87	0.23

The columns were aligned parallel to one another on a rack and connected to a compressed CO₂ tank and flushed for 12 hours with CO₂ at a rate of about 1 mL/min in order to enhance the saturation of the columns with synthetic OGI water (due to the increased solubility of CO₂ in water as opposed to air).

After the CO₂ flushing was complete, the columns were connected to a Harvard PHD2000 Programmable Multirack Pump (Harvard Apparatus), using six 10-mL Hamilton Gas-Tight syringes (Fisher Scientific). The system utilized a series of dual check valves supplied by Industrial Specialties Manufacturing, Inc. to check flow into the syringes from the reservoir and then into the columns. The reservoir for the synthetic OGI water was a 20 L polypropylene tank which could be easily refilled. All connections between reservoir, pump, and columns were established by lengths of PTFE tubing with an I.D. of 1/8" (Fisher Scientific). The system is depicted in figure 2.9.2.

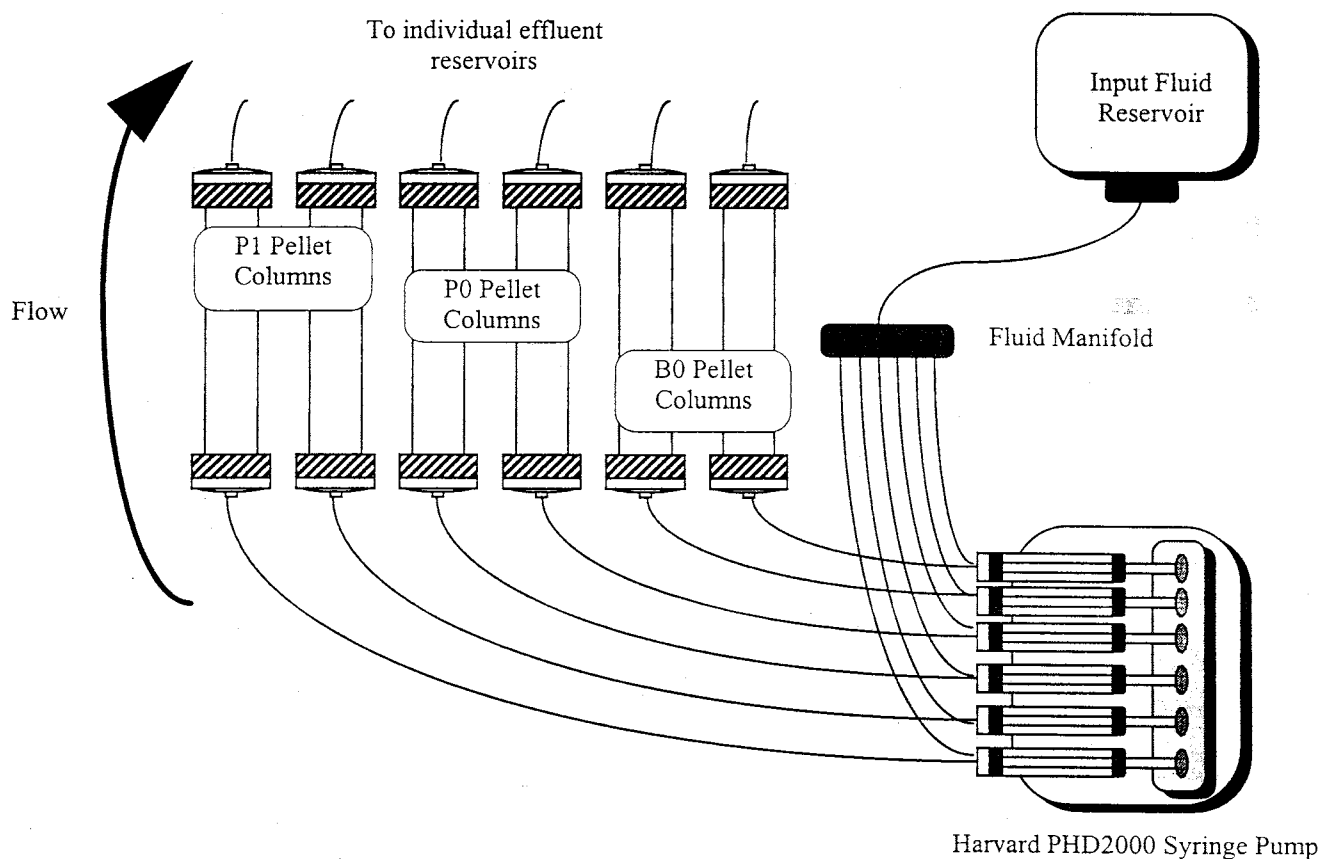


Figure 2.9.2. Chromate sorption/reduction column apparatus

Once the system was prepared and the columns had been flushed with CO₂, the Harvard pump was set at an infusion rate of 2.0 mL/min and a refill rate of 10 mL/min (per syringe) and flow of synthetic OGI water was initialized through the columns. The infusion rate was increased at random time intervals to 4, 6, 8, and 10 mL/min in order to investigate any leakage or mechanical failures at higher pressures and flow. In a previous column study with this same system and material and an infusion rate of 0.5 mL/min, I reached saturation in 7 days. After 12 days of monitoring column mass fluctuations by reweighing every 24 hours, at an infusion rate of 2 mL/min, I assumed the material had become saturated and proceeded with the contamination phase of the study after relatively small changes in column masses were noted.

2.9.2 Reactive Transport Study

20 liters of synthetic OGI water was contaminated with 41.8 ppm chromate by the addition of 1400 mg K₂CrO₄. The inlet line to the Harvard pump was then submerged into the contaminated water tank and the lines primed up through the pump and to the base of columns and out the three-way stop cocks. This was done to insure that there would be no dilution of the contaminant front (constant concentration input) and also to eliminate any lag time in the flow dynamics (i.e. contaminant flow begins at 0 pore volumes).

The outlet lines from the top of the columns (figure 2.9.2) were each run to a separate 500-mL polyallomer centrifuge tube. Each of the tubes was tared and then when filled with fluid through the experiment, were then reweighed in order to determine the total amount of effluent eluted throughout the experiment. After weighing, the waste solution was stored in a teflon waste bucket for later disposal.

Three separate column studies were run with the variables being the flow rate and the sampling intervals (i.e. faster flow rates required smaller sampling intervals). The three flow rates were 4, 2, and 0.6 mL/min. In the 4-mL/min study, each column was sampled every 10-12 minutes for the first 6 hours. The following 4 hours the columns were sampled every 30 minutes followed by 1 sample per hour until equilibrium was established. In the case of the 2 mL/min study, samples were taken again every 10-12 minutes for the first 1.5 hours, every 20 minutes for the next 3 hours, then 1 sample per hour until equilibrium was established. For the 0.6 mL/min study, samples were taken every 30 minutes for the first 2 hours, then 1 sample per hour until equilibrium was established.

Samples were taken with 1.0-mL plastic syringes (Fisher) at the outlet stopcock at each column in order to monitor the chromate concentration with time. 1 mL was drawn and placed in a 1-mL glass amber autosampler vial (Supelco) and stored for later analysis. The input concentration was monitored in the same manner, but taken from the inlet stopcock of each column. Input concentration samples were taken once per hour. The fluid reservoir was also sampled at random intervals to see how it compared to the input concentration at the inlet valves.

2.9.3 Tracer Study

A tracer study was also performed in order to determine some of the hydraulic properties of the columns. A 2-liter tracer solution was prepared by diluting a tritium stock solution 1:100. The count rate of this solution was 82800 cpm, and all sample concentrations were normalized to this amount. The tracer solution was introduced into

the column system in the same manner as the chromate solutions. The pump infusion rate was set at a rate of 2 mL/min. The inlet stopcocks were set to divert fluid out of the columns until the lines had become completely saturated. Once the lines had been saturated with the tracer solution, flow into the columns was initiated by opening the stopcocks. The outlet lines were again routed to waste reservoirs. The tracer solution was input into the system as a slug input rather than as a step input, which was the method used with the chromium solutions, with a total volume of 150 mL, this was equivalent to 1.05 to 1.54 pore volumes, depending on the column.

Sampling frequency was 1 sample every ten minutes. These samples were taken from the outlet stopcock with a 1 mL plastic syringe (Fisher Scientific) and added to 7 mL of scintillation cocktail (Ecolite Plus) in a 10 mL scintillation vial. The samples were then analyzed on a liquid scintillation counter with output in counts per minute.

2.10 Analytic Methods

2.10.1 Gas Chromatography

Chlorinated hydrocarbon quantification was performed on an Hewlett Packard 5890 GC with an HP-5 0.53 mm x 15 m capillary column and an FID detector. The gas pressures used in the analysis for compressed air, hydrogen, and helium (used as the carrier gas) were 250, 125, and 150 kPa respectively. The oven, injector and detector temperatures were 40°C, 240°C and 300°C. The retention times for PCE and TCE were 1.9 and 3.9 minutes, respectively. Sample injection volumes were 1 μ L.

2.10.2 High Pressure Liquid Chromatography

HDTMA

The quantification of HDTMA was determined by an HPLC method described by Helboe (1983) which employs a Nucleosil-CN column (Sigma Chemical Company). The column has the dimensions of 150 x 4.6 mm with a packing of bonded phase silica with CN groups at a 5 μ m diameter. The mobile phase required in this method is a 5 mM p-toluenesulphonic acid in a methanol:water solution at a 55:45 volumetric ratio. The mobile phase was obtained by dissolving 3.836 g of p-toluenesulphonic acid in 4 L of the methanol:water mix using degassed Millipore Milli-Q water.

The flow rate of 1 ml/min was controlled by a Waters 501 HPLC pump, through a UV-Vis Lambda Max 481 Spectrophotometer (Waters Associates) set at a detection wavelength of 254 nm. The detector actually detects the HDTMA-p-toluenesulphonic

acid ion pair in this case which eluted at about 5 minutes with an injection volume of 25 μ l.

Chromate

Aqueous chromate concentrations were determined by an HPLC method employing a Nova-Pak silica bonded C-18 reversed phase column (Waters Associates). The dimensions of the column are 150 x 2 mm. The column packing consisted of 4 μ m silica spheres to which were bonded C-18 chains. A 5 mM solution of tertbutylammonium hydrogen sulfate (TBAHS) in 10% CH₃CN was used for the liquid mobile phase. This solution was prepared by dissolving the TBAHS in 200 mL of CH₃CN and diluting everything to 2 L with Millipore Milli-Q degassed water.

The flow rate of 0.6 mL/min was controlled by a Waters 501 pump which yielded an average backpressure of 3000 psi. A Waters 994 UV-Vis detector was used to detect chromate concentrations at a wavelength of 365 nm at a retention time of 3.0 minutes with a 25 mL injection provide by a Waters 717 Plus Autosampler. Under these conditions, the run time was 4 minutes.

2.11 Transport and Reduction Modeling

2.11.1 CXTFIT 2.0

Various models were run using the mass transport code CXTFIT 2.0 (Toride et al, 1995), which is a model that addresses various solute transport problems by using a non-linear least-squares parameter optimization method. The CXTFIT 2.0 code may be used to solve either inverse problems or forward (direct) problems. When solving inverse problems, the code fits mathematical solutions of the theoretical models, which are based upon the advection/dispersion equation (ADE), to empirical data. By using this approach, transport parameters in the model can be estimated. When solving a direct problem, the concentration may be predicted as a function of time and position. CXTFIT 2.0 embodies three different one-dimensional transport models. These are the (a) conventional ADE, (b) the chemical and physical nonequilibrium ADE, and (c) the stochastic stream tube model.

The usage for CXTFIT 2.0 in this case was the determination of the hydrodynamic dispersion coefficient for each of the six separate columns based on data collected in a non-reactive tracer test (sections 2.9.3 and 3.6.4) in an inverse model approach. This parameter is then used in the reactive transport chromate study (sections 2.9.2 and 3.6.1-3.6.3) in order to extract values from additional inverse models for the decay and retardation coefficients.

2.11.2 Evaluation of Dispersivity

Using the results of the tritium tracer test, inverse models were run in order to obtain estimates for the longitudinal hydrodynamic dispersion coefficient for each column. In these cases, I assumed that there was no retardation and also no decay or production of the tritium in the system. For modeling purposes in CXTFIT 2.0, I ran an inverse deterministic equilibrium advection-dispersion equation (ADE) model (INVERSE = 1, MODE = 1) in order to obtain the estimate of the dispersion coefficient. This constant could then be used in equation 1.2.5 in order to obtain an estimate for the value of the dispersivity. The dispersivity could then be used again in equation 1.2.5 with the variable flow rates used in the reactive transport study, to obtain relative values for the hydrodynamic dispersion. The effective diffusion (D^*) of equation 1.2.5 is considered to be negligible in comparison to the dispersive influence caused by the high velocities in this investigation.

The inverse models for tritium dispersion assumed a retardation factor of 1.0 and employed the use of the deterministic equilibrium solution mode for the ADE (mode 1). All data used in the input file was normalized spatially and timewise making these parameters dimensionless. The concentration mode was set for flux-averaged concentration at the individual hydraulic lengths for each column (roughly 30 cm). Velocity values were based on the 2-mL/min volumetric flow rate, cross-sectional area, and porosity. No estimations were prescribed for the total mass input. Degradation was assumed to be 0 in this case. Based on this input format, values for the hydrodynamic

dispersion were fitted for each column. The complete CXTFIT 2.0 input files can be seen in appendices N through S of this report.

2.11.3 Evaluation of Decay and Retardation

Once the dispersion coefficients were determined, these values were assumed to be constants for each respective column system and treated as such in the inverse models for the reactive transport study. These models once again used the deterministic equilibrium ADE solution method with a flux-averaged concentration and conversions of D based on the respective volumetric flow velocities (4, 2, and 0.6 mL/min). 200 iterations maximum was again used with constraints on the fitted parameters. In this case, values for R and μ (decay) were fitted. In these cases, it was assumed that reduction occurred at significant levels only on the pellet surface with negligible decay occurring in the solution phase. The complete CXTFIT 2.0 input files can also be seen in appendices N through S of this report.

III.

Results and Discussion

3.1 Mechanical Stability Study

After a few initial isotherm studies with the Cercona pellets, it became obvious that there was a high degree of variability in the mechanical stability of the pellets. In some cases little or no change would be noted during surfactant modification while at other times there may have been a 20 to 50% reduction of the pellets to fines. In a few other cases, the pellets would become totally reduced to fines during the exposure to surfactant and shaking. This led to a study that would determine which pellet type is the most stable under the conditions I imposed upon it.

There were several variables involved in the process; iron to zeolite ratio, primary cation type, presence of a foaming agent, iron type present, grain size of the pellets, surfactant concentration, as well as shaking rate. After an initial test, it appeared that the most influential variables in this system were the primary cation type, presence of a foaming agent, surfactant concentration as well as the shaking rate. The surfactant concentration variation was eliminated since it is a constant in the batch and column studies contained in this work. I performed the initial tests with 100 mM HDTMA solutions.

Seventeen different pellet types were examined in this manner and what I determined was that those pellets that contained calcium as the primary cation, as opposed to sodium or ammonium, in combination with pellets that had not been subject to an increase in porosity by a foaming agent were, by far, mechanically the most stable.

Pellet types that contained sodium or ammonium as the primary cation were stable to some degree up to a rate of 75 rpm and then began to show significant

breakdown after one hour at a rate of 150 rpm, whereas the calcium pellets remained intact (estimated < 2% loss by mass). Pellet types that were foamed were found to be 100% unstable regardless of their cation types making them the least favorable pellet. These pellet types were completely broken down by the surfactant solution at even the slowest shaking rate of 75 rpm, although they were slightly more stable in pure water than in the surfactant solution. The pellet types tested and the results are briefly summarized below in Table 3.1.1.

Table 3.1.1. Summary of results from mechanical stability study

Description	Pellet Size	150 rpm Test	100 rpm Test	75 rpm Test
foamed/calcium form	-3 +8 mesh	U	U	NT
foamed/calcium form	-12 +20 mesh	U	U	NT
nonfoamed, porous/NH form/baked at 220°C	-3 +8 mesh	U	U	NT
nonfoamed, porous/NH form/baked at 220°C	-12 +20 mesh	U	U	NT
foamed/sodium form	-3 +8 mesh	U	U	U
foamed/sodium form	-8 +12 mesh	U	U	U
nonfoamed/sodium form	-12 +20 mesh	U	U	S
nonfoamed/sodium form	-3 +8 mesh	U	U	S
foamed/calcium form	-3 +8 mesh	S	S	U
nonfoamed/calcium form	-12 +20 mesh	S	S	S
nonfoamed/calcium form	-3 +8 mesh	S	S	S
higher density, nonfoamed/bimetallic iron media	-3 +8 mesh	S	S	S
higher density, nonfoamed/iron media	-3 +8 mesh	S	S	S
Type Z _{Na-1.10}	-3 +8 mesh	U	S	S
Type Z _{Na-1.2}	-3 +8 mesh	U	S	S
Type ZP _{NUSMC-1.2} /10 vol% iron	-3 +8 mesh	U	S	S
Type Z _{USMC-1.2} /50 vol% iron	-3 +8 mesh	U	S	S

U = unstable S = stable NT = not tested in these conditions

3.2 Surfactant Modifications

3.2.1 HDTMA Sorption Study

Isothermal batch studies were performed on both U0 pellets as well as P0 pellets. The surfactant loading for the U0 pellets was determined initially with duplicate samples containing 2.00 g (± 0.05 g) of the pellets and 20 mL of the initial conditions ranging from 1 to 28 mM HDTMA for a 1:10 solid to liquid ratio. Previous work by Whitworth (1997) and Anghel (1997) showed that the sorption of HDTMA onto raw zeolite surfaces containing mostly clinoptilolite, followed classical Langmuir type behavior which indicates some sorption maximum, or finite surfactant loading capacity. The data however, was examined for Langmuir behavior as well as Freundlich behavior which is common sorption behavior for cation exchange onto mixed silicate mineral surfaces (Fetter, 1993)

Figure 3.1.1 shows the empirical data obtained from the isothermal treatment of the U0 pellets. Here, C is the aqueous equilibrium concentration and S is the amount sorbed or the sorbed concentration. It is immediately obvious from the figure that the sorption behavior is not linear in this concentration range. In this figure we see an immediate high adsorption intensity out to approximately $C = 1$ mM at which point the sorption begins to approach its plateau at around 12 mmol/kg. This type of trend of sorption is typical of Langmuir behavior, but this may be tested further by linearizing the data set for Freundlich as well as for Langmuir isotherms. A comparison of the correlation coefficients will then give an indication of the sorption type.

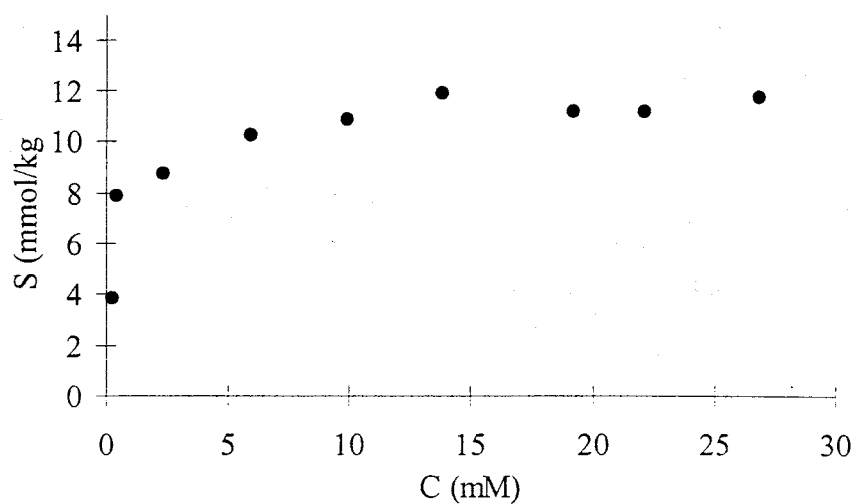


Figure 3.2.1. HDTMA sorption on U0 pellets at 25°C.

By plotting the $\log_{10} S$ as a function of $\log_{10} C$, and fitting the plot linearly, an indication of possible Freundlich behavior is obtained. In Figure 3.2.2 is shown the Freundlich linearization as described by equation 1.2.16.

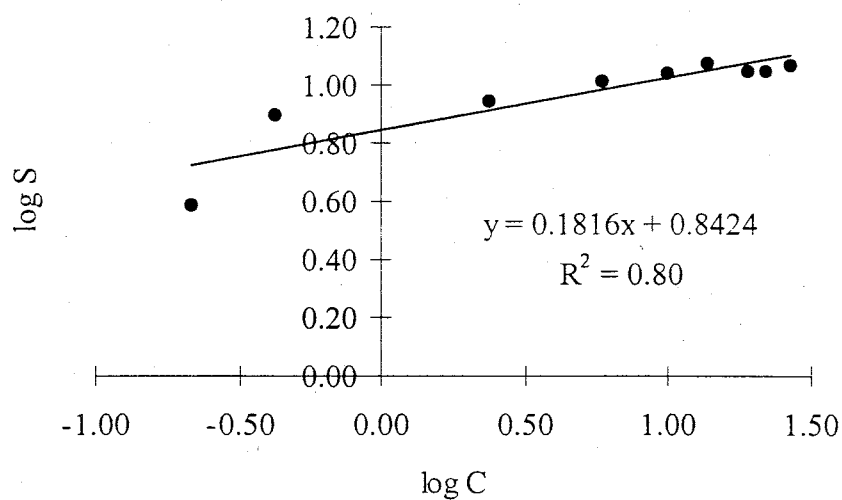


Figure 3.2.2. Freundlich linearization for U0 pellets sorption isotherm data at 25°C.

By plotting the ratio of the equilibrium solute concentration to the sorbed concentration as a function of the equilibrium solute concentration and fitting the plot linearly, an indication of possible Langmuir behavior can be obtained, as is indicated in equation 1.2.19. Figure 3.2.3 below shows the Langmuir linearized form of the sorption data.

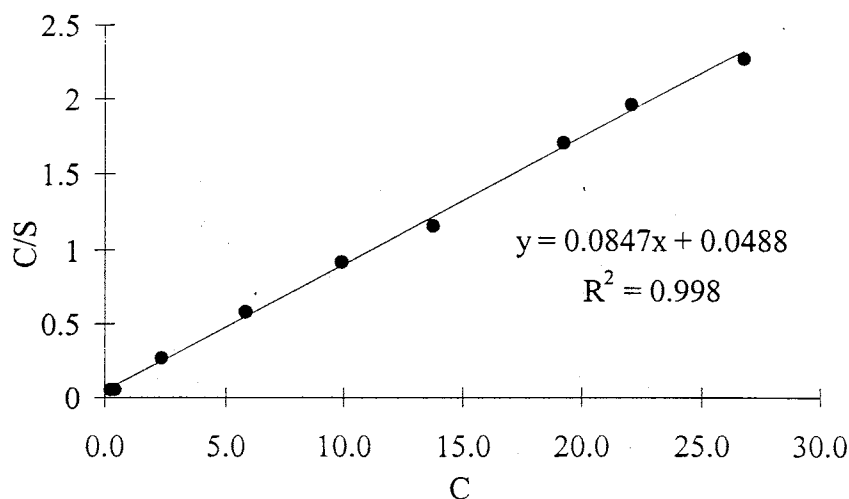


Figure 3.2.3. Langmuir linearization for U0 pellets sorption isotherm data at 25°C.

It is obvious by the comparison of the square of the correlation coefficients, that this sorption follows Langmuir behavior very strongly indicating some sorption maximum. From equation 1.2.19 and Figure 3.2.3 above, the value for M can be determined to be 11.81 mmol/kg which is in agreement with the plateau seen in figure 3.2.1 K_L , the Langmuir constant, comes out to be 1.736 L/mmol for the U0 pellets.

When the pellets containing Peerless 76D iron, P0 pellets, with the maintained calcium form and nonfoaming were characterized, slightly different results were found. Each sample batch contained 1.5 g (± 0.05 g) of the pellets and using the same initial conditions (1 to 28 mM HDTMA), 20 mL of solution was added for a 1:13.3 solid to

liquid ratio. This ratio was increased from the U0 pellet study to allow for any significantly greater sorption behavior. Figure 3.2.4. below shows the sorption isotherm of HDTMA onto P0 pellets after a 12 hour equilibration at 25°C. The sorption capacity appears to be in the neighborhood of 25 mmol/kg. It is evident from this data set that the P0 pellets have at least twice the sorption capacity for HDTMA over the U0 pellets, although this is still on the order of 12 to 17% of the sorption capacity of raw zeolite which has been seen between 140 mmol/kg (Haggerty and Bowman, 1994) up to 220 mmol/kg (Whitworth, 1997).

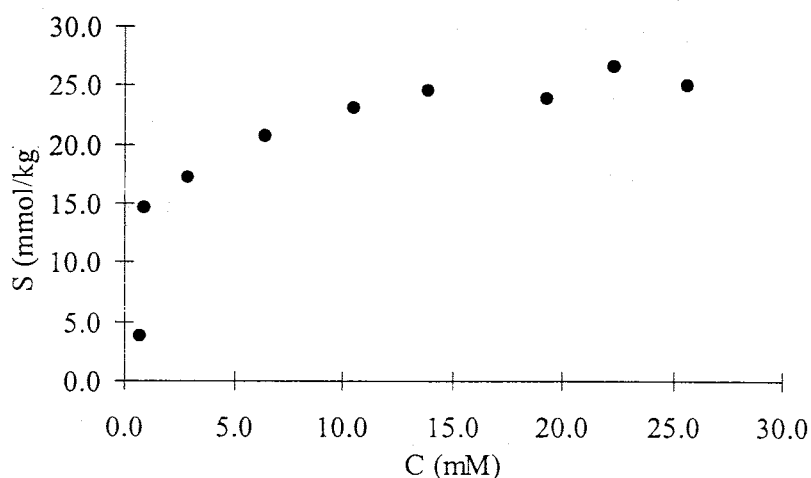


Figure 3.2.4. HDTMA sorption on P0 pellets at 25°C.

Figure 3.2.5 shows the Freundlich linearization of data and Figure 3.2.6 gives the Langmuir linearization.

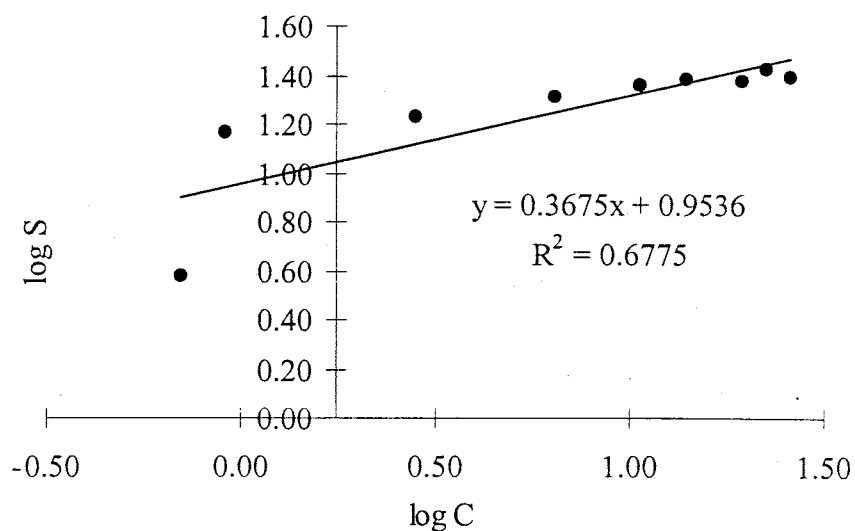


Figure 3.2.5. Freundlich linearization for P0 pellets sorption isotherm data at 25°C

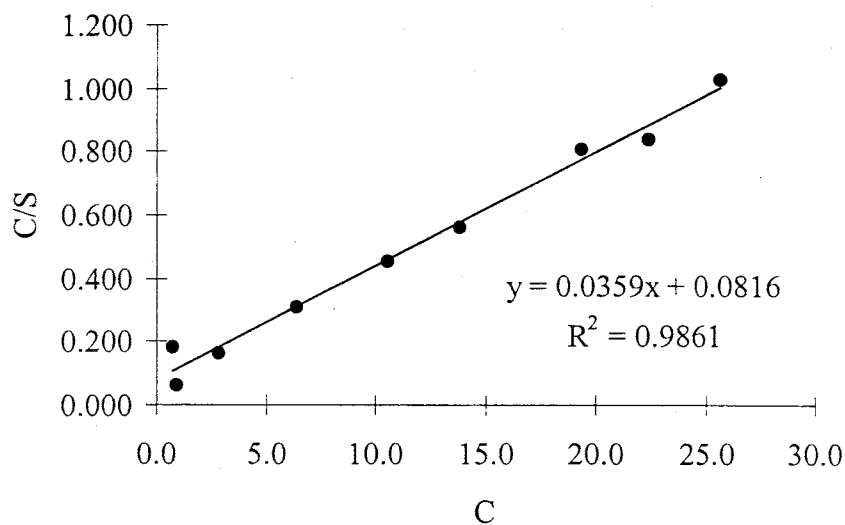


Figure 3.2.6. Langmuir linearization for P0 sorption isotherm data at 25°C.

As in the U0 pellet study, it is once again evident that the P0 pellets strongly exhibit Langmuir type sorption by comparing the coefficients of determination. The Langmuir sorption maximum for this case came out to be 27.9 mmol/kg. The Langmuir constant

was determined to be 0.440 L/mmol. Given the previously mentioned ranges for sorption of HDTMA onto a raw zeolite surface (140 - 220 mmol), I would expect a maximum sorption on these pellets in the range of 30 to 40 mmol/kg with a simple mass comparison of the actual zeolite present in the pellets (20%). However, this estimate is based on the assumption that all the exchangeable sites of the zeolite are available -- this of course is not the case. In the pelletization process, the iron powder is added as well as the binding material and then is hardened into a pellet greatly reducing the number of available exchange sites. In accordance with this, the values of the sorption maximums of 11.8 mmol/kg for the U0 pellets and 27.9 mmol/kg for the P0 pellets, are reasonable values.

As to the difference of a factor of two between the two pellets, I assume it is do to the basic difference in size of the type of irons used which is the only variable in these two pellet types. The US Metals iron is obtained from that company directly by Cercona and is a fine iron powder (-50 mesh) which also has the potential to "coat" the zeolite itself as I witnessed in a previous test that I performed using an unconsolidated mixture of this same iron and zeolite. The iron essentially coated the zeolite when mixed, possibly through simple coulombic interactions. The iron used in the P0 pellets is actually a steel fines product which is quite a bit larger than the US Metals iron powder. Upon visual inspection of the pellets themselves, these physical differences become even more evident. The U0 pellets appeared like small, homogeneous, iron balls while the P0 pellets exhibited some heterogeneity with patches of zeolite and iron present throughout, thus allowing for a greater exposed zeolitic surface area and hence a greater exchange capacity.

The binder used in the pellets itself also likely has some degree of cation exchange capacity. Differences in sorption capacity may be seen here as well because of differences in the amount or type of binder material used for the two separate pellet batches. The data from these two experiments may be found in appendices B and C of this report.

3.2.2 Pellet Surface Modification

The U0 and U1 pellets were used initially in this work which were followed later by the P0 and P1 pellets. From the HDTMA equilibrium and washoff concentrations, some quantifications can be made about the surface coverage of the pellet batches.

The U0 treatment revealed a HDTMA loss to sorption from the initial concentration of about 19.0 % or about 13.9 mmol/kg present on the pellet surface. This is in fairly close agreement with the isotherm data which showed a coverage of 11.8 mmol/kg. This number may be slightly higher given the case that all the nonsorbed HDTMA was not washed off in the treatment process.

In the case of the P0 pellets, a 46.9% loss of the initial surfactant present was noted, equating to a surface coverage of 27.75 mmol/kg which is virtually what I determined in the isotherm study (27.85 mmol/kg).

Another important factor to note here is that during the treatment process, not only does the P0 pellets have twice the sorption capacity of the U0, the P0 version is much more stable during the surface modification. Roughly 30% of the U0 may be lost as fines in pellet breakdown, whereas little to no breakdown is seen in the P0 pellets.

3.3 Hydraulic Characterizations

3.3.1 Gravimetric Water Content Analysis

The gravimetric water content study was performed as described in section 2.6 at a constant temperature of 105°C. The results of the study are summarized below in table 3.3.1. The complete results are listed in appendix D of this report.

Table 3.3.1. Summary of gravimetric water content study results

Pellet Type	GWC
	(% water by mass)
U0	1.22
U1	1.34
P0	1.69
P1	1.89
B0	4.55

Note in this result summary that in both cases, the U1 as well as the P1, the surfactant-modified pellets had a greater weight loss in the range of 0.1 to 0.2% of the total mass. This is likely due to a change in the hydrophyllicity after HDTMA modification; however, since this assumption was not tested nor confirmed, the actual percent values that were determined in this study were used to make adjustments in the column calculations.

3.3.2 Saturated Hydraulic Conductivity Study

In this conductivity test, three measurements were made for each column. From each of these measurements, a saturated hydraulic conductivity, K_s , was determined and the results averaged. The complete data set is shown in data appendix E and the results are summarized below in table 3.3.2.

Table 3.3.2 Summary of saturated hydraulic conductivity results

Column	Saturated Hydraulic Conductivity, K_s (cm/min)
Column A - P1	2.53 (± 0.02)
Column B - P1	1.24 (± 0.02)
Column C - P0	2.47 (± 0.02)
Column D - P0	1.62 (± 0.02)
Column E - B0	2.09 (± 0.02)
Column F - B0	3.31 (± 0.02)

Saturated hydraulic conductivity can vary in a range of over 13 orders of magnitude and given the type of material (i.e. sand vs. clay), it can vary 3 or 4 orders of magnitude (Freeze and Cherry, 1979). So comparatively, these differences in K_s can be considered relatively minor and are due most likely to the inhomogeneity of the columns due to the pellet size distribution and packing method. It is also likely that differences in

endplates as well as valve volumes and fittings may have caused slight differences in the experimentally determined values for K_s .

3.4 PCE Sorption/Reduction Batch Studies

3.4.1 Iron characterization

Upon analysis of the sacrificed samples of the iron characterization study, the following three data representations were developed. The first set, Figures 3.4.1 and 3.4.2 illustrates the loss of PCE through reductive dechlorination on a normal and logarithmic scale. The second set, Figures 3.4.3 and 3.4.4, show the production and reduction of trichloroethylene (TCE) in the same system. The third data representation, illustrates the simultaneous PCE reduction as compared to the TCE production and reduction for each individual iron type. This is illustrated in Figures 3.4.5 through 3.4.7. The data sets shown in the figures below are averages of triplicates, as described in section 2.7.1.

Figure 3.4.1 shows the normalized data set for the loss of PCE in each of the three systems. There does seem to be a bit of scatter, particularly at the 16 hour data set, but an overall trend can be seen from which some basic assumptions can be made. There doesn't seem to be a large reduction potential in the Fisher or US Metals iron as displayed by the data. Only about a 30-40% reduction in PCE levels was noted after 16 hours for these two iron types; although at later times, specifically 35 hours, the PCE levels begin to become comparable to those found in the Peerless batch system. The US Metals iron illustrates a slightly higher capacity for PCE reduction showing a 45-50% reduction at 8 hours and then about 70% at 32 hours. In this case, the Peerless 76D iron seems to illustrate the highest potential for PCE reduction. The initial intensity appears significantly higher than either the Fisher or US Metals, degrading approximately 70% of the PCE within the first hour.

One anomaly noted in this experiment was the generation of gas, probably CO_2 , in the Fisher batch system. The gas evolution was significant enough in volume to pressurize the head space vials and cause the septum to bubble. Considering this, Fisher was henceforth eliminated from the characterization process. If this iron type were to be used in a column study the evolution of gas could adversely effect the hydraulics of the system causing desaturation and blockage creating preferential flow paths and a heterogeneous flow regime.

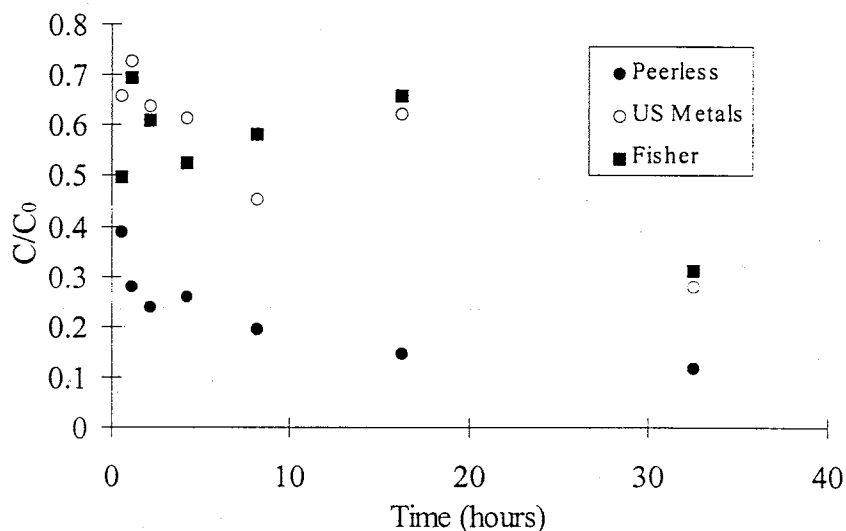
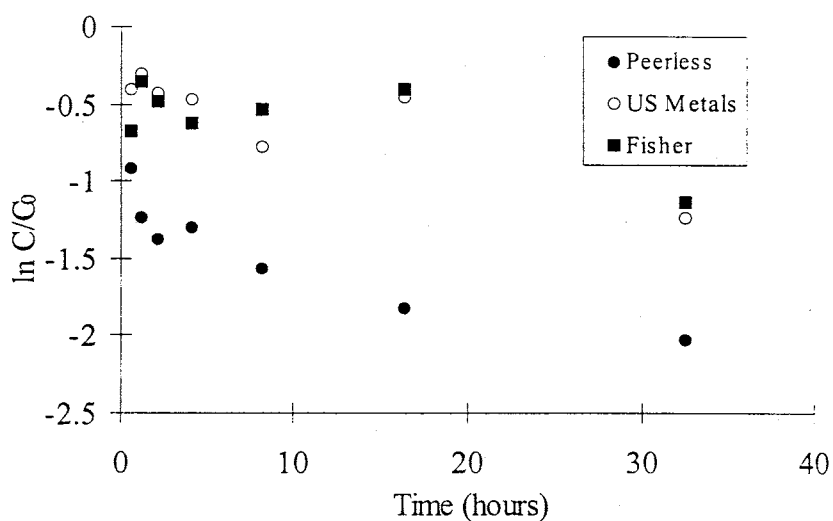


Figure 3.4.1 Relative decay of PCE by various zero valent iron (ZVI) sources

The logarithmically transformed data set shown in Figure 3.4.2 is what would normally be used to determine rate constants. Given the nonlinear behavior of this data, it would however be difficult to put an accurate fit to the data since there seem to be two definable kinetic regions, but only one hypothesized reduction process. One possibility to this dual region behavior is the actual sorption of PCE to the iron surface as described by Burris (1995). Burris noted that after accounting for the mass of PCE (as well as TCE)

that had sorbed to the nonreactive sites of the iron, the reduction rates were first order. This could be the case here. The initial intensities for PCE disappearance are quite different, but following this the decay seems to be quite similar for all three situations based on visual comparison.

