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Performance Evaluation of Granular Activated Carbon System at Pantex: Rapid Small-Scale Column Tests to Simulate Removal of High Explosives from Contaminated Groundwater

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A Report on

Performance Evaluation of Granular Activated Carbon System at Pantex: Rapid Small-Scale Column Tests to Simulate Removal of High Explosives from Contaminated Groundwater

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EXECUTIVE SUMMARY

BACKGROUND

A granular activated carbon (GAC) system is now in operation at Pantex to treat groundwater from the perched aquifer that is contaminated with high explosives. The main chemicals of concern are RDX and HMX. The system consists of two GAC columns in series (see Figure 1.4 for a system schematic). Each column is charged with 10,000 pounds of Northwestern LB-830 GAC. At the design flow rate of 325 gpm, the hydraulic loading is 6.47 gpm/ft^2, and the empty bed contact time is 8.2 minutes per column. Currently, the system is operating at less than 10% of its design flow rate, although flow rate increases are expected in the relatively near future.

Operation of full-scale GAC columns can be simulated by laboratory-scale experiments known as rapid small scale column tests (RSSCTs). RSSCTs are of short duration and require a relatively small volume of water. Full-scale columns are scaled down based on the fundamental concepts of mass transfer in GAC systems. Several scaling relationships permit the design of a small-scale column to simulate the performance (i.e., the breakthrough curve) of the corresponding full-scale column. RSSCTs have been used successfully in a variety of applications as design and operating tools for GAC systems.

OBJECTIVES

This study had several objectives:

- Estimate the service life of the GAC now in use at Pantex;
- Screen several GACs to provide a recommendation on the best GAC for use at Pantex when the current GAC is exhausted and is replaced;
- Determine the extent to which natural organic matter in the Pantex groundwater "fouls" GAC adsorption sites, thereby decreasing the adsorption capacity for high explosives;
- Determine if computer simulation models could match the experimental results, thereby providing another tool to follow system performance.

EXPERIMENTAL APPROACH

Water was shipped from Pantex to the University of Texas, where the RSSCT experiments were performed. Most of the groundwater had some RDX and HMX contamination; the concentrations were supplemented, as needed, to reach target influent concentrations. One batch of water was uncontaminated, and this batch was used to study the impact of natural organic matter on RDX and HMX adsorption. Most experiments were run with influent concentrations of 350 µg/L HMX and 2200 µg/L RDX. In selected experiments, the HMX concentration was raised to 1100 µg/L and the RDX concentration to 4500 µg/L. Effluent samples were collected from the RSSCTs to define the breakthrough curve. Two service times were noted: the time required to reach 26 µg/L RDX (the treatment goal) and the time required for complete breakthrough (influent and effluent concentrations were equal). These service times can also be equivalently represented as volumes of water treated. The average loading of RDX and HMX on the GAC (mg/g GAC) was also calculated at the corresponding service times.

GAC SCREENING EXPERIMENTS

RDX is less adsorbable than HMX; therefore, RDX breaks through first and controls the GAC service life. As such, much more attention was focused on RDX than on HMX. Five GACs were evaluated in the screening studies: Norit H3000 and H4000, Calgon F300 and F400, and Northwestern LB-830 (now in use at Pantex). Calgon F400 was the best of the five, and Northwestern LB-830 was the second best. F400 had the longest service life until the treatment goal of 26 µg /L RDX was exceeded and the largest average RDX loading. F400 and LB-830 were selected for thorough evaluation in subsequent RSSCT experiments.

OPERATION OF GAC SYSTEM

A GAC system consisting of two columns can be operated in a variety of ways, and the choice of operating modes can have a significant impact on service life, chemical loading on the GAC at exhaustion, and GAC utilization rates (i.e., lb GAC/1000 gal treated). Two columns can be operated in series or parallel. With parallel operation, the GAC in each column is replaced at the same time, and the average loading is lower than possible with series operation. In series operation, GAC replacement usually occurs when the effluent concentration from the second column in the series exceeds the treatment goal. Only the GAC in the first column is usually replaced, and the order of the columns is then switched. In this way, only the most highly loaded GAC is replaced at any time, producing the smallest possible GAC utilization rate. With this operating scheme, the service life until the first GAC replacement is shorter than that for all subsequent replacements. The information presented in this executive summary assumes series operation, replacement of one GAC column at a time, and switching of column order upon replacement. The information developed in this research, however, can be used to estimate the service life for any series or parallel operating scheme desired.

GAC SERVICE LIFE ESTIMATES

The GAC service life was estimated for F400 and LB-830 using influent concentrations of 2300 µg/L RDX and 350 µg/L HMX. The RSSCT was designed to simulate the design flow rate and EBCT. A summary of the service life, represented in terms of volume treated, and average RDX loading at exhaustion is provided in Table ES-1. The RSSCTs clearly demonstrate the superiority of F400 over LB-830; 40-45% more water can be treated with F400 in comparison to LB-830. Even so, at the current flow rate of 20 gpm the RSSCT results indicate that the GAC treatment system with LB-830 should be able to operate on the order of 4 years before GAC replacement is required.

Table ES-1: Volume Treated and Average RDX Loading at the End of the Service Life[1]

GAC	Volume Treated (million gallons)[2]		Average RDX Loading (mg/g)[3]
	First Replacement	Subsequent Replacements	
Calgon F400	65	106	108
Northwestern LB-830	45	75	82

1. Flow rate is 325 gpm; influent concentrations are 2300 µg/L RDX and 350 µg/L HMX.
2. Volume treated until RDX concentration equals 26 µg/L in second column effluent.
3. Average loading on GAC in first column at time of replacement.

Additional RSSCT experiments were run at elevated RDX and HMX concentrations to determine the impact of influent concentration on service life. Increased concentrations of RDX and HXM in the contaminated groundwater significantly decreased the service life of Calgon F400 GAC. Decreases were as large as 78% when the RDX influent concentration was increased from 2300 to 4500 μg/L. An increase in the HMX concentration from 350 to 1100 μg/L similarly produced an 80% decrease in service life. In this case, increased competition for adsorption sites from the larger HMX influent concentration caused RDX to break through earlier. These results highlight the importance of tracking influent concentrations over time, so that service life estimates can be refined based on actual operating conditions.

FOULING BY NATURAL ORGANIC MATTER

"Pre-loading" RSSCT experiments were conducted in which the GAC was first exposed to uncontaminated Pantex groundwater for various time periods, followed by exposure to contaminated groundwater. "Preloading" simulates the actual operation of GAC columns in that natural organic matter is much less adsorbable than RDX and HMX; therefore, the GAC is already exposed to (or pre-loaded with) natural organic matter prior to the arrival of the RDX and HMX adsorption fronts at any location in the GAC column. The duration of this pre-exposure time increases in going from the influent to effluent end of the column and in going from the first to second column. In many applications, the duration of pre-exposure to natural organic matter has been related to decreased adsorption capacity for target chemicals, and is termed fouling.

Adsorption of RDX and HMX was significantly hindered by the fouling caused by pre-loading with natural organic matter. The estimated service lives of an 8.2-min EBCT column packed with F400 were 81, 74 and 34 days (at a design flow of 325 gpm) based on pre-loading times of 37, 112, and 261 days. Clearly, natural organic matter had a substantial impact on adsorption capacity. Fouling is very difficult to account for in estimating GAC service life; however, the estimates provided in Table ES-1 must be viewed as accounting for fouling to only a minimal extent. Therefore, actual service life could be substantially smaller. Because of the detrimental impact of fouling on adsorption capacity, steps to minimize fouling should be considered. In particular, bypassing the second column in the series until breakthrough of RDX is observed from the first column might substantially lessen the effect of fouling in the second column.

COMPUTER SIMULATIONS

Computer simulations of the RSSCT experiments were performed using the computer program *PCsorb*. *PCsorb* was developed at the University of Texas and is an implementation of the homogenous surface diffusion model, which has been widely used for many years in adsorption modeling. *PCsorb* predicted longer service lives for GAC columns than were experimentally determined with RSSCTs. The breakthrough curves produced by *PCsorb* were steeper than the experimental breakthrough curves. Although the agreement between the computer model and experimental data is somewhat disappointing, the computer model may still be useful in tracking the operation of the Pantex GAC system, especially if the influent concentrations change over time. Changing influent concentrations are easily accommodated in the model, and not so easily accommodated in RSSCT experiments.

RECOMMENDATIONS

- Calgon F400 GAC performed the best of the five GACs evaluated; F400 is the recommended GAC as future purchases are needed.
- The GAC service life is significantly affected by the influent RDX and HMX concentrations; therefore, influent concentrations should be tracked over time to increase the accuracy of GAC service life estimates.
- Fouling of the GAC with natural organic matter is significant and may substantially decrease the adsorption capacity for high explosives. To minimize fouling, the second column in the series should be bypassed until RDX begins to break through the first column.
- If significant changes in influent concentration are experienced over time, use of the computer model is recommended to provide rough estimates of the expected GAC service life.

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Performance Evaluation of Granular Activated Carbon System at Pantex: Rapid Small-Scale Column Tests to Simulate Removal of High Explosives from Contaminated Groundwater

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Abstract

The U.S. Department of Energy Pantex plant near Amarillo, Texas, performs operations that include creation of high explosives components for nuclear weapons and assembly and disassembly of nuclear weapons.

The high explosives HMX and RDX have been detected in groundwater samples from the perched aquifer below the Pantex Plant. The contamination is a result of past waste disposal procedures at the facility. Granular activated carbon (GAC) adsorption is a treatment option for remediating the high explosives. A pilot-scale, dual-phase extraction system has been installed at Pantex to investigate the effectiveness of GAC adsorption for removal of these contaminants.

The goals of this study were to provide support and guidance for the operation of the pilot-scale system at Pantex through laboratory testing. Rapid small-scale column tests (RSSCTs) were performed with explosive-contaminated groundwater from Pantex to accomplish this task. Five different carbons were evaluated, and service life versus empty bed contact time (EBCT) curves were developed for the two best performing carbons. Further analyses evaluated the effect of increased influent concentration and "fouling" caused by preloading with natural organic matter. Modeling of the experimental data was also performed using PCsorb.

Results of this research indicate that series operation of GAC columns produced extended service lives relative to parallel operation. Calgon F400 GAC produced longer service lives than the Northwestern LB-830 GAC currently in use at Pantex and should be considered as an option for GAC replacement. Effects of preloading should be considered to minimize "fouling" by background organic matter. Influent concentration ranges should be defined to more accurately predict GAC service life.

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1. INTRODUCTION

In the manufacture of high explosives and the activities that load, assemble, and pack (LAP) explosives into military ordnance, wastewaters contaminated with explosives are produced and can be released into the environment. Energetic material waste and solid waste contaminated with energetic material are also produced during munitions-related manufacture. From past disposal practices of these materials, soil and groundwater contamination has occurred.

Past waste handling procedures for explosive-contaminated wastewater included using unlined lagoons or pits for holding the wastewater. From these lagoons, high explosives have migrated into the subsurface and contaminated the soil and groundwater. Open burning and open detonation of energetic material has also led to soil contamination and air pollution.

Two common high explosives that are prevalent in munitions manufacturing waste include HMX (Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) and RDX (Hexahydro-1,3,5-hexanitro-1,3,5-triazine). The current treatment practices for process wastewaters containing HMX and RDX include activated carbon adsorption. The concentrations of high explosives in the process wastewaters are higher than that in contaminated groundwater, but it has been demonstrated that activated carbon adsorption can be applied to treat explosive contaminated groundwater.

RDX has been classified by the USEPA as a possible human carcinogen (Class C Carcinogen) and is toxic at 0.25 mg/L, while HMX has not been classified as to human carcinogeneity (Class D Carcinogen) (McLellan et al., 1992; US Department of Health and Human Services, 1994). Inhalation exposure to RDX can lead to several toxic effects, especially on the central nervous system. These include nausea, irritability, convulsions, and unconsciousness (McLellan et al., 1992; Rosenblatt, et al., 1991). Drinking water health advisories have been proposed at 2 µg/L and 400 µg/L for RDX and HMX, respectively.

To alleviate the potential for adverse human health effects and the migration of high explosives contamination from the perched aquifer at the Pantex Plant, research was conducted to characterize the treatability of explosive contaminated groundwater at the Pantex Plant. This chapter describes the Pantex facility and high explosive contamination evident at Pantex. It also presents the objectives and approach of this research.

1.1 PANTEX PLANT

This section gives a short description of the Pantex Plant. Site history as well as groundwater monitoring data are presented. Some of the subsurface properties including the hydrogeology are also included. A more comprehensive description of the Pantex facility is located elsewhere (Batelle Pantex, 1996).

1.1.1 Plant History

The Pantex Plant is a U.S. Department of Energy (DOE) facility, located approximately 17 miles northeast of Amarillo in the Texas Panhandle (Figure 1.1). The plant consists of approximately 10,000 acres. An additional 6,000 acres are leased from Texas Tech University to serve as a security buffer zone. Primarily agricultural lands surround the Pantex Plant.

The original Pantex Plant was constructed in 1942 to serve the manufacture of conventional ammunition and bombs. During 1951, the operations shifted to nuclear weapons operations as arranged by the Atomic Energy Commission, which later became the DOE. In 1989, the storage of plutonium pits from nuclear weapons was included in the operations done by the Pantex Plant. Currently, the primary operations that occur at Pantex include the assembly and disassembly of weapons, evaluation of weapons, plutonium pit storage, and research and development of high explosives (Batelle Pantex, 1996).

The major areas of the facility are designated by zone number as shown in Figure 1.1. The areas that overlie the perched aquifer with the highest known levels of explosive contamination include Zone 11 and Zone 12. Zone 11 is the experimental explosives development area, while Zone 12 is the weapons assembly and disassembly area.

1.1.2 Hydrogeology

Below the Pantex site, the subsurface geology consists of the Blackwater Draw Formation, comprised of interbedded silty clays with caliche and very fine sands with caliche (Batelle Pantex, 1996). The Ogallala Formation lies under the Blackwater Draw Formation. In the Ogallala Formation, there are two water bearing members. These include discontinuous perched aquifers and the main Ogallala aquifer.

The discontinuous perched aquifer is underlain by a clayey layer that has low permeability. This fine-grained layer is 25 to 40 feet thick and serves as a vertical barrier between the perched aquifer and the Ogallala aquifer. The thickness of the saturation in the perched aquifer can vary by as much as 100 feet, and depths from the ground surface to the perched aquifer can range from 209 to 280 feet (Batelle Pantex, 1996). The lateral extent of the confining layers, and thus the perched aquifers, is unknown, but it is known that the groundwater flow in the perched aquifer flows in a southeastern and southwestern direction below Zone 12. This flow pattern is due to the decrease in the elevation of the fine-grained layer from the northwestern to southeastern corner of the area encompassed by Zones 11 and 12.

The Ogallala aquifer lies below the confining layer of these perched water zones. This aquifer is a principal water supply on the High Plains and can produce high quality groundwater. The groundwater flow of the Ogallala aquifer beneath the Pantex Plant is from the southwest to the northeast, in the direction of the City of Amarillo well field. The well field northeast of the plant is located within a paleovalley of the Ogallala Formation where the Ogallala aquifer is thickest.

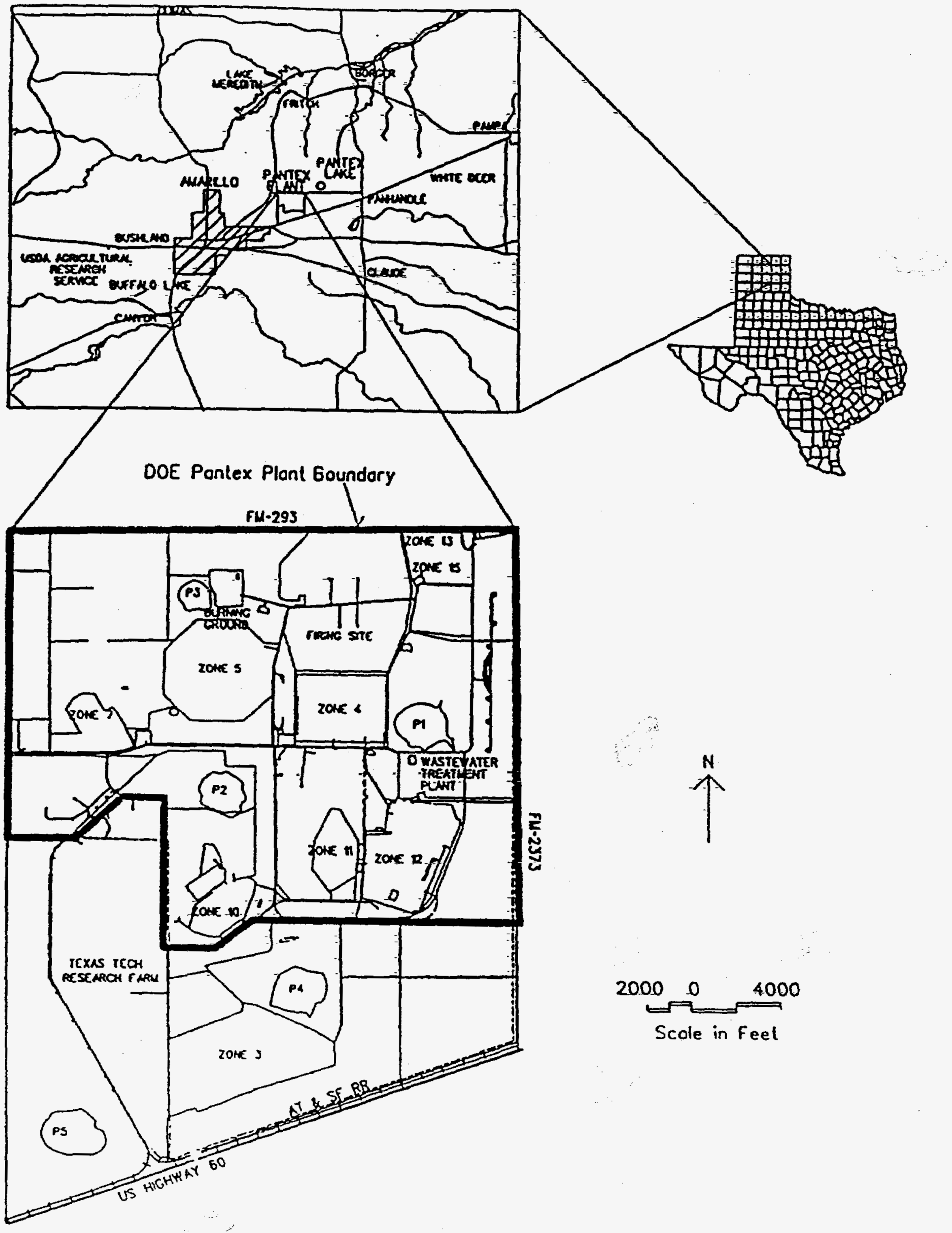

Figure 1.1: Pantex Plant Location and Layout (Source: Batelle Pantex, 1996)

1.1.3 Zone 12 Contamination History

Various chemicals have been used for weapon assembly and disassembly in Zone 12. As a result, process wastes were generated, and past disposal practices most likely caused contamination of the perched water zones. A landfill located east of Zone 12 was used for explosive process waste. A major surface drainage channel ran adjacent to the landfill. When the drainage channel would fill with water, it infiltrated and migrated through the landfill. Leaching of the explosive contaminated waste occurred and the contaminants were transported to the perched aquifer. Furthermore, discharge and runoff that accumulate in the region's playas can infiltrate into the perched aquifers. Thus, any contamination in these runoff waters will then be transported to the perched aquifers (Batelle Pantex, 1996). It is probable that this mechanism of contaminant transport is responsible for the high explosives as well as the TCE and chromium contamination in the perched aquifer. To date, no contamination has been detected in the Ogallala aquifer in this region.

Both the high explosives RDX and HMX have been detected at significant concentrations in the perched aquifer. From the 1995 Environmental Report for Pantex Plant, the maximum concentration values detected for RDX and HMX were 2.47 mg/L and 1.06 mg/L, respectively (Batelle Pantex, 1996). These levels for RDX and HMX are well above the risk reduction levels of 26 µg/L RDX and 5.11 mg/L HMX developed for the Pantex Plant. Figure 1.2 shows the RDX concentration contours for the perched aquifer while Figure 1.3 contains the HMX concentration contours. Operations still continue that produce hazardous wastes at Pantex, but proper disposal methods are now employed.

1.1.4 Current GAC Treatment System

A GAC pilot treatment system for high explosive removal is currently in place at Pantex. It is part of the pilot-scale dual-phase extraction system installed to the southeast of Zone 12 at the Pantex Plant in the fall of 1995 as a part of the Zone 12 treatability study. The GAC portion of the treatment system consists of two GAC columns in series and the system is used to treat any produced groundwater from perched aquifer investigations. The treated water can then be reinjected into the subsurface. The operation of the treatment system is not continuous; it is only operated when perched aquifer testing is being conducted.

Figure 1.4 shows a schematic of the GAC treatment system at Pantex. The flow to the system is 325 gpm and the GAC vessels have an 8 ft diameter. Ten-thousand pounds of Northwestern LB-830 GAC are in each column. The calculated empty bed contact time (EBCT) for each column is 8.2 min, and the hydraulic loading rate is 6.47 gpm/ft^2.

1.2 GROUNDWATER TREATMENT OPTIONS

The occurrence of high explosives as groundwater contaminants and the potential for adverse human health effects from this contamination have prompted investigations to remediate explosive-laden groundwater. The current treatment technology for explosive-contaminated wastewaters is granular activated carbon (GAC) adsorption. This process seems feasible to remediate explosive contaminated groundwater even though the explosive concentration in the groundwater is lower than that in waste process waters. Other treatment options, including direct chemical hydrolysis, ultraviolet radiation, polymeric adsorption, and biological degradation have been evaluated for high explosives remediation, but activated carbon adsorption remains the most widely applied technique.

For activated carbon adsorption to be effective as a remediation alternative, several operational conditions and parameters need to be considered. Granular activated carbon adsorption is a competitive process and the competition produced among adsorbing constituents must be taken into account. Also, the competition derived from any background organic matter must also be considered because it could reduce the expected capacity of the carbon. Taking all these concerns into account, GAC adsorption can be evaluated to be a viable treatment option for remediating explosive contaminated groundwater.

1.3 RESEARCH APPROACH AND OBJECTIVES

The research presented in this thesis was comprised of laboratory studies to determine the treatability of groundwater contaminated with explosives from the Pantex Plant utilizing GAC adsorption. Activated carbon adsorption of high explosives has been demonstrated to be an appropriate treatment technology, and the application of this technology has been documented.

The primary goals of this research include the following:

- determine the best performing GACs for explosive removal from contaminated Pantex groundwater using commercially available GACs, develop service life versus empty bed contact time (EBCT) curves for the best performing GACs,
- determine the effect of varying high explosive influent concentration on the competition for adsorption sites,
- determine the degree of competition presented by background organic matter present in the Pantex groundwater, and
- perform computer modeling to determine the applicability of current computer models to the present treatability study.

Once these objectives were met, the results were used to develop service life predictions and recommendations for GAC replacement options for Pantex. The results will also be used in future work relating to the biodegradation of high explosives adsorbed to GAC.

The background information, experimental procedures, and results of the adsorption studies are presented in the succeeding chapters. Chapter Two contains the background information on rapid small-scale column tests and information on previous explosive adsorption research while Chapter 3 describes the methodology used in performing the experiments. Chapter 4 presents the experimental and computer modeling results; conclusions and recommendations are found in Chapter 5.

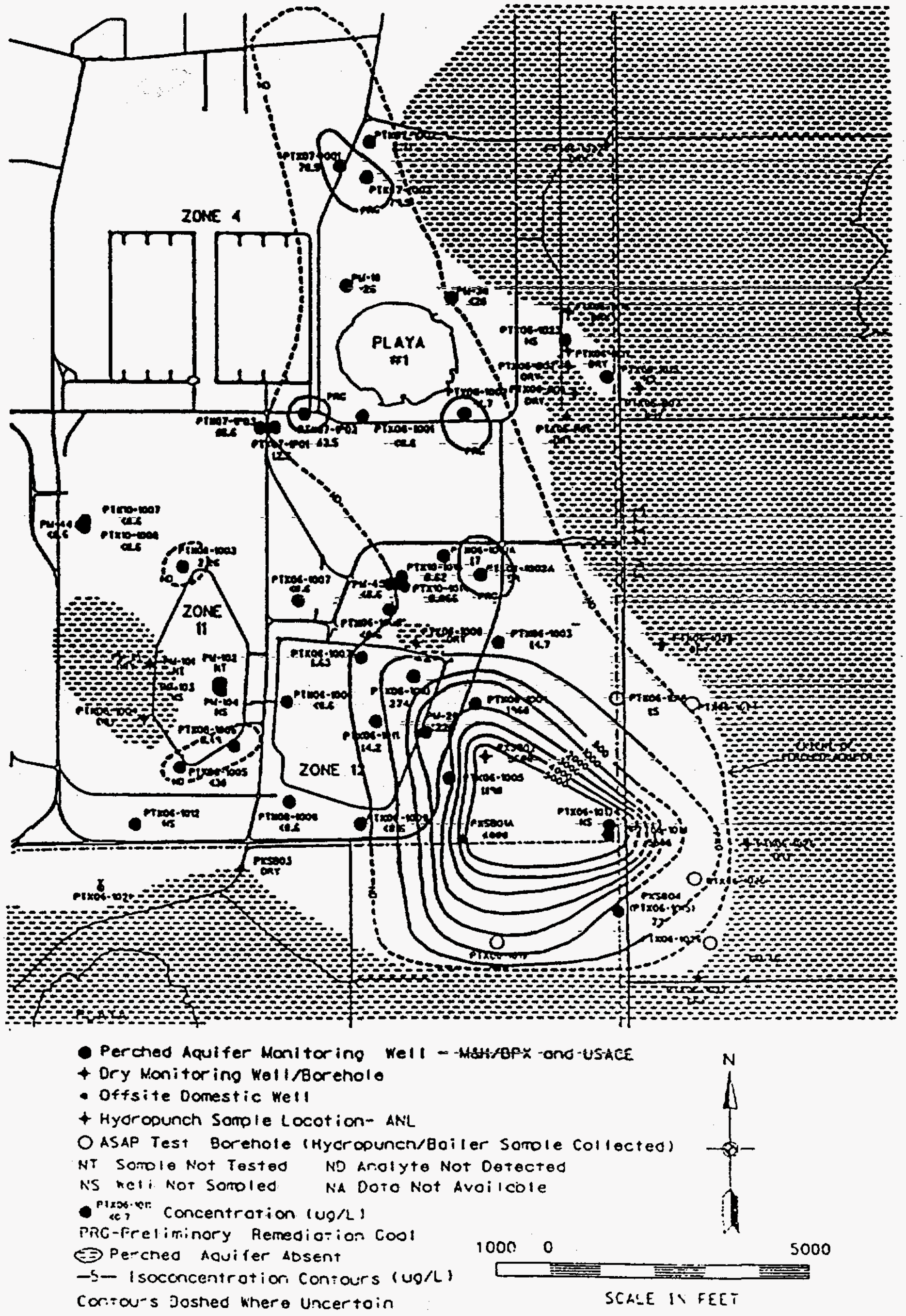

Figure 1.2: RDX Concentration Contours in the Perched Aquifer
(Source: Batelle Pantex, 1996)

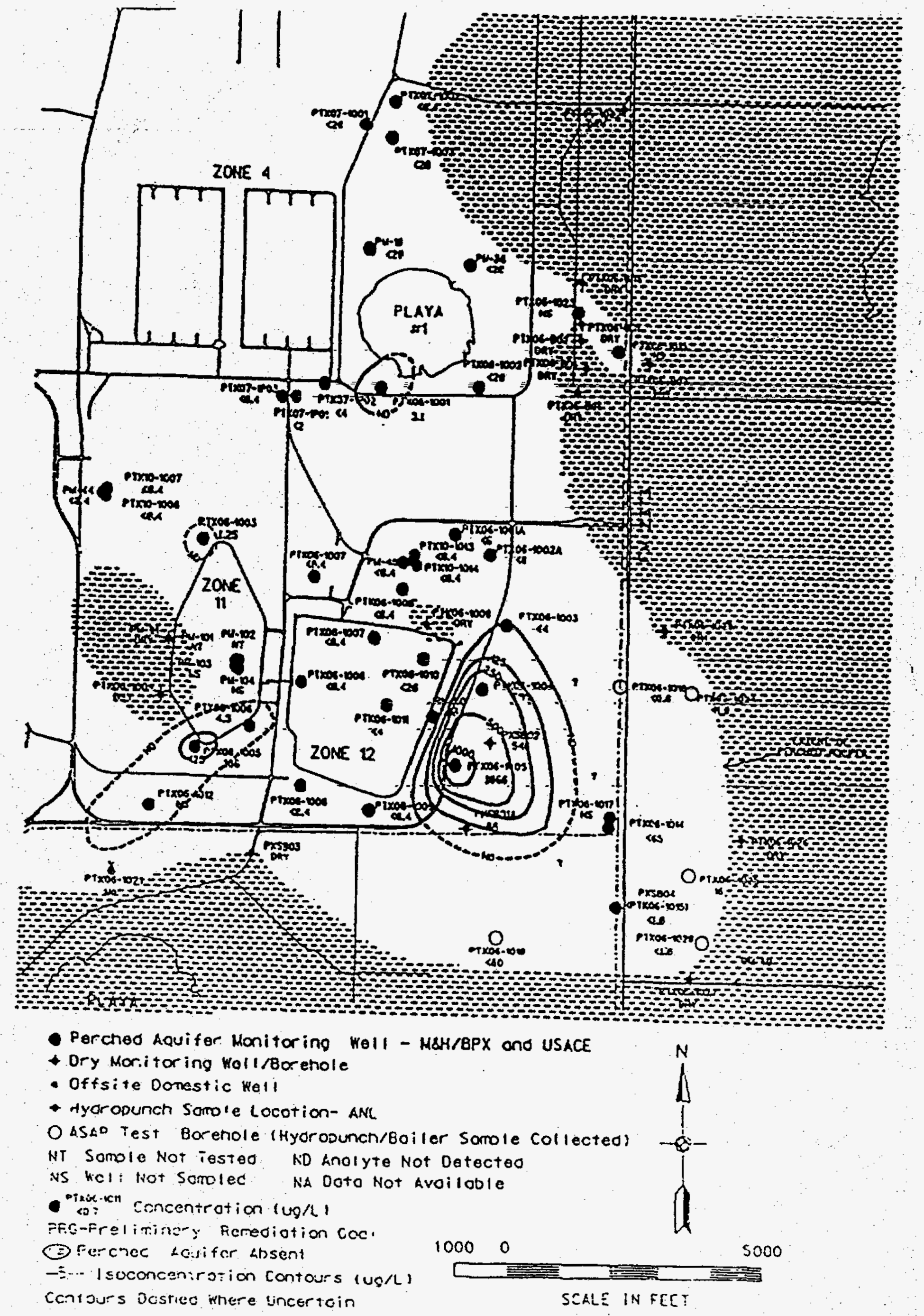

Figure 1.3: HMX Concentration Contours in the Perched Aquifer
(Source: Batelle Pantex, 1996)

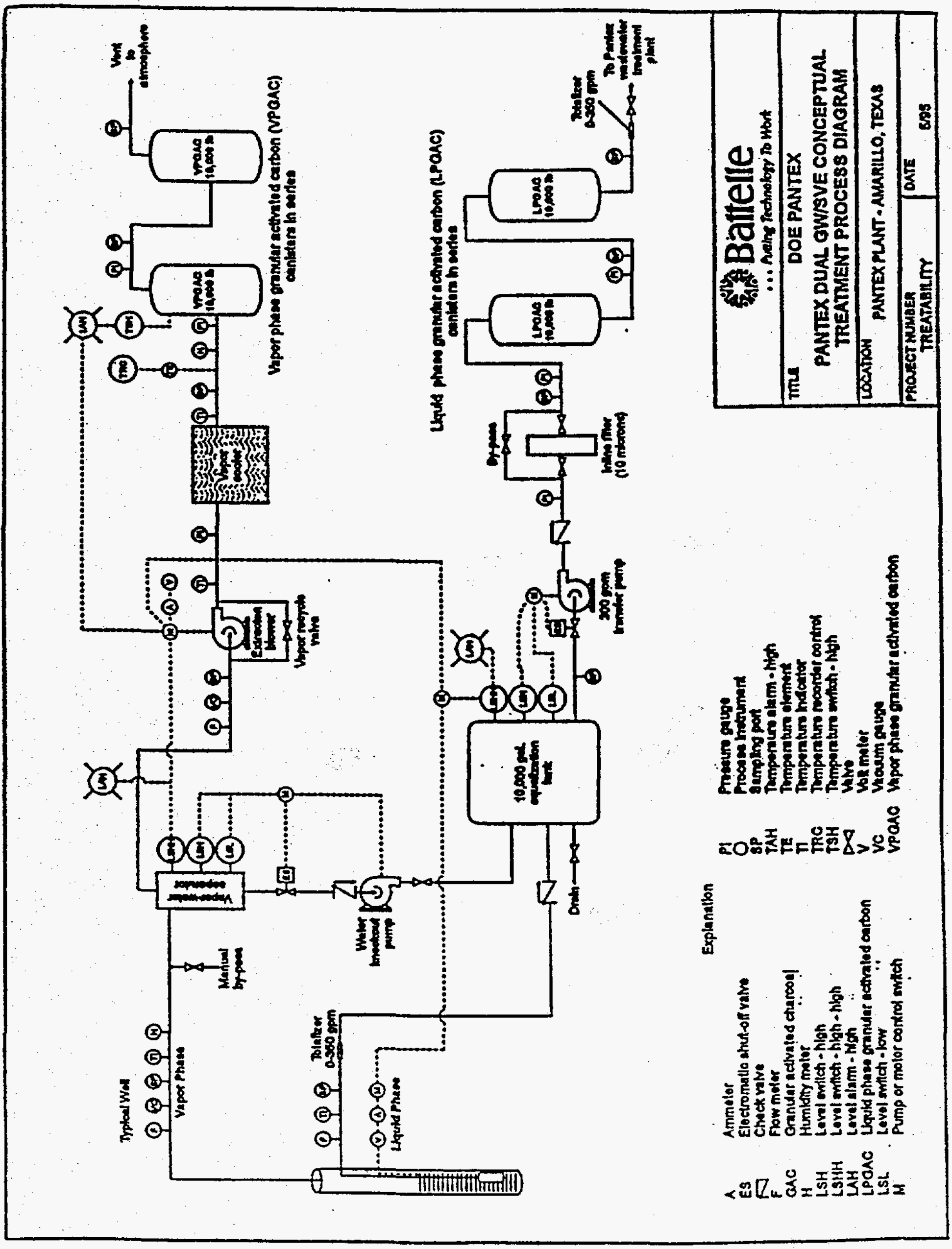

Figure 1.4: GAC Treatment System Currently in Place at Pantex

2. LITERATURE REVIEW

2.1 INTRODUCTION

Adsorption of mixtures of high explosives onto GAC has been a common method for treating explosives-contaminated water. Characterizing the adsorption of a mixture of chemicals is difficult because of competition for sites on the GAC. Thus, changes in the influent concentration of one chemical can affect not only its removal but also the removal of other chemicals in the mixture. Various treatability studies can be used to characterize adsorbability and predict treatment performance. These include a variety of experimental and computer modeling approaches such as single and multi-component isotherm experiments, batch adsorption kinetic experiments, rapid small-scale column tests (RSSCTs), and multi-component and kinetic computer simulation models. For a defined mixture, RSSCTs are a quick and accurate technique for defining treatability (Crittenden et al., 1986).

This chapter first presents important background information on the development of RSSCTs. Scaling principles and equations used to design an RSSCT are included. Previous work on GAC adsorption of high explosives is also covered. Information on the effects of the competition presented by natural organic matter in the source water is discussed in the pre-loading section. The use of computer models to predict adsorption performance is then discussed.

2.2 RAPID SMALL SCALE COLUMN TESTS (RSSCT)

Rapid small-scale column tests are continuous-flow column tests conducted at small-scale in the laboratory. Three primary advantages stem from performing RSSCTs rather than conducting other experimental procedures. An RSSCT may be conducted in a fraction of the time required to conduct pilot studies, and unlike mathematical models, extensive isotherm or kinetic studies are not required to obtain a full-scale performance prediction. Furthermore, a small volume of water is required to conduct the test, which can be transported to a central laboratory for evaluation (Crittenden et al., 1986).

2.2.1 RSSCT Approach

Using similitude to a full-scale column, mathematical models have been used to scale down the full-scale adsorber to a small column. By selecting the proper particle size, hydraulic loading, and empty bed contact time (EBCT) of the small-scale adsorber, the effluent breakthrough curve of the RSSCT will be similar to that of the full-scale column. To simulate full-scale adsorber performance, the amount of spreading in the breakthrough curve as compared to the column depth must be identical for the RSSCT and the full-scale column (Crittenden et al., 1991). Thus, no changes in the mechanisms that cause spreading can occur with changes in process size. The mechanisms that cause spreading include transport of the chemical from the bulk liquid to the liquid film, liquid film transport, adsorption onto the GAC surface, and diffusion within the GAC particle (Montgomery, 1985). An illustration of these mechanisms is included in Figure 2.1. The transport from the bulk liquid to the liquid film and the adsorption onto the GAC surface are typically rapid; the overall rate of adsorption is usually controlled by either the liquid film transport or diffusion within the GAC particle.

In theoretical adsorption models (Hand et al., 1983, Crittenden et al., 1986), adsorption is characterized by key dimensionless parameters. By maintaining the dimensionless parameters that describe the spreading mechanisms constant when the process is scaled down, similarity between the two systems (full-scale and small-scale) is maintained. Therefore, adsorption theory provides a way to design laboratory experiments that should simulate performance of full-scale columns well.

2.2.2 Development of Scaling Relationships for RSSCTs

Scaling equations for RSSCTs are developed by requiring that the dimensionless parameters of the small-scale and the full-scale adsorber be equal. The dimensionless parameters of interest include the solute distribution parameter (D_g), the surface diffusion modulus (E_d), the Stanton number (St), and the Reynolds number (Re). By setting the dimensionless parameters of the RSSCT equal to those of a large scale column, relationships between important design variables can be determined (Crittenden et al., 1986). The solute distribution parameter (D_g) describes the relative adsorbability of a chemical at equilibrium with the influent concentration; it is defined by the following equation:

$$D_g = \frac{\rho_a q_e (1-\varepsilon)}{\varepsilon C_o}$$

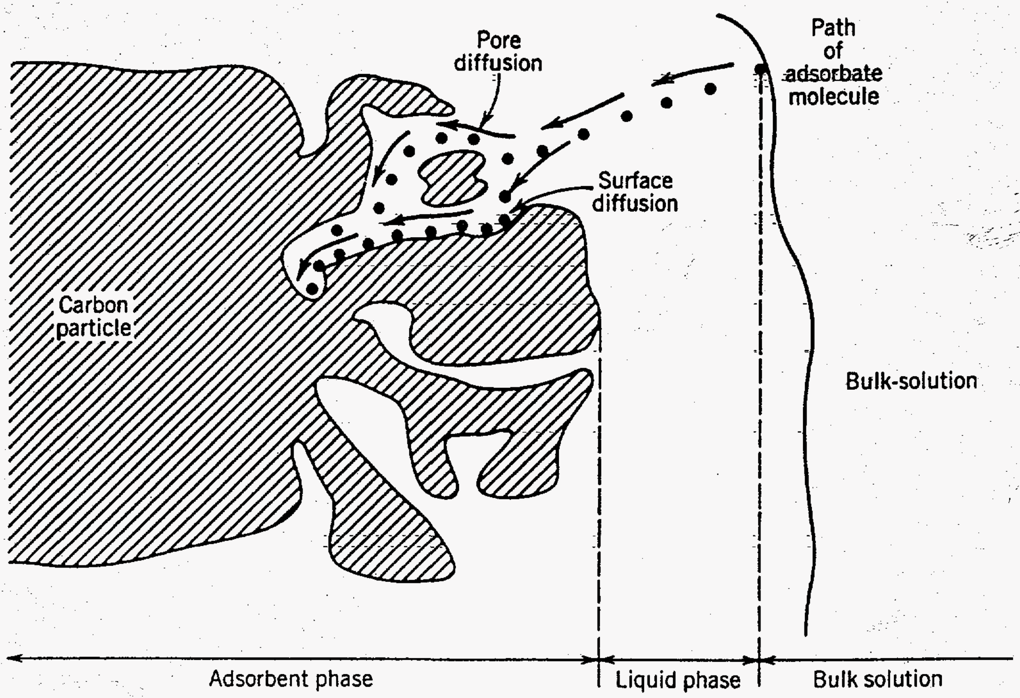

Figure 2.1: Mechanisms of Adsorption onto Granular Activated Carbon. (Hand et al. 1983)

where:

ρ_a = apparent density of the GAC (g/cm^3)
q_e = Freundlich equilibrium mass loading of contaminant on the adsorbent (mg chemical/g GAC)
ε = packed bed porosity
C_o = influent chemical concentration (mg/L)

The surface diffusion modulus (E_d) is a ratio of the diffusive mass transfer in the GAC to the rate of advection through the column. The equation that defines E_d is shown below. When diffusion controls adsorption rates, E_d relates the mass transfer zone length to the column's total length.

$$E_d = \frac{D_s D_g \tau}{R^2}$$

where:

D_s = surface diffusion coefficient (cm^2/sec)
D_g = solute distribution parameter
τ = packed bed contact time (min)
R = GAC radius (cm)

The Stanton number (S_t) is a ratio of the liquid film mass transfer to the rate of advection through the column. If liquid film transport controls the rate of adsorption, S_t relates the length of the mass transfer zone to the total column length. The Stanton number is defined by the following equation.

$$St = \frac{k_f \tau (1-\varepsilon)}{\varepsilon R}$$

where:

k_f = liquid film transfer coefficient (cm/sec)
τ = packed bed contact time (min)
ε = packed bed porosity
R = GAC radius (cm)

The Reynolds number (Re) describes the flow regime that exists in the GAC column as a ratio of the inertial to viscous forces. It is defined by the following equation:

$$Re = \frac{2R v_s}{\nu}$$

where:

R = GAC radius (cm)
v_s = interstitial velocity (cm/sec)
ν = kinematic viscosity (cm^2/sec)

To match the spreading due to intraparticle mass-transfer resistance, (intraparticle diffusion) the surface diffusivity modulus, E_d, of the small-scale and large-scale columns are equated. This produces a relationship between the EBCT values of the two columns, as shown below. This relationship incorporates the possible dependence of the intraparticle diffusivity on GAC particle size with the variable X.

$$\frac{EBCT_{SC}}{EBCT_{LC}} = \left(\frac{R_{SC}}{R_{LC}}\right)^{2-X} = \frac{t_{SC}}{t_{LC}}$$

where:

$EBCT_{SC}$, $EBCT_{LC}$ = empty bed contact time of small and large columns (min)
R_{SC}, R_{LC} = GAC radius of small and large GAC (cm)
t_{SC}, t_{LC} = elapsed time to conduct the test for small and large columns (min)
X = 0, for no dependence of intraparticle diffusivity on particle size 1, for linear dependence of intraparticle diffusivity on particle size

The relationship between the hydraulic loading rates for each column is determined by equating the Stanton and Reynolds numbers for both the small-scale and full-scale columns. This ensures that the external mass-transfer and dispersion contributions to spreading in the breakthrough curve are equal. The equation relating the hydraulic loading rates for each column is shown below:

$$\frac{V_{SC}}{V_{LC}} = \frac{R_{SC}}{R_{LC}}$$

where:

V_{SC}, V_{LC} = hydraulic loading rates of the small and large columns (gpm/ft^2)

R_{SC}, R_{LC} = radius of small and large GAC (cm)

If this relationship is applied to design an RSSCT using the proportional diffusivity relationship (X=1), a column equal in length to the full-scale column would result, producing an unacceptable pressure drop and influent volume requirement for an RSSCT. The proposed solution to this problem was developed by Crittenden et al. (1987) with the following equation.

$$\frac{V_{SC}}{V_{LC}} = \frac{R_{SC}}{R_{LC}} \times \frac{Re_{SC,Min}}{Re_{LC}}$$

where:

V_{SC}, V_{LC} = hydraulic loading rates of the small and large columns (gpm/ft^2)

R_{SC}, R_{LC} = radius of small and large GAC (cm)

$Re_{SC,Min}$ = minimum Re applied to the small column

Re_{LC} = Re applied to the large column

In this approach, the Re of the small column is decreased so that the length of the column is decreased. Since the liquid film transport resistance is typically a small fraction of the mechanism for spreading of the mass transfer zone, reduction of the Re should not present a problem. Crittenden et al. (1987) suggests values for $Re_{SC,Min}$ of 0.13, 0.05, 0.03, and 0.023 for organic compounds with molecular weights of 100-300, 1000, 5000, and 10,000, respectively.

