MODELING NATURAL ATTENUATION OF PETROLEUM HYDROCARBON CONTAMINATION IN GROUNDWATER USING ALTERNATE ELECTRON ACCEPTORS

By

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NOMENCLATURE

Acronyms:

BGS	below ground surface
BTEX	benzene, toluene, ethylbenzene, and xylene
C-C	carbon to carbon bond
COCs	chemicals of concern
EPA	Environmental Protection Agency
MCLs	Maximum Contaminant Levels
MW	monitoring well
NAPLs	non-aqueous phase liquids
OAC	Oklahoma Administrative Code
OCC	Oklahoma Corporation Commission
ODOT	Oklahoma Department of Transportation
PC	personal computer
RA	risk assessment
TOC	total organic carbon
USGS	United States Geological Survey

Units of Measure:

g	gram
mg	milligrams
kg	kilogram
L	liters

mL	milliliter
ATM	atmospheres
d	day
ft	foot or feet
yr	year
m	meter
m^3	cubic meter
°C	degrees Celsius
ft	feet
cm	centimeter
cm^3	cubic centimeter
s	second

1.0 INTRODUCTION

Contamination of groundwater supplies by gasoline and other petroleum-derived hydrocarbons is a serious and widespread environmental problem. Releases from underground storage tanks (USTs) and associated piping due to corrosion, ground movement, and poor installation practices are a prime source of hydrocarbon contamination. Approximately two million underground tanks stored gasoline in the United States (U.S.) in 1990, and 90,000 confirmed releases were reported between 1989 and 1990 (Kao and Borden, 1997). The leaking UST at the automobile service station on Patrick Air Force Base in Cocoa Beach, Florida provides a typical example of groundwater contamination resulting from a hydrocarbon release. Approximately 700 gallons of gasoline were released into the subsurface, and oily-phase residue continued to release water-soluble fuel hydrocarbons into the aquifer for more than eight years. Many such sites exist around the country with varying levels of contamination (Wiedemeier et al., 1995).

Gasoline is a complex mixture of many organic chemicals which have individual properties and behavior when in contact with soils and water (Nyer, 1993a). The aromatic group, composed of benzene, toluene, ethylbenzene, and xylene (BTEX), is typically the focus of concern at hydrocarbon contamination sites due to the physical properties and toxic nature of these chemicals. These water soluble components of gasoline have relatively high pollution potential due to their significant concentrations in gasoline, relatively high water solubility, and chronic toxicity. All BTEX compounds are powerful depressants to the central nervous system, and benzene is a confirmed carcinogen which can cause leukemia in humans (Beller et al., 1992).

Traditional processes for removing BTEX from aquifers include excavation, product skimming, pump and treat, in situ thermal or chemical treatment, soil venting, and engineered bioremediation. All of these options require equipment, materials, and manhours and may be quite costly to implement. BTEX compounds may be difficult to pump from an aquifer due to a tendency to sorb to the aquifer material. Other options, such as treatment with activated carbon or air strippers, merely transfer the contaminants from one phase to another without converting them into less hazardous components (Corseuil and Alvarez, 1996). Natural attenuation has recently emerged as an acceptable and less costly alternative to traditional treatment (Odermatt, 1997).

Mathematical models are becoming more commonly used by environmental consultants and scientists to simulate and predict the effectiveness of natural attenuation and to predict remediation costs and timetables. The use of these models is associated with a national move toward applying "risk management" strategy, rather than the "site remediation" strategy that was prevalent in the last decade. Computer modeling can be used to supplement risk assessments (RAs) to show the viability of using natural attenuation to remediate sites where immediate threats to human health, safety and the environment do not exist, and the chemicals of concern (COCs) are unlikely to impact a receptor. Provided that sufficient site characterization data are available, computer modeling can be used to predict the time required for natural attenuation to occur and any potential for contaminants to migrate off-site (Odermatt, 1997).

Several analytical and numerical computer models are currently available for simulating groundwater fate and transport. Of these models, relatively few incorporate biodegradation. The majority of the models incorporating biodegradation utilize first-order or Monod kinetics to approximate reactions. Recent developments in bioremediation modeling allow the use of instantaneous reactions in place of first-order or Monod kinetics. The use of instantaneous reactions has been shown to be very effective for simulating aerobic biodegradation (Rifai et al., 1995). With the development of the BIOSCREEN analytical model in 1996, the instantaneous reaction assumption was expanded to include simulation of anaerobic biodegradation utilizing alternate electron acceptor processes (Newell et al., 1996). Less than one year ago, a new numerical model incorporating instantaneous reactions and alternate electron acceptor simulation became available. This new model, BIOPLUME III, has not yet been applied to field data other than those utilized for model validation during the development phase (Rifai et al., 1998). The feasibility of using BIOPLUME III to support risk-based closure at typical petroleum contamination sites should be assessed. This endeavor will require an impartial comparison with a similar model, such as BIOSCREEN. Small petroleum contamination sites such as ODOT facilities often lack extensive site characterization data. The effects of limited input data on the accuracy and predictive capability of both BIOSCREEN and BIOPLUME III should be investigated.

This study evaluates the ability of BIOSCREEN and BIOPLUME III to simulate natural attenuation of petroleum contamination in groundwater at an Oklahoma Department of Transportation (ODOT) Residency Facility located in Edmond, Oklahoma (Site). Soil and groundwater at the Site are contaminated with petroleum hydrocarbons, specifically BTEX, which leaked from a fuel dispenser line. Analyses of groundwater samples from on-site monitoring wells show that both aerobic and anaerobic biodegradation are occurring at the Site, which indicates that natural attenuation models incorporating sequential electron acceptor processes are most applicable to this data (Caldwell, 1996). Limited Site characterization data are available to develop input data for the models.

This document discusses the current status of natural attenuation as a remediation technology and the physical and chemical processes associated with natural attenuation. The various natural attenuation models currently available are presented and categorized, and the state of the practice in bioremediation modeling is discussed. BIOSCREEN and BIOPLUME III are discussed in detail. The use of physical and chemical data for the ODOT Residency Facility to calibrate each model to match existing Site conditions is documented, and the natural attenuation predictions of each model are presented. The sensitivity, limitations, and predictive capability of each model are discussed. Ultimately, the feasibility of utilizing BIOSCREEN and

BIOPLUME III to simulate natural attenuation via alternate electron acceptor processes at limited-data petroleum contamination sites is evaluated.

2.0 REVIEW OF THE LITERATURE

Until recently, regulatory agencies and environmental groups tended to consider natural attenuation a "no action" remediation alternative. The body of technical literature documenting the function, versatility, and applicability of natural attenuation has grown, and the use of this approach for site management and remediation has increased in popularity. For example, "Intrinsic Bioremediation/Natural Attenuation" was selected as a topic area for the *Petroleum Hydrocarbons and Organic Chemicals in Ground Water: Prevention, Detection, and Remediation* conference in Houston, Texas, in November, 1996.

Natural attenuation has several advantages over traditional remediation processes, as follows (Corseuil and Alvarez, 1996):

- transforms contaminants to innocuous products,
- requires minimal disturbance of the site,
- avoids dewatering of the aquifer due to excessive pumping,
- travels with the contamination,
- involves no worker exposure to contaminants and no releases to the atmosphere,
- can be demonstrated through relatively inexpensive field and laboratory analytical methods,
- is very effective for BTEX, which are the constituents of regulatory concern at petroleum release sites,
- is generally less costly than traditional treatment processes, and
- biodegradation actually reduces the mass and concentration of petroleum contamination through microbial metabolization, instead of transferring the contamination from one phase to another.

Natural attenuation also has the following limitations (Corseuil and Alvarez, 1996 and Beller et al., 1995):

- May be sensitive to natural or man-induced changes in local hydrogeologic conditions and site operations,
- Typically requires a longer time period for remediation than more traditional techniques described in Section 1.0,
- May be viewed as a "do nothing" alternative by the public,
- Requires consistent site conditions,
- Requires definition of the groundwater plume, understanding of the site hydrogeology, and availability of groundwater data, and
- May require sampling and analysis to demonstrate that decreases in contaminant concentrations are the result of biological metabolism of compounds (rather than abiotic processes) in order to show that contaminants are actually being destroyed, rather than simply diluted or sorbed to aquifer material.

The advantages listed above have contributed to the increasing use of natural attenuation as a remediation alternative, particularly at sites contaminated with petroleum hydrocarbons. The current regulatory trend is toward development of risk-based cleanup levels using site-specific data, an evaluation of contaminant toxicity, and possible receptor exposure. When receptor exposure pathways do not exist, regulatory agencies are increasingly receptive to the use of natural attenuation remediation approaches, particularly in light of high capital costs required for active remediation alternatives (Morin and Henry, 1998). Implementation of natural attenuation as a plume management strategy in combination with risk assessment requires the following:

- site characterization;
- determination of whether contaminants are being attenuated and/or removed from the aquifer;

- modeling of the fate and transport of the dissolved groundwater plume; and
- long-term monitoring to confirm and ensure protection of human health and the environment.

The site characterization should provide data on the location and extent of the contaminant source(s), the extent and distribution of the dissolved contaminants, groundwater geochemical data, geologic data, and hydrogeologic parameters. The results of the site characterization are analyzed to identify and quantify the extent of natural attenuation occurring at the site. Three indicators primarily associated with biodegradation typically used to make this determination are (1) contaminant disappearance, (2) loss of electron acceptors, and (3) accumulation of degradation products. The site characterization data is also utilized during fate and transport modeling, which can be performed using numerical or analytical models. Following implementation of a natural attenuation site management program, groundwater monitoring should be conducted to track contaminant remediation and document success of the program (Rifai et al., 1995).

Site characteristics typical to successful implementation of natural attenuation include a homogeneous and permeable aquifer, contamination from a single source, low groundwater gradient, no free product, no soil contamination, and an easily degraded, extracted, or immobilized contaminant. Rarely will a contaminated site meet these ideal criteria for natural attenuation. However, each of the processes associated with natural attenuation may be described and approximated using educated engineering assumptions to accurately model remediation (Sims et al., 1992).

2.1 Natural Attenuation Processes

Naturally attenuating plumes may reach a quasi-steady-state condition at which the plume no longer grows in extent and begins to shrink somewhat over time. The major processes controlling the size of a steady-state plume include release of dissolved contaminants from the source area, downgradient transport of contaminants and mixing with uncontaminated groundwater, volatilization, and abiotic and biologically mediated transformations of the COCs. (Rifai et al., 1995).

The principle mechanisms of natural attenuation include dispersion, adsorption, volatilization, and biodegradation. BTEX compounds tend to be soluble and volatile due to relatively high solubilities and Henry's Law constants, respectively. Benzene has a moderate adsorption capacity, and all four compounds have specific gravities less than one. BTEX compounds are also biodegradable. The physical properties which dictate the behavior of BTEX compounds in groundwater are shown in Table 1. BTEX compounds are typically subject to the dispersion, adsorption, volatilization, and biodegradation mechanisms of natural attenuation, as discussed below.

2.1.1 Dispersion

Hydrodynamic dispersion is a process which includes molecular diffusion and mechanical dispersion and decreases contaminant concentrations through dilution. It is the process by which a contaminant plume spreads out in directions longitudinal and transverse to the direction of normal flow. Molecular diffusion, typically governed by Fick's law, is the molecular movement of a chemical in response to concentration gradients. Molecular diffusion is considered independent of groundwater flow and insignificant relative to mechanical dispersion, except in no-flow or low-flow groundwater situations. Mechanical dispersion is the spreading of molecules in the longitudinal and transverse directions due to interactions between advective movement of the chemical and the porous structure of the medium (ASTM, 1996).

2.1.2 Adsorption

Adsorption retards the advance of contaminant plumes relative to the groundwater flow velocity, thereby reducing the contaminant concentration in groundwater without decreasing the total

Table 1. Physical Properties of BTEX[1]

Chemical	Formula	Molar Weight	Solubility (mg/L)	Specific Gravity	K_{ow}	K_{oc}	Henry's Law Constant* (atm)	Adsorption Capacity at 500 ppb (mg-compound/g-carbon)
Benzene	C_6H_6	78.12	1.75×10^3	0.879	1.3×10^2	38 - 97	230	80
Toluene	$C_6H_5CH_3$	92.15	5.35×10^2	0.866	1.3×10^2	242	217	20
Ethylbenzene	$C_6H_5CH_2CH_3$	106.18	1.52×10^2	0.867	1.4×10^3	622	359	18
O-Xylene	$C_6H_4(CH_3)_2$	106.18	1.75×10^2	0.880	8.9×10^2	570	266	75

*at water temperature of 68°F

[1] From Nyer et al., 1993b and Yang et al., 1995

contaminant mass. It is considered a physical process because it does not irreversibly alter the contaminant. This process is an interphase interaction of a chemical between the water and the soil. Adsorption is primarily controlled by organic matter on the soil particle surface and the presence of clay minerals. A high fraction of organic carbon in the soil (f_{oc}) generally results in increased adsorption. The Langmuir, Freundlich, and linear isotherms are typically used to describe the relationship between the concentration of the contaminant sorbed on the soil and the equilibrium concentration remaining in groundwater. The slope of an adsorption isotherm is called the distribution coefficient, K_d, which is a ratio of sorbed to dissolved contaminant concentrations. Sorption of a chemical is directly proportional to the distribution coefficient, which is constant when described by the linear isotherm. The linear adsorption assumption typically fails in cases of low f_{oc}, large amounts of mineral clays, or for polar organic compounds. K_d can typically be estimated using the organic carbon partition coefficient (K_{oc}) and the f_{oc} for the soil (ASTM, 1996). K_{oc} is a measurement of the tendency of an organic compound to be adsorbed by the soil. The higher the K_{oc} value for a compound, the lower its motility and the higher its adsorption potential. K_{oc} values for benzene, toluene, and o-xylene were reported as 50, 339, and 255, respectively (Nyer et al., 1993a), and K_{oc} values reported for benzene range from 38 to 97 for benzene (Nyer et al., 1993b, Yang et al., 1995, and Newell et al., 1996). Adsorptive processes are typically described by a retardation factor which accounts for the bulk density of the soil, the distribution coefficient, and the effective porosity (ASTM, 1996).

2.1.3 Volatilization

Volatilization transfers contaminants from the groundwater to the atmosphere, provided appropriate conditions exist. It typically includes volatilization of the contaminant from soil and groundwater to soil gas and transfer of the soil gas to the atmosphere. Volatilization depends on both chemical-specific factors and media-specific conditions, and it is typically governed by Henry's law:

$$C_a = HC_w$$

Where: C_a = Concentration in air (g/cm^3-vapor)

H = Henry's law constant (dimensionless)

C_w = Concentration in water (g/cm^3-water)

Volatilization tends to contribute most to contaminant mass loss at sites where the water table is shallow or highly fluctuating (ASTM, 1996).

2.1.4 Biodegradation

Biodegradation is typically the principal mechanism for mass loss from BTEX plumes (Ollila, 1996). Intrinsic bioremediation can be defined as the transformation of a contaminant into innocuous products by indigenous microorganisms. Some requirements of intrinsic bioremediation processes include the following (Corseuil and Alvarez, 1996):

- Presence of microorganisms with potential to biodegrade the target compounds,
- Accessibility of target pollutants to the microorganisms,
- Adequate pH,
- Induction of appropriate degradative enzymes,
- Availability of electron acceptors,
- Availability of inorganic nutrients,
- Adequate temperature,
- Absence of toxic substances, and
- Faster biodegradation than migration rate.

Of these requirements for intrinsic bioremediation, the distribution and availability of electron acceptors are considered to have the most influence on the rate of in situ biodegradation. In fact, other factors rarely limit the amount of biodegradation occurring at petroleum release sites (Rifai et al., 1998).

2.1.4.1 Microorganisms

A wide variety of microorganisms typically accompany natural organics present in both soil and groundwater. Although microorganisms may exist even in areas that have low natural organic material, the rhizosphere (root zone) typically contains the greatest variety and largest number of microorgansims. Several genera of natural bacteria and fungi present in soil and groundwater are capable of degrading hydrocarbon substrates. The most prevalent hydrocarbon degrading bacteria are *Achromobacter, Alcaligenes, Arthrobacter, Bacillus, Flavorbacterium, Nocardia, Pseudomonas, Corynebacterium,* and *Micrococcus*, and typical fungi include *Trichoderma, Penicillum, Asperigillus, Mortierella, and Phanerochaete.* Any of these typically occurring bacteria and fungi are capable of degrading BTEX (Bowlen, 1995 and Nyer et al., 1996). Surface soil typically contains 0.1 to 1 billion cells per gram of soil. Subsurface soil concentrations range between 1,000 and 10,000,000 cells per gram of soil, and groundwater typically contains 100 to 200,000 bacterial cells per milliliter of water (Nyer et al., 1996). Field studies have shown BTEX degrading bacteria concentrations in groundwater on the order of 10^2 to 10^3 (Troy et al., 1995).

Intrinsic biodegradation is the process in which indigenous microorganisms convert or degrade natural and man-made organic compounds, with no man-induced process alterations, to obtain energy conserved in the carbon to carbon (C-C) bonds of the compounds (Nyer et al., 1996). Microorganisms obtain energy for cell production and maintenance by facilitating the transfer of electrons from electron donors to electron acceptors, which results in the oxidation of the electron donor and the reduction of the electron acceptor (Wiedemeier et al, 1995).

2.1.4.2 Accessibility of Contaminant

A common limitation of natural degradative processes is the lack of adequate contact between pollutants and microorganisms. In order for complete degradation by membrane-bound enzymes to occur, the contaminant molecule must be small enough to enter the microbial cell. Very large contaminant molecules are often recalcitrant to biodegradation. Enzyme attack can be impeded by the number, length, or location of functional groups. Strong sorption to aquifer material can also hinder enzyme attack and reduce effectiveness of intrinsic bioremediation. BTEX molecules are small, relatively soluble, and tend to be readily available for biodegradation in most subsurface systems (Godsy, 1994).