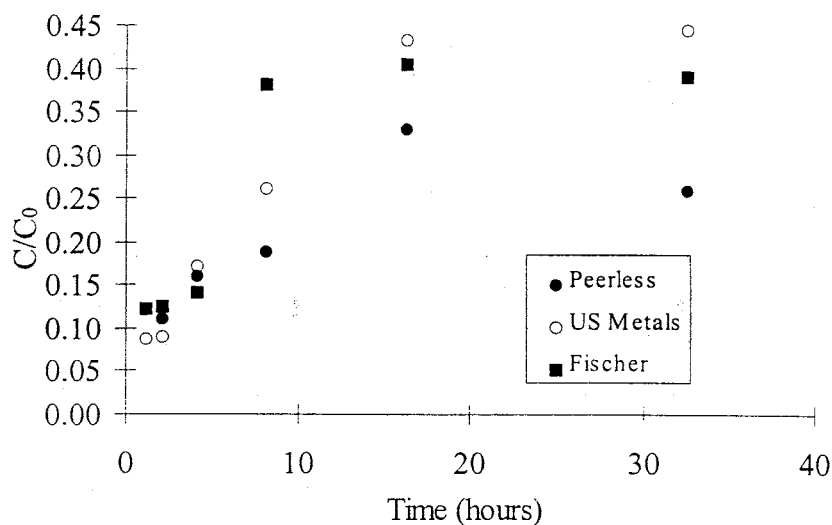


3.4.2 Relative decay of PCE by various ZVI sources (logarithmically transformed)

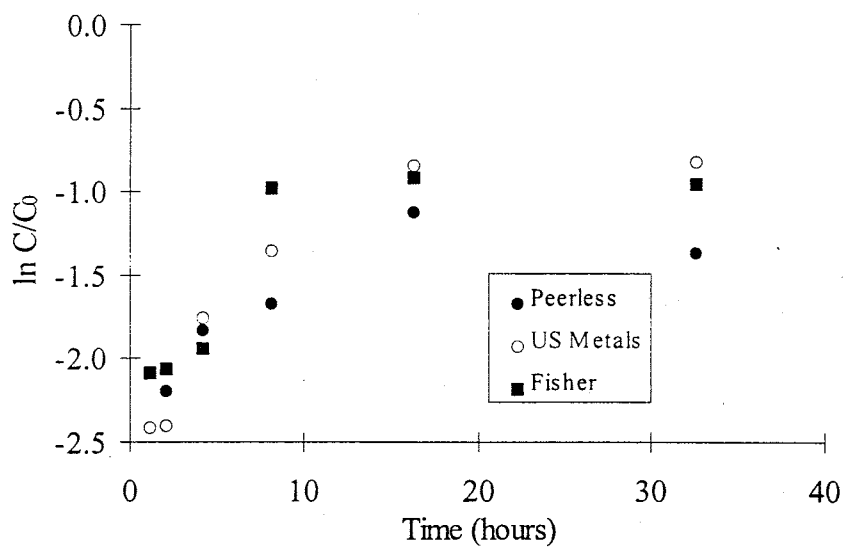
As mentioned, the production of TCE was also monitored in this experiment. Both peaks were clearly eluted on the same GC method, which made analysis simple and timely, which is important when dealing with volatile organic compounds. Figure 3.4.3 below shows the evolution of TCE from the dechlorination process of PCE by reduction. It can also be seen that after about 16 hours, the TCE concentrations begin to become

reduced as well (a complete reduction in the TCE concentrations is not illustrated in this data as this data set is a byproduct of the PCE trends). The three dichloroethylene (DCE) isomers as well as vinyl chloride were not detectable by this GC method and were therefore not quantified.

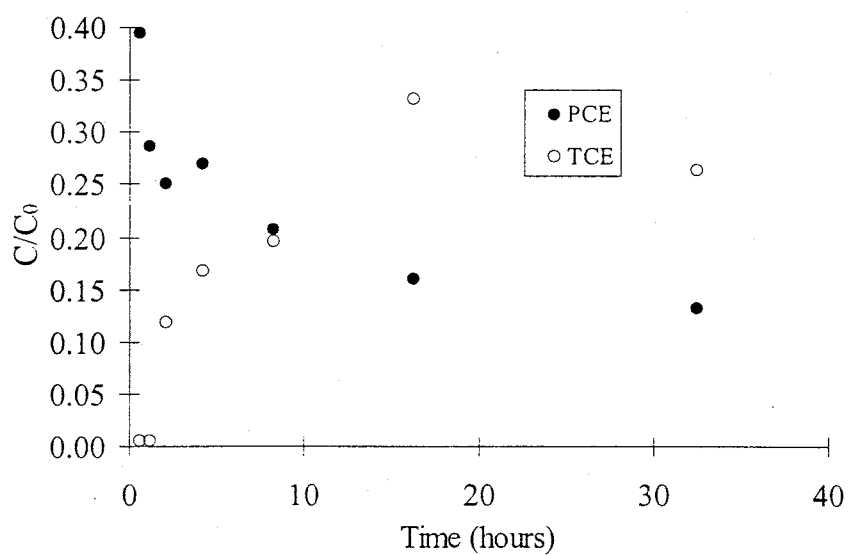
It can be seen as well from this data set that TCE production began about the same time and at comparable rates. The decrease in TCE concentration at later times is consistent with more rapid dechlorination of TCE by the Peerless iron, as is the case with PCE. Again the logarithmically transformed data set is shown in 3.4.4. In Figures 3.4.5 through 3.4.7 is shown the overlay of PCE reduction versus TCE reduction for each of the three individual iron sources.



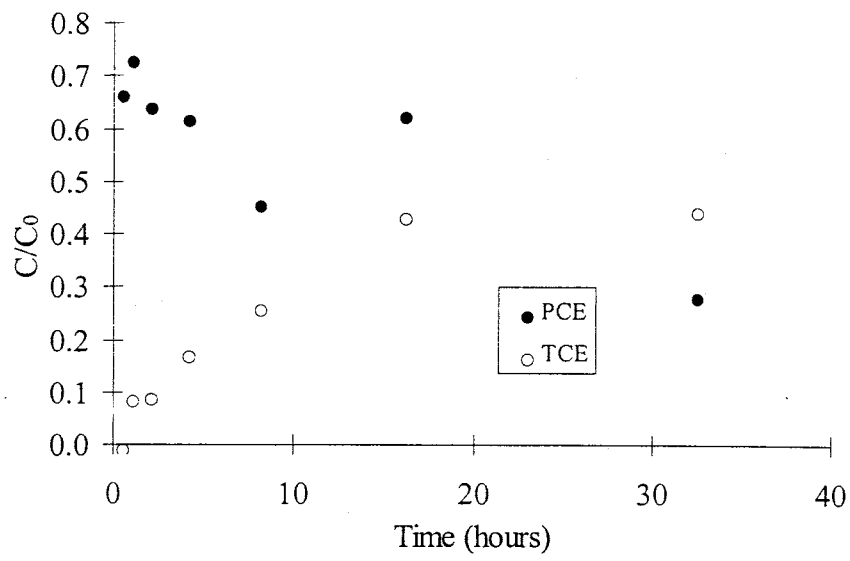
**3.4.3 TCE appearance due to dechlorination
by various ZVI sources**



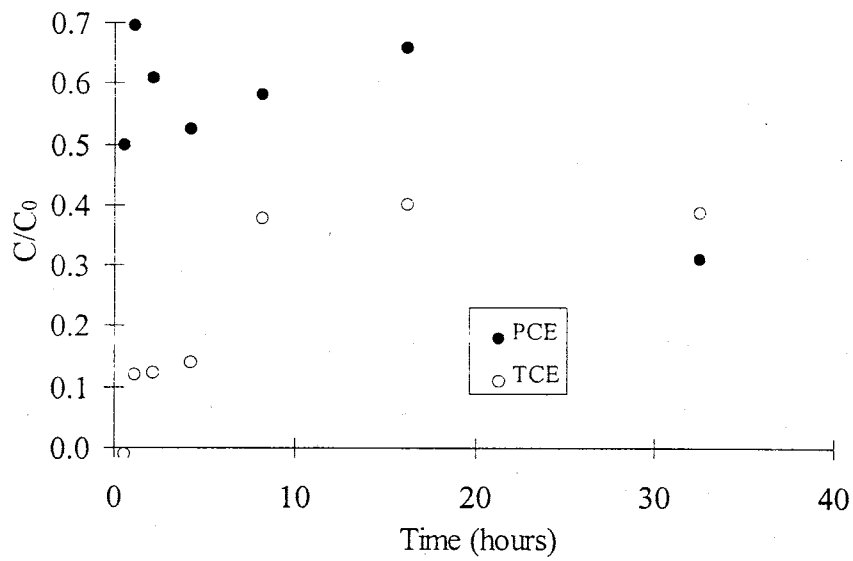
3.4.4 TCE appearance due to dechlorination by various ZVI sources (logarithmically transformed)



3.4.5 Dechlorination of PCE by Peerless 76D ZVI



3.4.6 Dechlorination of PCE by US Metals ZVI



3.4.7 Dechlorination of PCE by Fisher ZVI

No accurate rate constant could be extracted from these data due to the regional behavior and scatter. Any attempt to fit the data would have been subjective and would not have shown a true representation of the actual rate constant. Although no accurate rate constant could be defined in this data, by visual inspection, it appears as though the Peerless 76D iron showed the greatest potential for the reduction of PCE in this batch system, followed by the US Metals iron. The Fisher iron was least effective of the three in its reduction capabilities and also displayed gas evolution, as mentioned, which is highly undesirable.

The US Metals iron was actually chosen in the end for continued use. This choice was based mostly on cost and availability. US Metals iron is the iron used on site at the Cercona facility and can also be obtained at a lower cost than the Peerless 76D iron.

The complete data set from this experiment may be found in appendix F of this report.

3.4.2 US Metals Study

The same sort of experiment, as in 3.4.1, was performed again for the US Metals products in order to gain some baseline comparisons as to the effects of each of the components in the pellet system. The same sort of data is presented below for the US Metals products as was presented in 3.4.1 for the iron characterization test. Figures 3.4.8 and 3.4.9 depict the dechlorination process of PCE as seen in the US Metals study and the appearance and subsequent reduction of TCE is again exhibited in figures 3.4.10 and 3.4.11

It can be seen again from these figures that the US Metals iron powder is a strong reducing agent for PCE and TCE. Once again there is a good amount of scatter in the data, but some generalizations on overall trends can still be made. In figures 3.4.8 and 3.4.9, the control data shows that approximately 30% of the PCE was lost due to processes other than either sorption or reductive dechlorination. This loss is probably due to the volatilization of PCE through the septum, as opposed to volatilization during sampling times, since it seems to show a decrease with time. The remaining three sample sets show an approximate decrease in PCE by about 80% ($\pm 5\%$) after 80 hours of exposure to the iron products. The difference here again is in the initial time regions. After one hour of exposure, the Fe powder has degraded about 65% of the PCE present and the U0 pellets have eliminated about 50% of the hydrocarbon, while the surfactant modified U1 pellets have degraded about 75% of the PCE in the system. The loss of up to 30% of the PCE mass due to volatilization must be considered here as well, but the relative differences in degradation between the pellet types are noted. Considering the same data set at 5 hours, the PCE in the Fe powder system has been lowered by 45%, 70% in the Fe/zeolite system, and over 80% in the Fe/SMZ system.

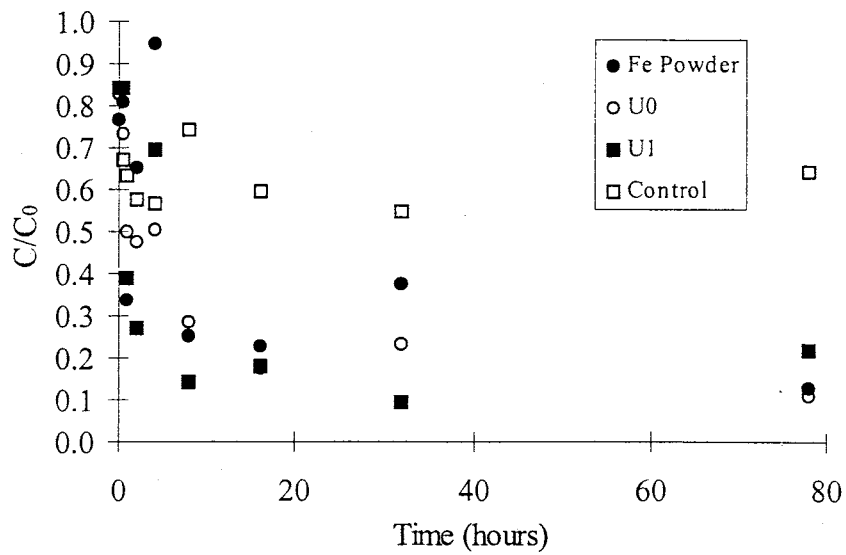


Figure 3.4.8 Relative decay of PCE by US Metals Products

In figure 3.4.9 is shown the log transform of the data. Again here, a reasonable fit to the data could not be determined due to scatter and the varying process regions of the curves. The complete data set from this experiment may be found in appendix G of this report.

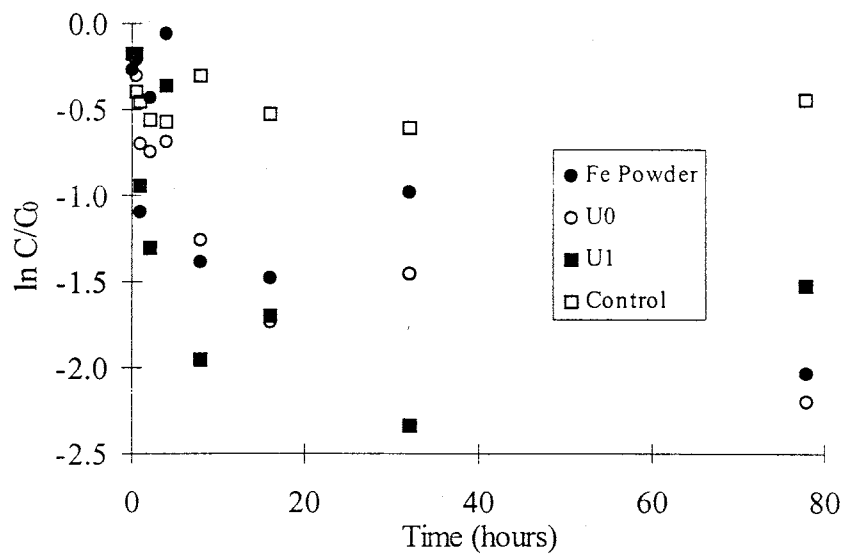
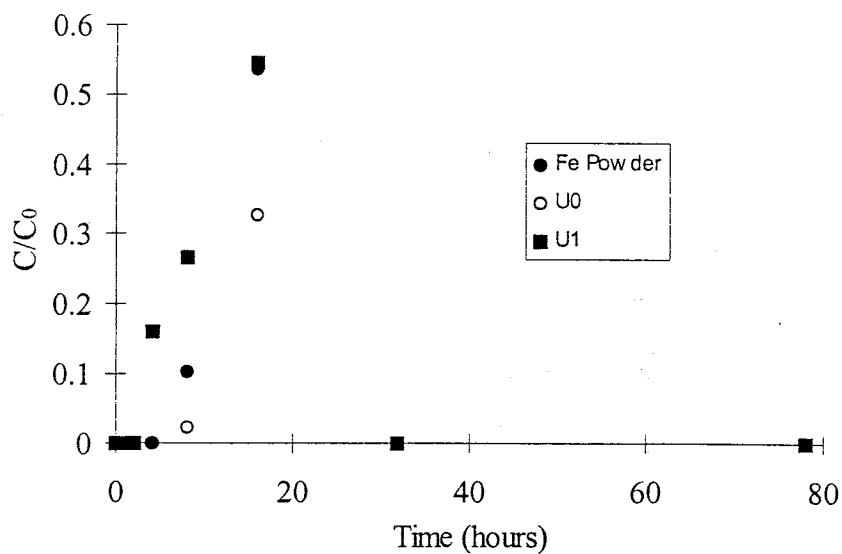


Figure 3.4.9 Relative decay of PCE by US Metals Products (logarithmically transformed)



3.4.10 TCE appearance due to dechlorination by US Metals products

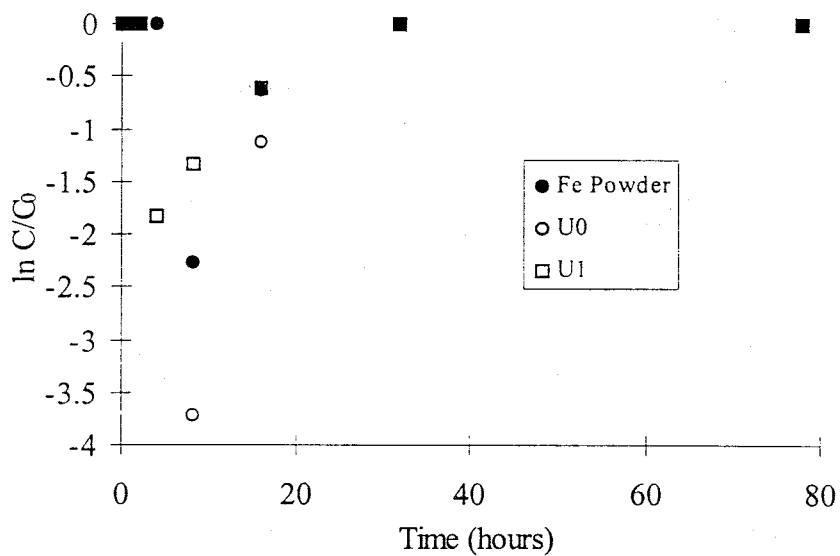


Figure 3.4.11 TCE appearance due to dechlorination by US Metals products (logarithmically transformed)

3.5 Chromate Sorption/Reduction Batch Studies

3.5.1 US Metals Study

This portion of work was performed in order to evaluate the ability of the Cercona pellet to anionically sorb and chemically reduce the toxic oxyanion chromate, CrO_4^{2-} . In figure 3.5.1 below are shown the kinetic results of the US Metals product study. This figure displays solid trends depicting the differences in degradation processes from the U1 pellet and the three controls.

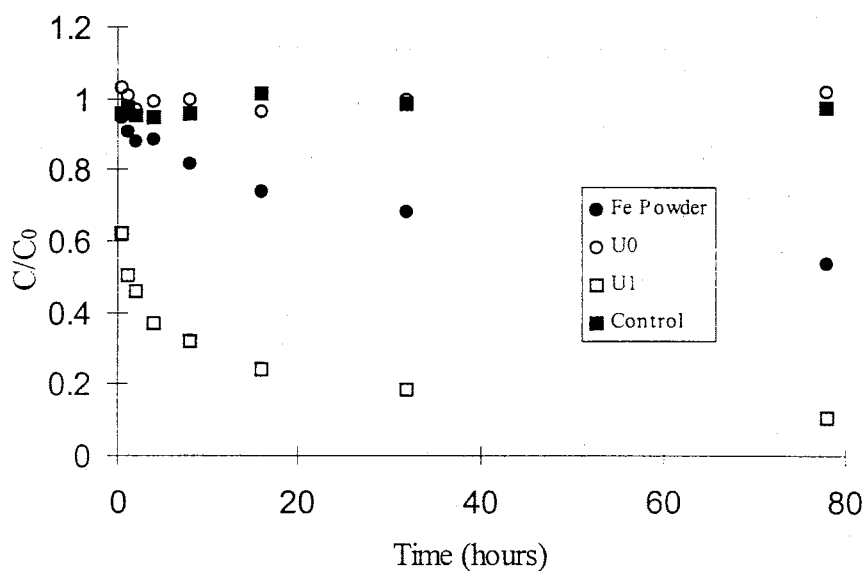


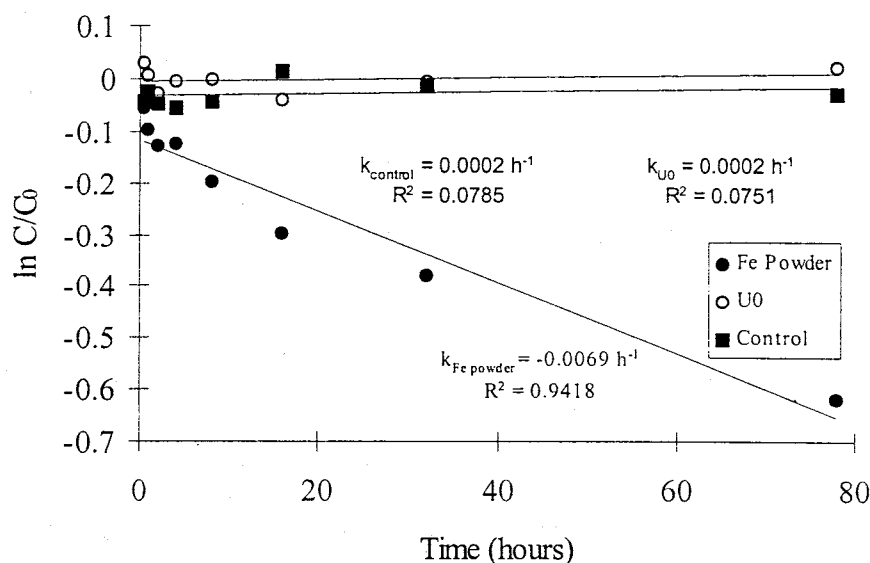
Figure 3.5.1 Chromate degradation by US Metals products

The control shows no significant loss of chromate in this data set, indicating that processes other than sorption or reduction were not occurring. It would be reasonable to expect a slight drop in chromate concentration in the U0 pellets since there potentially would exist some degree of chemical reduction occurring. The data doesn't seem to

present a noticeable amount of reduction in chromate levels. This is due probably to the reduced number of available reactive iron sites. The reduction of these sites is, once again, a product of the added binding material in the pelletization process. With fewer sites available, it also becomes statistically less likely that the anions will come into contact with these available sites.

In the Fe powder situation, there is a strong amount of degradation occurring. Once again, the controlling process is chemical reduction, but in this case the surface area is much greater than in the U0 pellet allowing for a far greater amount of available reactive iron sites. This greatly increases the statistical likelihood that the anions will come into contact with an available site.

In the final situation, the U1 pellets, we see the most favorable response. In this case we again have a decreased surface area, but the addition of the surfactant completely changes the dynamics of the situation. Through anion exchange, the surfactant bilayer is providing the residence time required for the chemical reduction process to adequately take place. The reduction process, at this point, is no longer dependent on the statistics involved in the meeting of reactive site and an anion, but on the meeting of the anion with the entire organic layer. This higher reduction potential is clearly shown in the U1 pellet data set in figure 3.5.1.

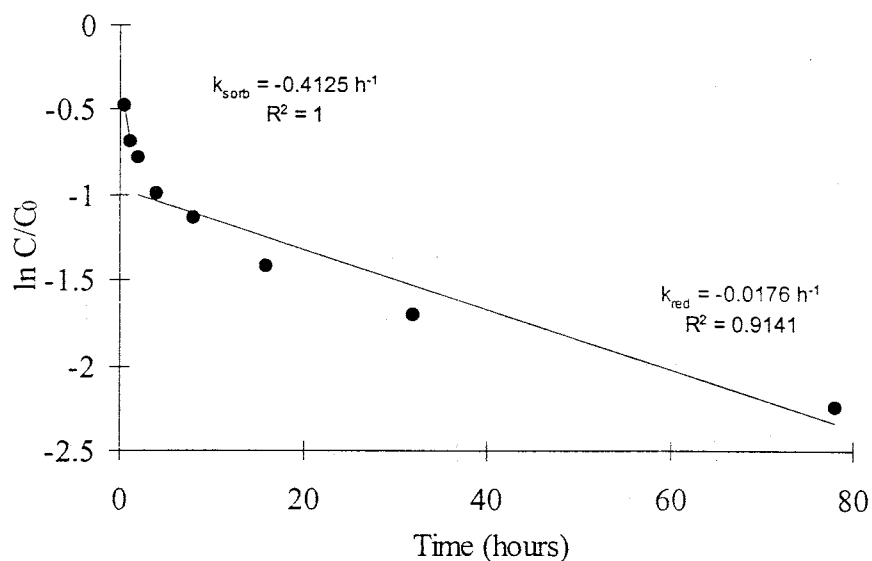


3.5.2 Chromate degradation by US Metals products (logarithmically transformed)

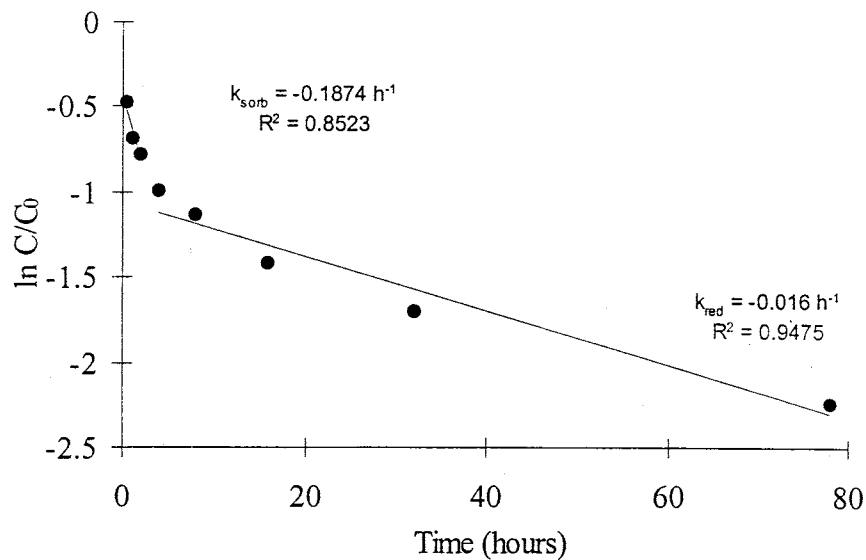
In figure 3.5.2, the natural logarithm of the concentration is plotted against the elapsed time in hours. By performing a linear fit to the data, the first order decay constant can be extracted from the data with units of h^{-1} , which is equal to the slope of the linear fit. Figure 3.5.2 depicts the control, Fe powder, and U0 pellet situations. As mentioned there does not seem to be much of a difference between the control and the U0 pellet, which is quantified here. Both cases yielded an extremely small decay constant of 0.0002 h^{-1} . The decay constant for the Fe powder was determined to be 0.0069 h^{-1} . The increased surface area of the Fe powder over the U0 pellets increased the decay constant by about 35 times; a rather significant difference.

The U1 pellet data was handled differently. As mentioned in the previous section (section 3.4) due to the scatter and the multi-degradation process regions for PCE, a reasonable fit to the transformed data could not be performed. The scatter in the chromate data is very low and we are looking at two process regions so a reasonable estimate to the

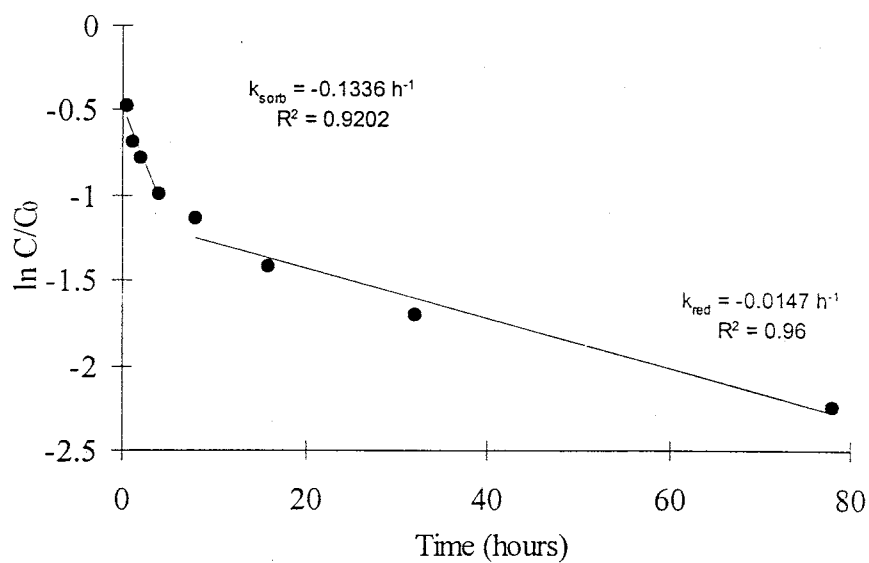
decay constant can be made. The initial region of the curve represents the higher intensity region of sorption through anion exchange. The sorption rate constant for this region is given as k_{sorb} . The lower intensity, later portion is the region where chemical reduction is most likely occurring. The reduction rate constant for this region is given as k_{red} . Since it is not fully clear when sorption ends and reduction begins, a series of dual region best fits were created by comparing different time regions to each other. The dual fit that gave fits for processes closest to $R^2=1.0$ was used as the representative fit from which the decay constant was determined. It should be noted that this is a best guess method and the actual decay will lay some where close to the given value. Figures 3.5.3 through 3.5.6 below illustrate four different time region differentiations and their respective rate constants.



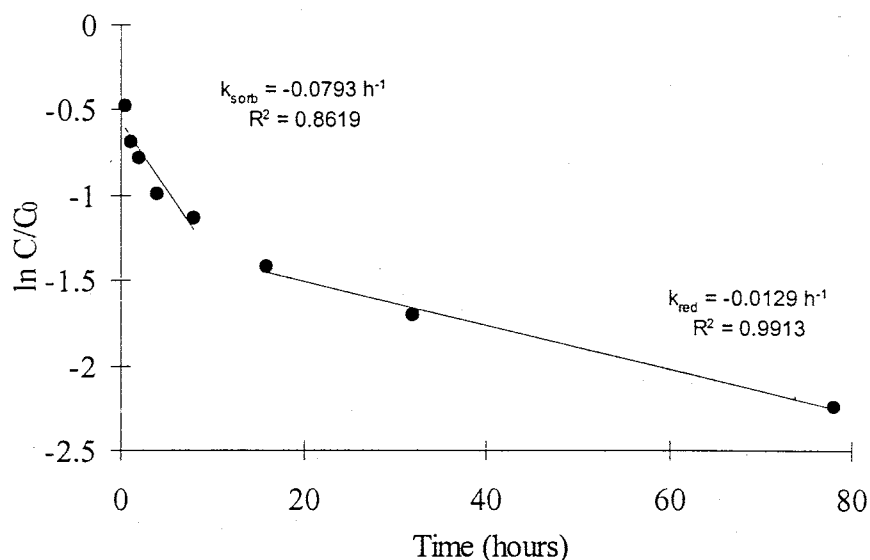
3.5.3 Chromate degradation by U1 Pellets – Fit I
(logarithmically transformed)



3.5.4 Chromate degradation by U1 Pellets – Fit II (logarithmically transformed)



3.5.5 Chromate degradation by U1 Pellets – Fit III (logarithmically transformed)



3.5.6 Chromate degradation by U1 Pellets – Fit IV (logarithmically transformed)

These figures depict a progressively longer in time sorption with decreasing intensity. The decrease in time and intensity for the reduction is only relative since this experiment was terminated at 78 hours which is before the complete elimination of chromate from the system. The k_{sorb} values vary by a factor of 5.2 while the k_{red} values vary by a factor of about 1.3. This would indicate that the estimate for the k_{red} value is much more accurate than the k_{sorb} estimate. Statistically, given the four dual fits, figure 3.5.5 probably gives the best estimate to the first order decay constants. In this case, k_{sorb} is estimated at 0.1336 h^{-1} and the estimate for k_{red} is 0.0147 h^{-1} . Here, the sorption mechanism is about 9 times faster than the chemical reduction mechanism.

Comparing the results of the U1 pellets to the U0 pellets and Fe powder will give an even better idea of how these modified pellets compare. The initial simple sorption process is approximately 670 times faster than the reduction occurring in the U0 pellets

and about 19 times faster than the reduction process in the Fe powder system. The subsequent chemical reduction rate is still 74 times greater than the UO pellet's and about 2 times greater than the Fe powder.

Another alternative in looking at this data is coming up with a time-weighted average for an overall process decay constant. In the case of Fit III (figure 3.5.5), about 5.1% of the reduction can be attributed to sorption and the remaining 94.9% to chemical reduction. The weighted average of the decay constant based on this division would be $k_{avg} = 0.0208 \text{ h}^{-1}$, which is still 104 times faster than the reduction occurring in the Fe/zeolite and about three times as fast as the raw iron.

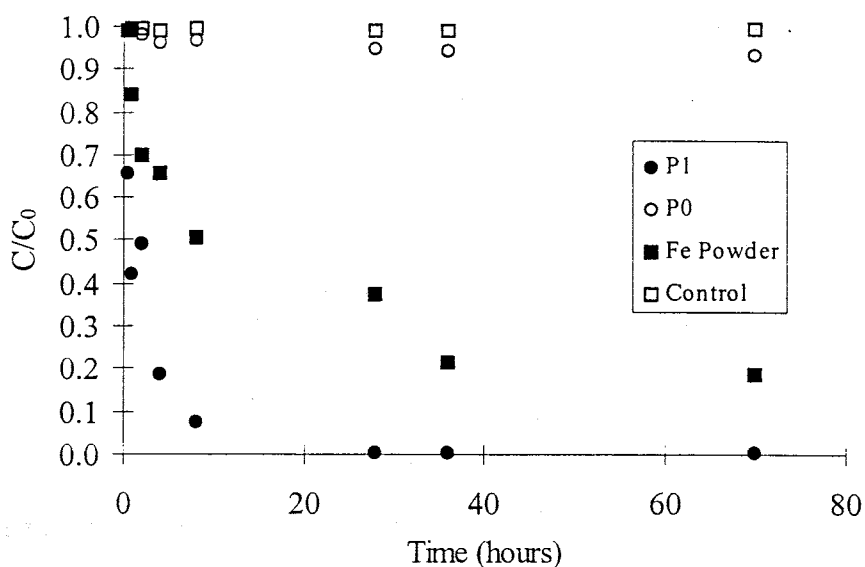
The raw data from this experiment may be found in appendix H of this report.

3.5.2 Peerless Study

An experiment similar to that described in 3.5.1 was performed using the pellets containing the Peerless iron powder. The results of the kinetic study are shown in figure 3.5.7 that once again show solid trends of chromate degradation in solution.

The data set follows the same sort of trend for each of the pellet types and the control. Once again we see that losses of chromate due to processes outside of chemical reduction and anion exchange are virtually negligible from the control data. There are, however, two major differences worth noting in this data set as compared to the US Metals data. First, there does appear to be more of a differentiation in the control data and the P0 pellet data. Active degradation is occurring with the P0 pellets, although still not on the same level with the Fe powder and P1 pellets. Secondly, after 28 hours the chromate has been almost completely eliminated from solution in the P1 pellet system

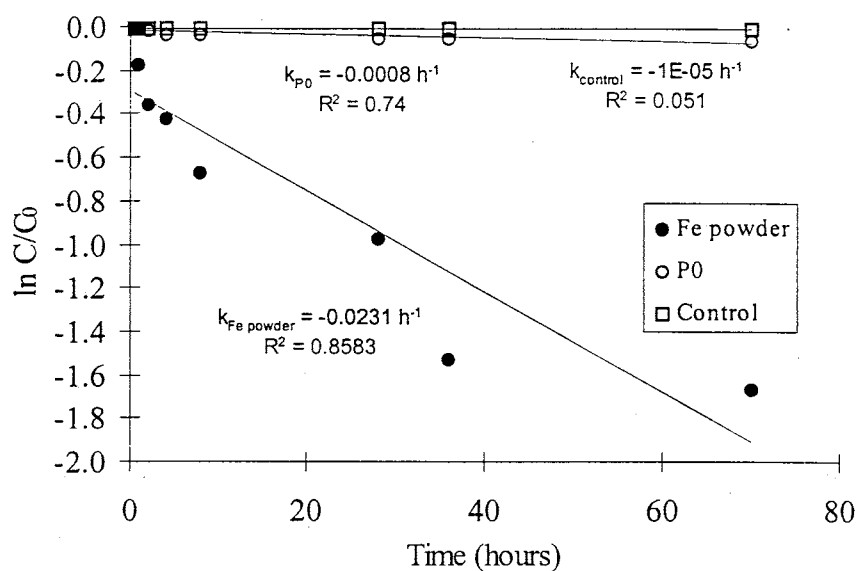
and the Fe powder itself is showing an increased potential for chromate by a factor of about three. So overall it appears that the Peerless iron products have a stronger reduction potential for chromate than was indicated by the US Metals iron products, which is consistent with the observed PCE reduction capabilities of these two iron sources.



3.5.7 Chromate reduction by Peerless products

Taking a closer look at the data, once again a plot of the natural logarithm of the concentration as a function of time is shown in figure 3.5.8. Note that in figure 3.5.7, there are no significant chromium levels seen after 28 hours. In order to give a more valid analysis of the rate constants for the P1 pellet, only the data from $t = 0$ to $t = 28$ will be used in that determination. The P1 pellet data has been separated out in the same manner and is shown in figures 3.5.9 through 3.5.11. The control data set in this scenario gives a negligible decay constant of $1.0\text{E-}5 \text{ h}^{-1}$ indicating once again that the initial condition is fairly constant. As mentioned, there is a noticeable amount of decay in the P0 system

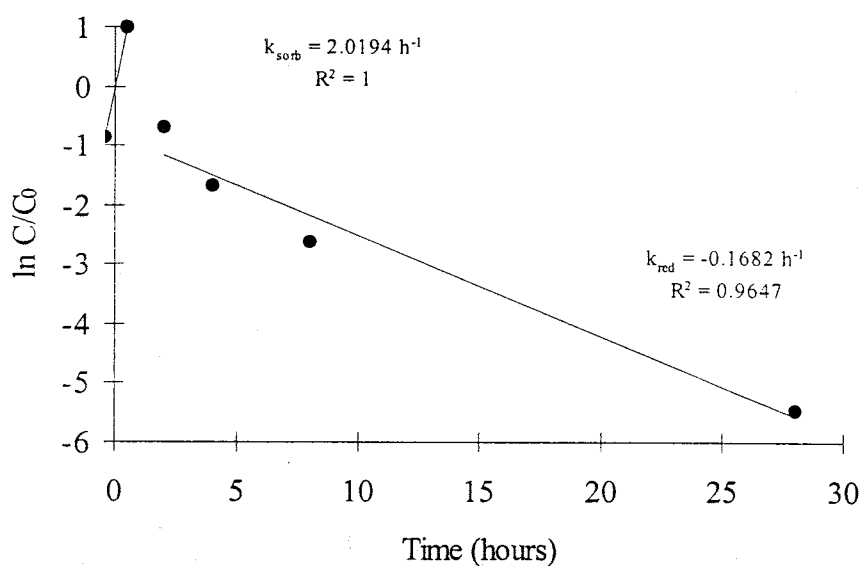
showing a decay constant of 0.0008 h^{-1} . The rate constant for the P0 pellets in this system is, therefore, about 4 times that found in the U0 results. We see the increasingly better results in the Peerless Fe powder data displayed as a rate constant of 0.0231 h^{-1} which is greater than the US Metals result by a factor of three. This rate constant is also on the same order as the weighted average, k_{avg} , determined for the U1 pellet.