Even though the reduction of the Re was formulated for proportional diffusivity, if the flow rate and volume of treated water are too large for an RSSCT designed with constant diffusivity using matching Re, the same rationale could be applied to reduce the Re for constant diffusivity tests (Speitel, 1997).

Based on the preceding equations, the only information needed to design the RSSCT are the large scale EBCT, GAC radius, and hydraulic loading rate. Other specific operational parameters, including the flow rate applied to the small column (Q_{SC}), the mass of GAC used during an RSSCT, and the column length, are determined from the following equations:

$$Q_{SC} = A \times V_{SC}$$

where:

Q_{SC} = flow rate of the small column (mL/min)

A = cross-sectional area of the small column (cm^2)

V_{SC} = hydraulic loading rate of the small column (cm/min)

$$M_{SC} = EBCT_{SC} \times Q_{SC} \times \rho_b$$

where:

M_{SC} = mass of GAC in the small column (g)

$EBCT_{SC}$ = empty bed contact time of the small column (min)

Q_{SC} = flow rate of the small column (mL/min)

ρ_b = bulk density of the full-scale column GAC (g/cm^3)

$$L_{SC} = V_{SC} \times EBCT_{SC}$$

where:

L_{SC} = length of the small column (cm)

V_{SC} = loading rate of the small column (cm/min)

$EBCT_{SC}$ = empty bed contact time of the small column (min)

The time and volume of water required for exhaustion of the RSSCT can be estimated if single-component isotherm parameters are known. These can be calculated applying the following equations.

$$t_{SC} = \varepsilon \times \left(D_g + 1\right) \times EBCT_{SC}$$

where:

t_{SC} = time to exhaust the small column (min)
ε = porosity
D_g = solute distribution parameter
$EBCT_{SC}$ = empty bed contact time of the small column (min)

$$Vol_{SC} = Q_{SC} \times t_{SC}$$

where:

Vol_{SC} = water volume to exhaust the small column (min)
Q_{SC} = flow rate of the small column (mL/min)
t_{SC} = time to exhaust the small column (min)

Previous RSSCT work has concentrated on removing volatile organic chemicals (VOCs) and disinfection byproduct (DBP) precursors from drinking water sources. Summers et al. (1995) confirmed that the RSSCT can predict breakthrough behavior of a full-scale column. In that study, removal of DBP precursors by GAC adsorption from six source waters was examined by operating RSSCTs. Pilot-scale and full-scale contactors were also run to verify the ability of the RSSCTs to predict full-scale operation.

Crittenden et al. (1989) did extensive work on the application of RSSCTs for the prediction of GAC performance. In this work, RSSCTs were compared to pilot studies for two sources of water. Studies were conducted with both constant diffusivity (X = 0) and proportional diffusivity (X = 1) designs. From the work, it was determined that the adsorption capacity of the GACs used in the RSSCTs and pilot columns were identical based on the batch isotherm results. Less capacity was observed, though, in the RSSCTs and pilot columns, for specific target organic chemicals when dissolved organic carbon (DOC) was present as compared to the case when DOC was absent.

Other conclusions were made on kinetics. When the contaminants of concern are more highly concentrated than the DOC of unidentified background, surface diffusion usually controls the intraparticle mass transfer rate. In this case, external mass transfer is important and any changes with the surface diffusion coefficient with particle size may be ignored when selecting RSSCT operating parameters (Crittenden et al., 1989). This would suggest that, for a contaminated groundwater with low TOC concentration, a constant diffusivity RSSCT design can be applied.

The RSSCT has recently been implemented as a part of the monitoring and testing for the Information Collection Rule (ICR) (Westrick, et al., 1996). The ICR resulted from an action to control microbial contaminants and disinfection byproducts in drinking water supplies. RSSCTs are required to be conducted by water utilities to examine the application of GAC treatment for removal of DBP precursors. The results of these tests would provide the water utilities with information to assess the feasibility of advanced treatment processes such as GAC adsorption to reduce DBP precursor levels (Westrick, 1996).

2.2.3 Further Considerations When Operating RSSCTs

Even though RSSCTs are a powerful experimental tool, they should be complemented by other experimental and analytical approaches. The primary difficulty in applying results from an RSSCT is determining the proper scaling relationship. As mentioned earlier, more than one set of scaling relationships exist for scaling RSSCT performance to larger scale performance (Crittenden et al., 1986, 1987). It is difficult to select the suitable scaling relationship without supporting experiments. Further, each RSSCT defines treatability only for one set of influent conditions and EBCT. The treatability of a source water can dramatically change if the influent concentration of the contaminants change. Thus, a representative sample of batch influent for the RSSCT is essential for good predictions (Summers et al., 1995).

To support RSSCT experiments, several other experimental analyses can be performed. Batch kinetic tests help define scaling relationships, while single and multi-component isotherm experiments provide more adsorption equilibrium information. The combination of the data from the RSSCT, batch tests, and isotherm tests can be evaluated with computer simulation models. When confidence in the models is attained, the models can be used to predict how changes in the influent conditions will affect performance. Thus, the models impart greater capabilities to extend the experimental results to other situations without having to experimentally define them.

2.3 PREVIOUS WORK ON ADSORPTION OF HIGH EXPLOSIVES

Adsorption onto GAC is the current industrial method for treating wastewaters contaminated with high explosives (pink water); it is being evaluated as a treatment alternative for explosive-contaminated groundwater. This section reviews some of the previous and current work on the adsorption of high explosives onto GAC. Various types of studies including isotherm development and pilot-treatment system evaluation are included in this compilation.

Adsorption isotherms characterize the equilibrium of a chemical between the water and activated carbon phase. The most commonly used isotherm is the Freundlich isotherm. It is given by the following equation:

$$q_e = KC_e^{1/n}$$

where:

q_e = mass loading of contaminant on the adsorbent (mg/g)
K = adsorption capacity at unit concentration (mg/g) $(L/mg)^{1/n}$
C_e = equilibrium concentration in the water (mg/L)
1/n = adsorption intensity

An isotherm can provide good information about the adsorbability of a chemical. More adsorbable chemicals have higher K and lower 1/n values.

Burrows (1982, 1984) conducted batch GAC adsorption studies to test the general feasibility of applying GAC treatment to remove munitions compounds from wastewater. Experiments using Calgon F300 were performed to develop single and multi-component isotherms. The single-component isotherm parameters produced from this study are shown in Table 2.1. The applicable concentration range for HMX was 0.234 mg/L (detection limit) to 5.2 mg/L; the concentration range for RDX was 0.264 mg/L

Table 2.1: Single-Component Isotherm Parameters for Calgon F300 (Burrows, 1982, 1984)

	K (mg HE/g GAC (L/mg)$^{1/n}$	1/n
HMX	168.2	0.461
RDX	118.8	0.340

Table 2.2: Isotherm Parameters for Contaminated Groundwater at Milan Army Ammunition Plant (MAAP)

	K (mg RDX/g GAC)(L/mg)$^{1/n}$	1/n
Calgon Filtrasorb 200	52	0.535
Calgon Filtrasorb 300	31	0.413
Calgon Filtrasorb 400	49	0.555
Norit Hydroarco 4000	1.2	0.100
Atochem, Inc. GAC 830	45	0.630

(detection limit) to 21.0 mg/L. The values of the Freundlich isotherm parameters indicate that removal of RDX and HMX from a contaminated water by GAC adsorption is feasible. Both HMX and RDX have high adsorption capacities (K isotherm parameter). The adsorption intensity (1/n) is fairly low, which also favors adsorption. However, RDX was deemed to be less adsorbable than HMX. When evaluated in a mixture, Burrows determined that competition for adsorption sites was evident; the log-log plots of Freundlich isotherms for HMX and RDX in a mixture and singly were parallel, but the intercepts for each of the components in the mixture was reduced. Therefore, in a mixture, HMX and RDX had similar adsorptive intensity (1/n) values as compared to the single-component system, but the adsorptive capacity (K) was reduced.

Bricka and Sharp (1992) and Bricka and Fleming (1995) investigated GAC to remove low levels of RDX from a drinking water source. The target treatment level in this study for RDX was less than 1 µg/L; the health advisory for RDX is 2 µg/L. Five GACs including Calgon F200 and F300, Norit ROW 0.8 and H4000, and Westates CC-601 were evaluated. Isotherm experiments were conducted with contaminated groundwater that had HMX and RDX concentrations of 1.4 µg/L and 5.5 µg/L, respectively. Based on previous work that did not experience good removal of contaminants at GAC dosages of 10 mg/L, increased GAC dosages of 10, 100, 500, 1000, and 10,000 mg/L were used in the isotherm experiments. For all of the GACs, at each dosage, the resulting RDX concentration after equilibration was below the detection limit, so no Freundlich isotherm parameters could be calculated. However, Calgon F200 and Norit H4000 were selected for pilot testing. Contaminated water was fed at a flow rate of 1.5 L/min to an upflow column system of 2 sets of 4 columns in series. Each column in the series had an EBCT of 5.4 min, producing a cumulative contact time for the series of 21.7 min. After continuous operation for six months, breakthrough in the first column of either set of columns had not been detected. At this point, the H4000 set of columns was modified, and sampling ports were attached every six inches on the first column of the series. Samples were taken, and it was concluded that the mass transfer zone was contained within the bottom 36 inches of the 48 inch column. The top 12 inches of the GAC had not yet been exposed to RDX. It was determined that the RDX loading on the GAC was 0.135 g RDX per pound of GAC (H4000).

The results of the isotherm tests show that all of the GACs tested can remove low levels of RDX from groundwater. Based on the preliminary results of the pilot-column studies, it seems that the GAC has a sorbative affinity for the low levels of contaminants present in the groundwater.

In a study conducted by Wujcik et al. (1992), preliminary batch (isotherm) tests were performed and followed with continuous-flow column testing to determine the feasibility of using GAC to treat groundwater contaminated with explosives. Several explosives including TNT, HMX, RDX, Tetryl, 2,4-DNT, 2,6-DNT, 1,3-DNB, 1,3,5-TNB, and NB were assessed in the study. The contaminated groundwaters used in this study were from the Badger Army Ammunition Plant (BAAP) and the Milan Army Ammunition Plant (MAAP). At BAAP, isotherms were developed for 2,4-DNT and 2,6-DNT while at MAAP, isotherms were developed for TNT and RDX.
The isotherm testing was comprised of batch adsorption experiments in which contaminated groundwater from each plant was treated with varying GAC dosages. For the isotherm experiments performed for MAAP, five GACs were evaluated, and the isotherm parameters were determined for each GAC in the 0.01 mg/L to 1.0 mg/L concentration range for RDX. These isotherm parameters are summarized in Table 2.1 compiled from the Wujcik (1992) study. Based on the results from the Wujcik study, two GACs, Calgon F300 and Atochem, Inc. 830, were selected for use in the continuous flow column studies. Three continuous-flow column tests were performed; each used two GAC column trains. Two of the column tests were stopped after 7.6 days and 14.5 days because breakthrough had not yet occurred. In the third column test, operation ceased after 54.5 days. At this point, the RDX concentration was 315 μg/L for the Atochem, Inc. 830 GAC and 344 μg/L for the F300 GAC. The average influent RDX concentration was 549 μg/L. In this test, the apparent breakthrough for both GACs occurred at approximately the same throughput volume of 12,000 gallons (8,144 bed volumes).

From the results of the column tests, both the Atochem, Inc. 830 GAC and the Calgon F300 GAC appear to be equivalent in meeting effluent goals for TNT and RDX. It was concluded that GAC was capable of removing explosives from contaminated groundwater to 1 μg/L at two Army ammunition plants. For contaminated groundwater at MAAP, concurrent removal of a mixture of explosives including TNT, HMX, RDX, Tetryl, 2,4-DNT, 2,6-DNT, 1,3-DNB, 1,3,5-TNB, and NB was possible.

Several other researchers have performed isotherm experiments with high explosives. These include the work by Haberman (1983) investigating the competition between TNT and RDX for adsorption sites. Hinshaw et al. (1987) investigated competitive adsorption of HMX, RDX, TNT, and 2,4-DNT on different GACs. Other effects from temperature, actual versus synthetic pink water, and acetone spiking were also evaluated in that study. Dennis et al. (1990) presented isotherm parameters that were determined for MAAP contaminated groundwater and used in the previously discussed Wujcik (1992) work. Most recently, Lee (1996) completed competitive isotherm modeling work using a mixture of HMX and RDX. In that work, a compilation of the previous single component and competitive batch isotherm parameters is presented.

2.4 PRE-LOADING THEORY

Naturally occurring organic matter (NOM) in a water source can have a significant impact on the adsorption of synthetic organic chemicals (Speth and Miltner, 1989). NOM, in an explosive-contaminated groundwater, can compete with the high explosives for adsorption sites and thus "foul" the GAC with the high molecular weight organics that comprise the background organic matter. Thus, the capacity for adsorption of the high explosives is reduced. Several researchers have investigated the effects of background organic matter on GAC adsorption and the adjustments that must be made to models to account for the effect of preloading with NOM. This section presents some of the relevant research that investigates preloading of GAC.

Speth and Miltner (1989) investigated the scale-up assumptions of equal capacities in small-scale columns and field columns to determine if preloading the GAC with a natural water greatly reduces the carbon's capacity for contaminant removal. RSSCTs and pilot column experiments were performed as well as isotherm experiments. Short-bed adsorber tests were also conducted to study adsorption kinetics. The carbon used in this study was Calgon F400, and the compound of interest was *cis*-1,2-dichloroethene (DCE). The source water was from the Great Miami Aquifer (GMA) in Ohio.

GAC was preloaded by feeding a column unspiked GMA water. This GAC was used in preloaded isotherm studies. Breakthrough curves were developed and compared for the pilot column and RSSCT. The capacity of both the pilot column and the RSSCT were determined by performing a mass balance around each column. These capacities were compared with those predicted by the GMA water isotherms. Speth and Miltner determined that the RSSCT capacity was on the upper 95 percent confidence band of the GMA water isotherm while the pilot column capacity was on the lower 95 percent confidence band. Thus, the capacities were statistically different, and the assumption of equal capacities in the scale-up procedure was violated. In the pilot column, the GAC near the effluent end of the column was exposed to NOM for an extended time period while the DCE front moved through the column; on the contrary, in the micro-column, the time to exhaustion was less than a day, which allowed for no preloading. Thus, it was determined that the reduction in capacity is consistent with the idea that preloading with NOM decreases the GAC capacity. This fact was also evident in the isotherm results. The preloaded GAC isotherms had a reduced capacity when compared to the GMA water isotherm and the distilled water isotherm.

Summers et al. (1989) also investigated the influence of background organic matter on GAC adsorption. This study probed the impact that natural organic matter in the Rhine River would have on GAC adsorption of trichloroethene (TCE) and the biodegradation of 1,2,4-trichlorobenzene (TCB). The effect on the small-scale column tests was also investigated. Pilot columns fed water spiked with TCE and TCB were run along with a column of unspiked water. To assess the reduction of the adsorption capacity, GAC samples were taken from the column receiving unspiked water at designated time intervals; TCE adsorption isotherms were performed with this GAC and compared to those done with fresh GAC. Small-scale columns were also fed TCE spiked water and unspiked water for further comparisons.

The results of these experiments showed that the amount of TCE adsorbed in the pilot column was significantly less than predicted from the batch isotherm study with fresh GAC. The isotherms run with GAC from the preloaded GAC columns showed reduced adsorptive capacity of the GAC as compared to the capacity of fresh GAC. For the small-scale column tests, breakthrough occurred much earlier for the full-scale column as compared to the scaled-up small-scale column results. Summers et al. (1989) found this to be true for both the constant diffusivity and particle-size dependent diffusivity cases. Thus, the reduction in adsorption capacity is not properly accounted for by either the isotherm based modeling approach or the small-scale column approach.

To overcome the disparity in the adsorption capacity predictions, Summers et al. (1989) proposed two alternatives. One approach applies the isotherm data from the preloaded GAC and combines it with the homogeneous surface diffusion model (HSDM) to predict loading capacity. The other proposed alternative is to preload the small GAC particles and then perform a small-scale column test. One drawback of initial preloading of the GAC particles for column tests is determining the appropriate preloading time. Complications arise because the scale-up procedure does not directly model the reduction of adsorption capacity. Therefore, Summers et al. (1989) indicated that kinetic information is required to accurately apply the scale-up procedure to predict full-scale column behavior.

2.5 COMPUTER MODELING WITH *PCSORB*

The *PCsorb* computer model is an interactive program for simulating adsorption of organic chemicals on granular activated carbon in continuous-flow columns (Dvorak, 1990). Solutions to either the Homogeneous Surface Diffusion Model (HSDM) or the Pore Surface Diffusion Model (PSDM) (Friedman, 1984) are provided by *PCsorb*.

In the development of the HSDM, three mechanisms of contaminant transport are considered. These include bulk liquid transport, liquid film transport, and diffusion within the adsorbent particle. The Freundlich isotherm parameters and Ideal Adsorption Solution Theory (IAST) describe the adsorption equilibria. IAST predicts multi-component equilibria using single-component isotherms.

Hand et al. (1984) identifies several assumptions that are incorporated into the solution of the HSDM. These include the following ideas. Plug flow exists in the bed, and the hydraulic loading is constant. The surface of the adsorbent is homogeneous and surface diffusion is the predominant intraparticle mass transfer mechanism. A liquid film mass transfer resistance exists external to the GAC particles. Mass transfer across the liquid film is described by a linear driving force expression, using the liquid film coefficient, k_f. The adsorbent is in a fixed position in the bed and backwashing is not considered. The only concentration gradients in the bed exist in the axial direction for the liquid phase and in the radial direction for the GAC particle.

Use of the PSDM is considered for systems with both weakly and strongly adsorbing chemicals. For the weaker adsorbing chemical, pore diffusion may be the primary transport mechanism due to surface diffusion blockage from the stronger adsorbing chemical (Dvorak, 1990). The mechanisms of contaminant transport included in the PSDM are identical to those for the HSDM, but pore diffusion within the GAC particles is now included.

The solution of the HSDM and PSDM involves performing mass balances on the two phases (liquid and GAC) for the contaminant.

A system of partial differential equations is created and cannot be solved analytically. Numerical methods with corresponding boundary conditions and initial conditions must be used. *PCsorb* uses orthogonal collocation to convert the system of partial differential equations to a system of first-order ordinary differential equations. These ordinary differential equations can be solved readily by Gear's method (Dvorak, 1990).

3. MATERIALS AND METHODS

3.1 INTRODUCTION

The major goal of this research was to characterize the treatability of groundwater contaminated with the high explosives HMX and RDX, using GAC adsorption. This goal was formulated to investigate the use of various GACs and to determine the effect, if any, that background organic matter has on the adsorption of high explosives. To address the goals of this research, RSSCTs were performed to characterize the treatability.

This chapter describes the analytical techniques and equipment that were implemented throughout this study. A description of the RSSCT experimental procedure is presented. Sampling practices and analytical methods are then described. The experimental plan for the entirety of this research follows.

3.2 RAPID SMALL-SCALE COLUMNS TESTS

Rapid small-scale column tests (RSSCTs) were conducted in which dissolved HMX and RDX were removed from contaminated groundwater using GAC. The RSSCT consisted of a continuous-flow GAC column from which effluent samples were taken.

3.2.1 GAC Preparation

The preparation of the GAC followed that described in other RSSCT work (Crittenden et al.,1989; Summers, 1996). The mesh size used for this RSSCT work was 80x100-mesh GAC. This size was acquired by crushing either 12x40-mesh GAC or 8x30-mesh GAC, depending on the GAC type. A representative sample of the full scale GAC was obtained and crushed. This sample was then sieved using a shaker table. Any of the GAC that did not pass through the upper sieve was returned and crushed again until all of the GAC passed through the upper sieve. The required sieve fraction was removed and stored in a beaker covered with aluminum foil until washed.

Washing was required to remove fines from the crushed GAC. The GAC was placed in a clean beaker filled with Milli-Q, deionized water. This was stirred with a glass rod and allowed to settle. An ultrasonic bath was used initially for 10 seconds to remove the fines. The ultrasonic bath was only repeated once during GAC washing to prevent more fines from being formed. After allowing the GAC particles to settle for 1-3 min, the supernatant was poured off and new Milli-Q water was added. Using fresh Milli-Q water, the stirring and settling process was continued until the supernatant was clear. The wet GAC was then placed in an oven that was maintained at 105°C to dry. Once the GAC was dried, it was removed from the oven and stored in dark amber bottles with Teflon lined caps in a cool, dark place.

3.2.2 Apparatus and Materials

All laboratory column experiments were conducted at room temperature. The materials used in the experimental apparatus were of glass, Teflon, or stainless steel. These materials were used to minimize adsorption of the high explosives by material other than the GAC.

A diagram of the RSSCT experimental apparatus is shown in Figure 3.1. Standard chromatography glass columns (Part No. 5795-04, Ace Glass, Inc.) with inner diameters of 0.8 cm were used in the RSSCT studies. Plastic safety shields (Part No. 5798-32, Ace Glass, Inc.) were used around the glass column. Channeling effects and wall effects were avoided because the ratio of column diameter to GAC particle diameter was at least 50 (Crittenden et al., 1989). Teflon end adapters (Part No. 5802-08, Ace Glass, Inc.) were used on the column ends to ensure a tight seal. The GAC bed was supported by a 100 mesh stainless-steel screen, a layer of glass beads (250 µM - 500 µM), a layer of glass wool, and another 100 mesh stainless-steel screen. Glass beads were also placed above the GAC to aid in producing plug flow through the GAC bed. All of these materials were cleaned thoroughly before use. A piston pump driver (Part No. H-07104-02, Fluid Metering, Inc.) equipped with ceramic piston pump heads of 1/4” and 1/8” (Part Nos. H-07014-56, H-07014-66, Fluid Metering, Inc.) were used to supply the required flow rate and pressure to the columns. A pulse dampener (Part No. H-07115-50, Fluid Metering, Inc.) was also used to minimize flow pulsing that was produced from the piston pump. Swage-lok fittings were used to connect the 1/8 inch 316 stainless steel tubing to the end adapters and to the piston pumps.

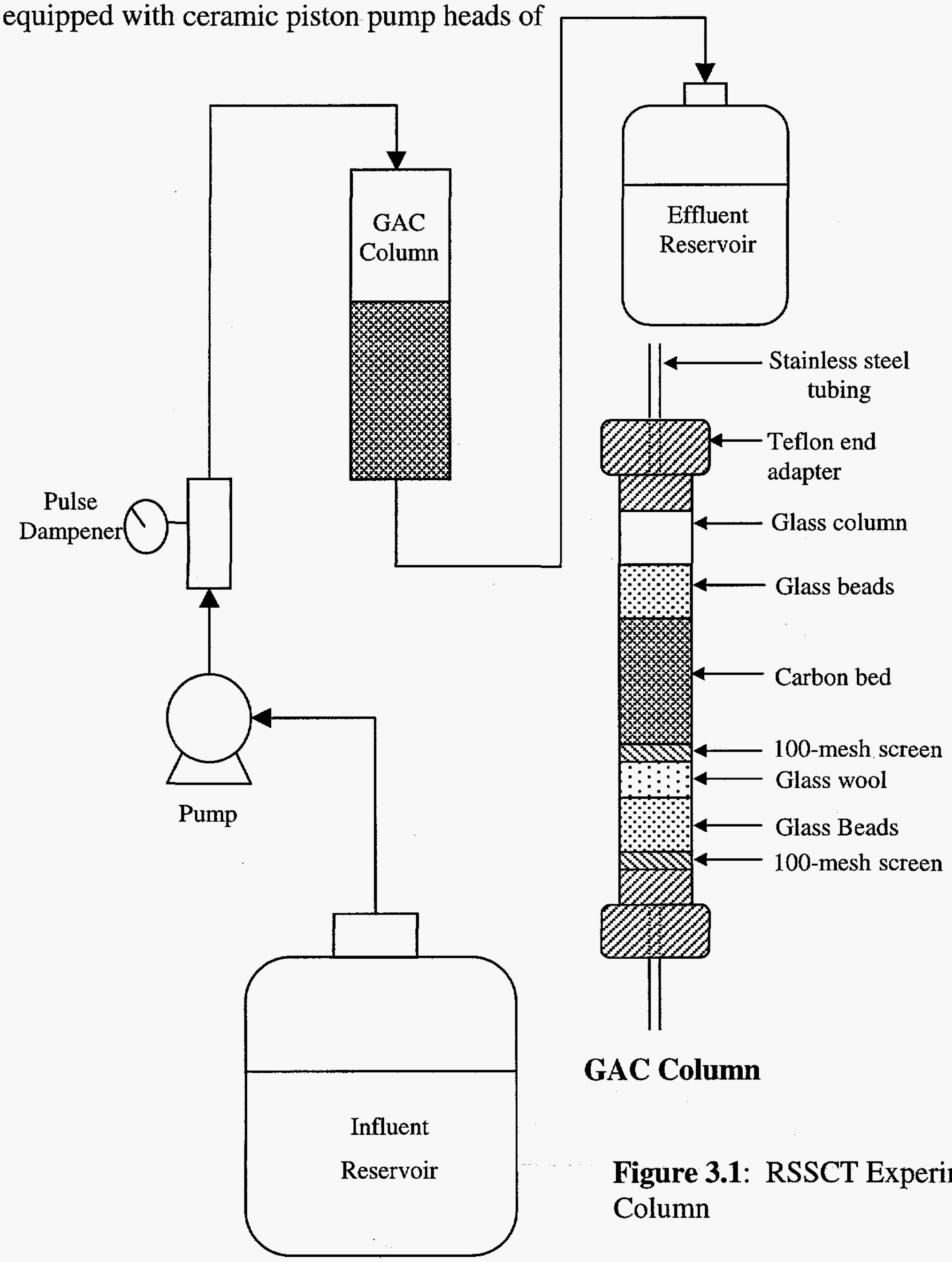

Figure 3.1: RSSCT Experimental Apparatus and Column

3.2.3 Influent Preparation

The influent used for most of the experiments was contaminated groundwater obtained from wells at the Pantex Plant. This water was shipped in 55 gallon drums and stored at room temperature until used. For the experiments conducted with spiked Pantex water, the groundwater was spiked with powdered high explosives and mixed for 24 hours with a large mixer before use.

3.2.4 Operation

A spreadsheet program was used to design the RSSCT experiments. Samples of this spreadsheet program are shown in Appendix A. The RSSCT is designed based on the specifications of a full-scale adsorption column. Using scaling equations developed from dimensional analysis, similitude to the full-scale column is preserved. The inputs into the spreadsheet include GAC properties, the full-scale loading rate, the empty bed contact time (EBCT) of the large column being modeled, and single component adsorption isotherm information. The output of the spreadsheet is given for designated GAC mesh sizes. The output information includes the amount of GAC required for the experiment as well as the flow rate and volume of water to exhaust the GAC. The length of time that the experiment will run is determined by the flow rate applied to the small column and the volume of water required to exhaust the GAC.

For each of the RSSCTs that was performed, the assumption of constant diffusivity was applied; the constant diffusivity design required less water to perform an RSSCT and could be performed in a reasonable amount of time as compared to the proportional diffusivity design. The Reynolds number that was used in the design had to produce a mass of at least 1 g of GAC. Initial tests were performed with a mass less than 1 g of GAC, and it was determined that the GAC bed was too short to contain the mass transfer zone of the contaminants.

The appropriate mass of dried GAC, taken from the dark amber bottles, was weighed and then pre-wetted with Milli-Q water. This wetting was done to pack the column as a slurry. Loading of the column was assisted by using a laboratory spatula to transfer the wetted GAC to the column. As the column was loaded, the column was tapped lightly to pack the GAC particles. Also, the GAC bed was submerged with Milli-Q water during and after the packing process.

Once the column was packed with GAC, the RSSCT system was tested for leaks by running Milli-Q water through it. After resolving any problems, the influent reservoir containing the contaminated water was connected and any air in the influent line was purged. The flow rate was set at the desired level and the pulse produced from the piston pump was minimized by adjusting the pulse dampener. The flow rate to the RSSCT was checked twice daily and was maintained within 1% of the desired flow rate.

3.2.5 Sampling

Influent samples as well as effluent samples were taken for explosives and TOC analysis. Column effluent samples were collected from the effluent line discharging from the bottom of the GAC column. Samples for explosives analysis were collected in 7 mL vials with Teflon lined caps and stored in the dark until analysis. Samples for TOC analysis were collected in 50 mL vials with screw tops; two drops of phosphoric acid were added to the sample as a preservative. The samples were capped and stored at 4°C until analysis.

3.3 ANALYTICAL TECHNIQUES

The analytical techniques chosen for examining the experimental results were High Performance Liquid Chromatography (HPLC) for explosives analysis and the use of the Dohrmann DC-180 Total Organic Carbon Analyzer for TOC analysis.

3.3.1 High Performance Liquid Chromatography (HPLC)

Liquid phase concentrations of HMX and RDX were determined with a Waters Model 440 HPLC with a Model M6000A pump. The Waters HPLC was equipped with an absorbance detector using a mercury lamp at a wavelength of 254 nm and the Waters 717Wisp Autosampler; data acquisition hardware and software were also linked to the Waters HPLC. The analytical column chosen for use with the HPLC was a 5 µm Phenomenex Ultracarb 5 ODS 20 column. The column had an inner diameter of 4.6 mm and a length of 250 mm. A model CH-30 Eppendorf column heater was used to maintain the column temperature at 28°C. A pre-filter and a 5 µm Phenomenex Ultracarb 5 ODS 20 guard column (30 x 4.6 mm) were placed before the analytical column to filter any particles that might have otherwise entered the analytical column.

The analytical method used was a variation on the EPA SW-846 Method 8330. Direct injection of the samples without dilution or concentration was used as the injection method instead of using the salting-out procedure for low concentration samples as outlined by Method 8330. This alteration to Method 8330 was done because of the small sample size taken during an RSSCT. A mobile phase of 55% methanol and 45% Milli-Q water at a flow rate of 0.6 mL/min was used. This produced retention times for HMX and RDX of 6.7 min and 10.2 min, respectively. The sample volume injected was 100 µL, and the detection limit for both HMX and RDX was 20 µg/L. A sample chromatogram is shown in Figure 3.2, while Table 3.1 summarizes the operational parameters for controlling the HPLC.

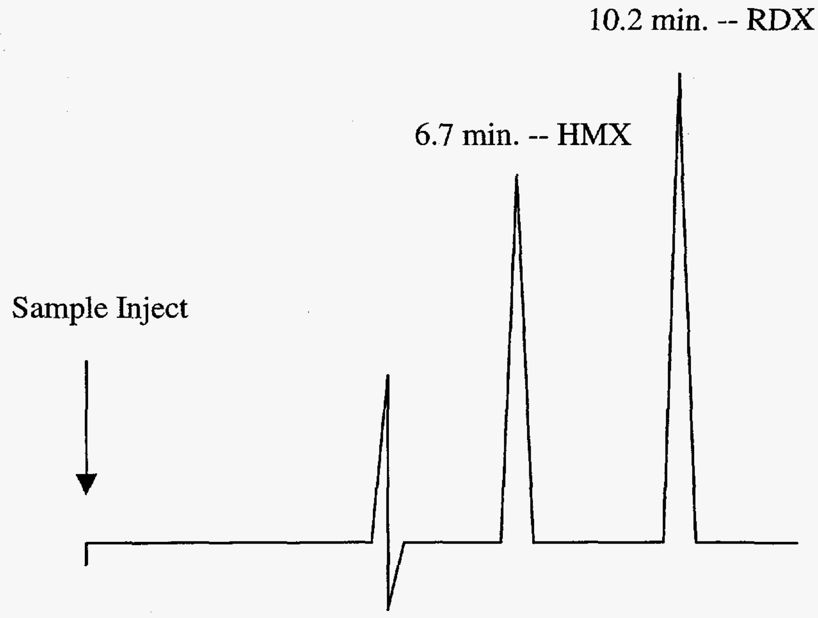

Figure 3.2: Sample Chromatogram for HPLC Analysis of HMX and RDX

Table 3.1: Waters HPLC Operating Parameters

Parameter	Description
Detector	Absorbance Detector at 254 nm
Pump	M6000A
Column	5µm Phenomenex Ultracarb 5 ODS 20, 250 x 4.6 mm
Column Heater	Eppendorf CH-30
Column Temperature	28°C
Pre-Filter	Yes
Guard Column	5µm Phenomenex Ultracarb 5 ODS 20, 30 x 4.6 mm
Mobile Phase	55% methanol, 45% Milli-Q water
Flow Rate	0.6 mL/min
Sample Injection Volume	100 µL
Sample Run Time	13.2 min

Table 3.2: Stock Solution Amounts Used in Standard Preparation

Standard Concentration (µg/L)	Stock Solution Amount (5 mg/L)
20	40 µL
50	100 µL
100	200 µL
200	400 µL
500	1 mL
1000	2 mL
1500	3 mL
2000	4 mL
2500	5 mL

A stock solution of HMX and RDX at 5 mg/L was prepared for making standards. This stock was made by placing 1 mL each of HMX and RDX of a 1000 µg/mL ampule (Supelco) into a 200-mL volumetric flask; the flask was then filled with Milli-Q water and mixed. The stock solution was stored in the dark and was discarded after 1 month of storage time.

Two calibration curves were used in the analysis of HMX and RDX since the range of explosives concentration could extend from below the detection limit (20 µg/L) to 1100 µg/L for HMX and 5000 µg/L for RDX. The two calibration curve ranges are 20 µg/L - 500 µg/L and 500 µg/L - 2500 µg/L. For samples that had a concentration higher than 2500 µg/L, a sample injection of 50 µL was used rather than 100 µL to avoid overloading the column.

The standards were made with Milli-Q water and the 5 mg/L stock solution in 10-mL volumetric flasks. Table 3.2 summarizes the dose amount of stock solution for each standard. To prepare the standards, the stock solution was either measured with a 100-µL syringe or a 5-mL graduated pipet and placed in the volumetric flask. Milli-Q water was then added to make 10 mL. The volumetric flask was capped and inverted several times to ensure thorough mixing. One mL of each standard was transferred to an autosampler vial for analysis by HPLC. An example of all calibration curves for HMX and RDX is shown in Appendix A. As shown in Appendix A, the calibration curves for the two concentration ranges for both HMX and RDX are linear.

3.3.2 TOC Analysis

TOC analyses were done to measure the natural background organic matter in the Pantex groundwater. The TOC analysis procedure followed that outlined in the Persulfate-Ultraviolet Oxidation Method (Standard Method No. 5310C, APHA, 1995). The non-purgeable organic carbon content of each sample was analyzed using UV-promoted persulfate oxidation. Organic carbon was measured on a Dohrmann DC-180 Total Organic Carbon Analyzer. The DC-180 was equipped with a multi-sampler and was totally automated in operation. Concentration was determined from a calibration curve obtained by injections of standard solution at 1, 2, 3, and 5 mg/L organic carbon.

3.4 EXPERIMENTAL PLAN

The experimental plan for this research consisted of five major tasks. A description of each of these tasks follows.

3.4.1 GAC Screening Tests

The GAC screening tests were conducted initially to determine which of the five GACs (Calgon F300 and F400, Norit H3000 and H4000, and Northwestern LB-830) performed the best in an RSSCT. For each of the GAC screening tests, the full scale design EBCT was 4.1 min and the full scale loading rate was 6.47 gpm/ft^2. This EBCT is one-half of the actual EBCT (8.2 min) of one of the columns currently used in the treatability study at the Pantex Plant and was chosen because these screening tests could be conducted quickly with the shorter design EBCT. This loading rate was calculated based on the parameters of the system currently in place at Pantex. The actual flow rate supplied to the columns and the column size were used in the calculation. Loading rates that are used in current practice range from 2 - 10 gpm/ft^2, so the design value of 6.47 gpm/ft^2 falls within this range. Influent concentrations of 350 µg/L HMX and 2200 µg/L RDX were used to design the columns. Table 3.3 summarizes the operational parameters for the screening tests for each GAC. A more detailed design description from the output of the spreadsheet program is shown for each GAC in Appendix A.

3.4.2 Service Life versus EBCT Curve Development

Once the two best performing GACs were determined from the screening tests, further RSSCTs were performed at a range of EBCTs to produce a service life versus EBCT curve for each GAC. The EBCTs used in this portion of the testing were 4.1 min, 8.2 min, 12.3 min, and 16.4 min. Because RDX is less adsorbable than HMX, the service life ended when the RDX concentration rose to 26 µg/L, the Pantex risk-reduction level. The full-scale loading rate for these experiments was again 6.47 gpm/ft^2, and the influent concentrations were 350 µg/L HMX and 2200 µg/L RDX.

Table 3.3: Operational Parameters for GAC Screening Tests

	Calgon F300	Calgon F400	Norit H3000	Norit H4000	Northwestern LB-830
GAC Mass (g)	0.98	1.09	1.01	1.09	0.99
Water Required (L)	65	66	60	66	66
Flow rate (mL/min)	43.14	22.86	35.51	26.63	34.61

Table 3.4: Operational Parameters for Service Life versus EBCT Curve Development Tests

	Calgon F400				Northwestern LB-830			
EBCT (min)	4.1	8.2	12.3	16.4	4.1	8.2	12.3	16.4
GAC Mass (g)	1.09	1.09	1.09	1.45	0.99	0.99	1.19	1.19
Water Required (L)	66	66	66	88	66	66	79	79
Flow rate (mL/min)	22.86	11.43	7.62	7.62	34.61	17.3	13.84	10.38

Table 3.5: Operational Parameters for Variable Concentration Ratio Tests Using Calgon F400

	HMX = 1100 μg/L, RDX = 1900 μg/L		HMX = 350 μg/L, RDX = 4500 μg/L	
EBCT (min)	8.2	12.3	8.2	12.3
GAC Mass (g)	1.09	1.09	1.09	1.09
Water Required (L)	66	66	41	41
Flow rate (mL/min)	11.43	7.62	11.43	7.62

A summary of the operational parameters for the service life versus EBCT curve development experiments is shown in Table 3.4. Additional information is also provided in Appendix A.

3.4.3 Variable Concentration Ratio Tests

The next set of experiments investigated the effect of different proportions of HMX and RDX on the extent of competition and treatability. The Calgon F400 and Northwestern LB-830 GACs were deemed to perform the best in the GAC screening tests and were utilized for the service life versus EBCT experiments. In these experiments, RSSCTs were run to model full-scale EBCTs of 8.2 min and 12.3 min. One set of experiments had an increased HMX concentration of 1100 μg/L while the RDX concentration remained at 1900 μg/L.