2.1.4.3 pH

Near-neutral aquifer pH values between 6.5 and 7.5 are typically optimum for the biodegradation of contaminant organic material, although most microorganisms can perform well within a pH range of 5 to 9. The hydrogen ion concentration of groundwater is governed by the types of compounds produced by bacterial activity, and it is controlled by CO_3^{2-}:HCO_3^-:CO_2 equilibrium rates. Because hydrogen ion transfer is commonly involved in electron transport, pH and redox potential are interdependent. Redox potential is extremely important in the biotransformation of contaminants, as described below (Godsy, 1994).

2.1.4.4 Energetics and Electron Transfer

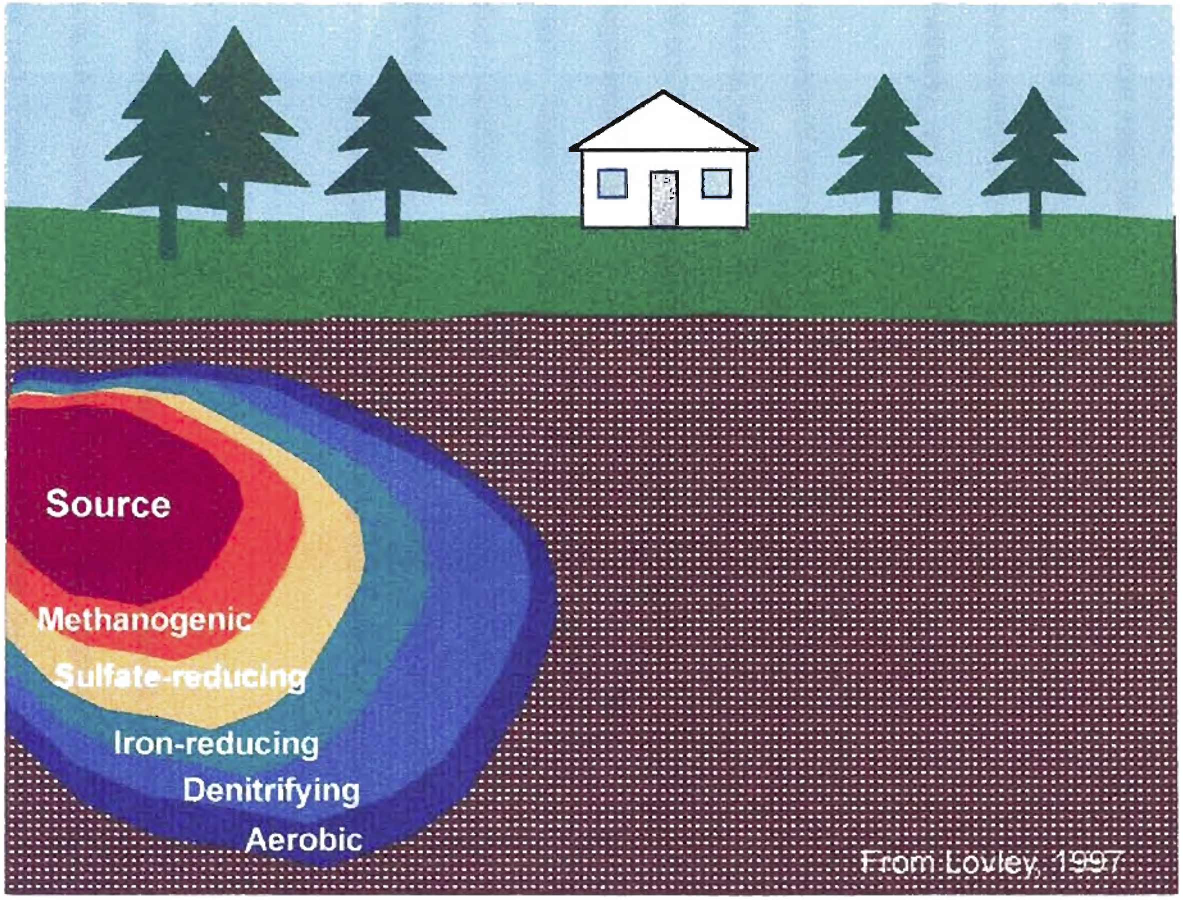
All living organisms must replenish enzymatic systems and maintain the oxidation-reduction power cycle. This involves the reduction of oxidized compounds by the addition of electrons released from compounds oxidized during energy production. Electron acceptors can be either organic or inorganic compounds. Oxygen, nitrate, iron(III) oxides, and sulfate have all been identified as potential electron acceptors in the biochemical pathway for hydrocarbon degradation (Borole et al., 1996). The respiration processes microorganisms use to bring about a reduction in total contaminant mass in groundwater are aerobic respiration, denitrification, iron or manganese reduction, sulfate reduction, and methanogenesis (Kampbell et al., 1996). Typical reactions for biodegradation of benzene are as follows (from Kampbell et al., 1996):

- Aerobic respiration $7.5O_2 + C_6H_6 = 6CO_{2,g} + 3H_2O$
- Denitrification $6NO_3^- + 6H^+ + C_6H_6 = 6CO_{2,g} + 6H_2O + 3N_{2,g}$
- Iron reduction $60H^+ + 30Fe(OH)_3 + C_6H_6 = 6CO_{2,g} + 30Fe^{2+} + 78\ H_2O$

- Sulfate reduction $7.5H^{+} + 3.75SO_4^{2-} + C_6H_6 = 6CO_{2,g} + 3.75H_2S^0 + 3\ H_2O$
- Methanogenesis $4.5H_2O + C_6H_6 = 2.25CO_{2,g} + 3.75CH_4$

In aerobic respiration, the final electron acceptor is O_2. The final reduced substrate in aerobic respiration is H_2O and the final oxidized compound respired from energy production is CO_2. Petroleum hydrocarbons are readily biodegradable at background dissolved oxygen levels above 2 mg/L. However, a heavily contaminated site will typically be oxygen-depleted in the source zone due to ongoing bacterial respiration. Although aerobic biodegradation proceeds at relatively higher rates than anaerobic processes, it is generally limited by the oxygen supply. Respiration in oxygen-poor conditions (less than 1 to 2 mg/L oxygen) tends to favor the most oxidized compounds, which have the highest redox potential. The resultant sequential utilization scheme is as follows: O_2, NO_3^-, Fe^{3+}, SO_4^{2-}, CO_2 (Rifai et al., 1995). Environmental conditions and microbial competition will ultimately determine which processes will dominate at a given site (Wiedemeier et al., 1995). Zonation of electron acceptor utilization in the direction of groundwater flow typically results, as shown in Figure 1. However, field studies have shown that biochemical mechanisms with similar energy potentials, such as aerobic oxidation and nitrate reduction, may occur simultaneously when electron acceptor concentrations are reduced, rather than completely depleted (Rifai et al., 1998).

Denitrification is a process promoted by facultative anaerobes, which are bacteria that can thrive under either aerobic or anaerobic conditions. These microbes can use O_2 as the terminal electron acceptor when it is available, or use NO_3^- as the terminal electron acceptor in the absence of oxygen. Toluene and o-xylene biodegradation have been conclusively shown under denitrifying conditions (Evans et al., 1991). Other work documents the degradation of BTEX under nitrate reducing conditions (Anid et al., 1993 and Zeyer et al., 1986). When oxidation-reduction potentials within soils are even lower, other inorganic compounds are used by specific groups of bacteria as terminal electron acceptors. Several common alternative electron



From Lovley, 1997

Figure 1. Theoretical Zonation of Terminal Electron Acceptor Processes

acceptors and associated bacterial groups include ferric iron (iron reducers), SO_4^{2-} (sulfate reducers), and CO_2 (methanogens). The predominant form of microbially reducible Fe (III) in most soils and sediments is poorly crystalline iron (III) oxides. These iron (III) oxides are highly insoluble (Coates et al., 1996). BTEX reduction under sulfate-reducing conditions has been studied in detail (Coates et al., 1996; Edwards et al., 1992; and Beller et al., 1996), and toluene and xylene are most likely to degrade under these conditions. Sulfanogenic and methanogenic bacteria tend to be extremely sensitive to oxygen (Godsy, 1994 and Nyer et al., 1996). Anaerobic biodegradation of aromatic hydrocarbons is associated with the production of fatty acids, methane, and carbon dioxide; solubilization of iron; and reduction of nitrate and sulfate.

The occurrence of intrinsic biodegradation of dissolved BTEX plumes using oxygen, nitrate, iron, and sulfate as terminal electron acceptors has been widely documented in the literature (Rifai et al., 1995 and Lovley, 1997). Utilization of carbon dioxide as a terminal electron acceptor during methanogenesis has also been documented for BTEX biodegradation (Lovley, 1997 and Borden et al., 1997). These studies, which include both laboratory and field data, have shown not only sequential utilization of electron acceptors, but also a distinct order of biodegradation. Toluene and o-xylene tend to degrade more quickly than m-xylene, p-xylene, and benzene, and ethylbenzene tends to be the least biodegradable (Edwards and Grbic-Galic, 1992).

2.1.4.5 Nutrients

Nutrient elements are critical components of genetic material, structural molecules, enzymes, and intracellular plasma that compose bacteria, as illustrated by typical composition of a bacterial cell (Table 2). Note that Table 2 represents each component on a dry weight basis. Water constitutes 80 to 90% of cellular weight and is always a major requirement for growth. Although the proportion of nutrient elements required for growth may vary widely among different types of bacteria, bacteria require carbon, hydrogen, sulfur, nitrogen, and phosphorous. Carbon

Table 2. Typical Molecular Composition of a Bacterial Cell[1]

Element	Dry Weight %
Carbon	50
Oxygen	20
Nitrogen	14
Hydrogen	8
Phosphorous	3
Sulfur	1
Potassium	1
Sodium	1
Calcium	0.5
Magnesium	0.5
Chlorine	0.5
Iron	0.2
Others	0.3

[1] From Nyer et al., 1996

and hydrogen are major components of organic compounds and are typically present in adequate quantities for growth, as is sulfur. Nitrogen and phosphorous are typically the growth-limiting elements. A typically recommended carbon/nitrogen/phosphorous ratio (C/N/P) is 300 to 100:10:1 to 0.05 (Godsy, 1994 and Nyer et al., 1996).

2.1.4.6 Temperature

Groundwater temperature is an important factor in controlling microbial activity and rates of organic matter decomposition. Chemical and enzymatic reaction rates in a microbial cell increase as the temperature rises. Low temperatures reduce the fluidity and permeability of the cellular membrane, which hinders nutrient and contaminant uptake (Corseuil and Alvarez, 1996 and Nyer et al., 1996). Rates of enzymatic degradation and bacterial metabolism typically double for every 10°C increase in temperature up to inhibitory temperatures, which are 40 to 50°C for most bacteria. However, bacteria are generally capable of degradation at most ambient temperatures, and biological reactions will generally occur year-round in an aquifer. Temperature can also affect biodegradation rates by changing the physical properties, bioavailability, or toxicity of the contaminant. For example, an increased temperature may increase sorption to aquifer materials (Godsy, 1994).

2.1.4.7 Toxic Materials

Conditions that restrict life or inactivate microbial enzymes are incompatible with intrinsic bioremediation. For example, if aquifer microorganisms encounter potentially toxic contaminants, such as high concentrations of heavy metals, bacterial growth will be impeded. Chemical agents of this sort can disrupt cellular activity by interfering with protein function. Typical BTEX plumes do not exhibit significant toxic effects on indigenous microorganisms unless other more toxic contaminants are present (Godsy, 1994).

2.1.4.8 Biodegradation Rate

In order to insure that the contaminant plume will recede, rather than spread, the rate of biodegradation must exceed the rate of plume migration. Biodegradation can be measured by the loss of original substrate, consumption of electron acceptors, or the production of by-products. Biodegradation rates can be dictated by factors such as the rate of substrate and electron acceptor movement in the aquifer and the rate that electron acceptors are utilized. In comparison to the rate of movement by advection, oxygen and nitrate utilization can be considered to be instantaneous. The rates of these two processes are then dictated by the rate of electron acceptor movement in the aquifer. Rates of sulfate, iron, and carbon dioxide utilization may be governed by the biochemical reaction rate (Nyer et al., 1996) or by instantaneous reactions (Newell et al., 1996), depending on site-specific conditions. Biodegradation rates are site-specific and difficult to compare for various sites, and biodegradation rates in the field consistently tend to be much lower than the same rates quantified during laboratory simulations (Edwards and Grbic-Galic, 1992). Studies have indicated first-order BTEX decay rates in the laboratory of approximately 0.016 to 0.045 d^{-1} and field decay rates ranging from approximately 0.0002 to 0.038 d^{-1} for various sites (Borden et al., 1997, Hutchins et al., 1991, and Wiedemeier et al., 1996).

Laboratory studies have shown that degradation rates can be sensitive to the presence of readily degradable co-substrates and geochemical factors. For example, consider the sequential degradation of BTEX compounds: degradation of toluene, p-xylene, o-xylene, and ethylbenzene typically precede benzene degradation except in aerobic conditions. Ethylbenzene degrades more rapidly in nitrate-reducing conditions than in sulfate-reducing conditions (Reinhard et al., 1997).

2.2 Modeling Bioremediation

When evaluating natural attenuation as a potential remediation alternative, the time required for remediation and predicted migration of the plume should both be determined. Several analytical and numerical fate and transport models are available to determine these parameters by simulating advection, dispersion, sorption, and source dissolution in contaminated aquifers. Analytical models are typically simple to use, but they are limited to simulation of simplified hydrogeologic scenarios. Numerical models can simulate heterogeneous systems and complex hydrogeologic and contaminant scenarios, but they tend to be more complicated and require more extensive input data. Of the many groundwater transport models available, relatively few also incorporate a component to simulate biodegradation. Table 3 lists models which are capable of simulating biodegradation.

The most common method for simulating biodegradation utilized by older models such as ULTRA, developed in 1986, and the original Domenico model, developed in 1987, is by use of a first-order decay equation of the form:

$$C = C_0 e^{-kt}$$

where C is the biodegraded concentration of the chemical, C_0 is the initial chemical concentration, and k is the rate of decrease of the chemical (Rifai and Bedient, 1995). The COC is assumed to biodegrade exponentially, and the first-order decay constant is specified by the modeler. This constant is typically modified to achieve model calibration. Although current scientific literature documents many first-order decay constants, they are specific to both the site and the contaminant. The use of this method can overestimate the effect of biodegradation on a given system because electron acceptor limitations are not accounted for. Alternatives to the first-order decay model are available (Rifai et al., 1995).

In 1988, a one-dimensional finite difference model titled BIO1D was developed to simulate biodegradation and sorption. BIO1D incorporates the Monod kinetic expression, which describes microbial growth and is composed of first-order, mixed-order, and zero-order regions.

Table 3. Groundwater Transport Models Capable of Simulating Biochemical Reactions

Model	Release Date	Multiple Electron Acceptor?	Contact Information
PORFLO	1985	N	N.W. Kline; Boeing Computer Services; P.O. Box 300, Richland, WA 99352
BIOPLUME I	1986	N	H.S. Rifai; Rice University, Dept. of Environmental Sciences and Engineering, P.O. Box 1892, Houston, TX 77251
AT123D	1987	N	G.T. Yeh; Dept. of Civil Engineering, Pennsylvania State University, University Park, PA 16802
BIOPLUME II (v. 1.1)	1989	N	H.S. Rifai; Rice University, Dept. of Environmental Sciences and Engineering, P.O. Box 1892, Houston, TX 77251
MT3D (v. 1.11)	1992	N	C. Zheng; S.S. Papadopulos & Assoc., Inc., 7944 Wisconsin Ave., Bethesda, MD 20814
BioF&T 3D		Y	Scientific Software Group; P.O.Box 23041, Washington, DC 20026-3041
BIOSCREEN (v. 1.4)	1997	Y	J.T. Wilson; Subsurface Protection and Remediation Division, National Risk Management Research Laboratory, Ada, Oklahoma 74820
BIO1D (v. 1.2)	1989	N	P. Srinivasan and J. W. Mercer, GeoTrans, Inc., 250 Exchange Place, Suite A, Herndon, VA 22070
BIOMOD-3D		N	Scientific Software Group; P.O.Box 23041, Washington, DC 20026-3041
2DFATMIC (v. 1.0)	1997	N	G.T. Yeh; Dept. of Civil Engineering, Pennsylvania State University, University Park, PA 16802
3DFATMIC (v. 1.0)	1997	N	G.T. Yeh; Dept. of Civil Engineering, Pennsylvania State University, University Park, PA 16802
SEAM3D	1998	Y	Mark A. Widdowson, Department of Civil Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0105
BIOPLUME III (v 1.0)	1998	Y	H.S. Rifai; Rice University, Dept. of Environmental Sciences and Engineering, P.O. Box 1892, Houston, TX 77251
RT3D	1998	Y	Brian Hooker, Pacific Northwest National Laboratory, or BOSS International, www.bossintl.com

The Monod equation is as follows:

$$\mu = \mu_{max} [C / (K_c + C)]$$

where μ is the growth rate ($time^{-1}$), μ_{max} is the maximum specific growth rate ($time^{-1}$), and C is the concentration of the growth-limiting substrate (mg/L). K_c is the half-saturation constant or the growth-limiting substrate concentration which allows the microorganism to grow at half the maximum specific growth rate (Rifai and Bedient, 1995).