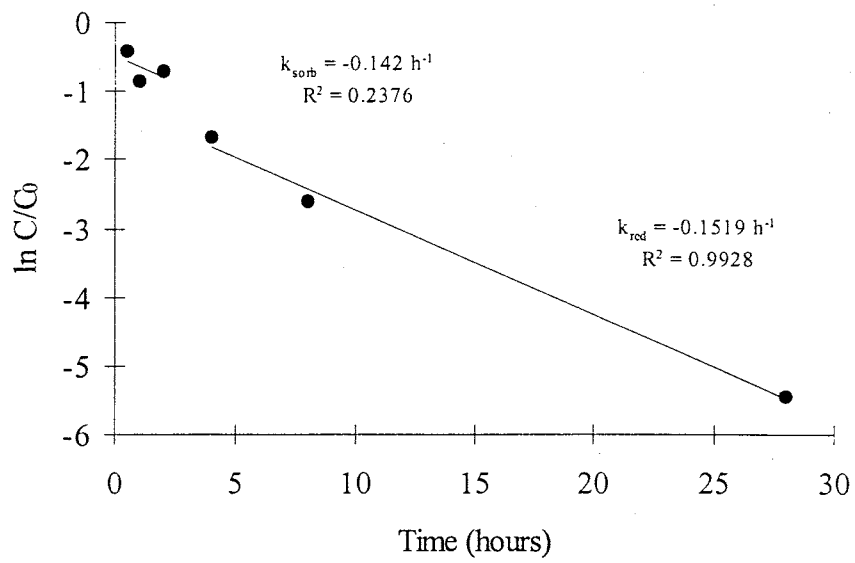
3.5.8 Chromate degradation by Peerless products (logarithmically transformed)

Following is the P1 pellet data in the differentiated time region plots with the dual fits. It appears that in this case that Fit III displayed in figure 3.5.12 shows the best dual fit situation. If this estimate is indeed close to the actual value, it may indicate that sorption is a more important process in this system than in the U1 system. This may be true since the P0 pellets showed a higher sorption capacity for HDTMA than the U0 pellets did. Recall that the U0 isotherm data showed a sorption maximum of around 12 mmol/kg while the sorption maximum for the P0 pellets was more than twice that at around 28 mmol/kg.

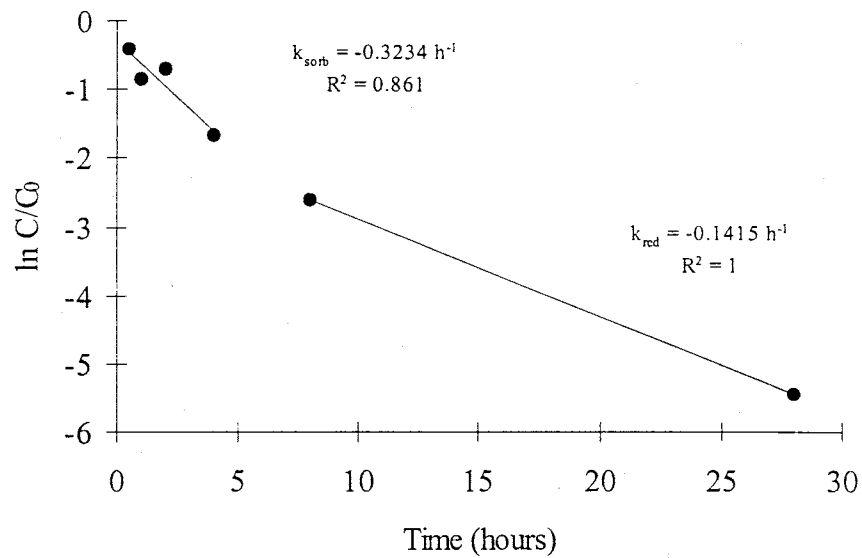
Fit I in figure 3.5.9 is not being considered because of the positive slope for k_{sorb} , which would indicate production rather than reduction. These data set shows a much smaller range in rate constant than those seen in the US Metals product study. The k_{sorb} values for the P1 pellets vary by a factor of 2.2 while the k_{red} values varied by a factor of 1.2. Using figure 3.5.11 as the representative plot for chromate decay by the P1 pellets, the k_{sorb} value is estimated at 0.32 h^{-1} and the k_{red} value is estimated to be 0.14 h^{-1} . In comparison to the U1 pellets, the sorption process decay constant for the P1 pellets is about 2.4 times greater and the reduction process decay constant is about 9.5 times greater.



**3.5.9 Chromate degradation by P1 Pellets – Fit I
(logarithmically transformed)**



3.5.10 Chromate degradation by P1 Pellets – Fit II (logarithmically transformed)



3.5.11 Chromate degradation by P1 Pellets – Fit III (logarithmically transformed)

Computing the time weighted average in the same manner will again give an overall estimate of the decay rate. In this case, 14.3% of the degradation is attributed to sorption while the remaining 85.7% is attributed to chemical reduction. By using this weighted scheme, an estimate of 0.1657 h^{-1} for the entire degradation process is derived. This time weighted average is approximately eight times that estimated for the U1 pellets.

The raw data from this experiment may be found in appendix I of this report.

3.6 Chromate Sorption/Reduction Hydrodynamic Study

The hydrodynamic portion of the study was done in two phases. In the first phase, the reactive transport of chromate through the columns was investigated. The concentration of dissolved chromate in the system was held constant; however, the input flow velocity was changed in each of three situations. Initially, the flow was set at 4 mL/min, then lowered to 2 mL/min, and then finally to 0.6 mL/min. The experiment was performed at three velocities primarily to obtain a statistical evaluation of the dynamic parameter of retardation as well as the decay coefficient. This, in theory, would give accurate estimates of the actual values. The second phase, which employed a conservative tracer, was performed in order to determine the effects of hydrodynamic dispersion in each column as described by equation 1.2.5. In this case, tritium was used as a tracer which theoretically should be conservative in the system. By using an inert species such as tritium, the hydrodynamic dispersion coefficient can be quantified. This value was then used in the CXTFIT 2.0 transport model from which values of the decay coefficients for the system were determined. In the inverse model simulations of ^3H transport, a value of 1 for R was assumed, meaning that the ^3H is uninhibited in its transport.

Effluent chromate concentration versus time analysis of the chromate breakthrough curve was performed for each of the three experiments. Aqueous chromate concentrations were evaluated chromatographically as described in section 2.10.2 of this report.

The raw data for these four investigations can be found in the corresponding sections of appendices J through M of this report.

3.6.1 4 mL/min Study

In figures 3.6.1 through 3.6.3 below are illustrated the individual step input breakthrough curves of chromate for each column. Each of these figures shows good reproducibility in the data sets. Figure 3.6.4 is a comparative figure showing all of the data. The columns containing the B0 pellets should theoretically show no capacity for chromate reduction as is displayed in figure 3.6.3. Along with that, it can be seen that the P0 columns in figure 3.6.2 display the same behavior as the B0 pellet columns. Although the P0 pellets did show some capacity for reduction in the batch studies previously described (sections 2.8 and 3.5), they are apparently ineffective at the high flow velocity here, which does not allow sufficient residence time for reduction to occur. The P1 pellet system, however, in figure 3.6.1 shows an approximate reduction of 5 to 8% of the original concentration at this high flow velocity.

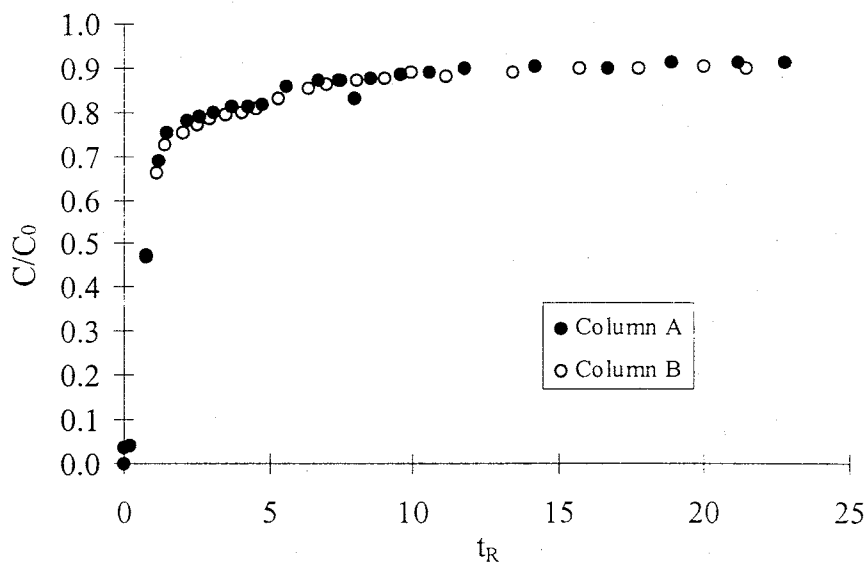


Figure 3.6.1 CrO_4^{2-} step input breakthrough curves for P1 columns at 4 mL/min

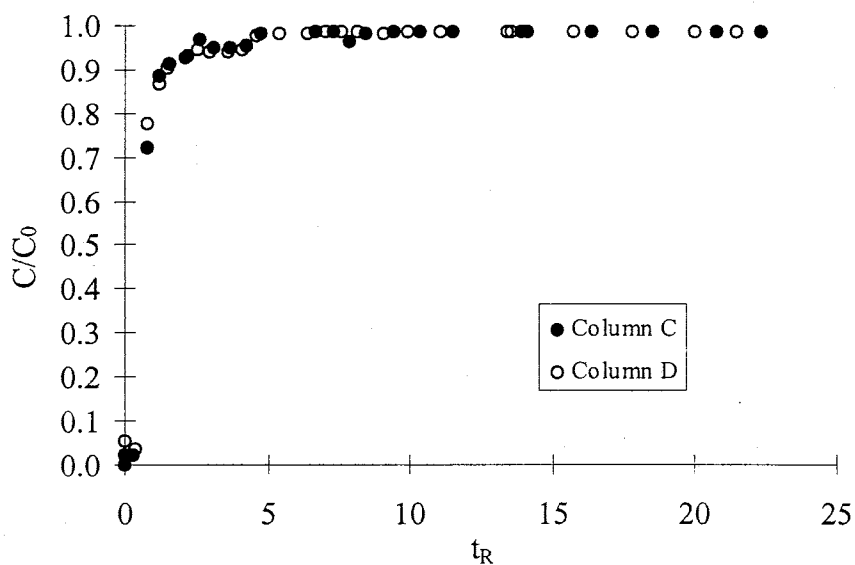


Figure 3.6.2 CrO_4^{2-} step input breakthrough curves for P0 columns at 4 mL/min

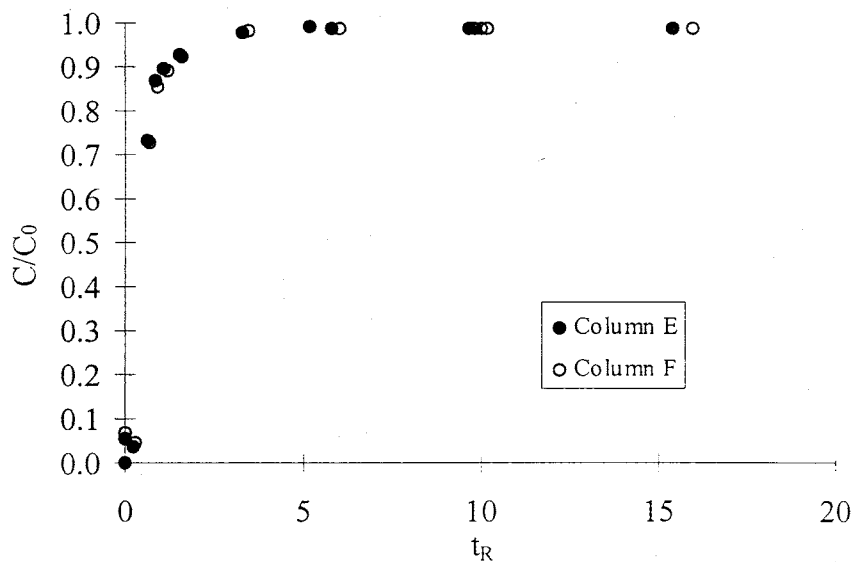


Figure 3.6.3 CrO_4^{2-} step input breakthrough curves for B0 columns at 4 mL/min

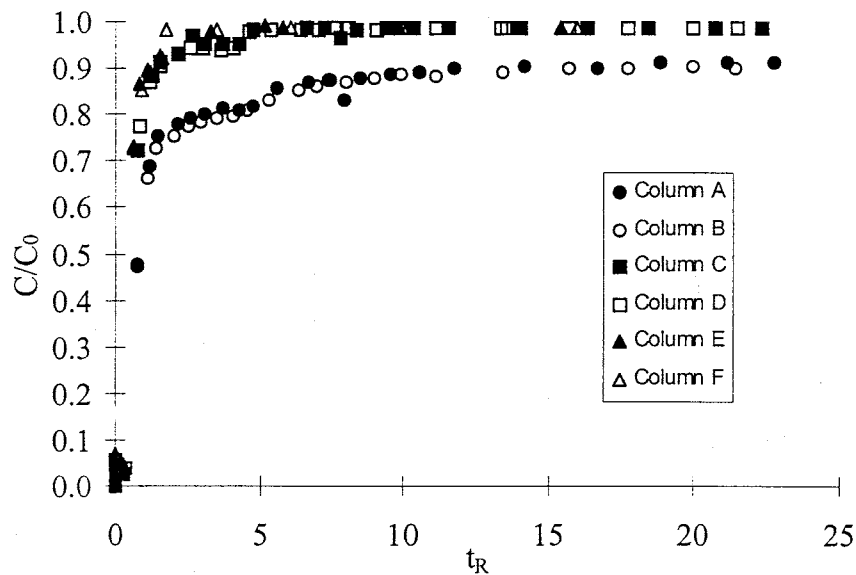


Figure 3.6.4 Comparative CrO_4^{2-} step input breakthrough curves for 4 mL/min study

3.6.2 2 mL/min Study

Figures 3.6.5 through 3.6.8 illustrate the breakthrough curve results of the 2 mL/min study in the same manner. In this situation, the behavior between the P0 pellet columns and the B0 pellet columns are essentially the same showing no significant retardation or reduction which is once again being caused, in the P0 pellet system, by high flow velocity and low residence time. When looking to the P1 pellet system this time, significant differences in the retardation appear and roughly a 2 to 5% difference in the reduced concentration is noted. The chromate is being retarded by about 5 pore volumes when compared to the transport in the B0 pellet system.

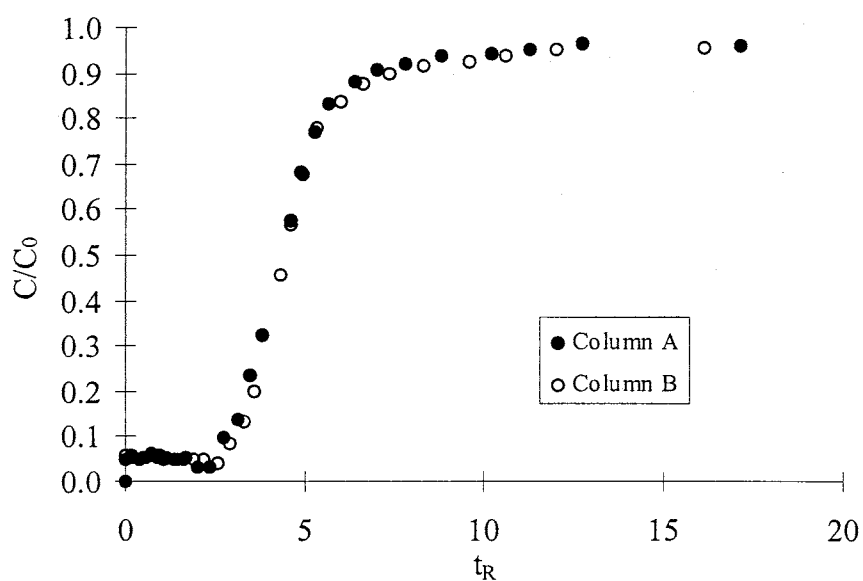


Figure 3.6.5 CrO_4^{2-} step input breakthrough curves for P1 columns at 2 mL/min

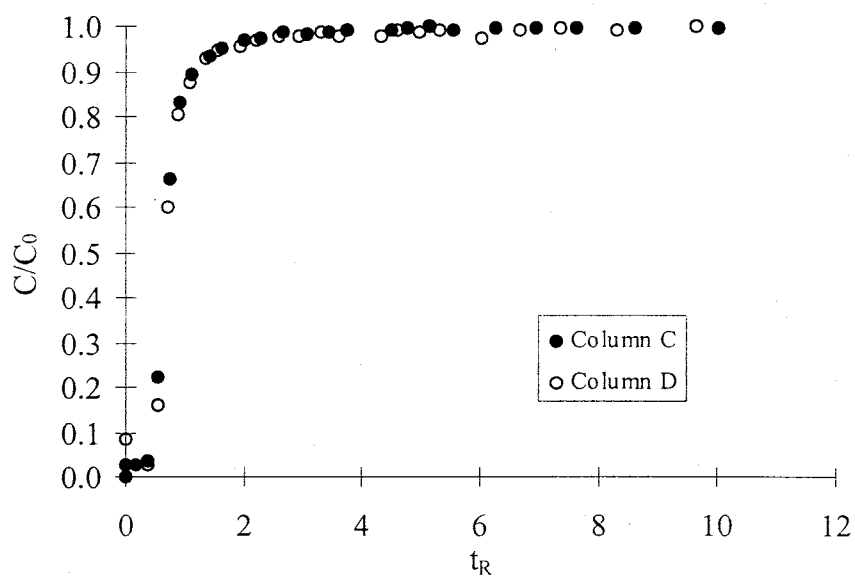


Figure 3.6.6 CrO_4^{2-} step input breakthrough curves for P0 columns at 2 mL/min

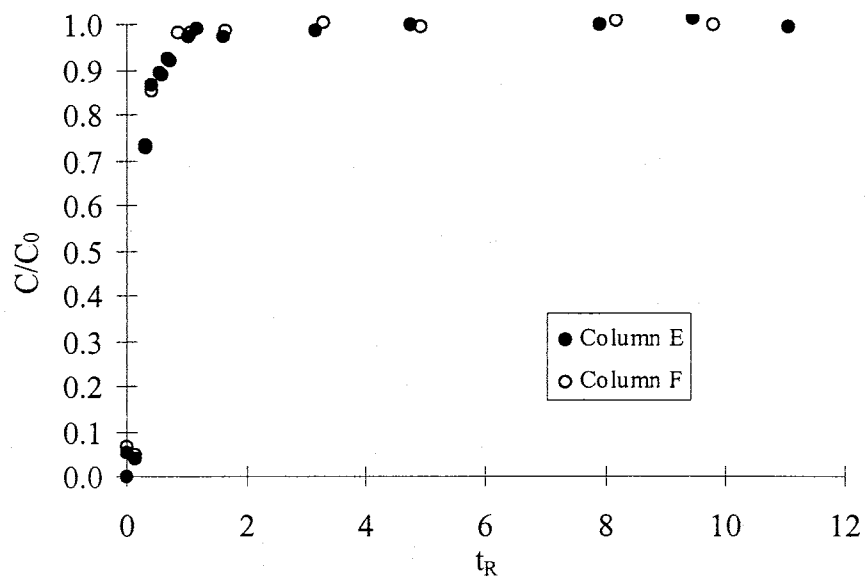


Figure 3.6.7 CrO_4^{2-} step input breakthrough curves for B0 columns at 2 mL/min

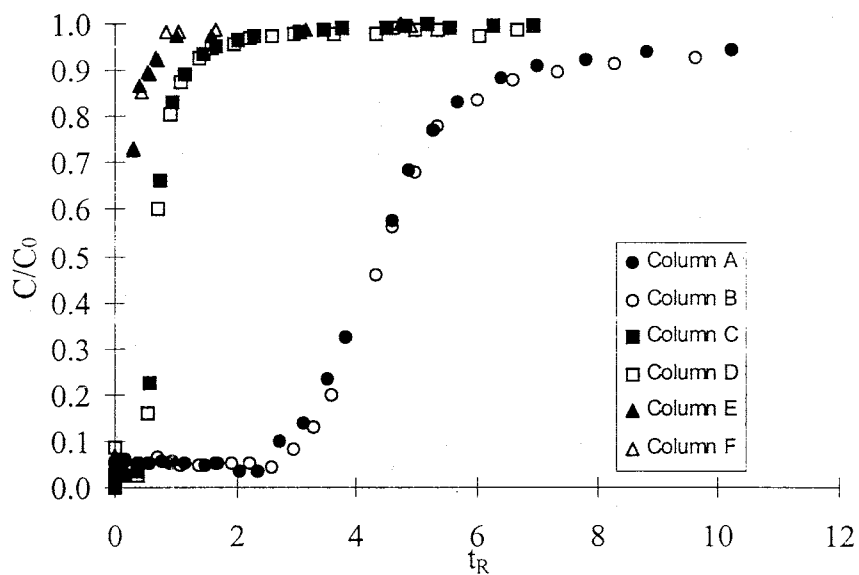


Figure 3.6.8 Comparative CrO_4^{2-} step input breakthrough curves for 2 mL/min study

3.6.3 0.6 mL/min Study

The 0.6 mL/min data is shown here in figures 3.6.9 through 3.6.12. Even larger and more significant differences are seen here in chromate behavior. Retardation is still not a factor in the P0 pellet system (figure 3.6.10) as expected due to the lack of anion exchange capability, but because of the lowered flow rate and subsequent extended residence times, reduction becomes evident in the non-modified system. Reduction in this system is on the order of 10-12% of the original concentration. In the P1 pellet system, chromate transport is retarded by 6 pore volumes and the reduction is close to 25% of the initial concentration.

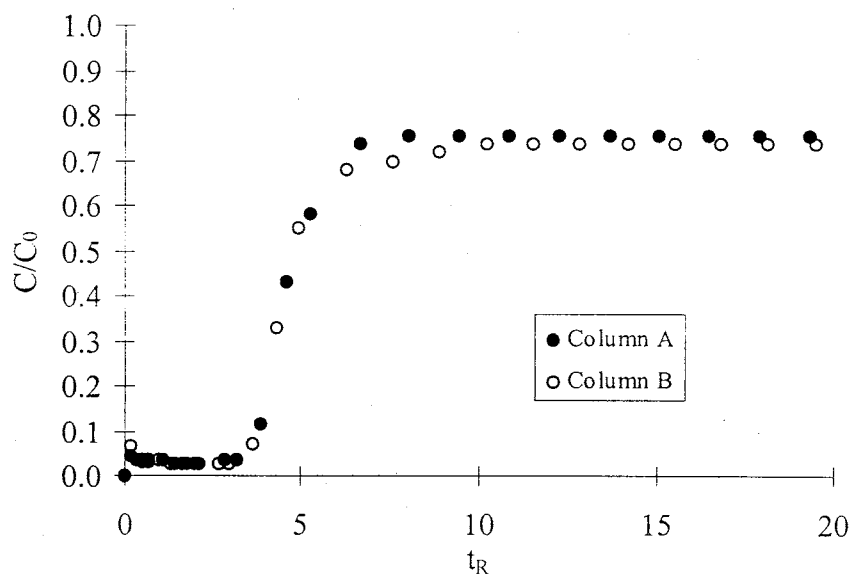


Figure 3.6.9 CrO_4^{2-} step input breakthrough curves for P1 columns at 0.6 mL/min

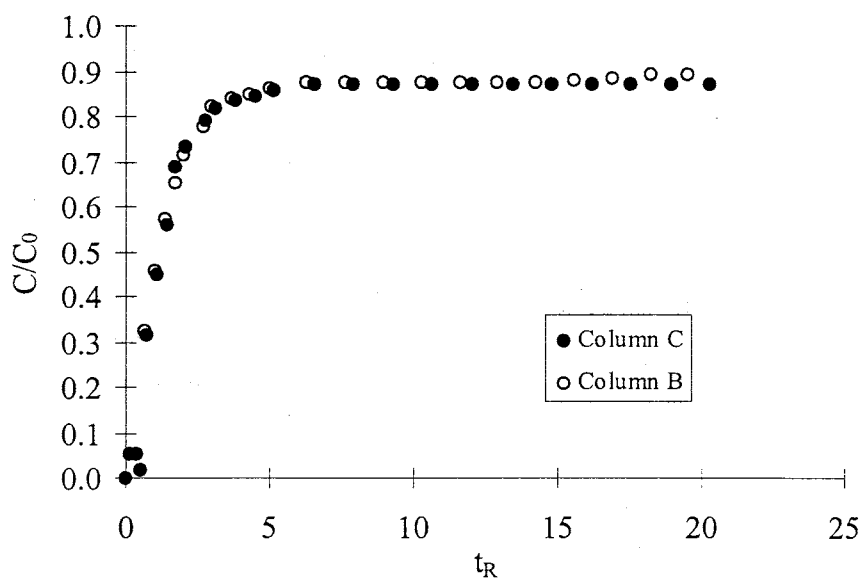


Figure 3.6.10 CrO_4^{2-} step input breakthrough curves for P0 columns at 0.6 mL/min

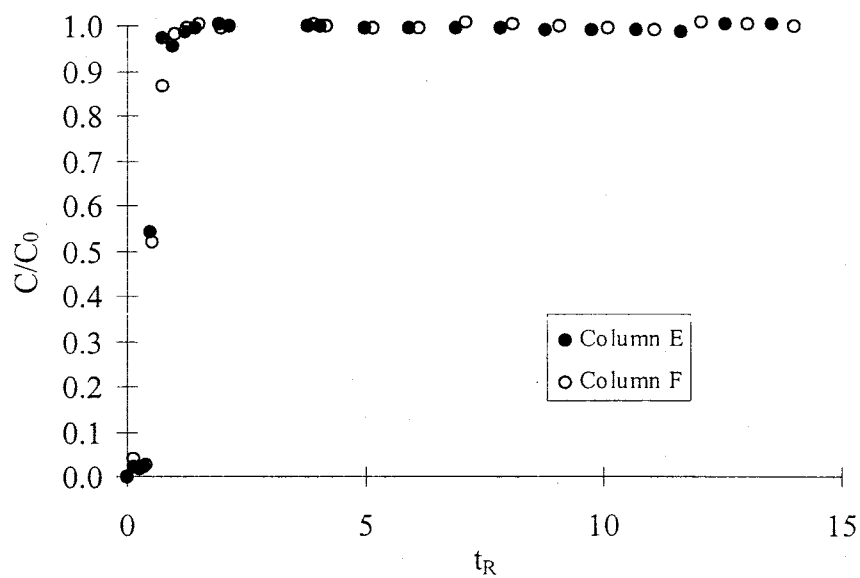


Figure 3.6.11 CrO_4^{2-} step input breakthrough curves for B0 columns at 0.6 mL/min

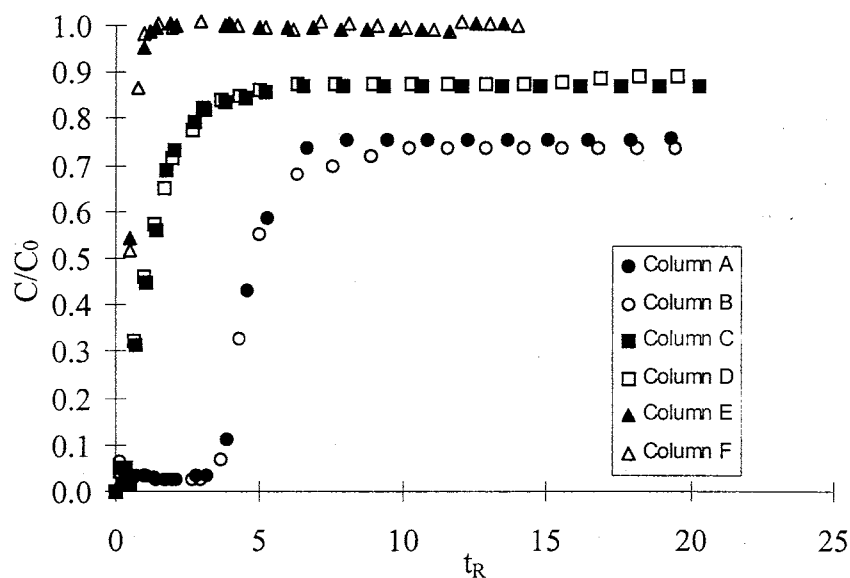


Figure 3.6.12 Comparative CrO_4^{2-} step input breakthrough curves for 0.6 mL/min study

3.6.4 Tracer Study

In order to determine the hydrodynamic properties of the three pellet types (P1, P0, and B0), tritium (^3H) was employed as a conservative tracer in a non-reactive transport study at a volumetric flow rate of 2 mL/min. In this case, a slug input was employed rather than a stepwise input. Figures 3.6.13 through 3.6.15 depict the individual column results and figure 3.6.16 shows the comparative results. Figure 3.6.16 shows good reproducibility between the column duplicates and an overall similar trend in the transport of tritium in the columns.

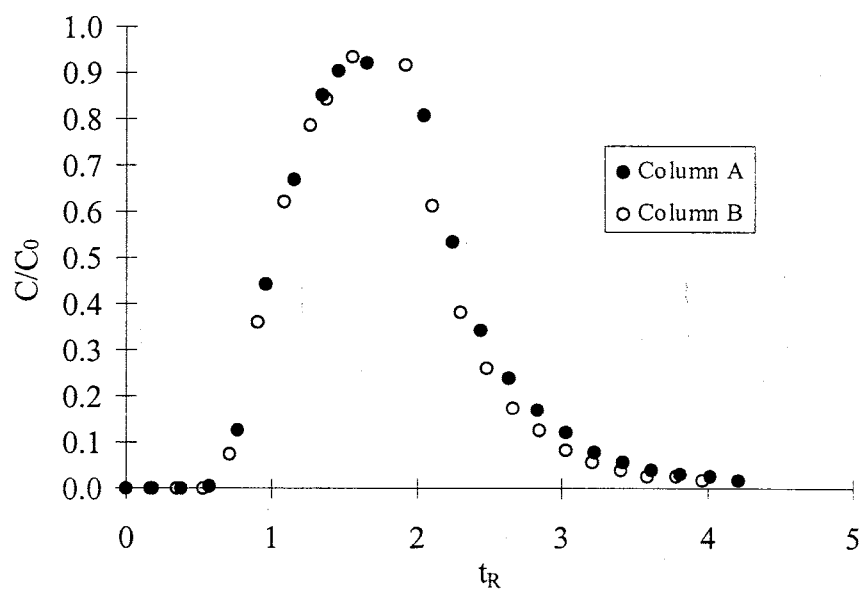


Figure 3.6.13 ^3H slug input breakthrough curves for P1 columns at 2 mL/min

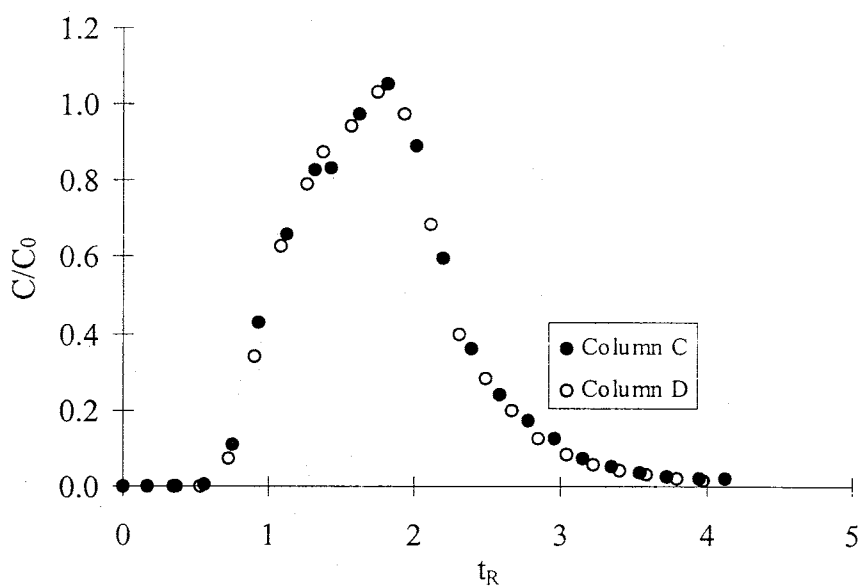


Figure 3.6.14 ^3H slug input breakthrough curves for P0 columns at 2 mL/min

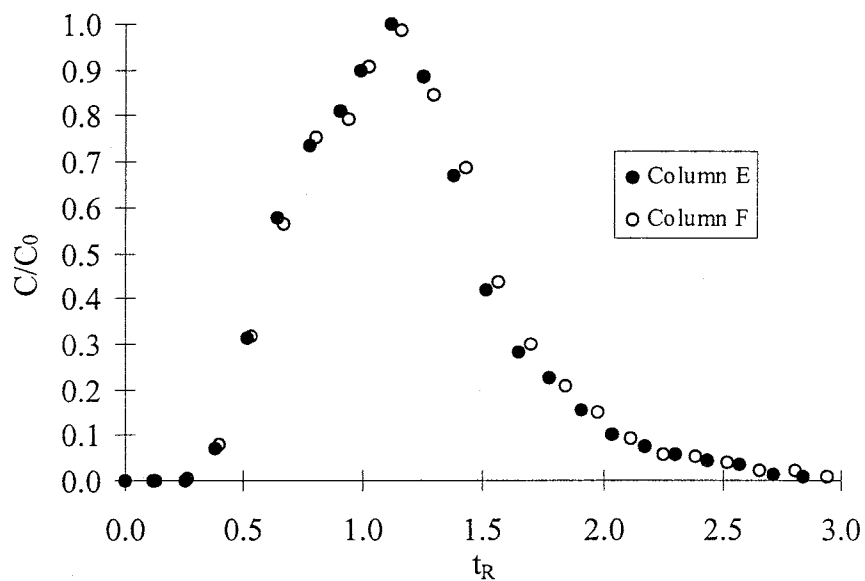


Figure 3.6.15 ^3H slug input breakthrough curves for B0 columns at 2 mL/min

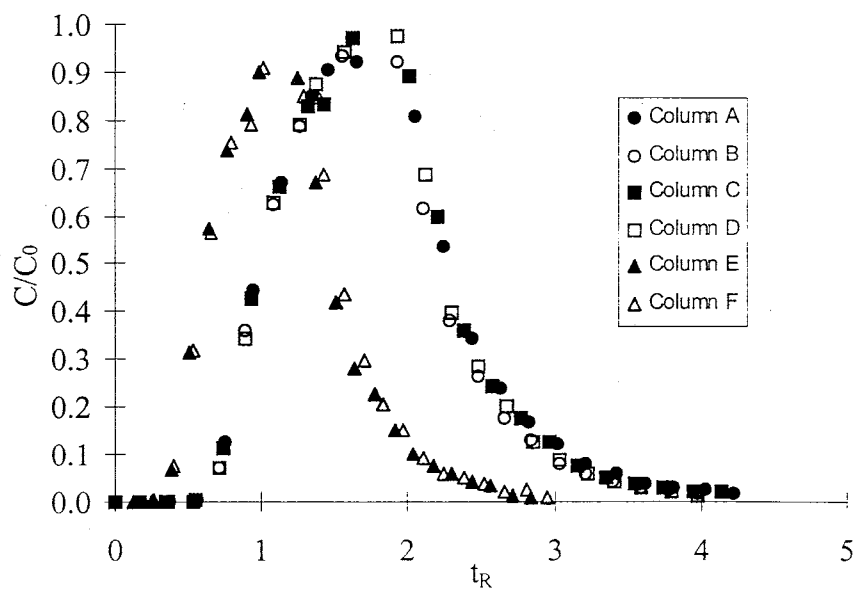


Figure 3.6.16 Comparative ^3H slug input breakthrough curves for tracer study

3.7 Transport/Reduction Modeling

3.7.1 P1 Pellet System

Figures 3.7.1 and 3.7.2 below show the results of the inverse modeling attempts of the P1 pellet system. The results for these two columns are fairly similar showing good representation of the empirical data by the models, except for the 4 mL/min case which only show slight digressions. As described in section 2.11 of this report, the dispersivity for each column was determined by fitting the dispersion coefficient to the tritium data with a retardation factor value of 1. The dispersivity value was then determined using equation 1.2.5, assuming molecular diffusion was negligible. The value was then used in conjunction with the fluid velocity for each column in order to calculate a value for the dispersion coefficient at each of the three experimental velocities. Using the estimated dispersion coefficient and the mean pore water velocity as fixed values, the retardation factor as well as the decay constant in each system could be fitted giving reasonable estimates for those parameters.

Based on the model results in part (a) of each of the figures below, the dispersivity was calculated. For column A the resulting dispersivity was 2.32 cm based on a dispersion coefficient of 85.62 cm²/hr and a similar result of 2.16 cm based on a dispersion coefficient of 73.54 cm²/hr was determined for column B. These constants were used in order to calculate the dispersion coefficients for the remaining three inverse models for the reactive transport portion of the experiment.