The other set of experiments were performed with the HMX concentration maintained at 350 µg/L but with an increased RDX concentration of 4500 µg/L. Table 3.5 provides a summary of the operational parameters for these experiments. Supplemental information is included in Appendix A.

3.4.4 Pre-loading Experiments

Pre-loading experiments were conducted to determine the effect of background organic matter on the adsorption of HMX and RDX. For these tests, three RSSCTs were performed; the full-scale design EBCT was 8.2 min and the loading rate was 6.47 gpm/ft^2. The three columns were first pre-loaded with uncontaminated groundwater from Pantex. The RSSCTs using explosive-contaminated groundwater were then run for each column. The pre-loading times for the three columns were 1 day, 3 days, and 7 days. These times corresponded to 37 days, 112 days, and 261 days of full-scale operation. The influent concentrations of HMX and RDX applied for these experiments were 300 µg/L and 2200 µg/L, respectively. A summary of the experimental parameters is given in Table 3.6 while Appendix A contains a more thorough experimental design.

3.4.5 Computer Modeling

Computer modeling was performed using the computer program *PCsorb* (Dvorak, 1990) to model the RSSCT as well as full-scale adsorber performance for several of the experimental cases. Input parameters, such as the isotherm parameters, were derived from other research work or from other literature sources. A sensitivity analysis was performed to determine a range of variations in the isotherm parameters that would produce acceptable results for predictive modeling.

Table 3.6: Operational Parameters for Pre-Loading Experiments Using Calgon F400 (EBCT = 8.2 min)

Preloading Time	**1 day**	**3 days**	**7 days**
GAC Mass (g)	1.09	1.09	1.09
Uncontaminated Water Required (L)	16	49	115
Contaminated Water Required (L)	66	66	66
Flow rate (mL/min)	11.43	11.43	11.43

4. RESULTS AND DISCUSSION

4.1 INTRODUCTION

Results of the rapid small-scale column tests performed for this feasibility study are presented in this chapter. The results include the GAC screening tests to identify the best GACs and service life versus empty bed contact time curves. The effects of varying high explosive influent concentration and preloading tests are also reported. Modeling results using *PCsorb* then follow.

4.2 GAC SCREENING TESTS

The initial RSSCTs were performed using five different GACs. The five GACs evaluated included Calgon F300 and F400, Norit H3000 and H4000, and Northwestern LB-830. These GACs included those used in other research work on adsorption of high explosives and the GAC currently used in the pilot treatment plant at Pantex (Northwestern LB-830).

Preliminary screening tests were run to model an EBCT of 4.1 min for a full-scale column. This EBCT was chosen because it was one-half of the actual EBCT of one of the columns in series at Pantex and results could be obtained in a short amount of time. As the column tests were run, effluent samples were taken and analyzed for HMX and RDX; breakthrough curves were developed for each GAC. The influent concentration was also monitored throughout the experiment. Data and experimental breakthrough curves for each GAC are presented in Appendix B.

The purpose of these experiments was to evaluate the five GACs and determine which performed best in adsorbing the high explosives HMX and RDX in a mixture. To accomplish this task, the breakthrough curves from each RSSCT for each GAC were compared to decide which GAC most effectively removed the high explosives from contaminated Pantex groundwater. One could also interpret the relative adsorbability between HMX and RDX from the breakthrough curves. HMX was more adsorbable than RDX for all GACs as shown by a later breakthrough time. This fact has been demonstrated by other researchers in high explosive adsorption work (Burrows, 1984; Wujcik et al., 1992).

The experimental breakthrough curve for each GAC consists of a plot of high explosive concentration versus operation time. Figure 4.1 shows the breakthrough curve for the Norit H4000 GAC. The breakthrough curves for other GACs are shown in Appendix B. The influent concentrations for each experiment were 2300 μg/L RDX and 350 μg/L HMX. As mentioned before, HMX was more highly adsorbed as compared to RDX. This is evident in a comparison of the breakthrough times for HMX and RDX for Norit H4000 GAC in Figure 4.1. The breakthrough of RDX occurred between 5 and 15 hours of operation. The adsorptive capacity of the column for RDX was exhausted in 20 hours when the effluent concentration reached the influent concentration. The HMX concentration never reached the influent concentration during this experiment, so the GAC had more capacity available for the more adsorbable HMX. Because RDX is less adsorbable than HMX and the health advisory for RDX is much lower than for HMX (2 μg/L for RDX versus 400 μg/L for HMX), most of this research was based on evaluating the breakthrough curve of RDX. Further, the risk-reduction level set by Pantex for RDX was 26 μg/L, while the HMX level is higher at 5.11 mg/L.

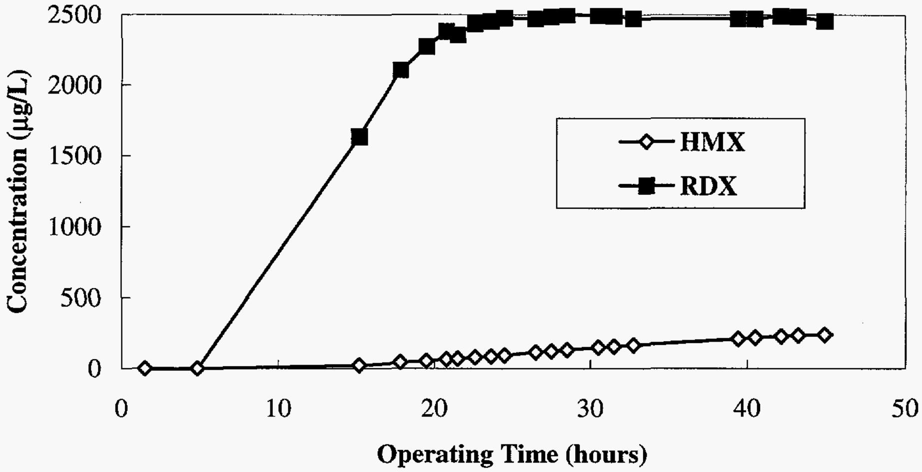

Figure 4.1: Experimental Breakthrough Curve for Norit H4000 GAC in the Screening Tests at EBCT = 4.1 min

This, too, drove the research effort to more thoroughly interpret results using RDX breakthrough data. HMX concentration data were still analyzed, but RDX received the major emphasis for removal purposes.

Once each individual GAC's breakthrough curve was developed, the average mass loading of RDX, *q* (mg RDX/g GAC), on the carbon was calculated. The experimental breakthrough curve results were scaled to model the full-scale adsorber with an EBCT of 4.1 min. The scaling equations for the constant diffusivity case as developed by Crittenden et al. (1986) were used to accomplish this. From these equations, the full scale operating time was determined by $t_{LC} = T_{SC} (EBT_{LC}/EBCT_{SC})$. A comparison of the experimentally predicted full-scale breakthrough curves for RDX for all of the five GACs for an EBCT of 4.1 min is shown in Figure 4.2. The contaminant mass loadings for each carbon are shown in Table 4.1.

It is evident that the two Norit GACs, H3000 and H4000, have the least adsorptive capacity for RDX since their breakthrough profiles rose quickly to the fluent concentration. The full scale breakthrough in time was 4 days and 8 days for H3000 and H4000, respectively. However, it is interesting to note that these two GACs performed so similarly.

The breakthrough time of RDX was determined when RDX reached a concentration of 26 µg/L, the Pantex risk reduction level. To see that time more clearly, the breakthrough curves for the five carbons are shown on a smaller time scale Figure 4.3. The predicted breakthrough time of RDX for the Calgon F300 GAC was less than 3 days while the Calgon F400 breakthrough time was 13 days and Northwestern LB-830 was 7 days.

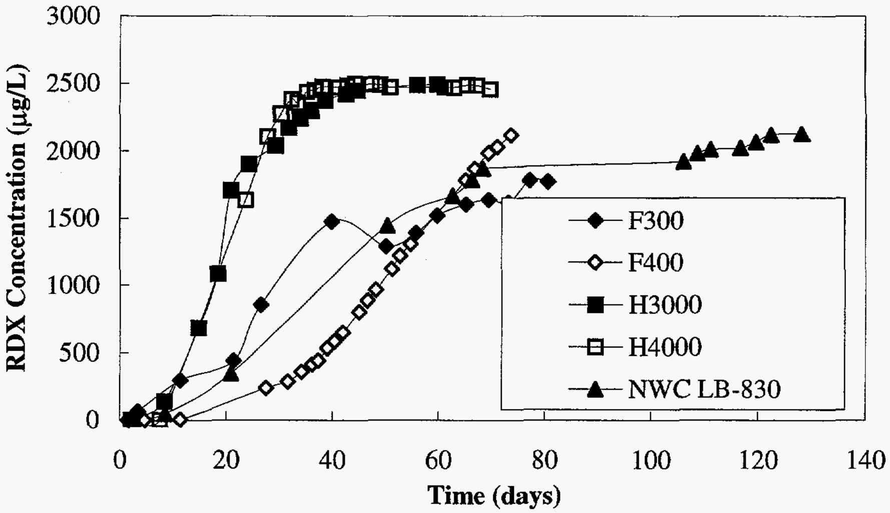

Figure 4.2: Full-scale Predicted Breakthrough Curves for the Five GACs in the Screening Tests at EBCT = 4.1 min

Table 4.1: Average RDX Mass Loadings for the Five GACs in the Screening Tests

Carbon	**Average Mass Loading (mg RDX/g GAC)**
Calgon F300	80
Calgon F400	96
Norit H3000	44
Norit H4000	44
Northwestern LB-830	91

The effluent concentration of RDX for the two Calgon GACs and the Northwestern GAC never reached the influent concentration during the experiment. If the experiment had been extended, it is believed that these GAC columns would have been fully exhausted with respect to RDX as were the Norit GACs. These experiments were all performed with the same batch of influent water and therefore had the same concentrations of HMX and RDX. Therefore, comparisons can be made among all of the GACs. Based on the breakthrough times and profiles for all five GACs, the two GACs that performed the best were the Calgon F400 and the Northwestern LB-830.

The shape of each breakthrough curve was also evaluated. The degree of spreading in the breakthrough curve correlates to spreading of the mass transfer zone (MTZ). For the two Norit GACs, there was less spreading as compared to the other GACs breakthrough curves. The lesser degree of spreading in the Norit breakthrough curves demonstrates that the MTZ for RDX for each Norit GAC is smaller than the MTZ for the other GACs. Typically, a shorter mass transfer zone is desired because breakthrough

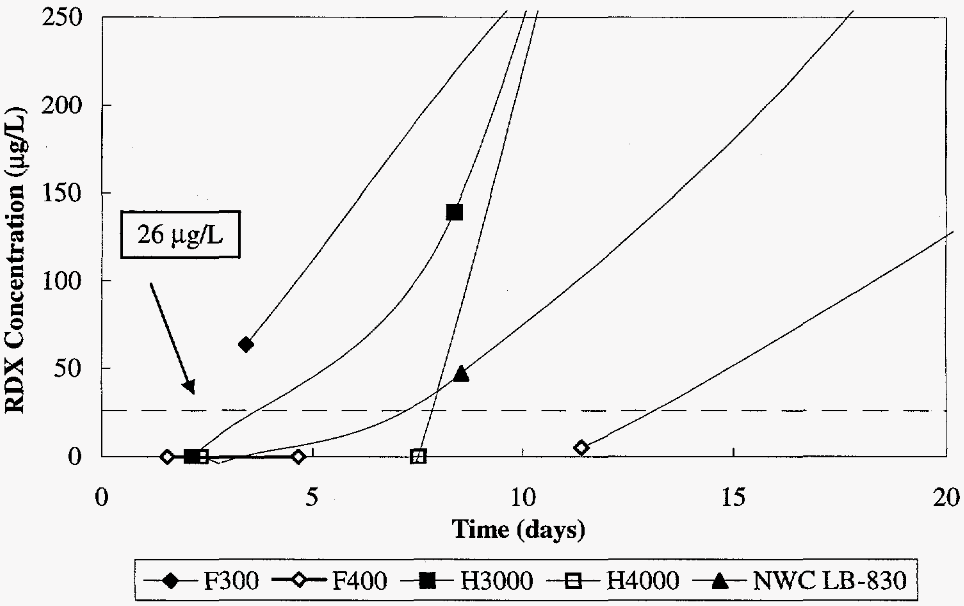

Figure 4.3: Full-scale Predicted Breakthrough Curves for the Five GACs in the Screening Tests at EBCT = 4.1 min for a Small Time Scale

occurs earlier if the mass transfer zone is more spread out. However, the adsorptive capacity of each GAC is also important and in this case was the controlling factor. Clearly, as shown in Table 4.1, the Norit GACs had significantly less adsorptive capacity than the other three GACs.

Each of the five GACs evaluated was capable of removing the high explosives RDX and HMX from contaminated groundwater, but based on the comparison breakthrough time and adsorptive capacity for each GAC, the Calgon F400 and the Northwestern LB-830 outperformed the remaining GACs. These two GACs were then used in subsequent experiments to further characterize the adsorption of HMX and RDX.

4.3 DETAILED RSSCT EXPERIMENTS WITH CALGON F400 AND NORTHWESTERN LB-830

Once two GACs were chosen for additional experiments to characterize the adsorptive behavior of the HMX and RDX in a mixture, RSSCTs were performed to develop a service life versus EBCT curve. RDX mass loadings were also determined from the RSSCT results. The service life versus EBCT curve can aid in evaluating the treatability of a contaminated water with GAC adsorption. For a range of EBCT values, the service life of a column is determined from an experimentally developed breakthrough curve and is then plotted versus the corresponding EBCT. The relationship between EBCT and service life is unique for each GAC evaluated, and this curve can be further applied to determine the service life of an EBCT that was not experimentally defined. However, the service life determined by the service life versus EBCT curve is for a single column configuration and not two columns in series. The service life for columns in series also can be calculated, however, through further analysis of the RSSCT breakthrough curves. The service life versus EBCT relationship for any column configuration is the most important information for cost estimations in GAC adsorption.

For each of the two chosen GACs, Calgon F400 and Northwestern LB-830, RSSCTs were run to model full scale EBCTs of 4.1 min, 8.2 min, 12.3 min, and 16.4 min. The same influent was used in all of these experiments; the RDX and HMX concentrations were 2300 μg/L and 350 μg/L, respectively. Effluent samples were taken at specified times, and the influent concentration was also monitored. Experimental breakthrough curves for each GAC were developed for RDX and HMX. The experimental data and small-scale breakthrough curves are included in Appendix C. These curves are presented there as a plot of the effluent explosive concentration versus operating time for each GAC. Figure 4.4 contains the scaled-up RDX breakthrough curves for Calgon F400 for all of the EBCTs modeled. Only RDX effluent concentrations are presented since it is the constituent of primary interest for these experiments. The HMX breakthrough curve was not fully developed during these experiments. As expected, the breakthrough time increased with increasing EBCT. A comparison of the breakthrough curves from each of the RSSCTs shows that, as the full-scale modeled EBCT increased, the amount of spreading in the breakthrough curve also increased. The breakthrough curves have shallower slopes for the increasing EBCTs. The decrease in the slope suggests that the reduction of the Re in the design of the RSSCT may not be valid as Crittenden et al. (1987) suggested. For the increases in EBCT, the Re of the RSSCT was decreased to reduce the amount of source water required and to allow the RSSCTs to be run in a timely manner. Another possibility for the shallower slopes is competition with NOM, which typically increases as EBCT increases. From each of the breakthrough curves, the amount of time for the RDX effluent concentration to reach 26 μg/L was noted and was deemed the service life that was determined for each column. The average RDX mass loading for each breakthrough curve was also determined. Figure 4.5 shows the breakthrough curves for Calgon F400 GAC on a smaller scale, which was used to determine the service life for each EBCT.

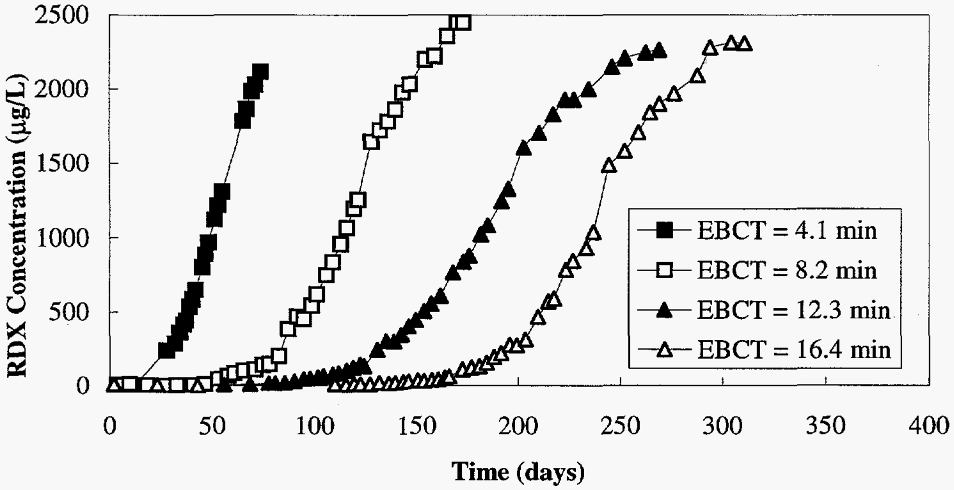

Figure 4.4: Comparison of Full-scale Breakthrough Curves at a Range of EBCTs for Calgon F400 GAC

Table 4.2 shows the service life and average RDX mass loading that was determined for each of the four EBCTs for Calgon F400. It should be noted that the *q* for the 4.1 min EBCT is low in comparison to the *q* from other EBCTs because the column was not fully exhausted. A plot of the corresponding service lives and EBCTs for Calgon F400 is shown in Figure 4.6. This figure shows a good linear fit to the data; therefore, service lives for EBCTs not determined experimentally can be calculated by applying the equation of the best fit line determined for the experimental data. It is evident that a minimum EBCT is necessary for any removal of RDX or for a service life to be determined. This is the case because for very short EBCTs, the MTZ of the adsorbing chemical is not contained within the length of the GAC bed and breakthrough occurs immediately. The minimum EBCT for RDX at the conditions applied for these experiments is 3.1 min.

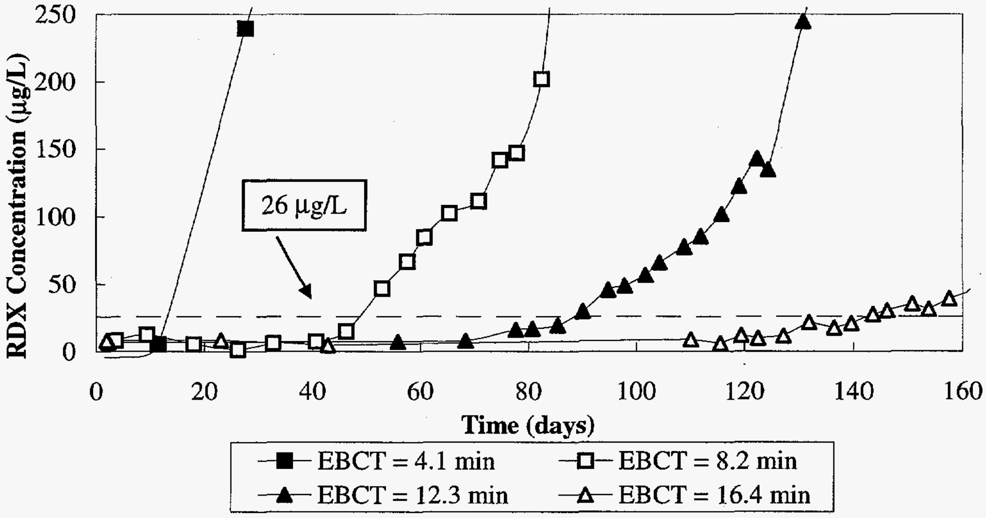

Figure 4.5: Comparison of Full-scale Breakthrough Curves at a Range of EBCTs for Calgon F400 GAC for a Small Time Scale

Table 4.2: Service Life and Average RDX Loading for a Range of EBCTs for Calgon F400 GAC

EBCT (min)	Service Life (days)	Average Loading (mg/g)
4.1	13	96
8.2	49	110
12.3	88	117
16.4	139	112

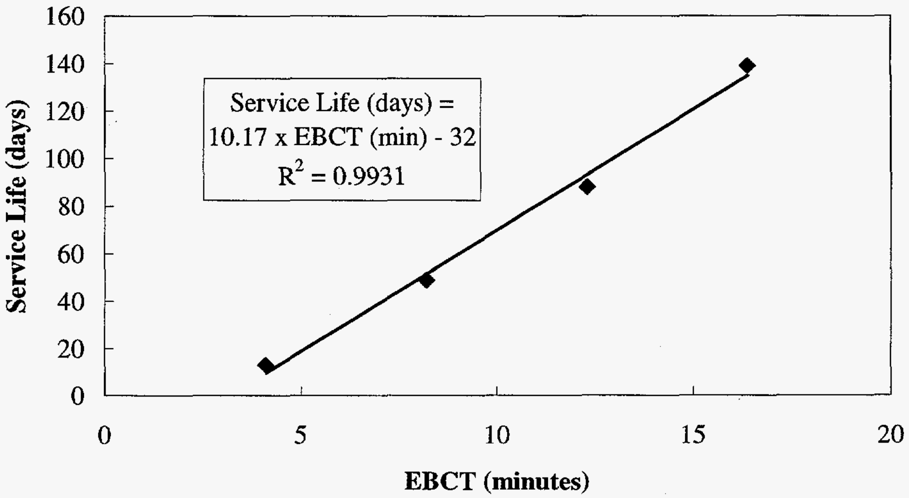

Figure 4.6: Service Life versus EBCT for Calgon F400

Similar experiments were performed with the Northwestern LB-830 GAC. The full scale breakthrough curves for RDX as predicted from applying the scaling equations to the experimental curves are shown in Figure 4.7. The breakthrough times increase with increasing EBCT. As with the Calgon F400 GAC breakthrough curves for RDX, the breakthrough curves for Northwestern LB-830 GAC follow a similar trend of increased spreading with increased EBCTs. The service life to reach 26 μg/L RDX and average RDX loading at each EBCT were graphically determined from each breakthrough curve. Figure 4.8 shows the full-scale breakthrough curves for Northwestern LB-830 with smaller time and concentration scales for the determination of the service life for each modeled EBCT.

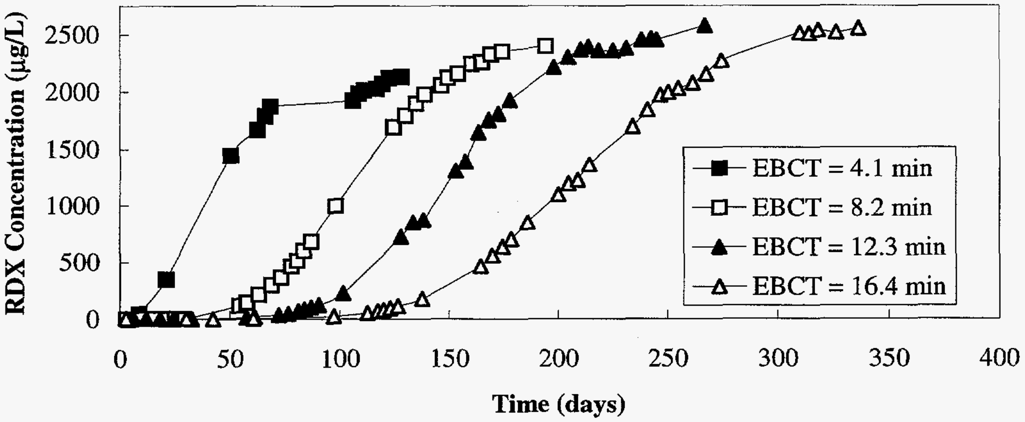

Figure 4.7: Comparison of Full-scale Breakthrough Curves at a Range of EBCTs for Northwestern LB-830 GAC

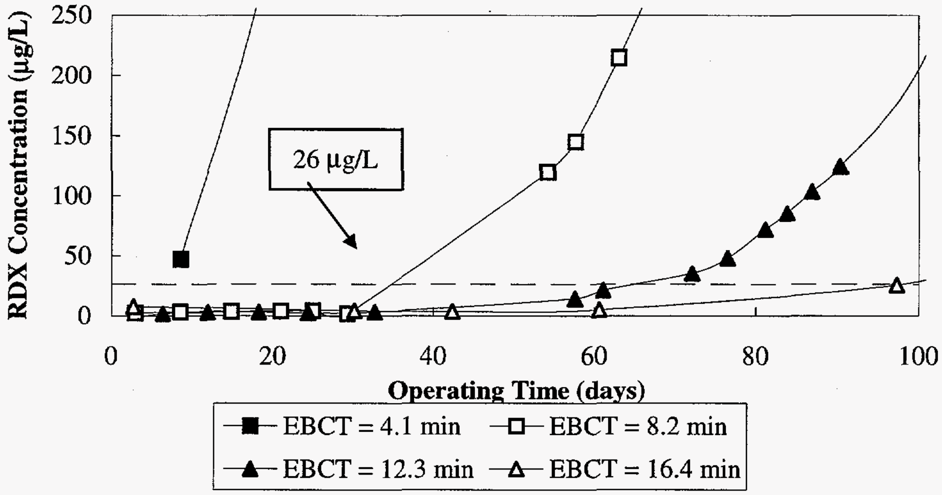

Figure 4.8: Comparison of Full-scale Breakthrough Curves at a Range of EBCTs for Northwestern LB-830 GAC for a Small Time Scale

Table 4.3 presents the service life and average RDX loading determined for each of the four experimentally modeled EBCTs for Northwestern LB-830. Figure 4.9 contains the service life versus EBCT curve for Northwestern LB-830. These data also have a good linear fit, and the minimum EBCT to produce any RDX removal is estimated to be 3.2 min from the best-fit line.

Table 4.3: Service Life and Average RDX Loading for a Range of EBCTs for Northwestern LB-830 GAC

EBCT (min)	Service Life (days)	Average Loading (mg/g)
4.1	7	91
8.2	34	95
12.3	61	88
16.4	97	90

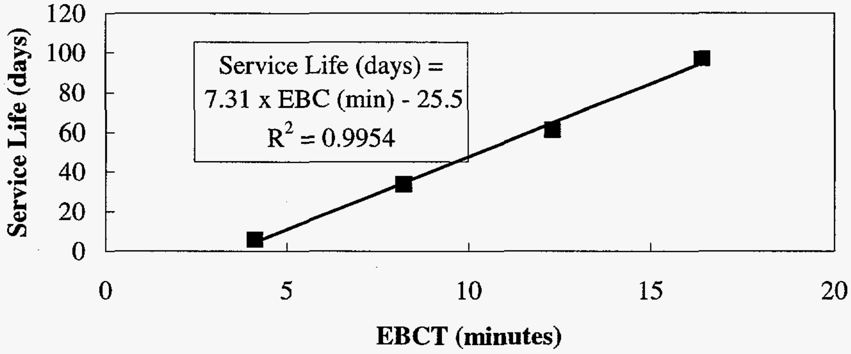

Figure 4.9: Service Life versus EBCT for Northwestern LB-830

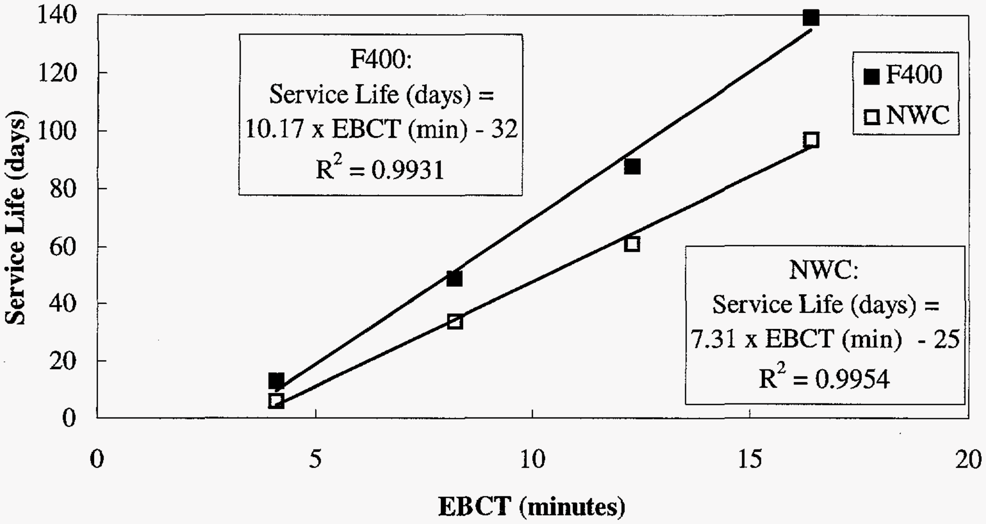

Figure 4.10: Comparison of the Service Life versus EBCT for Calgon F400 and Northwestern LB-830

Comparisons can be made between the performance of the Calgon F400 and the Northwestern LB-830 GAC based on the service life versus EBCT curves and the RDX mass loadings. The comparisons focused on two operating configurations: two columns in parallel and two columns in series. The Pantex plant now operates two columns in series but has the capability to operate in either mode. Three operating scenarios were evaluated for these system configurations. The different configurations demonstrated that either equilibrium or kinetics considerations can control the service life. The service life for two columns in parallel is kinetically controlled, while equilibrium considerations dominate for two columns in series.

For the two columns in parallel, direct comparison of the service life versus EBCT curves for the GACs can be done (Figure 4.10). The slope of the Calgon F400 line is 10.17 while the Northwestern LB-830 line's slope is 7.31. The ratio of these two slopes is 1.5; thus, for EBCTs typically used in practice, the service life for the Calgon F400 GAC is 50% greater than that of the Northwestern GAC.

For columns in series, the first column is replaced when the second column breaks through. The second column then becomes the first column, and the scenario is repeated. Only one column is replaced at a time, versus two replaced at a time for parallel operation. For one of the series operating scenarios, it was assumed that the MTZ of RDX was contained within the column (full-exhaustion of the column could be achieved). This system is completely equilibrium limited and represents the maximum possible GAC service life. In the second series operating scenario, the MTZ of RDX was not contained within the column, making this system both kinetically and equilibrium controlled. The RSSCT data indicate that the second operating scenario is expected in the Pantex GAC system.

The service life and average RDX mass loadings at the end of the service life are shown in Table 4.4 for the columns in series configuration. The service life shown for the series operation is given for replacement time

Table 4.4: Service Life and Average Mass Loading at the end of the Service Life for Calgon F400 and Northwestern LB-830 for Various Column Configurations

	F400		LB-830	
Operating Scenario	Average Loading (mg/g)	Approximate Service Life (days)	Average Loading (mg/g)	Approximate Service Life (days)
Two Columns in Parallel	66	139*	43	90*
Two Columns in Series				
Equilibrium and Kinetically Controlled	108	227**	82	160**
Equilibrium Controlled	113	240**	91	212**

*This is the service life of each column; replacement of both columns is required at the same time.

**This is the service life of each column, replacement of the columns alternates. Both columns are not replaced at the same time.

after the first GAC replacement is made. The columns are then in the alternating replacement schedule as described before. Data for the two columns in parallel are also shown for comparative purposes. If the service lives of two columns in parallel using each GAC are compared, the Calgon F400 GAC clearly outperforms the Northwestern LB-830 GAC, as noted before and is shown in Figure 4.10. The system in this case is kinetically controlled. Furthermore, if the columns were operated in series, the Calgon F400 still performs better than the Northwestern GAC although the difference in service life is not as great (54% versus 39%). Complete equilibrium control is achieved when the MTZ of RDX is contained within the column. With complete equilibrium control, the greatest service life and RDX mass loading are produced. The current system at Pantex would behave like the series column configuration that is both kinetically and equilibrium controlled; therefore, somewhat less than the maximum possible service life would be achieved. This analysis also demonstrates that series operation is superior to parallel operation. The much larger average RDX loading on the GAC in series operation should make this operating configuration significantly more economical. Because Calgon F400 produced longer service lives and greater mass loadings for the same EBCT, it was selected as the GAC for additional RSSCT experiments to investigate the effects of different influent concentrations and the effect of preloading with background organic matter.

4.4 VARIABLE CONCENTRATION RATIO TESTS

RSSCTs are quick and accurate experiments for characterizing the treatability of a source water (Crittenden at al., 1986). However, they can only predict the treatability for the experimental conditions tested. To further define the treatability for other influent conditions, additional RSSCTs must be performed that mimic the other influent possibilities. Varying influent conditions are likely when treating a contaminated groundwater. Depending on the location of the extraction wells, the plume extent and variability, and the subsurface properties, the contaminant concentration can range from low levels below the detection limit of the analytical instruments (water from the plume's edge) to highly concentrated contaminant levels (water from the plume center). To predict the treatability of the contaminated groundwater with GAC properly, the effect of various influent contaminant concentrations should be considered. Therefore, experiments with elevated explosive concentrations were performed. The elevated concentrations applied were the maximum level of contaminant concentrations currently known at Pantex.

RSSCTs were completed with higher concentrations of both HMX and RDX. One set of experiments was done with an HMX concentration of 1100 µg/L while the RDX concentration remained at 2300 µg/L. Two different full scale EBCTs were modeled with these experiments, 8.2 min and 12.3 min. The 8.2 min EBCT was selected because it is the EBCT of one of the columns in series in the system at Pantex. The 12.3 min EBCT is 1.5 times greater than the 8.2 min EBCT and was selected for comparison purposes. In a second set of experiments, the RDX concentration was raised to 4500 µg/L while the HMX concentration was kept at 350 µg/L. The EBCTs of 8.2 min and 12.3 min were also evaluated for the increased RDX concentration tests.

Experimental breakthrough curves for each of the RSSCTs were developed for HMX and RDX concentrations as a function of operating time. These curves are included in Appendix D. Figure 4.11 provides a comparison of the RDX breakthrough curves for the initial conditions and for the increased HMX concentration experiments for the 8.2 min and the 12.3 min EBCTs. The initial conditions are the conditions evaluated during the service life versus EBCT curve development with RDX and HMX concentrations of 2300 µg/L and 350 µg/L. From this figure, it is evident that the higher HMX concentration produced greater competition with RDX for adsorption sites; RDX broke through earlier with the higher HMX concentration. The breakthrough curves are shown in Figure 4.12 at a smaller time scale to see the difference in service life. Table 4.5 shows a comparison of service life and average RDX mass loading at breakthrough for initial experiments and the higher HMX concentration experiments. The service life was reduced by 80% for both the 8.2 min EBCT and the 12.3 min EBCT. The RDX mass loading was decreased by 84% for the 8.2 min EBCT and 82% for the 12.3 min EBCT. Note that this represents parallel or single column operation, not columns in series. Service life for columns in series also would decrease, because any increase in influent concentration decreases service life.

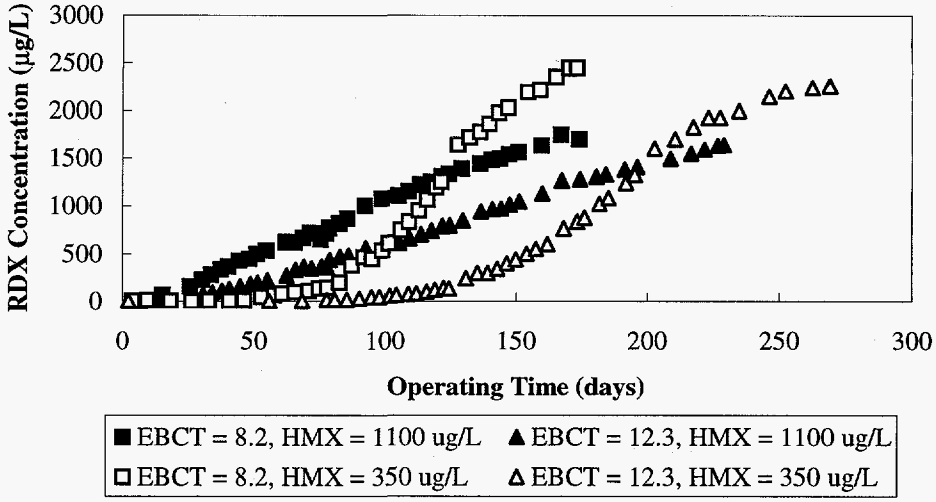

Figure 4.11: Curves for Initial Screening Tests and Increased HMX Influent Concentration at RDX Breakthrough EBCT = 8.2 min, 12.3 min

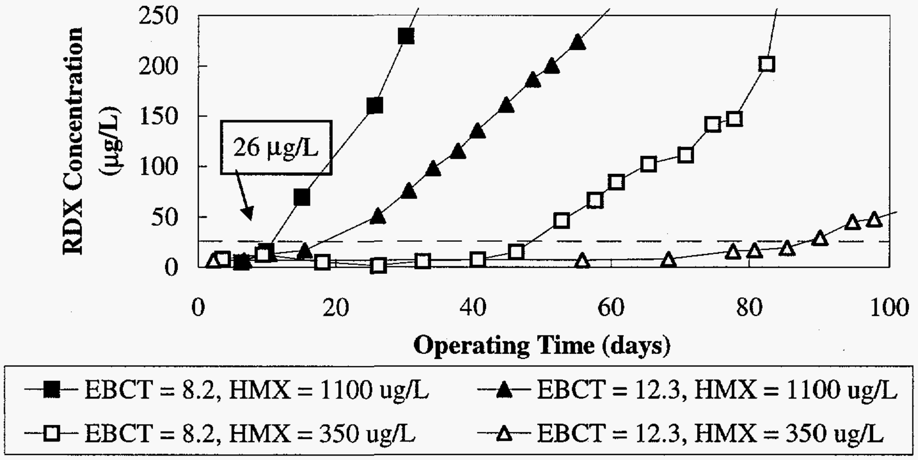

Figure 4.12: RDX Breakthrough Curves for Initial Screening Tests and Increased HMX Influent Concentration at EBCT = 8.2 min, 12.3 min at Small Time Scales

Table 4.5: Service Life and RDX Mass Loading of GAC Columns from Initial Screening Tests and Increased HMX Concentration

	HMX = 350 μg/L		HMX = 1100 μg/L	
EBCT (min)	Service Life (days)	RDX Loading* (mg/g)	Service Life (days)	RDX Loading* (mg/g)
8.2	49	50	10	8
12.3	88	55	18	10

* Average GAC loading when effluent concentration = 26 μg/L RDX.

Similar results were obtained with the RSSCTs examining the increased RDX concentration. Figure 4.13 compares the initial RDX breakthrough curves for EBCTs of 8.2 min and 12.3 min with the corresponding RDX breakthrough curves for increased RDX concentrations, and Figure 4.14 shows the breakthrough curves at a smaller time scale for better examination of the resulting service lives. The service life for each EBCT is once again reduced with the higher influent contaminant concentration; the increased RDX concentration exhausted the GAC more quickly. A comparison of the predicted service life and RDX mass loading for the initial experiments and the higher RDX concentration experiments is presented in Table 4.6. The reduction in service life due to the increased RDX concentration was 67% and 78% for EBCTs of 8.2 min and 12.3 min, respectively. The mass loading comparison shows a reduction in the RDX loading of 44% and 55% for EBCTs of 8.2 min and 12.3 min, respectively. Once again, these reductions are for single column operation, but a reduction in service life would also be experienced in a series configuration due to the increased influent concentration.

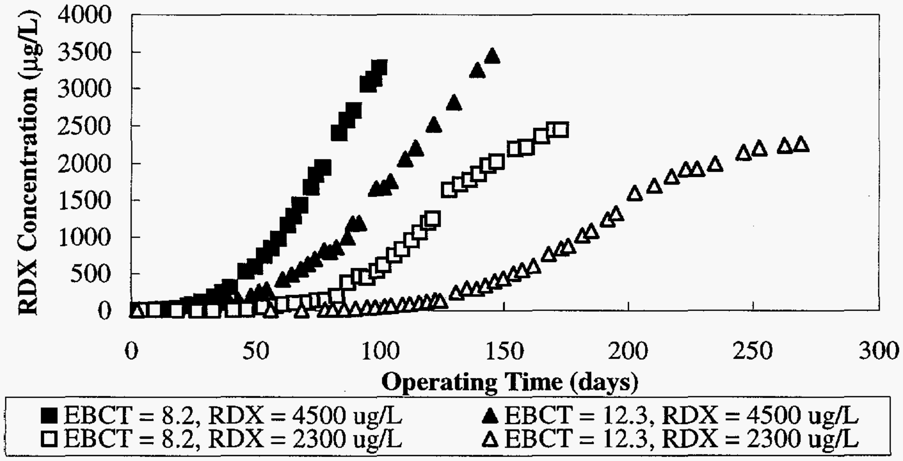

Figure 4.13: RDX Breakthrough Curves for Initial Screening Tests and Increased RDX Influent Concentration at EBCT = 8.2 min, 12.3 min

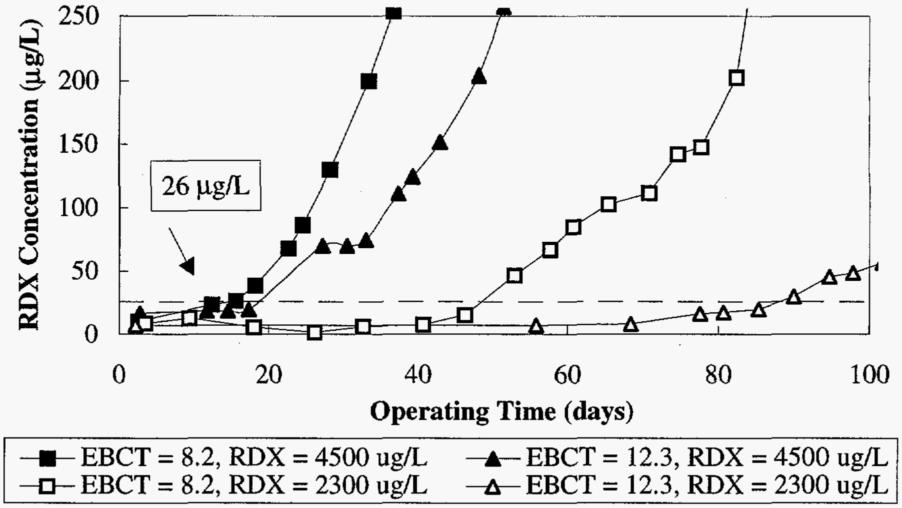

Figure 4.14: RDX Breakthrough Curves for Initial Screening Tests and Increased HMX Influent Concentration at EBCT = 8.2 min, 12.3 min at Small Time Scales

Table 4.6: Service Life and RDX Mass Loading of GAC Columns from Initial Screening Tests and Increased HMX Concentration

	RDX = 2300 µg/L		RDX = 4500 µg/L	
EBCT (min)	Service Life (days)	RDX Loading* (mg/g)	Service Life (days)	RDX Loading* (mg/g)
8.2	49	50	16	28
12.3	88	55	19	25

*Average GAC loading when effluent concentration = 26 µg/L RDX.