One of the first alternatives to utilizing first-order or Monod decay to model biodegradation is the use of an instantaneous reaction assumption. The BIOPLUME II model incorporates this assumption by combining the basis of an earlier model, BIOPLUME I, with the USGS two-dimensional solute transport model and adding superimposed oxygen and hydrocarbon plumes. The original BIOPLUME model was developed in 1986 and based on modifications to the U.S. Geologic Survey (USGS) Method of Characteristics Model. It is capable of simulating aerobic biodegradation as an instantaneous microbial reaction that is limited by the amount of electron acceptor available. Anaerobic biodegradation is simulated as first-order decay in hydrocarbon concentrations, and specific anaerobic decay reactions are not addressed (Rifai et al., 1998). BIOPLUME II is a two-dimensional numerical model capable of simulating advection, dispersion, mixing, and retardation, in addition to oxygen-limited biodegradation conditions. This model provides for simulation of a heterogeneous aquifer system with a variable flow field. Instantaneous reactions between oxygen and hydrocarbons are assumed, and the transport equation is solved twice to simulate these two superimposed plumes. Anaerobic biodegradation is simulated as first-order decay in hydrocarbon concentrations. BIOPLUME II is currently being used by Environmental Protection Agency (EPA) regional offices, U.S. Air Force facilities, and by consulting firms (Rifai et al., 1995). Both BIOPLUME and BIOPLUME II have been successfully calibrated to field sites (Rifai et al., 1998).

Recently-developed bioremediation modeling software incorporates simulation of anaerobic biodegradation utilizing sequential electron acceptor processes. As shown in Table 3, bioremediation models developed in 1997 and 1998 (BIOSCREEN, BIOPLUME III, SEAM3D, and RT3D) are capable of simulating alternate electron acceptor processes.

BIOSCREEN is based on the 1987 Domenico three-dimensional analytical solute transport model. BIOSCREEN adapts the original Domenico model to allow simulation of transport with no decay, transport with first-order decay, or transport with instantaneous biodegradation reactions. In addition to aerobic biodegradation, BIOSCREEN simulates anaerobic processes using nitrate, ferric iron, sulfate, and carbon dioxide as electron acceptors. The source term and dispersivity are used as calibration parameters, which allows a more refined calibration than a first-order simulation. BIOSCREEN is spreadsheet-based and relatively simple, compared to numerical models (Newell et al., 1996). Spreadsheet analytical models of this type were compared to BIOPLUME II and found to produce consistent results, although limited in prediction ability for complex flow paths in heterogeneous aquifers (Ollila, 1996 and Rifai et al., 1998).

BIOPLUME III became available from the EPA website in February, 1998. It is a two-dimensional numerical model capable of simulating groundwater transport and biodegradation utilizing first-order, Monod, or instantaneous reaction assumptions. The instantaneous reaction can be applied to both aerobic and anaerobic biodegradation if the microbial reaction is assumed to occur at a much faster rate than the rate of electron acceptor replenishment via flowing groundwater. This reaction assumes biodegradation is limited by the amount of electron acceptor available (Rifai et al., 1998). This assumption is valid, based on studies showing complete anaerobic biodegradation of BTEX in 10 to 72 days (Edwards et al., 1992 and Reinhard et al., 1997). BIOPLUME III also provides for anaerobic biodegradation simulation with sequential utilization of nitrate, ferric iron, sulfate, and carbon dioxide as electron acceptors. Six plumes are tracked simultaneously: hydrocarbon, oxygen, nitrate, ferrous iron, sulfate, and carbon dioxide. During development of the BIOPLUME III model, it was tested by comparing various single-electron-acceptor simulations to BIOPLUME II predictions. Eight sets of data for field sites were used to calibrate the model during development (Rifai et al., 1998). Aside from the *BIOPLUME III User's Manual*, no published literature was located describing field-scale application of the software.

All of the models discussed above treat the petroleum hydrocarbon as a single compound by combining BTEX into one parameter. Two additional models, RT3D and SEAM3D, developed in 1998, are capable of simulating transport and biodegradation of multiple constituents in three dimensions, utilizing sequential electron acceptors. SEAM3D is a block-centered, finite-difference computer algorithm which interfaces with the groundwater flow model MODFLOW. SEAM3D assumes Monod kinetics for biodegradation, modified to include effects of electron acceptor and nutrient availability, inhibition, and threshold concentrations. SEAM3D includes manganese as an electron acceptor, whereas BIOPLUME III and BIOSCREEN do not, but it does not incorporate instantaneous reactions. To date, the theoretical model supporting SEAM3D and hypothetical demonstration scenarios have been documented in scientific literature. No field-scale analyses have been conducted utilizing SEAM3D (Waddill and Widdowson, 1998).

RT3D is based on the 1997 version of MT3D and incorporates three-dimensional reactive groundwater transport. Multiple sorbed and aqueous phase contaminants and reactions can be defined, and user-defined kinetic expressions can be employed. Instantaneous reactions utilizing oxygen, nitrate, ferric iron, sulfate, and carbon dioxide as electron acceptors are an option (BOSS International, 1998). RT3D results were compared to actual natural attenuation field data during model validation efforts conducted by researchers at Pacific Northwest National Laboratory. Although field results were matched exactly during model validation, other field-scale applications of RT3D have not been published (K.S.B., 1997).

3.0 METHODOLOGY

The methodology for this project included selecting modeling software packages based on a review of the available models, gathering and summarizing available data for the study Site, modeling and comparing actual data from the study Site, and evaluating results. Each of these tasks is discussed in greater detail in the following sections.

3.1 Modeling Software Packages Selected

The selected software packages are BIOSCREEN and BIOPLUME III, which are both Natural Attenuation Decision Support Systems produced by the EPA Office of Research and Development. These models were selected based upon the capability to simulate natural attenuation utilizing instantaneous reactions and bioremediation via alternate electron acceptor processes. BIOSCREEN is an analytical model, and BIOPLUME III is a numerical model, which allows a comparison between the two model types and complexities to be made. The limitations of the two models do not preclude the ODOT Residency Facility, and both models were readily available. The two models were compared and evaluated based on the following criteria:

- ability to model natural attenuation,
- ability to simulate advection, dispersion, and adsorption,
- ability to model alternate electron acceptor processes,
- mathematical basis of model,
- limitations,
- input data required,
- complexity,
- availability, and
- cost.

Tables 4 and 5 summarize the applicability of these criteria to each model.

Table 4. BIOSCREEN Evaluation Criteria

Criteria	Applicability to BIOSCREEN
Ability to model natural attenuation:	BIOSCREEN simulates natural attenuation.
Ability to simulate advection, dispersion, and adsorption:	BIOSCREEN simulates advection, dispersion, and adsorption.
Ability to model alternate electron acceptor processes:	BIOSCREEN simulates oxygen, nitrate, ferric iron, sulfate, and carbon dioxide electron acceptor processes.
Mathematical basis of model:	BIOSCREEN is based on the Domenico analytical solute transport model. It can simulate both aerobic and anaerobic decay. Groundwater transport can be modeled in the x-direction with first-order, instantaneous, or no decay biodegradation. Three-dimensional dispersion can be simulated.
Limitations:	BIOSCREEN assumes simple groundwater flow conditions. It is a screening tool that makes simplifying assumptions, and is not intended to produce extremely detailed and accurate natural attenuation data for complex sites.
Input data required:	BIOSCREEN requires seepage velocity; hydraulic conductivity; hydraulic gradient; effective porosity; longitudinal, transverse, and vertical dispersivity; estimated plume length; retardation factor; soil bulk density; organic carbon partition coefficient; fraction organic carbon; first-order decay coefficient; dissolved plume solute half-life; delta oxygen; delta nitrate; observed ferrous iron; delta sulfate; observed methane; model area length and width; simulation time; source thickness in saturated zone; source zone width; source zone concentration; and soluble mass in source zone.
Complexity:	BIOSCREEN is a user-friendly screening level tool which incorporates simplifying assumptions.
Availability:	BIOSCREEN is readily available for download from the EPA internet site.
Cost:	BIOSCREEN is free.

Table 5. BIOPLUME III Evaluation Criteria

Criteria	Applicability to BIOPLUME III
Ability to model natural attenuation:	BIOPLUME III simulates natural attenuation.
Ability to simulate advection, dispersion, and adsorption:	BIOPLUME III simulates advection, dispersion, and adsorption.
Ability to model alternate electron acceptor processes:	BIOPLUME III simulates oxygen, nitrate, ferric iron, sulfate, and carbon dioxide electron acceptor processes.
Mathematical basis of model:	BIOPLUME III is a two-dimensional natural attentuation model that can simulate sequential biological decay via first-order, Monod, or instantaneous reactions. The principle of superposition is used to combine the hydrocarbon plume with the electron acceptor plume(s), and the transport equation is solved six times to account for the electron acceptors. BIOPLUME III is based on BIOPLUME II, which is based on the USGS Method of Characteristics Model dated July, 1989. Three-dimensional dispersion can be simulated.
Limitations:	BIOPLUME III is two-dimensional and is a simplification of complex redox reactions. The model does not account for selective or competitive biodegradation of hydrocarbons, so BTEX compounds are simulated as a lumped parameter.
Input data required:	BIOPLUME III requires definition of the model grid and simulation time; porosity; longitudinal dispersivity; storativity; dispersivity ratio; transmissivity; recharge; aquifer thickness; constant head and constant flux boundaries; initial water table; initial concentration of contaminants, oxygen, nitrate, ferrous iron, ferric iron, sulfate, and carbon dioxide; source/sink parameters; aquifer bulk density; sorption coefficient; kinetic model identifiers for each electron acceptor; concentration of microorganisms in the aquifer; microbial retardation coefficient; half-saturation constant for contaminant and electron acceptor; numerical parameter definitions; and output control parameters
Complexity:	BIOPLUME III is user-friendly due to the Windows interface and Environmental Information System (EIS) Graphical User Interface Platform. It is a numerical model that requires significant input data.
Availability:	BIOPLUME III is readily available for download from the EPA internet site.
Cost:	BIOPLUME III is free.

3.1.1 BIOSCREEN

BIOSCREEN is a Microsoft® Excel spreadsheet screening model which simulates natural attenuation of dissolved hydrocarbons at petroleum fuel release sites. It is a user-friendly, simple package, and it does not have any extraordinary personal computer (PC) requirements. This model is readily available for download from the EPA internet site (www.epa.gov) at no charge.

As described above, BIOSCREEN is based on the Domenico analytical model and is able to simulate advective transport, three-dimensional dispersion, and adsorption. Solute transport with instantaneous biodegradation reactions uses a superposition method to account for electron acceptor limitations. The BIOSCREEN version of the Domenico equation, including the instantaneous reaction superposition algorithm, is in Appendix A. As shown in Appendix A, BIOSCREEN assumes a fully penetrating vertical plane source oriented perpendicular to groundwater flow to simulate the release of organics to moving groundwater (Newell et al., 1996).

Aerobic or anaerobic biodegradation can be simulated with BIOSCREEN, assuming sequential utilization of electron acceptors such as nitrate, ferric iron, sulfate, and carbon dioxide. Biodegradation reactions can be simulated as first-order decay or instantaneous reactions. To apply an electron-acceptor-limited kinetic model, such as the instantaneous reaction, the amount of biodegradation that can be supported by the groundwater moving through the source zone must be calculated. The conceptual model used in BIOSCREEN is as follows (Newell et al., 1996 and Rifai et al., 1998):

- Groundwater upgradient of the source contains electron acceptors.
- Non-aqueous phase liquids (NAPLs) and contaminated soil release BTEX as upgradient groundwater moves through the source zone.

- Biological reactions occur until the available electron acceptors in groundwater are consumed.
- The total amount of electron acceptors available can be calculated by measuring differences between upgradient and source zone concentrations.
- A utilization factor based on stoichiometric relationships can be developed to show the ratio of electron acceptor consumed (or metabolic by-product produced) to the mass of dissolved hydrocarbon degraded. BIOSCREEN assumes the following utilization factors for combined BTEX in (g/g):

  O_2 - 3.14 NO_3^- - 4.9 Fe^{3+} - 21.8 SO_4^{2-} - 4.7 CO_2 - 2.17

  These utilization factors represent the grams of electron acceptor utilized for each gram of hydrocarbon degraded.
- The potential biodegradation capacity of an aquifer depends on the utilization factor specified for each electron acceptor. Dividing the background concentration of an electron acceptor by its utilization factor provides an estimate (in concentration units) of the assimilative capacity of the aquifer by that mode of biodegradation.

Because it incorporates simplifying assumptions, BIOSCREEN is not considered a substitute for detailed mathematical model analysis which may be necessary to make final regulatory decisions at complex sites. This package is intended to be used as a screening tool to determine whether full-scale site characterization and mathematical modeling are appropriate at a particular site. The BIOSCREEN model may also be applicable at small sites with simple subsurface conditions and limited data. The model should not be applied where pumping systems create a complicated flow field, where vertical flow gradients affect contaminant transport, or where hydrogeologic conditions change dramatically over the simulation domain (Newell et al., 1996).

BIOSCREEN simulations require hydrogeologic, dispersion, adsorption, and biodegradation data in addition to general information about the contamination source. The input data required by BIOSCREEN varies according to the simulation type chosen. For example, first-order decay requires a first-order decay coefficient, whereas the instantaneous reaction model requires specific electron acceptor information instead. Certain parameters required by the model may be entered directly or calculated by the software, depending on which data are available. The following data are required by BIOSCREEN (Newell et al., 1996):

- Seepage velocity *or* hydraulic conductivity, hydraulic gradient, and effective porosity;
- Longitudinal, transverse, and vertical dispersivity *or* estimated plume length;
- Retardation factor *or* soil bulk density, organic carbon partition coefficient, and fraction of organic carbon;
- First-order decay coefficient *or* dissolved plume solute half-life for first-order biodegradation, *or* the reduction in oxygen, sulfate, and nitrate in addition to the source area concentrations of ferrous iron and methane for alternate electron acceptor biodegradation;
- model area length and width and simulation time; and
- source area dimensions, concentration, and mass of contaminants in the source zone.

These BIOSCREEN input parameters are listed according to data type and defined in Appendix B. Site-specific values used in model simulations for this study are discussed in Section 3.3.1 below.

3.1.2 BIOPLUME III

BIOPLUME III is a detailed stand-alone numerical model that operates in the Microsoft® Windows 95 environment. Although the software is user-friendly, development of an accurate simulation requires considerable familiarity with the program and the *User's Manual*. This program does not require any extraordinary personal computer (PC) hardware to operate. This model is readily available for download from the EPA internet site (www.epa.gov) at no charge.

BIOPLUME III is a two-dimensional, finite-difference model for simulating biodegradation of hydrocarbons in groundwater. This program is able to simulate advective transport, dispersion, adsorption, ion exchange, and biodegradation using alternate electron acceptor processes. BIOPLUME III incorporates the following assumptions (Rifai et al., 1998):

- Darcy's law is valid and hydraulic head gradients are the only driving mechanism for flow.
- The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.
- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- No chemical reactions occur that affect the fluid properties or the aquifer properties.
- Ionic and molecular diffusion are negligible contributors to the total dispersive flux.
- Vertical variations in head and concentration are negligible.
- The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

BIOPLUME III is capable of simulating bioremediation using first-order decay, instantaneous reactions, or Monod kinetics. As described above for BIOSCREEN, the biodegradation capacity of the aquifer must be calculated by the model in order to apply an electron-acceptor-limited kinetic model such as the instantaneous reaction. The conceptual model utilized by BIOPLUME III is identical to that described above for BIOSCREEN (Rifai et al., 1998).

BIOPLUME III is based on simplifications of the complex biologically mediated redox reactions that occur in the subsurface. Aerobic and anaerobic biodegradation processes are simulated utilizing oxygen, nitrate, ferric iron, sulfate, and carbon dioxide as electron acceptors. Manganese is not included. Ferric iron is simulated based on the production and transport of ferrous iron, which is a soluble by-product of the iron reaction. The model solves the transport equation six times to determine the fate and transport of the hydrocarbons and electron acceptors or reaction by-products. The BIOPLUME III equations and associated variables are in Appendix C, and the BIOPLUME II equations are provided for comparison. BIOPLUME III does not account for selective or competitive biodegradation of hydrocarbons; rather, BTEX is simulated as a single organic compound due to the difficulty of determining how much electron acceptor is available for each individual component (Rifai et al., 1998).

Numerical models typically require that the modeler determine what data are required and how to incorporate the field data into the modeling process. Typical data requirements include estimates of aquifer thickness, matrix conductivity, porosity, and sorptive characteristics. A description of the hydraulic and hydrologic behavior of the system, including boundary conditions or recharge data, is also required, and the source representation and electron acceptor availability must also be determined. Numerical models must be calibrated to match existing site hydraulics and contamination conditions (Rifai et al., 1995). In accordance with typical numerical models, the input data required by BIOPLUME III are used for discretization of time and space, setting boundary and initial conditions, describing hydrogeologic characteristics of the aquifer, sources and sinks, sorption, source decay, radioactive decay, ion exchange, biodegradation, and defining numerical and output control parameters. All of the possible BIOPLUME III input parameters are described in Appendix D. The input data required by BIOPLUME III varies according to the simulation type chosen. For example, first-order decay requires a first-order decay coefficient, whereas the instantaneous reaction model requires specific electron acceptor information instead (Rifai et al., 1998). Input data used in model simulations for the ODOT Residency Facility are discussed in Section 3.3.2 below.

3.2 Site Description

The Oklahoma Department of Transportation (ODOT) Edmond Residency Facility (Facility) was used for this study. The Facility serves as an office for ODOT personnel working on projects in Logan County and north Oklahoma County. The Site is located approximately 1,000 feet northwest of the intersection of Interstate 35 (I-35) and Memorial Road in Edmond, Oklahoma, as shown on Figure 2. The property surrounding the Facility is commercial and residential, and an ODOT Maintenance Facility is adjacent to the Facility on the east (Caldwell, 1996). The Facility layout is shown on Figure 3, Site Map.