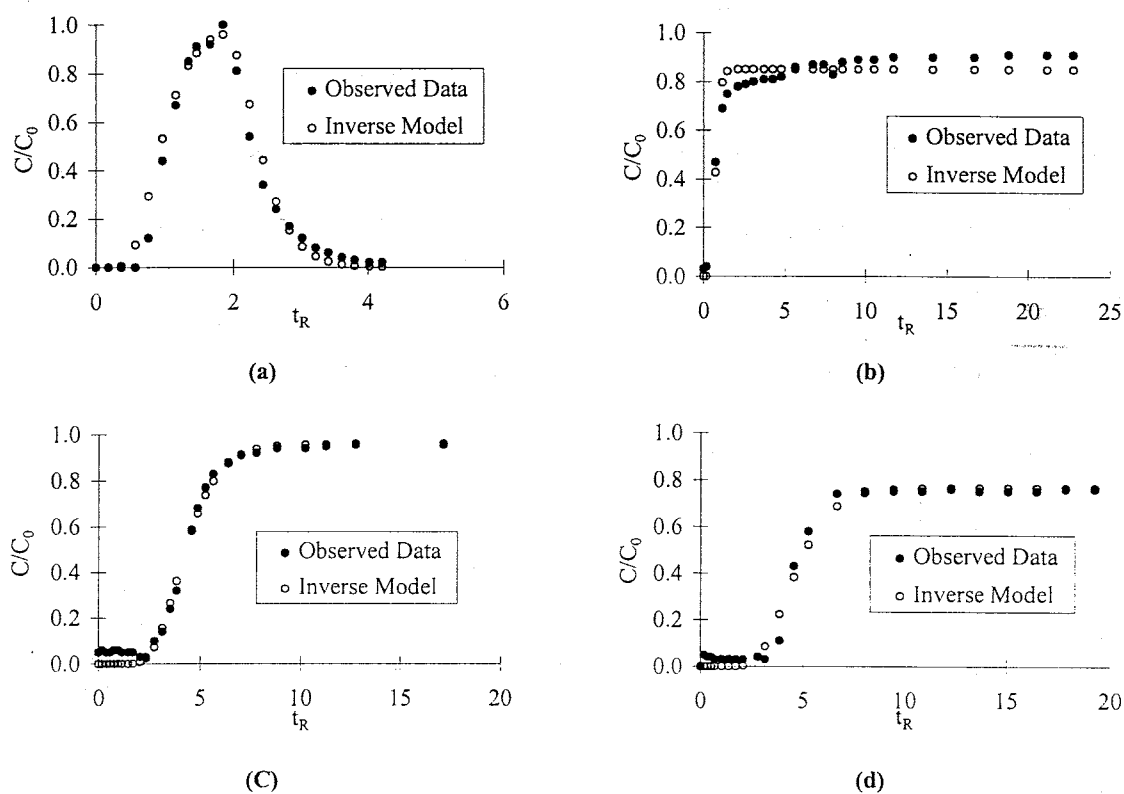


Figure 3.7.1 P1 pellet empirical data and model fits for Column A. (a) Tritium tracer at 2 mL/min, and Cro_4^{2-} at (b) 4 mL/min (c) 2 mL/min (d) 0.6 mL/min

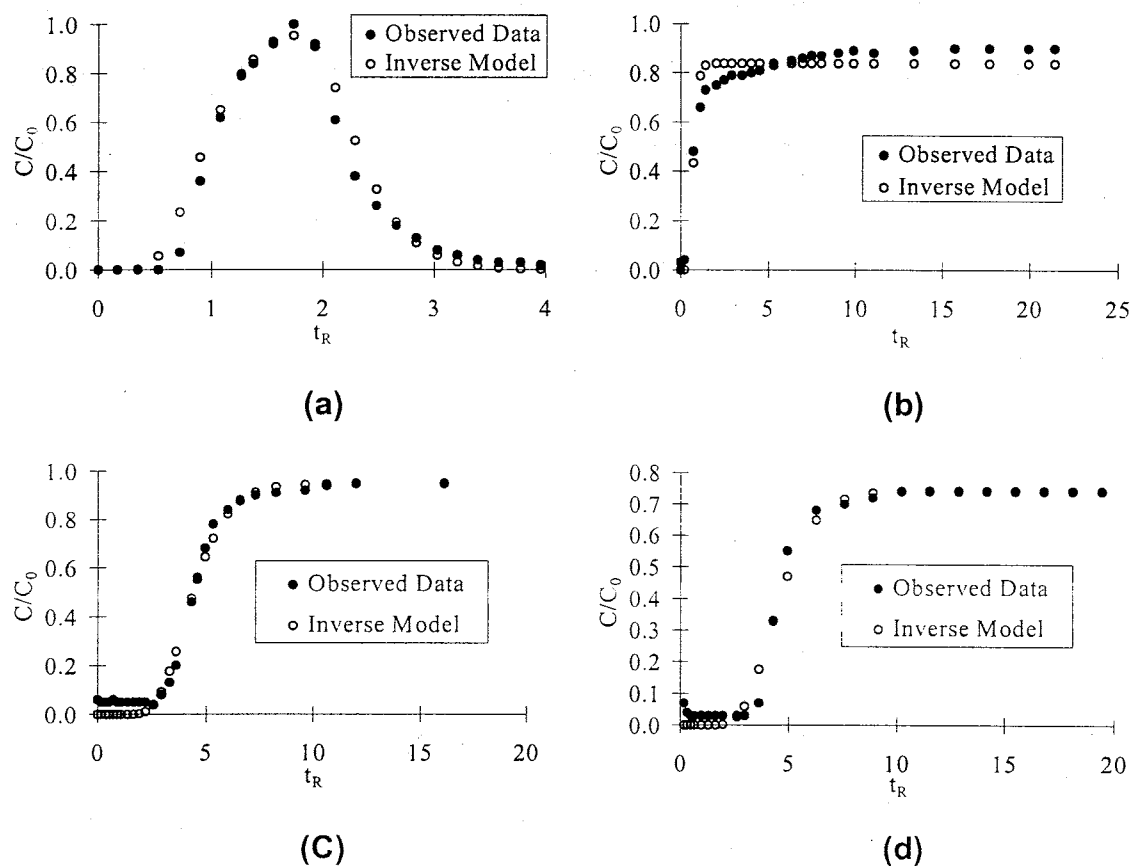


Figure 3.7.2 P1 pellet empirical data and model fits for Column B. (a) Tritium tracer at 2 mL/min, and Cro_4^{2-} at (b) 4 mL/min (c) 2 mL/min (d) 0.6 mL/min

3.7.2 P0 Pellet System

This section represents the same sort of data, as previous, for the P0 (non-surfactant-modified) pellets. Figures 3.7.3 and 3.7.4 again show good simulations of the experimental data by the models. The dispersion values from the tracer study were once again used in order to determine the dispersivity values for each of the two non-modified columns. For column C the resulting dispersivity was 2.00 cm based on a dispersion coefficient of 73.38 cm²/hr and a similar result of 1.63 cm based on a dispersion coefficient of 58.90 cm²/hr was determined for column D.

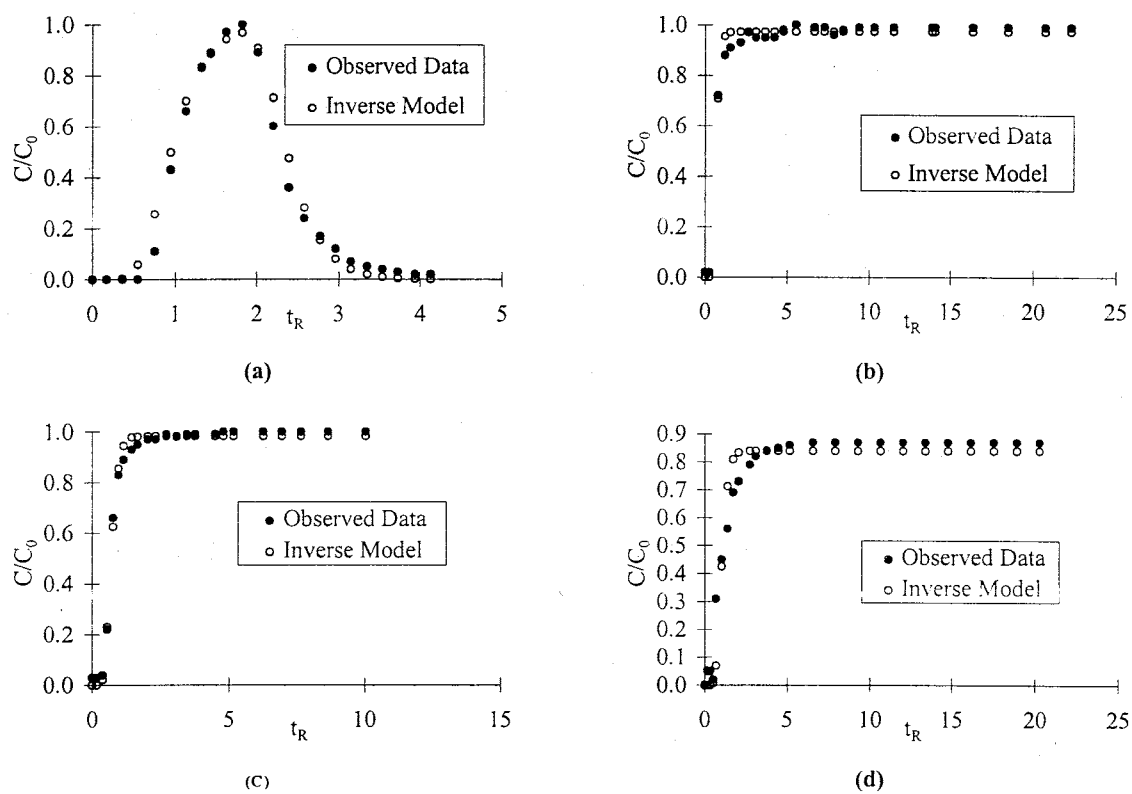


Figure 3.7.3 P0 pellet empirical data and model fits for Column C. (a) Tritium tracer at 2 mL/min, and Cro_4^{2-} at (b) 4 mL/min (c) 2 mL/min (d) 0.6 mL/min

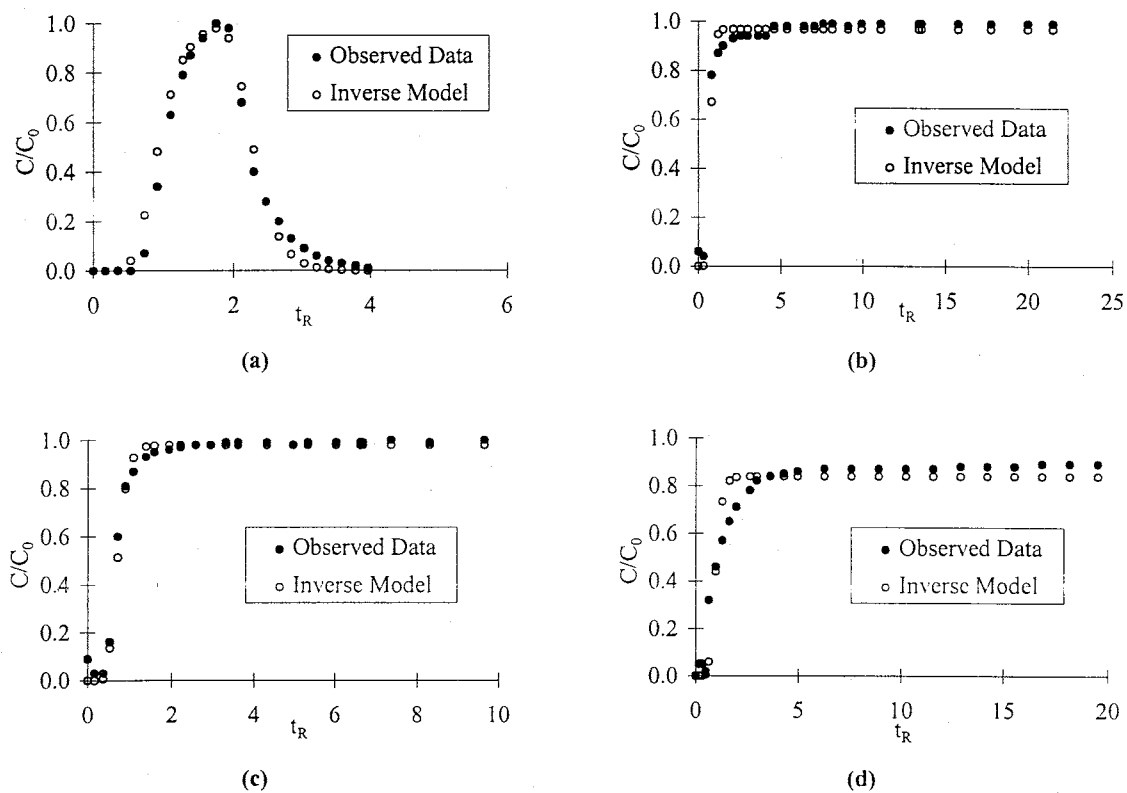


Figure 3.7.4 P0 pellet empirical data and model fits for Column D. (a) Tritium tracer at 2 mL/min, and CrO_4^{2-} at (b) 4 mL/min (c) 2 mL/min (d) 0.6 mL/min

3.7.3 B0 Pellet System

This section represents the blank pellet results. Figures 3.7.5 and 3.7.6 again show good simulation of the experimental data by the models in both cases. The dispersion values from the tracer study were once again used in order to determine the dispersivity values for each of the two non-modified columns. For column E the resulting dispersivity was 4.16 cm based on a dispersion coefficient of $108.80 \text{ cm}^2/\text{hr}$ and a similar result of 4.00 cm based on a dispersion coefficient of $108.40 \text{ cm}^2/\text{hr}$ was determined for column F. Since there are no reducing agents in these two systems, there is no calculation for the decay coefficient ($\mu=0$).

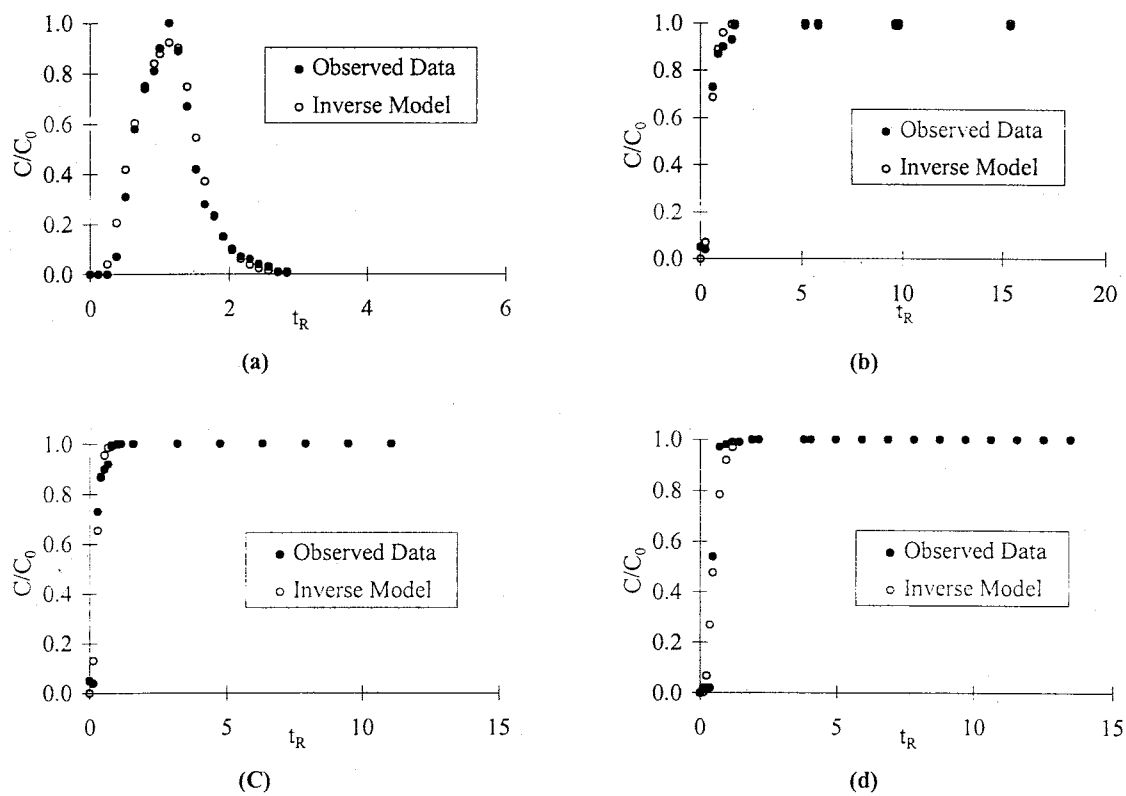


Figure 3.7.5 B0 pellet empirical data and model fits for Column E. (a) Tritium tracer at 2 mL/min, and CrO_4^{2-} at (b) 4 mL/min (c) 2 mL/min (d) 0.6 mL/min

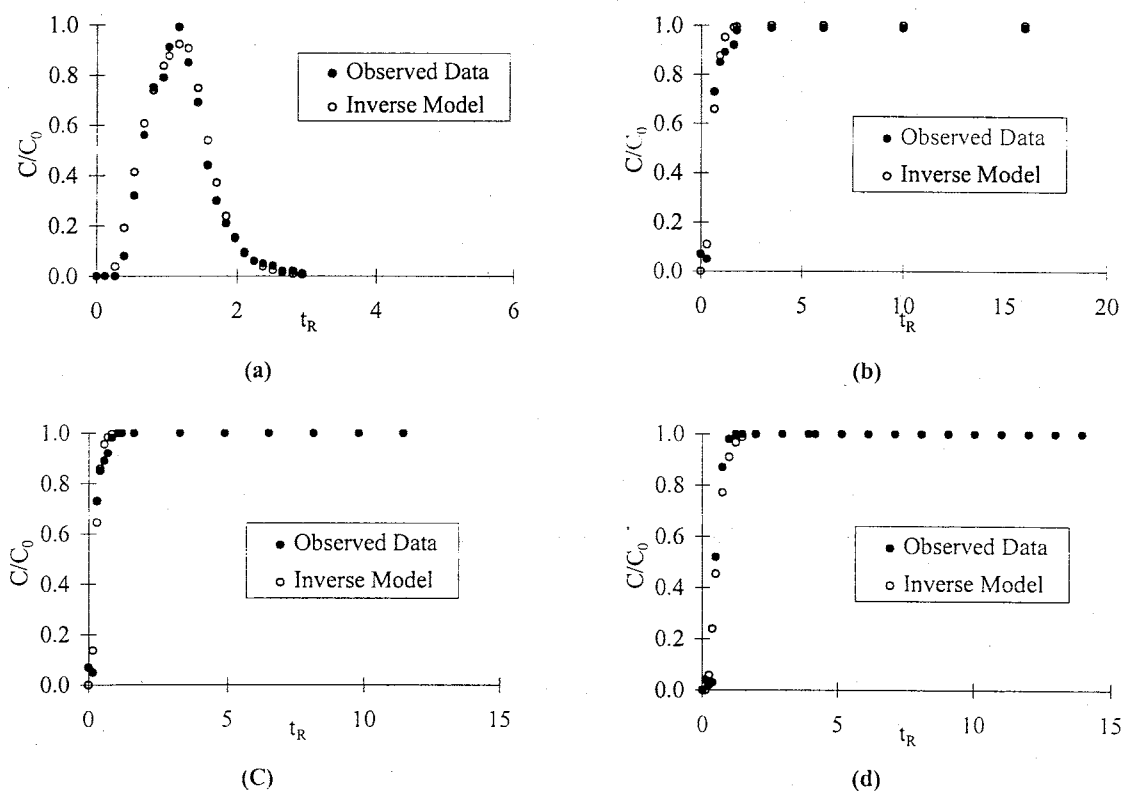


Figure 3.7.6 B0 pellet empirical data and model fits for Column F. (a) Tritium tracer at 2 mL/min, and Cro_4^{2-} at (b) 4 mL/min (c) 2 mL/min (d) 0.6 mL/min

3.7.4 Model Input/Output Results Summary

Table 3.7.1 below summarizes the results of the tritium slug test with the calculated pore water velocities and the resultant dispersivity values (using equation 1.2.5). Following, in table 3.7.2, are the subsequently determined values for the pore water velocities and dispersion coefficients that were used as fixed parameters in order to fit the retardation factors and decay constants in the inverse models.

Table 3.7.1 Resultant values from tritium slug test

Column	n	Slug Volume (PV)	D_t (cm ² /h)	V_t (cm/h)	α (cm)
A	0.17	1.46	85.62	36.88	2.32
B	0.18	1.38	73.54	34.01	2.16
C	0.17	1.43	73.38	36.66	2.00
D	0.17	1.38	58.9	36.23	1.63
E	0.23	0.99	108.8	26.16	4.16
F	0.23	1.02	108.4	27.09	4.00

Table 3.7.2 Modeled pore water velocity and dispersion coefficient values

Column	V_4 (cm/h)	D_4 (cm ² /h)	V_2 (cm/h)	D_2 (cm ² /h)	$V_{0.6}$ (cm/h)	$D_{0.6}$ (cm ² /h)
A	73.76	171.24	36.88	85.62	11.06	25.69
B	68.03	147.10	34.01	73.55	10.20	22.06
C	73.32	146.76	36.66	73.38	11.00	22.01
D	72.46	117.80	36.23	58.90	10.87	17.67
E	52.33	217.60	26.16	108.80	7.85	32.64
F	54.18	216.80	27.09	108.40	8.13	32.52

Tables 3.7.3 and 3.7.4 below were generated using the output results from the inverse CXTFIT 2.0 models. Table 3.7.3 summarizes the retardation factor results for each of the three column experiments. The third column of this table also lists the retardation factor values used in the tritium slug models that were used in order to fit the

dispersion coefficients for the study. Note that columns A, B, C, and D all have retardation values of 1.000 which is representative of a conservative tracer. This was the constant value for each column (it was not fitted). However, columns E and F have fitted values of 0.633 and 0.660 respectively. When the tritium data for these two columns was modeled with CXTFIT 2.0, the slug width was greatly increased and the breakthrough curve only reached about 70% of the initial concentration. The only way this problem was resolved was by allowing the retardation factor value to be fitted. This pseudo-early breakthrough is probably a result of the fact that this model mode cannot handle some of the hydrodynamic phenomena that are occurring in these two systems. With a larger pore space and difference in hydrophobicity in these columns, there is the possibility of a significant amount of immobile water in the system.

Table 3.7.3 Fitted values for retardation factors

Column	Pellet	Retardation Factor, R (%)			
	Type	2 mL/min ^3H	4 mL/min	2 mL/min	0.6 mL/min
A	P1	1.000	1.205	6.785	7.510
B	P1	1.000	1.149	6.780	7.209
C	P0	1.000	1.020	1.030	1.578
D	P0	1.000	1.000	1.000	1.390
E	B0	0.633	0.540	0.268	0.543
F	B0	0.660	0.598	0.281	0.580

It can be seen clearly from this data as well that even though there is surfactant present in the P1 pellets, velocity is still a large factor in the amount of retardation that occurs. The faster velocity experiment with 4 mL/min shows very little retardation in comparison to the slower 0.6 mL/min experiment which is about 7 to 8 times that of the faster experiment. Retardation in the P0 is very low to negligible as would be expected

since there is no surfactant present. Once again we see the faster breakthrough anomalies with the B0 pellets with retardation factor values below 1.

Table 3.7.4 summarizes the results of the decay constants from the three column studies. The constant that is shown here in table 3.7.4 is the lumped decay constant that is shown in equation 1.2.23 and further defined in equation 1.2.24. This decay constant is a function of the decay occurring in liquid phase as well as the sorbed phase. The third column once again shows the values that were used in the tritium study. Since tritium is inert in this system and there is no decay within this short time frame, all decay constant values were set to 0.

Table 3.7.4 Fitted values for decay constants

Column	Pellet Type	Decay Constant, k (1/hr)			
		2 mL/min ^3H	4 mL/min	2 mL/min	0.6 mL/min
A	P1	0.000	4.863	4.681	5.032
B	P1	0.000	4.812	4.628	4.998
C	P0	0.000	4.507	4.492	4.723
D	P0	0.000	4.339	4.323	4.535
E	B0	0.000	0.000	0.000	0.000
F	B0	0.000	0.000	0.000	0.000

The primary reason that there were three different reactive transport studies done at three different flow rates was to get a small distribution on results so that a better interpretation of the results might be possible. In this manner, a statistical average of the decay constant for each column may be used instead of relying on a single value as an empirical result. Of course, three duplicate data sets does not supply a very large statistical population and a larger series of studies would have better defined these hydrodynamic parameters; however, this was not possible logistically. However, the

results found showed good reproducibility giving a higher level of confidence in the data. In table 3.7.5, the arithmetic mean of the decay constant for each column are tabulated giving an overall or final value, the material mean. As can be seen, the modified material is about 1.11 times faster under the same conditions.

Table 3.7.5 Mean decay constant results for reactive transport study

Pellet Type	Decay Constant, k (1/hr)			
	4 mL/min	2 mL/min	0.6 mL/min	Material Mean
P1	4.838	4.655	5.015	4.836
P0	4.423	4.4075	4.629	4.487

IV.
Concluding Remarks

4.1 Conclusions

This work was aimed at characterizing the degradation ability of a pelletized zero valent iron/surfactant-modified zeolite material at the laboratory level. It is thought by combining the effects of sorption and chemical degradation, a more time effective and cost efficient material might be derived for use as a permeable barrier material for in-situ groundwater remediation. Within the framework of the mechanical stability study, HDTMA loading study, iron and pellet characterization studies for PCE and chromate degradation, and the series of solute transport studies, the following conclusions were derived.

- Pellet types that contained sodium or ammonium as the primary cation were stable to some degree up to a rate of 75 rpm and then began to show significant breakdown after one hour at a rate of 150 rpm, whereas the calcium pellets remained intact (estimated < 2% loss by mass).
- Pellet types that were foamed were found to be 100% unstable regardless of their cation types, making them the least favorable pellet. These pellet types were completely broken down by the surfactant solution at even the slowest shaking rate of 75 rpm, although they were slightly more stable in pure water than in the surfactant solution.
- Both the US Metals and Peerless pellets had finite loading capacities for HDTMA which were well described by the Langmuir sorption isotherm model. The US Metals (UO) pellets displayed a maximum loading capacity of 11.8 mmol/kg and a Langmuir

constant of 1.736 L/mmol. The Peerless (P0) pellets showed a maximum sorption capacity of 27.9 mmol/kg and a Langmuir constant of 0.440 L/mmol.

- The saturated hydraulic conductivity of the material when tested with a constant head apparatus varied from column to column slightly but remained in the 1 to 4 cm/min range. The iron-bearing pellets showed a water loss of 2% (by total mass) while the blank zeolite pellet contained almost 5% water by mass. This water-mass loss was noted at a temperature of 105°C.
- In testing US Metals, Fisher, and Peerless irons for the degradation properties for PCE, the following were noted:
 - Fisher iron evolved gas (probably CO₂) in the presence of PCE making it unsuitable for further study. Gas evolution could significantly upset the equilibrium of an aqueous system.
 - Peerless iron gave slightly better results than the US Metals within a 32 hour time frame, meaning it has a greater decay constant. This constant could not be quantified defensibly because it contained three process regions (nonreactive iron site sorption, organic partitioning, and reduction) and a good deal of scatter with low resolution.
 - TCE was produced in the system, as a product of reductive dechlorination, and then subsequently eliminated.
- In testing US Metals and Peerless pellet products in batch kinetic studies for the ability to remove and degrade chromate, the following were noted:
 - The Fe powder and the non-surfactant-modified pellets each displayed a single process (reduction) which yielded decay constants of 0.0002 h⁻¹ for the UO

pellets and 0.0069 h^{-1} for the US Metals iron powder and 0.0008 h^{-1} for the P0 pellets and 0.0231 h^{-1} for the Peerless iron powder.

- The surfactant modified pellets displayed a dual process region (anion exchange and reduction) for both iron types with a weighted average decay constant of 0.0208 h^{-1} for the U1 pellets based on a k_{sorb} of 0.1336 h^{-1} and a k_{red} of 0.0147 h^{-1} . The P1 pellets showed a weighted average decay constant of 0.0416 h^{-1} based on a k_{sorb} of 0.2861 h^{-1} and a k_{red} of 0.01 h^{-1} .
- Dispersivities in the six column system ranged between 1.6 and 4.2 cm.
- In the reactive transport study, each column type and its respective duplicate emulated each other well and were therefore good scientific duplicates.
- The material mean decay constant for the P1 pellets was estimated at 4.998 h^{-1} and 4.487 h^{-1} for the P0 pellets.

4.2 Suggestions for Future Work

Based on my experiences in this work, shortcomings and successes, I recommend the following as some possible points to be covered and/or further addressed if this work is continued.

- Further study should be done to better define the exact mechanism by which perchloroethylene is reduced by metallic iron. By further understanding this process, tighter controls on experimental procedures could yield more desirable results in the economic use of this material for groundwater remediation.
- Other clay minerals in combination with iron should be investigated to find a possibly more effective pellet/material for contaminant degradation.
- Reproducibility in pellet production was a significant problem in this research. Minor changes in physical properties caused significant differences in chemical behavior. This is a primary issue that needs to be addressed before any further work be done in this field or large undertakings with this material are performed. Time should be spent on the quality development of this material if it is to be effectively used in research and/or industry.
- It may also be reasonable to not only vary the material used in the pelletization process, but also to try an assortment of surfactants. A different surfactant type may better function in the formation of a bilayer which is necessary for anion exchange. A different surfactant type may display a more favorable interaction in the presence of metallic iron.

- Much of the scatter in the PCE data is most likely due to experimental error in the handling of the sample from the time it is sacrificed to the time of injection. Further thought needs to be given to this work in order to eliminate much of the error. An extraction method was initially tried in the early stages of this work but the extraction matrix interfered with the detection of PCE and dechlorination products. It may be worth investigating an extraction method for the HPLC method or even switch to a completely or more closed analysis system (i.e. purge and trap).
- Additional statistical modeling may have been a good route to follow in this research, but would have required much more data. A larger series of volumetric flow rates might have been used by which more distributions would have been generated. This could have been subjected to a series of calibrated Monte-Carlo simulations that would then give a more rigorously statistical approach to the estimation of the decay constants.
- Although the data generated in the blank B0 pellet columns was not quantitatively used in any calculations, it would be better in the future to find the appropriate model that simulates this apparent early breakthrough data well.
- A better modeling approach should be found as well that has a better conceptual approach as to why the retardation factor is such a strong apparent function of flow rate, which is not completely sensible in this model. The model being used in this work assumes complete chemical equilibrium. This study shows that the process of chromate sorption is not instantaneous. The high flow rate data presented in this work should be simulated with a model that includes the sorption kinetics that are taking place in the system.

V. References

References

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VI.

Appendices of Data

Appendix A
Cercona Pellet Mechanical Stability

Description	Pellet Size	150 rpm Test	100 rpm Test	75 rpm Test
foamed/calcium form	-3 +8 mesh	U	U	NT
foamed/calcium form	-12 +20 mesh	U	U	NT
nonfoamed, porous/NH ₃ form/baked at 220°C	-3 +8 mesh	U	U	NT
nonfoamed, porous/NH ₃ form/baked at 220°C	-12 +20 mesh	U	U	NT
foamed/sodium form	-3 +8 mesh	U	U	U
foamed/sodium form	-8 +12 mesh	U	U	U
nonfoamed/sodium form	-12 +20 mesh	U	U	S
nonfoamed/sodium form	-3 +8 mesh	U	U	S
foamed/calcium form	-3 +8 mesh	S	S	U
nonfoamed/calcium form	-12 +20 mesh	S	S	S
nonfoamed/calcium form	-3 +8 mesh	S	S	S
higher density, nonfoamed/bimetallic iron media	-3 +8 mesh	S	S	S
higher density, nonfoamed/iron media	-3 +8 mesh	S	S	S
Type Z _{Na-1:10}	-3 +8 mesh	U	S	S
Type Z _{Na-1:2}	-3 +8 mesh	U	S	S
Type ZP _{NUSMC-1:2} /10 vol% iron	-3 +8 mesh	U	S	S
Type Z _{USMC-1:2} /50 vol% iron	-3 +8 mesh	U	S	S

*U = unstable**S = stable**NT = not tested in these conditions*

Appendix B
HDTMA Sorption Isotherm for UO Pellets

Batch A

Sample Mass (g)	Initial Concentration (mM)	Peak Height	Dilute Equilibrium Conc (mM)	C (mM)	S (mM/kg)
2.042	1.00	0.0	0.0	0.0	4.9
2.025	2.03	20403.0	0.2	0.2	8.9
2.026	4.14	196199.9	2.3	2.3	9.2
2.020	8.00	510350.1	5.9	5.9	10.4
2.038	12.15	852027.3	9.8	9.8	11.3
2.034	16.21	1205338.0	13.9	13.9	11.3
2.031	21.15	1663140.0	19.2	19.2	11.0
2.033	24.36	1919542.0	22.2	22.2	10.8
2.029	28.29	2402451.0	27.7	27.7	2.7

Batch B

Sample Mass (g)	Initial Concentration (mM)	Peak Height	Dilute Equilibrium Conc (mM)	C (mM)	S (mM/kg)
2.023	1.00	37178.2	0.4	0.4	2.8
2.045	2.03	52853.9	0.6	0.6	6.9
2.046	4.14	212179.4	2.5	2.5	8.3
2.049	8.00	513600.8	5.9	5.9	10.1
2.027	12.15	867367.5	10.0	10.0	10.5
2.043	16.21	1182063.0	13.7	13.7	12.5
2.039	21.15	1662822.0	19.2	19.2	11.5
2.031	24.36	1903626.0	22.0	22.0	11.7
2.037	28.29	2241329.0	25.9	25.9	11.8

Mean Values		Langmuir Lineraized		Freudlich Lineraized	
C (mM)	S (mM/kg)	C (mM)	C/S	log C	log S
0.2	3.9	0.2	0.055634682	-0.67	0.59
0.4	7.9	0.4	0.05353874	-0.37	0.90
2.4	8.8	2.4	0.269395972	0.37	0.94
5.9	10.3	5.9	0.576326538	0.77	1.01
9.9	10.9	9.9	0.908635631	1.00	1.04
13.8	11.9	13.8	1.159659404	1.14	1.08
19.2	11.3	19.2	1.707210558	1.28	1.05
22.1	11.2	22.1	1.965212202	1.34	1.05
26.8	11.8	26.8	2.272542201	1.43	1.07

Appendix C

HDTMA Sorption Isotherm for PO Pellets

Batch A				
Sample Mass (g)	Initial Conc (mM)	Peak Height	C (mM)	S (mM/kg)
1.524	1.00	367379.0	6.1	-66.8
1.527	2.03	42885.0	0.7	17.3
1.523	4.14	156586.5	2.6	20.3
1.528	8.00	357203.7	5.9	27.2
1.531	12.15	608725.7	10.1	27.0
1.519	16.21	812780.6	13.5	36.1
1.521	21.15	1120068.0	18.6	34.1
1.507	24.36	1347073.0	22.3	27.1
1.515	28.29	1507644	25.0	43.7

Batch B				
Sample Mass (g)	Initial Conc (mM)	Peak Height	C (mM)	S (mM/kg)
1.519	1.00	42874.4	0.7	3.8
1.519	2.03	66565.7	1.1	12.2
1.497	4.14	185848.0	3.1	14.2
1.530	8.00	417709.8	6.9	14.1
1.151	12.15	666263.9	11.0	19.3
1.540	16.21	864039.5	14.3	24.6
1.514	21.15	1213965.0	20.1	13.7
1.516	24.36	1350817.0	22.4	26.1
1.525	28.29	1593531	26.4	24.7

Mean Values		Langmuir Lineraized		Freudlich Lineraized	
C (mM)	S (mM/kg)	C (mM)	C/S	log C	log S
0.7	3.8	0.7	0.184	-0.15	0.58
0.9	14.7	0.9	0.061	-0.04	1.17
2.8	17.2	2.8	0.165	0.45	1.24
6.4	20.7	6.4	0.311	0.81	1.32
10.6	23.1	10.6	0.457	1.02	1.36
13.9	24.6	13.9	0.565	1.14	1.39
19.3	23.9	19.3	0.810	1.29	1.38
22.4	26.6	22.4	0.841	1.35	1.42
25.7	25.0	25.7	1.028	1.41	1.40

Appendix D

Gravimetric Water Content Analysis

Pellet Type	Sample	Wet Mass (g)	Dry Mass (g)	Water Mass (g)	GWC (% water by mass)
U1	a	7.060	6.963	0.097	1.374
U1	b	6.940	6.849	0.091	1.311
U0	a	10.443	10.314	0.129	1.235
U0	b	9.397	9.283	0.114	1.213
P1	a	6.506	6.384	0.122	1.875
P1	b	6.793	6.663	0.130	1.914
P0	a	7.726	7.596	0.130	1.683
P0	b	10.738	10.555	0.183	1.704
B0	a	4.582	4.372	0.210	4.583
B0	b	6.123	5.847	0.276	4.508

Pellet Type	Average GWC (% water by mass)
U1	1.343
U0	1.224
P1	1.894
P0	1.693
B0	4.545

Appendix E
Saturated Hydraulic Conductivity Study

Column A - P1

Test	V (mL)	t (min)	A (cm ²)	L (cm)	h (cm)	K _s (cm/min)
1	100	1.83	19.6	31.5	34.75	2.527
2	100	1.86	19.6	31.5	34.75	2.486
3	100	1.80	19.6	31.5	34.75	2.569
Average K _s =						2.528

Column B - P1

Test	V (mL)	t (min)	A (cm ²)	L (cm)	h (cm)	K _s (cm/min)
1	100	3.68	19.6	31.5	35.0	1.248
2	100	3.70	19.6	31.5	35.0	1.241
3	100	3.78	19.6	31.5	35.0	1.215
Average K _s =						1.235

Column C - P0

Test	V (mL)	t (min)	A (cm ²)	L (cm)	h (cm)	K _s (cm/min)
1	100	1.87	19.6	32.0	35.25	2.477
2	100	1.87	19.6	32.0	35.25	2.477
3	110	2.07	19.6	32.0	35.25	2.461
Average K _s =						2.472

Column D - P0

Test	V (mL)	t (min)	A (cm ²)	L (cm)	h (cm)	K _s (cm/min)
1	100	2.83	19.6	32.8	35.75	1.654
2	100	2.90	19.6	32.8	35.75	1.614
3	100	2.95	19.6	32.8	35.75	1.587
Average K _s =						1.618

Column E - B0

Test	V (mL)	t (min)	A (cm²)	L (cm)	h (cm)	K_s (cm/min)
1	100	2.17	19.6	33.2	36.25	2.153
2	100	2.37	19.6	33.2	36.25	1.972
3	100	2.18	19.6	33.2	36.25	2.143

Average K_s = 2.089**Column F - B0**

Test	V (mL)	t (min)	A (cm²)	L (cm)	h (cm)	K_s (cm/min)
1	100	1.43	19.6	32.8	35.95	3.255
2	110	1.48	19.6	32.8	35.95	3.460
3	100	1.45	19.6	32.8	35.95	3.210

Average K_s = 3.308

Appendix F

Iron Characterization

Time (hours)	Relative Peak Height (RPH) for Aqueous PCE Concentration								
	Peerless			USMetals			Fischer		
	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>
0.5	946	1260	1340	1724	1856	2382	1756	1450	1323
1	655	1057	856	1459	2355	2747	1416	2348	2498
2	463	884	885	1557	2360	1857	1728	1943	1840
4	857	767	786	1841	2189	1510	1559	1519	1679
8	693	552	596	1168	1696	1241	1858	1403	1993
16	379	489	538	2160	1324	2138	1682	2281	1975
32	506	356	288	936	680	947	1077	846	926

Time (hours)	Average RPH for Aqueous PCE Concentration		
	Peerless	US Metals	Fischer
0.5	1182	1987	1510
1	856	2187	2087
2	744	1925	1837
4	803	1847	1586
8	614	1368	1751
16	469	1874	1979
32	383	854	950

Time (hours)	Normalized RPH for Aqueous PCE Concentration					
	Peerless	ln P	US Metals	Ln USM	Fischer	Ln F
0.5	0.394	-0.9314	0.66244	-0.4118	0.50322	-0.6867
1	0.28533	-1.2541	0.729	-0.3161	0.69578	-0.3627
2	0.248	-1.3943	0.64156	-0.4439	0.61233	-0.4905
4	0.26778	-1.3176	0.61556	-0.4852	0.52856	-0.6376
8	0.20456	-1.5869	0.45611	-0.785	0.58378	-0.5382
16	0.15622	-1.8565	0.62467	-0.4705	0.65978	-0.4159
32	0.12778	-2.0575	0.28478	-1.256	0.31656	-1.1503

Time (hours)	Relative Peak Height (RPH) for Aqueous TCE Concentration								
	Peerless			USMetals			Fischer		
	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>
0.5	0	0	0	0	0	0	0	0	0
1	0	0	0	317	240	281	320	449	385
2	375	344	315	387	214	246	289	425	462
4	459	548	479	604	579	411	378	542	404
8	361	715	663	1141	631	610	913	1445	1095
16	574	1353	1049	1539	1344	1030	1279	997	1381
32	599	943	811	1665	-	1013	1128	1372	1031

Time (hours)	Average RPH for Aqueous PCE Concentration		
	Peerless	US Metals	Fischer
0.5	0	0	0
1	0	279	385
2	345	282	392
4	495	531	441
8	580	794	1151
16	992	1304	1219
32	784	1339	1177

Time (hours)	Normalized RPH for Aqueous TCE Concentration					
	Peerless	ln P	US Metals	Ln USM	Fischer	Ln F
0.5	-	-	-	-	-	-
1	-	-	0.093	-2.374	0.128	-2.054
2	0.115	-2.164	0.094	-2.363	0.131	-2.035
4	0.165	-1.801	0.177	-1.731	0.147	-1.917
8	0.193	-1.644	0.265	-1.329	0.384	-0.958
16	0.331	-1.107	0.435	-0.833	0.406	-0.901
32	0.261	-1.342	0.446	-0.807	0.392	-0.936