A comparison of the breakthrough curves for HMX also indicates the competition with increased concentration of contaminants. Figure 4.15 shows a comparison of the HMX breakthrough curves for the increased HMX concentration and the initial conditions. With an increased concentration of the more adsorbable HMX, the time to breakthrough of HMX is significantly reduced for each EBCT as seen in Figure 4.15. The comparison of the HMX breakthrough curves for increased RDX concentration and the initial conditions is shown in Figure 4.16. Typically, an increased concentration of the least adsorbable chemical does not greatly affect the adsorption of the more adsorbable chemical. This is evident in Figure 4.16 since the breakthrough curve of HMX with higher RDX influent concentration at each EBCT is not affected as much as the RDX breakthrough curve is with higher HMX influent concentration (Figure 4.11).

From the results produced by the varying concentration RSSCTs, it is evident that increased concentration of HMX and RDX significantly reduce the service life of the GAC with respect to RDX. Thus, a thorough characterization of the range of concentrations that a GAC column in a treatment system at a facility like Pantex would experience should be performed. This characterization would more accurately predict the service life of the column. Also, a study could be performed to investigate

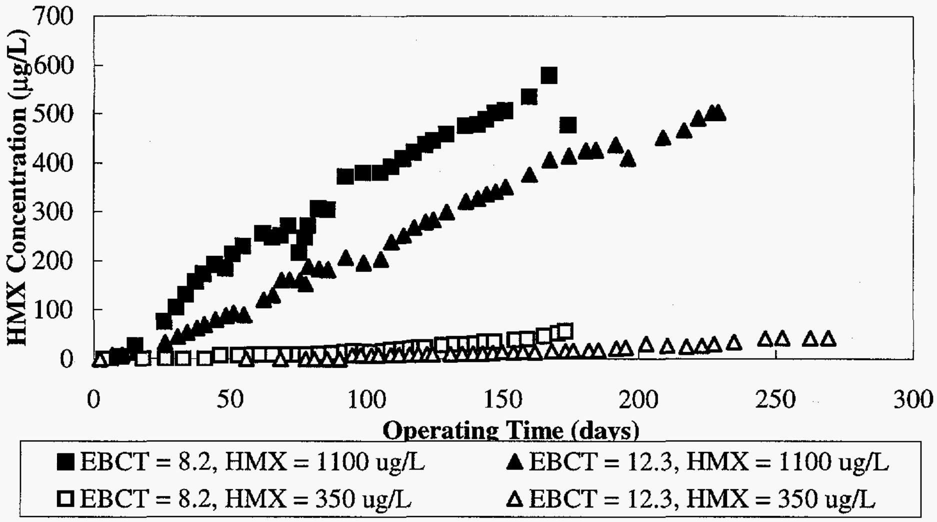

Figure 4.15: HMX Breakthrough Curves for Initial Screening Tests and Increased HMX Influent Concentration at EBCT = 8.2 min, 12.3 min

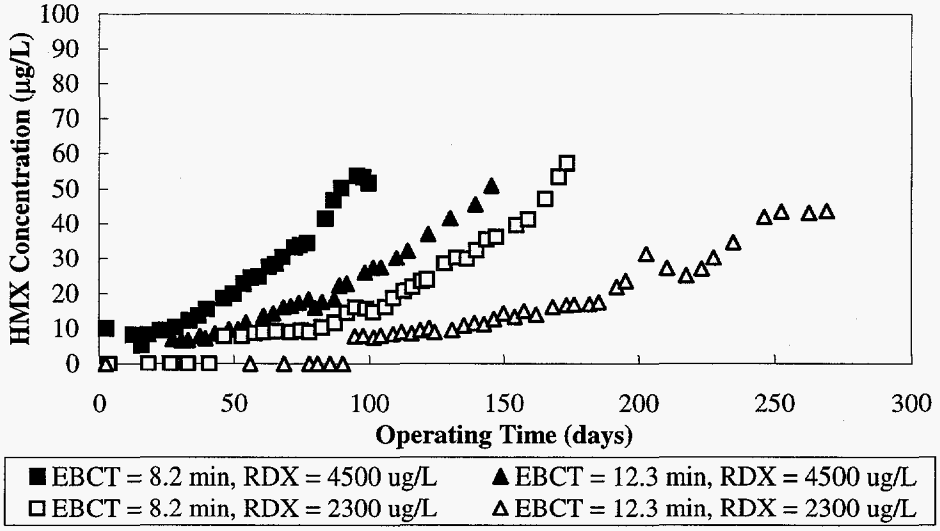

Figure 4.16: HMX Breakthrough Curves for Initial Screening Tests and Increased RDX Influent Concentration at EBCT = 8.2 min, 12.3 min

various configurations (parallel versus series operation) of the GAC columns to optimize treatment.

4.5 PRE-LOADING TESTS

The adsorption capacity of GAC for synthetic organic chemicals can be reduced by the presence of naturally occurring background organic matter. This reduction is not well described by competitive adsorption theories, and "fouling" of the GAC occurs (Summers et al., 1989). Essentially, fouling can cause a decrease in adsorption capacity for the target chemicals and slow adsorption kinetics, which results in broadening MTZs over time. The effect of preloading, and thus fouling by background organic matter on the application of the scaling procedure for an RSSCT, is not well understood. Various approaches have been attempted to enhance the ability to predict the capacity of GAC affected by preloading. One such approach is to use preloaded GAC for isotherms to predict capacity (Summers et al., 1989), and another includes varying input parameters for models that predict full scale behavior (Speth and Miltner, 1989).

The purpose of preloading experiments for this study was to evaluate the effect of background organic matter on the adsorption of HMX and RDX from Pantex contaminated groundwater. Three RSSCTs were performed to investigate preloading phenomena. The three columns used in this study were each preloaded with uncontaminated (RDX- and HMX-free) groundwater from Pantex for different times, and then the column tests were performed using explosive contaminated groundwater as the influent. Calgon F400 was used as the GAC in these tests and the preloading times for the three columns were 1, 3, and 7 days, respectively. The corresponding full scale modeled EBCT was 8.2 min. The influent concentrations of HMX and RDX in the contaminated groundwater were 300 μg/L and 2200 μg/L, respectively.

The TOC concentration of the uncontaminated groundwater was measured, as was that of the effluent for each of the preloaded columns before starting the RSSCT with contaminated water. A comparison of these measurements shows the varying degrees of TOC loading on the columns. Breakthrough curves for each of these RSSCTs were developed as a plot of RDX concentration versus operating time. The experimental data and breakthrough curves for the preloading experiments are included in Appendix E.

Influent and effluent TOC concentrations of the uncontaminated groundwater as well as the average TOC mass loading on the GAC are shown in Table 4.7 for each of the preloaded columns. Since the effluent TOC concentration is highest for the 7-day preloaded column at 0.21 mg/L, it is apparent that the TOC breakthrough curve has progressed further than that of the 3-day or 1-day preloaded columns. The same is true for the 3-day preloaded column (0.16 mg/L TOC) as compared to the 1-day (0.12 mg/L TOC) column.

The TOC mass loading on the GAC was determined by assuming that the difference in the influent and effluent mass of TOC was adsorbed to the GAC. This mass loading was calculated by determining the area under the TOC concentration versus preloading time curve and subtracting that from the total mass of TOC that was applied to the column. Figure 4.17 shows the graph constructed to determine the TOC mass loading on the GAC in each of the preloading tests. The area was multiplied by the flow rate (11.43 mL/min) supplied to the GAC column to calculate the TOC mass loaded on the GAC, and then it was then divided by the mass of GAC in the column to produce the TOC mass loading. Other assumptions were made to perform this calculation. Since TOC concentration effluent samples were not taken for the duration of preloading, it was assumed that the singular effluent TOC concentrations from the 1, 3, and 7-day preloading times could represent effluent samples for TOC concentration as in a breakthrough curve. The effluent TOC concentration at time zero was interpolated back to time zero from the other

Table 4.7: Influent and Effluent TOC Concentrations for the Preloading Tests

	TOC Concentration (mg/L)	Average Mass Loading (mg/g)
Influent	0.63	
Effluent: 1-day preloaded	0.12	7.5
Effluent: 3-day preloaded	0.16	22.6
Effluent: 7-day preloaded	0.21	49.6

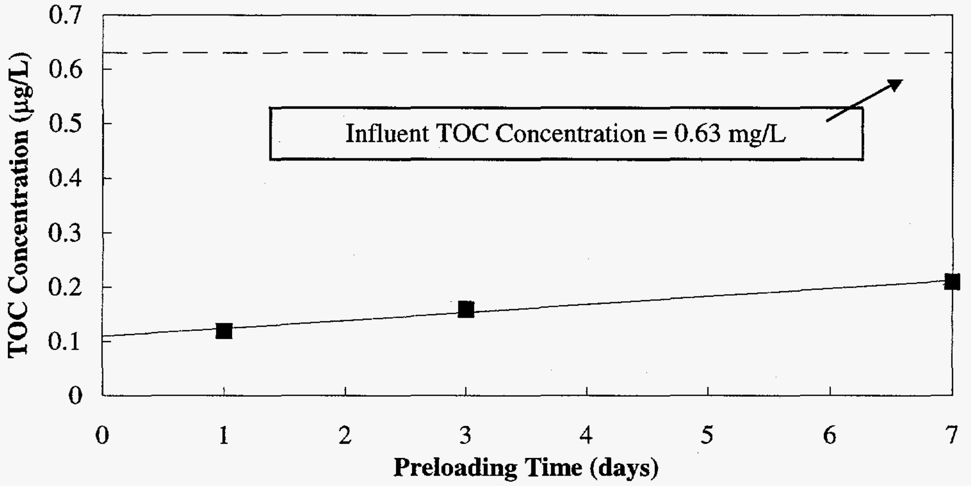

Figure 4.17: TOC Concentration versus Preloading Time for Determining TOC Mass Loading on GAC in Preloading Tests

data points. This interpolation was done because of the strong possibility that there was a fraction of non-adsorbable TOC in the influent. Varying degrees of exhaustion with respect to TOC were obtained by preloading with uncontaminated groundwater. Figure 4.18 shows the comparison of the scaled-up breakthrough curves for RDX for the preloading experiments. The breakthrough curve for no preloading, as developed in the previous section, is not included here because the influent water was from a different batch and could not be reliably compared to the preloading results. As expected, the time for RDX to break through decreased with increasing time of preloading, thereby reducing the capacity for adsorption of RDX. The predicted times for the service life with respect to RDX are 81, 74, and 34 days for 1-day, 3-day, and 7-day preloading, respectively. The 1, 3, and 7 days of preloading scale-up to full-scale operation times of 37, 112, and 261 days, respectively. Figure 4.19 graphically shows the extent of reduction in service life for the successive increases in preloading.

It is evident that the amount of preloading affects the adsorptive capacity of the columns. This complicates the use of current models to predict the behavior of a full scale adsorption column. Preloading effects could have the greatest impact with variable influent concentration, especially when the contaminant concentration is low. To alleviate problems produced by preloading, a series GAC column configuration could be utilized with subsequent columns being added to minimize capacity reductions from preloading (Speth and Miltner, 1989). To implement this at the Pantex facility, the second column series of the treatment system could be bypassed until breakthrough was first experienced in the first column. This would protect the second GAC column from fouling.

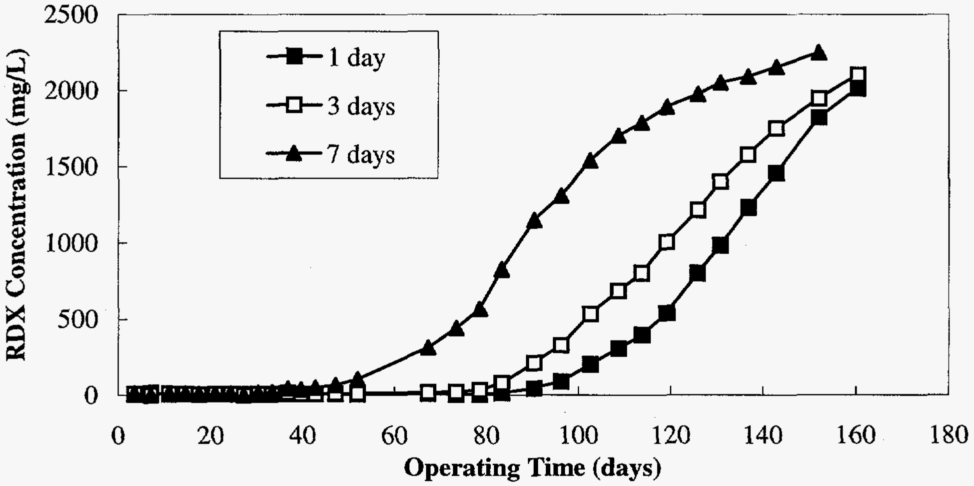

Figure 4.18: Breakthrough Curves from Preloading Experiments with Preloading Times of 1, 3, and 7 days for EBCT = 8.2 min

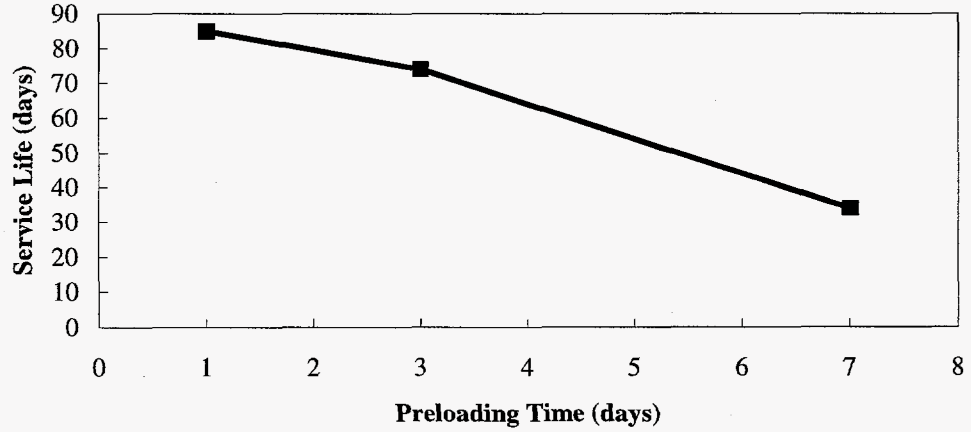

Figure 4.19: Service Life for Increasing Times of Preloading as Demonstrated in the Preloading Experiments

4.6 MODELING WITH *PCSORB*

Computer modeling was done with *PCsorb* to model the RSSCTs as well as full-scale adsorber performance using Calgon F400. Both the RSSCT experimental data and the predicted full-scale performance were modeled because all the dimensionless parameters (e.g. Stanton Number) used to design the RSSCT did not match the full-scale parameters. Constraints were placed on the design of the RSSCT that required alteration of the dimensionless parameters for the small-scale. The Homogeneous Surface Diffusion Model (HSDM) was used for all breakthrough curve simulations. Results using the Pore Surface Diffusion Model did not vary much from the HSDM predictions, so the HSDM was used as the model of choice. The input parameters for the computer model were single-component Freundlich isotherm parameters. These parameters were determined from isotherm tests that were performed in buffered Milli-Q water at the University of Texas. Other input parameters such as the liquid film transfer coefficient, k_f, and the surface diffusion coefficient, D_S, were estimated using the autocalculate option in *PCsorb*. A correlation developed by Williamson et al. (1963) was used for the calculation of k_f. A correlation for the calculation of D_s was developed by Crittenden et al. (1987). The value of the free liquid diffusivity, D_L, was assumed to be 7.5 x 10^{-6} cm^2/sec. This value is based on typical values for synthetic organic chemicals. Insufficient information was available to use the correlation for D_L. Table 4.8 summarizes the general input parameters for *PCsorb*. A more detailed summary is included with the output for each run in Appendix F. The modeling compared the experimental RDX breakthrough curves with model predicted breakthrough curves.

Table 4.8: Input Parameters for PCsorb

Parameter	Value
K_{RDX}	260 µM/g $(L/\mu M)^{1/n}$
1/n $_{RDX}$	0.286
K_{HMX}	543 µM/g $(L/\mu M)^{1/n}$
1/n $_{RDX}$	0.241
HMX	1.18 µM/L (350 µg/L)
RDX	10.36 µM/L (2300 µg/L)
Temperature	20° C
D_L*	7.5 x 10^{-6} cm^2/sec
PSDFR**	6.58
k_f	autocalculated, Williamson et al. (1963)
D_s	autocalculated, Crittenden et al. (1987)

*D_L = free liquid diffusivity, used by *PCsorb* to autocalculate the liquid film transport coefficient and the surface diffusion coefficient

**PSFDR = Pore Surface Diffusion Flux Ratio

4.6.1 RSSCT Modeling

Modeling of the four RSSCTs EBCTs used in developing the service life versus EBCT curve for Calgon F400 was done using *PCsorb*. Figure 4.20 shows the experimental data and the model-predicted simulations for each EBCT. The model predicts a sharper breakthrough curve (shorter mass transfer zone) for each of the EBCTs. More spreading is evident in the RSSCT curves as compared to the model-predicted breakthrough curves, especially for the larger EBCTs. It is unclear why the fit of the model to the experimental data is not better. Several possibilities exist. The increased spreading in the RSSCT breakthrough curves could be attributed to the reduced Re for the larger EBCTs. The Re was reduced so that influent water usage would be minimized. It seems that the statement by Crittenden et al. (1987) that Re can be reduced without affecting the adsorption kinetics is not consistent in this case. With the lower Re (higher EBCT), more spreading of the MTZ was produced. Although possible, it is not believed that the spreading is due to fouling of the GAC because the exposure time to the natural background organic matter was minimal for the short duration of the RSSCTs. Another potential source of error to produce a poor fit to the data could be from an inaccurate estimate of the kinetic coefficients. The service life for each of the four model predicted RSSCTs was determined at an RDX effluent concentration of 26 μg/L, and a service life versus EBCT relationship was developed. Figure 4.21 shows a comparison of the experimental and the model-predicted service life versus EBCT curves. The *PCsorb* predicted curve lies above the experimental curve. Thus, for any EBCT, *PCsorb* predicted greater service lives than were experienced in the RSSCTs. The ratio of the slopes of the two lines is 1.85. From the comparison of the *PCsorb* and the RSSCT service life prediction, the RSSCT was more conservative in predicting the service life for a GAC column.

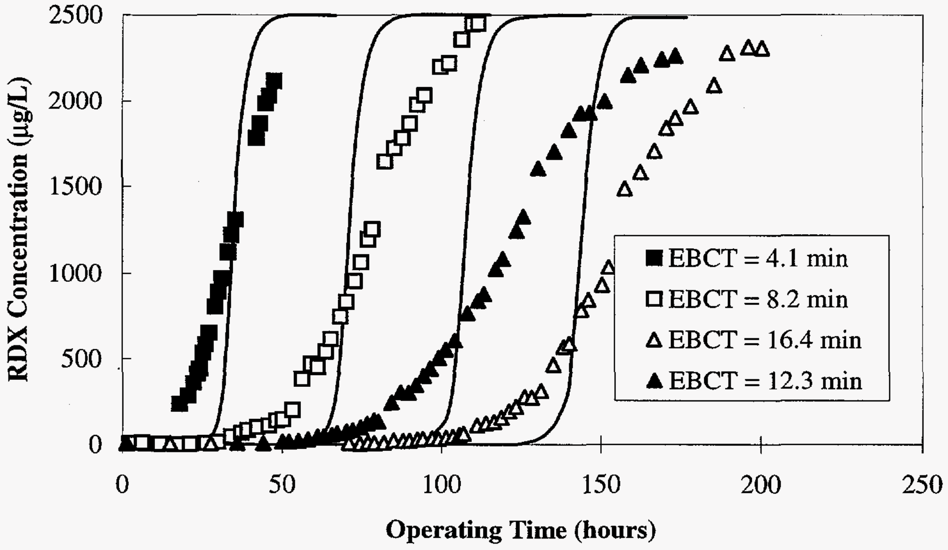

Figure 4.20: Comparison of Small-scale Experimental and *PCsorb* Predicted Breakthrough Curves for RDX for Calgon F400 GAC

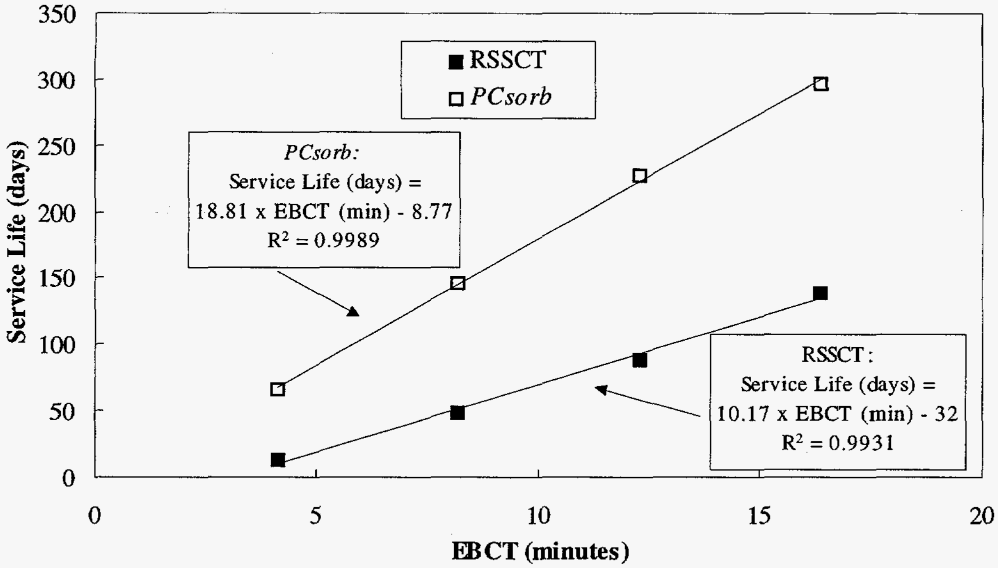

Figure 4.21: Service Life versus EBCT for RSSCT and Small-Scale *PCsorb* Predictions

4.6.2 Full-Scale Adsorber Modeling

PCsorb runs were also performed at each EBCT to model full-scale breakthrough curves as predicted by scaling up the RSSCT breakthrough curves. Figure 4.22 shows the comparison of the *PCsorb* predicted curves and the scaled-up RSSCT curves. A good fit of the experimental data is not evident from comparing the breakthrough curves. This is expected because the actual RSSCT data was not modeled well. The model overpredicts the service life, and there is less spreading in the model predicted breakthrough curves than the experimental curves. As mentioned before, it is not known why the model prediction does not produce a better fit for the experimental data. The service life for each full-scale column for the *PCsorb* runs was determined, and a service life versus EBCT curve was developed. Figure 4.23 shows a comparison of this curve with the experimental predicted curve for Calgon F400. The curve for the *PCsorb* full-scale column lies above the RSSCT predicted curve, so the service lives are higher if predicted with PCsorb. The ratio of the PCsorb slope to the RSSCT slope is 1.38. This difference is attributed to the variance in the dimensionless parameters (and thus the kinetics) between the small-scale and full-scale designs.

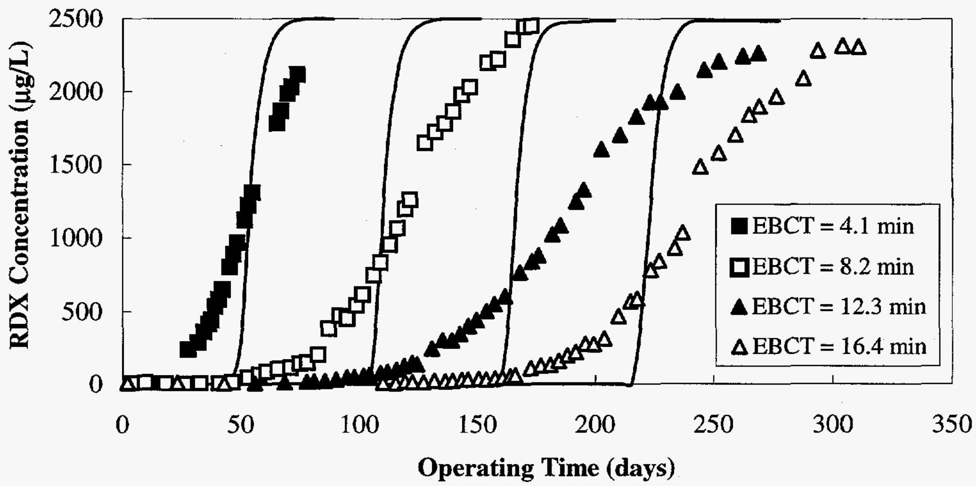

Figure 4.22: Comparison of Full-scale Experimental and *PCsorb* Predicted Breakthrough Curves for RDX

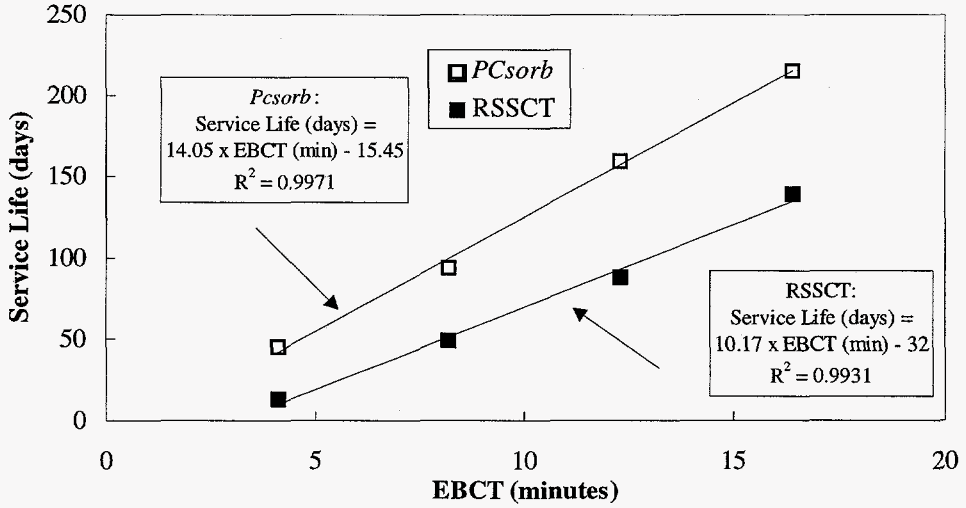

Figure 4.23: Service Life versus EBCT for RSSCT and Full-Scale *PCsorb* Predictions

4.6.3 Preloading Modeling

Modeling of the preloading experiments was done to investigate the reduction in the capacity of the carbon after preloading with uncontaminated Pantex groundwater. The three breakthrough curves for the preloading set of experiments were modeled. Each was performed at an EBCT of 8.2 min. The K isotherm value for RDX was varied until $C/C_o = 0.5$ ($C = 1150$ μg/L) for the model data matched the corresponding point on the experimental breakthrough curves. The K values that matched the preloading data were 320, 293, and 210 µM/mg(L/µM)$^{1/n}$ for the 1, 3, and 7 day curves, respectively. Figure 4.23 shows the experimental data for the preloading breakthrough curves along with the *PCsorb* predicted breakthrough curves. As noted with the other modeling for the RSSCTs and full-scale adsorbers, there is more spreading in the experimental breakthrough curves as compared to the model solutions. However, the curves presented in Figure 4.24 and the corresponding K values indicate that preloading with uncontaminated Pantex groundwater significantly reduces the adsorption capacity of the Calgon F400 GAC.

4.6.4 Sensitivity Analysis

A sensitivity analysis was performed for the EBCT of 8.2 min. Similar results can be expected at the other EBCTs. Three model input parameters were varied: the isotherm parameter K (for both RDX and HMX) and the kinetic parameters, k_f and D_s. Analyses were done for both modeling the RSSCTs and the full-scale adsorber. One parameter was varied singularly, and the RDX breakthrough curve for each case was plotted. The experimental data from the 8.2 min EBCT was included in each of the plots for the sensitivity analysis.

RSSCTs. The K isotherm value for RDX was varied at values of -10%, -5%, +5%, and +10% of the original K (260 µM/g (L/µM)$^{1/n}$). Figure 4.25 shows the results of varying the RDX K isotherm value. The HMX K isotherm parameter was also varied at the same percent differences as the RDX K value, and the RDX breakthrough curve was not appreciably affected from these variations.

The variation of the RDX K isotherm parameter produced variations in the service life of the column from 54 to 66 hours, for variations of -10% to +10%, respectively. These breakthrough times scale-up to 84 and 102 days, respectively. Since the variation of the K value does not affect spreading of the breakthrough curve and thus the MTZ, a better fit to the experimental data was not expected. However, Figure 4.25 does show the variation in the predicted service life for variations in the RDX K isotherm value.

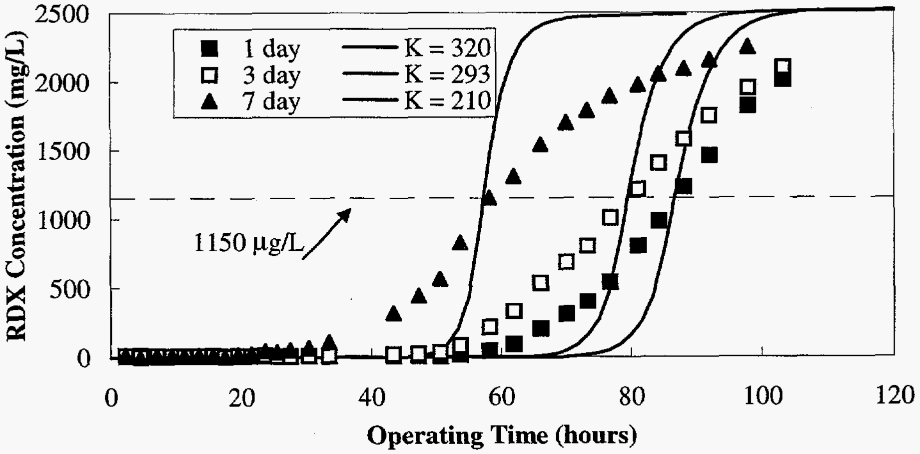

Figure 4.24: Experimental and *PCsorb* Predicted Breakthrough Curves for Preloading Experiments at EBCT = 8.2 min (K in units of µM/g (L/µM)$^{1/n}$)

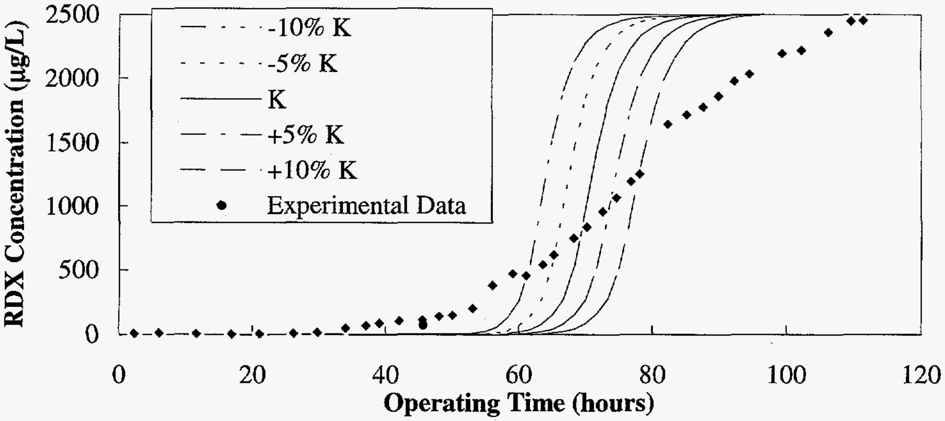

Figure 4.25: *PCsorb* Predicted RSSCT RDX Breakthrough Curves for EBCT = 8.2 min for Various K values for RDX (K = 260 μM/g $(L/\mu M)^{1/n}$)

The surface diffusion coefficient, D_s, was varied at values of -94%, -90%, -80%, -65%, -50%, and -20% of the original D_s. The variation was done for both RDX and HMX concurrently. The original values, as determined from the literature correlation from Crittenden et al.(1987), for D_s were 8.85 x 10^{-10} and 9.05 x 10^{-11} cm^2/sec for RDX and HMX, respectively. The surface diffusion coefficient was not varied to values larger than the one autocalculated by *PCsorb* because the model predicted kinetics faster than were observed in the RSSCTs. Increased values of the D_s would only further increase the kinetics. Figure 4.26 shows the resulting breakthrough curves for varying the surface diffusion coefficient, D_s. As D_s was decreased, spreading was more pronounced in the breakthrough curve. When the D_s was ultimately reduced by 94%, the service life predicted by *PCsorb* matched that as determined from the RSSCT for an EBCT = 8.2 min. However, the shape of the breakthrough curve was not represented well by any variation in D_s. The liquid film transport coefficient, k_f, was varied at values of -80%, -65%, -50%, and -20% of the k_f calculated by applying the literature correlation from Williamson et al. (1963). The value calculated by *PCsorb* for the 8.2 min EBCT was 1.08 x 10^{-2} cm/sec. As with the surface diffusion coefficient, values greater than the k_f predicted by *PCsorb* were not investigated since the kinetics predicted by *PCsorb* were faster than experienced in the RSSCTs. A larger value of k_f would increase the kinetics more. Figure 4.27 contains breakthrough curves from altering the liquid film coefficient, k_f. Variations in k_f produced breakthrough curves that were more similar in shape to the experimental data. A k_f value of 2.16 x 10^{-3} cm/sec (-80%) produced the best fit for the experimental data. At k_f values smaller than 2.16 x 10^{-3} cm/sec, *PCsorb* would not run because the differential equations become too stiff for the numerical methods solution; therefore, it could not be determined if an even lower k_f would fit the data better. The variation of k_f produced the greatest effect on the resulting service life of the GAC column. Comparing the service lives for the original k_f and the -80% variation, the service life was reduced from 45

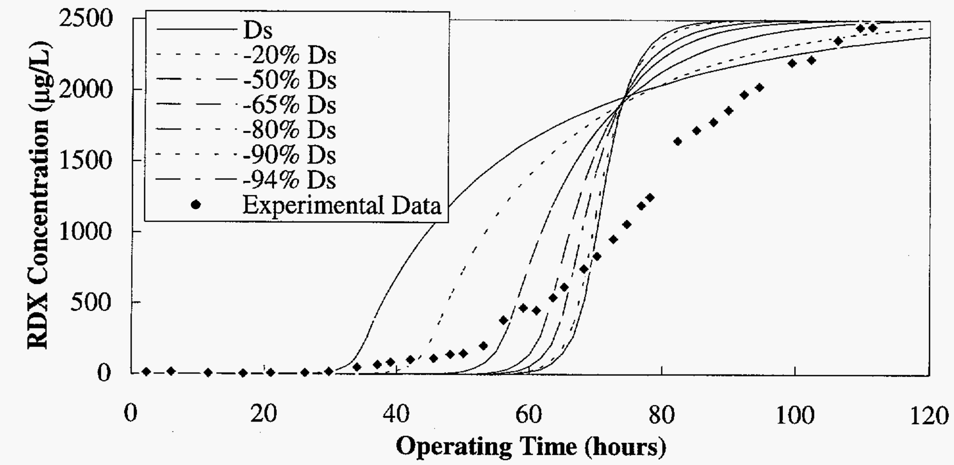

Figure 4.26: *PCsorb* Predicted RSSCT RDX Breakthrough Curves for EBCT = 8.2 min for Various D_s values (RDX: $D_s = 8.85 \times 10^{-10}$ cm^2/s, HMX: $D_s = 9.05 \times 10^{-11}$ cm^2/s)

to 26 hours. This corresponds to a reduction from 70 to 41 days for scaled-up operation.

Full-scale adsorbers. Similar sensitivity analyses were done for the full-scale adsorber. The K isotherm value for RDX was varied at values of -10%, -5%, +5%, and +10% of the original K (260 µM/g (L/µM)$^{1/n}$. The results of the variance in the RDX K are shown in Figure 4.28 Variances in the HMX K isotherm parameter were also done, and they did not substantially affect column performance with respect to RDX breakthrough.

Variations of 94 to 114 days in the service life of the full-scale GAC column with respect to RDX were predicted for the 8.2 min EBCT for changes of -10% and +10% in the RDX K isotherm value. As stated for the RSSCT analyses of varying the RDX K isotherm parameter, the changes in K will not change the spreading of the breakthrough curve. They can, however, give a better understanding of how variances in the isotherm parameters will affect system performance. As done for the RSSCT sensitivity analysis, the surface diffusion coefficient, D_s, was varied at values of -94%, -90%, -80%, -65%, -50%, and -20% of the original D_s. Variation of the RDX and HMX surface diffusion coefficient was done for each *PCsorb* run. The original (from literature correlation) values for D_s were 8.85 x 10^{-10} and 9.05 x 10^{-11} cm^2/s for RDX and HMX, respectively. The surface diffusion coefficient was only varied to values smaller than the one autocalculated by *PCsorb* to examine slower kinetics. Figure 4.29 shows the resulting breakthrough curves for varying the surface diffusion coefficient, D_s. The results from varying the D_s for the full-scale column are similar to those from the RSSCT analyses. At a reduction of 94% of the D_s, the service life of the full-scale column is decreased to correspond to the service life produced from the scaled-up RSSCT. The shape of the breakthrough curves for variances in D_s do not agree with the experimental data.

Variation of the liquid film transport coefficient for full-scale analyses done at the same values at applied for the RSSCT analyses. These included the values of -88%, -80%, -65%, -50%, and -20% of the k_f

calculated with the literature correlation. The value calculated by *PCsorb* for the 8.2 min EBCT was 3.42 x 10^{-3} cm/sec. Similarly to the other investigation of varying k_f for RSSCT analyses, only smaller values of k_f were considered. Figure 4.30 contains breakthrough curves from altering the liquid film coefficient, k_f. Reductions in k_f produced breakthrough curves with more spreading as a result of the slower kinetics. The k_f value of 4.10 x 10^{-4} cm/sec (-88%) best matches the experimental data.