In early 1991, a leak was discovered in a dispenser line which was used to transfer fuel from a 12,000 gallon underground storage tank (UST) to pumps located beneath the canopy on the east side of the Facility building. It is unknown when the line began to leak and how much fuel was lost. The leak resulted in a release of fuel to the soil and groundwater. Figure 3 shows the location of the dispenser line and UST relative to the building. The fuel dispenser line was removed on February 1, 1992, along with soil containing BTEX concentrations exceeding Oklahoma Corporation Commission (OCC) Category I cleanup levels, which are 5, 400, 150, and 1000 ppm for benzene, toluene, ethylbenzene, and xylene, respectively. The UST was removed on September 19, 1994. In accordance with Oklahoma Administrative Code (OAC 165:25) and OCC requirements, an Initial Response, Initial Abatement Measures and Site Check, Initial Site Characterization, and a Risk Assessment (RA) were conducted for the Site. The document summarizing the RA also describes background information, physical and chemical data, remediation activities conducted, and the regulatory history for the Site (Caldwell, 1996).

The RA reported that soil borings were drilled, and monitoring wells were installed during Site characterization activities. According to the soil boring data, the Site is underlain by approximately one to five feet of brown to red silty clay, reddish brown silty clayey sand, and brown to red fine grained sand. The upper soil layer is underlain by weathered Permian age Garber Sandstone (bedrock) composed of light red, very fine to fine grained, moderately well sorted sandstone with some siltstone and shale. According to regional geologic information, the bedrock dips to the southwest at approximately 40 feet per mile. During the investigation, groundwater was present in the uppermost Garber Sandstone aquifer at an approximate depth of

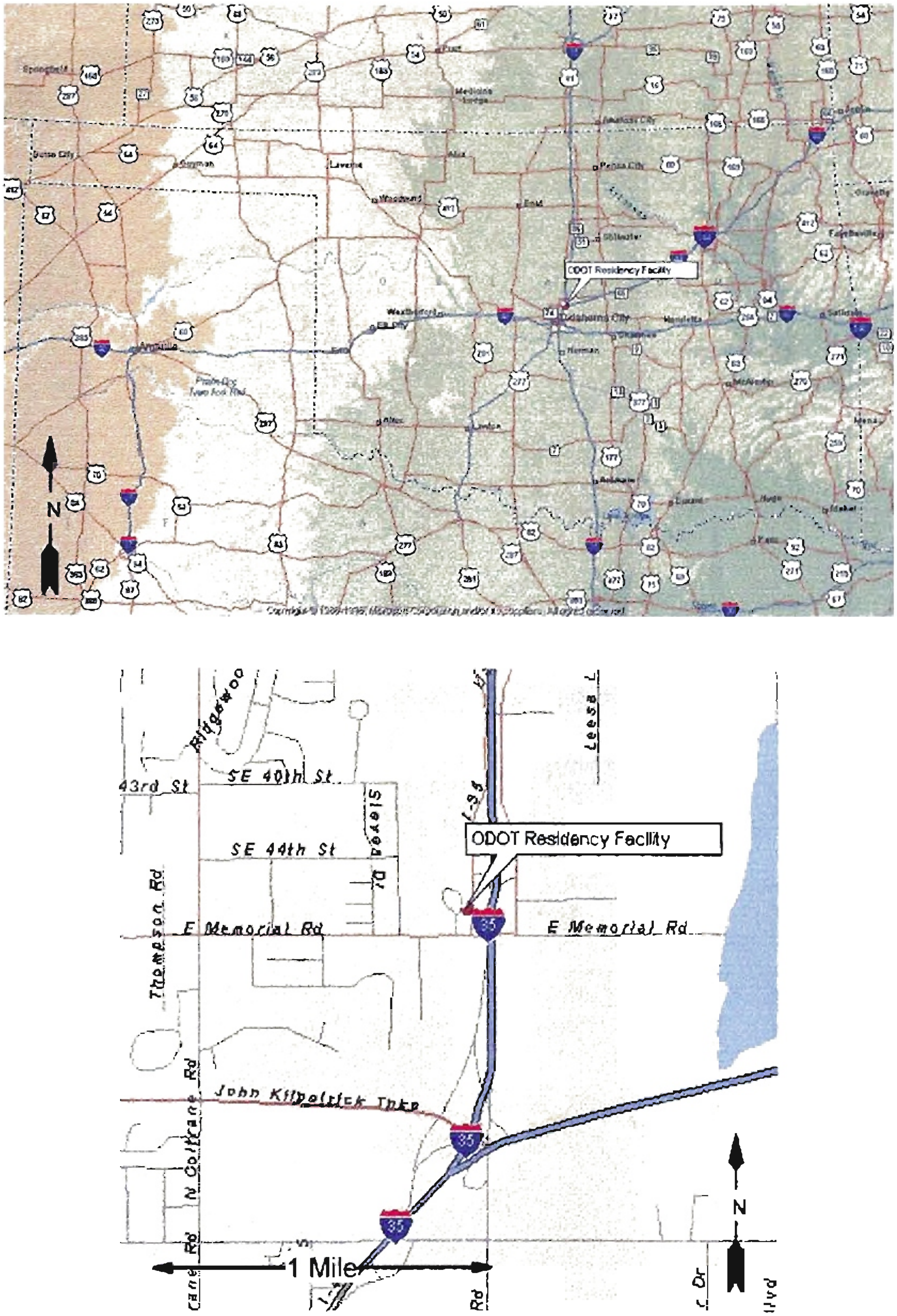


Figure 2. ODOT Residency Facility Location Map

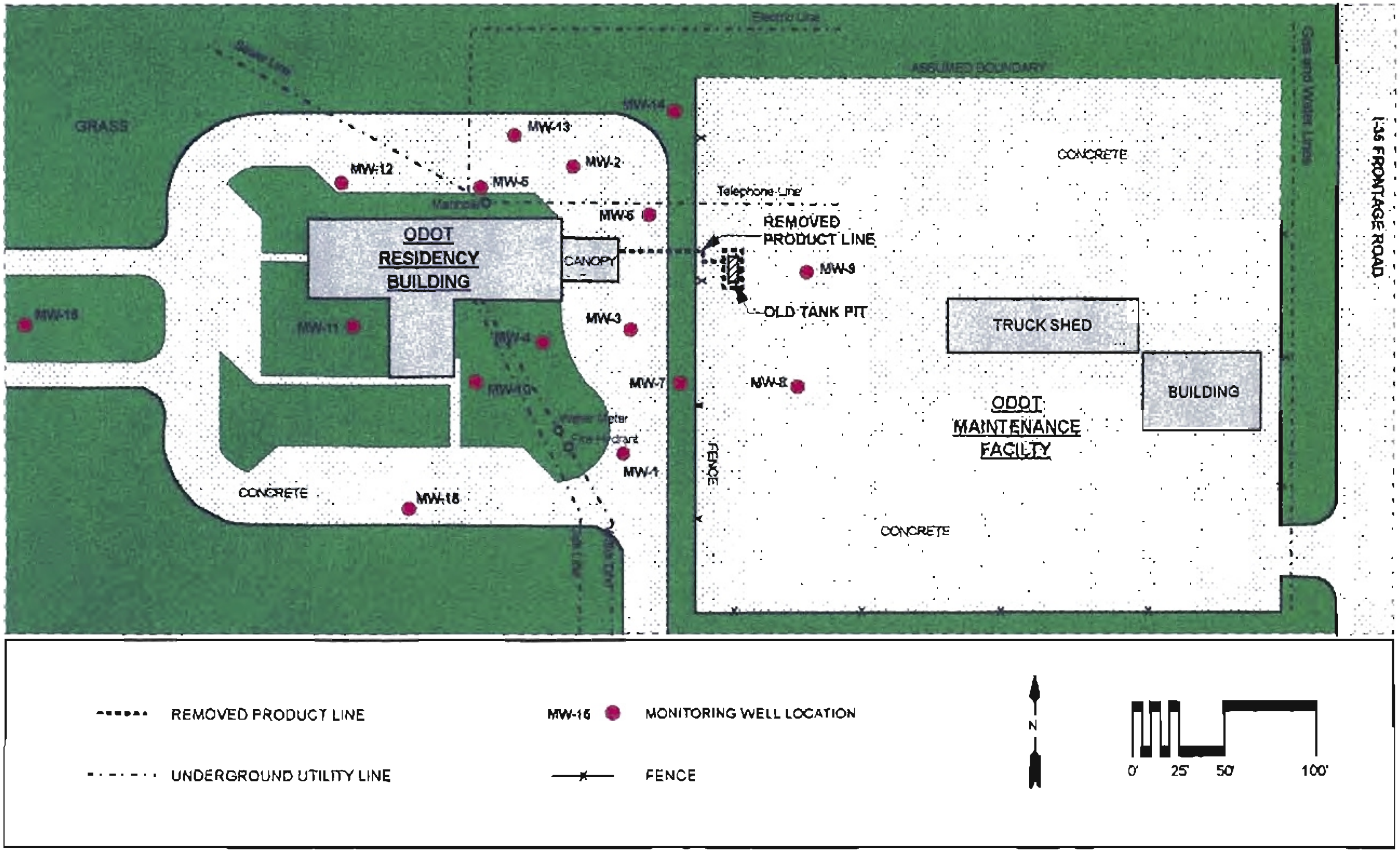


Figure 3. ODOT Residency Facility Site Map

25 feet below ground surface (BGS). Sandstone typically has a porosity of 0.005 to 0.10, which is much lower than typical porosity values for clay, silt, sand, and gravel. Due to the presence of siltstone and shale lenses, the porosity of the aquifer material may actually range between 0.1 and 0.2. Sandstone is also estimated to have a very low fraction of organic carbon and a bulk density of approximately 2.1 g/cm^3. Based on the potentiometric surface estimated from depth to groundwater measurements conducted in October, 1995, the hydraulic gradient (i) is approximately 0.005 to 0.006 toward the west-southwest, as shown on Figure 4. Aquifer slug tests performed on monitoring wells MW-2 and MW-3 showed the hydraulic conductivity (K) to be approximately 6.3×10^{-4} cm/s, which falls within the published range of 9.4×10^{-4} to 1.7×10^{-3} cm/sec for the Garber-Wellington aquifer (Caldwell, 1996). The low hydraulic gradient, hydraulic conductivity, and low porosity indicate that groundwater is moving slowly in the aquifer beneath the Site.

Although no free product was identified in monitoring wells or soil borings, analytical data from groundwater sampling events delineated a plume of dissolved petroleum hydrocarbons located under and to the west of the dispenser line leak. The initial contamination occurred to the upper three meters of saturated, fine grained, moderate to loosely cemented sandstone with lenses of shale and siltstone (Caldwell, 1996). BTEX concentrations in groundwater between July, 1994 and February, 1998 are summarized in Appendices E - H, respectively. These data were obtained from Caldwell (1996) and Akins (1998). Isopleths for each sampling date are also included in the respective appendices to show the extent of each contaminant plume with time. The isopleths were constructed using Surfer® 6.0 software for both Kriging and triangulation methods to demonstrate that a range of accuracy exists for estimation of the plume boundary and concentrations. Kriging is a geostatistical gridding method capable of smoothing data and incorporating anisotropy and underlying trends in data. The triangulation interpolator draws lines between three input data points and creates triangular planes that closely match input data without incorporating smoothing techniques, anisotropy, or trends in data.

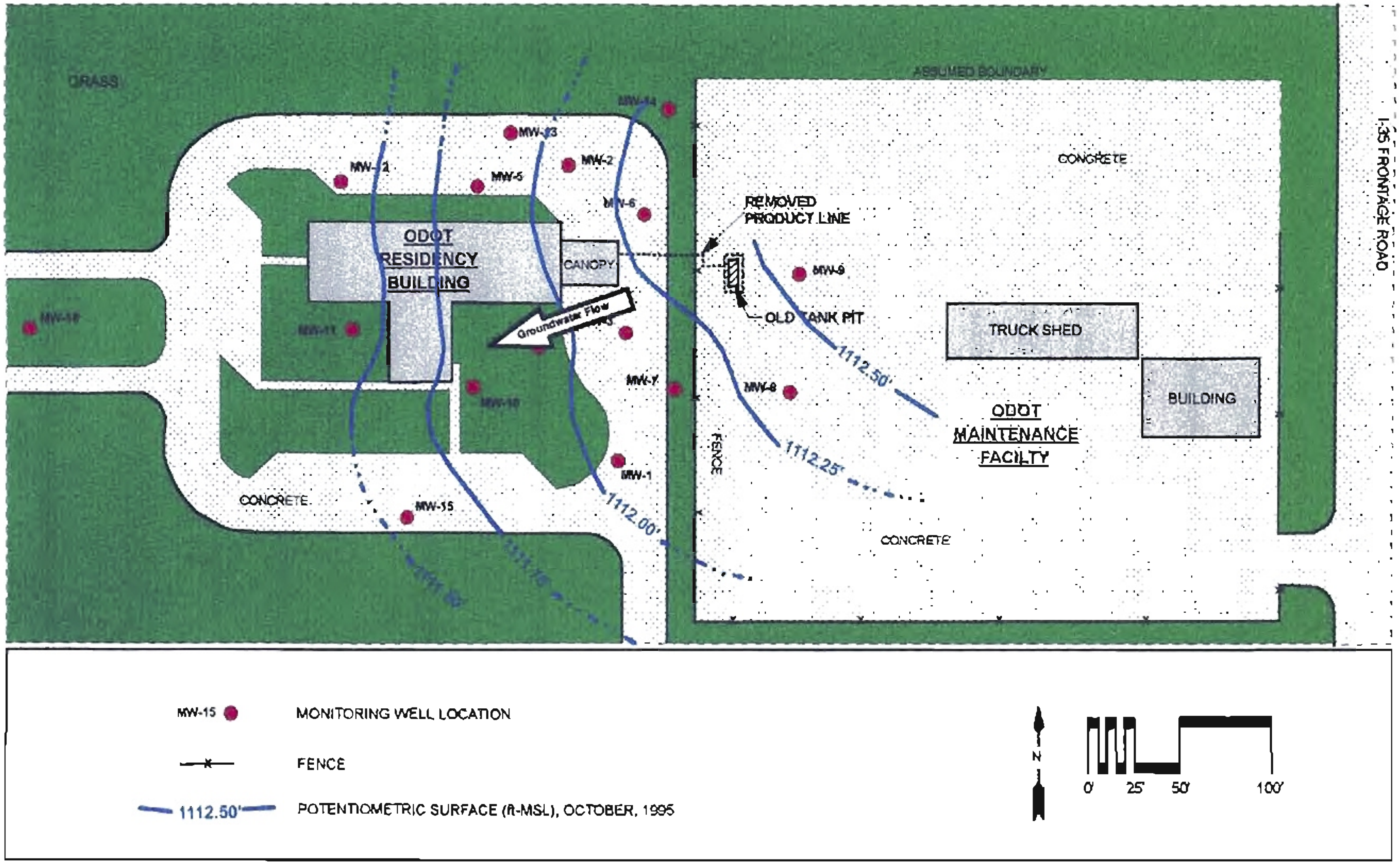


Figure 4. Potentiometric Surface Map (ft-MSL)

The EPA has established National Primary Drinking Water Standards which specify Maximum Contaminant Levels (MCLs) for BTEX of 0.005, 1.0, 0.7, and 10 mg/L, respectively. MCLs represent the maximum amount of a chemical that may be present in drinking water without posing a threat to human health. The July 1994 analytical results identified BTEX concentrations which exceeded MCLs for all four chemicals. However, the risk of this BTEX plume contaminating any drinking water supply is negligible. As discussed above, groundwater is moving very slowly beneath the Site, which will increase the time required for contaminants to reach the property boundary. In addition, the City of Edmond requires municipal water supplies to be used for drinking water; private drinking water wells are not permitted. Based on all the background, physical, analytical, and risk data available for the Site, an OCC Remediation Index score of 47 points was calculated for the Site during the RA. According to this Index, OCC Category II Soil and Groundwater Cleanup Levels were determined to be the applicable remediation goal for the Site, rather than MCLs. OCC Category II Cleanup levels for BTEX are 0.05, 10, 7, and 100 mg/L, respectively. No groundwater containing BTEX concentrations exceeding OCC Category II cleanup levels traveled beyond the ODOT property boundary, although benzene and toluene concentrations were initially in excess of the Category II cleanup levels (Caldwell, 1996).

The source of contamination at the Site was eliminated when the fuel dispenser line and the UST were excavated and removed. Because there is no continuing source, petroleum contamination at the Site appears to have reached equilibrium with the exception of biodegradation, adsorption, and desorption processes. The fuel remaining at the Site from the dispenser line leak is present in the following phases:

- as vapor in the unsaturated zone,
- in the vadose zone in the form of free product adhering to the individual soil grains, and
- dissolved in groundwater.

The petroleum release occurred beneath a concrete and asphalt covered driveway and parking lot. The pavement effectively seals the ground surface and prevents the escape of fuel vapors (Caldwell, 1996). Any free product in the vadose zone will not be flushed into groundwater because infiltration is eliminated by the sealed ground surface. Product present in the vadose zone may dissolve in groundwater during periods of high water table elevation (Caldwell, 1996). Groundwater elevations have not been tracked regularly for the Site, and subsequently, groundwater fluctuations and any resultant potential increase in dissolved BTEX have not been quantified. Groundwater fluctuations are assumed to be negligible based on the low hydraulic gradient, hydraulic conductivity, and low Darcy velocity for the Site. Contribution from product present in the vadose zone is also expected to be minimal because soil contaminated above OCC Category I levels was excavated. Without significant contribution from the unsaturated and vadose zones, concentrations of BTEX dissolved in groundwater are decreasing due to natural attenuation, adsorption, and desorption processes (Caldwell, 1996).

3.3 Modeling Practices and Input Data

Benzene is more soluble than toluene, ethylbenzene, and xylene, which typically causes it to spread the most quickly in groundwater (Verschuren, 1983 and Bowlen, 1995). Comparisons of BTEX isopleths for October, 1994 (see Appendices E - H) revealed that the benzene extended further than TEX contamination in groundwater, as expected. Figure 5 shows this relationship. Benzene isopleths were used to delineate the extent of the contaminant plume, defined as the line of zero concentration. Figure 6 shows the approximate plume boundary in October 1994, and in October 1997, according to the Caldwell (1996) data and the Akins (1998) data, respectively. Figure 6 also indicates the plume orientation relative to the direction of groundwater flow and the assumed source location.