Peak Height

Time (hours)	Peerless		US Metals		Fisher	
	PCE	TCE	PCE	TCE	PCE	TCE
0.5	1182	0	1987	0	1510	0
1	856	0	2187	279	2087	385
2	744	345	1925	282	1837	392
4	803	495	1847	531	1586	441
8	614	580	1368	794	1751	1151
16	469	992	1874	1304	1979	1219
32	383	784	854	1339	950	1177

Normalized

Time (hours)	Peerless		US Metals		Fisher	
	PCE	TCE	PCE	TCE	PCE	TCE
0.5	0.394	0.000	0.662	0.000	0.503	0.000
1	0.285	0.000	0.729	0.093	0.696	0.128
2	0.248	0.115	0.642	0.094	0.612	0.131
4	0.268	0.165	0.616	0.177	0.529	0.147
8	0.205	0.193	0.456	0.265	0.584	0.384
16	0.156	0.331	0.625	0.435	0.660	0.406
32	0.128	0.261	0.285	0.446	0.317	0.392

Appendix G
US Metals PCE Sorption/Reduction Batch Study

US Metals Iron Powder							
Time (hours)	Area Response			PCE (ppm)			Average
	a	b	c	a	b	c	
0	6200	6152	6432	26.6	26.4	27.6	26.9
0.5	5547.3	6349.2	7900.1	23.8	27.3	33.9	28.3
1	2643.2	2214.0	3355.2	11.3	9.5	14.4	11.8
2	2724.9	6986.1	6198.5	11.7	30.0	26.6	22.8
4	6512.0	11853.9	4815.0	28.0	50.9	20.7	33.2
8	1855.0	2308.2	2000.0	8.0	9.9	8.6	8.8
16	1904.5	1800.0	1850.0	8.2	7.7	7.9	7.9
32	803.4	2528.3	5911.9	3.4	10.9	25.4	13.2
78	1054.6	1000.0	1147.9	4.5	4.3	4.9	4.6

UO Pellets							
Time (hours)	Area Response			PCE (ppm)			Average
	a	b	c	a	b	c	
0	7500	6325	6498	32.2	27.2	27.9	29.1
0.5	5859.6	3789.3	8343.4	25.2	16.3	35.8	25.7
1	3476.3	5255.1	3508.5	14.9	22.6	15.1	17.5
2	4984.0	3506.1	3165.1	21.4	15.1	13.6	16.7
4	4911.0	4000.0	3425.4	21.1	17.2	14.7	17.7
8	2000.0	2710.4	2279.1	8.6	11.6	9.8	10.0
16	1770.1	1031.5	1500.0	7.6	4.4	6.4	6.2
32	2060.7	2181.4	1500.0	8.8	9.4	6.4	8.2
78	705.0	1724.2	273.7	3.0	7.4	1.2	3.9

U1 Pellets							
Time (hours)	Area Response			PCE (ppm)			Average
	a	b	c	a	b	c	
0	6952	6523	7123	29.8	28.0	30.6	29.5
0.5	6494.9	6110.8	8041.5	27.9	26.2	34.5	29.5
1	1854.5	5443.3	2264.2	8.0	23.4	9.7	13.7
2	1880.8	2449.0	2349.6	8.1	10.5	10.1	9.6
4	6000.0	6000.0	5000.0	25.8	25.8	21.5	24.3
8	1227.9	1156.9	1101.1	5.3	5.0	4.7	5.0
16	1900.0	2032.2	534.0	8.2	8.7	2.3	6.4
32	1000.0	783.5	589.4	4.3	3.4	2.5	3.4
78	1130.2	2327.5	1863.0	4.9	10.0	8.0	7.6

US Metals Iron Powder							
Time (hours)	Area Response			TCE (ppm)			Average
	a	b	c	a	b	c	
0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	333.9	0.0	313.9	3.2	0.0	3.0	2.1
16	999.0	1072.0	1245.0	9.7	10.4	12.1	10.7
32	0.0	0.0	0.0	0.0	0.0	0.0	0.0
78	0.0	0.0	0.0	0.0	0.0	0.0	0.0

U0 Pellets							
Time (hours)	Area Response			TCE (ppm)			Average
	a	b	c	a	b	c	
0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	0.0	0.0	150.0	0.0	0.0	1.5	0.5
16	605.0	707.0	711.0	5.9	6.9	6.9	6.5
32	0.0	0.0	0.0	0.0	0.0	0.0	0.0
78	0.0	0.0	0.0	0.0	0.0	0.0	0.0

U1 Pellets							
Time (hours)	Area Response			TCE (ppm)			Average
	a	b	c	a	b	c	
0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	343.0	348.0	303.0	3.3	3.4	2.9	3.2
8	500.0	495.6	650.0	4.8	4.8	6.3	5.3
16	920.0	1295.1	1165.0	8.9	12.5	11.3	10.9
32	0.0	0.0	0.0	0.0	0.0	0.0	0.0
78	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Time (hours)	Controls				Average
	C1	C2	C1	C2	
	Area Response		PCE (ppm)		
0.5	6458.3	4519.7	27.7	19.4	23.6
1	6100.0	4253.7	26.2	18.3	22.2
2	6000.0	3367.2	25.8	14.5	20.1
4	6000.0	3221.0	25.8	13.8	19.8
8	5500.0	6580.2	23.6	28.2	25.9
16	4500.0	5200.0	19.3	22.3	20.8
32	5525.0	3400.0	23.7	14.6	19.2
78	5000.0	5515.0	21.5	23.7	22.6

Appendix H
US Metals Chromate Sorption/Reduction Batch Study

US Metals Fe Powder						
Time (hours)	a	b (ppm)	c	average	C/C ₀	ln C/C ₀
0.5	96.5	109.1	107.2	104.3	0.94788	-0.0535
1	98.7	97.3	103.4	99.8	0.90727	-0.0973
2	94.8	97	98.9	96.9	0.88091	-0.1268
4	100.1	97.5	93.9	97.2	0.88333	-0.1241
8	91.1	90.5	88.9	90.2	0.8197	-0.1988
16	86.3	81.8	76.7	81.6	0.74182	-0.2987
32	76.4	70.9	78.2	75.2	0.68333	-0.3808
78	60.9	47.6	69.2	59.2	0.53848	-0.619

U1 Pellets						
Time (hours)	a	b (ppm)	c	average	C/C ₀	ln C/C ₀
0.5	71	70.7	63.8	68.5	0.62273	-0.4736
1	53.8	59.1	54.3	55.7	0.50667	-0.6799
2	51.1	49.3	51.3	50.6	0.4597	-0.7772
4	41.9	35.9	44.5	40.8	0.37061	-0.9926
8	34.4	33.8	37.7	35.3	0.32091	-1.1366
16	27.9	19.2	32.8	26.6	0.24212	-1.4183
32	24.9	14.5	20.9	20.1	0.18273	-1.6998
78	11.8	8.2	15.2	11.7	0.10667	-2.238

U0 Pellets						
Time (hours)	a	b (ppm)	c	average	C/C ₀	ln C/C ₀
0.5	110	120.2	109.8	113.3	1.0303	0.02985
1	107.4	116.3	109.2	111.0	1.00879	0.00875
2	107.5	107.5	105.9	107.0	0.97242	-0.028
4	108.9	110.3	108.9	109.4	0.99424	-0.0058
8	104.1	117.4	107.9	109.8	0.99818	-0.0018
16	107.1	98.8	111.7	105.9	0.96242	-0.0383
32	110.1	110.3	108.7	109.7	0.99727	-0.0027
78	107.16	118.1	111.9	112.4	1.0217	0.02146

P1 Pellets				
t (hours)	RPA	C (ppm)	C/C ₀	ln C/C ₀
0.5	424718.7	12.74	0.657	-0.42
1	274018.9	8.22	0.424	-0.86
2	318919.3	9.57	0.493	-0.71
4	120783.8	3.62	0.187	-1.68
8	47374.6	1.42	0.073	-2.61
28	2796.7	0.08	0.004	-5.44
36	2047.6	0.06	0.003	-5.76
70	1699.8	0.05	0.003	-5.94

Peerless Iron Powder				
t (hours)	RPA	C (ppm)	C/C ₀	ln C/C ₀
0.5	640367.4	19.21	0.990	-0.01
1	543400.8	16.30	0.840	-0.17
2	452003.6	13.56	0.699	-0.36
4	424575.9	12.74	0.657	-0.42
8	328476.4	9.85	0.508	-0.68
28	243142.9	7.29	0.376	-0.98
36	139846.8	4.20	0.216	-1.53
70	122188.1	3.67	0.189	-1.67

P0 Pellets				
t (hours)	RPA	C (ppm)	C/C ₀	ln C/C ₀
0.5	641854.5	19.26	0.993	-0.01
1	642331.0	19.27	0.993	-0.01
2	635766.8	19.07	0.983	-0.02
4	623230.4	18.70	0.964	-0.04
8	624347.1	18.73	0.965	-0.04
28	614183.3	18.43	0.950	-0.05
36	609220.9	18.28	0.942	-0.06
70	605651.4	18.17	0.937	-0.07

t (hours)	Control			
	RPA	C	C/C ₀	ln C
0.5	641899.5	19.26	0.993	-0.01
1	642362.0	19.27	0.993	-0.01
2	642566.2	19.28	0.994	-0.01
4	641466.3	19.24	0.992	-0.01
8	643523.1	19.31	0.995	0.00
28	641021.9	19.23	0.991	-0.01
36	640735.4	19.22	0.991	-0.01
70	642352.9	19.27	0.993	-0.01

Appendix J
Chromate Sorption/Reduction Hydrodynamic Study
4 mL/min

Column A - P1 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	04/28/98 08:37	517	0	0	0	0.00	0	0	0
027	04/28/98 08:37	517	0	0	4	0.00	330496.5	33.92	0.89
028	04/28/98 08:37	517	0	0	4	0.00	3381.7	1.21	0.03
029	04/28/98 08:42	522	5	5	4	0.19	5943.3	1.46	0.04
030	04/28/98 08:56	536	14	19	4	0.74	156124.2	16.48	0.47
031	04/28/98 09:07	547	11	30	4	1.17	232026.80	24.07	0.69
032	04/28/98 09:15	555	8	38	4	1.48	254959.50	26.37	0.75
033	04/28/98 09:32	572	17	55	4	2.14	263528.30	27.27	0.78
034	04/28/98 09:39	579	7	62	4	2.42	321899.50	33.11	0.95
035	04/28/98 09:44	584	5	67	4	2.61	267692.90	27.69	0.79
036	04/28/98 09:56	596	12	79	4	3.08	271093.80	28.03	0.80
037	04/28/98 10:12	612	16	95	4	3.70	275213.20	28.44	0.81
038	04/28/98 10:26	626	14	109	4	4.25	274666.70	28.38	0.81
039	04/28/98 10:39	639	13	122	4	4.76	276974.20	28.62	0.82
040	04/28/98 11:01	661	22	144	4	5.61	291193.10	30.04	0.86
041	04/28/98 11:29	689	28	172	4	6.70	296059.40	30.52	0.87
042	04/28/98 11:46	706	17	189	4	7.37	296206.10	30.54	0.87
043	04/28/98 11:50	710	4	193	4	7.52	340176.00	34.94	1.00
044	04/28/98 12:01	721	11	204	4	7.95	281941.50	29.11	0.83
045	04/28/98 12:16	736	15	219	4	8.54	298298.10	30.75	0.88
046	04/28/98 12:42	762	26	245	4	9.55	300902.10	31.01	0.89
047	04/28/98 13:07	787	25	270	4	10.53	302834.80	31.20	0.89
048	04/28/98 13:38	818	31	301	4	11.73	305434.30	31.46	0.90
049	04/28/98 14:40	880	62	363	4	14.15	307067.10	31.62	0.90
050	04/28/98 14:45	885	5	368	4	14.35	341274.20	35.05	1.00
051	04/28/98 15:45	945	60	428	4	16.68	303986.30	31.32	0.90
052	04/28/98 16:40	1000	55	483	4	18.83	310342.30	31.95	0.91
053	04/28/98 17:40	1060	60	543	4	21.17	310002.80	31.92	0.91
054	04/28/98 18:21	1101	41	584	4	22.77	345180.40	35.44	1.01
055	04/29/98 18:21	1101	0	584	4	22.77	310390.90	31.96	0.91

Column B - P1 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t_R	RPA	CrO_4^{2-} (ppm)	C/C ₀
Time Zero	04/28/98 08:37	517	0	0	0	0.00	0	0	0
027	04/28/98 08:37	517	0	0	4	0.00	326830.2	33.55	0.88
028	04/28/98 08:37	517	0	0	4	0.00	3381.7	1.21	0.03
029	04/28/98 08:43	523	6	6	4	0.22	4921.3	1.36	0.04
030	04/28/98 08:57	537	14	20	4	0.73	157629.9	16.63	0.48
031	04/28/98 09:08	548	11	31	4	1.14	223680.80	23.24	0.66
032	04/28/98 09:16	556	8	39	4	1.43	246123.50	25.48	0.73
033	04/28/98 09:33	573	17	56	4	2.05	254270.50	26.34	0.75
034	04/28/98 09:39	579	6	62	4	2.27	336293.90	34.55	0.99
035	04/28/98 09:45	585	6	68	4	2.49	261491.80	27.07	0.77
036	04/28/98 09:57	597	12	80	4	2.93	265729.40	27.49	0.79
037	04/28/98 10:13	613	16	96	4	3.52	268730.90	27.79	0.79
038	04/28/98 10:27	627	14	110	4	4.03	270237.10	27.94	0.80
039	04/28/98 10:40	640	13	123	4	4.51	273590.70	28.28	0.81
040	04/28/98 11:02	662	22	145	4	5.32	281864.10	29.10	0.83
041	04/28/98 11:30	690	28	173	4	6.34	289246.00	29.84	0.85
042	04/28/98 11:47	707	17	190	4	6.97	292763.30	30.19	0.86
043	04/28/98 11:50	710	3	193	4	7.08	336282.90	34.55	0.99
044	04/28/98 12:01	721	11	204	4	7.48	296326.50	30.55	0.87
045	04/28/98 12:16	736	15	219	4	8.03	295824.50	30.50	0.87
046	04/28/98 12:43	763	27	246	4	9.02	297893.20	30.71	0.88
047	04/28/98 13:07	787	24	270	4	9.90	301814.40	31.10	0.89
048	04/28/98 13:39	819	32	302	4	11.08	299428.70	30.86	0.88
049	04/28/98 14:42	882	63	365	4	13.39	302198.10	31.14	0.89
050	04/28/98 14:46	886	4	369	4	13.53	337364.30	34.65	0.99
051	04/28/98 15:45	945	59	428	4	15.70	299090.30	30.83	0.90
052	04/28/98 16:40	1000	55	483	4	17.71	306112.60	31.53	0.90
053	04/28/98 17:41	1061	61	544	4	19.95	306815.70	31.60	0.90
053	04/28/98 18:22	1102	41	585	4	21.45	338373.90	34.76	0.99
054	04/29/98 18:22	1102	0	585	4	21.45	306377.90	31.56	0.90

Column C - P0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	04/28/98 08:37	517	0	0	0	0.00	0	0	0
027	04/28/98 08:37	517	0	0	4	0.00	316881.9	32.56	0.86
028	04/28/98 08:37	517	0	0	4	0.00	0	0.87	0.02
029	04/28/98 08:44	524	7	7	4	0.27	0	0.87	0.02
030	04/28/98 08:58	538	14	21	4	0.80	243949.6	25.26	0.72
031	04/28/98 09:09	549	11	32	4	1.22	300772.40	30.95	0.88
032	04/28/98 09:17	557	8	40	4	1.53	311265.60	32.00	0.91
033	04/28/98 09:34	574	17	57	4	2.18	316366.90	32.55	0.93
034	04/28/98 09:40	580	6	63	4	2.41	339923.40	34.91	1.00
035	04/28/98 09:46	586	6	69	4	2.64	329520.30	33.87	0.97
036	04/28/98 09:58	598	12	81	4	3.10	323911.30	33.31	0.95
037	04/28/98 10:13	613	15	96	4	3.67	323411.30	33.26	0.95
038	04/28/98 10:28	628	15	111	4	4.24	324767.80	33.39	0.95
039	04/28/98 10:42	642	14	125	4	4.78	335066.30	34.42	0.98
040	04/28/98 11:02	662	20	145	4	5.54	339830.00	34.90	1.00
041	04/28/98 11:31	691	29	174	4	6.65	336369.60	34.55	0.99
042	04/28/98 11:47	707	16	190	4	7.26	335842.90	34.50	0.99
043	04/28/98 11:53	713	6	196	4	7.49	340038.80	34.92	1.00
044	04/28/98 12:02	722	9	205	4	7.84	328404.70	33.76	0.96
045	04/28/98 12:17	737	15	220	4	8.41	334987.80	34.42	0.98
046	04/28/98 12:43	763	26	246	4	9.40	336108.30	34.53	0.99
047	04/28/98 13:07	787	24	270	4	10.32	336108.30	34.53	0.99
048	04/28/98 13:38	818	31	301	4	11.51	336108.30	34.53	0.99
049	04/28/98 14:40	880	62	363	4	13.88	336108.30	34.53	0.99
050	04/28/98 14:45	885	5	368	4	14.07	336108.30	34.53	0.99
051	04/28/98 15:45	945	60	428	4	16.36	336108.30	34.53	0.99
052	04/28/98 16:40	1000	55	483	4	18.47	336108.30	34.53	0.99
053	04/28/98 17:40	1060	60	543	4	20.76	336108.30	34.53	0.99
054	04/28/98 18:21	1101	41	584	4	22.33	336108.30	34.53	0.99
055	04/29/98 18:21	1101	0	584	4	22.33	336108.30	34.53	0.99

Column D - P0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	04/28/98 08:37	517	0	0	0	0.00	0	0	0
027	04/28/98 08:37	517	0	0	4	0.00	327897.4	33.66	0.89
028	04/28/98 08:37	517	0	0	4	0.00	11160.1	1.99	0.06
029	04/28/98 08:46	526	9	9	4	0.33	4683.3	1.34	0.04
030	04/28/98 08:59	539	13	22	4	0.81	262609.6	27.13	0.78
031	04/28/98 09:10	550	11	33	4	1.21	295098.90	30.38	0.87
032	04/28/98 09:18	558	8	41	4	1.51	307242.90	31.59	0.90
033	04/28/98 09:35	575	17	58	4	2.13	315988.10	32.52	0.93
034	04/28/98 09:40	580	5	63	4	2.32	337292.90	34.65	0.99
035	04/28/98 09:47	587	7	70	4	2.58	321098.30	33.03	0.94
036	04/28/98 09:58	598	11	81	4	2.98	320498.40	32.97	0.94
037	04/28/98 10:15	615	17	98	4	3.61	320007.90	32.92	0.94
038	04/28/98 10:28	628	13	111	4	4.08	321218.40	33.04	0.94
039	04/28/98 10:42	642	14	125	4	4.60	332656.80	34.18	0.98
040	04/28/98 11:03	663	21	146	4	5.37	334421.50	34.36	0.98
041	04/28/98 11:31	691	28	174	4	6.40	335187.10	34.44	0.98
042	04/28/98 11:48	708	17	191	4	7.03	335371.10	34.45	0.98
043	04/28/98 11:53	713	5	196	4	7.21	342390.10	35.16	1.00
044	04/28/98 12:03	723	10	206	4	7.58	335782.10	34.50	0.99
045	04/28/98 12:18	738	15	221	4	8.13	336381.20	34.56	0.99
046	04/28/98 12:44	764	26	247	4	9.09	334898.90	34.41	0.98
047	04/28/98 13:07	787	23	270	4	9.93	336381.20	34.56	0.99
048	04/28/98 13:38	818	31	301	4	11.07	336381.20	34.56	0.99
049	04/28/98 14:40	880	62	363	4	13.36	336381.20	34.56	0.99
050	04/28/98 14:45	885	5	368	4	13.54	336381.20	34.56	0.99
051	04/28/98 15:45	945	60	428	4	15.75	336381.20	34.56	0.99
052	04/28/98 16:40	1000	55	483	4	17.77	336381.20	34.56	0.99
053	04/28/98 17:40	1060	60	543	4	19.98	336381.20	34.56	0.99
054	04/28/98 18:21	1101	41	584	4	21.49	336381.20	34.56	0.99
055	04/29/98 18:21	1101	0	584	4	21.49	336381.20	34.56	0.99

Column E - B0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	04/28/98 08:37	517	0	0	0	0.00	0	0	0
027	04/28/98 08:37	517	0	0	4	0.00	333193.5	34.19	0.90
028	04/28/98 08:37	517	0	0	4	0.00	10345.8	1.90	0.05
029	04/28/98 08:46	526	9	9	4	0.24	4751.9	1.34	0.04
030	04/28/98 09:00	540	14	23	4	0.61	247609.3	25.63	0.73
031	04/28/98 09:10	550	10	33	4	0.87	294825.40	30.35	0.87
032	04/28/98 09:19	559	9	42	4	1.11	304758.80	31.35	0.90
033	04/28/98 09:36	576	17	59	4	1.55	315173.10	32.44	0.93
034	04/28/98 09:41	581	5	64	4	1.68	337738.20	34.69	0.99
035	04/28/98 10:42	642	61	125	4	3.29	332863.40	34.20	0.98
037	04/28/98 11:54	714	72	197	4	5.18	337585.30	34.68	0.99
038	04/28/98 12:18	738	24	221	4	5.82	336401.40	34.56	0.99
039	04/28/98 14:44	884	146	367	4	9.66	336401.40	34.56	0.99
040	04/28/98 14:50	890	6	373	4	9.82	336401.40	34.56	0.99
041	04/28/98 18:23	1103	213	586	4	15.42	336401.40	34.56	0.99

Column F - B0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	04/28/98 08:37	517	0	0	0	0.00	0	0	0
027	04/28/98 08:37	517	0	0	4	0.00	291059.8	29.98	0.79
028	04/28/98 08:37	517	0	0	4	0.00	15215	2.39	0.07
029	04/28/98 08:48	528	11	11	4	0.30	7982.7	1.67	0.05
030	04/28/98 09:01	541	13	24	4	0.65	246478.5	25.52	0.73
031	04/28/98 09:11	551	10	34	4	0.93	290251.70	29.89	0.85
032	04/28/98 09:20	560	9	43	4	1.17	303321.70	31.20	0.89
033	04/28/98 09:36	576	16	59	4	1.61	313619.70	32.28	0.92
034	04/28/98 09:41	581	5	64	4	1.74	335214.00	34.44	0.98
035	04/28/98 10:44	644	63	127	4	3.46	334700.20	34.39	0.98
037	04/28/98 11:55	715	71	198	4	5.39	339788.10	34.90	1.00
038	04/28/98 12:19	739	24	222	4	6.05	336660.20	34.58	0.99
039	04/28/98 14:44	884	145	367	4	10.00	336660.20	34.58	0.99
040	04/28/98 14:50	890	6	373	4	10.16	336660.20	34.58	0.99
041	04/28/98 18:24	1104	214	587	4	15.99	336660.20	34.58	0.99

Appendix K
Chromate Sorption/Reduction Hydrodynamic Study
2 mL/min

Column A - P1 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/18/98 15:00	900	0	0	0	0.00	0	0	0
001	05/18/98 15:00	900	0	0	2	0.00	312362.1	32.09	0.97
002	05/18/98 15:00	900	0	0	2	0.00	39831.6	4.84	0.05
003	05/18/98 15:09	909	9	9	2	0.18	10827.4	1.94	0.06
004	05/18/98 15:20	920	11	20	2	0.39	8226.2	1.68	0.05
005	05/18/98 15:29	929	9	29	2	0.57	8649.90	1.72	0.05
006	05/18/98 15:39	939	10	39	2	0.76	9958.10	1.85	0.06
007	05/18/98 15:49	949	10	49	2	0.96	10002.00	1.85	0.06
008	05/18/98 15:59	959	10	59	2	1.15	8472.70	1.70	0.05
009	05/18/98 16:15	975	16	75	2	1.46	7347.40	1.59	0.05
010	05/18/98 16:26	986	11	86	2	1.68	8522.20	1.71	0.05
011	05/18/98 16:30	990	4	90	2	1.75	314529.80	32.31	0.98
012	05/18/98 16:45	1005	15	105	2	2.05	2356.40	1.09	0.03
013	05/18/98 17:00	1020	15	120	2	2.34	2356.40	1.09	0.03
014	05/18/98 17:20	1040	20	140	2	2.73	23724.80	3.23	0.10
015	05/18/98 17:40	1060	20	160	2	3.12	36873.40	4.54	0.14
016	05/18/98 18:00	1080	20	180	2	3.51	69223.80	7.78	0.24
017	05/18/98 18:16	1096	16	196	2	3.82	98034.20	10.66	0.32
018	05/18/98 18:55	1135	39	235	2	4.58	181947.60	19.05	0.58
019	05/18/98 19:10	1150	15	250	2	4.87	216601.30	22.51	0.68
020	05/18/98 19:30	1170	20	270	2	5.26	245887.60	25.44	0.77
021	05/18/98 19:50	1190	20	290	2	5.65	266364.70	27.49	0.83
022	05/18/98 20:28	1228	38	328	2	6.39	282238.00	29.08	0.88
023	05/18/98 21:00	1260	32	360	2	7.02	291365.90	29.99	0.91
024	05/18/98 21:03	1263	3	363	2	7.08	335728.00	34.43	1.04
025	05/18/98 21:40	1300	37	400	2	7.80	295355.90	30.39	0.92
026	05/18/98 22:32	1352	52	452	2	8.81	300974.80	30.95	0.94
027	05/18/98 23:45	1425	73	525	2	10.23	302560.40	31.11	0.94
028	05/19/98 00:44	44	54	579	2	11.29	304984.20	31.35	0.95
029	05/19/98 02:00	120	76	655	2	12.77	309171.20	31.77	0.96
030	05/19/98 05:45	345	225	880	2	17.15	308374.10	31.69	0.96

Column B - P1 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/18/98 15:00	900	0	0	0	0.00	0	0	0
001	05/18/98 15:00	900	0	0	2	0.00	323198.80	33.17	1.01
002	05/18/98 15:00	900	0	0	2	0.00	10154.5	1.87	0.06
003	05/18/98 15:09	909	9	9	2	0.17	9376.1	1.79	0.05
004	05/18/98 15:20	920	11	20	2	0.37	8155.9	1.67	0.05
005	05/18/98 15:29	929	9	29	2	0.53	8467.80	1.70	0.05
006	05/18/98 15:39	939	10	39	2	0.72	12595.90	2.11	0.06
007	05/18/98 15:49	949	10	49	2	0.90	8467.00	1.70	0.05
008	05/18/98 15:59	959	10	59	2	1.08	7872.20	1.64	0.05
009	05/18/98 16:15	975	16	75	2	1.38	7877.30	1.64	0.05
010	05/18/98 16:26	986	11	86	2	1.58	315987.00	32.45	0.98
011	05/18/98 16:30	990	4	90	2	1.65	8041.80	1.66	0.05
012	05/18/98 16:45	1005	15	105	2	1.93	8041.80	1.66	0.05
013	05/18/98 17:00	1020	15	120	2	2.20	8041.80	1.66	0.05
014	05/18/98 17:20	1040	20	140	2	2.57	5251.20	1.38	0.04
015	05/18/98 17:40	1060	20	160	2	2.93	19240.90	2.78	0.08
016	05/18/98 18:00	1080	20	180	2	3.30	34923.00	4.35	0.13
017	05/18/98 18:16	1096	16	196	2	3.59	57181.20	6.57	0.20
018	05/18/98 18:55	1135	39	235	2	4.31	142518.90	15.11	0.46
019	05/18/98 19:10	1150	15	250	2	4.58	177714.00	18.63	0.56
020	05/18/98 19:30	1170	20	270	2	4.95	215157.00	22.37	0.68
021	05/18/98 19:50	1190	20	290	2	5.32	248050.70	25.66	0.78
022	05/18/98 20:28	1228	38	328	2	6.01	267555.20	27.61	0.84
023	05/18/98 21:00	1260	32	360	2	6.60	280898.70	28.94	0.88
024	05/18/98 21:03	1263	3	363	2	6.66	332972.40	34.15	1.03
025	05/18/98 21:40	1300	37	400	2	7.33	287623.10	29.62	0.90
026	05/18/98 22:32	1352	52	452	2	8.29	293131.90	30.17	0.91
027	05/18/98 23:45	1425	73	525	2	9.63	296661.90	30.52	0.92
028	05/19/98 00:44	44	54	579	2	10.62	300689.00	30.92	0.94
029	05/19/98 02:00	120	76	655	2	12.01	305501.10	31.40	0.95
030	05/19/98 05:45	345	225	880	2	16.14	306497.80	31.50	0.95

Column C - P0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/18/98 15:00	900	0	0	0	0.00	0	0	0
001	05/18/98 15:00	900	0	0	2	0.00	317943.8	32.65	0.99
002	05/18/98 15:00	900	0	0	2	0.00	0	0.85	0.03
003	05/18/98 15:09	909	9	9	2	0.17	0	0.85	0.03
004	05/18/98 15:20	920	11	20	2	0.38	3272.7	1.18	0.04
005	05/18/98 15:29	929	9	29	2	0.55	65322.80	7.39	0.22
006	05/18/98 15:39	939	10	39	2	0.75	209733.50	21.83	0.66
007	05/18/98 15:49	949	10	49	2	0.94	265921.40	27.45	0.83
008	05/18/98 15:59	959	10	59	2	1.13	286012.60	29.46	0.89
009	05/18/98 16:15	975	16	75	2	1.43	299855.80	30.84	0.93
010	05/18/98 16:26	986	11	86	2	1.64	306012.30	31.46	0.95
011	05/18/98 16:30	990	4	90	2	1.72	325918.70	33.45	1.01
012	05/18/98 16:45	1005	15	105	2	2.01	310742.90	31.93	0.97
013	05/18/98 17:00	1020	15	120	2	2.29	313060.40	32.16	0.97
014	05/18/98 17:20	1040	20	140	2	2.68	316588.30	32.51	0.99
015	05/18/98 17:40	1060	20	160	2	3.06	316296.30	32.48	0.98
016	05/18/98 18:00	1080	20	180	2	3.44	317207.30	32.57	0.99
017	05/18/98 18:16	1096	16	196	2	3.75	318021.80	32.66	0.99
018	05/18/98 18:55	1135	39	235	2	4.49	318612.50	32.72	0.99
019	05/18/98 19:10	1150	15	250	2	4.78	320543.90	32.91	1.00
020	05/18/98 19:30	1170	20	270	2	5.16	321382.60	32.99	1.00
021	05/18/98 19:50	1190	20	290	2	5.54	318596.80	32.71	0.99
022	05/18/98 20:28	1228	38	328	2	6.27	320462.80	32.90	1.00
023	05/18/98 21:00	1260	32	360	2	6.88	328354.70	33.69	1.02
024	05/18/98 21:03	1263	3	363	2	6.94	319992.50	32.85	1.00
025	05/18/98 21:40	1300	37	400	2	7.65	320700.30	32.92	1.00
026	05/18/98 22:32	1352	52	452	2	8.64	320094.40	32.86	1.00
027	05/18/98 23:45	1425	73	525	2	10.04	319953.60	32.85	1.00

Column D - P0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/18/98 15:00	900	0	0	0	0.00	0	0	0
001	05/18/98 15:00	900	0	0	2	0.00	325006.4	33.35	1.01
002	05/18/98 15:00	900	0	0	2	0.00	19736.7	2.83	0.09
003	05/18/98 15:09	909	9	9	2	0.17	0	0.85	0.03
004	05/18/98 15:20	920	11	20	2	0.37	0	0.85	0.03
005	05/18/98 15:29	929	9	29	2	0.53	44649.30	5.32	0.16
006	05/18/98 15:39	939	10	39	2	0.72	189844.90	19.84	0.60
007	05/18/98 15:49	949	10	49	2	0.90	257159.60	26.57	0.81
008	05/18/98 15:59	959	10	59	2	1.09	280039.50	28.86	0.87
009	05/18/98 16:15	975	16	75	2	1.38	297803.80	30.63	0.93
010	05/18/98 16:26	986	11	86	2	1.58	303897.00	31.24	0.95
011	05/18/98 16:30	990	4	90	2	1.66	334501.30	34.30	1.04
012	05/18/98 16:45	1005	15	105	2	1.93	307297.20	31.58	0.96
013	05/18/98 17:00	1020	15	120	2	2.21	310773.10	31.93	0.97
014	05/18/98 17:20	1040	20	140	2	2.58	313404.80	32.19	0.98
015	05/18/98 17:40	1060	20	160	2	2.94	313689.50	32.22	0.98
016	05/18/98 18:00	1080	20	180	2	3.31	316954.10	32.55	0.99
017	05/18/98 18:16	1096	16	196	2	3.61	314715.30	32.33	0.98
018	05/18/98 18:55	1135	39	235	2	4.32	314732.80	32.33	0.98
019	05/18/98 19:10	1150	15	250	2	4.60	319173.60	32.77	0.99
020	05/18/98 19:30	1170	20	270	2	4.97	316464.70	32.50	0.98
021	05/18/98 19:50	1190	20	290	2	5.33	317818.30	32.64	0.99
022	05/18/98 20:28	1228	38	328	2	6.03	312938.40	32.15	0.97
023	05/18/98 21:00	1260	32	360	2	6.62	335440.00	34.40	1.04
024	05/18/98 21:03	1263	3	363	2	6.68	317844.30	32.64	0.99
025	05/18/98 21:40	1300	37	400	2	7.36	320130.00	32.87	1.00
026	05/18/98 22:32	1352	52	452	2	8.31	318228.80	32.68	0.99
027	05/18/98 23:45	1425	73	525	2	9.66	320835.60	32.94	1.00

Column E - B0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/18/98 15:00	900	0	0	0	0.00	0	0	0
001	05/18/98 15:00	900	0	0	2	0.00	333193.5	34.17	0.90
002	05/18/98 15:00	900	0	0	2	0.00	10345.8	1.89	0.05
003	05/18/98 15:11	911	11	11	2	0.14	4751.9	1.33	0.04
004	05/18/98 15:22	922	11	22	2	0.29	247609.3	25.61	0.73
005	05/18/98 15:31	931	9	31	2	0.41	294825.40	30.34	0.87
006	05/18/98 15:41	941	10	41	2	0.54	304758.80	31.33	0.90
007	05/18/98 15:51	951	10	51	2	0.67	315173.10	32.37	0.92
008	05/18/98 16:01	961	10	61	2	0.80	337738.20	34.63	0.99
009	05/18/98 16:17	977	16	77	2	1.01	332863.40	34.14	0.98
010	05/18/98 16:27	987	10	87	2	1.14	337585.30	34.61	0.99
011	05/18/98 17:00	1020	33	120	2	1.58	332307.20	34.08	0.97
012	05/18/98 19:00	1140	120	240	2	3.16	337029.10	34.56	0.99
013	05/18/98 21:00	1260	120	360	2	4.74	341751.00	35.03	1.00
014	05/18/98 23:00	1380	120	480	2	6.32	346472.90	35.50	1.01
015	05/19/98 01:00	60	120	600	2	7.90	341194.80	34.97	1.00
016	05/19/98 03:00	180	120	720	2	9.47	345916.70	35.45	1.01
017	05/19/98 05:00	300	120	840	2	11.05	340638.60	34.92	1.00

Column F - B0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/18/98 15:00	900	0	0	0	0.00	0	0	0
001	05/18/98 15:00	900	0	0	2	0.00	291059.8	29.96	0.79
002	05/18/98 15:00	900	0	0	2	0.00	15215	2.38	0.07
003	05/18/98 15:11	911	11	11	2	0.15	7982.7	1.65	0.05
004	05/18/98 15:22	922	11	22	2	0.30	246478.5	25.50	0.73
005	05/18/98 15:31	931	9	31	2	0.42	290251.70	29.88	0.85
006	05/18/98 15:41	941	10	41	2	0.56	303321.70	31.19	0.89
007	05/18/98 15:51	951	10	51	2	0.69	313619.70	32.22	0.92
008	05/18/98 16:01	961	10	61	2	0.83	335214.00	34.38	0.98
009	05/18/98 16:17	977	16	77	2	1.05	334700.20	34.32	0.98
010	05/18/98 16:27	987	10	87	2	1.19	339788.10	34.83	1.00
011	05/18/98 17:00	1020	33	120	2	1.63	336660.20	34.52	0.99
012	05/18/98 19:00	1140	120	240	2	3.27	343532.30	35.21	1.01
013	05/18/98 21:00	1260	120	360	2	4.90	340404.40	34.89	1.00
014	05/18/98 23:00	1380	120	480	2	6.54	347276.50	35.58	1.02
015	05/19/98 01:00	60	120	600	2	8.17	344148.60	35.27	1.01
016	05/19/98 03:00	180	120	720	2	9.81	341020.70	34.96	1.00
017	05/19/98 05:00	300	120	840	2	11.44	347892.80	35.64	1.02

Appendix L
Chromate Sorption/Reduction Hydrodynamic Study
0.6 mL/min

Column A - P1 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/28/98 14:00	840	0	0	0	0.00	0	0	0
001	05/29/98 14:00	840	0	0	0.6	0.00	521060	37.07	0.98
002	05/28/98 14:30	870	30	30	0.6	0.18	16521	1.75	0.05
003	05/28/98 15:00	900	30	60	0.6	0.35	10841	1.35	0.04
004	05/29/98 15:30	930	30	90	0.6	0.53	10819	1.35	0.04
005	05/28/98 16:00	960	30	120	0.6	0.70	9683	1.27	0.03
006	05/28/98 17:00	1020	90	180	0.6	1.05	542140	38.54	1.01
007	05/29/98 17:00	1020	0	180	0.6	1.05	9988	1.29	0.03
008	05/28/98 18:00	1080	60	240	0.6	1.40	5989	1.01	0.03
009	05/28/98 19:00	1140	60	300	0.6	1.75	6307	1.04	0.03
010	05/28/98 20:00	1200	60	360	0.6	2.11	5899	1.01	0.03
011	05/28/98 21:00	1260	120	480	0.6	2.81	10712	1.34	0.04
012	05/28/98 22:00	1320	60	540	0.6	3.16	10031	1.30	0.03
013	05/29/98 00:00	0	120	660	0.6	3.86	53510	4.31	0.11
014	05/28/98 02:00	120	120	780	0.6	4.56	224932	16.31	0.43
015	05/29/98 04:00	240	120	900	0.6	5.26	309107	22.20	0.58
016	05/29/98 08:00	480	240	1140	0.6	6.67	391459	27.97	0.74
017	05/29/98 12:00	720	240	1380	0.6	8.07	401354	28.66	0.75
018	05/29/98 16:00	960	240	1620	0.6	9.47	401459	28.67	0.75
019	05/29/98 20:00	1200	240	1860	0.6	10.88	401011	28.64	0.75
020	05/30/98 00:00	0	240	2100	0.6	12.28	402563	28.74	0.76
021	05/30/98 04:00	240	240	2340	0.6	13.68	401658	28.68	0.75
022	05/30/98 08:00	480	240	2580	0.6	15.09	401459	28.67	0.75
023	05/30/98 12:00	720	240	2820	0.6	16.49	401378	28.66	0.75
024	05/30/98 16:00	960	240	3060	0.6	17.89	401953	28.70	0.76
025	05/30/98 20:00	1200	240	3300	0.6	19.30	402659	28.75	0.76