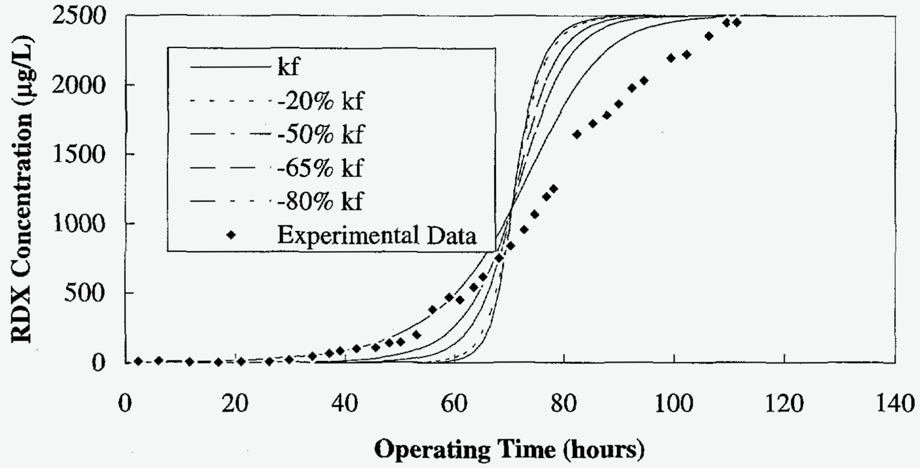

Figure 4.27: *PCsorb* Predicted RSSCT RDX Breakthrough Curves for EBCT = 8.2 min for Various k_f Values (k_f = 1.08 x 10^{-2} cm/s)

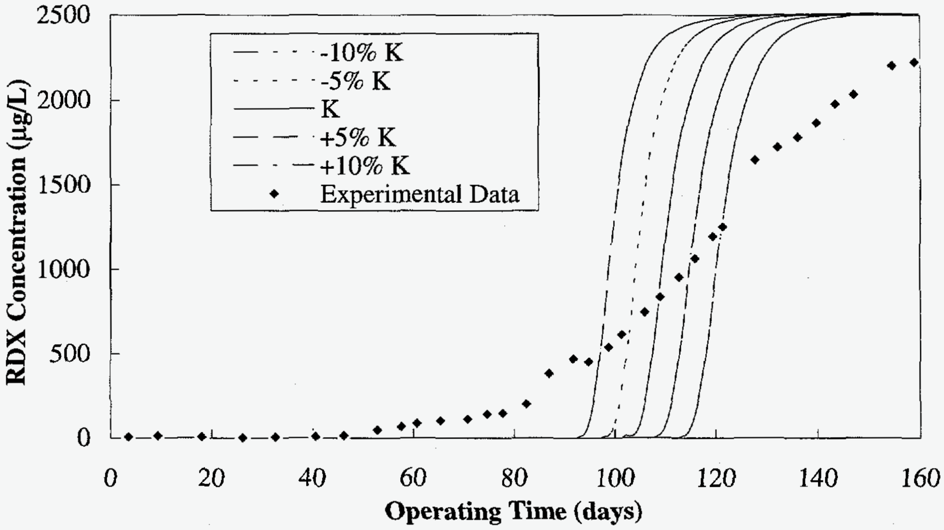

Figure 4.28: *PCsorb* Predicted Full-Scale RDX Breakthrough Curves for EBCT = 8.2 min for Various K Values for RDX (K = 260 μM/g $(L/\mu M)^{1/n}$)

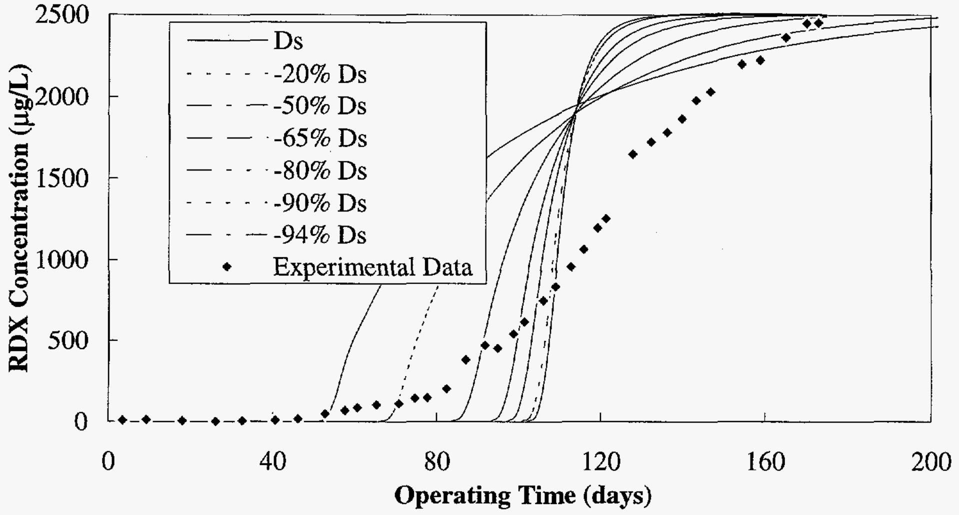

Figure 4.29: *PCsorb* Predicted Full-Scale RDX Breakthrough Curves for EBCT = 8.2 min for Various D_s Values (RDX: $D_s = 8.85 \times 10^{-10}$ cm^2/s, HMX: $D_s = 9.05 \times 10^{-11}$ cm^2/s)

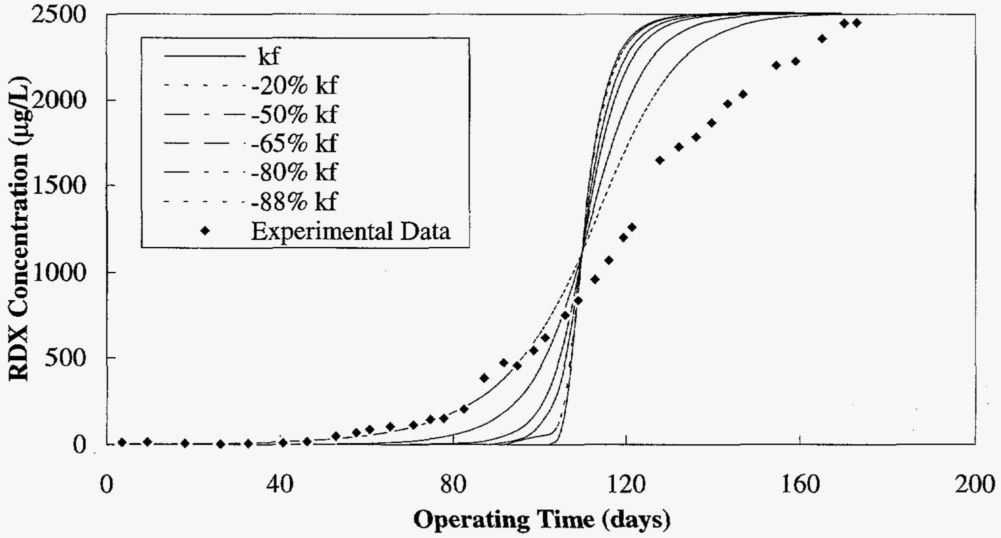

Figure 4.30: *PCsorb* Predicted Full-Scale RDX Breakthrough Curves for EBCT = 8.2 min for Various k_f Values ($k_f = 3.42 \times 10^{-3}$ cm/s)

For all of the experimental cases, the model *PCsorb* overpredicts the service life using measured equilibrium parameters and literature correlations for calculation of the kinetic parameters. An improvement can be made in the prediction of the model by applying a simultaneous reduction of k_f and D_s. The liquid film coefficients that represented the experimental data well, especially at early times, were quite small (4.10×10^{-4} cm/sec) and are not realistic for practical application.

5. CONCLUSIONS AND RECOMMENDATIONS

The overall goals of this research were to conduct laboratory studies to evaluate the treatability of explosive-contaminated groundwater at Pantex with granular activated carbon adsorption. Results of this research will be used to support the current operation of the pilot-scale GAC adsorption system installed as part of the Zone 12 Treatability Study at Pantex. This chapter summarizes the research findings and conclusions. Recommendations for operation options for the pilot treatment system at Pantex are also included.

5.1 CONCLUSIONS

Of the five GACs evaluated in this work, Calgon F400 and Northwestern LB-830 (currently in use at Pantex) outperformed the other GACs in effectively removing HMX and RDX from contaminated groundwater at Pantex. Further analyses of the Calgon F400 and Northwestern LB-830 GACs in RSSCTs showed that a single GAC column packed with Calgon F400 had approximately a 50% greater service life than a column packed with the Northwestern LB-830. If the current treatment system at Pantex were operated as two columns in parallel, the service life of the entire system would be 97 days for Northwestern LB-830 and 139 days for Calgon F400 for continuous operation at the design flow rate of 325 gpm and influent concentrations of 350 μg/L HMX and 2300 μg/L RDX. When predicting the service life of two columns operated in series as they currently are at Pantex, the service life can be increased to 160 days for Northwestern LB-830 and 227 days for Calgon F400. These service lives are valid for GAC replacement after the first column has been exhausted and replaced; the GAC columns will then be in the alternating replacement pattern. The service life for the first column when the system is first started up is 97 days for Northwestern LB-830 and 139 days for Calgon F-400. The MTZ of RDX is not completely contained within one column; therefore, the predicted service life is somewhat less than the maximum possible service life. If the GAC treatment system is operated intermittently or at less than the design flow, the services lives noted above can be adjusted in proportion to the total volume treated (e.g., the 160-day service life for LB-830 corresponds to treating approximately 75 million gallons of water).

Additional evaluation of the Calgon F400 GAC produced the following findings. Increased concentrations of HMX and RDX in the contaminated groundwater significantly reduced the service life of a Calgon F400 column. Reductions were as great as 78% for an RDX increase from 2300 μg/L to 4500 μg/L; increases from 350 μg/L to 1100 μg/L HMX produce a 80% reduction in service life. These reductions are for a single column; reductions in the service life for series operation can also be expected.

Adsorption of RDX and HMX was significantly hindered by fouling caused by preloading with natural organic matter. The service lives of a 8.2 min EBCT full-scale column of Calgon F400 were 81, 74, and 34 days for preloading times of 1, 3, and 7 days, respectively. The respective full-scale preloading times for these service lives are 37, 112, and 261 days.

The RSSCTs were more conservative in predicting the service life as compared to the modeled predictions from the computer model *PCsorb*. *PCsorb* predicted longer service lives for GAC columns than were experimentally determined with RSSCTs. The breakthrough curves produced by *PCsorb* were steeper than the experimental breakthrough curves. Thus, the MTZ predicted by *PCsorb* had less spreading than the experimentally defined MTZ. Only variations in the liquid film transport coefficient (k_f) produced model predicted breakthrough curves that more closely matched the RSSCTs. However, combinations of varying both k_f and D_s simultaneously might produce a better model prediction of the experimental breakthrough curve data.

The mismatch between the experimental data and modeling is a cause for some concern about the accuracy of service life predictions. HSDM does not fully account for observed behavior in RSSCTs. Because scaling relationships are based on HSDM concepts, the service life predicted by the scaling approach may by subject to some error. The source of error might arise from fouling by NOM, inaccuracies in mass transfer kinetic correlations, and the smaller Reynolds number in the RSSCT compared to that required to match the Re in the full-scale column.

5.2 RECOMMENDATIONS

For the GAC in use at Pantex (Northwestern LB-830), the service life of a two column parallel system based on the RSSCT experiments can be calculated by the equation: Service Life (days) = 7.31 x EBCT (min) - 25. The Calgon F400 service life is determined by the equation: Service Life (days) = 10.17 x EBCT (min) - 32. In this configuration as well as the other configurations studied, the use of Calgon F400 produced a longer service life and should be considered as an option for GAC replacement when the current GAC becomes exhausted.

The current operation at Pantex of two columns in series clearly produces extended service lives relative to parallel operation, so it is recommended that series operation continue. Considerations should be given, however, to approaches for minimizing the "fouling" of GAC by background organic matter. The second column in the series could be by-passed until breakthrough occurs in the first column. This would minimize the exposure of the second column to background organic matter and probably extend the GAC service life. The range of influent concentrations expected over the operating time of the GAC treatment system should also be defined to aid in more accurately predicting GAC service life. The HSDM can be used with a fair degree of accuracy to predict effects of changing influent concentration on service life. RSSCTs at elevated influent concentration also provide guidance on service life with changing influent concentration.

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APPENDIX A

EXPERIMENT DESIGN

Design for GAC screening tests using Calgon F400 GAC for EBCT = 4.1 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:			
K =	101.9	$mg/g(L/mg)^{1/n}$	
1/n =	0.344		
V_{lc} =	6.47	or	0.439 cm /sec.
$(EBCT)_{lc}$ =	4.1	min	
(GAC mesh)$_{lc}$ =	12x40		Calgon F400
(GAC rad.)$_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data
(bulk dens.)$_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)
(serv. life)$_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.73	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.41		Bed porosity (about 0.4)
C_o =	2.2	mg/L	
Column ID =	0.8	cm	
COLUMN CALCULATIONS:			
D_g =	63565		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	10.58		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	**80x100**	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	**0.00822**	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	**3.00**	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	**0**	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	**11.2**	5.6	3.7	4.9
Q_{sc} (mL/min)	62.51	11.32	5.91	80.61	**22.86**	11.43	7.62	9.94
GAC $Mass_{sc}$ (g)	4.95	0.94	0.47	3.84	**1.09**	0.54	0.36	0.28
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.18	0.18	0.18	0.11	**0.11**	0.11	0.11	0.07
length (cm)	22.9	4.3	2.2	17.8	**5.0**	2.5	1.7	1.3
t^*_{sc} (min)	4814	4814	4814	2895	**2895**	2895	2895	1700
t^*_{sc} (hr)	80	80	80	48	**48**	48	48	28
Qt^*_{sc} (L)	301	57	28	233	**66**	33	22	17
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	**56.4**	56.4	56.4	33.1

Equations used in spreadsheet calculations:

$Re_{lc} = 2 * \text{GAC Rad.} * Vs_{lc} * \text{Liq. Dens.}/(\text{Visc.} * \text{porosity})$

$V_{sc} = V_{lc} * (\text{GAC Rad.}_{lc}/\text{GAC Rad.}_{sc}) * (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} * A$

$\text{GAC Mass}_{sc} = EBCT_{lc} * (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)} * Q_{sc} * \text{bulk dens.}_{lc}$

$EBCT_{sc} = EBCT_{lc} * (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)}$

$\text{length} = V_{sc} * EBCT_{sc}$

$t^*_{sc} = (\text{porosity}) * (Dg + 1) * EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for GAC screening tests using Norit H3000 GAC for EBCT = 4.1 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	$mg/g(L/mg)^{1/n}$		
1/n =	0.344			
V_{lc} =	6.47	gpm/ft^2	or	0.439 cm /sec.
$(EBCT)_{lc}$ =	4.1	min		
$(GAC\ mesh)_{lc}$ =	8x30		Hydrodarco 3000	
$(GAC\ rad.)_{lc}$ =	0.06	cm	GAC particle radius from manufacturer's data	
$(bulk\ dens.)_{lc}$ =	0.37	g/cm^3	Bulk GAC density (0.4-0.5)	
$(serv.\ life)_{lc}$ =	75	days	Service life of large column to be simulated by RSSCT (optional)	
Viscosity =	1.0087	centipoise		
Liq. Density =	0.99823	g/cm^3		
apparent dens. =	0.71	g/cm^3	Apparent density of the GAC (<1)	
porosity =	0.48		Bed porosity (about 0.4)	
C_o =	2.2	mg/L		
Column ID =	0.8	cm		

COLUMN CALCULATIONS:

D_g =	46938		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	10.90		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	10.90	2.00	1.00	10.90	4.00	2.00	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	36.6	6.7	3.4	47.2	17.3	8.7	4.3	5.7
Q_{sc} (mL/min)	75.01	13.77	6.88	96.73	35.51	17.76	8.88	11.58
GAC $Mass_{sc}$ (g)	3.55	0.65	0.33	2.75	1.01	0.51	0.25	0.19
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.13	0.13	0.13	0.08	0.08	0.08	0.08	0.05
length (cm)	19.1	3.5	1.8	14.8	5.4	2.7	1.4	1.0
t^*_{sc} (min)	2876	2876	2876	1730	1730	1730	1730	1016
t^*_{sc} (hr)	48	48	48	29	29	29	29	17
Qt^*_{sc} (L)	216	40	20	167	61	31	15	12
Serv. $life_{sc}$ (hr)	56.2	56.2	56.2	33.8	33.8	33.8	33.8	19.8

Equations used in spreadsheet calculations:

$Re_{lc} = 2 * GAC\ Rad. * Vs_{lc} * Liq.\ Dens./(Visc. * porosity)$

$V_{sc} = V_{lc} * (GAC\ Rad._{lc} / GAC\ Rad._{sc}) * (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} * A$

$GAC\ Mass_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)} * Q_{sc} * bulk\ dens._{lc}$

$EBCT_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)}$

$length = V_{sc} * EBCT_{sc}$

$t^*_{sc} = (porosity) * (Dg + 1) * EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
   A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
   These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet.
   The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for GAC screening tests using Norit H4000 GAC for EBCT = 4.1 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K = 101.9 mg/g(L/mg)$^{1/n}$
$1/n$ = 0.344
V_{lc} = 6.47 gpm/ft^2 or 0.439 cm/sec.
$(EBCT)_{lc}$ = 4.1 min
$(\text{GAC mesh})_{lc}$ = 8x30 **Hydroarco 4000**
$(\text{GAC rad.})_{lc}$ = 0.05 cm GAC particle radius from manufacturer's data
$(\text{bulk dens.})_{lc}$ = 0.37 g/cm^3 Bulk GAC density (0.4-0.5)
$(\text{serv. life})_{lc}$ = 75 days Service life of large column to be simulated by RSSCT (optional)
Viscosity = 1.0087 centipoise
Liq. Density = 0.99823 g/cm^3
apparent dens. = 0.71 g/cm^3 Apparent density of the GAC (<1)
porosity = 0.48 Bed porosity (about 0.4)
C_o = 2.2 mg/L
Column ID = 0.8 cm

COLUMN CALCULATIONS:

D_g = 46938
Max. GAC Rad. = 0.008 cm 1% of column diameter
Re_{lc} = 9.08

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	9.08	2.00	1.00	9.08	3.00	2.00	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	6.7	3.4	39.4	13.0	8.7	4.3	5.7
Q_{sc} (mL/min)	62.51	13.77	6.88	80.61	26.63	17.76	8.88	11.58
GAC Mass_{sc} (g)	4.26	0.94	0.47	3.31	1.09	0.73	0.36	0.28
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.18	0.18	0.18	0.11	0.11	0.11	0.11	0.07
length (cm)	22.9	5.0	2.5	17.8	5.9	3.9	2.0	1.5
t^*_{sc} (min)	4142	4142	4142	2491	2491	2491	2491	1463
t^*_{sc} (hr)	69	69	69	42	42	42	42	24
Qt^*_{sc} (L)	259	57	29	201	66	44	22	17
Serv. life_{sc} (hr)	80.9	80.9	80.9	48.6	48.6	48.6	48.6	28.6

Equations used in spreadsheet calculations:

$Re_{lc} = 2 \cdot \text{GAC Rad.} \cdot Vs_{lc} \cdot \text{Liq. Dens.}/(\text{Visc.} \cdot \text{porosity})$

$V_{sc} = V_{lc} \cdot (\text{GAC Rad.}_{lc}/\text{GAC Rad.}_{sc}) \cdot (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} \cdot A$

$\text{GAC Mass}_{sc} = EBCT_{lc} \cdot (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)} \cdot Q_{sc} \cdot \text{bulk dens.}_{lc}$

$EBCT_{sc} = EBCT_{lc} \cdot (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)}$

$\text{length} = V_{sc} \cdot EBCT_{sc}$

$t^*_{sc} = (\text{porosity}) \cdot (Dg + 1) \cdot EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. life_{sc} = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet.
The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for GAC screening tests using Northwestern LB-830 GAC for EBCT = 4.1 min.

RSSCT Design Spreadsheet
Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)
Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	111.8	mg/g(L/mg)$^{1/n}$	
1/n =	0.34		
V_{lc} =	6.47	gpm/ft^2	or 0.439 cm /sec.
$(EBCT)_{lc}$ =	4.1	min	
$(GAC\ mesh)_{lc}$ =	8x30		NWC LB-830
$(GAC\ rad.)_{lc}$ =	0.0675	cm	GAC particle radius from manufacturer's data
$(bulk\ dens.)_{lc}$ =	0.47	g/cm^3	Bulk GAC density (0.4-0.5)
$(serv.\ life)_{lc}$ =		days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.75	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.37		Bed porosity (about 0.4)
C_o =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	83646		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	15.72		

INPUTS:

GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	15.72	2.00	1.00	15.72	5.00	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	41.2	5.2	2.6	53.1	16.9	5.1	3.4	4.4
Q_{sc} (mL/min)	84.39	10.73	5.37	108.82	34.61	10.38	6.92	9.03
GAC $Mass_{sc}$ (g)	4.01	0.51	0.26	3.11	0.99	0.30	0.20	0.15
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.10	0.10	0.10	0.06	0.06	0.06	0.06	0.04
length (cm)	17.0	2.2	1.1	13.2	4.2	1.3	0.8	0.6
t^*_{sc} (min)	3157	3157	3157	1899	1899	1899	1899	1115
t^*_{sc} (hr)	53	53	53	32	32	32	32	19
Qt^*_{sc} (L)	266	34	17	207	66	20	13	10
Serv. $life_{sc}$ (hr)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Equations used in spreadsheet calculations:

$Re_{lc} = 2 \cdot \text{GAC Rad.} \cdot Vs_{lc} \cdot \text{Liq. Dens.}/(\text{Visc.} \cdot \text{porosity})$

$V_{sc} = V_{lc} \cdot (\text{GAC Rad.}_{lc}/\text{GAC Rad.}_{sc}) \cdot (Re_{sc}/Ro_{lc})$

$Q_{sc} = V_{sc} \cdot A$

$\text{GAC Mass}_{sc} = EBCT_{lc} \cdot (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)} \cdot Q_{sc} \cdot \text{bulk dens.}_{lc}$

$EBCT_{sc} = EBCT_{lc} \cdot (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)}$

$\text{length} = V_{sc} \cdot EBCT_{sc}$

$t^*_{sc} = (\text{porosity}) \cdot (Dg + 1) \cdot EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for service life versus EBCT tests using Calgon F400 GAC for EBCT = 8.2 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.L. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	mg/g(L/mg)$^{1/n}$	
1/n =	0.344		
V_{lc} =	6.47	or	0.439 cm/sec.
$(EBCT)_{lc}$ =	8.2	min	
$(GAC\ mesh)_{lc}$ =	12x40		Calgon F400
$(GAC\ rad.)_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data
$(bulk\ dens.)_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)
$(serv.\ life)_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.73	g/cm^3	*Apparent density of the GAC* (<1)
porosity =	0.41		Bed porosity (about 0.4)
C_0 =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	63565		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	10.58		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	**80x100**	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	**0.00822**	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	3.00	**1.50**	1.00	1.00
X (See Note 1)	0	0	0	0	0	**0**	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	**5.6**	3.7	4.9
Q_{sc} (mL/min)	62.51	11.82	5.91	80.61	22.86	**11.43**	7.62	9.94
GAC $Mass_{sc}$ (g)	9.91	1.87	0.94	7.68	2.18	**1.09**	0.73	0.56
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.37	0.37	0.37	0.22	0.22	**0.22**	0.22	0.13
length (cm)	45.8	8.7	4.3	35.5	10.1	**5.0**	3.4	2.6
t^*_{sc} (min)	9627	9627	9627	5789	5789	**5789**	5789	3401
t^*_{sc} (hr)	160	160	160	96	96	**96**	96	57
Qt^*_{sc} (L)	602	114	57	467	132	**66**	44	34
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	**56.4**	56.4	33.1

Equations used in spreadsheet calculations:

Re_{lc} = 2 * GAC Rad. * Vs_{lc} * Liq. Dens./(Visc. * porosity)

V_{sc} = V_{lc} * (GAC $Rad._{lc}$ /GAC $Rad._{sc}$) * (Re_{sc}/Re_{lc})

Q_{sc} = V_{sc} * A

GAC $Mass_{sc}$ = $EBCT_{lc}$ * (GAC $Rad._{sc}$/GAC $Rad._{lc}$)$^{(2-X)}$ * Q_{sc} * bulk $dens._{lc}$

$EBCT_{sc}$ = $EBCT_{lc}$ * (GAC $Rad._{sc}$/GAC $Rad._{lc}$)$^{(2-X)}$

length = V_{sc} * $EBCT_{sc}$

t^*_{sc} = (porosity) * (Dg + 1) * $EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
   A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
   These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for service life versus EBCT tests using Calgon F400 GAC for EBCT = 12.3 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9 mg/g(L/mg)$^{1/n}$	
1/n =	0.344	
V_{lc} =	6.47	or 0.439 cm /sec.
$(EBCT)_{lc}$ =	12.3 min	
$(GAC\ mesh)_{lc}$ =	12x40	Calgon F400
$(GAC\ rad.)_{lc}$ =	0.05 cm	GAC particle radius from manufacturer's data
$(bulk\ dens.)_{lc}$ =	0.43 g/cm^3	Bulk GAC density (0.4-0.5)
$(serv.\ life)_{lc}$ =	87 days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087 centipoise	
Liq. Density =	0.99823 g/cm^3	
apparent dens. =	0.73 g/cm^3	Apparent density of the GAC (<1)
porosity =	0.41	Bed porosity (about 0.4)
C_0 =	2.2 mg/L	
Column ID =	0.8 cm	

COLUMN CALCULATIONS:

D_g =	63565	
Max. GAC Rad.=	0.008 cm	1% of column diameter
Re_{lc} =	10.58	

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	**80x100**	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	**0.00822**	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	3.00	1.50	**1.00**	1.00
X (See Note 1)	0	0	0	0	0	0	**0**	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	5.6	**3.7**	4.9
Q_{sc} (mL/min)	62.51	11.82	5.91	80.61	22.86	11.43	**7.62**	9.94
GAC $Mass_{sc}$ (g)	14.86	2.81	1.40	11.52	3.27	1.63	**1.09**	0.83
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.55	0.55	0.55	0.33	0.33	0.33	**0.33**	0.20
length (cm)	68.7	13.0	6.5	53.3	15.1	7.6	**5.0**	3.9
t^*_{sc} (min)	14441	14441	14441	8684	8684	8684	**8684**	5101
t^*_{sc} (hr)	241	241	241	145	145	145	**145**	85
Qt^*_{sc} (L)	903	171	85	700	198	99	**66**	51
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	56.4	**56.4**	33.1

Equations used in spreadsheet calculations:

Re_{lc} = 2 * GAC Rad. * Vs_{lc} * Liq. Dens./(Visc. * porosity)

V_{sc} = V_{lc} * (GAC $Rad._{lc}$/GAC $Rad._{sc}$) * (Re_{sc}/Re_{lc})

Q_{sc} = V_{sc} * A

GAC $Mass_{sc}$ = $EBCT_{lc}$ * (GAC $Rad._{sc}$/GAC $Rad._{lc}$)$^{(2-X)}$ * Q_{sc} * bulk $dens._{lc}$

$EBCT_{sc}$ = $EBCT_{lc}$ * (GAC $Rad._{sc}$/GAC $Rad._{lc}$)$^{(2-X)}$

length = V_{sc} * $EBCT_{sc}$

t^*_{sc} = (porosity) * (Dg + 1) * $EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for service life versus EBCT tests using Calgon F400 GAC for EBCT = 16.4 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	$mg/g(L/mg)^{1/n}$	
1/n =	0.344		
V_{lc} =	6.47	or	0.439 cm/sec.
$(EBCT)_{lc}$ =	16.4	min	
$(GAC\ mesh)_{lc}$ =	12x40		Calgon F400
$(GAC\ rad.)_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data
$(bulk\ dens.)_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)
$(serv.\ life)_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.73	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.41		Bed porosity (about 0.4)
C_o =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	63565		
Max. GAC Rad. =	0.008	cm	1% of column diameter
Re_{lc} =	10.58		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	**80x100**	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	**0.00822**	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	3.00	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	5.6	3.7	4.9
Q_{sc} (mL/min)	62.51	11.82	5.91	80.61	22.36	11.43	7.62	9.94
GAC $Mass_{sc}$ (g)	19.81	3.75	1.87	15.36	4.36	2.18	1.45	1.11
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.74	0.74	0.74	0.44	0.44	0.44	0.44	0.26
length (cm)	91.7	17.3	8.7	71.1	20.2	10.1	6.7	5.1
t^*_{sc} (min)	19255	19255	19255	11579	11579	11579	11579	6802
t^*_{sc} (hr)	321	321	321	193	193	193	193	113
Qt^*_{sc} (L)	1204	228	114	933	265	132	88	68
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	56.4	56.4	33.1

Equations used in spreadsheet calculations:

$Re_{sc} = 2 \cdot GAC\ Rad. \cdot Vs_{sc} \cdot Liq.\ Dens./(Visc. \cdot porosity)$

$V_{sc} = V_{lc} \cdot (GAC\ Rad._{sc}/GAC\ Rad._{lc}) \cdot (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} \cdot A$

$GAC\ Mass_{sc} = EBCT_{lc} \cdot (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)} \cdot Q_{sc} \cdot bulk\ dens._{lc}$

$EBCT_{sc} = EBCT_{lc} \cdot (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)}$

$length = V_{sc} \cdot EBCT_{sc}$

$t^*_{sc} = (porosity) \cdot (Dg + 1) \cdot EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. *The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.* A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size. These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for service life versus EBCT tests using Northwestern LB-830 GAC for EBCT = 8.2 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	111.8	mg/g(L/mg)$^{1/n}$	
1/n =	0.34		
V_{lc} =	6.47	gpm/ft^2	or 0.439 cm /sec.
$(EBCT)_{lc}$ =	8.2	min	
$(GAC\ mesh)_{lc}$ =	8x30		NWC LB-830
$(GAC\ rad.)_{lc}$ =	0.0675	cm	GAC particle radius from manufacturer's data
$(bulk\ dens.)_{lc}$ =	0.47	g/cm^3	Bulk GAC density (0.4-0.5)
$(serv.\ life)_{lc}$ =		days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.75	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.37		Bed porosity (about 0.4)
C_0 =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	83646		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	15.72		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	**80x100**	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	**0.00822**	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	15.72	2.00	1.00	15.72	**2.50**	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	**0**	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	41.2	5.2	2.6	53.1	**8.4**	5.1	3.4	4.4
Q_{sc} (mL/min)	84.39	10.73	5.37	108.82	**17.30**	10.38	6.92	9.03
$GAC\ Mass_{sc}$ (g)	8.02	1.02	0.51	6.22	**0.99**	0.59	0.40	0.30
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.20	0.20	0.20	0.12	**0.12**	0.12	0.12	0.07
length (cm)	33.9	4.3	2.2	26.3	**4.2**	2.5	1.7	1.3
t^*_{sc} (min)	6315	6315	6315	3797	3797	3797	3797	2231
t^*_{sc} (hr)	105	105	105	63	**63**	63	63	37
Qt^*_{sc} (L)	533	68	34	413	**66**	39	26	20
$Serv.\ life_{sc}$ (hr)	0.0	0.0	0.0	0.0	**0.0**	0.0	0.0	0.0

Equations used in spreadsheet calculations:

$Re_{lc} = 2 * GAC\ Rad. * Vs_{lc} * Liq.\ Dens./(Visc. * porosity)$

$V_{sc} = V_{lc} * (GAC\ Rad._{lc}/GAC\ Rad_{sc}) * (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} * A$

$GAC\ Mass_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)} * Q_{sc} * bulk\ dens._{lc}$

$EBCT_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)}$

$length = V_{sc} * EBCT_{sc}$

$t^*_{sc} = (porosity) * (Dg + 1) * EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

$Serv.\ life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
   A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
   These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for service life versus EBCT tests using Northwestern LB-830 GAC for EBCT = 12.3 min.

RSSCT Design Spreadsheet
Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)
Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	111.8	mg/g(L/mg)$^{1/n}$	
1/n =	0.34		
V_{lc} =	6.47	gpm/ft^2	or 0.439 cm /sec.
$(EBCT)_{lc}$ =	12.3	min	
$(\text{GAC mesh})_{lc}$ =	8x30		NWC LB-830
$(\text{GAC rad.})_{lc}$ =	0.0675	cm	GAC particle radius from manufacturer's data
$(\text{bulk dens.})_{lc}$ =	0.47	g/cm^3	Bulk GAC density (0.4-0.5)
$(\text{serv. life})_{lc}$ =		days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.75	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.37		Bed porosity (about 0.4)
C_o =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	83646		
Max. GAC Rad. =	0.008	cm	1% of column diameter
Re_{lc} =	15.72		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	15.72	2.00	1.00	15.72	2.00	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	41.2	5.2	2.6	53.1	6.8	5.1	3.4	4.4
Q_{sc} (mL/min)	84.39	10.73	5.37	108.82	13.84	10.38	6.92	9.03
GAC Mass_{sc} (g)	12.03	1.53	0.77	9.33	1.19	0.89	0.59	0.45
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.30	0.30	0.30	0.18	0.18	0.18	0.18	0.11
length (cm)	50.9	6.5	3.2	39.5	5.0	3.8	2.5	1.9
t^*_{sc} (min)	9472	9472	9472	5696	5696	5696	5696	3346
t^*_{sc} (hr)	158	158	158	95	95	95	95	56
Qt^*_{sc} (L)	799	102	51	620	79	59	39	30
Serv. life_{sc} (hr)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Equations used in spreadsheet calculations:

$Re_{lc} = 2 * \text{GAC Rad.} * Vs_{lc} * \text{Liq. Dens.}/(\text{Visc.} * \text{porosity})$

$V_{sc} = V_{lc} * (\text{GAC Rad.}_{lc} / \text{GAC Rad.}_{sc}) * (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} * A$

$\text{GAC Mass}_{sc} = EBCT_{lc} * (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)} * Q_{sc} * \text{bulk dens.}_{lc}$

$EBCT_{sc} = EBCT_{lc} * (\text{GAC Rad.}_{sc}/\text{GAC Rad.}_{lc})^{(2-X)}$

$\text{length} = V_{sc} * EBCT_{sc}$

$t^*_{sc} = (\text{porosity}) * (Dg + 1) * EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. life_{sc} = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used. A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size. These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for service life versus EBCT tests using Northwestern LB-830 GAC for EBCT = 16.4 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	111.8	mg/g(L/mg)$^{1/n}$	
1/n =	0.34		
V_{lc} =	6.47	gpm/ft^2	or 0.439 cm/sec.
$(EBCT)_{lc}$ =	16.4	min	
$(\text{GAC mesh})_{lc}$ =	8x30		NWC LB-830
$(\text{GAC rad.})_{lc}$ =	0.0675	cm	GAC particle radius from manufacturer's data
$(\text{bulk dens.})_{lc}$ =	0.47	g/cm^3	Bulk GAC density (0.4-0.5)
$(\text{serv. life})_{lc}$ =		days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.75	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.37		Bed porosity (about 0.4)
C_o =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	83646		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	15.72		

INPUTS:								
GAC mesh sizes	60x80	60x30	60x80	80x100	80x100	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	15.72	2.00	1.00	15.72	2.00	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	41.2	5.2	2.6	53.1	6.8	5.1	3.4	4.4
Q_{sc} (mL/min)	84.39	10.73	5.37	108.82	13.84	10.38	6.92	9.03
GAC $Mass_{sc}$ (g)	16.04	2.04	1.02	12.44	1.58	1.19	0.79	0.61
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.40	0.40	0.40	0.24	0.24	0.24	0.24	0.14
length (cm)	67.9	8.6	4.3	52.7	6.7	5.0	3.3	2.6
t^*_{sc} (min)	12630	12630	12630	7595	7595	7595	7595	4461
t^*_{sc} (hr)	210	210	210	127	127	127	127	74
Qt^*_{sc} (L)	1066	136	68	827	105	79	53	40
Serv. $life_{sc}$ (hr)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Equations used in spreadsheet calculations:

Re_{lc} = 2 • GAC Rad. • Vs_{lc} • Liq. Dens./(Visc. • porosity)

V_{sc} = V_{lc} • (GAC $Rad._{lc}$ /GAC $Rad._{sc}$) • (Re_{sc}/Re_{lc})

Q_{sc} = V_{sc} • A

GAC $Mass_{sc}$ = $EBCT_{lc}$ • (GAC $Rad._{sc}$/GAC $Rad._{lc}$)$^{(2-X)}$ • Q_{sc} • bulk $dens._{lc}$

$EBCT_{sc}$ = $EBCT_{lc}$ • (GAC $Rad._{sc}$/GAC $Rad._{lc}$)$^{(2-X)}$

length = V_{sc} • $EBCT_{sc}$

t^*_{sc} = (porosity) • (Dg + 1) • $EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or proportional diffusivity assumption is to be used. A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size. These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for variable concentration tests using Calgon F400 GAC for EBCT = 8.2 min.

RSSCT Design Spreadsheet
Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)
Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	$mg/g(L/mg)^{1/n}$	
1/n =	0.344		
V_{lc} =	6.47		or 0.439 cm /sec.
$(EBCT)_{lc}$ =	8.2	min	
$(GAC\ mesh)_{lc}$ =	12x40		Calgon F400
$(GAC\ rad.)_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data
$(bulk\ dens.)_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)
$(serv.\ life)_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.73	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.41		Bed porosity (about 0.4)
C_o =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	63565		
Max. GAC Rad. =	0.008	cm	1% of column diameter
Re_{lc} =	10.58		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	**80x100**	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	**0.00822**	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	3.00	**1.50**	1.00	1.00
X (See Note 1)	0	0	0	0	0	**0**	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	**5.6**	3.7	4.9
Q_{sc} (mL/min)	62.51	11.82	5.91	80.61	22.86	**11.43**	7.62	9.94
GAC $Mass_{sc}$ (g)	9.91	1.87	0.94	7.68	2.18	**1.09**	0.73	0.56
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.37	0.37	0.37	0.22	0.22	**0.22**	0.22	0.13
length (cm)	45.8	8.7	4.3	35.5	10.1	**5.0**	3.4	2.6
t^*_{sc} (min)	9627	9627	9627	5789	5789	**5789**	5789	3401
t^*_{sc} (hr)	160	160	160	96	96	**96**	96	57
Qt^*_{sc} (L)	602	114	57	467	132	**66**	44	34
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	**56.4**	56.4	33.1

Equations used in spreadsheet calculations:

$Re_{lc} = 2 * GAC\ Rad. * Vs_{lc} * Liq.\ Dens./(Visc. * porosity)$

$V_{sc} = V_{lc} * (GAC\ Rad._{lc} / GAC\ Rad_{sc}) * (Re_{sc} / Re_{lc})$

$Q_{sc} = V_{sc} * A$

GAC $Mass_{sc} = EBCT_{lc} * (GAC\ Rad._{sc} / GAC\ Rad._{lc})^{(2-X)} * Q_{sc} * bulk\ dens._{lc}$

$EBCT_{sc} = EBCT_{lc} * (GAC\ Rad._{sc} / GAC\ Rad._{lc})^{(2-X)}$

$length = V_{sc} * EBCT_{sc}$

$t^*_{sc} = (porosity) * (Dg + 1) * EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used. A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size. These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for variable concentration tests using Calgon F400 GAC for EBCT = 12.3 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	mg/g(L/mg)$^{1/n}$	
1/n =	0.344		
V$_{lc}$ =	6.47		or 0.439 cm /sec.
(EBCT)$_{lc}$ =	12.3	min	
(GAC mesh)$_{lc}$ =	12x40		Calgon F400
(GAC rad.)$_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data
(bulk dens.)$_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)
(serv. life)$_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.73	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.41		Bed porosity (about 0.4)
C$_o$ =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D$_g$ =	63565		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re$_{lc}$ =	10.58		

INPUTS:

GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	0.00822	0.0063
Re$_{sc}$ (1 to Re$_{lc}$)	10.58	2.00	1.00	10.58	3.00	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V$_{sc}$ (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	5.6	3.7	4.9
Q$_{sc}$ (mL/min)	62.51	11.82	5.91	80.61	22.86	11.43	7.62	9.94
GAC Mass$_{sc}$ (g)	14.86	2.81	1.40	11.52	3.27	1.63	1.09	0.83
ADDITIONAL OUTPUT CALCULATIONS:								
EBCT$_{sc}$ (min)	0.55	0.55	0.55	0.33	0.33	0.33	0.33	0.20
length (cm)	68.7	13.0	6.5	53.3	15.1	7.6	5.0	3.9
t$^*_{sc}$ (min)	14441	14441	14441	8684	8684	8684	8684	5101
t$^*_{sc}$ (hr)	241	241	241	145	145	145	145	85
Qt$^*_{sc}$ (L)	903	171	85	700	198	99	66	51
Serv. life$_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	56.4	56.4	33.1

Equations used in spreadsheet calculations:

Re$_{sc}$ = 2 * GAC Rad. * Vs$_{lc}$ * Liq. Dens./(Visc. * porosity)

V$_{sc}$ = V$_{lc}$ * (GAC Rad.$_{lc}$ /GAC Rad.$_{sc}$) * (Re$_{sc}$/Re$_{lc}$)

Q$_{sc}$ = V$_{sc}$ * A

GAC Mass$_{sc}$ = EBCT$_{lc}$ * (GAC Rad.$_{sc}$/GAC Rad.$_{lc}$)$^{(2-X)}$ * Q$_{sc}$ * bulk dens.$_{lc}$

EBCT$_{sc}$ = EBCT$_{lc}$ * (GAC Rad.$_{sc}$/GAC Rad.$_{lc}$)$^{(2-X)}$

length = V$_{sc}$ * EBCT$_{sc}$

t$^*_{sc}$ = (porosity) * (Dg + 1) * EBCT$_{sc}$

(Qt*)$_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. life$_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
   A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
   These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for variable concentration tests using Calgon F400 GAC for EBCT = 8.2 min.