3.3.1 BIOSCREEN Input Data and Simulations

The plume dimensions and location were used to select the modeled area dimensions. An area

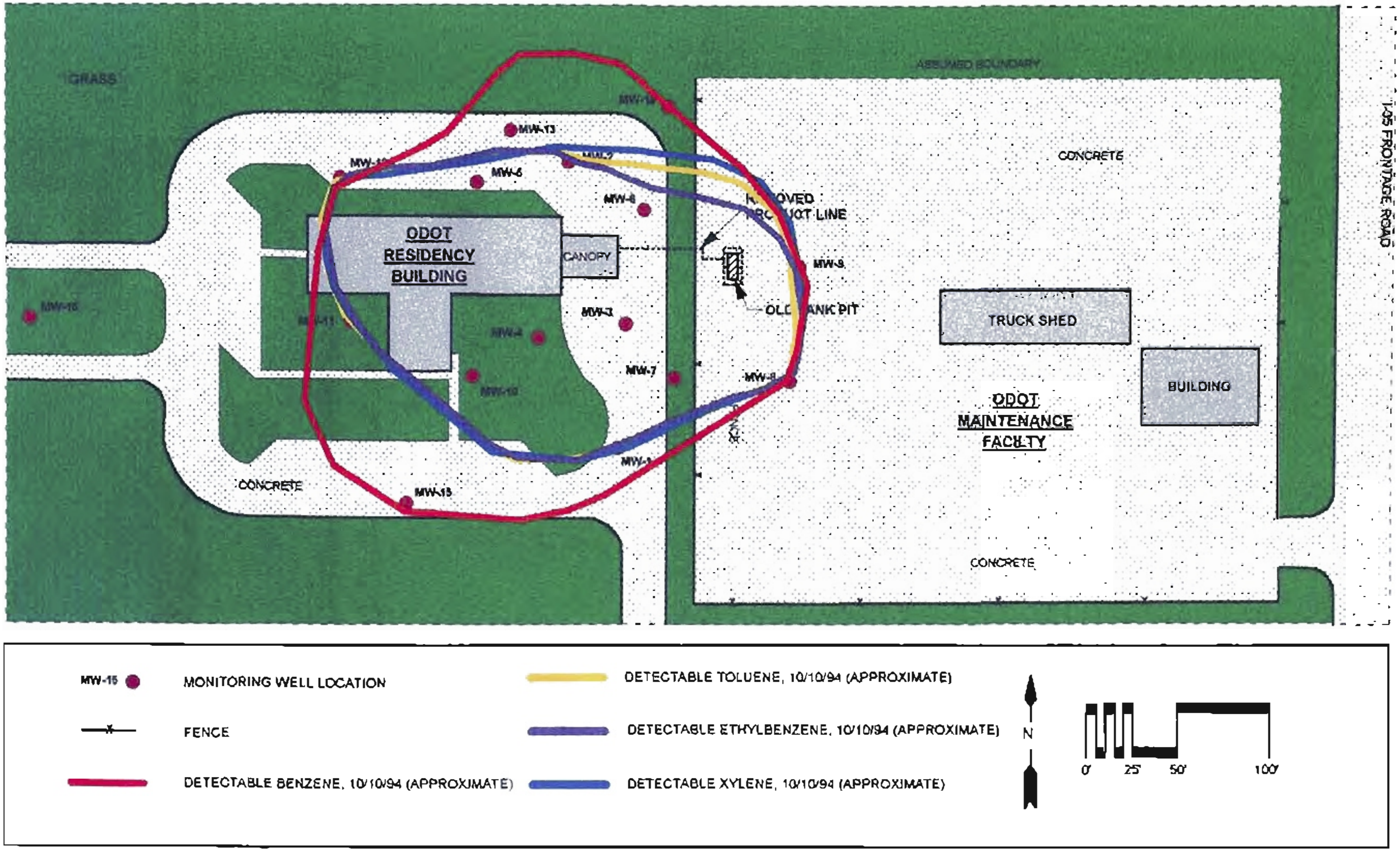


Figure 5. Comparison of BTEX Isopleths, October 1994

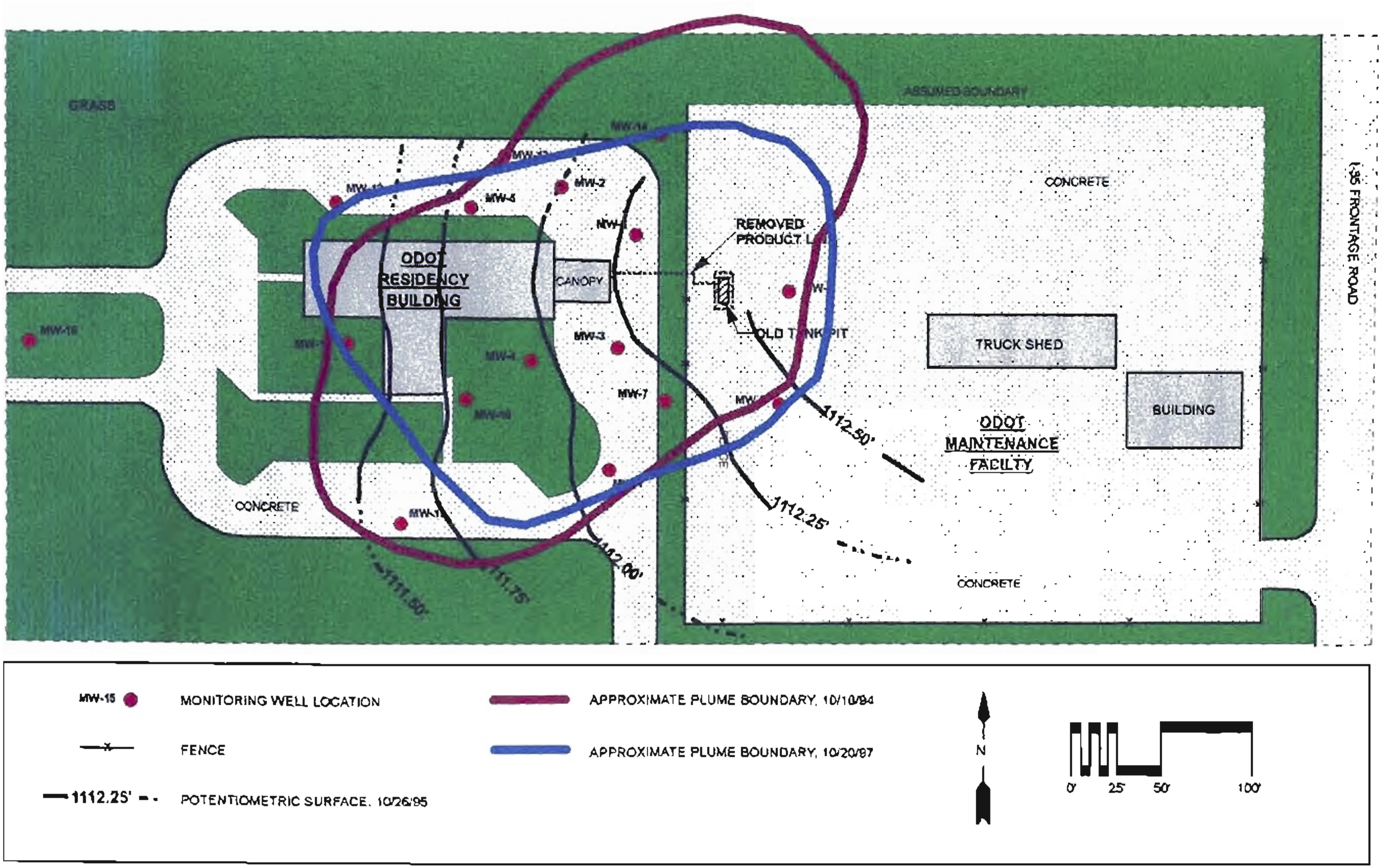


Figure 6. Approximate Plume Boundary

approximately 300 feet long by 300 feet wide was selected to accommodate the contaminant plume and monitoring wells used to gather data. As shown on Figure 7, the BIOSCREEN modeling area was oriented to correspond with the plume direction and groundwater flow. Dispersion data required by BIOSCREEN included estimates of longitudinal, transverse, and vertical dispersivity. Longitudinal dispersivity corresponds to the x-axis, which is defined as the direction of groundwater flow, as shown on Figure 8. Data from October 1997 were used to estimate the length of the plume in the longitudinal direction (L_p) to be 150 feet. Longitudinal dispersivity (α_x) was estimated to range between 9.3 and 15 feet according to methods discussed by Newell et al. (1996) which were developed by Pickens and Grisak, and Xu and Eckstein, as follows:

$$\text{Longitudinal dispersivity, } \alpha_x = 0.1\ L_p = 0.1\ (150 \text{ feet}) = 15 \text{ feet,}$$

or

$$\text{Longitudinal dispersivity, } \alpha_x = 3.28\ (0.83)\ [\log\ (L_p\ /\ 3.28)]^{2.414} = 9.3 \text{ feet.}$$

Transverse dispersivity corresponds to the y-axis, which is perpendicular to groundwater flow. Transverse dispersivity (α_y) was estimated to range between 0.9 and 4.9 feet, according to methods referenced by Newell et al. (1996) which were developed by the ASTM, and Gelhar et al., as follows:

$$\text{Transverse dispersivity, } \alpha_y = 0.33\ \alpha_x = 0.33\ (15 \text{ feet}) = 4.9 \text{ feet.}$$

or

$$\text{Transverse dispersivity, } \alpha_y = 0.1\ \alpha_x = 0.1\ (9.3 \text{ feet}) = 0.9 \text{ feet.}$$

The transverse dispersivity estimated from the October 1997 plume is 0.34, which suggests that the Gelhar method may be the most applicable at the Site. Vertical dispersivity corresponds to the z-axis, which is downward. Vertical dispersivity (α_z) is typically assumed to be very low or zero, based on conservative estimates (Newell et al., 1996).

Using hydrogeologic data for the Site, (see Section 3.2 above), the seepage velocity (V) was calculated to range between 17.9 and 35.9 ft/yr, as follows:

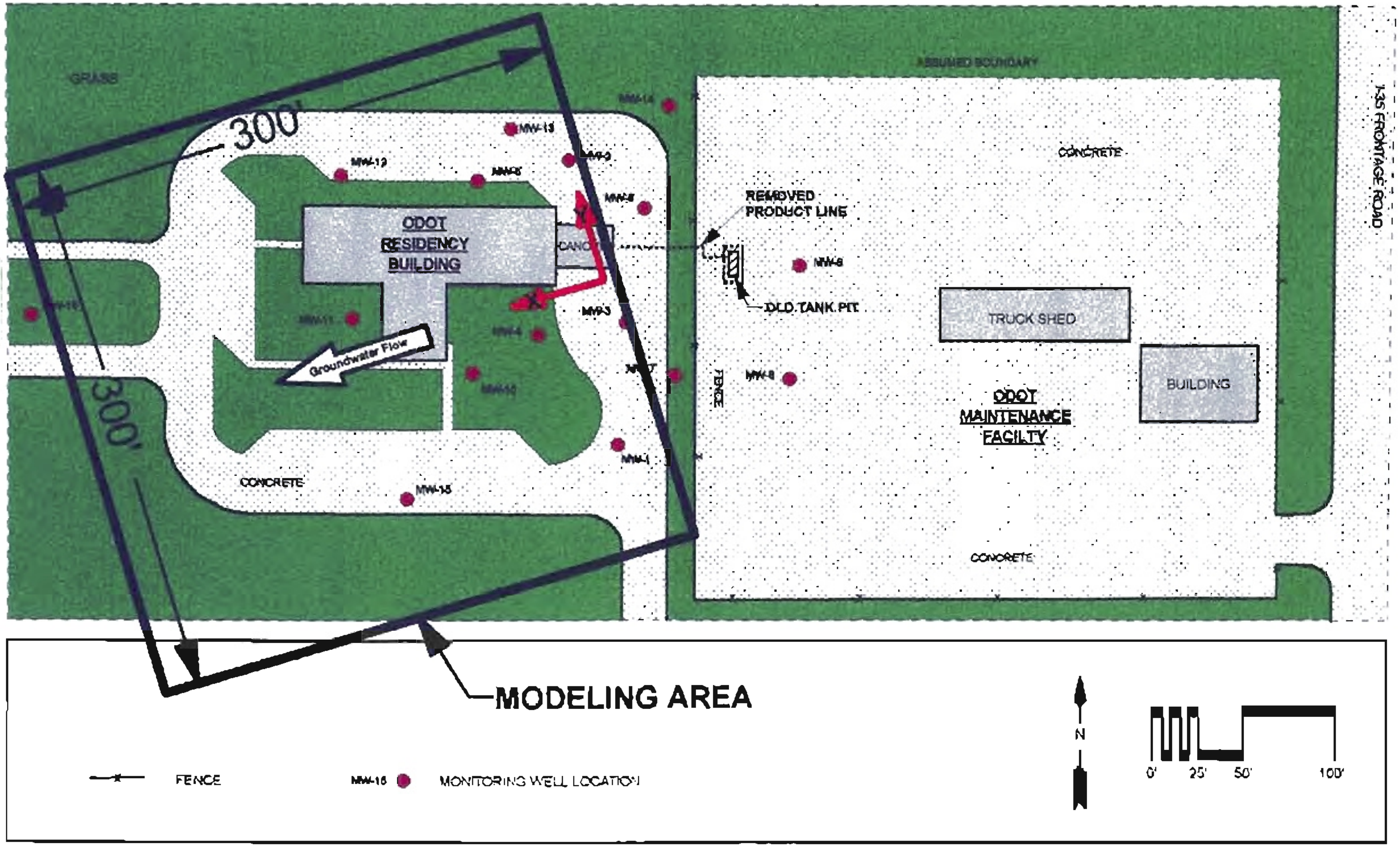


Figure 7. BIOSCREEN Modeling Area Orientation

K = hydraulic conductivity = 6.3×10^{-4} cm/s = 652.26 ft/yr

i = hydraulic gradient = 0.0055 ft/ft

η = effective porosity = 0.1 to 0.2 (dimensionless)

V = seepage velocity = Ki/η = (652.26 ft/yr) x (0.0055 ft/ft) / 0.1 = 35.9 ft/yr, or

(652.26 ft/yr) x (0.0055 ft/ft) / 0.2 = 17.9 ft/yr.

Using data discussed in previous sections, the retardation factor was estimated to be approximately 1.1, as follows:

ρ_b = Bulk density of the aquifer material = 2.1 kg/L (or g/cm^3)

K_{oc} = Organic carbon partition coefficient = 38 L/kg

f_{oc} = Fraction of organic carbon = 0.0002

η_e = Effective porosity (dimensionless) = 0.1 to 0.2

Retardation factor, $R = 1 + [(\rho_b)(K_{oc})(f_{oc}) / \eta_e] = 1 + [(2.1)(38)(0.0002) / 0.1] = 1.16$, or

$1 + [(2.1)(38)(0.0002) / 0.2] = 1.08$.

Retardation factors typically used to simulate natural attenuation of BTEX in shallow aquifers range between 1.0 and 2.0 (Newell et al., 1996).

To estimate biodegradation according to the instantaneous reaction model, BIOSCREEN requires estimates of electron acceptor utilization, defined as background concentrations minus source area concentrations for oxygen, nitrate, and sulfate (referenced as ΔO_2, ΔNO_3, and ΔSO_4). Dissolved oxygen, nitrate, ferrous iron, and sulfate data for the site are presented in both tabular and isopleth format in Appendices I-L, respectively. Sulfate concentrations at the Site exceeded even the highest typical values reported in the literature (Sublette et al., 1997). The wells with the highest concentrations (MW-2, MW-5, MW-6, and MW-13) are located north of the Facility building, as shown on Figure 3. Sulfate concentrations in MW-16, which is downgradient from the four affected wells, were also higher than typical. Nitrate concentrations were also elevated near wells MW-2 and MW-5. Dissolved oxygen was distributed as expected, with background concentrations of approximately 5 mg/L present at the outer edges of the BTEX plume and reduced concentrations present in the center of the plume. The wells in the area of elevated sulfate and nitrate concentrations are located near an underground sanitary sewer line. Total organic carbon (TOC) data were reviewed (see Appendix M) to evaluate the possibility of a sewer line leak, but the TOC isopleths did not indicate any unusually high concentrations of organic carbon near the affected wells. The land directly upgradient from the affected wells is open field, which suggests that elevated concentrations of nitrate may be present due to fertilizer application and infiltration. However, the cause of the elevated concentrations of sulfate and nitrate was not conclusively determined. A second set of isopleths were constructed for nitrate and sulfate, excluding the unusually high values. These isopleths appeared to be representative of expected conditions at the Site, as shown in Appendix N. Based on the revised isopleths, values for ΔO_2, ΔNO_3, and ΔSO_4 were estimated for October 1997, as follows:

- MW-16 was considered representative of background DO concentrations, and MW-6 and MW-7 data were averaged to obtain the source area concentration. $\Delta O_2 = 5.37 - 0.21 = 5.16$ mg/L.
- Data from MW-13, MW-5, and MW-2 were averaged to estimate the background nitrate concentration. MW-3 was selected to represent the source zone concentration. $\Delta NO_3 = 25.0 - 0.04 = 24.96$ mg/L.
- MW-7 was considered representative of background sulfate concentrations, and MW-4 was used for the source area concentration. $\Delta SO_4 = 212.4 - 7.71 = 204.69$ mg/L.