Column B - P1 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/28/98 14:00	840	0	0	0	0.00	0	0	0
001	05/29/98 14:00	840	0	0	0.6	0.00	528362	37.58	0.99
002	05/28/98 14:30	870	30	30	0.6	0.17	27330	2.51	0.07
003	05/28/98 15:00	900	30	60	0.6	0.33	11943	1.43	0.04
004	05/29/98 15:30	930	30	90	0.6	0.50	8851	1.21	0.03
005	05/28/98 16:00	960	30	120	0.6	0.66	7983	1.15	0.03
006	05/28/98 17:00	1020	90	180	0.6	0.99	525206	37.36	0.98
007	05/29/98 17:00	1020	0	180	0.6	0.99	9714	1.28	0.03
008	05/28/98 18:00	1080	60	240	0.6	1.32	6994	1.08	0.03
009	05/28/98 19:00	1140	60	300	0.6	1.65	6185	1.03	0.03
010	05/28/98 20:00	1200	60	360	0.6	1.98	5362	0.97	0.03
011	05/28/98 21:00	1260	120	480	0.6	2.64	5616	0.99	0.03
012	05/28/98 22:00	1320	60	540	0.6	2.97	5227	0.96	0.03
013	05/29/98 00:00	0	120	660	0.6	3.63	29875	2.66	0.07
014	05/28/98 02:00	120	120	780	0.6	4.29	170587	12.51	0.33
015	05/29/98 04:00	240	120	900	0.6	4.95	290588	20.91	0.55
016	05/29/98 08:00	480	240	1140	0.6	6.27	361736	25.89	0.68
017	05/29/98 12:00	720	240	1380	0.6	7.59	371736	26.59	0.70
018	05/29/98 16:00	960	240	1620	0.6	8.91	381736	27.29	0.72
019	05/29/98 20:00	1200	240	1860	0.6	10.23	391736	27.99	0.74
020	05/30/98 00:00	0	240	2100	0.6	11.55	391856	28.00	0.74
021	05/30/98 04:00	240	240	2340	0.6	12.87	391896	28.00	0.74
022	05/30/98 08:00	480	240	2580	0.6	14.19	391902	28.00	0.74
023	05/30/98 12:00	720	240	2820	0.6	15.51	391956	28.00	0.74
024	05/30/98 16:00	960	240	3060	0.6	16.83	392035	28.01	0.74
025	05/30/98 20:00	1200	240	3300	0.6	18.15	392065	28.01	0.74
026	05/31/98 00:00	0	240	3540	0.6	19.47	392062	28.01	0.74

Column C - P0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t_R	RPA	CrO_4^{2-} (ppm)	C/C_0
Time Zero	05/28/98 14:00	840	0	0	0	0.00	0	0	0
001	05/29/98 14:00	840	0	0	0.6	0.00	568477	40.39	1.01
002	05/28/98 14:30	870	30	30	0.6	0.17	21141	2.07	0.05
003	05/28/98 15:00	900	30	60	0.6	0.34	21140	2.07	0.05
004	05/29/98 15:30	930	30	90	0.6	0.52	1898	0.73	0.02
005	05/28/98 16:00	960	30	120	0.6	0.69	171281	12.58	0.31
006	05/28/98 17:00	1020	90	180	0.6	1.03	550554	39.13	0.98
007	05/29/98 17:00	1020	0	180	0.6	1.03	247397	17.91	0.45
008	05/28/98 18:00	1080	60	240	0.6	1.38	311650	22.41	0.56
009	05/28/98 19:00	1140	60	300	0.6	1.72	384717	27.53	0.69
010	05/28/98 20:00	1200	60	360	0.6	2.06	409691	29.27	0.73
011	05/28/98 21:00	1260	120	480	0.6	2.75	444354	31.70	0.79
012	05/28/98 22:00	1320	60	540	0.6	3.10	459494	32.76	0.82
013	05/29/98 00:00	0	120	660	0.6	3.78	469907	33.46	0.84
014	05/28/98 02:00	120	120	780	0.6	4.47	475323	33.84	0.85
015	05/29/98 04:00	240	120	900	0.6	5.16	482873	34.37	0.86
016	05/29/98 08:00	480	240	1140	0.6	6.54	489129	34.80	0.87
017	05/29/98 12:00	720	240	1380	0.6	7.91	489563	34.83	0.87
018	05/29/98 16:00	960	240	1620	0.6	9.29	489596	34.84	0.87
019	05/29/98 20:00	1200	240	1860	0.6	10.67	489129	34.80	0.87
020	05/30/98 00:00	0	240	2100	0.6	12.04	489206	34.81	0.87
021	05/30/98 04:00	240	240	2340	0.6	13.42	489256	34.81	0.87
022	05/30/98 08:00	480	240	2580	0.6	14.79	489289	34.82	0.87
023	05/30/98 12:00	720	240	2820	0.6	16.17	489299	34.82	0.87
024	05/30/98 16:00	960	240	3060	0.6	17.55	489160	34.81	0.87
025	05/30/98 20:00	1200	240	3300	0.6	18.92	489101	34.80	0.87
026	05/31/98 00:00	0	240	3540	0.6	20.30	489305	34.82	0.87

Column D - P0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/28/98 14:00	840	0	0	0	0.00	0	0	0
001	05/29/98 14:00	840	0	0	0.6	0.00	538477	38.29	0.98
002	05/28/98 14:30	870	30	30	0.6	0.17	21141	2.07	0.05
003	05/28/98 15:00	900	30	60	0.6	0.33	21140	2.07	0.05
004	05/29/98 15:30	930	30	90	0.6	0.50	1898	0.73	0.02
005	05/28/98 16:00	960	30	120	0.6	0.66	171281	12.58	0.32
006	05/28/98 17:00	1020	90	180	0.6	0.99	550554	39.13	1.00
007	05/29/98 17:00	1020	0	180	0.6	0.99	247397	17.91	0.46
008	05/28/98 18:00	1080	60	240	0.6	1.32	311650	22.41	0.57
009	05/28/98 19:00	1140	60	300	0.6	1.66	354717	25.43	0.65
010	05/28/98 20:00	1200	60	360	0.6	1.99	389691	27.87	0.71
011	05/28/98 21:00	1260	120	480	0.6	2.65	424354	30.30	0.78
012	05/28/98 22:00	1320	60	540	0.6	2.98	449494	32.06	0.82
013	05/29/98 00:00	0	120	660	0.6	3.64	459907	32.76	0.84
014	05/28/98 02:00	120	120	780	0.6	4.30	465323	33.14	0.85
015	05/29/98 04:00	240	120	900	0.6	4.97	472873	33.67	0.86
016	05/29/98 08:00	480	240	1140	0.6	6.29	479129	34.10	0.87
017	05/29/98 12:00	720	240	1380	0.6	7.62	479199	34.11	0.87
018	05/29/98 16:00	960	240	1620	0.6	8.94	479256	34.11	0.87
019	05/29/98 20:00	1200	240	1860	0.6	10.26	479299	34.12	0.87
020	05/30/98 00:00	0	240	2100	0.6	11.59	479389	34.12	0.87
021	05/30/98 04:00	240	240	2340	0.6	12.91	479456	34.13	0.88
022	05/30/98 08:00	480	240	2580	0.6	14.24	479800	34.15	0.88
023	05/30/98 12:00	720	240	2820	0.6	15.56	482300	34.33	0.88
024	05/30/98 16:00	960	240	3060	0.6	16.89	485623	34.56	0.89
025	05/30/98 20:00	1200	240	3300	0.6	18.21	488453	34.76	0.89
026	05/31/98 00:00	0	240	3540	0.6	19.54	489222	34.81	0.89

Column E - B0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	RPA	CrO ₄ ²⁻ (ppm)	C/C ₀
Time Zero	05/28/98 14:00	840	0	0	0	0.00	0	0	0
001	05/29/98 14:00	840	0	0	0.6	0.00	545698.4	38.79	0.99
002	05/28/98 14:30	870	30	30	0.6	0.12	3063.6	0.81	0.02
003	05/28/98 15:00	900	30	60	0.6	0.24	3807.5	0.86	0.02
004	05/29/98 15:30	930	30	90	0.6	0.36	2904	0.80	0.02
005	05/28/98 16:00	960	30	120	0.6	0.47	294763.20	21.23	0.54
006	05/28/98 17:00	1020	90	180	0.6	0.71	547598.80	38.93	1.00
007	05/29/98 17:00	1020	0	180	0.6	0.71	532871.90	37.90	0.97
008	05/28/98 18:00	1080	60	240	0.6	0.95	522669.20	37.18	0.95
009	05/28/98 19:00	1140	60	300	0.6	1.18	540703.80	38.44	0.99
010	05/28/98 20:00	1200	60	360	0.6	1.42	545160.90	38.76	0.99
011	05/28/98 21:00	1260	120	480	0.6	1.89	550317.40	39.12	1.00
012	05/28/98 22:00	1320	60	540	0.6	2.13	549560.60	39.06	1.00
013	05/29/98 05:00	300	240	960	0.6	3.79	548803.80	39.01	1.00
014	05/29/98 09:00	540	60	1020	0.6	4.03	548047.00	38.96	1.00
015	05/29/98 13:00	780	240	1260	0.6	4.97	547290.20	38.91	1.00
016	05/29/98 17:00	1020	240	1500	0.6	5.92	546533.40	38.85	1.00
017	05/29/98 21:00	1260	240	1740	0.6	6.87	545776.60	38.80	0.99
018	05/30/98 01:00	60	240	1980	0.6	7.82	545019.80	38.75	0.99
019	05/30/98 05:00	300	240	2220	0.6	8.76	544263.00	38.69	0.99
020	05/30/98 09:00	540	240	2460	0.6	9.71	543506.20	38.64	0.99
021	05/30/98 13:00	780	240	2700	0.6	10.66	542749.40	38.59	0.99
022	05/30/98 17:00	1020	240	2940	0.6	11.61	541992.60	38.53	0.99
023	05/28/98 21:00	1260	240	3180	0.6	12.55	551235.80	39.18	1.00
024	05/29/98 01:00	60	240	3420	0.6	13.50	550479.00	39.13	1.00

Column F - B0 Pellets

Sample ID	Time	Minutes	Time Interval (min)	Elapsed Minutes	Flow Rate (mL/min)	t_R	RPA	CrO_4^{2-} (ppm)	C/C_0
Time Zero	05/28/98 14:00	840	0	0	0	0.00	0	0	0
001	05/29/98 14:00	840	0	0	0.6	0.00	541426	38.49	1.01
002	05/28/98 14:30	870	30	30	0.6	0.12	14384	1.60	0.04
003	05/28/98 15:00	900	30	60	0.6	0.25	1977	0.73	0.02
004	05/29/98 15:30	930	30	90	0.6	0.37	5415	0.97	0.03
005	05/28/98 16:00	960	30	120	0.6	0.49	273221	19.72	0.52
006	05/28/98 17:00	1020	90	180	0.6	0.74	547124	38.89	1.02
007	05/29/98 17:00	1020	0	180	0.6	0.74	462594	32.98	0.87
008	05/28/98 18:00	1080	60	240	0.6	0.98	525854	37.40	0.98
009	05/28/98 19:00	1140	60	300	0.6	1.23	532688	37.88	1.00
010	05/28/98 20:00	1200	60	360	0.6	1.47	536856	38.17	1.00
011	05/28/98 21:00	1260	120	480	0.6	1.96	531065	37.77	0.99
012	05/29/98 01:00	60	240	720	0.6	2.94	539013	38.33	1.01
013	05/29/98 05:00	300	240	960	0.6	3.92	536961	38.18	1.00
014	05/29/98 09:00	540	60	1020	0.6	4.17	534909	38.04	1.00
015	05/29/98 13:00	780	240	1260	0.6	5.15	532857	37.90	1.00
016	05/29/98 17:00	1020	240	1500	0.6	6.13	530805	37.75	0.99
017	05/29/98 21:00	1260	240	1740	0.6	7.11	538753	38.31	1.01
018	05/30/98 01:00	60	240	1980	0.6	8.09	536701	38.16	1.00
019	05/30/98 05:00	300	240	2220	0.6	9.07	534649	38.02	1.00
020	05/30/98 09:00	540	240	2460	0.6	10.05	532597	37.88	1.00
021	05/30/98 13:00	780	240	2700	0.6	11.03	530545	37.73	0.99
022	05/30/98 17:00	1020	240	2940	0.6	12.01	538493	38.29	1.01
023	05/28/98 21:00	1260	240	3180	0.6	12.99	536441	38.15	1.00
024	05/29/98 01:00	60	240	3420	0.6	13.97	534389	38.00	1.00

Appendix M

Tracer Study

Column A

Type	Column + Stopcock Mass (g)	Column+Stopcock +Pellet Mass (g)	Pellet Mass (g)	Minus GWC (g)	Column+Stopcock +Pellet+H ₂ O Mass (g)	Fluid Length (cm)	PV (mL)	Cross Sectional Area (cm ²)	Porosity (PV/AL)
P1	459.53	729.47	269.94	264.83	826.97	31.5	102.61	19.6	0.17

Sample ID	Time	Minutes	Time Interval(min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	C/C ₀
Time Zero	06/02/94 08:41	521	0	0	0	0.00	0.00
001	06/03/94 08:50	530	9	9	2	0.18	0.00
002	06/04/94 09:00	540	10	19	2	0.37	0.00
003	06/05/94 09:10	550	10	29	2	0.57	0.00
004	06/06/94 09:20	560	10	39	2	0.76	0.12
005	06/07/94 09:30	570	10	49	2	0.96	0.44
006	06/08/94 09:40	580	10	59	2	1.15	0.67
007	06/09/94 09:50	590	10	69	2	1.34	0.85
008	06/10/94 10:00	600	6	75	2	1.46	0.91
009	06/11/94 10:10	610	10	85	2	1.66	0.92
010	06/12/94 10:20	620	10	95	2	1.85	1.02
011	06/13/94 10:30	630	10	105	2	2.05	0.81
012	06/14/94 10:40	640	10	115	2	2.24	0.54
013	06/15/94 10:50	650	10	125	2	2.44	0.34
014	06/16/94 11:00	660	10	135	2	2.63	0.24
015	06/17/94 11:10	670	10	145	2	2.83	0.17
016	06/18/94 11:20	680	10	155	2	3.02	0.12
017	06/19/94 11:30	690	10	165	2	3.22	0.08
018	06/20/94 11:40	700	10	175	2	3.41	0.06
019	06/21/94 11:50	710	10	185	2	3.61	0.04
020	06/22/94 12:00	720	10	195	2	3.80	0.03
021	06/24/94 12:20	740	10	206	2	4.02	0.02
022	06/25/94 12:30	750	10	216	2	4.21	0.02

Column B

Type	Column + Stopcock Mass (g)	Column+Stopcock+ Pellet Mass (g)	Pellet Mass (g)	Minus GWC (g)	Column+Stopcock +Pellet+H ₂ O Mass (g)	Fluid Length (cm)	PV (mL)	Cross Sectional Area (cm ²)	Porosity (PV/AL)
P1	464.33	732.16	267.83	262.76	836.16	31.5	109.07	19.6	0.18

Sample ID	Time	Minutes	Missing Time (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	C/C ₀
Time Zero	06/02/94 08:41	521	0	0	0	0.00	0.00
001	06/03/94 08:50	530	9	9	2	0.17	0.00
002	06/04/94 09:00	540	10	19	2	0.35	0.00
003	06/05/94 09:10	550	10	29	2	0.53	0.00
004	06/06/94 09:20	560	10	39	2	0.72	0.07
005	06/07/94 09:30	570	10	49	2	0.90	0.36
006	06/08/94 09:40	580	10	59	2	1.08	0.62
007	06/09/94 09:50	590	10	69	2	1.27	0.79
008	06/10/94 10:00	600	6	75	2	1.38	0.84
009	06/11/94 10:10	610	10	85	2	1.56	0.93
010	06/12/94 10:20	620	10	95	2	1.74	1.07
011	06/13/94 10:30	630	10	105	2	1.93	0.92
012	06/14/94 10:40	640	10	115	2	2.11	0.61
013	06/15/94 10:50	650	10	125	2	2.29	0.38
014	06/16/94 11:00	660	10	135	2	2.48	0.26
015	06/17/94 11:10	670	10	145	2	2.66	0.18
016	06/18/94 11:20	680	10	155	2	2.84	0.13
017	06/19/94 11:30	690	10	165	2	3.03	0.08
018	06/20/94 11:40	700	10	175	2	3.21	0.06
019	06/21/94 11:50	710	10	185	2	3.39	0.04
020	06/22/94 12:00	720	10	195	2	3.58	0.03
021	06/24/94 12:20	740	10	206	2	3.78	0.03
022	06/25/94 12:30	750	10	216	2	3.96	0.02

Column C

Type	Column + Stopcock Mass (g)	Column+Stopcock+ Pellet Mass (g)	Pellet Mass (g)	Minus GWC (g)	Column+Stopcock +Pellet+H ₂ O Mass (g)	Fluid Length (cm)	PV (mL)	Cross Sectional Area (cm ²)	Porosity (PV/AL)
P0	469.08	689.30	220.22	216.49	790.20	32.0	104.63	19.6	0.167

Sample ID	Time	Minutes	Missing Time (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	C/C ₀
Time Zero	06/02/94 08:41	521	0	0	0	0.00	0.00
001	06/03/94 08:50	530	9	9	2	0.17	0.00
002	06/04/94 09:00	540	10	19	2	0.36	0.00
003	06/05/94 09:10	550	10	29	2	0.55	0.00
004	06/06/94 09:20	560	10	39	2	0.75	0.11
005	06/07/94 09:30	570	10	49	2	0.94	0.43
006	06/08/94 09:40	580	10	59	2	1.13	0.66
007	06/09/94 09:50	590	10	69	2	1.32	0.83
008	06/10/94 10:00	600	6	75	2	1.43	0.83
009	06/11/94 10:10	610	10	85	2	1.62	0.97
010	06/12/94 10:20	620	10	95	2	1.82	1.05
011	06/13/94 10:30	630	10	105	2	2.01	0.89
012	06/14/94 10:40	640	10	115	2	2.20	0.60
013	06/15/94 10:50	650	10	125	2	2.39	0.36
014	06/16/94 11:00	660	10	135	2	2.58	0.24
015	06/17/94 11:10	670	10	145	2	2.77	0.17
016	06/18/94 11:20	680	10	155	2	2.96	0.12
017	06/19/94 11:30	690	10	165	2	3.15	0.07
018	06/20/94 11:40	700	10	175	2	3.35	0.05
019	06/21/94 11:50	710	10	185	2	3.54	0.04
020	06/22/94 12:00	720	10	195	2	3.73	0.03
021	06/24/94 12:20	740	10	206	2	3.94	0.02
022	06/25/94 12:30	750	10	216	2	4.13	0.02

Column D

Type	Column + Stopcock Mass (g)	Column+Stopcock +Pellet Mass (g)	Pellet Mass (g)	Minus GWC (g)	Column+Stopcock +Pellet+H ₂ O Mass (g)	Fluid Length (cm)	PV (mL)	Cross Sectional Area (cm ²)	Porosity (PV/AL)
P0	435.77	667.10	231.33	227.41	771.90	32.8	108.72	19.6	0.169

Sample ID	Time	Minutes	Missing Time (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	C/C ₀
Time Zero	06/02/94 08:41	521	0	0	0	0.00	0.00
001	06/03/94 08:50	530	9	9	2	0.17	0.00
002	06/04/94 09:00	540	10	19	2	0.35	0.00
003	06/05/94 09:10	550	10	29	2	0.53	0.00
004	06/06/94 09:20	560	10	39	2	0.72	0.07
005	06/07/94 09:30	570	10	49	2	0.90	0.34
006	06/08/94 09:40	580	10	59	2	1.09	0.63
007	06/09/94 09:50	590	10	69	2	1.27	0.79
008	06/10/94 10:00	600	6	75	2	1.38	0.87
009	06/11/94 10:10	610	10	85	2	1.56	0.94
010	06/12/94 10:20	620	10	95	2	1.75	1.03
011	06/13/94 10:30	630	10	105	2	1.93	0.98
012	06/14/94 10:40	640	10	115	2	2.12	0.68
013	06/15/94 10:50	650	10	125	2	2.30	0.40
014	06/16/94 11:00	660	10	135	2	2.48	0.28
015	06/17/94 11:10	670	10	145	2	2.67	0.20
016	06/18/94 11:20	680	10	155	2	2.85	0.13
017	06/19/94 11:30	690	10	165	2	3.04	0.09
018	06/20/94 11:40	700	10	175	2	3.22	0.06
019	06/21/94 11:50	710	10	185	2	3.40	0.04
020	06/22/94 12:00	720	10	195	2	3.59	0.03
021	06/24/94 12:20	740	10	206	2	3.79	0.02
022	06/25/94 12:30	750	10	216	2	3.97	0.01

Column E

Column + Stopcock Mass (g)	Column+Stopcock +Pellet Mass (g)	Pellet Mass (g)	Minus GWC (g)	Column+Stopcock +Pellet+H ₂ O Mass (g)	Fluid Length (cm)	PV (mL)	Cross Sectional Area (cm ²)	Porosity (PV/AL)
452.24	586.34	134.10	128.01	732.24	33.2	151.99	19.6	0.234

Sample ID	Time	Minutes	Missing Time (min)	Elapsed Minutes	Flow Rate (mL/min)	tR	C/C0
Time Zero	06/02/94 08:41	521	0	0	0	0.00	0.00
001	06/03/94 08:50	530	9	9	2	0.12	0.00
002	06/04/94 09:00	540	10	19	2	0.25	0.00
003	06/05/94 09:10	550	10	29	2	0.38	0.07
004	06/06/94 09:20	560	10	39	2	0.51	0.31
005	06/07/94 09:30	570	10	49	2	0.64	0.58
006	06/08/94 09:40	580	10	59	2	0.78	0.74
007	06/09/94 09:50	590	10	69	2	0.91	0.81
008	06/10/94 10:00	600	6	75	2	0.99	0.90
009	06/11/94 10:10	610	10	85	2	1.12	1.00
010	06/12/94 10:20	620	10	95	2	1.25	0.89
011	06/13/94 10:30	630	10	105	2	1.38	0.67
012	06/14/94 10:40	640	10	115	2	1.51	0.42
013	06/15/94 10:50	650	10	125	2	1.64	0.28
014	06/16/94 11:00	660	10	135	2	1.78	0.23
015	06/17/94 11:10	670	10	145	2	1.91	0.15
016	06/18/94 11:20	680	10	155	2	2.04	0.10
017	06/19/94 11:30	690	10	165	2	2.17	0.07
018	06/20/94 11:40	700	10	175	2	2.30	0.06
019	06/21/94 11:50	710	10	185	2	2.43	0.04
020	06/22/94 12:00	720	10	195	2	2.57	0.03
021	06/24/94 12:20	740	10	206	2	2.71	0.01
022	06/25/94 12:30	750	10	216	2	2.84	0.01

Column F

Type	Column + Stopcock Mass (g)	Column+Stopcock +Pellet Mass (g)	Pellet Mass (g)	Minus GWC (g)	Column+Stopcock +Pellet+H ₂ O Mass (g)	Fluid Length (cm)	PV (mL)	Cross Sectional Area (cm ²)	Porosity (PV/AL)
B0	466.47	601.51	135.04	128.90	742.24	33.2	146.87	19.6	0.226

Sample ID	Time	Minutes	Missing Time (min)	Elapsed Minutes	Flow Rate (mL/min)	t _R	C/C ₀
Time Zero	06/02/94 08:41	521	0	0	0	0.00	0.00
001	06/03/94 08:50	530	9	9	2	0.12	0.00
002	06/04/94 09:00	540	10	19	2	0.26	0.00
003	06/05/94 09:10	550	10	29	2	0.39	0.08
004	06/06/94 09:20	560	10	39	2	0.53	0.32
005	06/07/94 09:30	570	10	49	2	0.67	0.56
006	06/08/94 09:40	580	10	59	2	0.80	0.75
007	06/09/94 09:50	590	10	69	2	0.94	0.79
008	06/10/94 10:00	600	6	75	2	1.02	0.91
009	06/11/94 10:10	610	10	85	2	1.16	0.99
010	06/12/94 10:20	620	10	95	2	1.29	0.85
011	06/13/94 10:30	630	10	105	2	1.43	0.69
012	06/14/94 10:40	640	10	115	2	1.57	0.44
013	06/15/94 10:50	650	10	125	2	1.70	0.30
014	06/16/94 11:00	660	10	135	2	1.84	0.21
015	06/17/94 11:10	670	10	145	2	1.97	0.15
016	06/18/94 11:20	680	10	155	2	2.11	0.09
017	06/19/94 11:30	690	10	165	2	2.25	0.06
018	06/20/94 11:40	700	10	175	2	2.38	0.05
019	06/21/94 11:50	710	10	185	2	2.52	0.04
020	06/22/94 12:00	720	10	195	2	2.66	0.02
021	06/24/94 12:20	740	10	206	2	2.81	0.02
022	06/25/94 12:30	750	10	216	2	2.94	0.01

Appendix N
Column A:CXTFIT 2.0 Input and Output Files

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column A - Tritium Tracer Study - 2 mL/min
INVERSE  MODE  NREDU
1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
1      31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
V      D      R      Mu
36.88  1      1.00  0
0      1      0      0
0.00   0.00   1.0   0.00
0.00   1000.0 5.0   1.00
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
3
1.0  1.46
*** 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
31.5
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.00
0.18  0.00
0.37  0.00
0.57  0.00
0.76  0.12
0.96  0.44
1.15  0.67
1.34  0.85
1.46  0.91
1.66  0.92
1.85  1.00
2.05  0.81
2.24  0.54
2.44  0.34
2.63  0.24
2.83  0.17
3.02  0.12
3.22  0.08
3.41  0.06
3.61  0.04
3.80  0.03
4.02  0.02
4.21  0.02
0 0 0

```

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column A - Tritium Tracer Study - 2 mL/min
*
* DATA INPUT FILE: at.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.3688E+02	N		
D.....	.1000E+01	Y	.0000E+00	.1000E+04
R.....	.1000E+01	N		
mu.....	.0000E+00	N		

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
SINGLE PULSE OF CONC. = 1.0000 & DURATION = 1.4600
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

ITER	SSQ	D....
0	.7114E+00	.100E+01
1	.5622E+00	.372E+01
2	.3412E+00	.147E+02
3	.1455E+00	.429E+02
4	.9499E-01	.726E+02
5	.9139E-01	.840E+02
6	.9134E-01	.855E+02
7	.9134E-01	.856E+02

8 .9134E-01 .856E+02

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .96809990
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

		95% CONFIDENCE LIMITS		
NAME	VALUE	S.E.COEFF.	LOWER	UPPER
D....	.8562E+02	.6444E-01	.8548E+02	.8575E+02

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

		CONCENTRATION			RESI-	
\$	NO	DISTANCE	TIME	OBS	FITTED	DUAL
	1	31.5000	.0000	.0000	.0000	
	2	31.5000	.1800	.0000	.0000	
	3	31.5000	.3700	.0000	.0052	-.0052
	4	31.5000	.5700	.0000	.0927	-.0927
	5	31.5000	.7600	.1200	.2934	-.1734
	6	31.5000	.9600	.4400	.5313	-.0913
	7	31.5000	1.1500	.6700	.7113	-.0413
	8	31.5000	1.3400	.8500	.8326	.0174
	9	31.5000	1.4600	.9100	.8838	.0262
	10	31.5000	1.6600	.9200	.9384	-.0184
	11	31.5000	1.8500	1.0000	.9589	.0411
	12	31.5000	2.0500	.8100	.8737	-.0637
	13	31.5000	2.2400	.5400	.6735	-.1335
	14	31.5000	2.4400	.3400	.4427	-.1027
	15	31.5000	2.6300	.2400	.2710	-.0310
	16	31.5000	2.8300	.1700	.1519	.0181
	17	31.5000	3.0200	.1200	.0843	.0357
	18	31.5000	3.2200	.0800	.0441	.0359
	19	31.5000	3.4100	.0600	.0234	.0366
	20	31.5000	3.6100	.0400	.0119	.0281
	21	31.5000	3.8000	.0300	.0062	.0238
	22	31.5000	4.0200	.0200	.0029	.0171
	23	31.5000	4.2100	.0200	.0015	.0185

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column A - 4 mL/min
INVERSE MODE  NREDU
1      1      3
MODC    ZL(BLANK IF MODE=NREDU=1)
1      31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT    ILMT  MASS
200    1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
V      D      R      Mu
73.76  171.24  1.00  1.0
0      0      1      1
0      0      1.00  1.0
0      0      2.00  5.0
*** BLOCK D: BVP; MODB= 0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB           =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
2
38.0
*** 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
31.5
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.03
0.19  0.04
0.74  0.47
1.17  0.69
1.48  0.75
2.14  0.78
2.61  0.79
3.08  0.80
3.70  0.81
4.25  0.81
4.76  0.82
5.61  0.86
6.70  0.87
7.37  0.87
7.95  0.83
8.54  0.88
9.55  0.89
10.53 0.89
11.73 0.90
14.15 0.90
16.68 0.90
18.83 0.91
21.17 0.91
22.77 0.91

```

000

\$

```

*****
*                               *
*   CXTFIT VERSION 2.0 (1/2/95)   *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE   *
*   NON-LINEAR LEAST-SQUARES ANALYSIS   *
*                               *
*   CERCONA PELLET STUDY   *
*   Column A - 4 mL/min   *
*                               *
*   DATA INPUT FILE: a6.in   *
*                               *
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.7376E+02	N		
D.....	.1712E+03	N		
R.....	.1000E+01	Y	.1000E+01	.2000E+01
mu.....	.1000E+01	Y	.1000E+01	.5000E+01

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

ITER	SSQ	R....	mu...
0	.4097E+04	.100E+01	.100E+01
1	.5802E+03	.111E+01	.207E+01
2	.7089E+02	.120E+01	.316E+01
3	.6082E+01	.126E+01	.411E+01
4	.2581E+00	.125E+01	.469E+01
5	.6329E-01	.122E+01	.485E+01
6	.6263E-01	.121E+01	.486E+01
7	.6262E-01	.121E+01	.486E+01

8 .6262E-01 .121E+01 .486E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

R.... mu...
R.... 1.000
mu... -.156 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .95413809
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS

NAME	VALUE	S.E.	COEFF.	T-VALUE	LOWER	UPPER
R....	.1205E+01	.5401E-01	.2232E+02	.1093E+01	.1317E+01	
mu...	.4863E+01	.5401E-01	.9005E+02	.4751E+01	.4975E+01	

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

\$	NO	DISTANCE	TIME	CONCENTRATION		RESI-	DUAL
				OBS	FITTED		
	1	31.5000	.0000	.0300	.0000	.0300	
	2	31.5000	.1900	.0400	.0000	.0400	
	3	31.5000	.7400	.4700	.4282	.0418	
	4	31.5000	1.1700	.6900	.7964	-.1064	
	5	31.5000	1.4800	.7500	.8420	-.0920	
	6	31.5000	2.1400	.7800	.8505	-.0705	
	7	31.5000	2.6100	.7900	.8506	-.0606	
	8	31.5000	3.0800	.8000	.8506	-.0506	
	9	31.5000	3.7000	.8100	.8506	-.0406	
	10	31.5000	4.2500	.8100	.8506	-.0406	
	11	31.5000	4.7600	.8200	.8506	-.0306	
	12	31.5000	5.6100	.8600	.8506	.0094	
	13	31.5000	6.7000	.8700	.8506	.0194	
	14	31.5000	7.3700	.8700	.8506	.0194	
	15	31.5000	7.9500	.8300	.8506	-.0206	
	16	31.5000	8.5400	.8800	.8506	.0294	
	17	31.5000	9.5500	.8900	.8506	.0394	
	18	31.5000	10.5300	.8900	.8506	.0394	
	19	31.5000	11.7300	.9000	.8506	.0494	
	20	31.5000	14.1500	.9000	.8506	.0494	
	21	31.5000	16.6800	.9000	.8506	.0494	
	22	31.5000	18.8300	.9100	.8506	.0594	
	23	31.5000	21.1700	.9100	.8506	.0594	
	24	31.5000	22.7700	.9100	.8506	.0594	

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column A - 2 mL/min
INVERSE MODE NREDU
  1      1      3
MODC    ZL(BLANK IF MODE=NREDU=1)
  1      31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V      D      R      Mu
36.88  85.62  1.00  1.0
  0      0      1      1
  0      0      1.00  1.0
  0      0      10.00 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
  38.0
*** 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
  31.5
TIME    CONC    (Give "0 0 0" after last data set.)
0.00  0.05
0.18  0.06
0.39  0.05
0.57  0.05
0.76  0.06
0.96  0.06
1.15  0.05
1.46  0.05
1.68  0.05
2.05  0.03
2.34  0.03
2.73  0.10
3.12  0.14
3.51  0.24
3.82  0.32
4.58  0.58
4.87  0.68
5.26  0.77
5.65  0.83
6.39  0.88
7.02  0.91
7.80  0.92
8.81  0.94
10.23 0.94

```

11.29 0.95
12.77 0.96
17.15 0.96
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column A - 2 mL/min
*
* DATA INPUT FILE: a3.in
*
*****

```

MODEL DESCRIPTION

DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
 FLUX-AVERAGED CONCENTRATION
 REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.3688E+02	N		
D.....	.8562E+02	N		
R.....	.1000E+01	Y	.1000E+01	.1000E+02
mu.....	.1000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

STEP INPUT OF CONC. = 38.0000
 SOLUTE FREE INITIAL CONDITION
 NO PRODUCTION TERM

PARAMETER ESTIMATION MODE

MAXIMUM NUMBER OF ITERATIONS = 200

ITER	SSQ	R....	mu...
0	.4373E+04	.100E+01	.100E+01
1	.6407E+03	.114E+01	.209E+01
2	.8721E+02	.131E+01	.324E+01
3	.1168E+02	.156E+01	.432E+01
4	.3117E+01	.201E+01	.510E+01
5	.2055E+01	.287E+01	.533E+01
6	.9154E+00	.442E+01	.514E+01
7	.8165E-01	.635E+01	.481E+01

8 .3320E-01 .682E+01 .468E+01
 9 .3307E-01 .678E+01 .468E+01
 10 .3307E-01 .679E+01 .468E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

R.... mu...
 R.... 1.000
 mu... -.474 1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99217229
 (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS

NAME	VALUE	S.E.COEFF.	T-VALUE	LOWER	UPPER
R....	.6785E+01	.4131E-01	.1643E+03	.6700E+01	.6871E+01
mu...	.4681E+01	.4131E-01	.1133E+03	.4596E+01	.4766E+01

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

\$	NO	DISTANCE	TIME	CONCENTRATION		RESI-	DUAL
				OBS	FITTED		
1	31.5000	.0000	.0500	.0000	.0500		
2	31.5000	.1800	.0600	.0000	.0600		
3	31.5000	.3900	.0500	.0000	.0500		
4	31.5000	.5700	.0500	.0000	.0500		
5	31.5000	.7600	.0600	.0000	.0600		
6	31.5000	.9600	.0600	.0000	.0600		
7	31.5000	1.1500	.0500	.0000	.0500		
8	31.5000	1.4600	.0500	.0001	.0499		
9	31.5000	1.6800	.0500	.0009	.0491		
10	31.5000	2.0500	.0300	.0076	.0224		
11	31.5000	2.3400	.0300	.0245	.0055		
12	31.5000	2.7300	.1000	.0738	.0262		
13	31.5000	3.1200	.1400	.1569	-.0169		
14	31.5000	3.5100	.2400	.2660	-.0260		
15	31.5000	3.8200	.3200	.3618	-.0418		
16	31.5000	4.5800	.5800	.5853	-.0053		
17	31.5000	4.8700	.6800	.6564	.0236		
18	31.5000	5.2600	.7700	.7362	.0338		
19	31.5000	5.6500	.8300	.7984	.0316		
20	31.5000	6.3900	.8800	.8764	.0036		
21	31.5000	7.0200	.9100	.9134	-.0034		
22	31.5000	7.8000	.9200	.9372	-.0172		
23	31.5000	8.8100	.9400	.9500	-.0100		
24	31.5000	10.2300	.9400	.9552	-.0152		
25	31.5000	11.2900	.9500	.9561	-.0061		
26	31.5000	12.7700	.9600	.9565	.0035		
27	31.5000	17.1500	.9600	.9565	.0035		

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column A - 0.6 mL/min
INVERSE MODE  NREDU
1      1      3
MODC    ZL(BLANK IF MODE=NREDU=1)
1      31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT    ILMT  MASS
200    1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
V      D      R      Mu
11.06  25.69  1.0  1.0
0      0      1      1
0      0      1.0  1.0
0      0      20.0 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB    =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
2
38.0
*** 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
31.5
TIME    CONC    (Give "0 0 0" after last data set.)
0.00 0.00
0.18 0.05
0.35 0.04
0.53 0.04
0.70 0.03
1.05 0.03
1.40 0.03
1.75 0.03
2.11 0.03
2.81 0.04
3.16 0.03
3.86 0.11
4.56 0.43
5.26 0.58
6.67 0.74
8.07 0.75
9.47 0.75
10.88 0.75
12.28 0.76
13.68 0.75
15.09 0.75
16.49 0.75
17.89 0.76
19.30 0.76

```

000

S

```

*****
*                                     *
*   CXTFIT VERSION 2.0 (1/2/95)       *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE       *
*   NON-LINEAR LEAST-SQUARES ANALYSIS *
*                                     *
*   CERCONA PELLET STUDY             *
*   Column A - 0.6 mL/min            *
*                                     *
*   DATA INPUT FILE: a1.in          *
*                                     *
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.1106E+02	N		
D.....	.2569E+02	N		
R.....	.1000E+01	Y	.1000E+01	.2000E+02
mu.....	.1000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

ITER	SSQ	R....	mu...
0	.3858E+04	.100E+01	.100E+01
1	.5682E+03	.114E+01	.209E+01
2	.7788E+02	.130E+01	.326E+01
3	.1013E+02	.156E+01	.438E+01
4	.2190E+01	.204E+01	.523E+01
5	.1315E+01	.298E+01	.554E+01
6	.6935E+00	.451E+01	.540E+01
7	.7227E-01	.687E+01	.513E+01

```

8 .3584E-01 .761E+01 .503E+01
9 .3527E-01 .749E+01 .503E+01
10 .3523E-01 .751E+01 .503E+01
11 .3523E-01 .751E+01 .503E+01

```

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

=====
R.... mu...
R.... 1.000
mu... -.310 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98756746
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```

=====
                        95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R.... .7510E+01 .4209E-01 .1784E+03 .7422E+01 .7597E+01
mu... .5032E+01 .4209E-01 .1195E+03 .4944E+01 .5119E+01