RSSCT Design Spreadsheet
Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)
Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	$mg/g(L/mg)^{1/n}$		
1/n =	0.344			
V_{lc} =	6.47		or	0.439 cm /sec.
$(EBCT)_{lc}$ =	8.2	min		
$(GAC\ mesh)_{lc}$ =	12x40		Calgon F400	
$(GAC\ rad.)_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data	
$(bulk\ dens.)_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)	
$(serv.\ life)_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)	
Viscosity =	1.0087	centipoise		
Liq. Density =	0.99823	g/cm^3		
apparent dens. =	0.73	g/cm^3	Apparent density of the GAC (<1)	
porosity =	0.41		Bed porosity (about 0.4)	
C_0 =	4.5	mg/L		
Column ID =	0.8	cm		

COLUMN CALCULATIONS:

D_g =	39750		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	10.58		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	3.00	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	5.6	3.7	4.9
Q_{sc} (mL/min)	62.51	11.82	5.91	80.61	22.86	11.43	7.62	9.94
GAC $Mass_{sc}$ (g)	9.91	1.87	0.94	7.68	2.18	1.09	0.73	0.56
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.37	0.37	0.37	0.22	0.22	0.22	0.22	0.13
length (cm)	45.8	8.7	4.3	35.5	10.1	5.0	3.4	2.6
t^*_{sc} (min)	6020	6020	6020	3620	3620	3620	3620	2127
t^*_{sc} (hr)	100	100	100	60	60	60	60	35
Qt^*_{sc} (L)	376	71	36	292	83	41	28	21
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	56.4	56.4	33.1

Equations used in spreadsheet calculations:

$Re_{lc} = 2 * GAC\ Rad. * Vs_{lc} * Liq.\ Dens./(Visc. * porosity)$

$V_{sc} = V_{lc} * (GAC\ Rad._{lc}/GAC\ Rad._{sc}) * (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} * A$

$GAC\ Mass_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)} * Q_{sc} * bulk\ dens._{lc}$

$EBCT_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)}$

$length = V_{sc} * EBCT_{sc}$

$t^*_{sc} = (porosity) * (Dg + 1) * EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used. A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size. These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for variable concentration tests using Calgon F400 GAC for EBCT = 12.3 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	$mg/g(L/mg)^{1/n}$		
1/n =	0.344			
V_{lc} =	6.47		or	0.439 cm /sec.
$(EBCT)_{lc}$ =	12.3	min		
$(GAC\ mesh)_{lc}$ =	12x40		Calgon F400	
$(GAC\ rad.)_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data	
$(bulk\ dens.)_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)	
$(serv.\ life)_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)	
Viscosity =	1.0087	centipoise		
Liq. Density =	0.99823	g/cm^3		
apparent dens. =	0.73	g/cm^3	Apparent density of the GAC (<1)	
porosity =	0.41		Bed porosity (about 0.4)	
C_o =	4.5	mg/L		
Column ID =	0.8	cm		

COLUMN CALCULATIONS:

D_g =	39750		
Max. GAC Rad.=	0.008	cm	1% of column diameter
Re_{lc} =	10.58		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	80x100	**80x100**	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	0.00822	**0.00822**	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	3.00	1.50	**1.00**	1.00
X (See Note 1)	0	0	0	0	0	0	**0**	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	5.6	**3.7**	4.9
Q_{sc} (mL/min)	62.51	11.82	5.91	80.61	22.36	11.43	**7.62**	9.94
GAC $Mass_{sc}$ (g)	14.86	2.81	1.40	11.52	3.27	1.63	**1.09**	0.83
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.55	0.55	0.55	0.33	0.33	0.33	**0.33**	0.20
length (cm)	68.7	13.0	6.5	53.3	15.1	7.6	**5.0**	3.9
t^*_{sc} (min)	9031	9031	9031	5431	5431	5431	**5431**	3190
t^*_{sc} (hr)	151	151	151	91	91	91	**91**	53
Qt^*_{sc} (L)	565	107	53	438	124	62	**41**	32
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	56.4	**56.4**	33.1

Equations used in spreadsheet calculations:

$Re_{lc} = 2 * GAC\ Rad. * Vs_{lc} * Liq.\ Dens./(Visc. * porosity)$

$V_{sc} = V_{lc} * (GAC\ Rad._{lc}/GAC\ Rad_{sc}) * (Re_{sc}/Re_{lc})$

$Q_{sc} = V_{sc} * A$

$GAC\ Mass_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad_{lc})^{(2-X)} * Q_{sc} * bulk\ dens._{lc}$

$EBCT_{sc} = EBCT_{lc} * (GAC\ Rad._{sc}/GAC\ Rad._{lc})^{(2-X)}$

$length = V_{sc} * EBCT_{sc}$

$t^*_{sc} = (porosity) * (Dg + 1) * EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
   A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
   These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

Design for pre-loading tests using Calgon F400 GAC for EBCT = 8.2 min.

RSSCT Design Spreadsheet

Valid for Both Constant and Proportional Diffusivity Assumptions (X = 0 and 1, respectively)

Created by B.I. Dvorak and G.E. Speitel Jr. (May 1992, June 1996)

INPUTS:

K =	101.9	$mg/g(L/mg)^{1/n}$	
1/n =	0.344		
V_{lc} =	6.47		or 0.439 cm/sec.
$(EBCT)_{lc}$ =	8.2	min	
$(GAC\ mesh)_{lc}$ =	12x40		**Calgon F400**
$(GAC\ rad.)_{lc}$ =	0.05	cm	GAC particle radius from manufacturer's data
$(bulk\ dens.)_{lc}$ =	0.43	g/cm^3	Bulk GAC density (0.4-0.5)
$(serv.\ life)_{lc}$ =	87	days	Service life of large column to be simulated by RSSCT (optional)
Viscosity =	1.0087	centipoise	
Liq. Density =	0.99823	g/cm^3	
apparent dens. =	0.73	g/cm^3	Apparent density of the GAC (<1)
porosity =	0.41		Bed porosity (about 0.4)
C_o =	2.2	mg/L	
Column ID =	0.8	cm	

COLUMN CALCULATIONS:

D_g =	63565		
Max. GAC Rad. =	0.008	cm	1% of column diameter
Re_{lc} =	10.58		

INPUTS:								
GAC mesh sizes	60x80	60x80	60x80	80x100	80x100	**80x100**	80x100	100x140
GAC rad. (cm)	0.0106	0.0106	0.0106	0.00822	0.00822	**0.00822**	0.00822	0.0063
Re_{sc} (1 to Re_{lc})	10.58	2.00	1.00	10.58	3.00	1.50	1.00	1.00
X (See Note 1)	0	0	0	0	0	0	0	0
OUTPUTS:								
V_{sc} (gpm/ft^2)	30.5	5.8	2.9	39.4	11.2	5.6	3.7	4.9
Q_{sc} (mL/min)	62.51	11.82	5.91	80.61	22.36	11.43	7.62	9.94
GAC $Mass_{sc}$ (g)	9.91	1.87	0.94	7.68	2.18	1.09	0.73	0.56
ADDITIONAL OUTPUT CALCULATIONS:								
$EBCT_{sc}$ (min)	0.37	0.37	0.37	0.22	0.22	0.22	0.22	0.13
length (cm)	45.8	8.7	4.3	35.5	10.1	5.0	3.4	2.6
t^*_{sc} (min)	9627	9627	9627	5789	5789	5789	5789	3401
t^*_{sc} (hr)	160	160	160	96	96	96	96	57
Qt^*_{sc} (L)	602	114	57	467	132	66	44	34
Serv. $life_{sc}$ (hr)	93.8	93.8	93.8	56.4	56.4	56.4	56.4	33.1

Equations used in spreadsheet calculations:

Re_{lc} = 2 * GAC Rad. * Vs_{lc} * Liq. Dens./(Visc. * porosity)

$V_{sc} = V_{lc}$ * (GAC $Rad._{lc}$ /GAC $Rad._{sc}$) * (Re_{sc}/Re_{lc})

$Q_{sc} = V_{sc}$ * A

GAC $Mass_{sc}$ = $EBCT_{lc}$ * (GAC $Rad._{sc}$/GAC $Rad._{lc})^{(2-X)}$ * Q_{sc} * bulk $dens._{lc}$

$EBCT_{sc}$ = $EBCT_{lc}$ * (GAC $Rad._{sc}$/GAC $Rad._{lc})^{(2-X)}$

length = V_{sc} * $EBCT_{sc}$

t^*_{sc} = (porosity) * (Dg + 1) * $EBCT_{sc}$

$(Qt^*)_{sc}$ = volume of water for complete breakthrough based on single component equilibrium

Serv. $life_{sc}$ = RSSCT run time to achieve user-selected large scale service life

NOTES:

1. The X value denotes if the constant diffusivity or propotional diffusivity assumption is to be used.
   A X value of "0" denotes constant diffusivity and a X value of "1" proportional diffusivity.

2. Below are data for six common sieve sizes, with the log mean particle radius (cm) below the sieve size.
   These values can be copied into the RSSCT design cells (b29 to g30) when needed.

GAC mesh sizes	30x40	40x50	50x60	60x80	80x100	100x140
GAC rad. (cm)	0.0245	0.0177	0.0136	0.0106	0.00822	0.0063

3. This design method is based upon research performed at Michigan Tech. University by John Crittenden et al., and laboratory work performed at the Univerisity of Texas at Austin by the designers of this spreadsheet. The Crittenden research is outlined in the article "Predicting GAC Performace With Rapid Small-Scale Column Tests" by Crittenden et al., AWWA Journal, Jan. 1991, pp. 77-87.

APPENDIX B

GAC SCREENING TEST DATA

Experiment Number:	F3-1
Carbon:	F300
HMX (μg/L):	309
RDX (μg/L):	2364
EBCT LC (min):	4.1
EBCT SC (min):	0.05

Re:	5.5
Mass Carbon (g):	0.98
RSSCT Time (hr):	24
RSSCT Flowrate (mL/min):	43.14
Volume of Water (L):	63

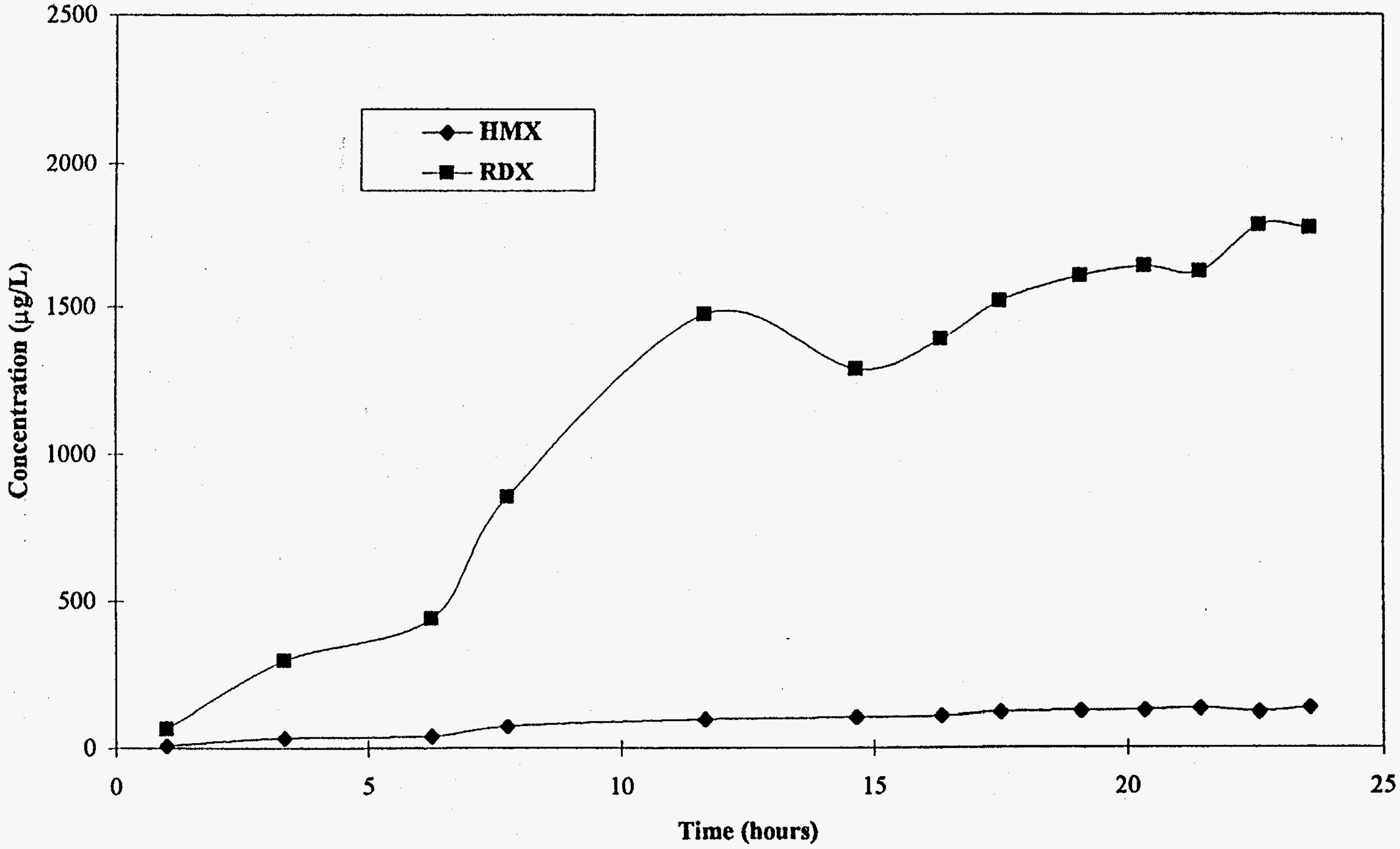
Experimental Results

Time (hr)	HMX (μg/L)	RDX (μg/L)
1.00	8	64
3.33	33	296
6.25	41	441
7.75	74	857
11.67	97	1476
14.67	103	1289
16.33	107	1392
17.50	120	1520
19.08	124	1606
20.33	126	1638
21.42	134	1619
22.58	119	1782
23.58	135	1772

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
82	8	64
273	33	296
513	41	441
636	74	857
957	97	1476
1203	103	1289
1339	107	1392
1435	120	1520
1565	124	1606
1667	126	1638
1756	134	1619
1852	119	1782
1934	135	1772

Experiment F3-1



Experiment Number:	F4-1
Carbon:	F400
HMX (µg/L):	320
RDX (µg/L):	2340
EBCT LC (min):	4.1
EBCT SC (min):	0.11

Re:	3
Mass Carbon (g):	1.09
RSSCT Time (hr):	48
RSSCT Flowrate (mL/min):	22.86
Volume of Water (L):	66

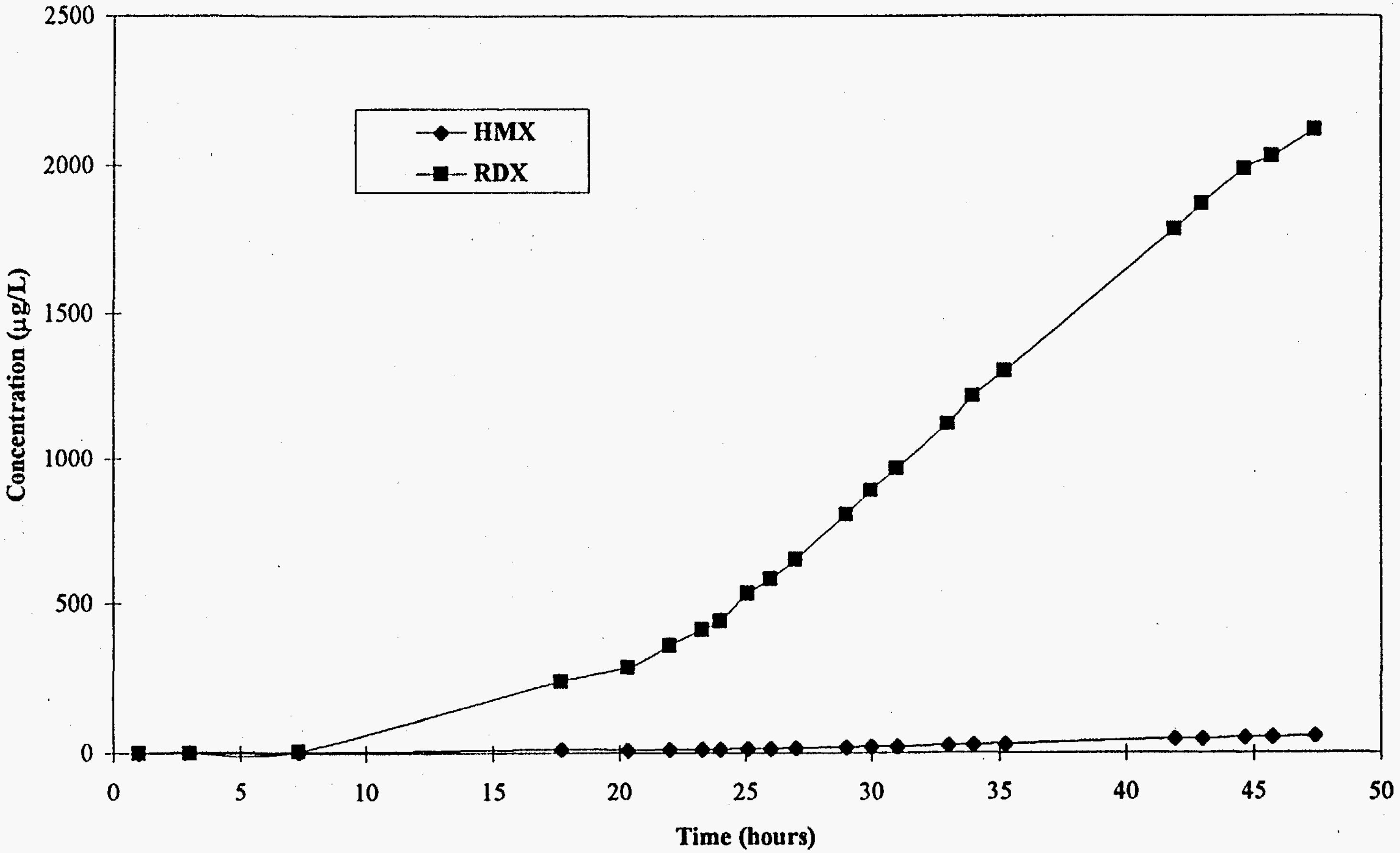
Experimental Results

Time (hr)	HMX	RDX
1.00	1	0
3.00	4	0
7.33	4	5
17.70	12	240
20.33	10	288
22.00	12	361
23.30	13	415
24.02	13	444
25.12	14	536
26.02	14	584
27.02	16	651
29.00	18	805
30.00	21	891
31.00	22	968
33.00	26	1124
34.00	28	1220
35.25	30	1308
41.92	46	1783
43.00	47	1868
44.67	51	1986
45.75	53	2031
47.42	56	2118

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
2	1	0
5	4	0
11	4	5
27	12	240
32	10	288
34	12	361
36	13	415
37	13	444
39	14	536
40	14	584
42	16	651
45	18	805
47	21	891
48	22	968
51	26	1124
53	28	1220
55	30	1308
65	46	1783
67	47	1868
69	51	1986
71	53	2031
74	56	2118

Experiment F4-1



Experiment Number: H3-1
Carbon: H3000
HMX (μg/L): 307
RDX (μg/L): 2392
EBCT LC (min): 4.1
EBCT SC (min): 0.08

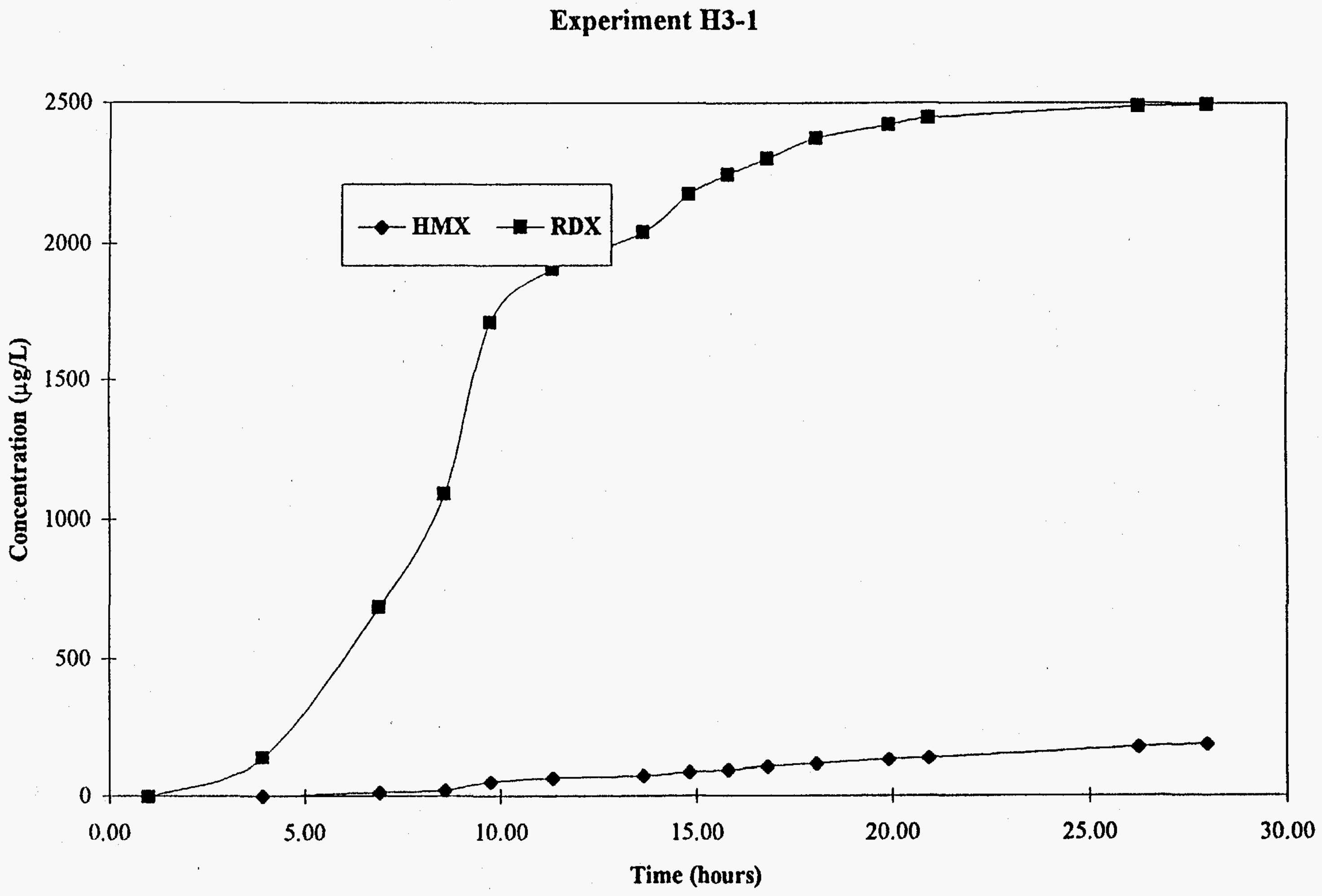
Re: 4
Mass Carbon (g): 1.01
RSSCT Time (hr): 28
RSSCT Flowrate (mL/min): 35.51
Volume of Water (L): 60

Experimental Results

Time (hr)	HMX	RDX
1.00	1	-4
3.92	1	139
6.92	13	685
8.58	22	1089
9.75	51	1708
11.33	65	1904
13.67	74	2040
14.83	87	2173
15.83	96	2244
16.83	108	2301
18.08	119	2374
19.92	133	2422
20.92	139	2448
26.25	178	2488
28.00	190	2493

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
2	1	-4
8	1	139
15	13	685
18	22	1089
21	51	1708
24	65	1904
29	74	2040
32	87	2173
34	96	2244
36	108	2301
39	119	2374
43	133	2422
45	139	2448
56	178	2488
60	190	2493


Experiment H3-1
HMX
RDX
Concentration (µg/L)
2500
2000
1500
1000
500
0
0.00
5.00
10.00
15.00
20.00
25.00
30.00
Time (hours)

Experiment Number:	H4-1
Carbon:	H4000
HMX (μg/L):	316
RDX (μg/L):	2388
EBCT LC (min):	4.1
EBCT SC (min):	0.11

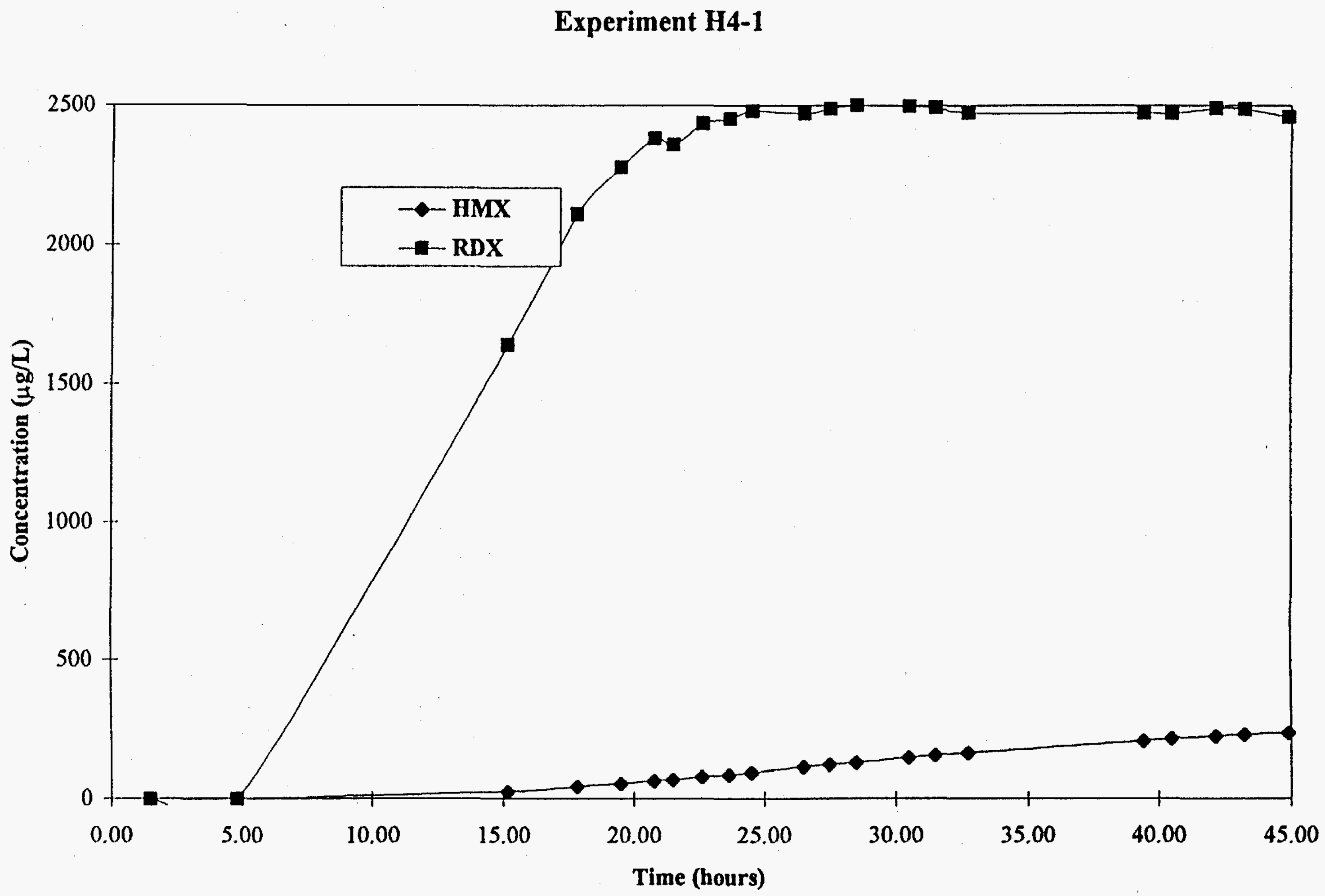
Re:	3
Mass Carbon (g):	1.09
RSSCT Time (hr):	42
RSSCT Flowrate (mL/min):	26.63
Volume of Water (L):	66

Experimental Results

Time (hr)	HMX	RDX
1.50	1	-4
4.83	1	-4
15.18	25	1636
17.83	45	2107
19.50	55	2273
20.78	66	2380
21.50	70	2356
22.62	81	2436
23.65	87	2452
24.50	94	2478
26.50	116	2471
27.50	124	2487
28.50	132	2499
30.50	150	2495
31.50	158	2492
32.75	166	2472
39.42	210	2473
40.50	219	2470
42.17	229	2490
43.25	234	2487
44.92	240	2457

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
56	1	-4
180	1	-4
566	25	1636
665	45	2107
727	55	2273
775	66	2380
801	70	2356
843	81	2436
882	87	2452
913	94	2478
988	116	2471
1025	124	2487
1062	132	2499
1137	150	2495
1174	158	2492
1221	166	2472
1469	210	2473
1510	219	2470
1572	229	2490
1612	234	2487
1674	240	2457


Experiment H4-1
HMX
RDX
Concentration (µg/L)
2500
2000
1500
1000
500
0
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
40.00
45.00
Time (hours)

Experiment Number: NWC-1
Carbon: NWC
HMX (µg/L): 298
RDX (µg/L): 2320
EBCT LC (min): 4.1
EBCT SC (min): 0.06

Re: 5
Mass Carbon (g): 0.99
RSSCT Time (hr): 32
RSSCT Flowrate (mL/min): 34.61
Volume of Water (L): 66

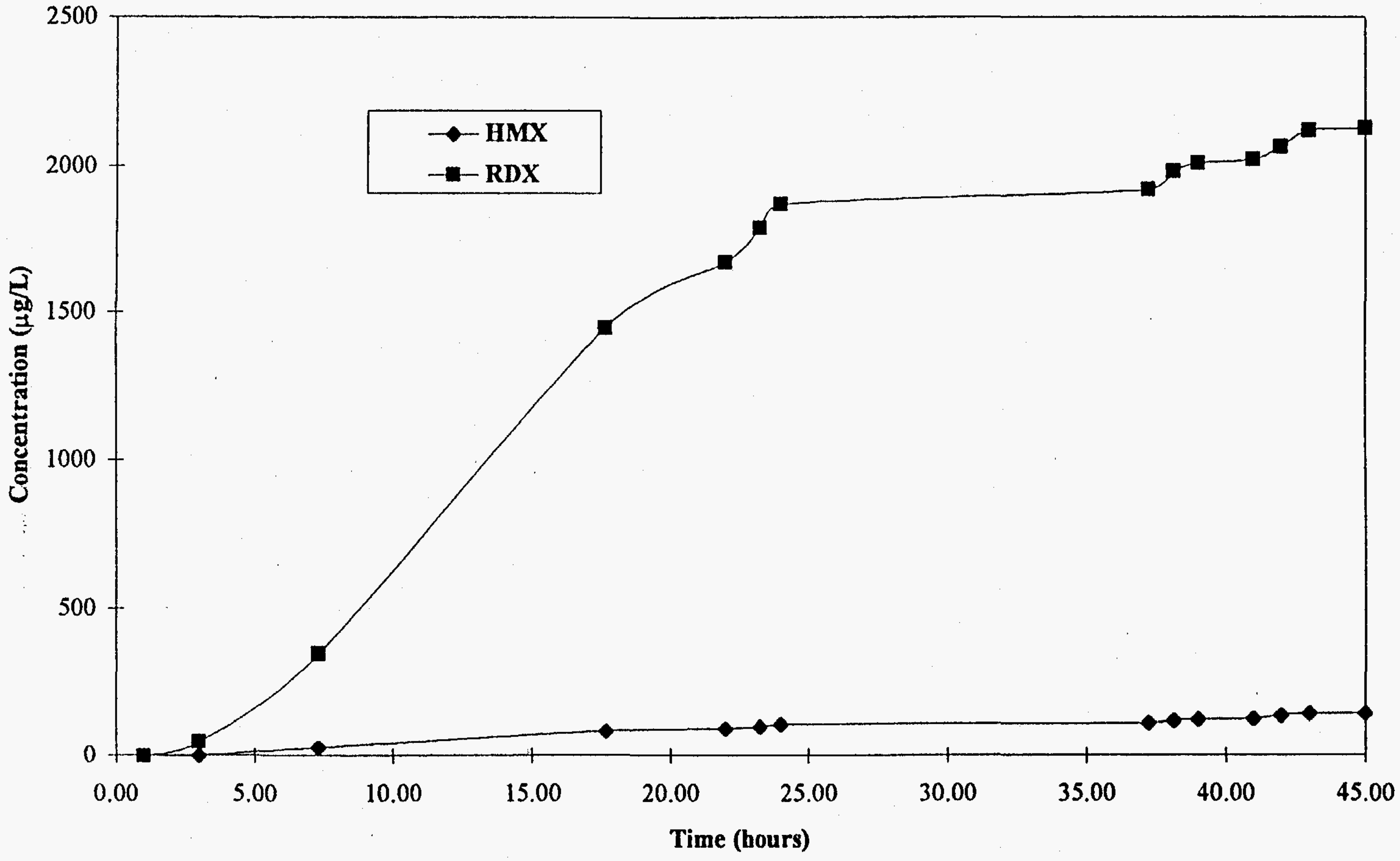
Experimental Results

Time (hr)	HMX	RDX
1.00	1	-4
3.00	1	47
7.33	27	347
17.68	84	1447
22.00	93	1670
23.27	99	1787
24.00	108	1871
37.25	112	1922
38.15	120	1984
39.02	124	2012
41.00	127	2024
42.00	136	2067
43.00	143	2120
45.00	144	2129

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
3	1	-4
9	1	47
21	27	347
50	84	1447
63	93	1670
66	99	1787
68	108	1871
106	112	1922
109	120	1984
111	124	2012
117	127	2024
120	136	2067
122	143	2120
128	144	2129

Experiment NWC-1



APPENDIX C

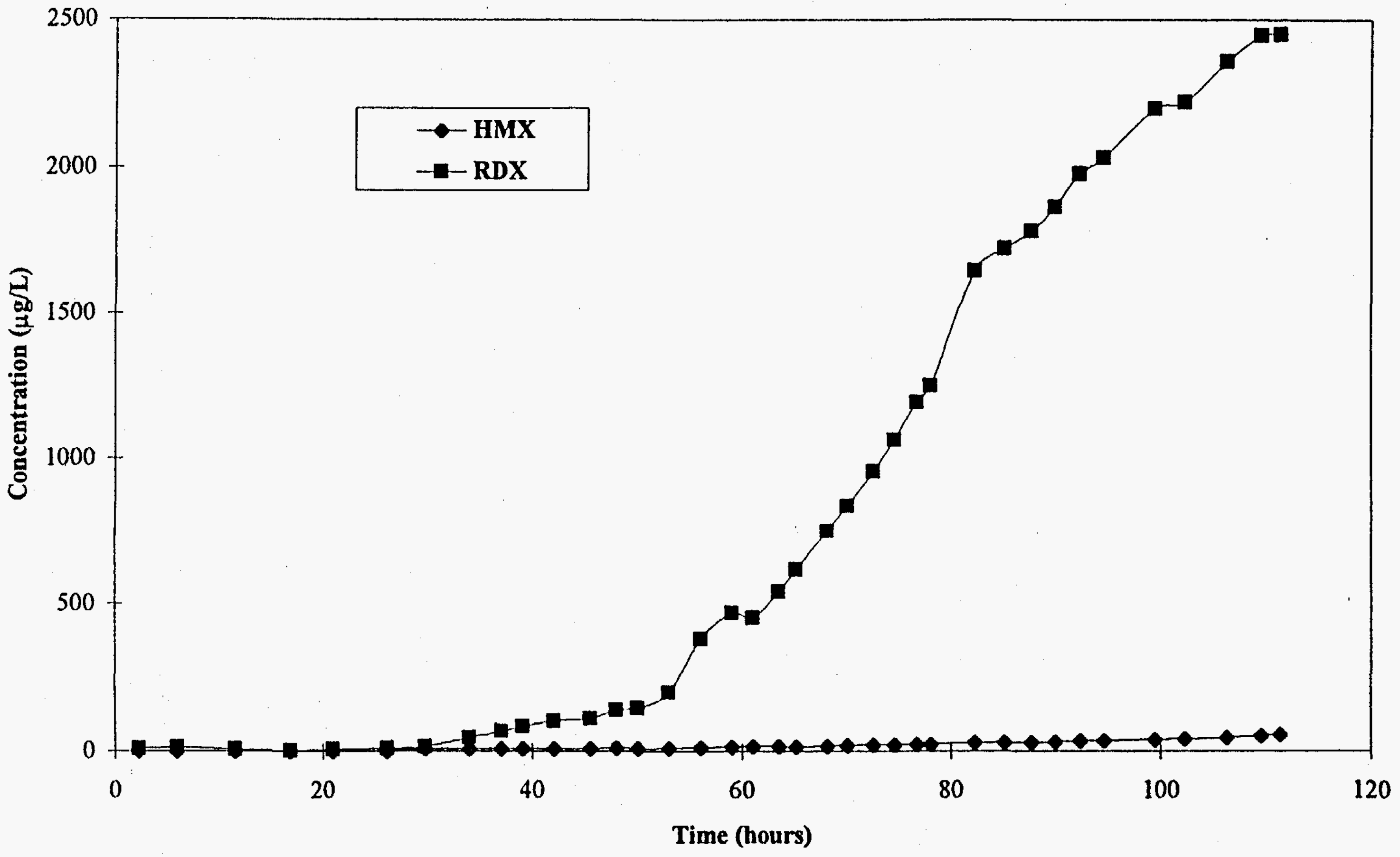
SERVICE LIFE VERSUS ECBT RSSCT DATA

Experiment Number:	F4-2
Carbon:	F400
HMX (mg/L):	309
RDX (mg/L):	2333
EBCT LC (min):	8.2
EBCT SC (min):	0.22

Re:	1.5
Mass Carbon (g):	1.09
RSSCT Time (hr):	96
RSSCT Flowrate (mL/min):	11.43
Volume of Water (L):	66

Experimental Results			Scaled Results		
Time (hr)	HMX (mg/L)	RDX (mg/L)	Time (d)	HMX: RSSCT	RDX: RSSCT
2.25		8	3		8
6.00		13	9		13
11.58		5	18		5
16.83		2	26		2
21.00		6	33		6
26.15		8	41		8
29.75	8	15	46	8	15
34.00	8	47	53	8	47
37.08	9	67	58	9	67
39.08	9	85	61	9	85
42.08	9	103	65	9	103
45.58	9	111	71	9	111
48.08	9	142	75	9	142
50.08	9	147	78	9	147
53.08	10	202	82	10	202
56.08	12	383	87	12	383
59.08	15	471	92	15	471
61.08	16	453	95	16	453
63.58	16	542	99	16	542
65.25	15	617	101	15	617
68.21	16	748	106	16	748
70.16	19	836	109	19	836
72.63	21	956	113	21	956
74.68	22	1066	116	22	1066
76.83	23	1197	119	23	1197
78.13	24	1255	121	24	1255
82.30	29	1646	128	29	1646
85.13	30	1723	132	30	1723
87.68	30	1781	136	30	1781
89.96	32	1865	140	32	1865
92.33	36	1978	143	36	1978
94.58	36	2033	147	36	2033
99.46	40	2199	154	40	2199
102.33	41	2223	159	41	2223
106.33	47	2360	165	47	2360
109.58	54	2448	170	54	2448
111.41	57	2452	173	57	2452

Experiment F4-2

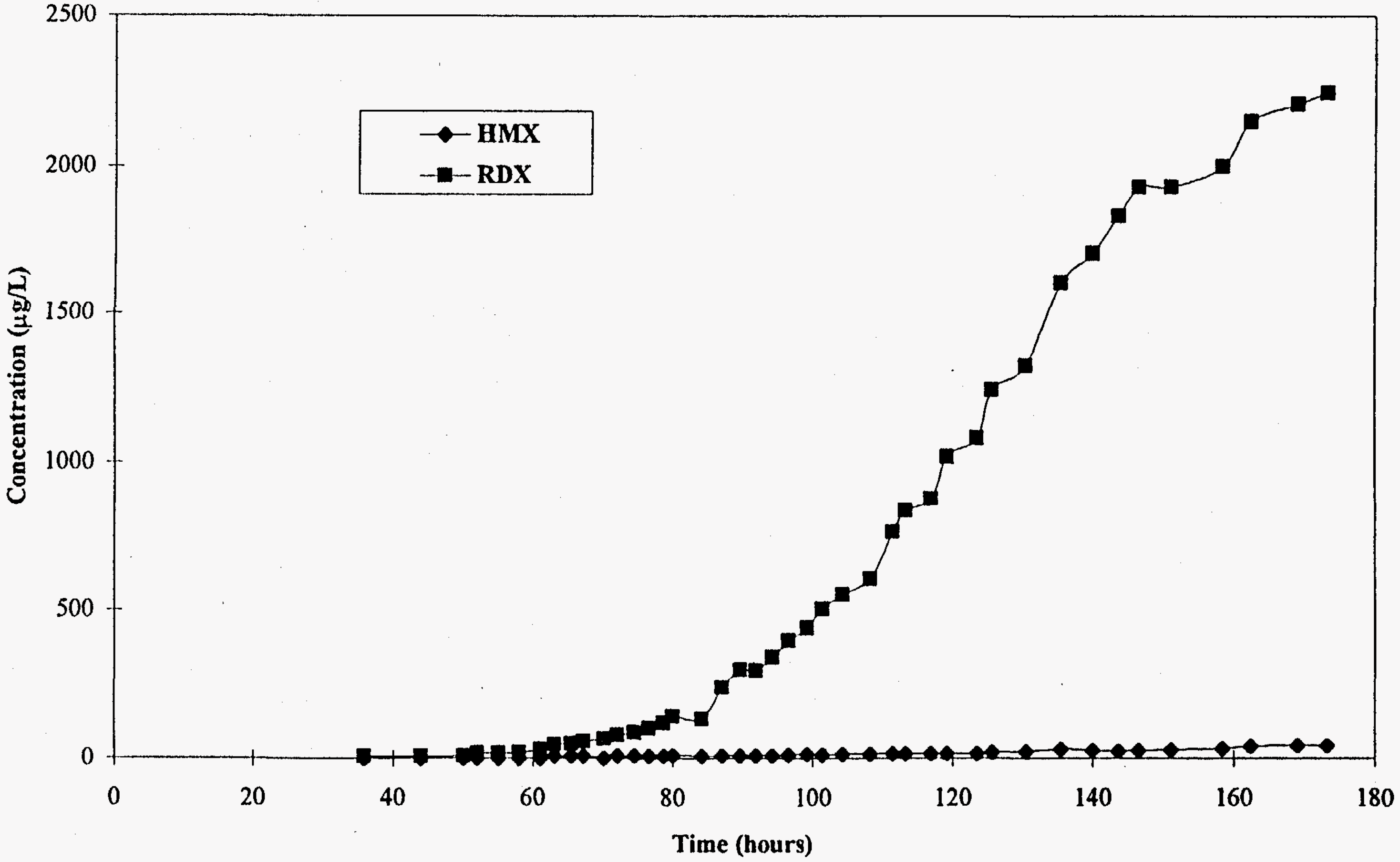


Experiment Number:	F4-3
Carbon:	F400
35455.75 HMX (mg/L):	302
RDX (mg/L):	2330
EBCT LC (min):	12.3
EBCT SC (min):	0.33

Re:	1
Mass Carbon (g):	1.09
RSSCT Time (hr):	145
RSSCT Flowrate (mL/min):	7.62
Volume of Water (L):	66