Concentrations of ferrous iron and methane present in the source area were also required as input data for BIOSCREEN. However, no methane data were available for the Site. As discussed in Section 2.1.4.4 above, methanogenesis is the last of the sequential electron acceptor processes to proceed because carbon dioxide has the lowest redox potential. Reduced concentrations of nitrate and sulfate and production of ferrous iron in the plume area indicate that anaerobic biodegradation processes are occurring at the Site. Methanogenesis could be occurring in the most concentrated area of the plume. However, the significance of the methanogenic process at the Site is currently unknown. Based on typical background concentrations of methane (less than 9.0 mg/L, (Rafai et al., 1998)), methane concentrations were conservatively assumed to be zero in the source area at this Site. No ferrous iron data were available for October 1997. A concentration of 1.0 mg/L was assumed in the source area, based on ferrous iron data for April 1998.

The source thickness was assumed to be approximately 10 feet, based on information provided in the RA for the Site. BIOSCREEN also requires source zone widths and concentrations and the soluble contaminant mass in soil. No soil sampling data were available, which eliminated the possibility of estimating the soluble mass of BTEX available in the source area. In absence of any soil data, any volume of fuel spilled, and the date the release began to occur, the source information for the Site became the primary calibration parameter. To investigate the effect of source definition on the model results, three simulations were performed for different source zone scenarios. These simulations are described below.

<u>BIOSCREEN Simulation #1</u>: The Hill Air Force Base example provided in the *BIOSCREEN User's Manual* provided guidance for sites lacking source data. Following this example, the soluble mass of BTEX in soil was assumed to be an infinite source, and the source area was placed in the highest BTEX concentration zone of the plume. Figure 6 shows the location of the source area. This location for the source area is logical, based upon the observed concentrations and the location of the assumed fuel leak point in the dispenser line. The plume length was measured from the source area. This source area was divided into three different concentration zones according to concentrations shown on the benzene isopleth from October 1997. The zone concentrations ranged from 1.0 to 9.0 mg/L. Based upon the history of the Site, the leak was assumed to occur one year prior to its discovery in 1991. As a result, a simulation

time of 7 years was selected, and the model was successfully calibrated to match the October 1997 benzene isopleth. The primary calibration parameters for the BIOSCREEN model are typically dispersivity and the source definition. Appendix O contains the input data utilized for Simulation #1 and the resultant two- and three-dimensional plume concentration graphs. As recommended by Newell et al. (1996), longitudinal dispersivity was utilized as the primary calibration parameter aside from the source term. The initial value of 9.3 ft was increased to 20.0 ft. Following calibration, the simulation time was extended to predict future attenuation. Utilizing the infinite soluble mass, the plume did not reduce with time. An infinite soluble mass is not representative of the existing Site conditions following removal of the fuel dispenser line. In order to approximate more realistic conditions, a finite source approximation was attempted. An assumed finite soluble mass of 12,500 kg produced results equivalent to the infinite source simulation for October 1997. This assumed finite source required 232 years to fully attenuate. A second set of assumptions was required to predict future attenuation. Utilizing the otherwise calibrated model, a soluble mass of 1000 kg was simulated to full attenuation over a total of 27 years following the assumed beginning of the fuel release in 1990. The plume was predicted to disappear by the year 2017.

<u>BIOSCREEN Simulation #2</u>: In place of the infinite soluble mass assumed in the source area soil for Simulation #1, a soluble contaminant mass of 6 kg and a three-zone, finite source with a maximum concentration of 30 mg/L were developed for Simulation #2. The model area, location of the source area, and the source thickness were unchanged from those used for Simulation #1. Rather than use October 1997 electron acceptor and plume data to calibrate the model as in Simulation #1, data used for this simulation were projected backward to represent conditions of the contaminant plume in 1990. The dimensions of the contaminant plume were reduced and the concentrations were increased. ΔO_2, and ΔNO_3, were recalculated, assuming less electron acceptor reduction. For this simulation, MW-2 was assumed to be representative of dissolved oxygen in the source zone, and MW-5 was used for nitrate data in the source zone. Longitudinal

dispersivity was again increased from 9.3 to 20 feet. In order to calibrate this simulation to the October 1997 data, a porosity of 0.17 and a retardation factor of 1.8 were used. Both of these values are within the ranges discussed above. The input data are in Appendix P. The model was successfully calibrated to match the October 1997 data at a simulation time of 7 years, as shown on the plume centerline plot in Appendix P. Because a finite source was initially assumed, no modification of the source data was required for the future attenuation projection. Over a twenty-year simulation period, the plume was predicted to simultaneously decrease in concentration and lengthen to approximately 210 feet, until entirely attenuated. Assuming that the fuel line leak began in 1990, the entire plume should disappear in 2010.

BIOSCREEN Simulation #3: Similar to Simulation #2, a finite soluble mass source was utilized and current plume boundary, concentration, and biodegradation process data were used to project these same parameters for 1987, when the fuel leak was estimated to begin. This simulation assumed that the source area was located at the assumed leak point in the fuel dispenser line, rather than downgradient where the BTEX concentrations were greatest in the plume, as shown on Figure 8. This scenario required that the plume concentrations be calibrated to first increase and then decrease with downgradient distance to represent a circular area of elevated concentration, as indicated on the BTEX isopleths. Calibration of this simulation required that porosity be increased to 0.2, which is the maximum value in the estimated range for the Site. The input data for Simulation #3 are in Appendix Q. A retardation factor of 1.8 was used, which is higher than the estimated value, but still within the typical range for BTEX sites. Longitudinal dispersivity was increased from 9.3 to 11 feet, which is a smaller increase than required for the previous two simulations. Biodegradation input data were consistent with those used for Simulation #2. The model was successfully calibrated to match the July 1994 benzene isopleth at a simulation time of 7 years, which assumes that the fuel line began to leak in 1987. This simulation predicted that the plume would travel downgradient, maintaining a relatively high concentration in the center, without spreading significantly in area.

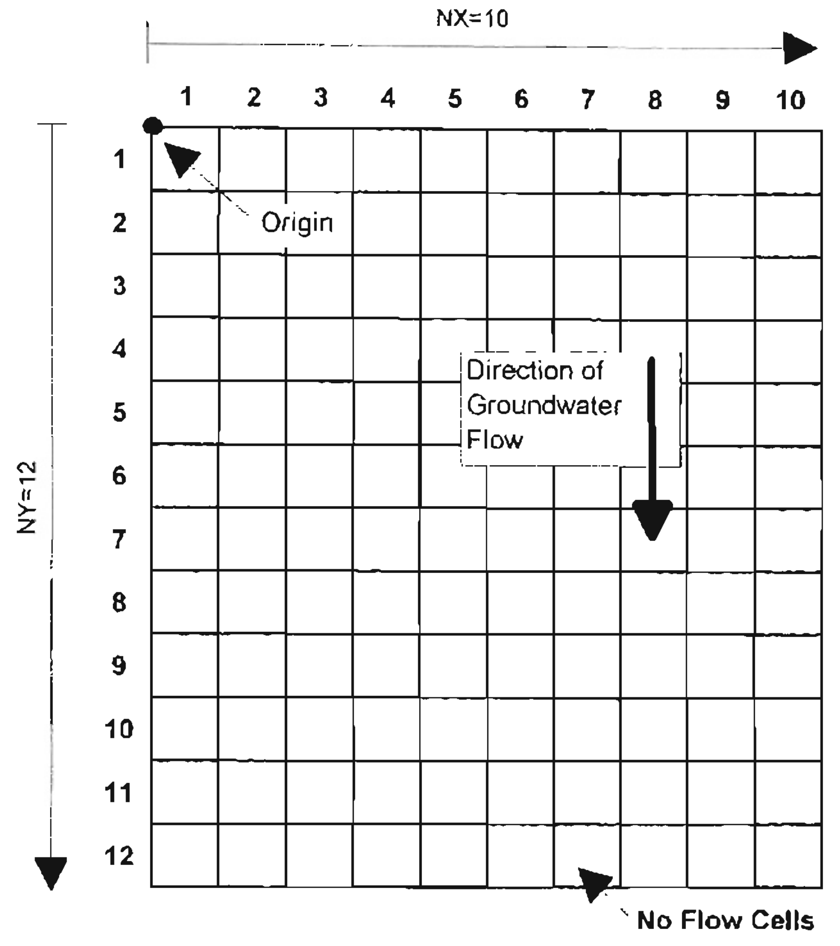
As shown on the plume centerline plot in Appendix Q, the model predicted the October 1997 plume dimensions fairly well, and continued to predict a decreasing contaminant plume traveling downgradient until completely disappearing in 47 years, or in 2034.

3.3.2 BIOPLUME III Input Data and Simulations

As described above for the BIOSCREEN simulations, the plume dimensions and location dictated the modeled area dimensions. An area approximately 450 feet long by 350 feet wide was selected to accommodate the plume, the monitoring well network, and to allow an outer row of grid cells to be defined as inactive, as required by the BIOPLUME III model. Figure 9 shows the orientation of the BIOPLUME III modeling grid aligned with the direction of groundwater flow. The second row of cells within the edge of the modeling grid was defined as a constant head area, as required by the model, to fix the water table elevation at a constant value in these cells throughout the simulation. This constant head assumption is applicable for this Site, based on the apparent stability of the water table, as described in Section 3.2 above. The start date for the BIOPLUME III simulations was set to January 1992, which is the year the leaking fuel dispenser line and contaminated soil were removed. Because soil containing concentrations of BTEX above OCC Category I levels was excavated in 1992, the dissolved BTEX plume was assumed to be the only significant component of contamination existing for the purposes of the BIOPLUME III simulations. No specific Site data are available prior to July 1994, so source area dimensions and concentrations were assumed. Both transient and steady-state flow analyses were performed.

<u>BIOPLUME III Simulation #1</u>: The concentrations assumed to exist in the plume area in 1992 were adjusted until the plume shape and concentrations matched the July 1994 benzene isopleth at a simulation time of two years. Appendix R contains tables and plots showing the concentrations defined for each cell of the modeling grid for the assumed source and the July 1994 calibration.

Figure 9. BIOPLUME III Modeling Grid Orientation



Longitudinal dispersivity was initially assumed to be equal to the average of the two values approximated in the previous section, or 12.1 feet. Unlike BIOSCREEN, BIOPLUME III requires dispersivity ratios, rather than approximated lengths in feet. A vertical dispersivity ratio of 0.00001 was assumed, and an approximate ratio of 0.33 was estimated to represent transverse dispersivity, based on the plume dimensions shown on Figure 6. Molecular diffusion data was not available for the Site. Because molecular diffusion is typically insignificant compared to mechanical dispersion (Rifai et al., 1998), it was assumed to be zero for BIOPLUME III simulations.

For the BIOSCREEN simulations, effective porosity was estimated to range between 0.1 and 0.2, based on Site characterization information. Rifai et al., 1998 reported a typical range of 0.005 to 0.10 for effective porosity values for sandstone. Based on these two approximated values, an effective porosity of 0.10 was used for BIOPLUME III simulations. For transient analysis, a storage coefficient equal to the specific storage multiplied by the aquifer thickness was required. Rifai et al., 1998 recommended that the storage coefficient be set equal to the effective porosity for unconfined aquifers. A storage coefficient of 0.10 was used. The Site-specific horizontal hydraulic conductivity (K) value of 2.07×10^{-5} ft/sec (6.3×10^{-4} cm/s) was used for the BIOPLUME III simulations.

A bulk density of 2.1 g/cm^3 was used for the aquifer matrix, and an anisotropy value of 1.0 was used to represent an isotropic aquifer with respect to vertical and horizontal hydraulic conductivity. No anisotropy data were available for the Site. Consistent with the BIOSCREEN model, BTEX was assumed to interact with soil according to the linear sorption isotherm. Linear sorption is considered to be appropriate for BTEX, except for subsurface materials with low f_{oc} values (ASTM, 1996). Although sandstone is assumed to have a very low f_{oc}, no lab data area available to indicate a typical distribution coefficient. Linear sorption is assumed to be appropriate at the Site in lieu of other data. The distribution coefficient, K_d, was estimated as described above by multiplying K_{oc} by f_{oc} to equal 0.0076. Ion exchange and infiltration were not included in BIOPLUME III simulations because ion exchange is not a significant process in sandstone, and infiltration is negligible through the asphalt and concrete parking lot.

Biodegradation was simulated according to the instantaneous reaction assumption and sequential utilization of oxygen, nitrate, and sulfate. No carbon dioxide data were available for the Site, and methanogenic biodegradation was not included in BIOPLUME III simulations. Data for MW-14 were utilized to represent background dissolved oxygen concentrations of 5.5 mg/L, based on October 1997 data. Background concentrations from MW-8 and MW-14 were averaged to approximate a background nitrate concentration of 18.2 mg/L. MW-12 data were initially assumed to be representative of background sulfate concentrations of approximately 244 mg/L. This background concentration proved to be unrealistic during model calibration. This high value caused the model to predict complete disappearance of the BTEX plume within one year of the simulation start date for both steady-state and transient model assumptions. In an attempt to utilize the original background concentration assumption, the applicability of first-order decay was evaluated for sulfate.

Following calibration of the assumed source, the electron acceptor utilization thresholds were adjusted until the predicted results for 1997 matched the concentrations shown on the October 1997 isopleths for dissolved oxygen and nitrate. The best match to the October 1997 data was achieved using a utilization threshold of 2.0 mg/L for oxygen and a threshold of 5.0 mg/L for nitrate. Sulfate could not be calibrated to match Site data using a background concentration of 244 mg/L for either first-order decay or an instantaneous reaction. Monod kinetics could not be applied due to lack of required input data. Based on the unexplainable elevated concentrations of sulfate in groundwater discussed in Section 3.3.1 above, the possibility that the background concentration had been overestimated was evaluated. Based on data collected for MW-15, a concentration of 62.7 mg/L was used to replace the previously selected 244 mg/L for the background concentration. Predicted sulfate concentrations were calibrated to match October, 1997 data with a threshold of 17 mg/L for sulfate. The sulfate data summary in Appendix L suggests that the utilization threshold could be lower than 17 mg/L; however, values below 17 mg/L caused the model to slightly overpredict the dimensions of the sulfate reduction zone.

BIOPLUME III Simulation #2: Although simulations of transient flow conditions initially appeared to most closely match the measured Site data, a second simulation was performed to attempt to calibrate BIOPLUME III to simulate steady-state conditions at the Site. Concentrations assumed to exist in the plume area in 1992 were re-adjusted until the plume shape and concentrations matched the July 1994 benzene isopleth at a simulation time of two years. Appendix S contains tables and plots showing the concentrations defined for each cell of the modeling grid for the assumed source and the July 1994 calibration. The steady-state simulation could not be accurately calibrated to simulate the February 1998 plume and electron acceptor data for the Site. The closest approximation, shown in Appendix S, was achieved assuming a longitudinal dispersivity of 1.0, which is significantly lower than previously assumed for the Site. Other input data were unchanged from Simulation #1, although variation in fraction of organic carbon, distribution coefficient, and retardation factor did not improve the simulation. Calibrated as shown in Appendix S, the model predicted that the plume would completely disappear within 10 years, or by 2002.

3.3.3 Additional BIOSCREEN Simulation

Following the BIOPLUME III simulations described above, an additional BIOSCREEN simulation was performed using the same input data defined for BIOPLUME III Simulation #1, which simulated transient flow conditions. This additional BIOSCREEN simulation was conducted so a direct comparison could be made between the two models. No additional BIOSCREEN simulation was conducted to match the second BIOPLUME III simulation because it could not be accurately calibrated.

The hydrogeologic, dispersivity, and adsorption data utilized in BIOPLUME III Simulation #1 were incorporated directly by BIOSCREEN, as was the assumed source thickness. However, BIOSCREEN required approximation of the source zone concentrations, arbitrary estimation of the soluble mass of BTEX remaining in soil, and approximation of required electron acceptor concentration differences. The input data and simulation results for BIOSCREEN Simulation #4 are in Appendix T. As the simulation results for this simulation show, the BIOSCREEN model underpredicted BTEX concentrations by approximately 8.8 mg/L at a distance of 65 feet downgradient from the assumed source zone location. This simulation predicted downgradient transport and reduction in plume concentration and size with time. In an attempt to more closely approximate July 1994 Site data, this BIOSCREEN simulation was calibrated by decreasing longitudinal dispersivity and f_{oc}. Other parameters were unchanged, as shown on the second input data summary in Appendix T. This calibration effort improved the approximation of the July 1994 Site data, but plume concentrations were still underpredicted at distances greater than 35 feet downgradient from the assumed source zone location. This simulation predicted downgradient transport and reduction in plume concentration and size with time. The plume was predicted to completely disappear within 10 years, or by 2002.

4.0 RESULTS AND DISCUSSION

Three BIOSCREEN model simulations were developed utilizing totally different source zone assumptions and relatively smaller variations in other input data. For each simulation, the model was successfully calibrated to match a specific benzene isopleth for the Site utilizing data within ranges estimated to be applicable to Site-specific conditions. Each simulation produced a very different prediction for the time to complete attenuation of the contaminant plume, indicating that predictive capability is strongly dependent on quality and accuracy of input data, particularly source definition.

Two BIOPLUME III model simulations were developed, one for transient and another for steady-state flow conditions. The transient simulation was calibrated to match the measured benzene plume in 1994 and 1997 as well as measured electron acceptor concentrations in 1997. This simulation predicted very little attenuation in an 80 year time period. The second BIOPLUME III simulation was performed using the steady-state flow option. This simulation could not be accurately calibrated to match two sets of benzene data, or measured electron acceptor concentrations. The model was calibrated to match only the 1994 benzene data, and the plume was predicted to disappear in ten years. The electron acceptor assumptions and measured data described in Section 3.3.2 were checked by comparing the zones of reduced electron acceptor concentrations predicted by the isopleths in Appendices I - L to theoretical zones (see Figure 1). The zones predicted from the measured data are shown in Figure 10. These measured and theoretical zones are generally similar in shape and order of occurrence. The assumptions used for the BIOPLUME III simulations appear to be valid.

An additional BIOSCREEN simulation was performed using the input data successfully calibrated for the BIOPLUME III transient flow simulation, but BIOSCREEN could not be exactly calibrated using identical input data. BIOSCREEN predicted a much quicker rate of attenuation and lower concentrations in the downgradient portions of the plume than the BIOPLUME III simulation. This additional BIOSCREEN simulation predicted that the plume would disappear in ten years.