```

```

-----ORDERED BY COMPUTER INPUT-----
CONCENTRATION  RESI-
$ NO  DISTANCE  TIME  OBS  FITTED  DUAL
1  31.5000  .0000  .0000  .0000  .0000
2  31.5000  .1800  .0500  .0000  .0500
3  31.5000  .3500  .0400  .0000  .0400
4  31.5000  .5300  .0400  .0000  .0400
5  31.5000  .7000  .0300  .0000  .0300
6  31.5000  1.0500  .0300  .0000  .0300
7  31.5000  1.4000  .0300  .0000  .0300
8  31.5000  1.7500  .0300  .0004  .0296
9  31.5000  2.1100  .0300  .0034  .0266
10 31.5000  2.8100  .0400  .0405  -.0005
11 31.5000  3.1600  .0300  .0853  -.0553
12 31.5000  3.8600  .1100  .2232  -.1132
13 31.5000  4.5600  .4300  .3837  .0463
14 31.5000  5.2600  .5800  .5223  .0577
15 31.5000  6.6700  .7400  .6858  .0542
16 31.5000  8.0700  .7500  .7428  .0072
17 31.5000  9.4700  .7500  .7590  -.0090
18 31.5000  10.8800  .7500  .7630  -.0130
19 31.5000  12.2800  .7600  .7640  -.0040
20 31.5000  13.6800  .7500  .7642  -.0142
21 31.5000  15.0900  .7500  .7642  -.0142
22 31.5000  16.4900  .7500  .7643  -.0143
23 31.5000  17.8900  .7600  .7643  -.0043
24 31.5000  19.3000  .7600  .7643  -.0043

```

Appendix O
Column B:CXTFIT 2.0 Input and Output Files

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column B - Tritium Tracer Study - 2 mL/min
INVERSE  MODE  NREDU
1      1      3
MODC    ZL(BLANK IF MODE=NREDU=1)
1      31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT     ILMT  MASS
200     1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
V       D      R    Mu
34.01   1      1.0  0
0       1      0    0
0       0.00   1.0  0.00
0       2000.0 1.0  0.00
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB     =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
3
1.0  1.38
*** 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
31.5
TIME  CONC  (Give "0 0 0" after last data set.)
0.00 0.00
0.17 0.00
0.35 0.00
0.53 0.00
0.72 0.07
0.90 0.36
1.08 0.62
1.27 0.79
1.38 0.84
1.56 0.93
1.74 1.00
1.93 0.92
2.11 0.61
2.29 0.38
2.48 0.26
2.66 0.18
2.84 0.13
3.03 0.08
3.21 0.06
3.39 0.04
3.58 0.03
3.78 0.03
3.96 0.02
0 0 0

```

\$

```

*****
*                                     *
*   CXTFIT VERSION 2.0 (1/2/95)       *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE       *
*   NON-LINEAR LEAST-SQUARES ANALYSIS *
*                                     *
*   CERCONA PELLET STUDY             *
*   Column B - Tritium Tracer Study - 2 mL/min *
*                                     *
*   DATA INPUT FILE: bt.in          *
*                                     *
*****

```

MODEL DESCRIPTION

DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
 FLUX-AVERAGED CONCENTRATION
 REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.3401E+02	N		
D.....	.1000E+01	Y	.0000E+00	.2000E+04
R.....	.1000E+01	N		
mu.....	.0000E+00	N		

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

SINGLE PULSE OF CONC. = 1.0000 & DURATION = 1.3800
 SOLUTE FREE INITIAL CONDITION
 NO PRODUCTION TERM

PARAMETER ESTIMATION MODE

MAXIMUM NUMBER OF ITERATIONS = 200

ITER	SSQ	D....
0	.9705E+00	.100E+01
1	.4484E+00	.879E+01
2	.2085E+00	.262E+02
3	.1014E+00	.552E+02
4	.9022E-01	.711E+02
5	.9005E-01	.734E+02
6	.9005E-01	.735E+02
7	.9005E-01	.735E+02

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .96849381
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

		95% CONFIDENCE LIMITS		
NAME	VALUE	S.E.COEFF.	LOWER	UPPER
D....	.7354E+02	.6398E-01	.7341E+02	.7367E+02

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

			CONCENTRATION	RESI-	
\$	NO	DISTANCE	TIME	OBS	FITTED DUAL
	1	31.5000	.0000	.0000	.0000
	2	31.5000	.1700	.0000	.0000
	3	31.5000	.3500	.0000	-.0023
	4	31.5000	.5300	.0000	-.0557
	5	31.5000	.7200	.0700	-.1641
	6	31.5000	.9000	.3600	-.0967
	7	31.5000	1.0800	.6200	-.0323
	8	31.5000	1.2700	.7900	-.0088
	9	31.5000	1.3800	.8400	-.0170
	10	31.5000	1.5600	.9300	.0095
	11	31.5000	1.7400	1.0000	.0461
	12	31.5000	1.9300	.9200	.0108
	13	31.5000	2.1100	.6100	-.1324
	14	31.5000	2.2900	.3800	-.1452
	15	31.5000	2.4800	.2600	-.0663
	16	31.5000	2.6600	.1800	-.0137
	17	31.5000	2.8400	.1300	.0202
	18	31.5000	3.0300	.0800	.0217
	19	31.5000	3.2100	.0600	.0287
	20	31.5000	3.3900	.0400	.0235
	21	31.5000	3.5800	.0300	.0217
	22	31.5000	3.7800	.0300	.0260
	23	31.5000	3.9600	.0200	.0179

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column B - 4 mL/min
INVERSE  MODE  NREDU
  1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
  1     31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V      D      R      Mu
68.03   147.10  1.00  1.0
  0      0      1      1
  0      0     1.00  1.0
  0      0    10.00 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB          =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
38.0
*** 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
  31.5
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.00
0.00  0.03
0.22  0.04
0.73  0.48
1.14  0.66
1.43  0.73
2.05  0.75
2.49  0.77
2.93  0.79
3.52  0.79
4.03  0.80
4.51  0.81
5.32  0.83
6.34  0.85
6.97  0.86
7.48  0.87
8.03  0.87
9.02  0.88
9.90  0.89
11.08 0.88
13.39 0.89
15.70 0.90
17.71 0.90
19.95 0.90

```

21.45 0.90
000

21.45 0.90
000

\$

```

*****
*                                     *
*   CXTFIT VERSION 2.0 (1/2/95)       *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE       *
*   NON-LINEAR LEAST-SQUARES ANALYSIS *
*                                     *
*   CERCONA PELLET STUDY             *
*   Column B - 4 mL/min              *
*                                     *
*   DATA INPUT FILE: b6.in          *
*                                     *
*****

```

MODEL DESCRIPTION

DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
 FLUX-AVERAGED CONCENTRATION
 REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.6803E+02	N		
D.....	.1471E+03	N		
R.....	.1000E+01	Y	.1000E+01	.1000E+02
mu.....	.1000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

STEP INPUT OF CONC. = 38.0000
 SOLUTE FREE INITIAL CONDITION
 NO PRODUCTION TERM

PARAMETER ESTIMATION MODE

MAXIMUM NUMBER OF ITERATIONS = 200

ITER	SSQ	R....	mu...
0	.4054E+04	.100E+01	.100E+01
1	.5709E+03	.110E+01	.206E+01
2	.6943E+02	.119E+01	.314E+01
3	.5949E+01	.123E+01	.408E+01
4	.2683E+00	.121E+01	.465E+01
5	.7812E-01	.117E+01	.480E+01
6	.7720E-01	.115E+01	.481E+01
7	.7716E-01	.115E+01	.481E+01

8 .7716E-01 .115E+01 .481E+01
 9 .7716E-01 .115E+01 .481E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

R.... mu...
 R.... 1.000
 mu... -.157 1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .95891384
 (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS
 NAME VALUE S.E.COEFF. T-VALUE LOWER UPPER
 R.... .1149E+01 .5865E-01 .1959E+02 .1027E+01 .1270E+01
 mu... .4812E+01 .5865E-01 .8205E+02 .4690E+01 .4933E+01

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

			CONCENTRATION	RESI-	
\$	NO	DISTANCE	TIME	OBS	FITTED DUAL
	1	31.5000	.0000	.0000	.0000
	2	31.5000	.0000	.0300	.0300
	3	31.5000	.2200	.0400	.0400
	4	31.5000	.7300	.4800	.4323 .0477
	5	31.5000	1.1400	.6600	.7878 -.1278
	6	31.5000	1.4300	.7300	.8306 -.1006
	7	31.5000	2.0500	.7500	.8386 -.0886
	8	31.5000	2.4900	.7700	.8387 -.0687
	9	31.5000	2.9300	.7900	.8387 -.0487
	10	31.5000	3.5200	.7900	.8387 -.0487
	11	31.5000	4.0300	.8000	.8387 -.0387
	12	31.5000	4.5100	.8100	.8387 -.0287
	13	31.5000	5.3200	.8300	.8387 -.0087
	14	31.5000	6.3400	.8500	.8387 .0113
	15	31.5000	6.9700	.8600	.8387 .0213
	16	31.5000	7.4800	.8700	.8387 .0313
	17	31.5000	8.0300	.8700	.8387 .0313
	18	31.5000	9.0200	.8800	.8387 .0413
	19	31.5000	9.9000	.8900	.8387 .0513
	20	31.5000	11.0800	.8800	.8387 .0413
	21	31.5000	13.3900	.8900	.8387 .0513
	22	31.5000	15.7000	.9000	.8387 .0613
	23	31.5000	17.7100	.9000	.8387 .0613
	24	31.5000	19.9500	.9000	.8387 .0613
	25	31.5000	21.4500	.9000	.8387 .0613

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column B - 2 mL/min
INVERSE  MODE  NREDU
1      1      3
MODC    ZL(BLANK IF MODE=NREDU=1)
1      31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT     ILMT  MASS
200     1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
V       D      R      Mu
34.01   73.55  1.00  1.0
0       0      1      1
0       0      1.00  1.0
0       0      10.00 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB          =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
2
38.0
*** 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
31.5
TIME    CONC  (Give "0 0 0" after last data set.)
0.00 0.06
0.17 0.05
0.37 0.05
0.53 0.05
0.72 0.06
0.90 0.05
1.08 0.05
1.38 0.05
1.65 0.05
1.93 0.05
2.20 0.05
2.57 0.04
2.93 0.08
3.30 0.13
3.59 0.20
4.31 0.46
4.58 0.56
4.95 0.68
5.32 0.78
6.01 0.84
6.60 0.88
7.33 0.90
8.29 0.91
9.63 0.92

```

10.62 0.94
12.01 0.95
16.14 0.95
0 0 0

\$

```

*****
*                                     *
*   CXTFIT VERSION 2.0 (1/2/95)       *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE       *
*   NON-LINEAR LEAST-SQUARES ANALYSIS *
*                                     *
*   CERCONA PELLET STUDY             *
*   Column B - 2 mL/min               *
*                                     *
*   DATA INPUT FILE: b3.in          *
*                                     *
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .3401E+02   N
D.....  .7355E+02   N
R.....  .1000E+01   Y  .1000E+01  .1000E+02
mu.....  .1000E+01   Y  .1000E+01  .1000E+02

```

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

```

ITER  SSQ    R....  mu...
0     .4298E+04 .100E+01 .100E+01
1     .6277E+03 .113E+01 .208E+01
2     .8563E+02 .129E+01 .322E+01
3     .1164E+02 .151E+01 .431E+01
4     .3183E+01 .191E+01 .510E+01
5     .2195E+01 .269E+01 .536E+01
6     .1146E+01 .414E+01 .517E+01
7     .1433E+00 .614E+01 .482E+01

```

```

8 .4167E-01 .686E+01 .462E+01
9 .4076E-01 .677E+01 .463E+01
10 .4075E-01 .678E+01 .463E+01
11 .4075E-01 .678E+01 .463E+01

```

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

=====
R.... mu...
R.... 1.000
mu... -.485 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98989235
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```

=====
                        95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R.... .6780E+01 .4618E-01 .1468E+03 .6685E+01 .6875E+01
mu... .4628E+01 .4618E-01 .1002E+03 .4533E+01 .4723E+01

```

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

S	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
1	31.5000	.0000	.0600	.0000	.0600	
2	31.5000	.1700	.0500	.0000	.0500	
3	31.5000	.3700	.0500	.0000	.0500	
4	31.5000	.5300	.0500	.0000	.0500	
5	31.5000	.7200	.0600	.0000	.0600	
6	31.5000	.9000	.0500	.0000	.0500	
7	31.5000	1.0800	.0500	.0000	.0500	
8	31.5000	1.3800	.0500	.0000	.0500	
9	31.5000	1.6500	.0500	.0004	.0496	
10	31.5000	1.9300	.0500	.0026	.0474	
11	31.5000	2.2000	.0500	.0101	.0399	
12	31.5000	2.5700	.0400	.0377	.0023	
13	31.5000	2.9300	.0800	.0916	-.0116	
14	31.5000	3.3000	.1300	.1756	-.0456	
15	31.5000	3.5900	.2000	.2566	-.0566	
16	31.5000	4.3100	.4600	.4751	-.0151	
17	31.5000	4.5800	.5600	.5514	.0086	
18	31.5000	4.9500	.6800	.6441	.0359	
19	31.5000	5.3200	.7800	.7207	.0593	
20	31.5000	6.0100	.8400	.8227	.0173	
21	31.5000	6.6000	.8800	.8758	.0042	
22	31.5000	7.3300	.9000	.9127	-.0127	
23	31.5000	8.2900	.9100	.9345	-.0245	
24	31.5000	9.6300	.9200	.9441	-.0241	
25	31.5000	10.6200	.9400	.9460	-.0060	
26	31.5000	12.0100	.9500	.9467	.0033	
27	31.5000	16.1400	.9500	.9469	.0031	

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column B - 0.6 mL/min
INVERSE  MODE  NREDU
  1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
  1     31.5
*** BLOCK B: INVERSE PROBLEM *****
MIT  ILMT  MASS
200   1    0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V    D    R    Mu
10.20 22.06  1.0  1.0
  0    0    1    1
  0    0    1.0  1.0
  0    0   20.0 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB           =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
38.0
*** 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
  31.5
TIME  CONC  (Give "0 0 0" after last data set.)
0.17 0.07
0.33 0.04
0.50 0.03
0.66 0.03
0.99 0.03
1.32 0.03
1.65 0.03
1.98 0.03
2.64 0.03
2.97 0.03
3.63 0.07
4.29 0.33
4.95 0.55
6.27 0.68
7.59 0.70
8.91 0.72
10.23 0.74
11.55 0.74
12.87 0.74
14.19 0.74
15.51 0.74
16.83 0.74
18.15 0.74
19.47 0.74

```

000

\$

```

*****
*                                     *
*   CXTFIT VERSION 2.0 (1/2/95)       *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE       *
*   NON-LINEAR LEAST-SQUARES ANALYSIS *
*                                     *
*   CERCONA PELLET STUDY             *
*   Column B - 0.6 mL/min            *
*                                     *
*   DATA INPUT FILE: b1.in          *
*                                     *
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .1020E+02  N
D.....  .2206E+02  N
R.....  .1000E+01  Y  .1000E+01  .2000E+02
mu.....  .1000E+01  Y  .1000E+01  .1000E+02

```

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

```

ITER  SSQ    R....  mu...
0  .3995E+04  .100E+01  .100E+01
1  .5845E+03  .113E+01  .209E+01
2  .7959E+02  .129E+01  .323E+01
3  .1021E+02  .154E+01  .434E+01
4  .2139E+01  .201E+01  .516E+01
5  .1273E+01  .290E+01  .546E+01
6  .6662E+00  .434E+01  .534E+01
7  .7112E-01  .653E+01  .509E+01

```

```

8 .3237E-01 .729E+01 .499E+01
9 .3202E-01 .720E+01 .500E+01
10 .3200E-01 .721E+01 .500E+01
11 .3200E-01 .721E+01 .500E+01

```

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

=====
R.... mu...
R.... 1.000
mu... -.295 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98797941
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```

=====
                        95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R.... .7209E+01 .3992E-01 .1806E+03 .7127E+01 .7292E+01
mu... .4998E+01 .3992E-01 .1252E+03 .4915E+01 .5081E+01

```

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

\$	NO	DISTANCE	CONCENTRATION		RESI-		DUAL
			TIME	OBS	FITTED		
	1	31.5000	.1700	.0700	.0000	.0700	
	2	31.5000	.3300	.0400	.0000	.0400	
	3	31.5000	.5000	.0300	.0000	.0300	
	4	31.5000	.6600	.0300	.0000	.0300	
	5	31.5000	.9900	.0300	.0000	.0300	
	6	31.5000	1.3200	.0300	.0000	.0300	
	7	31.5000	1.6500	.0300	.0001	.0299	
	8	31.5000	1.9800	.0300	.0016	.0284	
	9	31.5000	2.6400	.0300	.0256	.0044	
	10	31.5000	2.9700	.0300	.0592	-.0292	
	11	31.5000	3.6300	.0700	.1760	-.1060	
	12	31.5000	4.2900	.3300	.3276	.0024	
	13	31.5000	4.9500	.5500	.4692	.0808	
	14	31.5000	6.2700	.6800	.6482	.0318	
	15	31.5000	7.5900	.7000	.7159	-.0159	
	16	31.5000	8.9100	.7200	.7360	-.0160	
	17	31.5000	10.2300	.7400	.7412	-.0012	
	18	31.5000	11.5500	.7400	.7424	-.0024	
	19	31.5000	12.8700	.7400	.7427	-.0027	
	20	31.5000	14.1900	.7400	.7427	-.0027	
	21	31.5000	15.5100	.7400	.7427	-.0027	
	22	31.5000	16.8300	.7400	.7427	-.0027	
	23	31.5000	18.1500	.7400	.7427	-.0027	
	24	31.5000	19.4700	.7400	.7427	-.0027	

Appendix P
Column C:CXTFIT 2.0 Input and Output Files

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column C - Tritium Tracer Study - 2 mL/min
INVERSE MODE NREDU
1 1 3
MODC ZL(BLANK IF MODE=NREDU=1)
1 32.0
*** BLOCK B: INVERSE PROBLEM *****
MIT ILMT MASS
200 1 0
*** BLOCK C: TRANSPORT PARAMETERS *****
V D R Mu
36.66 1 1.00 0
0 1 0 0
36.66 0.00 1.0 0.00
36.66 20000 1.0 0.00
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
3
1.0 1.43
*** 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
32.0
TIME CONC (Give "0 0 0" after last data set.)
0.00 0.00
0.17 0.00
0.36 0.00
0.55 0.00
0.75 0.11
0.94 0.43
1.13 0.66
1.32 0.83
1.43 0.89
1.62 0.97
1.82 1.00
2.01 0.89
2.20 0.60
2.39 0.36
2.58 0.24
2.77 0.17
2.96 0.12
3.15 0.07
3.35 0.05
3.54 0.04
3.73 0.03
3.94 0.02
4.13 0.02
0 0 0

```

\$

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column C - Tritium Tracer Study - 2 mL/min
*
* DATA INPUT FILE: ct.in
*
*****

```

MODEL DESCRIPTION

DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
 FLUX-AVERAGED CONCENTRATION
 REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.3666E+02	N		
D.....	.1000E+01	Y	.0000E+00	.2000E+05
R.....	.1000E+01	N		
mu.....	.0000E+00	N		

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

SINGLE PULSE OF CONC. = 1.0000 & DURATION = 1.4300
 SOLUTE FREE INITIAL CONDITION
 NO PRODUCTION TERM

PARAMETER ESTIMATION MODE

MAXIMUM NUMBER OF ITERATIONS = 200

ITER	SSQ	D....
0	.8063E+00	.100E+01
1	.4980E+00	.475E+01
2	.2648E+00	.161E+02
3	.9876E-01	.432E+02
4	.6774E-01	.668E+02
5	.6661E-01	.729E+02
6	.6660E-01	.734E+02
7	.6660E-01	.734E+02

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97781497
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

		95% CONFIDENCE LIMITS		
NAME	VALUE	S.E.COEFF.	LOWER	UPPER
D....	.7338E+02	.5502E-01	.7327E+02	.7350E+02

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

		CONCENTRATION		RESI-	
\$	NO	DISTANCE	TIME	OBS	FITTED DUAL
	1	32.0000	.0000	.0000	.0000
	2	32.0000	.1700	.0000	.0000
	3	32.0000	.3600	.0000	-.0019
	4	32.0000	.5500	.0000	-.0582
	5	32.0000	.7500	.1100	-.1458
	6	32.0000	.9400	.4300	-.0680
	7	32.0000	1.1300	.6600	-.0397
	8	32.0000	1.3200	.8300	-.0043
	9	32.0000	1.4300	.8900	.0044
	10	32.0000	1.6200	.9700	.0284
	11	32.0000	1.8200	1.0000	.0321
	12	32.0000	2.0100	.8900	-.0174
	13	32.0000	2.2000	.6000	-.1126
	14	32.0000	2.3900	.3600	-.1149
	15	32.0000	2.5800	.2400	-.0416
	16	32.0000	2.7700	.1700	.0156
	17	32.0000	2.9600	.1200	.0396
	18	32.0000	3.1500	.0700	.0297
	19	32.0000	3.3500	.0500	.0310
	20	32.0000	3.5400	.0400	.0309
	21	32.0000	3.7300	.0300	.0257
	22	32.0000	3.9400	.0200	.0181
	23	32.0000	4.1300	.0200	.0191

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column C - 4 mL/min
INVERSE MODE NREDU
  1   1   3
MODC  ZL(BLANK IF MODE=NREDU=1)
  1  32.0
*** BLOCK B: INVERSE PROBLEM *****
MIT  ILMT  MASS
200   1    0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V    D    R    Mu
73.32 146.76 1.00 5.0
  0    0    1    1
  0    0    1.00 1.0
  0    0    2.00 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
38.0
*** 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
  32.0
TIME  CONC  (Give "0 0 0" after last data set.)
0.00 0.02
0.27 0.02
0.80 0.72
1.22 0.88
1.53 0.91
2.18 0.93
2.64 0.97
3.10 0.95
3.67 0.95
4.24 0.95
4.78 0.98
5.54 1.00
6.65 0.99
7.26 0.99
7.84 0.96
8.41 0.98
9.40 0.99
10.32 0.99
11.51 0.99
13.88 0.99
14.07 0.99
16.36 0.99
18.47 0.99
20.76 0.99

```

22.33 0.99
0 0 0

\$

```

*****
*                                     *
* CXTFIT VERSION 2.0 (1/2/95)         *
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE      *
* NON-LINEAR LEAST-SQUARES ANALYSIS                *
*                                     *
* CERCONA PELLET STUDY                     *
* Column C - 4 mL/min                       *
*                                     *
* DATA INPUT FILE: c6.in                  *
*                                     *
*****

```

MODEL DESCRIPTION

DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
 FLUX-AVERAGED CONCENTRATION
 REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.7332E+02	N		
D.....	.1468E+03	N		
R.....	.1000E+01	Y	.1000E+01	.2000E+01
mu.....	.5000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

STEP INPUT OF CONC. = 38.0000
 SOLUTE FREE INITIAL CONDITION
 NO PRODUCTION TERM

PARAMETER ESTIMATION MODE

MAXIMUM NUMBER OF ITERATIONS = 200

ITER	SSQ	R....	mu...
0	.1707E+01	.100E+01	.500E+01
1	.1323E+00	.103E+01	.440E+01
2	.1798E-01	.102E+01	.450E+01
3	.1787E-01	.102E+01	.451E+01
4	.1787E-01	.102E+01	.451E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

R.... mu...
R.... 1.000
mu... -.165 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98951517
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS

```

NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R.... .1020E+01 .2826E-01 .3609E+02 .9614E+00 .1078E+01
mu... .4507E+01 .2826E-01 .1595E+03 .4448E+01 .4565E+01

```

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

\$	NO	DISTANCE	CONCENTRATION		OBS	RESI- FITTED	DUAL
			TIME				
	1	32.0000	.0000	.0200	.0000	.0200	
	2	32.0000	.2700	.0200	.0005	.0195	
	3	32.0000	.8000	.7200	.7082	.0118	
	4	32.0000	1.2200	.8800	.9539	-.0739	
	5	32.0000	1.5300	.9100	.9701	-.0601	
	6	32.0000	2.1800	.9300	.9718	-.0418	
	7	32.0000	2.6400	.9700	.9718	-.0018	
	8	32.0000	3.1000	.9500	.9718	-.0218	
	9	32.0000	3.6700	.9500	.9718	-.0218	
	10	32.0000	4.2400	.9500	.9718	-.0218	
	11	32.0000	4.7800	.9800	.9718	.0082	
	12	32.0000	5.5400	1.0000	.9718	.0282	
	13	32.0000	6.6500	.9900	.9718	.0182	
	14	32.0000	7.2600	.9900	.9718	.0182	
	15	32.0000	7.8400	.9600	.9718	-.0118	
	16	32.0000	8.4100	.9800	.9718	.0082	
	17	32.0000	9.4000	.9900	.9718	.0182	
	18	32.0000	10.3200	.9900	.9718	.0182	
	19	32.0000	11.5100	.9900	.9718	.0182	
	20	32.0000	13.8800	.9900	.9718	.0182	
	21	32.0000	14.0700	.9900	.9718	.0182	
	22	32.0000	16.3600	.9900	.9718	.0182	
	23	32.0000	18.4700	.9900	.9718	.0182	
	24	32.0000	20.7600	.9900	.9718	.0182	
	25	32.0000	22.3300	.9900	.9718	.0182	

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column C - 2 mL/min
INVERSE  MODE  NREDU
  1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
  1     32.0
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V      D      R      Mu
36.66   73.38   1.0   1.0
  0      0      1      1
  0      0     1.0   1.0
  0      0    10.0  10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
  38.0
*** 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
  32.0
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.03
0.17  0.03
0.38  0.04
0.55  0.22
0.75  0.66
0.94  0.83
1.13  0.89
1.43  0.93
1.64  0.95
2.01  0.97
2.29  0.97
2.68  0.99
3.06  0.98
3.44  0.99
3.75  0.99
4.49  0.99
4.78  1.00
5.16  1.00
6.27  1.00
6.94  1.00
7.65  1.00
8.64  1.00
10.04 1.00
0 0 0

```

S

```

*****
*                                     *
* CXTFIT VERSION 2.0 (1/2/95)         *
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE      *
* NON-LINEAR LEAST-SQUARES ANALYSIS                *
*                                     *
* CERCONA PELLET STUDY                     *
* Column C - 2 mL/min                       *
*                                     *
* DATA INPUT FILE: c3.in                  *
*                                     *
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.3666E+02	N		
D.....	.7338E+02	N		
R.....	.1000E+01	Y	.1000E+01	.1000E+02
mu.....	.1000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

ITER	SSQ	R....	mu...
0	.3228E+04	.100E+01	.100E+01
1	.4433E+03	.109E+01	.204E+01
2	.5117E+02	.114E+01	.307E+01
3	.3825E+01	.114E+01	.392E+01
4	.1016E+00	.108E+01	.439E+01
5	.1336E-01	.104E+01	.449E+01
6	.1321E-01	.103E+01	.449E+01
7	.1320E-01	.103E+01	.449E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

R.... mu...
R.... 1.000
mu... -.228 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99507701
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```

          95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R.... .1030E+01 .2575E-01 .4000E+02 .9764E+00 .1084E+01
mu... .4492E+01 .2575E-01 .1744E+03 .4438E+01 .4545E+01

```

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

			CONCENTRATION	RESI-	
\$	NO	DISTANCE	TIME	OBS	FITTED DUAL
	1	32.0000	.0000	.0300	.0000 .0300
	2	32.0000	.1700	.0300	.0000 .0300
	3	32.0000	.3800	.0400	.0207 .0193
	4	32.0000	.5500	.2200	.2305 -.0105
	5	32.0000	.7500	.6600	.6249 .0351
	6	32.0000	.9400	.8300	.8551 -.0251
	7	32.0000	1.1300	.8900	.9448 -.0548
	8	32.0000	1.4300	.9300	.9777 -.0477
	9	32.0000	1.6400	.9500	.9811 -.0311
	10	32.0000	2.0100	.9700	.9819 -.0119
	11	32.0000	2.2900	.9700	.9820 -.0120
	12	32.0000	2.6800	.9900	.9820 .0080
	13	32.0000	3.0600	.9800	.9820 -.0020
	14	32.0000	3.4400	.9900	.9820 .0080
	15	32.0000	3.7500	.9900	.9820 .0080
	16	32.0000	4.4900	.9900	.9820 .0080
	17	32.0000	4.7800	1.0000	.9820 .0180
	18	32.0000	5.1600	1.0000	.9820 .0180
	19	32.0000	6.2700	1.0000	.9820 .0180
	20	32.0000	6.9400	1.0000	.9820 .0180
	21	32.0000	7.6500	1.0000	.9820 .0180
	22	32.0000	8.6400	1.0000	.9820 .0180
	23	32.0000	10.0400	1.0000	.9820 .0180

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column C - 0.6 mL/min
INVERSE MODE  NREDU
1 1 3
MODC  ZL(BLANK IF MODE=NREDU=1)
1 32.0
*** BLOCK B: INVERSE PROBLEM *****
MIT  ILMT  MASS
200  1  0
*** BLOCK C: TRANSPORT PARAMETERS *****
V    D    R    Mu
11.00 22.01 1.0 1.0
0 0 1 1
0 0 1.0 1.0
0 0 20.0 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
2
38.0
*** 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
32.0
TIME  CONC  (Give "0 0 0" after last data set.)
0.00 0.00
0.17 0.05
0.34 0.05
0.52 0.02
0.69 0.31
1.03 0.45
1.38 0.56
1.72 0.69
2.06 0.73
2.75 0.79
3.10 0.82
3.78 0.84
4.47 0.85
5.16 0.86
6.54 0.87
7.91 0.87
9.29 0.87
10.67 0.87
12.04 0.87
13.42 0.87
14.79 0.87
16.17 0.87
17.55 0.87
18.92 0.87

```

20.30 0.87
0 0 0

S

```

*****
*                                     *
*   CXTFIT VERSION 2.0 (1/2/95)       *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE       *
*   NON-LINEAR LEAST-SQUARES ANALYSIS *
*                                     *
*   CERCONA PELLET STUDY             *
*   Column C - 0.6 mL/min            *
*                                     *
*   DATA INPUT FILE: c1.in          *
*                                     *
*****

```

MODEL DESCRIPTION

DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
 FLUX-AVERAGED CONCENTRATION
 REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.1100E+02	N		
D.....	.2201E+02	N		
R.....	.1000E+01	Y	.1000E+01	.2000E+02
mu.....	.1000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

STEP INPUT OF CONC. = 38.0000
 SOLUTE FREE INITIAL CONDITION
 NO PRODUCTION TERM

PARAMETER ESTIMATION MODE

MAXIMUM NUMBER OF ITERATIONS = 200

ITER	SSQ	R....	mu...
0	.3783E+04	.100E+01	.100E+01
1	.5294E+03	.110E+01	.205E+01
2	.6420E+02	.121E+01	.311E+01
3	.5559E+01	.131E+01	.403E+01
4	.3092E+00	.140E+01	.458E+01
5	.1298E+00	.147E+01	.472E+01
6	.1270E+00	.152E+01	.473E+01
7	.1261E+00	.154E+01	.473E+01

```

8 .1259E+00 .156E+01 .472E+01
9 .1258E+00 .157E+01 .472E+01
10 .1258E+00 .158E+01 .472E+01
11 .1258E+00 .158E+01 .472E+01

```

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

=====
R.... mu...
R.... 1.000
mu... -.209 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .94773409
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```

=====
                      95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R.... .1578E+01 .7565E-01 .2086E+02 .1421E+01 .1734E+01
mu... .4723E+01 .7565E-01 .6243E+02 .4566E+01 .4879E+01

```

```

-----ORDERED BY COMPUTER INPUT-----
CONCENTRATION  RESI-
$ NO  DISTANCE  TIME  OBS  FITTED  DUAL
1  32.0000  .0000  .0000  .0000  .0000
2  32.0000  .1700  .0500  .0000  .0500
3  32.0000  .3400  .0500  .0000  .0500
4  32.0000  .5200  .0200  .0066  .0134
5  32.0000  .6900  .3100  .0693  .2407
6  32.0000  1.0300  .4500  .4247  .0253
7  32.0000  1.3800  .5600  .7124  -.1524
8  32.0000  1.7200  .6900  .8093  -.1193
9  32.0000  2.0600  .7300  .8329  -.1029
10 32.0000  2.7500  .7900  .8386  -.0486
11 32.0000  3.1000  .8200  .8387  -.0187
12 32.0000  3.7800  .8400  .8388  .0012
13 32.0000  4.4700  .8500  .8388  .0112
14 32.0000  5.1600  .8600  .8388  .0212
15 32.0000  6.5400  .8700  .8388  .0312
16 32.0000  7.9100  .8700  .8388  .0312
17 32.0000  9.2900  .8700  .8388  .0312
18 32.0000  10.6700 .8700  .8388  .0312
19 32.0000  12.0400 .8700  .8388  .0312
20 32.0000  13.4200 .8700  .8388  .0312
21 32.0000  14.7900 .8700  .8388  .0312
22 32.0000  16.1700 .8700  .8388  .0312
23 32.0000  17.5500 .8700  .8388  .0312
24 32.0000  18.9200 .8700  .8388  .0312
25 32.0000  20.3000 .8700  .8388  .0312

```

Appendix Q
Column D:CXTFIT 2.0 Input and Output Files

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column D - Tritium Tracer Study - 2 mL/min
INVERSE MODE NREDU
  1   1   3
MODC  ZL(BLANK IF MODE=NREDU=1)
  1  32.8
*** BLOCK B: INVERSE PROBLEM *****
MIT  ILMT  MASS
200   1   0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V   D   R   Mu
36.23  1   1.00  0
  0   1   0   0
36.23  0.00  1.0  0.00
36.23 20000  1.0  0.00
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  3
  1.0  1.38
*** 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
  31.5
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.00
0.17  0.00
0.35  0.00
0.53  0.00
0.72  0.07
0.90  0.34
1.09  0.63
1.27  0.79
1.38  0.87
1.56  0.94
1.75  1.00
1.93  0.98
2.12  0.68
2.30  0.40
2.48  0.28
2.67  0.20
2.85  0.13
3.04  0.09
3.22  0.06
3.40  0.04
3.59  0.03
3.79  0.02

```

3.97 0.01
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column D - Tritium Tracer Study - 2 mL/min
*
* DATA INPUT FILE: dt.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .3623E+02  N
D.....  .1000E+01  Y  .0000E+00  .2000E+05
R.....  .1000E+01  N
mu.....  .0000E+00  N

```

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
SINGLE PULSE OF CONC. = 1.0000 & DURATION = 1.3800
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

```

ITER  SSQ  D....
0  .7307E+00  .100E+01
1  .4689E+00  .436E+01
2  .2617E+00  .140E+02
3  .1131E+00  .368E+02
4  .8849E-01  .559E+02
5  .8815E-01  .590E+02

```

6 .8815E-01 .589E+02
 7 .8815E-01 .589E+02

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97090646
 (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS				
NAME	VALUE	S.E. COEFF.	LOWER	UPPER
D....	.5890E+02	.6330E-01	.5877E+02	.5903E+02

-----ORDERED BY COMPUTER INPUT-----						
		CONCENTRATION		RESI-		
\$	NO	DISTANCE	TIME	OBS	FITTED	DUAL
	1	31.5000	.0000	.0000	.0000	.0000
	2	31.5000	.1700	.0000	.0000	.0000
	3	31.5000	.3500	.0000	.0008	-.0008
	4	31.5000	.5300	.0000	.0405	-.0405
	5	31.5000	.7200	.0700	.2255	-.1555
	6	31.5000	.9000	.3400	.4812	-.1412
	7	31.5000	1.0900	.6300	.7111	-.0811
	8	31.5000	1.2700	.7900	.8509	-.0609
	9	31.5000	1.3800	.8700	.9041	-.0341
	10	31.5000	1.5600	.9400	.9554	-.0154
	11	31.5000	1.7500	1.0000	.9794	.0206
	12	31.5000	1.9300	.9800	.9395	.0405
	13	31.5000	2.1200	.6800	.7442	-.0642
	14	31.5000	2.3000	.4000	.4898	-.0898
	15	31.5000	2.4800	.2800	.2786	.0014
	16	31.5000	2.6700	.2000	.1376	.0624
	17	31.5000	2.8500	.1300	.0657	.0643
	18	31.5000	3.0400	.0900	.0286	.0614
	19	31.5000	3.2200	.0600	.0126	.0474
	20	31.5000	3.4000	.0400	.0054	.0346
	21	31.5000	3.5900	.0300	.0022	.0278
	22	31.5000	3.7900	.0200	.0008	.0192
	23	31.5000	3.9700	.0100	.0003	.0097

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column D - 4 mL/min
INVERSE MODE NREDU
1 1 3
MODC ZL(BLANK IF MODE=NREDU=1)
1 32.8
*** BLOCK B: INVERSE PROBLEM *****
MIT ILMT MASS
200 1 0
*** BLOCK C: TRANSPORT PARAMETERS *****
V D R Mu
72.46 117.80 1.00 5.0
0 0 1 1
0 0 1.00 1.0
0 0 2.00 10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac; =2 STEP; =3 A PULSE *****
MODB =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
2
38.0
*** 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
32.8
TIME CONC (Give "0 0 0" after last data set.)
0.00 0.06
0.33 0.04
0.81 0.78
1.21 0.87
1.51 0.90
2.13 0.93
2.58 0.94
2.98 0.94
3.61 0.94
4.08 0.94
4.60 0.98
5.37 0.98
6.40 0.98
7.03 0.98
7.58 0.99
8.13 0.99
9.09 0.98
9.93 0.99
11.07 0.99
13.36 0.99
13.54 0.99
15.75 0.99

```

17.77 0.99
19.98 0.99
21.49 0.99
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column D - 4 mL/min
*
* DATA INPUT FILE: d6.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .7246E+02  N
D.....  .1178E+03  N
R.....  .1000E+01  Y  .1000E+01  .2000E+01
mu.....  .5000E+01  Y  .1000E+01  .1000E+02

```

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

```

ITER  SSQ    R...  mu...
0  .3091E+01  .100E+01  .500E+01
1  .5806E+00  .100E+01  .413E+01
2  .3847E-01  .100E+01  .432E+01
3  .3749E-01  .100E+01  .434E+01
4  .3749E-01  .100E+01  .434E+01

```

COVARIANCE MATRIX FOR FITTED PARAMETERS

```
=====
R... mu...
R... 1.000
mu... -.160 1.000
```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97620698
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```
=====
                        95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R...  .1000E+01 .4090E-01 .2445E+02 .9154E+00 .1085E+01
mu...  .4339E+01 .4090E-01 .1061E+03 .4254E+01 .4423E+01
```

```
-----ORDERED BY COMPUTER INPUT-----
CONCENTRATION  RESI-
$ NO  DISTANCE  TIME  OBS  FITTED  DUAL
1  32.8000  .0000  .0600  .0000  .0600
2  32.8000  .3300  .0400  .0016  .0384
3  32.8000  .8100  .7800  .6708  .1092
4  32.8000  1.2100  .8700  .9465  -.0765
5  32.8000  1.5100  .9000  .9654  -.0654
6  32.8000  2.1300  .9300  .9672  -.0372
7  32.8000  2.5800  .9400  .9672  -.0272
8  32.8000  2.9800  .9400  .9672  -.0272
9  32.8000  3.6100  .9400  .9672  -.0272
10 32.8000  4.0800  .9400  .9672  -.0272
11 32.8000  4.6000  .9800  .9672  .0128
12 32.8000  5.3700  .9800  .9672  .0128
13 32.8000  6.4000  .9800  .9672  .0128
14 32.8000  7.0300  .9800  .9672  .0128
15 32.8000  7.5800  .9900  .9672  .0228
16 32.8000  8.1300  .9900  .9672  .0228
17 32.8000  9.0900  .9800  .9672  .0128
18 32.8000  9.9300  .9900  .9672  .0228
19 32.8000  11.0700  .9900  .9672  .0228
20 32.8000  13.3600  .9900  .9672  .0228
21 32.8000  13.5400  .9900  .9672  .0228
22 32.8000  15.7500  .9900  .9672  .0228
23 32.8000  17.7700  .9900  .9672  .0228
24 32.8000  19.9800  .9900  .9672  .0228
25 32.8000  21.4900  .9900  .9672  .0228
```

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column D - 2 mL/min
INVERSE  MODE  NREDU
  1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
  1     32.8
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V      D      R      Mu
36.23   58.90   1.0   1.0
  0      0      1      1
  0      0      1.0   1.0
  0      0     10.0  10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB          =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
  38.0
*** 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
  32.8
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.09
0.17  0.03
0.37  0.03
0.53  0.16
0.72  0.60
0.90  0.81
1.09  0.87
1.38  0.93
1.58  0.95
1.93  0.96
2.21  0.97
2.58  0.98
2.94  0.98
3.31  0.99
3.61  0.99
4.32  0.99
4.97  0.98
5.33  0.99
6.03  0.99
6.62  0.99
6.68  0.99
7.36  1.00