Experimental Results			**Scaled Results**		
Time (hr)	HMX (mg/L)	RDX (mg/L)	Time (d)	HMX: RSSCT	RDX: RSSCT
1.42		7	2		7
35.92		7	56		7
44.00		8	68		8
50.00		16	78		16
52.00		17	81		17
55.00		20	85		20
58.00		30	90		30
61.00	8	46	95	8	46
63.00	8	49	98	8	49
65.50	7	57	102	7	57
67.17		66	104	8	66
70.13	8	78	109	8	78
72.08	9	86	112	9	86
74.55	9	102	116	9	102
76.60	9	122	119	9	122
78.75	10	143	122	10	143
80.05	9	135	124	9	135
84.22	10	245	131	10	245
87.05	11	302	135	11	302
89.60	12	300	139	12	300
91.88	11	345	143	11	345
94.25	13	400	146	13	400
96.50	14	443	150	14	443
99.17	13	504	154	13	504
101.38	15	553	157	15	553
104.25	14	606	162	14	606
108.25	16	766	168	16	766
111.50	17	839	173	17	839
113.33	17	879	176	17	879
117.00	17	1023	182	17	1023
119.25	18	1083	185	18	1083
123.50	22	1244	192	22	1244
125.67	24	1326	195	24	1326
130.50	31	1606	203	31	1606
135.50	27	1704	210	27	1704
140.00	25	1831	217	25	1831
143.67	27	1930	223	27	1930
146.50	30	1930	228	30	1930
151.17	35	2000	235	35	2000
158.50	42	2151	246	42	2151
162.50	43	2209	252	43	2209
169.08	43	2245	263	43	2245
173.28	44	2264	269	44	2264

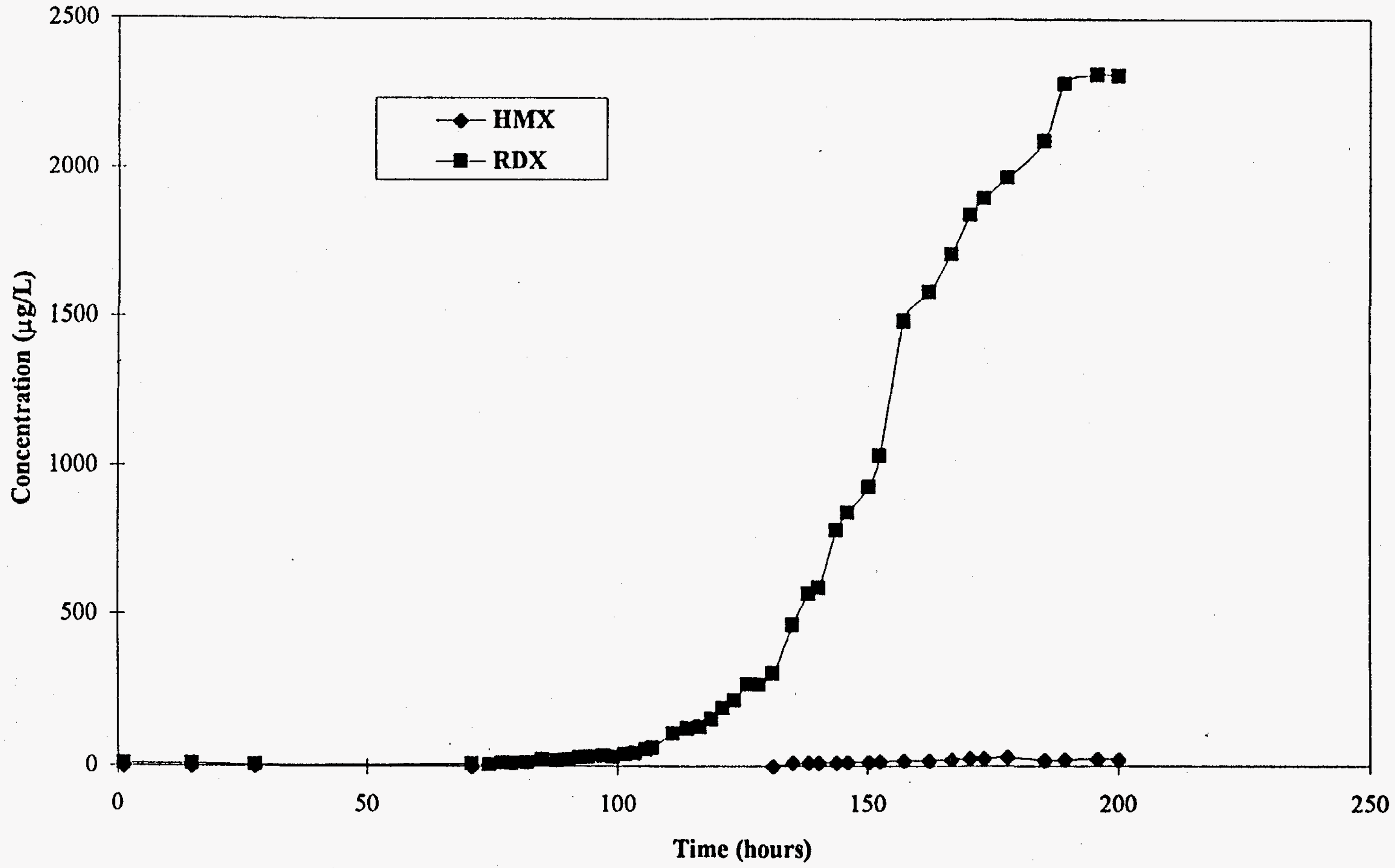
Experiment F4-3



Experiment Number:	F4-4	Re:	1
Carbon:	F400	Mass Carbon (g):	1.45
HMX (mg/L):	315	RSSCT Time (hr):	193
RDX (mg/L):	2350	RSSCT Flowrate (mL/min):	7.62
EBCT LC (min):	16.4	Volume of Water (L):	88
EBCT SC (min):	0.44		

Experimental Results			Scaled Results		
Time (hr)	HMX (mg/L)	RDX (mg/L)	Time (d)	HMX: RSSCT	RDX: RSSCT
1.21		8	2		8
14.81		8	23		8
27.55		5	43		5
70.88		9	110		9
74.38		6	116		6
76.88		12	119		12
78.88		10	123		10
81.88		12	127		12
84.88		22	132		22
87.88		18	136		18
89.88		21	140		21
92.38		28	143		28
94.05		31	146		31
97.01		35	151		35
98.96		31	154		31
101.43		39	158		39
103.48		44	161		44
105.63		56	164		56
106.93		62	166		62
111.10		110	173		110
113.93		124	177		124
116.48		132	181		132
118.76		157	184		157
121.13		195	188		195
123.38		220	192		220
126.05		277	196		277
128.26		275	199		275
131.13		314	204		314
135.13	12	468	210	12	468
138.38	13	570	215	13	570
140.21	11	589	218	11	589
143.88	13	785	223	13	785
146.13	15	844	227	15	844
150.38	15	932	234	15	932
152.55	17	1037	237	17	1037
157.38	19	1486	244	19	1486
162.38	19	1582	252	19	1582
166.88	23	1707	259	23	1707
170.55	26	1842	265	26	1842
173.38	26	1900	269	26	1900
178.05	30	1969	277	30	1969
185.38	21	2093	288	21	2093
189.38	23	2282	294	23	2282
195.96	24	2314	304	24	2314
200.16	23	2309	311	23	2309

Experiment F4-4



Experiment Number:	NWC-2
Carbon:	NWC
HMX (mg/L):	315
RDX (mg/L):	2397
EBCT LC (min):	8.2
EBCT SC (min):	0.12

Re:	2.5
Mass Carbon (g):	0.99
RSSCT Time (hr):	58
RSSCT Flowrate (mL/min):	17.3
Volume of Water (L):	60

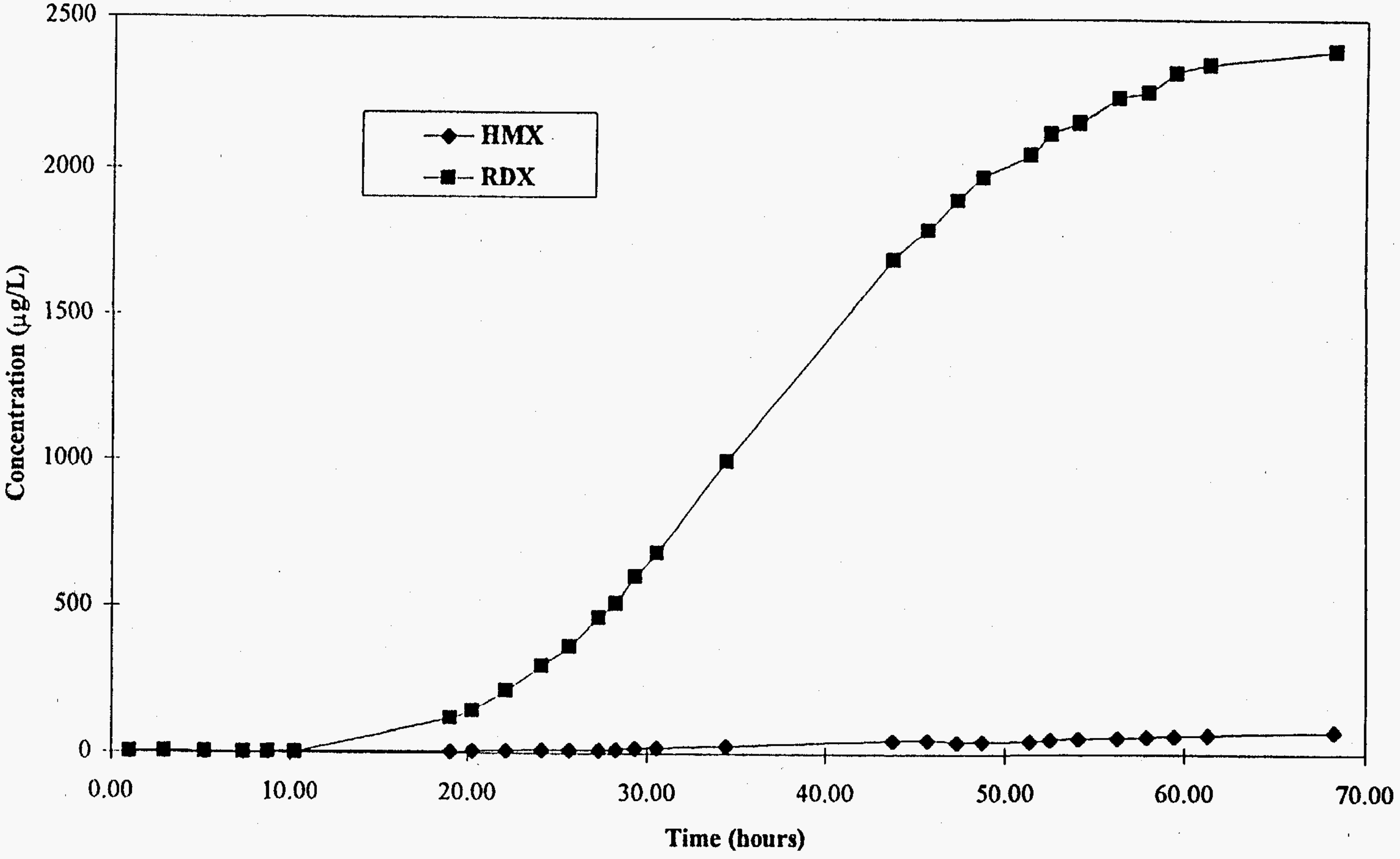
Experimental Results

Time (hr)	HMX (μg/L)	RDX (μg/L)
1.03	4	2
2.98	6	3
5.21	5	4
7.36	5	4
8.78	4	4
10.28	7	2
19.03	6	120
20.25	9	145
22.15	11	215
24.13	12	300
25.66	13	366
27.30	13	464
28.25	15	513
29.31	18	604
30.55	21	684
34.45	28	999
43.78	47	1693
45.70	48	1794
47.36	42	1897
48.75	44	1976
51.40	45	2053
52.51	50	2121
54.10	54	2157
56.28	58	2239
57.91	61	2257
59.43	63	2323
61.28	68	2350
68.28	78	2396

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
3	4	2
8	6	3
15	5	4
21	5	4
25	4	4
29	7	2
54	6	120
58	9	145
63	11	215
69	12	300
73	13	366
78	13	464
80	15	513
83	18	604
87	21	684
98	28	999
125	47	1693
130	48	1794
135	42	1897
139	44	1976
146	45	2053
150	50	2121
154	54	2157
160	58	2239
165	61	2257
169	63	2323
174	68	2350
194	78	2396

Experiment NWC-2



Experiment Number:	NWC-3
Carbon:	NWC
HMX (mg/L):	320
RDX (mg/L):	2427
EBCT LC (min):	12.3
EBCT SC (min):	0.18

Re:	2
Mass Carbon (g):	1.19
RSSCT Time (hr):	95
RSSCT Flowrate (mL/min):	13.84
Volume of Water (L):	79

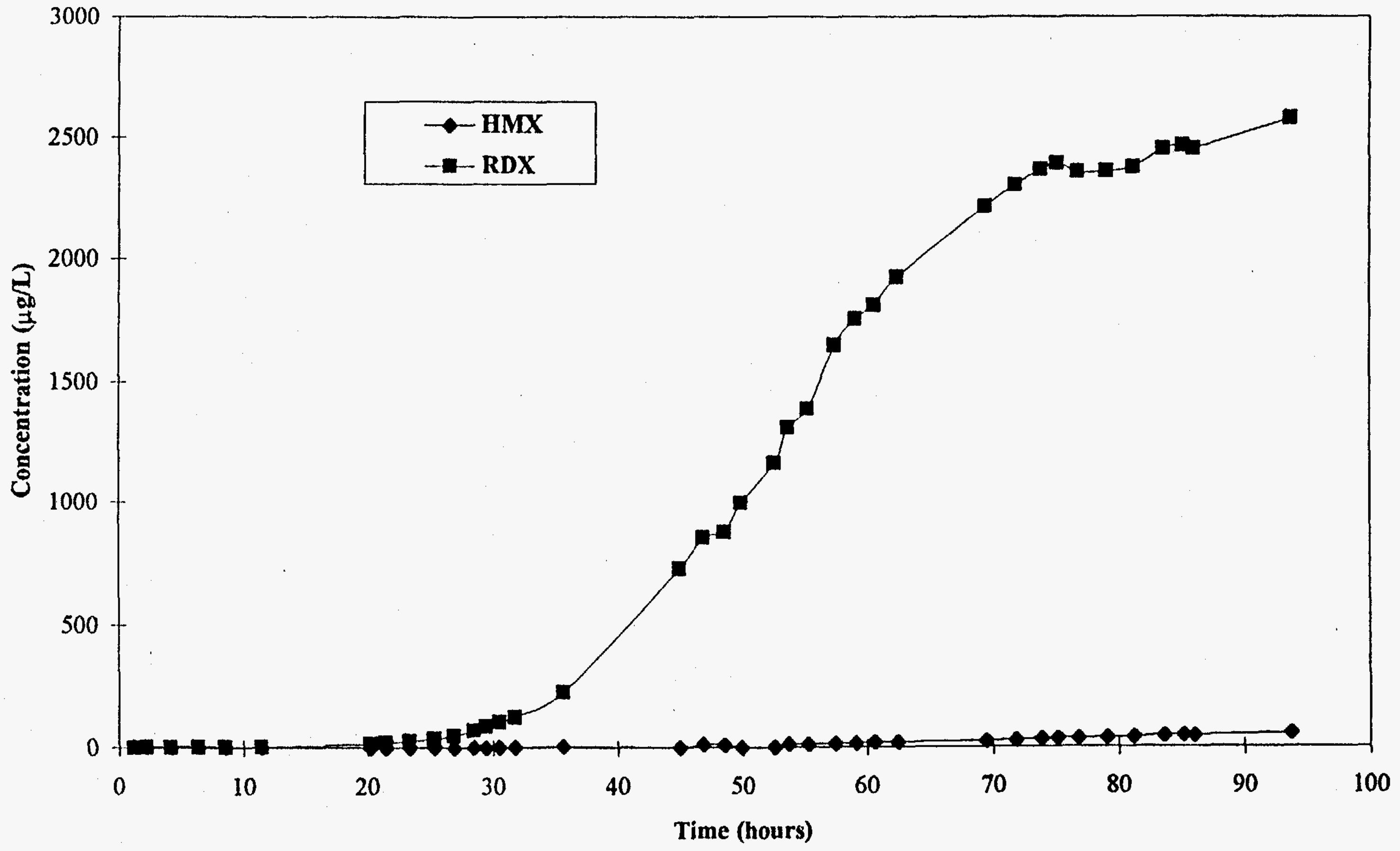
Experimental Results

Time (hr)	HMX (μg/L)	RDX (μg/L)
1.23	4	-1
2.23	4	2
4.18	4	3
6.41	5	3
8.56	3	3
11.48	4	3
20.23	1	14
21.45	1	21
23.35	1	25
25.33	3	35
26.86	1	48
28.50	3	72
29.45	1	85
30.51	4	104
31.75	4	124
35.65	6	226
44.98	1	725
46.90	12	850
48.56	10	872
49.95	1	994
52.60	1	1162
53.71	13	1308
55.30	12	1388
57.48	16	1648
59.11	16	1753
60.63	19	1808
62.48	21	1924
69.48	26	2213
71.86	29	2299
73.90	33	2366
75.15	35	2392
76.78	36	2357
79.06	39	2357
81.20	42	2377
83.65	46	2452
85.20	49	2464
86.03	46	2452
93.76	56	2577

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
4	4	-1
6	4	2
12	4	3
18	5	3
24	3	3
33	4	3
58	1	14
61	1	21
66	1	25
72	3	35
76	1	48
81	3	72
84	1	85
87	4	104
90	4	124
101	6	226
128	1	725
134	12	850
138	10	872
142	1	994
150	1	1162
153	13	1308
157	12	1388
164	16	1648
168	16	1753
173	19	1808
178	21	1924
198	26	2213
205	29	2299
210	33	2366
214	35	2392
219	36	2357
225	39	2357
231	42	2377
238	46	2452
243	49	2464
245	46	2452
267	56	2577

Experiment NWC-3



Experiment Number:	NWC-4
Carbon:	NWC
HMX (mg/L):	315
RDX (mg/L):	2397
EBCT LC (min):	16.4
EBCT SC (min):	0.24

Re:	1.5
Mass Carbon (g):	1.19
RSSCT Time (hr):	127
RSSCT Flowrate (mL/min):	10.38
Volume of Water (L):	79

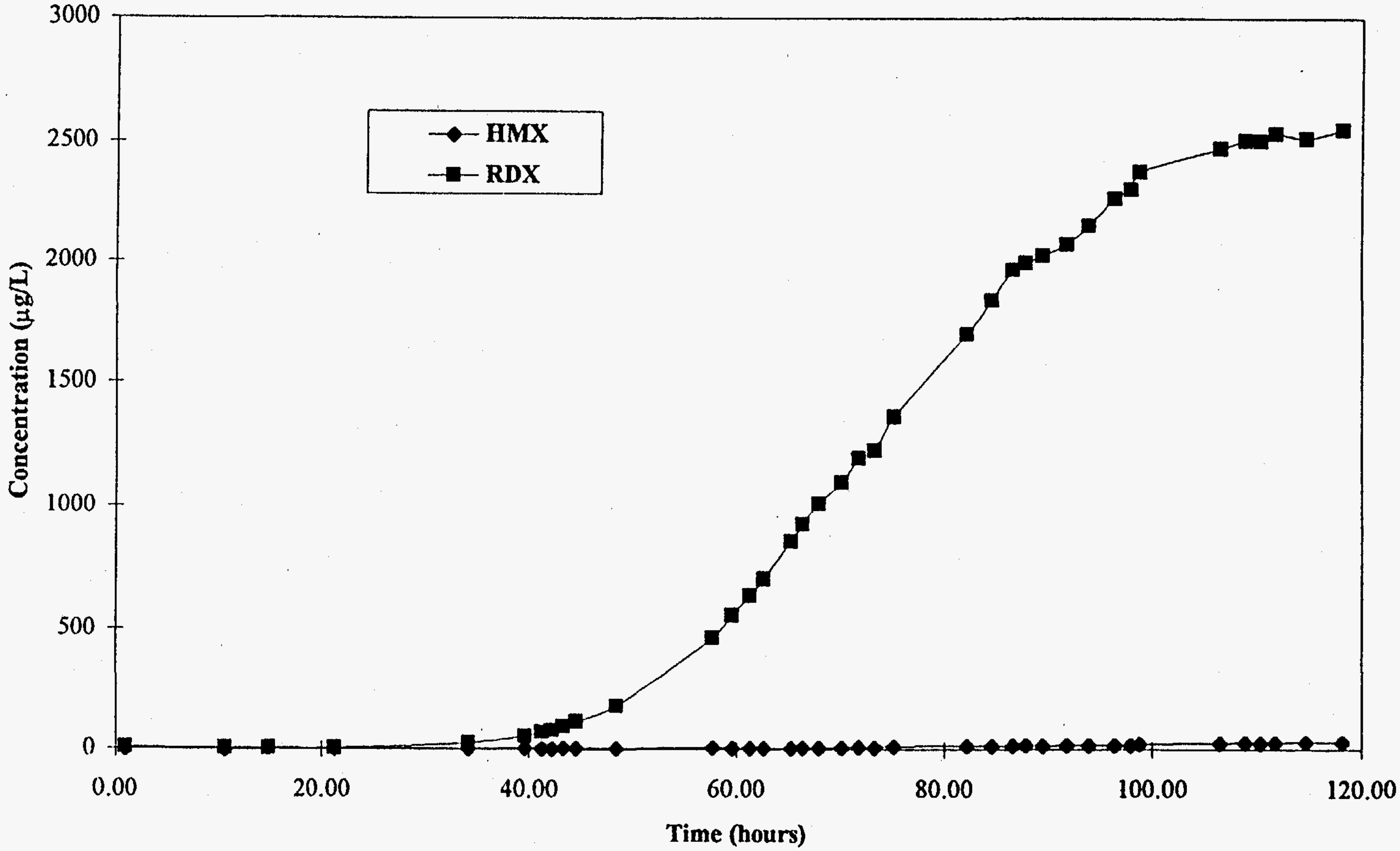
Experimental Results

Time (hr)	HMX (μg/L)	RDX (μg/L)
0.95	1	8
10.58	1	4
14.87	5	4
21.28	2	5
34.17	2	26
39.58	4	53
41.22	4	70
42.17	4	78
43.23	5	95
44.47	4	114
48.37	4	179
57.70	7	464
59.62	5	557
61.28	6	637
62.67	6	702
65.32	6	851
66.43	7	924
68.02	8	1010
70.20	8	1098
71.83	9	1198
73.35	9	1227
75.20	12	1364
82.20	14	1698
84.58	15	1842
86.62	16	1968
87.87	17	1995
89.50	15	2026
91.78	18	2075
93.92	18	2153
96.37	18	2267
97.92	19	2305
98.75	22	2379
106.48	24	2475
108.87	27	2509
110.37	27	2505
111.78	27	2535
114.70	30	2516
118.20	32	2551

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
3	1	8
30	1	4
42	5	4
61	2	5
97	2	26
113	4	53
117	4	70
120	4	78
123	5	95
127	4	114
138	4	179
164	7	464
170	5	557
174	6	637
178	6	702
186	6	851
189	7	924
194	8	1010
200	8	1098
205	9	1198
209	9	1227
214	12	1364
234	14	1698
241	15	1842
247	16	1968
250	17	1995
255	15	2026
261	18	2075
267	18	2153
274	18	2267
279	19	2305
281	22	2379
303	24	2475
310	27	2509
314	27	2505
318	27	2535
327	30	2516
337	32	2551

Experiment NWC-4



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APPENDIX D

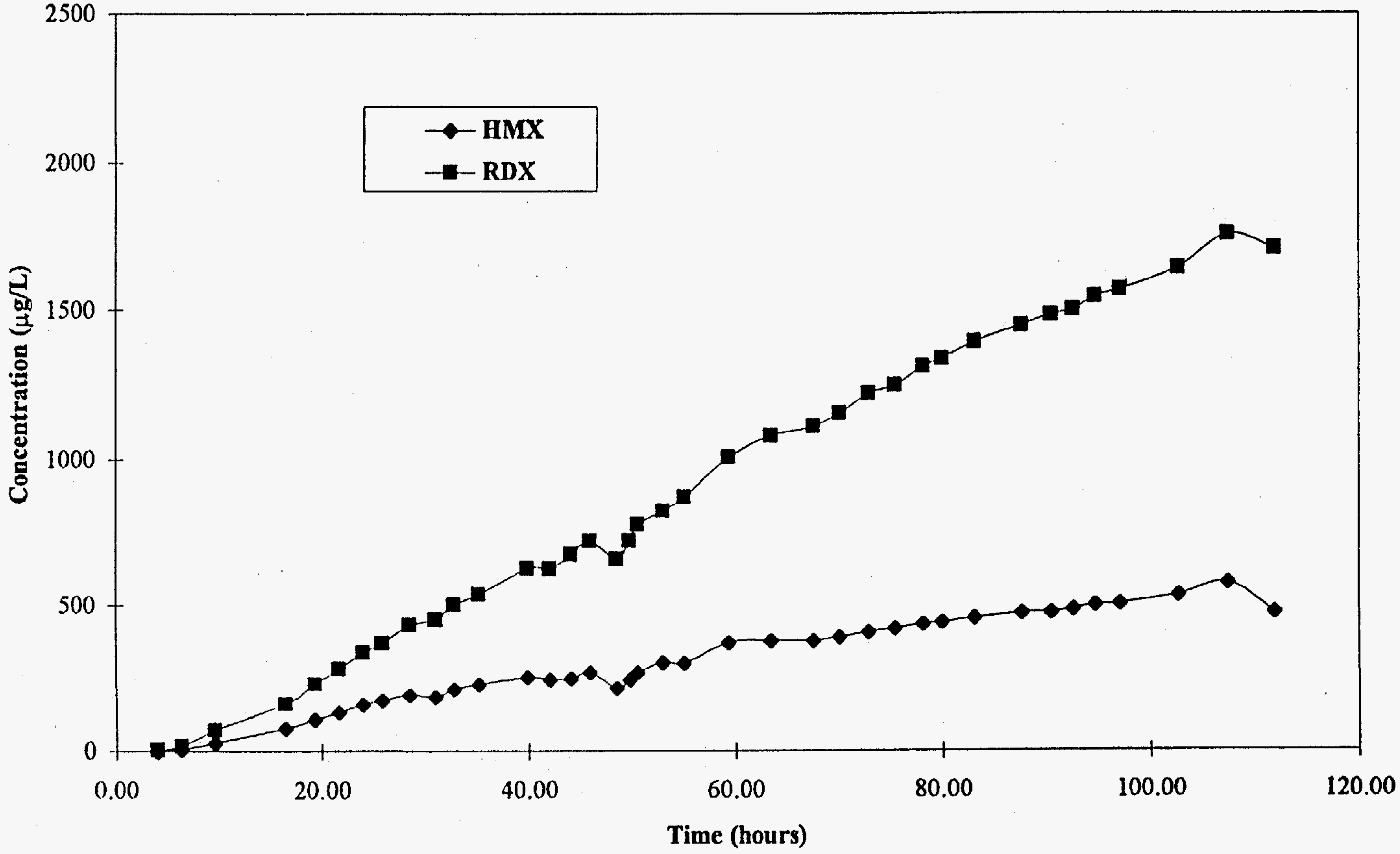
VARIABLE CONCENTRATION RSSCT DATA

Experiment Number:	H2 8.2
Carbon:	F400
HMX (mg/L):	1103
RDX (mg/L):	1933
EBCT LC (min):	8.2
EBCT SC (min):	0.22

Re:	1.5
Mass Carbon (g):	1.09
RSSCT Time (hr):	96
RSSCT Flowrate (mL/min):	11.43
Volume of Water (L):	66

Experimental Results			Scaled Results		
Time (hr)	HMX (μg/L)	RDX (μg/L)	Time (d)	HMX: RSSCT	RDX: RSSCT
4.00	**0**	**5**	6.21	**0**	**5**
6.33	**6**	**16**	9.84	**6**	**16**
9.67	28	70	15.01	28	70
16.50	76	161	25.63	76	161
19.38	106	230	30.10	106	230
21.67	131	283	33.65	131	283
24.00	158	341	37.27	158	341
25.83	173	373	40.12	173	373
28.50	193	433	44.26	193	433
31.00	185	451	48.14	185	451
32.75	214	503	50.86	214	503
35.17	230	539	54.61	230	539
39.88	256	627	61.94	256	627
42.03	248	625	65.28	248	625
44.12	252	673	68.51	252	673
45.92	272	718	71.31	272	718
48.50	217	659	75.32	217	659
49.77	248	720	77.29	248	720
50.50	272	775	78.43	272	775
53.00	307	821	82.31	307	821
55.08	304	872	85.55	304	872
59.33	373	1008	92.15	373	1008
63.50	380	1080	98.62	380	1080
67.58	381	1111	104.96	381	1111
70.12	393	1156	108.89	393	1156
72.95	409	1221	113.29	409	1221
75.50	422	1249	117.25	422	1249
78.20	437	1312	121.45	437	1312
80.00	445	1337	124.24	445	1337
83.17	459	1393	129.16	459	1393
87.67	476	1447	136.15	476	1447
90.50	478	1484	140.55	478	1484
92.58	489	1501	143.78	489	1501
94.75	502	1545	147.15	502	1545
97.08	507	1569	150.77	507	1569
102.75	536	1639	159.57	536	1639
107.50	580	1755	166.95	580	1755
112.00	477	1706	173.94	477	1706

Experiment H2 8.2

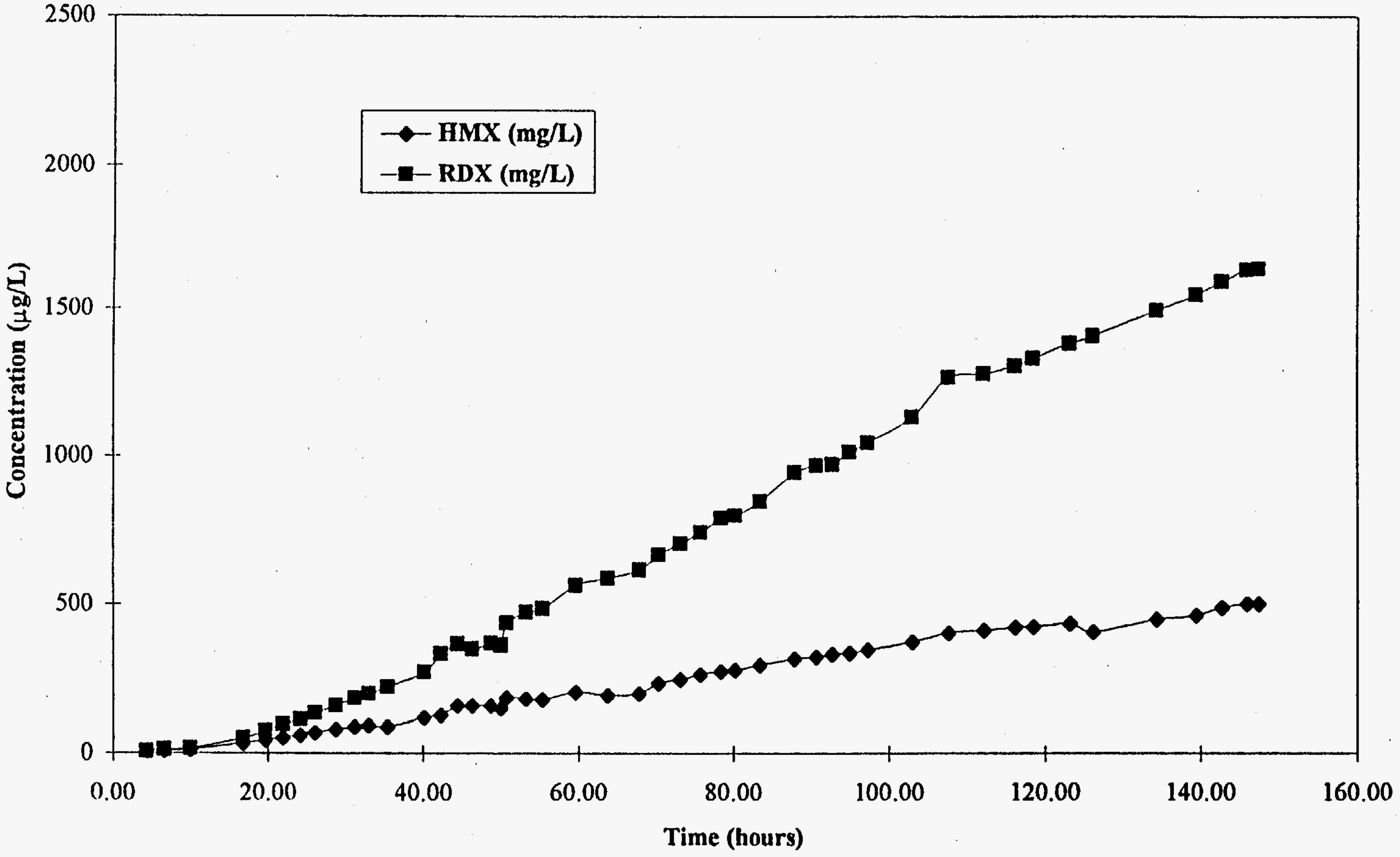


Experiment Number:	H2 12.3
Carbon:	F400
HMX (mg/L):	1105
RDX (mg/L):	1930
EBCT LC (min):	12.3
EBCT SC (min):	0.33

Re:	1
Mass Carbon (g):	1.09
RSSCT Time (hr):	96
RSSCT Flowrate (mL/min):	11.43
Volume of Water (L):	66

Experimental Results			Scaled Results		
Time (hr)	HMX (μg/L)	RDX (μg/L)	Time (d)	HMX: RSSCT	RDX: RSSCT
4.28	9	7	7	9	7
6.62	10	13	10	10	13
9.95	13	17	15	13	17
16.78	34	51	26	34	51
19.67	45	76	31	45	76
21.95	54	98	34	54	98
24.28	62	115	38	62	115
26.12	70	135	41	70	135
28.78	80	161	45	80	161
31.28	88	187	49	88	187
33.03	93	200	51	93	200
35.45	89	224	55	89	224
40.17	120	275	62	120	275
42.32	130	335	66	130	335
44.40	161	369	69	161	369
46.28	162	350	72	162	350
48.75	161	370	76	161	370
50.02	153	364	78	153	364
50.75	189	438	79	189	438
53.25	183	473	83	183	473
55.33	182	486	86	182	486
59.58	206	565	93	206	565
63.75	196	588	99	196	588
67.83	203	615	105	203	615
70.37	239	667	109	239	667
73.20	252	705	114	252	705
75.75	267	742	118	267	742
78.45	279	791	122	279	791
80.25	283	798	125	283	798
83.42	299	848	130	299	848
87.92	321	944	137	321	944
90.75	327	967	141	327	967
92.83	335	973	144	335	973
95.00	341	1014	148	341	1014
97.33	351	1047	151	351	1047
103.00	377	1132	160	377	1132
107.75	407	1268	167	407	1268
112.25	415	1281	174	415	1281
116.25	425	1308	181	425	1308
118.58	427	1333	184	427	1333
123.25	437	1383	191	437	1383
126.25	411	1409	196	411	1409
134.42	452	1496	209	452	1496
139.42	466	1550	217	466	1550
142.75	491	1595	222	491	1595
145.97	502	1635	227	502	1635
147.42	503	1641	229	503	1641

Experiment H2 12.3



Experiment Number:	R5 8.2
Carbon:	F400
HMX (mg/L):	350
RDX (mg/L):	4400
EBCT LC (min):	8.2
EBCT SC (min):	0.22

Re:	1.5
Mass Carbon (g):	1.09
RSSCT Time (hr):	60
RSSCT Flowrate (mL/min):	11.43
Volume of Water (L):	41

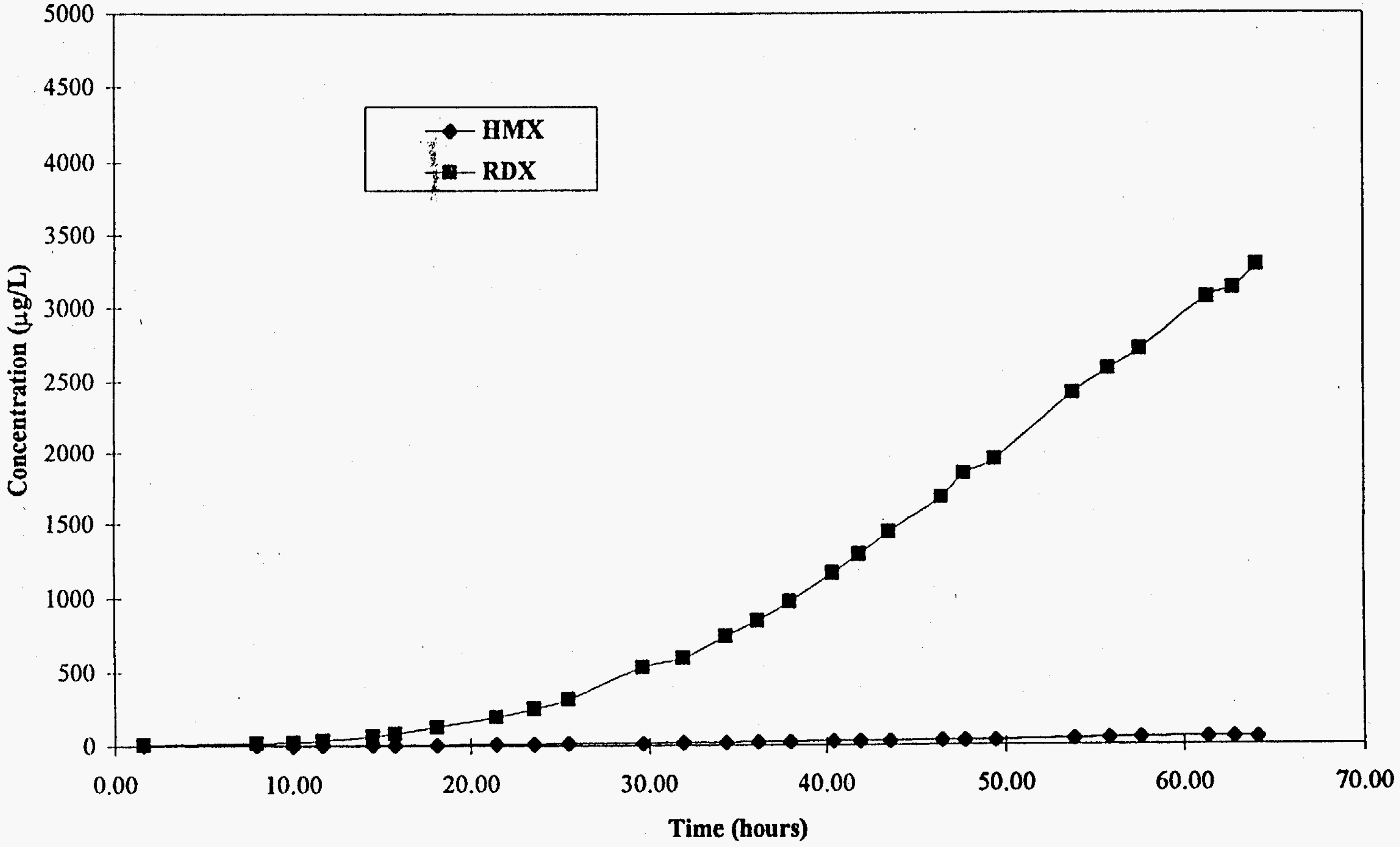
Experimental Results

Time (hr)	HMX (μg/L)	RDX (μg/L)
1.62	10	10
7.97	8	23
10.03	5	26
11.68	8	39
14.50	9	68
15.75	10	86
18.12	10	130
21.42	12	200
23.53	14	253
25.50	16	316
29.67	19	533
31.93	20	597
34.37	23	744
36.17	25	850
38.00	25	977
40.42	28	1167
41.93	28	1288
43.60	30	1442
46.50	33	1683
47.75	34	1852
49.47	35	1952
53.83	42	2413
55.83	47	2584
57.60	50	2718
61.33	54	3068
62.78	53	3134
64.08	52	3289

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
3	10	10
12	8	23
16	5	26
18	8	39
23	9	68
24	10	86
28	10	130
33	12	200
37	14	253
40	16	316
46	19	533
50	20	597
53	23	744
56	25	850
59	25	977
63	28	1167
65	28	1288
68	30	1442
72	33	1683
74	34	1852
77	35	1952
84	42	2413
87	47	2584
89	50	2718
95	54	3068
98	53	3134
100	52	3289

Experiment R5 8.2



Experiment Number:	R5 12.3
Carbon:	F400
HMX (mg/L):	372
RDX (mg/L):	4870
EBCT LC (min):	12.3
EBCT SC (min):	0.33

Re:	1
Mass Carbon (g):	1.09
RSSCT Time (hr):	91
RSSCT Flowrate (mL/min):	7.62
Volume of Water (L):	41