4.1 Comparison of Simulation Results

The lack of source information for the Site introduced considerable uncertainty in the simulations. The time period between the initial fuel dispenser line leak and the removal of the line is unknown, as is the volume of fuel released and the actual location of the leak. No soil data is available, so the soluble contaminant mass in the soil can not be estimated. Several different assumptions can be made about the source type, concentrations, and dimensions which

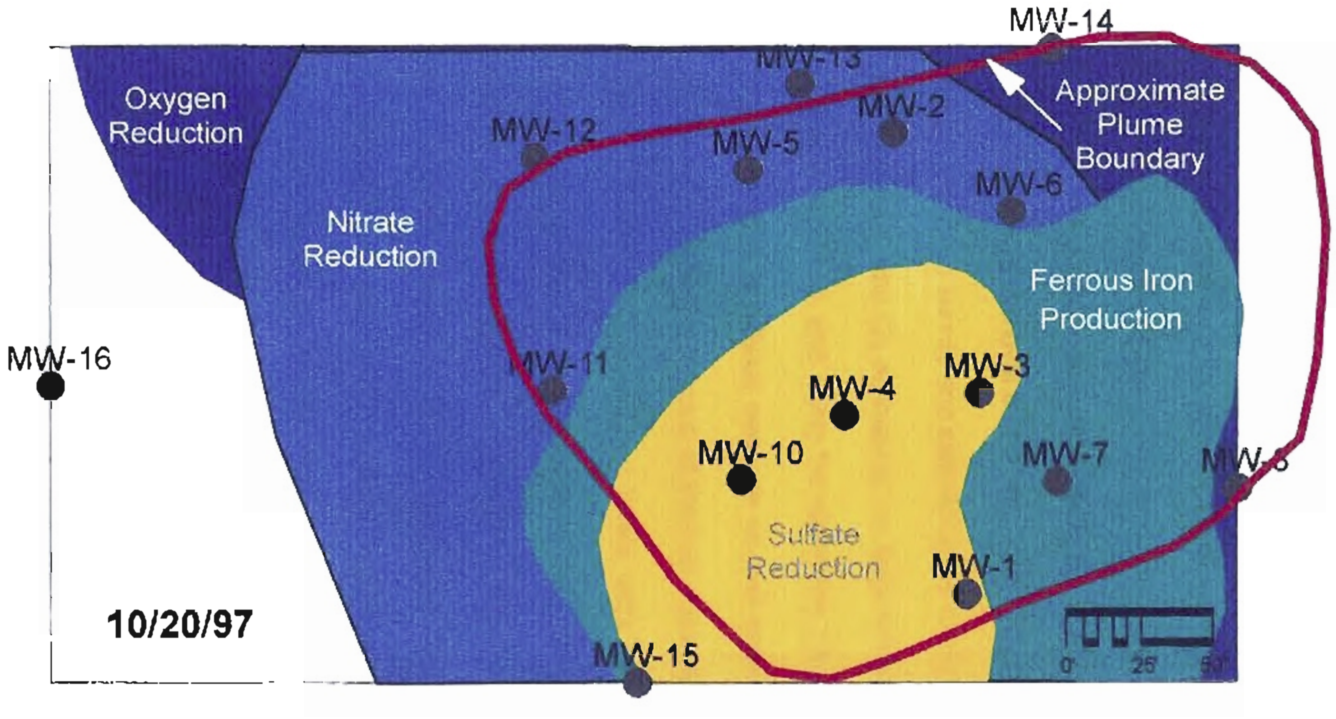


Figure 10. Measured Zonation of Terminal Electron Acceptor Processes

affect the time required to fully attenuate the Site and the behavior of the plume prior to complete attenuation.

According to the Hill Air Force Base example provided in the *BIOSCREEN User's Manual*, an infinite source can be conservatively assumed for sites lacking source data. BIOSCREEN Simulation #1 illustrated that the infinite soluble mass assumption is not valid for the Site following removal of the fuel dispenser line. The contaminant plume continued to expand and did not attenuate. It is more realistic to assume the source is infinite prior to removal of the fuel dispenser line and finite following removal of the line. This type of simulation would require (1) assuming an infinite soluble mass source and calibrating the model to match conditions when the fuel dispenser line is removed, and (2) estimating the finite soluble mass source present when the fuel dispenser line is removed, and using the otherwise calibrated model to predict future attenuation. This second step is difficult because no soil data are available to support any estimate of the soluble mass following removal of the fuel dispenser line. The RA does indicate that soils contaminated above OCC Category I levels were excavated, which suggests that remaining soils could conservatively be assumed to have 0.5, 40, 15, or 200 ppm BTEX, respectively. However, no dimensions are provided for the contaminated area. Assuming a contaminated area of 150 feet square by 10 feet deep, a soluble mass of 6.7 kg was estimated for benzene. Utilizing this value, the model predicted that the entire contaminant plume would be remediated in one year. The infinite soluble mass source assumption is not applicable to this Site, and changing the source type within a simulation introduces a second level of uncertainty in the model results.

A finite soluble mass source was assumed for BIOSCREEN Simulations #2 and #3, and the model results appear more realistic, although considerable uncertainty exists due to lack of Site data. The prime source of uncertainty for this simulation is the development of the assumed source. The plume dimensions and concentrations were projected backwards in time by assuming that the contaminated area would be relatively smaller and more highly concentrated closer to the time the leak began. The electron acceptor utilization zones were assumed to shrink as well, which required that wells located along the fringes of the plume in 1997 be used to represent the source area wells in 1990. This assumption resulted in decreases in both ΔO_2, and ΔNO_3 and elimination of any sulfate, iron, and methane data from the simulation, because oxygen and nitrate processes were assumed to dominate at that time. The model was successfully calibrated to match assumed field conditions exactly, as shown in Appendices P and Q. Aside from the biodegradation parameters, the input data remained within the original ranges estimated for the Site.

The BIOPLUME III model allows a more detailed source definition than BIOSCREEN, but simulation results are still highly dependent on the source area dimensions and concentrations used, as described above for BIOSCREEN. A second significant parameter for BIOPLUME III simulations is the type of flow modeled. BIOPLUME III was accurately calibrated to match field conditions, assuming transient groundwater flow. This transient simulation was calibrated using input data within ranges expected for the Site (discussed in Section 3.2 above). A second simulation assuming steady-state conditions could not be simulated to accurately match more than one date for benzene, and electron acceptor concentrations were not matched. Input data used for this simulation matched those used for the transient simulation, except for longitudinal dispersivity, which was decreased from 12.1 to 1.0 feet.

Steady-state conditions have been shown to exist by 3 to 7 years following gasoline releases at service stations with clay and silty clay subsurface materials, which indicates that the time required for typical BTEX plumes to reach steady-state conditions is reasonably short. (McAllister, 1996). If this report can be applied to sandstone aquifers, it is reasonable to assume that the Site conditions are also at steady-state. Rifai et al. (1998) also report that steady-state flow simulations are appropriate at most sites, unless pumping wells or other flowaltering factors are present. However, the transient simulation performed using BIOPLUME III did not incorporate any flow data except those defined for dispersivity, which was utilized as a calibration parameter. No Site data indicates that this type of transient simulation should not be used to approximate the existing Site conditions.

4.2 Model Sensitivity Analysis

4.2.1 BIOSCREEN

Following calibration of the model during Simulation #1, various input data were methodically altered to evaluate the sensitivity of the model to the variations. An increase in porosity resulted in a decrease in seepage velocity, which caused simulated contaminant concentrations to decrease more rapidly with distance from the source. Increased longitudinal dispersivity resulted in decreased plume concentrations midway between the source and the tip of the plume. An increased retardation factor caused the plume to shorten. With all other input data consistent, Simulation #1 was rerun with a fraction of organic carbon value of zero, rather than 0.0002. This change resulted in a retardation factor decrease from 1.2 to 1.0. To recalibrate the model, longitudinal dispersivity was increased by 4 feet. Both versions of this simulation were calibrated to closely match the October, 1997 data for the Site. No visible change in model results was caused by entering zeros for ΔO_2 and ΔNO_3 separately, although an increase in plume length with time was expected. The concentration of observed ferrous iron was varied from 0.0 to 3.0 without any visible effect. Reduction of ΔSO_4 to zero caused a significant increase in the plume length due to the large concentration of sulfate in the aquifer.

A comparison of the results of the three simulations indicates that the BIOSCREEN model is highly sensitive to the manner in which the source is defined and described. An infinite source resulted in no attenuation of the plume with time, and no method was available for converting the infinite source to a finite source following calibration of the model. Variations on a finite source assumption caused attenuation endpoints to range between 2000 and 2034. Considerable variability and uncertainty exist for sites lacking laboratory analytical data to quantify subsurface physical and chemical properties.

4.2.2 BIOPLUME III

Various modeling assumptions were investigated during calibration of the BIOPLUME III model, and several input parameters were systematically varied to determine the effect on simulation results. For BIOPLUME III Simulation #1, selection of sulfate background concentrations was the second most significant parameter in terms of model sensitivity, aside from source definition. Utilization of the originally assumed background concentration of 244 mg/L and the instantaneous reaction resulted in a prediction of complete disappearance of the BTEX plume by the year 1993, which is obviously inconsistent with site data. The best calibration for sulfate data was achieved by assuming that the background concentration of sulfate is approximately 63 mg/L, which is much lower than the originally assumed value of 244 mg/L. The sensitivity of the model to background sulfate concentrations was evaluated by methodically changing the concentration and evaluating the results. For steady-state and transient simulations, background sulfate concentrations above 150 mg/L resulted in a prediction of complete disappearance of the plume within one year. A background sulfate concentration of 100 mg/L resulted in reduction in the BTEX plume concentrations of approximately 50% within one year for the steady-state simulation and a 72% reduction within one year for the transient simulation. Both transient and steady-state simulations with a background concentration of 25 mg/L sulfate resulted in a 23% reduction in BTEX concentrations in the plume within one year. The steady-state and transient simulations appear to be equally affected by changes in background sulfate concentrations. BIOPLUME III appears to be sensitive to large background concentrations of electron acceptors.

Manipulation of utilization threshold values for dissolved oxygen, nitrate, and sulfate resulted in slight changes in the BTEX plume and electron acceptor concentrations, but the shape of the plume and zones of reduced electron acceptor concentrations were unchanged. Background concentrations of ferrous iron in the source zone were assumed to vary between 0 and 3 mg/L, without any visible effect on the plume dimensions. Variations in longitudinal dispersivity produced very little change in the simulation results; an increase of 10 feet resulted in a very slight (approximately 0.10 mg/L) concentration increase in the model grid cell containing the most concentrated area of the plume. No changes in plume shape or extent were observed. Variations in porosity also produced only very slight changes in plume concentrations.

Aside from the parameters discussed above, the selection of transient or steady-state flow conditions most affected the predictive capacity of BIOPLUME III. Identical input data were simulated for both steady-state and transient conditions, with and without biodegradation. A significant difference in simulation results was observed. The steady-state simulation predicted that the plume would travel farther downgradient with time, but attenuate much more rapidly than the transient simulation, even without biodegradation. The transient simulation predicted that the plume would remain in place as Site data indicate, but total attenuation time was predicted to be much longer than 80 years. Transient flow conditions could be calibrated to match measured Site data, whereas steady-state flow conditions could not be calibrated to match more than one date for benzene. During calibration of the steady-state simulation, longitudinal dispersivity was initially assumed to be equal to 12.1 feet, the value used in BIOPLUME III Simulation #1, but the plume was predicted to travel downgradient too rapidly. As discussed in Section 3.3.2 above, the model was calibrated using a value of 1.0. Appendix S shows the steady-state BIOPLUME III results assuming a longitudinal dispersivity of 12.1 feet. No other input parameters significantly affected the results of Simulation #2, following definition of the source.

4.3 Model Predictive Capabilities

The wide range in results for the simulations suggests that BIOSCREEN and BIOPLUME III have limited predictive capability unless site-specific data are available. BIOSCREEN simulations suggested a range of total attenuation times from 10 to 47 years, and the BIOPLUME III simulations ranged from 10 years to over 80 years. Ranges for physical and chemical data such as porosity and fraction of organic carbon can be used to predict a range for total attenuation time, but specific data delineating the dimensions of the source and contaminant concentrations in soil and groundwater play a key role in determining the total time for plume attenuation.

The predictive capability of the models is limited by the available electron acceptor information. All of the simulations described above most likely underpredict the time required for measurable concentrations of benzene to disappear because methanogenic and iron-reducing processes were not accounted for. Without soil data, concentrations of ferric iron which may be contributing to biodegradation are overlooked. Contributions from methanogenic processes are overlooked as well because no carbon dioxide or methane data are available for the Site. Part of the plume is also subject to elevated concentrations of sulfate which may also be contributing to the biodegradation of the plume.

5.0 SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

Although sufficient data were available to simulate natural attenuation at the ODOT facility using both BIOSCREEN and BIOPLUME III, the models predicted a wide range for the time period required for the BTEX plume to reach full attenuation. BIOSCREEN was simple to use and required basic Site information for input data. However, no information concerning the date the fuel dispenser line began to leak or the volume of fuel leaked is available for this site, so varied plausible source definitions were estimated for BIOSCREEN simulations. BIOSCREEN could be calibrated to match existing Site conditions, regardless of the source zone assumptions made, but predictions of total attenuation times varied widely. BIOPLUME III required additional input data to define the modeling grid and boundary conditions, and allowed more complex definitions of the hydrocarbon source and electron acceptors. However, this model was equally as sensitive as BIOSCREEN to the defined source concentrations and extent. Additionally, BIOPLUME III produced very different results for the transient and steady-state simulations. Steady-state conditions were expected to be most applicable to the Site, but the steady-state simulation could not be calibrated to match measured Site data very well. The transient flow simulation was calibrated to match not only hydrocarbon concentrations, but also electron acceptor data. However, this simulation predicted that the plume would be attenuated only slightly within 80 years, which is twice the longest time to complete plume disappearance predicted by BIOSCREEN. Use of a relatively more complex numerical model, BIOPLUME III, did not produce results which could be regarded with any more confidence than those produced by the steady-state analytical model, BIOSCREEN.

A recent study was conducted to compare model and parameter uncertainties in groundwater flow and solute transport predictions. The study illustrated that uncertainty and variability in model input parameters often outweigh error due to the type of model applied, which suggests that application of sophisticated computer models may not be warranted for sites with limited input data (Massman and Hagley, 1995). The results of this comparison between BIOSCREEN and BIOPLUME III support the premise that use of a complex model is not necessarily advisable for typical petroleum hydrocarbon sites with limited data. Modeling with BIOPLUME III may serve as a method for identifying those areas where detailed field information needs to be collected (Rifai et al., 1998), but typically, collection of large amounts of data is prohibitively expensive at sites such as the ODOT Edmond Residency Facility.

Both BIOSCREEN and BIOPLUME III predict that natural attenuation is taking place at the ODOT Residency Facility rapidly enough to prevent migration of any BTEX beyond the Facility property boundary. In spite of the widely varied results, all of the simulations described above are conservative and tend to underpredict bioremediation. Natural attenuation is generally considered to be acceptable support for risk-based closure provided that the contaminant plume is shrinking or stable, and there are no impacts to receptors (ASTM, 1996). These model results, in combination with documentation of biodegradation processes at the Facility, support risk-based closure by showing that biodegradation is taking place, and the plume will not migrate off-site where it could potentially impact receptors.

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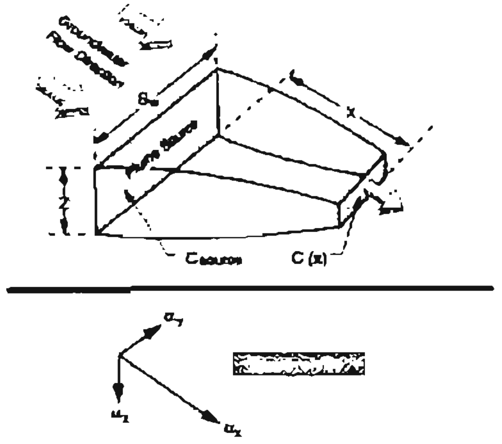
APPENDICES

APPENDIX A –

BIOSCREEN Equations

Domenico Model with Instantaneous Reaction Superposition Algorithm[1]

The 1987 Domenico analytical model utilized by BIOSCREEN is designed for the multidimensional transport of a decaying contaminant species. The model equation, boundary conditions, and assumptions are discussed below.



$$\frac{C(x,y,o,t)}{(Co+BC)} = \frac{1}{8}\exp\left[\frac{x}{\alpha_x 2}\left(1-\left(1+4\lambda\alpha_x/v\right)^{1/2}\right)\right]$$

$$erfc\left[\frac{\left(x-vt\left(1+4\lambda\alpha_x/v\right)^{1/2}\right)}{2\left(\alpha_x vt\right)^{1/2}}\right]$$

$$\left\{erf\left[\frac{(y+Y/2)}{2\left(\alpha_y x\right)^{1/2}}\right]-erf\left[\frac{(y-Y/2)}{2\left(\alpha_y x\right)^{1/2}}\right]\right\}$$

$$\left\{erf\left[\frac{(Z)}{2\left(\alpha_z x\right)^{1/2}}\right]-erf\left[\frac{(-Z)}{2\left(\alpha_z x\right)^{1/2}}\right]\right\}-BC$$

where: $v = \frac{K \cdot i}{\theta_e R}$ $\quad BC = \Sigma \frac{C(ea)_n}{UF_n}$

Definitions of Variables:

BC	Biodegradation capacity (mg/L)
C(x,y,z,t)	Concentration at distance x downstream of source and distance y off centerline of plume at time t (mg/L)
C_s	Concentration in Source Zone (mg/L)
C_o	Concentration in Source Zone at t=0 (mg/L)
x	Distance downgradient of source (ft)
y	Distance from plume centerline of source (ft)
z	Distance from surface to measurement point (assumed to be 0; concentration is always assumed to be at top of water table).
$C(ea)_n$	Concentration of electron acceptor n in groundwater (mg/L)
Uf_n	Utilization factor for electron acceptor n (i.e., mass ratio of electron acceptor to hydrocarbon consumed in biodegradation reaction)
α_x	Longitudinal groundwater dispersivity (ft)
α_y	Transverse groundwater dispersivity (ft)
α_z	Vertical groundwater dispersivity (ft)
θ_e	Effective Soil Porosity
λ	First-Order Degradation Rate (day^{-1})

[1] From Newell et al., 1996.