```

8.31 0.99
9.66 1.00
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column D - 2 mL/min
*
* DATA INPUT FILE: d3.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.3623E+02	N		
D.....	.5890E+02	N		
R.....	.1000E+01	Y	.1000E+01	.1000E+02
mu.....	.1000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

ITER	SSQ	R...	mu...
0	.3299E+04	.100E+01	.100E+01
1	.4448E+03	.107E+01	.202E+01
2	.5030E+02	.110E+01	.301E+01
3	.3652E+01	.108E+01	.381E+01
4	.1011E+00	.101E+01	.424E+01
5	.2609E-01	.100E+01	.432E+01

6 .2608E-01 .100E+01 .432E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

```
=====
R... mu...
R... 1.000
mu... -.220 1.000
```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99035409
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```
=====
                        95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R... .1000E+01 .3529E-01 .2833E+02 .9268E+00 .1073E+01
mu... .4323E+01 .3529E-01 .1225E+03 .4249E+01 .4396E+01
```

```
-----ORDERED BY COMPUTER INPUT-----
                        CONCENTRATION  RESI-
$ NO  DISTANCE  TIME  OBS  FITTED  DUAL
1  32.8000  .0000  .0900  .0000  .0900
2  32.8000  .1700  .0300  .0000  .0300
3  32.8000  .3700  .0300  .0064  .0236
4  32.8000  .5300  .1600  .1349  .0251
5  32.8000  .7200  .6000  .5135  .0865
6  32.8000  .9000  .8100  .7980  .0120
7  32.8000  1.0900  .8700  .9275  -.0575
8  32.8000  1.3800  .9300  .9733  -.0433
9  32.8000  1.5800  .9500  .9778  -.0278
10 32.8000  1.9300  .9600  .9788  -.0188
11 32.8000  2.2100  .9700  .9788  -.0088
12 32.8000  2.5800  .9800  .9788  .0012
13 32.8000  2.9400  .9800  .9788  .0012
14 32.8000  3.3100  .9900  .9788  .0112
15 32.8000  3.6100  .9900  .9788  .0112
16 32.8000  4.3200  .9900  .9788  .0112
17 32.8000  4.9700  .9800  .9788  .0012
18 32.8000  5.3300  .9900  .9788  .0112
19 32.8000  6.0300  .9900  .9788  .0112
20 32.8000  6.6200  .9900  .9788  .0112
21 32.8000  6.6800  .9900  .9788  .0112
22 32.8000  7.3600  1.0000  .9788  .0212
23 32.8000  8.3100  .9900  .9788  .0112
24 32.8000  9.6600  1.0000  .9788  .0212
```

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column D - 0.6 mL/min
INVERSE MODE NREDU
  1   1   3
MODC   ZL(BLANK IF MODE=NREDU=1)
  1   32.8
*** BLOCK B: INVERSE PROBLEM *****
MIT   ILMT  MASS
200   1     0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V     D     R     Mu
10.87  17.67  1.0  1.0
  0     0     1     1
  0     0     1.0  1.0
  0     0    10.0  10.0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac; =2 STEP; =3 A PULSE *****
MODB           =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
  38.0
*** 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
  32.8
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.00
0.17  0.05
0.33  0.05
0.50  0.02
0.66  0.32
0.99  0.46
1.32  0.57
1.66  0.65
1.99  0.71
2.65  0.78
2.98  0.82
3.64  0.84
4.30  0.85
4.97  0.86
6.29  0.87
7.62  0.87
8.94  0.87
10.26 0.87
11.59 0.87
12.91 0.88
14.24 0.88
15.56 0.88

```

16.89 0.89
18.21 0.89
19.54 0.89
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column D - 0.6 mL/min
*
* DATA INPUT FILE: d1.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .1087E+02  N
D.....  .1767E+02  N
R.....  .1000E+01  Y  .1000E+01  .1000E+02
mu.....  .1000E+01  Y  .1000E+01  .1000E+02

```

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

```

ITER  SSQ    R...  mu...
0  .3668E+04  .100E+01  .100E+01
1  .5034E+03  .108E+01  .203E+01
2  .5973E+02  .117E+01  .304E+01
3  .5030E+01  .124E+01  .391E+01
4  .3149E+00  .130E+01  .441E+01
5  .1694E+00  .133E+01  .453E+01

```

```

6 .1683E+00 .136E+01 .454E+01
7 .1680E+00 .137E+01 .454E+01
8 .1679E+00 .138E+01 .454E+01
9 .1679E+00 .139E+01 .454E+01
10 .1679E+00 .139E+01 .454E+01

```

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

=====
R... mu...
R... 1.000
mu... -.200 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .93086375
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```

=====
                        95% CONFIDENCE LIMITS
NAME  VALUE  S.E. COEFF. T-VALUE  LOWER  UPPER
R...  .1390E+01 .8718E-01 .1594E+02 .1209E+01 .1570E+01
mu...  .4535E+01 .8718E-01 .5202E+02 .4355E+01 .4716E+01

```

```

=====ORDERED BY COMPUTER INPUT=====

```

S	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
1	32.8000	.0000	.0000	.0000	.0000	
2	32.8000	.1700	.0500	.0000	.0500	
3	32.8000	.3300	.0500	.0000	.0500	
4	32.8000	.5000	.0200	.0044	.0156	
5	32.8000	.6600	.3200	.0587	.2613	
6	32.8000	.9900	.4600	.4399	.0201	
7	32.8000	1.3200	.5700	.7327	-.1627	
8	32.8000	1.6600	.6500	.8200	-.1700	
9	32.8000	1.9900	.7100	.8354	-.1254	
10	32.8000	2.6500	.7800	.8380	-.0580	
11	32.8000	2.9800	.8200	.8380	-.0180	
12	32.8000	3.6400	.8400	.8380	.0020	
13	32.8000	4.3000	.8500	.8380	.0120	
14	32.8000	4.9700	.8600	.8380	.0220	
15	32.8000	6.2900	.8700	.8380	.0320	
16	32.8000	7.6200	.8700	.8380	.0320	
17	32.8000	8.9400	.8700	.8380	.0320	
18	32.8000	10.2600	.8700	.8380	.0320	
19	32.8000	11.5900	.8700	.8380	.0320	
20	32.8000	12.9100	.8800	.8380	.0420	
21	32.8000	14.2400	.8800	.8380	.0420	
22	32.8000	15.5600	.8800	.8380	.0420	
23	32.8000	16.8900	.8900	.8380	.0520	
24	32.8000	18.2100	.8900	.8380	.0520	
25	32.8000	19.5400	.8900	.8380	.0520	

§

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column D - 0.6 mL/min
*
* DATA INPUT FILE: d1.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.1087E+02	N		
D.....	.1767E+02	N		
R.....	.1000E+01	Y	.1000E+01	.1000E+02
mu.....	.1000E+01	Y	.1000E+01	.1000E+02

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
STEP INPUT OF CONC. = 38.0000
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

ITER	SSQ	R...	mu...
0	.3668E+04	.100E+01	.100E+01
1	.5034E+03	.108E+01	.203E+01
2	.5973E+02	.117E+01	.304E+01
3	.5030E+01	.124E+01	.391E+01
4	.3149E+00	.130E+01	.441E+01
5	.1694E+00	.133E+01	.453E+01

6	.1683E+00	.136E+01	.454E+01
7	.1680E+00	.137E+01	.454E+01
8	.1679E+00	.138E+01	.454E+01
9	.1679E+00	.139E+01	.454E+01
10	.1679E+00	.139E+01	.454E+01

COVARIANCE MATRIX FOR FITTED PARAMETERS

```

=====
R.... mu...
R.... 1.000
mu... -.200 1.000

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .93086375
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

```

=====
                        95% CONFIDENCE LIMITS
NAME  VALUE  S.E.COEFF. T-VALUE  LOWER  UPPER
R.... .1390E+01 .8718E-01 .1594E+02 .1209E+01 .1570E+01
mu... .4535E+01 .8718E-01 .5202E+02 .4355E+01 .4716E+01

```

```

-----ORDERED BY COMPUTER INPUT-----
CONCENTRATION  RESI-
$ NO  DISTANCE  TIME  OBS  FITTED  DUAL
1  32.8000  .0000  .0000  .0000  .0000
2  32.8000  .1700  .0500  .0000  .0500
3  32.8000  .3300  .0500  .0000  .0500
4  32.8000  .5000  .0200  .0044  .0156
5  32.8000  .6600  .3200  .0587  .2613
6  32.8000  .9900  .4600  .4399  .0201
7  32.8000  1.3200  .5700  .7327  -.1627
8  32.8000  1.6600  .6500  .8200  -.1700
9  32.8000  1.9900  .7100  .8354  -.1254
10 32.8000  2.6500  .7800  .8380  -.0580
11 32.8000  2.9800  .8200  .8380  -.0180
12 32.8000  3.6400  .8400  .8380  .0020
13 32.8000  4.3000  .8500  .8380  .0120
14 32.8000  4.9700  .8600  .8380  .0220
15 32.8000  6.2900  .8700  .8380  .0320
16 32.8000  7.6200  .8700  .8380  .0320
17 32.8000  8.9400  .8700  .8380  .0320
18 32.8000  10.2600 .8700  .8380  .0320
19 32.8000  11.5900 .8700  .8380  .0320
20 32.8000  12.9100 .8800  .8380  .0420
21 32.8000  14.2400 .8800  .8380  .0420
22 32.8000  15.5600 .8800  .8380  .0420
23 32.8000  16.8900 .8900  .8380  .0520
24 32.8000  18.2100 .8900  .8380  .0520
25 32.8000  19.5400 .8900  .8380  .0520

```

Appendix R
Column E:CXTFIT 2.0 Input and Output Files

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column E - Tritium Tracer Study - 2 mL/min
INVERSE MODE NREDU
1 1 3
MODC ZL(BLANK IF MODE=NREDU=1)
1 33.2
*** BLOCK B: INVERSE PROBLEM *****
MIT ILMT MASS
200 1 0
*** BLOCK C: TRANSPORT PARAMETERS *****
V D R Mu
26.16 1 0.1 0
0 1 1 0
26.16 0.00 0.1 0.00
26.16 1000 1.0 0.00
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac; =2 STEP; =3 A PULSE *****
MODB =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
3
1.0 0.99
*** 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
33.2
TIME CONC (Give "0 0 0" after last data set.)
0.00 0.00
0.12 0.00
0.25 0.00
0.38 0.07
0.51 0.31
0.64 0.58
0.78 0.74
0.91 0.81
0.99 0.90
1.12 1.00
1.25 0.89
1.38 0.67
1.51 0.42
1.64 0.28
1.78 0.23
1.91 0.15
2.04 0.10
2.17 0.07
2.30 0.06
2.43 0.04
2.57 0.03
2.71 0.01

```

2.84 0.01
0 0 0

\$

```

*****
*                                     *
*   CXTFIT VERSION 2.0 (1/2/95)       *
*   ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE   *
*   NON-LINEAR LEAST-SQUARES ANALYSIS *
*                                     *
*   CERCONA PELLET STUDY               *
*   Column E - Tritium Tracer Study - 2 mL/min *
*                                     *
*   DATA INPUT FILE: et.in           *
*                                     *
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL POSITION(Z)
  (ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
CHARACTERISTIC LENGTH = 33.2000
FOR DIMENSIONLESS PARAMETERS

```

INITIAL VALUES OF COEFFICIENTS

NAME	INITIAL VALUE	FITTING	MIN VALUE	MAX VALUE
V.....	.2616E+02	N		
D.....	.1000E+01	Y	.0000E+00	.1000E+04
R.....	.1000E+00	Y	.1000E+00	.1000E+01
mu.....	.0000E+00	N		

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
SINGLE PULSE OF CONC. = 1.0000 & DURATION = .9900
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

ITER	SSQ	D....	R....
0	.6223E+01	.100E+01	.100E+00
1	.7174E+00	.100E+04	.100E+01
2	.4408E+00	.496E+03	.100E+01
3	.2996E+00	.495E+02	.508E+00
4	.9184E-01	.925E+02	.589E+00
5	.7210E-01	.105E+03	.626E+00

6 .7170E-01 .108E+03 .632E+00
 7 .7169E-01 .109E+03 .632E+00
 8 .7169E-01 .109E+03 .632E+00
 9 .7169E-01 .109E+03 .632E+00

COVARIANCE MATRIX FOR FITTED PARAMETERS

=====

D.... R....
 D.... 1.000
 R.... .350 1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97326935
 (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

=====

95% CONFIDENCE LIMITS

NAME	VALUE	S.E.COEFF.	T-VALUE	LOWER	UPPER
D....	.1088E+03	.6238E-01	.1745E+04	.1087E+03	.1090E+03
R....	.6325E+00	.6238E-01	.1014E+02	.5027E+00	.7622E+00

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

\$	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
1	33.2000	.0000	.0000	.0000	.0000	
2	33.2000	.1200	.0000	.0002	-.0002	
3	33.2000	.2500	.0000	.0409	-.0409	
4	33.2000	.3800	.0700	.2059	-.1359	
5	33.2000	.5100	.3100	.4191	-.1091	
6	33.2000	.6400	.5800	.6040	-.0240	
7	33.2000	.7800	.7400	.7488	-.0088	
8	33.2000	.9100	.8100	.8389	-.0289	
9	33.2000	.9900	.9000	.8782	.0218	
10	33.2000	1.1200	1.0000	.9227	.0773	
11	33.2000	1.2500	.8900	.9023	-.0123	
12	33.2000	1.3800	.6700	.7476	-.0776	
13	33.2000	1.5100	.4200	.5461	-.1261	
14	33.2000	1.6400	.2800	.3719	-.0919	
15	33.2000	1.7800	.2300	.2357	-.0057	
16	33.2000	1.9100	.1500	.1511	-.0011	
17	33.2000	2.0400	.1000	.0958	.0042	
18	33.2000	2.1700	.0700	.0603	.0097	
19	33.2000	2.3000	.0600	.0379	.0221	
20	33.2000	2.4300	.0400	.0238	.0162	
21	33.2000	2.5700	.0300	.0144	.0156	
22	33.2000	2.7100	.0100	.0087	.0013	
23	33.2000	2.8400	.0100	.0055	.0045	

1

*** BLOCK A: MODEL DESCRIPTION *****

CERCONA PELLET STUDY

Column E - 4 mL/min

INVERSE MODE NREDU

1 1 3

MODC ZL(BLANK IF MODE=NREDU=1)

1 33.2

*** BLOCK B: INVERSE PROBLEM *****

MIT ILMT MASS

200 1 0

*** BLOCK C: TRANSPORT PARAMETERS *****

V D R Mu

52.33 217.60 1.00 0

0 0 1 0

0 0 1.00 0

0 0 1.00 0

*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****

MODB =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY

2

1.0

*** 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

33.2

TIME CONC (Give "0 0 0" after last data set.)

0.00 0.05

0.24 0.04

0.61 0.73

0.87 0.87

1.11 0.90

1.55 0.93

1.68 0.99

5.18 0.99

5.82 0.99

9.66 0.99

9.82 0.99

15.42 0.99

0 0 0

\$

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column E - 4 mL/min
*
* DATA INPUT FILE: e6.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL POSITION(Z)
(ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
CHARACTERISTIC LENGTH = 33.2000
FOR DIMENSIONLESS PARAMETERS

```

INITIAL VALUES OF COEFFICIENTS

```

=====
NAME      INITIAL VALUE FITTING MIN VALUE  MAX VALUE
V.....  .5233E+02  N
D.....  .2176E+03  N
R.....  .1000E+01  Y  .1000E+01  .1000E+01
mu.....  .0000E+00  N

```

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 = 200

```

```

ITER  SSQ    R...
0  .4817E+00  .100E+01
1  .1451E-01  .557E+00
2  .1371E-01  .541E+00
3  .1371E-01  .540E+00
4  .1371E-01  .540E+00

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .99014855
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS				
NAME	VALUE	S.E.COEFF.	LOWER	UPPER
R...	.5402E+00	.3531E-01	.4625E+00	.6179E+00

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

\$	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
	1	33.2000	.0000	.0500	.0000	.0500
	2	33.2000	.2400	.0400	.0698	-.0298
	3	33.2000	.6100	.7300	.6876	.0424
	4	33.2000	.8700	.8700	.8898	-.0198
	5	33.2000	1.1100	.9000	.9595	-.0595
	6	33.2000	1.5500	.9300	.9936	-.0636
	7	33.2000	1.6800	.9900	.9963	-.0063
	8	33.2000	5.1800	.9900	1.0000	-.0100
	9	33.2000	5.8200	.9900	1.0000	-.0100
	10	33.2000	9.6600	.9900	1.0000	-.0100
	11	33.2000	9.8200	.9900	1.0000	-.0100
	12	33.2000	15.4200	.9900	1.0000	-.0100

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column E - 2 mL/min
INVERSE  MODE  NREDU
  1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
  1      33.2
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V      D      R      Mu
26.16   108.80  0.1    0
  0      0      1      0
  0      0      0.1    0
  0      0      10.0   0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB          =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
  1.0
*** 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
  33.2
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.05
0.14  0.04
0.29  0.73
0.41  0.87
0.54  0.90
0.67  0.92
0.80  0.99
1.01  1.00
1.14  1.00
1.58  1.00
3.16  1.00
4.74  1.00
6.32  1.00
7.90  1.00
9.47  1.00
11.05 1.00
0 0 0

```

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column E - 2 mL/min
*
* DATA INPUT FILE: e3.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL POSITION(Z)
(ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
CHARACTERISTIC LENGTH = 33.2000
FOR DIMENSIONLESS PARAMETERS

```

INITIAL VALUES OF COEFFICIENTS

```

=====
NAME      INITIAL VALUE FITTING MIN VALUE  MAX VALUE
V.....  .2616E+02  N
D.....  .1088E+03  N
R.....  .1000E+00  Y  .1000E+00  .1000E+02
mu.....  .0000E+00  N

```

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 = 200

```

```

ITER  SSQ    R....
0  .7211E+00  .100E+00
1  .3111E-01  .247E+00
2  .2370E-01  .270E+00
3  .2368E-01  .268E+00
4  .2368E-01  .268E+00

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98462272
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS
NAME VALUE S.E. COEFF. LOWER UPPER
R... .2684E+00 .3973E-01 .1837E+00 .3531E+00

-----ORDERED BY COMPUTER INPUT-----
CONCENTRATION RESI-
\$ NO DISTANCE TIME OBS FITTED DUAL
1 33.2000 .0000 .0500 .0000 .0500
2 33.2000 .1400 .0400 .1304 -.0904
3 33.2000 .2900 .7300 .6548 .0752
4 33.2000 .4100 .8700 .8675 .0025
5 33.2000 .5400 .9000 .9554 -.0554
6 33.2000 .6700 .9200 .9851 -.0651
7 33.2000 .8000 .9900 .9950 -.0050
8 33.2000 1.0100 1.0000 .9991 .0009
9 33.2000 1.1400 1.0000 .9997 .0003
10 33.2000 1.5800 1.0000 1.0000 .0000
11 33.2000 3.1600 1.0000 1.0000 .0000
12 33.2000 4.7400 1.0000 1.0000 .0000
13 33.2000 6.3200 1.0000 1.0000 .0000
14 33.2000 7.9000 1.0000 1.0000 .0000
15 33.2000 9.4700 1.0000 1.0000 .0000
16 33.2000 11.0500 1.0000 1.0000 .0000

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column E - 0.6 mL/min
INVERSE  MODE  NREDU
  1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
  1     33.2
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V      D      R      Mu
  7.85  32.64   0.1   0
  0      0      1      0
  0      0     0.1   0
  0      0    10.0   0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB          =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
  1.0
*** 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
  33.2
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.00
0.12  0.02
0.24  0.02
0.36  0.02
0.47  0.54
0.71  0.97
0.95  0.98
1.18  0.99
1.42  0.99
1.89  1.00
2.13  1.00
3.79  1.00
4.03  1.00
4.97  1.00
5.92  1.00
6.87  1.00
7.82  1.00
8.76  1.00
9.71  1.00
10.66 1.00
11.61 1.00
12.55 1.00

```

13.50 1.00
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column E - 0.6 mL/min
*
* DATA INPUT FILE: el.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL POSITION(Z)
(ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
CHARACTERISTIC LENGTH = 33.2000
FOR DIMENSIONLESS PARAMETERS

```

INITIAL VALUES OF COEFFICIENTS

NAME	INITIAL VALUE	FITTING	MIN VALUE	MAX VALUE
V.....	.7850E+01	N		
D.....	.3264E+02	N		
R.....	.1000E+00	Y	.1000E+00	.1000E+02
mu.....	.0000E+00	N		

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 = 200

```

ITER	SSQ	R...
0	.2600E+01	.100E+00
1	.1350E+01	.224E+00
2	.2129E+00	.436E+00
3	.1084E+00	.556E+00
4	.1074E+00	.539E+00
5	.1073E+00	.544E+00

6 .1073E+00 .543E+00
 7 .1073E+00 .543E+00

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .96673716
 (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS				
NAME	VALUE	S.E. COEFF.	LOWER	UPPER
R...	.5433E+00	.6983E-01	.3985E+00	.6882E+00

-----ORDERED BY COMPUTER INPUT-----						
		CONCENTRATION		RESI-		
\$	NO	DISTANCE	TIME	OBS	FITTED	DUAL
	1	33.2000	.0000	.0000	.0000	
	2	33.2000	.1200	.0200	.0008	.0192
	3	33.2000	.2400	.0200	.0681	-.0481
	4	33.2000	.3600	.0200	.2696	-.2496
	5	33.2000	.4700	.5400	.4764	.0636
	6	33.2000	.7100	.9700	.7853	.1847
	7	33.2000	.9500	.9800	.9191	.0609
	8	33.2000	1.1800	.9900	.9690	.0210
	9	33.2000	1.4200	.9900	.9886	.0014
	10	33.2000	1.8900	1.0000	.9984	.0016
	11	33.2000	2.1300	1.0000	.9994	.0006
	12	33.2000	3.7900	1.0000	1.0000	.0000
	13	33.2000	4.0300	1.0000	1.0000	.0000
	14	33.2000	4.9700	1.0000	1.0000	.0000
	15	33.2000	5.9200	1.0000	1.0000	.0000
	16	33.2000	6.8700	1.0000	1.0000	.0000
	17	33.2000	7.8200	1.0000	1.0000	.0000
	18	33.2000	8.7600	1.0000	1.0000	.0000
	19	33.2000	9.7100	1.0000	1.0000	.0000
	20	33.2000	10.6600	1.0000	1.0000	.0000
	21	33.2000	11.6100	1.0000	1.0000	.0000
	22	33.2000	12.5500	1.0000	1.0000	.0000
	23	33.2000	13.5000	1.0000	1.0000	.0000

\$

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column E - 0.6 mL/min
*
* DATA INPUT FILE: e1.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL POSITION(Z)
(ALL PARAMETERS EXCEPT D AND V ARE DIMENSIONLESS)
CHARACTERISTIC LENGTH = 33.2000
FOR DIMENSIONLESS PARAMETERS

```

INITIAL VALUES OF COEFFICIENTS

```

=====
NAME      INITIAL VALUE FITTING MIN VALUE  MAX VALUE
V.....  .7850E+01  N
D.....  .3264E+02  N
R.....  .1000E+00  Y  .1000E+00  .1000E+02
mu.....  .0000E+00  N

```

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 = 200

```

```

ITER  SSQ  R...
0  .2600E+01  .100E+00
1  .1350E+01  .224E+00
2  .2129E+00  .436E+00
3  .1084E+00  .556E+00
4  .1074E+00  .539E+00
5  .1073E+00  .544E+00

```

6 .1073E+00 .543E+00
 7 .1073E+00 .543E+00

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .96673716
 (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS				
NAME	VALUE	S.E.COEFF.	LOWER	UPPER
R...	.5433E+00	.6983E-01	.3985E+00	.6882E+00

-----ORDERED BY COMPUTER INPUT-----						
\$	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
	1	33.2000	.0000	.0000	.0000	.0000
	2	33.2000	.1200	.0200	.0008	.0192
	3	33.2000	.2400	.0200	.0681	-.0481
	4	33.2000	.3600	.0200	.2696	-.2496
	5	33.2000	.4700	.5400	.4764	.0636
	6	33.2000	.7100	.9700	.7853	.1847
	7	33.2000	.9500	.9800	.9191	.0609
	8	33.2000	1.1800	.9900	.9690	.0210
	9	33.2000	1.4200	.9900	.9886	.0014
	10	33.2000	1.8900	1.0000	.9984	.0016
	11	33.2000	2.1300	1.0000	.9994	.0006
	12	33.2000	3.7900	1.0000	1.0000	.0000
	13	33.2000	4.0300	1.0000	1.0000	.0000
	14	33.2000	4.9700	1.0000	1.0000	.0000
	15	33.2000	5.9200	1.0000	1.0000	.0000
	16	33.2000	6.8700	1.0000	1.0000	.0000
	17	33.2000	7.8200	1.0000	1.0000	.0000
	18	33.2000	8.7600	1.0000	1.0000	.0000
	19	33.2000	9.7100	1.0000	1.0000	.0000
	20	33.2000	10.6600	1.0000	1.0000	.0000
	21	33.2000	11.6100	1.0000	1.0000	.0000
	22	33.2000	12.5500	1.0000	1.0000	.0000
	23	33.2000	13.5000	1.0000	1.0000	.0000

Appendix S
Column F:CXTFIT 2.0 Input and Output Files

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column F - Tritium Tracer Study - 2 mL/min
INVERSE MODE NREDU
1 1 3
MODC ZL(BLANK IF MODE=NREDU=1)
1 32.8
*** BLOCK B: INVERSE PROBLEM *****
MIT ILMT MASS
200 1 0
*** BLOCK C: TRANSPORT PARAMETERS *****
V D R Mu
27.09 1 0.10 0
0 1 1 0
27.09 0.00 0.1 0.00
27.09 20000 1.0 0.00
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
3
1.0 1.02
*** 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
32.8
TIME CONC (Give "0 0 0" after last data set.)
0.00 0.00
0.12 0.00
0.26 0.00
0.39 0.08
0.53 0.32
0.67 0.56
0.80 0.75
0.94 0.79
1.02 0.91
1.16 0.99
1.29 0.85
1.43 0.69
1.57 0.44
1.70 0.30
1.84 0.21
1.97 0.15
2.11 0.09
2.25 0.06
2.38 0.05
2.52 0.04
2.66 0.02
2.81 0.02

```

2.94 0.01
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column F - Tritium Tracer Study - 2 mL/min
*
* DATA INPUT FILE: ft.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .2709E+02  N
D.....  .1000E+01  Y  .0000E+00  .2000E+05
R.....  .1000E+00  Y  .1000E+00  .1000E+01
mu.....  .0000E+00  N

```

BOUNDARY, INITIAL, AND PRODUCTION CONDITIONS

```

=====
SINGLE PULSE OF CONC. = 1.0000 & DURATION = 1.0200
SOLUTE FREE INITIAL CONDITION
NO PRODUCTION TERM

```

PARAMETER ESTIMATION MODE

```

=====
MAXIMUM NUMBER OF ITERATIONS = 200

```

```

ITER  SSQ    D.... R....
0  .6163E+01 .100E+01 .100E+00
1  .8004E+00 .114E+04 .100E+01
2  .4061E+00 .497E+03 .100E+01
3  .3141E+00 .316E+02 .543E+00
4  .9675E-01 .712E+02 .605E+00
5  .5738E-01 .988E+02 .646E+00

```

6 .5523E-01 .107E+03 .658E+00
 7 .5518E-01 .108E+03 .659E+00
 8 .5518E-01 .108E+03 .660E+00
 9 .5518E-01 .108E+03 .660E+00

COVARIANCE MATRIX FOR FITTED PARAMETERS

D.... R...
 D.... 1.000
 R.... .340 1.000

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97915183
 (COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS

NAME	VALUE	S.E.COEFF.	T-VALUE	LOWER	UPPER
D....	.1084E+03	.5450E-01	.1989E+04	.1083E+03	.1085E+03
R....	.6595E+00	.5450E-01	.1210E+02	.5462E+00	.7729E+00

ORDERED BY COMPUTER INPUT

\$	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
1	32.8000	.0000	.0000	.0000	.0000	
2	32.8000	.1200	.0000	.0001	-.0001	
3	32.8000	.2600	.0000	.0380	-.0380	
4	32.8000	.3900	.0800	.1918	-.1118	
5	32.8000	.5300	.3200	.4129	-.0929	
6	32.8000	.6700	.5600	.6061	-.0461	
7	32.8000	.8000	.7500	.7385	.0115	
8	32.8000	.9400	.7900	.8356	-.0456	
9	32.8000	1.0200	.9100	.8748	.0352	
10	32.8000	1.1600	.9900	.9223	.0677	
11	32.8000	1.2900	.8500	.9052	-.0552	
12	32.8000	1.4300	.6900	.7475	-.0575	
13	32.8000	1.5700	.4400	.5383	-.0983	
14	32.8000	1.7000	.3000	.3704	-.0704	
15	32.8000	1.8400	.2100	.2379	-.0279	
16	32.8000	1.9700	.1500	.1544	-.0044	
17	32.8000	2.1100	.0900	.0957	-.0057	
18	32.8000	2.2500	.0600	.0589	.0011	
19	32.8000	2.3800	.0500	.0374	.0126	
20	32.8000	2.5200	.0400	.0228	.0172	
21	32.8000	2.6600	.0200	.0140	.0060	
22	32.8000	2.8100	.0200	.0082	.0118	
23	32.8000	2.9400	.0100	.0052	.0048	

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column F - 4 mL/min
INVERSE  MODE  NREDU
1      1      3
MODC    ZL(BLANK IF MODE=NREDU=1)
1      32.8
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
V      D      R      Mu
54.18  216.80  1.00  0
0      0      1      0
0      0      1.00  0
0      0      1.00  0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
2
1.0
*** 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
32.8
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.07
0.30  0.05
0.65  0.73
0.93  0.85
1.17  0.89
1.61  0.92
1.74  0.98
3.46  0.99
6.05  0.99
10.00 0.99
15.99 0.99
0 0 0

```

\$

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column F - 4 mL/min
*
* DATA INPUT FILE: f6.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .5418E+02  N
D.....  .2168E+03  N
R.....  .1000E+01  Y  .1000E+01  .1000E+01
mu.....  .0000E+00  N

```

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 = 200

```

```

ITER  SSQ    R...
0  .3712E+00  .100E+01
1  .2439E-01  .615E+00
2  .2356E-01  .598E+00
3  .2356E-01  .598E+00

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98174740

(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

		95% CONFIDENCE LIMITS		
NAME	VALUE	S.E.COEFF.	LOWER	UPPER
R...	.5980E+00	.4854E-01	.4899E+00	.7062E+00

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

\$	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
	1	32.8000	.0000	.0700	.0000	.0700
	2	32.8000	.3000	.0500	.1093	-.0593
	3	32.8000	.6500	.7300	.6591	.0709
	4	32.8000	.9300	.8500	.8772	-.0272
	5	32.8000	1.1700	.8900	.9509	-.0609
	6	32.8000	1.6100	.9200	.9911	-.0711
	7	32.8000	1.7400	.9800	.9946	-.0146
	8	32.8000	3.4600	.9900	1.0000	-.0100
	9	32.8000	6.0500	.9900	1.0000	-.0100
	10	32.8000	10.0000	.9900	1.0000	-.0100
	11	32.8000	15.9900	.9900	1.0000	-.0100

1

*** BLOCK A: MODEL DESCRIPTION *****

CERCONA PELLET STUDY

Column F - 2 mL/min

INVERSE MODE NREDU

1 1 3

MODC ZL(BLANK IF MODE=NREDU=1)

1 32.8

*** BLOCK B: INVERSE PROBLEM *****

MIT ILMT MASS

200 1 0

*** BLOCK C: TRANSPORT PARAMETERS *****

V D R Mu

27.09 108.40 0.1 0

0 0 1 0

0 0 0.1 0

0 0 1.0 0

*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac; =2 STEP; =3 A PULSE *****

MODB =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY

2

1.0

*** 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

32.8

TIME CONC (Give "0 0 0" after last data set.)

0.00 0.07

0.15 0.05

0.30 0.73

0.42 0.85

0.56 0.89

0.69 0.92

0.83 0.98

1.05 1.00

1.19 1.00

1.63 1.00

3.27 1.00

4.90 1.00

6.54 1.00

8.17 1.00

9.81 1.00

11.44 1.00

0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column F - 2 mL/min
*
* DATA INPUT FILE: f3.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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 MIN VALUE  MAX VALUE
V.....  .2709E+02  N
D.....  .1084E+03  N
R.....  .1000E+00  Y  .1000E+00  .1000E+01
mu.....  .0000E+00  N

```

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 = 200

```

```

ITER  SSQ  R...
0  .7744E+00  .100E+00
1  .2925E-01  .273E+00
2  .2835E-01  .281E+00
3  .2835E-01  .281E+00
4  .2835E-01  .281E+00

```

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .98094987
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

95% CONFIDENCE LIMITS
NAME VALUE S.E.COEFF. LOWER UPPER
R.... .2810E+00 .4347E-01 .1883E+00 .3736E+00

-----ORDERED BY COMPUTER INPUT-----
CONCENTRATION RESI-
\$ NO DISTANCE TIME OBS FITTED DUAL
1 32.8000 .0000 .0700 .0000 .0700
2 32.8000 .1500 .0500 .1371 -.0871
3 32.8000 .3000 .7300 .6454 .0846
4 32.8000 .4200 .8500 .8593 -.0093
5 32.8000 .5600 .8900 .9549 -.0649
6 32.8000 .6900 .9200 .9846 -.0646
7 32.8000 .8300 .9800 .9951 -.0151
8 32.8000 1.0500 1.0000 .9992 .0008
9 32.8000 1.1900 1.0000 .9997 .0003
10 32.8000 1.6300 1.0000 1.0000 .0000
11 32.8000 3.2700 1.0000 1.0000 .0000
12 32.8000 4.9000 1.0000 1.0000 .0000
13 32.8000 6.5400 1.0000 1.0000 .0000
14 32.8000 8.1700 1.0000 1.0000 .0000
15 32.8000 9.8100 1.0000 1.0000 .0000
16 32.8000 11.4400 1.0000 1.0000 .0000

```

1
*** BLOCK A: MODEL DESCRIPTION *****
CERCONA PELLET STUDY
Column F - 0.6 mL/min
INVERSE  MODE  NREDU
  1      1      3
MODC     ZL(BLANK IF MODE=NREDU=1)
  1     32.8
*** BLOCK B: INVERSE PROBLEM *****
MIT      ILMT  MASS
200      1      0
*** BLOCK C: TRANSPORT PARAMETERS *****
  V      D      R      Mu
  8.13  32.52   0.1   0
  0      0      1      0
  0      0     0.1   0
  0      0     5.0   0
*** BLOCK D: BVP; MODB=0 ZERO; =1 Dirac ; =2 STEP; =3 A PULSE *****
MODB      =4 MULTIPLE; =5 EXPONENTIAL; =6 ARBITRARY
  2
  1.0
*** 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
  32.8
TIME  CONC  (Give "0 0 0" after last data set.)
0.00  0.00
0.12  0.04
0.25  0.02
0.37  0.03
0.49  0.52
0.74  0.87
0.98  0.98
1.23  1.00
1.47  1.00
1.96  1.00
2.94  1.00
3.92  1.00
4.17  1.00
5.15  1.00
6.13  1.00
7.11  1.00
8.09  1.00
9.07  1.00
10.05 1.00
11.03 1.00
12.01 1.00
12.99 1.00

```

13.97 1.00
0 0 0

S

```

*****
*
* CXTFIT VERSION 2.0 (1/2/95)
* ANALYTICAL SOLUTIONS FOR ONE-DIMENSIONAL CDE
* NON-LINEAR LEAST-SQUARES ANALYSIS
*
* CERCONA PELLET STUDY
* Column F - 0.6 mL/min
*
* DATA INPUT FILE: fl.in
*
*****

```

MODEL DESCRIPTION

```

=====
DETERMINISTIC EQUILIBRIUM CDE (MODE=1)
FLUX-AVERAGED CONCENTRATION
REDUCED TIME (T), DIMENSIONAL 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	MIN VALUE	MAX VALUE
V.....	.8130E+01	N		
D.....	.3252E+02	N		
R.....	.1000E+00	Y	.1000E+00	.5000E+01
mu.....	.0000E+00	N		

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 = 200

```

ITER	SSQ	R...
0	.2598E+01	.100E+00
1	.1494E+01	.216E+00
2	.2557E+00	.429E+00
3	.6712E-01	.582E+00
4	.6711E-01	.579E+00
5	.6710E-01	.580E+00

6 .6710E-01 .580E+00

RSQUARE FOR REGRESSION OF OBSERVED VS PREDICTED = .97886150
(COEFFICIENT OF DETERMINATION)

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

=====

95% CONFIDENCE LIMITS

NAME	VALUE	S.E.COEFF.	LOWER	UPPER
R...	.5798E+00	.5523E-01	.4652E+00	.6943E+00

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

\$	NO	DISTANCE	CONCENTRATION		RESI-	DUAL
			TIME	OBS	FITTED	
	1	32.8000	.0000	.0000	.0000	
	2	32.8000	.1200	.0400	.0397	
	3	32.8000	.2500	.0200	-.0383	
	4	32.8000	.3700	.0300	-.2095	
	5	32.8000	.4900	.5200	.0656	
	6	32.8000	.7400	.8700	.0981	
	7	32.8000	.9800	.9800	.0704	
	8	32.8000	1.2300	1.0000	.0335	
	9	32.8000	1.4700	1.0000	.0128	
	10	32.8000	1.9600	1.0000	.0018	
	11	32.8000	2.9400	1.0000	.0000	
	12	32.8000	3.9200	1.0000	.0000	
	13	32.8000	4.1700	1.0000	.0000	
	14	32.8000	5.1500	1.0000	.0000	
	15	32.8000	6.1300	1.0000	.0000	
	16	32.8000	7.1100	1.0000	.0000	
	17	32.8000	8.0900	1.0000	.0000	
	18	32.8000	9.0700	1.0000	.0000	
	19	32.8000	10.0500	1.0000	.0000	
	20	32.8000	11.0300	1.0000	.0000	
	21	32.8000	12.0100	1.0000	.0000	
	22	32.8000	12.9900	1.0000	.0000	
	23	32.8000	13.9700	1.0000	.0000	