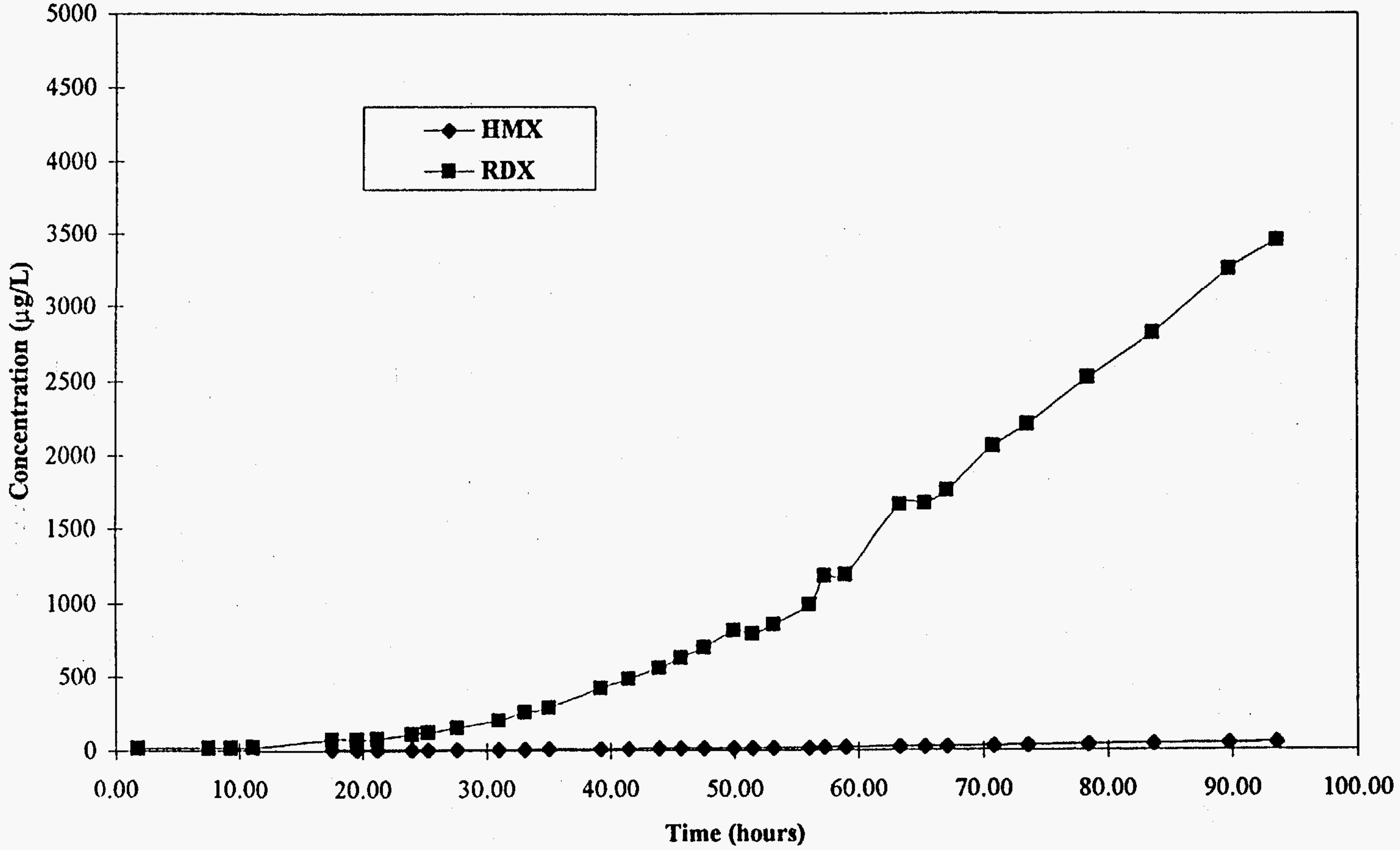
Experimental Results

Time (hr)	HMX (μg/L)	RDX (μg/L)
1.78		17
7.50		18
9.33		18
11.15		19
17.50	7	70
19.57	7	70
21.20	7	75
24.00	8	111
25.28	7	124
27.62	9	152
30.95	10	204
33.07	10	257
35.02	12	289
39.20	14	422
41.47	14	487
43.90	16	561
45.70	16	632
47.53	17	701
49.95	18	817
51.47	16	794
53.13	18	860
56.03	18	995
57.28	22	1188
59.00	23	1198
63.37	26	1667
65.37	27	1672
67.13	27	1761
70.87	30	2064
73.60	32	2212
78.47	37	2524
83.67	42	2819
89.75	46	3255
93.55	51	3455

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
3		17
12		18
14		18
17		19
27	7	70
30	7	70
33	7	75
37	8	111
39	7	124
43	9	152
48	10	204
51	10	257
54	12	289
61	14	422
64	14	487
68	16	561
71	16	632
74	17	701
78	18	817
80	16	794
83	18	860
87	18	995
89	22	1188
92	23	1198
98	26	1667
102	27	1672
104	27	1761
110	30	2064
114	32	2212
122	37	2524
130	42	2819
139	46	3255
145	51	3455

Experiment R5 12.3



APPENDIX E

PRE-LOADING RSSCT DATA AND CALIBRATION CURVES

Experiment Number:	PL1
Carbon:	F400
HMX (mg/L):	292
RDX (mg/L):	2267
EBCT LC (min):	8.2
EBCT SC (min):	0.22

Re:	1.5
Mass Carbon (g):	1.09
RSSCT Time (hr):	96
RSSCT Flowrate (mL/min):	11.43
Volume of Water (L):	66

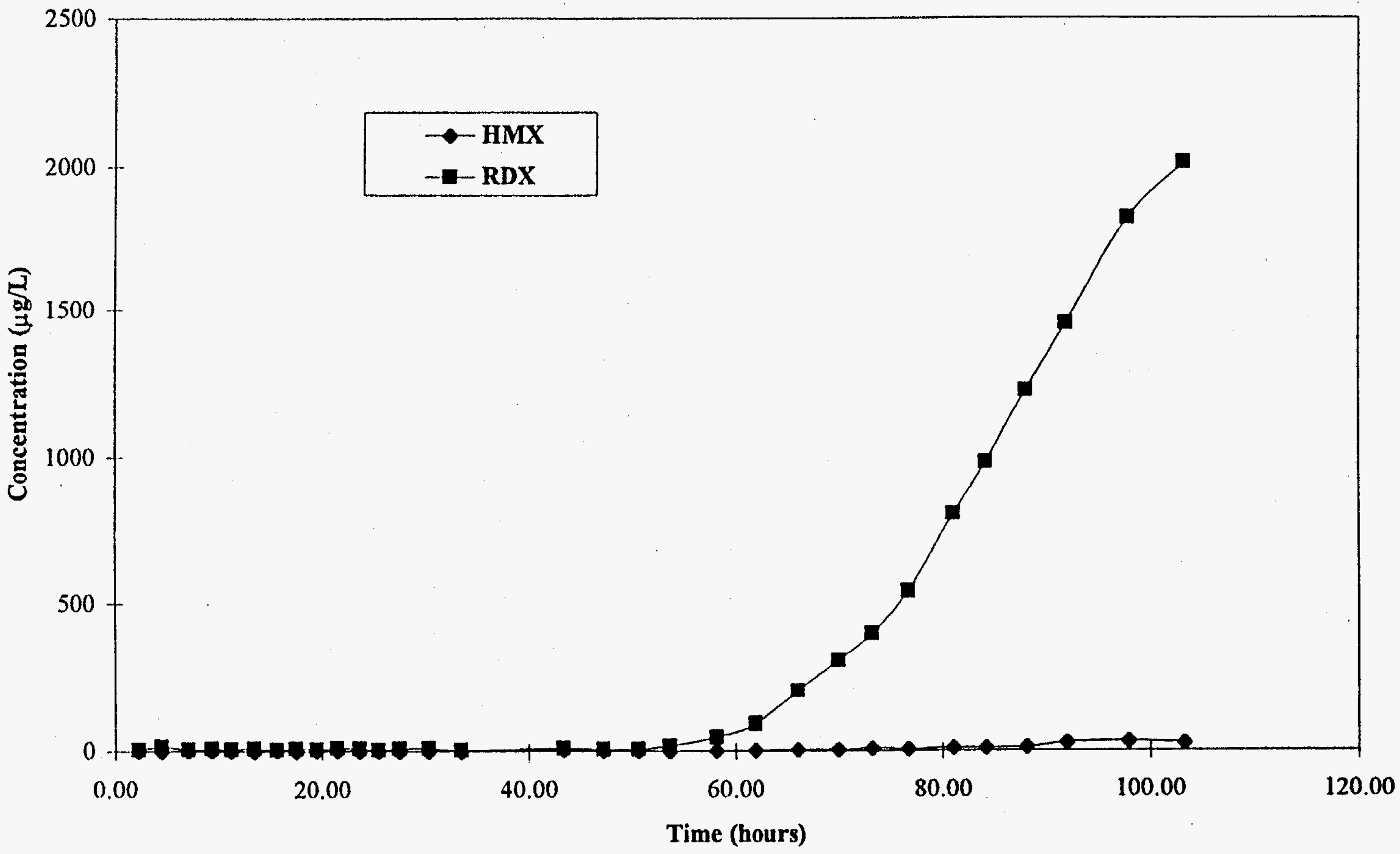
Experimental Results

Time (hr)	HMX (µg/L)	RDX (µg/L)
2.25	0	4
4.50	0	14
7.08	2	6
9.33	3	8
11.25	2	6
13.50	0	8
15.67	4	4
17.50	0	8
19.50	1	6
21.50	2	10
23.67	0	9
25.50	0	3
27.50	0	8
30.33	0	11
33.42	0	4
43.33	4	10
47.25	2	6
50.58	2	7
53.67	0	18
58.17	2	46
61.92	3	91
66.05	3	203
70.00	5	309
73.25	7	399
76.75	7	543
81.08	10	804
84.20	11	984
88.08	14	1229
92.00	27	1457
97.92	32	1824
103.25	24	2014

Scaled Results

Time (d)	HMX: RSSCT	RDX: RSSCT
3	0	4
7	0	14
11	2	6
14	3	8
17	2	6
21	0	8
24	4	4
27	0	8
30	1	6
33	2	10
37	0	9
40	0	3
43	0	8
47	0	11
52	0	4
67	4	10
73	2	6
79	2	7
83	0	18
90	2	46
96	3	91
103	3	203
109	5	309
114	7	399
119	7	543
126	10	804
131	11	984
137	14	1229
143	27	1457
152	32	1824
160	24	2014

Experiment PL1

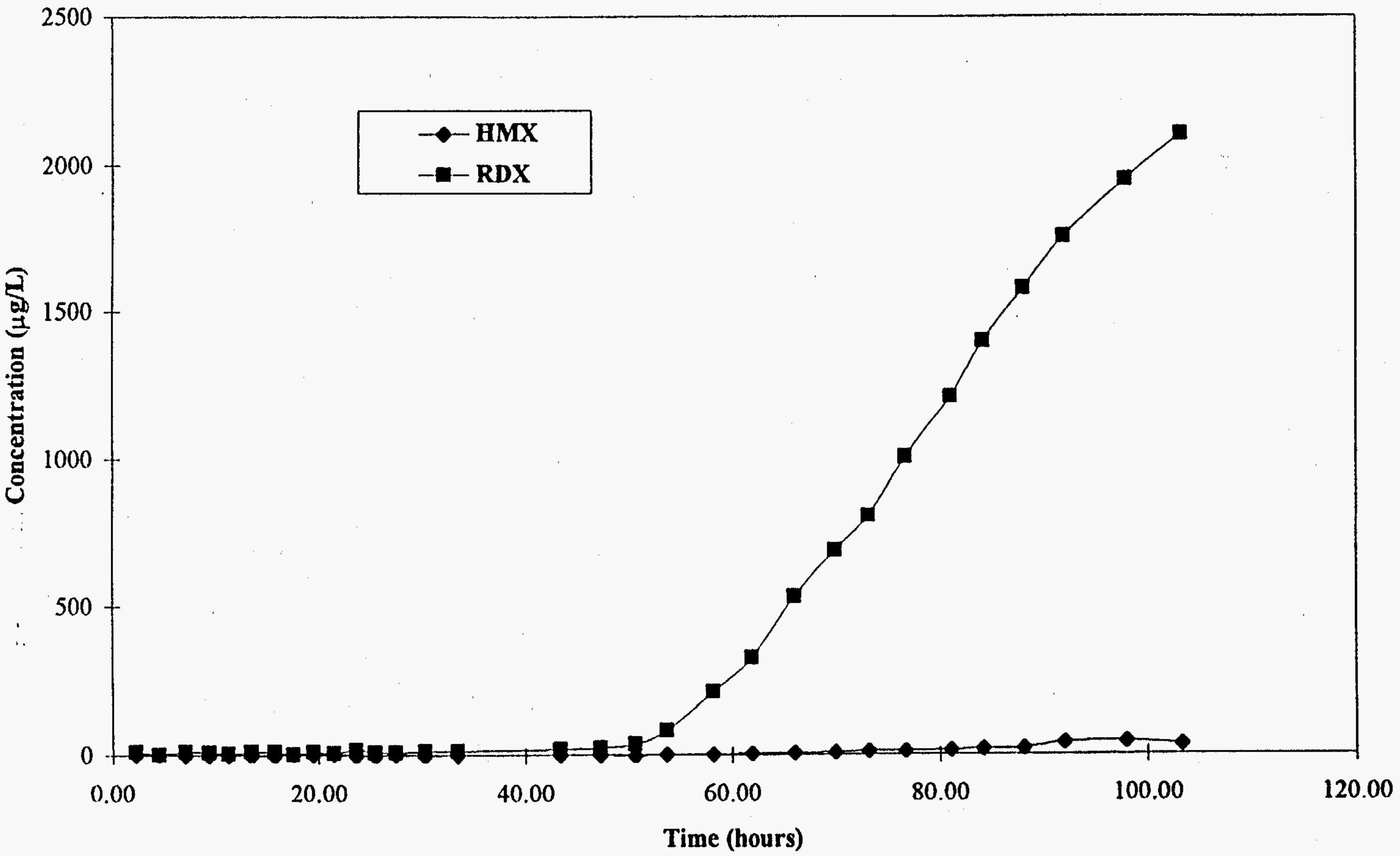


Experiment Number:	PL3
Carbon:	F400
HMX (mg/L):	296
RDX (mg/L):	2231
EBCT LC (min):	8.2
EBCT SC (min):	0.22

Re:	1.5
Mass Carbon (g):	1.09
RSSCT Time (hr):	96
RSSCT Flowrate (mL/min):	11.43
Volume of Water (L):	66

Experimental Results			Scaled Results		
Time (hr)	HMX (μg/L)	RDX (μg/L)	Time (d)	HMX: RSSCT	RDX: RSSCT
2.25	2	11	3	2	11
4.50	1	3	7	1	3
7.08	1	11	11	1	11
9.33	0	8	14	0	8
11.25	1	4	17	1	4
13.50	-2	10	21	-2	10
15.67	-2	11	24	-2	11
17.50	5	2	27	5	2
19.50	2	12	30	2	12
21.50	5	7	33	5	7
23.67	-2	16	37	-2	16
25.50	-2	8	40	-2	8
27.50	2	9	43	2	9
30.33	-2	12	47	-2	12
33.42	0	12	52	0	12
43.33	0	20	67	0	20
47.25	0	24	73	0	24
50.58	-2	36	79	-2	36
53.67	2	83	83	2	83
58.17	2	214	90	2	214
61.92	4	329	96	4	329
66.05	7	536	103	7	536
70.00	9	687	109	9	687
73.25	12	804	114	12	804
76.75	13	1007	119	13	1007
81.08	15	1214	126	15	1214
84.20	18	1401	131	18	1401
88.08	21	1577	137	21	1577
92.00	40	1751	143	40	1751
97.92	43	1949	152	43	1949
103.25	35	2102	160	35	2102

Experiment PL3



Experiment Number:	PL7
Carbon:	F400
HMX (mg/L):	318
RDX (mg/L):	2242
EBCT LC (min):	8.2
EBCT SC (min):	0.22

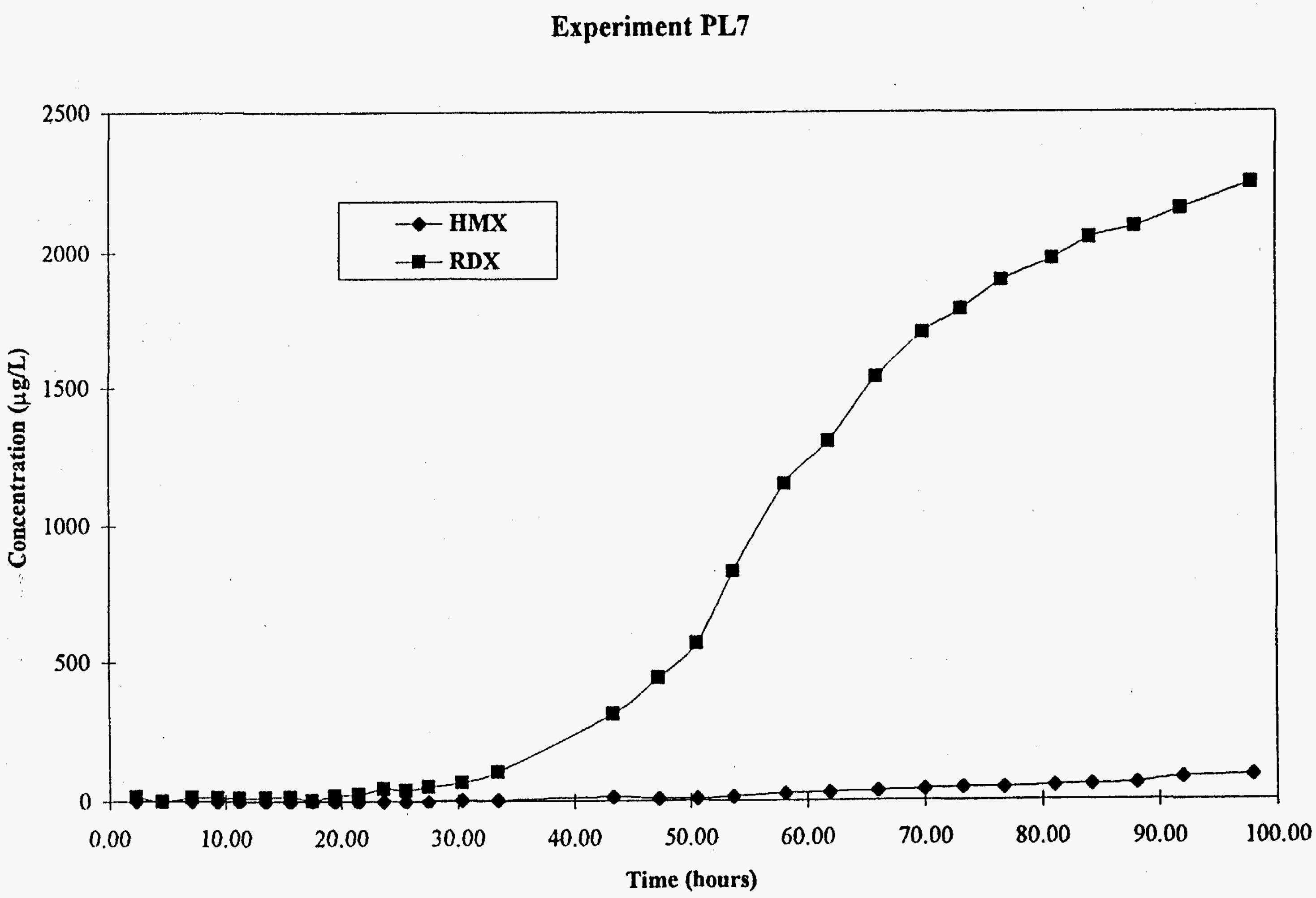
Re:	1.5
Mass Carbon (g):	1.09
RSSCT Time (hr):	96
RSSCT Flowrate (mL/min):	11.43
Volume of Water (L):	66

Experimental Results

Time (hr)	HMX (μg/L)	RDX (μg/L)
2.25	**3**	**16**
4.50	**1**	**1**
7.08	**3**	**14**
9.33	**0**	**12**
11.25	**-2**	**10**
13.50	**-2**	**13**
15.67	**-2**	**14**
17.50	**-2**	**1**
19.50	**-2**	**19**
21.50	**-2**	23
23.67	1	43
25.50	-2	38
27.50	-2	50
30.33	4	67
33.42	5	107
43.33	**14**	315
47.25	**8**	443
50.58	**8**	569
53.67	16	831
58.17	25	1150
61.92	29	1307
66.05	37	1539
70.00	41	1702
73.25	46	1790
76.75	47	1895
81.08	54	1977
84.20	58	2052
88.08	61	2091
92.00	82	2156
97.92	91	2249

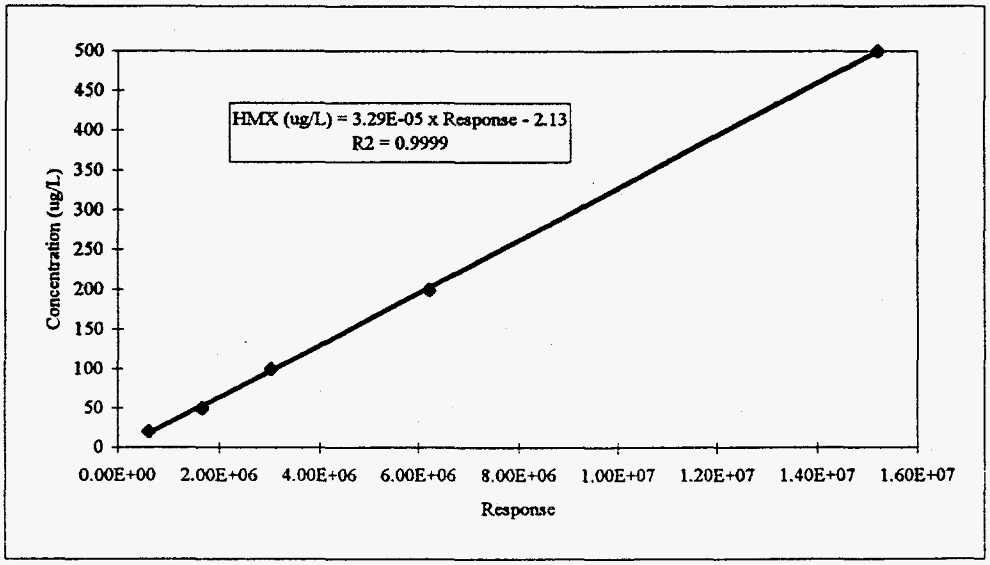
Scaled Results

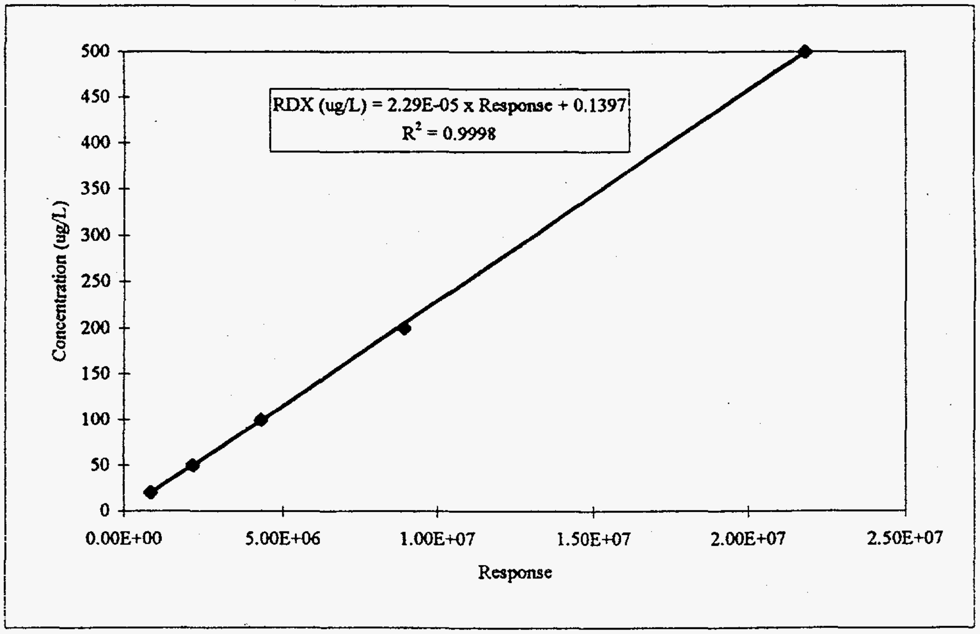
Time (d)	HMX: RSSCT	RDX: RSSCT
3	**3**	**16**
7	**1**	**1**
11	**3**	**14**
14	**0**	**12**
17	**-2**	**10**
21	**-2**	**13**
24	**-2**	**14**
27	**-2**	**1**
30	**-2**	**19**
33	**-2**	23
37	1	43
40	-2	38
43	-2	50
47	4	67
52	5	107
67	**14**	315
73	**8**	443
79	**8**	569
83	16	831
90	25	1150
96	29	1307
103	37	1539
109	41	1702
114	46	1790
119	47	1895
126	54	1977
131	58	2052
137	61	2091
143	82	2156
152	91	2249


Experiment PL7
HMX
RDX
2500
2000
1500
1000
500
0
Concentration (µg/L)
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00
90.00
100.00
Time (hours)

20 ug/L - 500 ug/L Concentration Range for Calibration Curves

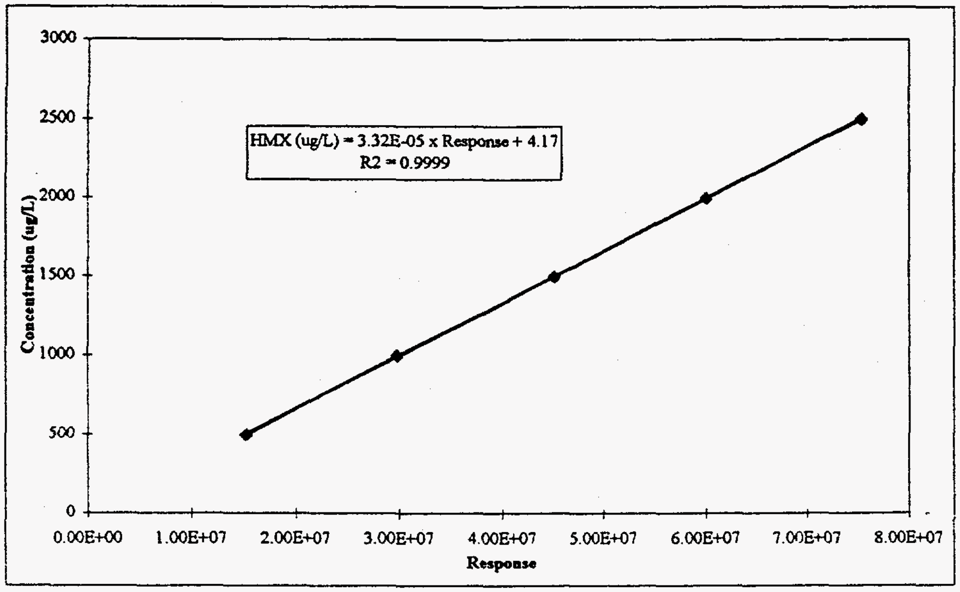
HMX Response	RDX Response	Standard Concentration (mg/L)
612238	835489	20
1655374	2149218	50
3029019	4298274	100
6205744	8937376	200
15203404	21799490	500

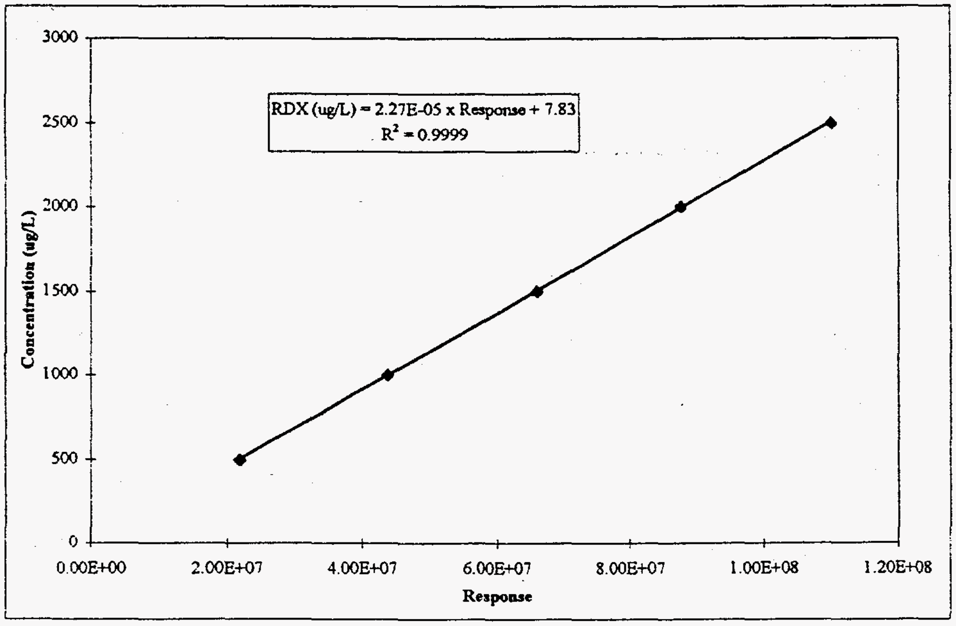




500 ug/L - 2500 ug/L Concentration Range Calibration Curves

HMX Response	RDX Response	Standard Concentration (µg/L)
15144777	21799490	500
29735230	43622776	1000
45073756	65879204	1500
60042724	87406816	2000
75292856	110069784	2500





APPENDIX F

PCSORB MODELING OUTPUT FILES

Model of RSSCT: EBCT = 4.1 min

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
                    HSDM
                SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =           3
NUMBER OF AXIAL COLLOCATION POINTS ....... =          12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =          94
GAC NAME................................ = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =     .82200E-02
MASS OF ADSORBENT,  (GRAMS)............... =    .10810E+01
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=    .73000E+00
LENGTH OF BED, (CM)...................... =    .50190E+01
DIAMETER OF BED, (CM).................... =    .79900E+00
VOID FRACTION OF BED, (DIM.)............. =    .41156E+00
FLOW RATE, (mL/MIN)...................... =    .22860E+02
SURFACE LOADING, (GPM/FT**2)............. =    .11189E+02
PACKED BED CONTACT TIME, (SEC)........... =    .27184E+01
EMPTY BED CONTACT TIME, (MIN)............ =    .11008E+00

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, ............................. = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)......................... =    .94566E+00
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .51105E+05
  BIOT NUMBER, (DIM.)............................ =    .45994E-02
  DIFFUSIVITY MODULUS, (DIM.).................... =    .20560E+03
  TARGET EFFLUENT CONC., (uM/L).................. =    .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, ............................. = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)......................... =    .94566E+00
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .49957E+06
  BIOT NUMBER, (DIM.)............................ =    .47052E-03
  DIFFUSIVITY MODULUS, (DIM.).................... =    .20098E+04
  TARGET EFFLUENT CONC., (uM/L).................. =    .23600E-01
```

Model of Full Scale: EBCT = 4.1

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
              HSDM
           SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =          3
NUMBER OF AXIAL COLLOCATION POINTS ....... =         12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =         94
GAC NAME................................. = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =    .50000E-01
MASS OF ADSORBENT,  (GRAMS)............... =   .21687E+07
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=    .73000E+00
LENGTH OF BED, (CM)...................... =   .10791E+03
DIAMETER OF BED, (CM).................... =   .24400E+03
VOID FRACTION OF BED, (DIM.)............. =   .41119E+00
FLOW RATE, (mL/MIN)...................... =   .12300E+07
SURFACE LOADING, (GPM/FT**2)............. =   .64560E+01
PACKED BED CONTACT TIME, (SEC)........... =   .10120E+03
EMPTY BED CONTACT TIME, (MIN)............ =   .41021E+01

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, ............................. = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =   .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =   .20000E-02
  STANTON NUMBER, (DIM.)........................ =   .57968E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =   .51184E+05
  BIOT NUMBER, (DIM.)........................... =   .27977E-01
  DIFFUSIVITY MODULUS, (DIM.)................... =   .20720E+03
  TARGET EFFLUENT CONC., (uM/L)................. =   .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, ............................. = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =   .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =   .20000E-02
  STANTON NUMBER, (DIM.)........................ =   .57968E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =   .50033E+06
  BIOT NUMBER, (DIM.)........................... =   .28620E-02
  DIFFUSIVITY MODULUS, (DIM.)................... =   .20254E+04
  TARGET EFFLUENT CONC., (uM/L)................. =   .23600E-01
```

Model of RSSCT: EBCT = 8.2

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
         HSDM
              SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =          3
NUMBER OF AXIAL COLLOCATION POINTS ....... =         12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =         94
GAC NAME................................ = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =    .82200E-02
MASS OF ADSORBENT, (GRAMS)............... =    .10800E+01
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=    .73000E+00
LENGTH OF BED, (CM)...................... =    .50190E+01
DIAMETER OF BED, (CM).................... =    .79900E+00
VOID FRACTION OF BED, (DIM.)............. =    .41210E+00
FLOW RATE, (mL/MIN)...................... =    .11430E+02
SURFACE LOADING, (GPM/FT**2)............. =    .55947E+01
PACKED BED CONTACT TIME, (SEC)............ =    .54439E+01
EMPTY BED CONTACT TIME, (MIN)............ =    .22017E+00

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, .............................. = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =    .18896E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .50991E+05
  BIOT NUMBER, (DIM.)........................... =    .45994E-02
  DIFFUSIVITY MODULUS, (DIM.)................... =    .41083E+03
  TARGET EFFLUENT CONC., (uM/L)................. =    .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, .............................. = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =    .18896E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .49845E+06
  BIOT NUMBER, (DIM.)........................... =    .47052E-03
  DIFFUSIVITY MODULUS, (DIM.)................... =    .40159E+04
  TARGET EFFLUENT CONC., (uM/L)................. =    .23600E-01
```

Model of Full Scale: EBCT = 8.2 min

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
                        HSDM
                  SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =          3
NUMBER OF AXIAL COLLOCATION POINTS ....... =         12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =         94
GAC NAME................................ = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =    .50000E-01
MASS OF ADSORBENT,  (GRAMS)............... =    .43441E+07
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=    .73000E+00
LENGTH OF BED, (CM)...................... =    .21615E+03
DIAMETER OF BED, (CM).................... =    .24393E+03
VOID FRACTION OF BED, (DIM.).............. =    .41089E+00
FLOW RATE, (mL/MIN)...................... =    .12300E+07
SURFACE LOADING, (GPM/FT**2).............. =    .64594E+01
PACKED BED CONTACT TIME, (SEC)............ =    .20247E+03
EMPTY BED CONTACT TIME, (MIN)............ =    .82125E+01

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, .............................. = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)......................... =    .11611E+02
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .51247E+05
  BIOT NUMBER, (DIM.)........................... =    .27977E-01
  DIFFUSIVITY MODULUS, (DIM.).................... =    .41503E+03
  TARGET EFFLUENT CONC., (uM/L).................. =    .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, .............................. = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)......................... =    .11611E+02
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .50095E+06
  BIOT NUMBER, (DIM.)........................... =    .28620E-02
  DIFFUSIVITY MODULUS, (DIM.).................... =    .40570E+04
  TARGET EFFLUENT CONC., (uM/L).................. =    .23600E-01
```

Model of RSSCT: EBCT = 12.3 min

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
              HSDM
          SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =          3
NUMBER OF AXIAL COLLOCATION POINTS ....... =         12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =         94
GAC NAME................................ = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =    .82200E-02
MASS OF ADSORBENT, (GRAMS)............... =    .10830E+01
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=    .73000E+00
LENGTH OF BED, (CM)...................... =    .49750E+01
DIAMETER OF BED, (CM).................... =    .80200E+00
VOID FRACTION OF BED, (DIM.)............. =    .40970E+00
FLOW RATE, (mL/MIN)...................... =    .76200E+01
SURFACE LOADING, (GPM/FT**2)............. =    .37020E+01
PACKED BED CONTACT TIME, (SEC)........... =    .81076E+01
EMPTY BED CONTACT TIME, (MIN)............ =    .32982E+00

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, .............................. = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L).......... =    .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.).......... =    .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)........... =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =    .28422E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.)......... =    .51500E+05
  BIOT NUMBER, (DIM.)........................... =    .45994E-02
  DIFFUSIVITY MODULUS, (DIM.)................... =    .61795E+03
  TARGET EFFLUENT CONC., (uM/L)................. =    .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, .............................. = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L).......... =    .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.).......... =    .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)........... =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =    .28422E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.)......... =    .50342E+06
  BIOT NUMBER, (DIM.)........................... =    .47052E-03
  DIFFUSIVITY MODULUS, (DIM.)................... =    .60406E+04
  TARGET EFFLUENT CONC., (uM/L)................. =    .23600E-01
```

Model of Full Scale: EBCT = 12.3 min

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
                    HSDM
                SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =            3
NUMBER OF AXIAL COLLOCATION POINTS ....... =           12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =          94
GAC NAME................................. = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =     .50000E-01
MASS OF ADSORBENT, (GRAMS)............... =    .65062E+07
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=     .73000E+00
LENGTH OF BED, (CM)...................... =    .32372E+03
DIAMETER OF BED, (CM).................... =     .24443E+03
VOID FRACTION OF BED, (DIM.)............. =     .41328E+00
FLOW RATE, (mL/MIN)...................... =    .12300E+07
SURFACE LOADING, (GPM/FT**2)............. =     .64331E+01
PACKED BED CONTACT TIME, (SEC)............ =     .30624E+03
EMPTY BED CONTACT TIME, (MIN)............ =     .12350E+02

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, ............................ = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =     .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =     .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =     .17391E+02
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =     .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .50745E+05
  BIOT NUMBER, (DIM.)........................... =    .27977E-01
  DIFFUSIVITY MODULUS, (DIM.)................... =    .62160E+03
  TARGET EFFLUENT CONC., (uM/L)................. =    .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, ............................ = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =     .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =     .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =     .17391E+02
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =     .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .49604E+06
  BIOT NUMBER, (DIM.)........................... =    .28620E-02
  DIFFUSIVITY MODULUS, (DIM.)................... =    .60763E+04
  TARGET EFFLUENT CONC., (uM/L)................. =    .23600E-01
```

Model of RSSCT = 16.4 min

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
           HSDM
        SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =          3
NUMBER OF AXIAL COLLOCATION POINTS ....... =         12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =         94
GAC NAME................................. = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =    .82200E-02
MASS OF ADSORBENT, (GRAMS)............... =    .14440E+01
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=    .73000E+00
LENGTH OF BED, (CM)...................... =    .66330E+01
DIAMETER OF BED, (CM).................... =    .80200E+00
VOID FRACTION OF BED, (DIM.).............. =    .40967E+00
FLOW RATE, (mL/MIN)...................... =    .76200E+01
SURFACE LOADING, (GPM/FT**2).............. =    .37020E+01
PACKED BED CONTACT TIME, (SEC)............ =    .10809E+02
EMPTY BED CONTACT TIME, (MIN)............ =    .43974E+00

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, .............................. = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =    .37896E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .51506E+05
  BIOT NUMBER, (DIM.)........................... =    .45994E-02
  DIFFUSIVITY MODULUS, (DIM.).................... =    .82394E+03
  TARGET EFFLUENT CONC., (uM/L).................. =    .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, .............................. = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)........................ =    .37896E+01
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .50349E+06
  BIOT NUMBER, (DIM.)........................... =    .47052E-03
  DIFFUSIVITY MODULUS, (DIM.).................... =    .80542E+04
  TARGET EFFLUENT CONC., (uM/L).................. =    .23600E-01
```

Model of Full Scale: EBCT = 16.4 min

```
MULTICOMPONENT PLUG FLOW HOMOGENEOUS SURFACE DIFFUSION MODEL
            HSDM
         SUMMARY OUTPUT FILE

NUMBER OF RADIAL COLLOCATION POINTS ...... =          3
NUMBER OF AXIAL COLLOCATION POINTS ....... =         12
TOTAL NO. OF DIFFERENTIAL EQUATIONS ...... =         94
GAC NAME................................ = Calgon F 400
RADIUS OF ADSORBENT PARTICLE, (CM)........ =    .50000E-01
MASS OF ADSORBENT, (GRAMS)............... =    .86750E+07
APPARENT PARTICLE DENSITY, (GM/CM**3) .....=    .73000E+00
LENGTH OF BED, (CM)...................... =    .43163E+03
DIAMETER OF BED, (CM).................... =    .24400E+03
VOID FRACTION OF BED, (DIM.).............. =    .41119E+00
FLOW RATE, (mL/MIN)...................... =    .12300E+07
SURFACE LOADING, (GPM/FT**2).............. =    .64560E+01
PACKED BED CONTACT TIME, (SEC)............ =    .40481E+03
EMPTY BED CONTACT TIME, (MIN)............. =    .16408E+02

PARAMETERS FOR COMPONENT 1
  COMPONENT NAME, .............................. = RDX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .10360E+02
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .25980E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .28620E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)......................... =    .23187E+02
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .51184E+05
  BIOT NUMBER, (DIM.)........................... =    .27977E-01
  DIFFUSIVITY MODULUS, (DIM.)................... =    .82880E+03
  TARGET EFFLUENT CONC., (uM/L).................. =    .21000E+00

PARAMETERS FOR COMPONENT 2
  COMPONENT NAME, .............................. = HMX
  INITIAL BULK CONCENTRATION, (uMOL/L)........... =    .11800E+01
  FREUNDLICH ISO. CAP., (uMOL/GM)/(uMOL/L)**XN .. =    .54270E+03
  FREUNDLICH ISOTHERM EXPONENT, (DIM.)........... =    .24100E+00
  FILM TRANSFER COEFFICIENT, (CM/SEC)............ =    .20000E-02
  STANTON NUMBER, (DIM.)......................... =    .23187E+02
  SURFACE DIFFUSION COEFFICIENT, (CM**2/SEC)..... =    .10000E-06
  SOLUTE DISTRIBUTION PARAMETER, (DIM.).......... =    .50033E+06
  BIOT NUMBER, (DIM.)........................... =    .28620E-02
  DIFFUSIVITY MODULUS, (DIM.)................... =    .81017E+04
  TARGET EFFLUENT CONC., (uM/L).................. =    .23600E-01
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