υ	Groundwater Seepage Velocity (ft/yr)
K	Hydraulic Conductivity (ft/yr)
R	Constituent retardation factor
i	Hydraulic Gradient (cm/cm)
Y	Source Width (ft)
Z	Source Depth (ft)

- The initial conditions are:
  1) $c(x, y, z, 0) = 0$ (Initial concentration = 0 for $x, y, z, > 0$)
  2) $c(0, Y, Z, 0) = C_0$ (Source concentration for each vertical plane source = C_0 at time 0)

- The key assumptions in the model are:
  1) The aquifer and flow field are homogeneous and isotropic.
  2) The groundwater velocity is fast enough that molecular diffusion in the dispersion terms can be ignored (may not be appropriate for simulation of transport through clays).
  3) Adsorption is a reversible process represented by a linear isotherm.

- The key limitations to the model are:
  1) The model should not be applied where pumping systems create a complicated flow field.
  2) The model should not be applied where vertical flow gradients affect contaminant transport.
  3) The model should not be applied where hydrogeologic conditions change dramatically over the simulation domain.

- The most important modifications to the original Domenico model are:
  1) The addition of "layer cake" source terms where three Domenico models are superimposed one on top of another to yield the 5-source term used in BIOSCREEN.

  2) Addition of the instantaneous reaction term using the superposition algorithm. For the instantaneous reaction assumption, the source concentration is assumed to be an "effective source concentration" (Coe) equal to the observed concentration in the source zone plus the biodegradation capacity.

APPENDIX B –

BIOSCREEN Input Parameters

DEFINITIONS OF BIOSCREEN INPUT PARAMETERS

Hydrogeologic Data:

- Seepage velocity (**V_s**), ft/yr - Actual interstitial groundwater velocity equal to Darcy velocity divided by effective porosity.
- Hydraulic conductivity (**K**), cm/s - Horizontal hydraulic conductivity of the saturated porous medium.
- Hydraulic gradient (I), ft/ft - The slope of the potentiometric surface, which is equivalent to the slope of the water table in unconfined aquifers.
- Effective porosity (η) - Dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer matrix.

Dispersion Data:

- Longitudinal, transverse, and vertical dispersivity (**alpha x, alpha y, and alpha z**), ft - An estimation of the tendency of a plume to spread out in the longitudinal direction (parallel to groundwater flow), the transverse direction (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion.
- Estimated plume length (**L_p**), ft - Estimated length of the existing or hypothetical groundwater plume.

Adsorption Data:

- Retardation factor (**R**) - Dimensionless rate at which dissolved contaminants moving through an aquifer can be reduced by sorption of contaminants to the solid aquifer matrix.

Adsorption Data, Cont'd:

- Soil bulk density (ρ_b), kg/L or g/cm^3 - The bulk density of the aquifer matrix.
- Organic carbon partition coefficient (K_{oc}), L/kg or mL/g - Chemical-specific partition coefficient between soil organic carbon and the aqueous phase.
- Fraction of organic carbon (f_{oc}) - Dimensionless fraction of the aquifer soil matrix comprised of natural organic carbon in uncontaminated areas.

Biodegradation Data:

- First-order decay coefficient (λ), yr^{-1} - Rate coefficient describing first-order decay process for dissolved constituents.
- Dissolved plume solute half-life ($t_{1/2}$), yr - Time for dissolved plume concentrations to decay by one half as contaminants migrate through the aquifer.
- Delta oxygen (ΔO_2), mg/L - The average background concentration of oxygen minus the lowest observed concentration of oxygen in the source area.
- Delta nitrate (ΔNO_3), mg/L - The average background concentration of nitrate minus the lowest observed concentration of nitrate in the source area.
- Observed ferrous iron (Fe^{2+}), mg/L - The average observed concentration of ferrous iron found in the source area.
- Delta sulfate (ΔSO_4), mg/L - The average background concentration of sulfate minus the lowest observed concentration of sulfate in the source area.
- Observed methane (CH_4), mg/L - The average observed concentration of methane found in the source area.

General Data:

- Model area length and width (**L and W**), ft - Physical dimensions of the rectangular area to be modeled.

- Simulation time (**t**), yr - Time for which concentrations are to be calculated.

Source Data:

- Source thickness in saturated zone (**z**), ft - The thickness of the contaminated groundwater zone, measured down from the top of the water table.
- Source zone width, ft - The horizontal width, perpendicular to groundwater flow, of the source area, divided into one, three, or five zones.
- Source zone concentration, mg/L - Concentrations of contaminant within each source zone.
- Soluble mass in source zone, kg - The best estimate of dissolvable organics present in the source zone.

APPENDIX C –

BIOPLUME III Equations

BIOPLUME III Equation Formulation

Rifai et al. (1988) incorporated the conclusions developed by Borden and Bedient (1986) into the USGS two-dimensional solute transport model more commonly referred as the Method of Characteristics (MOC) model. The MOC model was modified from a single particle mover to a dual particle mover model to simulate the transport of hydrocarbon and oxygen. The system of transport equations solved in BIOPLUME II is given by:

$$\frac{\partial Hb}{\partial t} = \frac{1}{R_h}\left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial H}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(bHV_i)\right) - \frac{H'W}{n}$$

$$\frac{\partial Ob}{\partial t} = \left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial O}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(bOV_i)\right) - \frac{O'W}{n}$$

where

H = concentration of hydrocarbon
O = concentration of oxygen
H' = concentration of hydrocarbon in source or sink fluid
O' = concentration of oxygen in source or sink fluid
n = effective porosity
b = saturated thickness
W = volume flux per unit area
V_i = seepage velocity in the direction of x_i
R_h = retardation factor for hydrocarbon
D_{ij} = coefficient of hydrodynamic dispersion

Much like the approach used in developing BIOPLUME II, the 1989 version of the MOC model was modified to become a six-component particle mover model to simulate the transport of hydrocarbon, oxygen, nitrate, iron(II), sulfate and carbon dioxide. Since the biodegradation of hydrocarbon uses iron (III) as an electron acceptor, iron (III) concentrations are simulated as an initial concentration of ferric iron that is available in each cell. Once the iron (III) is consumed, hydrocarbon concentrations are reduced and ferrous iron is produced. The resulting ferrous iron is then transported in the aquifer. The BIOPLUME III equations include:

$$\frac{\partial Hb}{\partial t} = \frac{1}{R_h}\left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial H}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(bHV_i)\right) - \frac{H'W}{n}$$

$$\frac{\partial Ob}{\partial t} = \left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial O}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(bOV_i)\right) - \frac{O'W}{n}$$

$$\frac{\partial Nb}{\partial t} = \left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial N}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(bNV_i)\right) - \frac{N'W}{n}$$

$$\frac{\partial Fb}{\partial t}=\left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial F}{\partial x_j}\right)-\frac{\partial}{\partial x_i}(bFV_i)\right)-\frac{F'W}{n}$$

$$\frac{\partial Sb}{\partial t}=\left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial S}{\partial x_j}\right)-\frac{\partial}{\partial x_i}(bSV_i)\right)-\frac{S'W}{n}$$

$$\frac{\partial Cb}{\partial t}=\left(\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right)-\frac{\partial}{\partial x_i}(bCV_i)\right)-\frac{C'W}{n}$$

where

N = concentration of nitrate
N' = concentration of nitrate in source or sink fluid
F = concentration of iron (II)
F' = concentration of iron (II) in source or sink fluid
S = concentration of sulfate
S' = concentration of sulfate in source or sink fluid
C = concentration of carbon dioxide
C' = concentration of carbon dioxide in source or sink fluid
All other parameters as defined previously.

The biodegradation of hydrocarbon using the aerobic and anaerobic electron acceptors is simulated using the principle of superposition and the following equations:

$H(t+1) = H(t) - R_{HO} - R_{HN} - R_{HFe} - R_{HS} - R_{HC}$

$O(t+1) = O(t) - R_{OH}$

$N(t+1) = N(t) - R_{NH}$

$Fe(t+1) = Fe(t) - R_{FeH}$
$F(t+1) = R\ FeH$

$S(t+1) = S(t) - R_{SH}$

$C(t+1) = C(t) - R_{CH}$

where R_{HO}, R_{HN}, R_{HFe}, R_{HS}, R_{HC} are the hydrocarbon concentration losses due to biodegradation using oxygen, nitrate, ferric iron, sulfate and carbon dioxide as electron acceptors, respectively. The terms R_{OH}, R_{NH}, R_{FeH}, R_{SH}, R_{CH} are the corresponding concentration losses in the electron acceptors. These reaction terms are computed using one of the three biodegradation expressions: first-order, instantaneous or Monod. For example, and for the instantaneous model, the reaction terms are computed as follows:

$R_{HO} = O(t)/F_O$
$R_{HN} = N(t)/F_N$
$R_{HFe} = Fe(t)/F_{Fe}$
$R_{HS} = S(t)/F_S$
$R_{HC} = C(t)/F_C$

$R_{OH} = H(t) \bullet F_O$
$R_{NH} = H(t+1)^1 \bullet F_N$

$R_{FeH} = H(t+1)^2 \bullet F_{Fe}$
$R_{SH} = H(t+1)^3 \bullet F_S$
$R_{CH} = H(t+1)^4 \bullet F_C$

where F_O, F_N, F_{Fe}, F_S, and F_C are the stoichiometric ratios for each of the electron acceptors, respectively, and $H(t+1)^1$, $H(t+1)^2$, $H(t+1)^3$, and $H(t+1)^4$ are the hydrocarbon concentrations modified by loss due to the reaction with oxygen; oxygen and nitrate; oxygen, nitrate and iron; and oxygen, nitrate, iron and sulfate; respectively in the given time step.

For each of the electron acceptors, the following constraints are applied:

$H(t+1)^1 = 0$ where $O(t) > H(t) \bullet F_O$
$O(t+1) = 0$ where $H(t) > O(t)/F_O$

$H(t+1)^2 = 0$ where $N(t) > H(t+1)^1 \bullet F_N$
$N(t+1) = 0$ where $H(t+1)^1 > N(t)/F_N$

$H(t+1)^3 = 0$ where $Fe(t) > H(t+1)^2 \bullet F_{Fe}$
$Fe(t+1) = 0$ where $H(t+1)^2 > Fe(t)/F_{Fe}$

$H(t+1)^4 = 0$ where $S(t) > H(t+1)^3 \bullet F_S$
$S(t+1) = 0$ where $H(t+1)^3 > S(t)/F_S$

$H(t+1) = 0$ where $C(t) > H(t+1)^4 \bullet F_C$
$C(t+1) = 0$ where $H(t+1)^4 > C(t)/F_C$

Furthermore, these reaction terms are subject to additional constraints. For first-order decay, instantaneous and Monod kinetic models:

$R_{HN} = 0$ if $O(t+1) > O$

$R_{HFe} = 0$ if $O(t+1) > O_{min}$
or $N(t+1) > N_{min}$

$R_{HS} = 0$ if $O(t+1) > O_{min}$
or $N(t+1) > N_{min}$
or $Fe(t+1) > Fe_{min}$

$R_{HC} = 0$ if $O(t+1) > O_{min}$
or $N(t+1) > N_{min}$
or $Fe(t+1) > Fe_{min}$
or $S(t+1) > S_{min}$

where O_{min}, N_{min}, Fe_{min}, S_{min}, C_{min} are the threshold concentrations for the corresponding electron acceptor below which no biodegradation will take place.

For the first-order decay and Monod kinetic models, the reaction terms are compared to the concentration of the electron acceptor:

$R_{HO} < O(t)/F_O$
$R_{HN} < N(t)/F_N$
$R_{HFe} < Fe(t)/F_{Fe}$
$R_{HS} < S(t)/F_S$
$R_{HC} < C(t)/F_C$

APPENDIX D --

BIOPLUME III Input Parameters

BIOPLUME III INPUT DATA

The BIOPLUME III input data are described in the following sections.

1.0 Discretization of Space

The first step in applying the BIOPLUME III model to a field site involves selecting the size of the model grid and the number of cells contained within the grid. Four variables are used to define the selected grid: NX, NY, XDEL and YDEL. The number of grid cells in the x- and y- directions are defined in NX and NY, respectively and the size of the individual cells are defined in XDEL and YDEL, respectively.

Since the model requires that no- flow boundaries be specified around the site, "extra" cells need to be incorporated into the grid design. In other words, if an "active" domain of 12 x 12 cells is needed, a 14 x 14 grid is specified in order to allow for the outer rows and columns to serve as no-flow boundaries.

There are a number of conventions used in the model which are useful to note. First, flow is generally along the y- direction. The origin is designated at the upper left- hand corner of the grid (this means that flow is essentially "down the page"). The x- cells are then counted starting with 1 at the origin and through NX moving to the right of the origin. Similarly, the y- cells are counted starting with 1 at the origin and through NY moving downwards from the origin. These conventions may be changed but caution needs to be exercised in entering the input data and analyzing the resulting output to avoid confusion.

2.0 Discretization of Time

BIOPLUME III uses three variables to define simulation time in the model: NTIM, PINT and NPMP.

NTIM - is defined as the number of times in a given simulation period that the user may receive model results.

PINT - is defined as the length of time in a given simulation period.

NPMP - defines the number of pumping periods to be simulated. A pumping period is defined as a specified length of time during which the hydrologic conditions at the site remain unchanged.

3.0 Hydrogeologic Characteristics of the Aquifer

A number of variables are used in BIOPLUME III to identify the hydrogeologic characteristics of the aquifer. These include: porosity (POROS), longitudinal dispersivity (BETA), storativity (S), ratio of transverse to longitudinal dispersivity (DLTRAT), ratio of longitudinal transmissivity to transverse transmissivity (ANFCTR), transmissivity (VPRM), recharge (RECH) and thickness of the aquifer (THCK).

POROS - (effective porosity) is the dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer solids. The porosity is obtained from site specific measurements or from literature values.

BETA - (longitudinal dispersivity) defines the longitudinal spreading of a plume in the direction of flow. Selection of dispersivity values is difficult because of the impracticability of measuring dispersion in the field. Values for BETA may be obtained using:

- ☐ Data compiled from 50 sites by Gelhar et al. (1985);
- ☐ Data from recent field studies;
- ☐ Using the relationship suggested by Pickens and Grisak (1981):

BETA = 0.1 Lp, where Lp is the plume length or distance to measurement point in ft

S - (storativity) is the product of the specific storage and the thickness of the aquifer, where the specific storage is defined as the volume of water that a unit volume of aquifer releases from storage when the pressure head in the unit volume changes a unit amount. Storativity is only used for transient flow analyses and is estimated from pump tests conducted at the site.

DLTRAT - is the ratio of transverse to longitudinal dispersivity. Much like the longitudinal dispersivity, this variable is difficult to estimate. One of the following relationships may be used:

DLTRAT = 0.33 (Gelhar et al., 1992)
DLTRAT = 0. 1 (U. S. Environmental Protection Agency, 1986)

ANFCTR - (ratio of longitudinal transmissivity to transverse transmissivity) is rarely characterized at field sites and is mostly set to 1.

VPRM - (transmissivity) is the product of the hydraulic conductivity and the thickness of the aquifer. VPRM can be obtained from slug tests or pump tests at the site or from published literature values for the hydraulic conductivity.

RECH - (recharge) is generally obtained from rainfall data and soil infiltration characteristics. This variable is rarely, if ever, measured at field sites. It is usually estimated from local or regional data published by the USGS and the Soil Conservation Service, or calibrated.

THCK - (aquifer thickness) is generally obtained from well logs, soil borings and other geologic characterization efforts at the site.

Note: The last three parameters: VPRM, RECH and THCK, may be specified as a constant for the whole site or as a spatially variable parameter such that a different value is entered for each cell in the model grid.

4.0 Boundary Conditions

In order to simulate a field site with the BIOPLUME III model, it is necessary to identify the hydrogeologic conditions that prevail around the site. These hydrogeologic conditions are referred to as *boundary conditions.* The two types of boundary conditions that can be simulated with BIOPLUME III include: *constant head* and *constant flux* .

Constant head boundaries refer to cells where the water level is constant throughout the simulation. The head or water level value is specified by the user at the constant head boundaries.

Constant flux boundaries, on the other hand, refer to cells that allow water (and possibly contaminants and electron acceptors) to flow through. In this case, the user specifies the rate of water flow (or flux of water) through the cell and specifies whether the cell is also a source of contamination or electron acceptor(s).

A number of variables in BIOPLUME III allow the user to specify the boundary conditions for the site. These include: NCODES, the NODEID matrix, and the parameters ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD.

The NCODES variable is used to define the number of boundary condition types to be used in the model. For example, if constant head boundary conditions without chemical concentration inflow are to be used for the site, then the NCODES variable is set to one. If, on the other hand, constant head boundaries without chemical concentration inflow are to be used in one portion of the site and constant head boundaries with chemical concentrations inflow are to be used in another portion of the site, then the NCODES variable is set to two.

The NODEID matrix is used to specify the cells at which the boundary conditions will be designated. The NODEID matrix can be thought of as an ON/OFF switch designator. If BIOPLUME III encounters a number between 1 to 9 at any of the cells, the model interprets that as "an ON switch" for additional boundary condition information. BIOPLUME III anticipates that more data would be provided for those cells. The data include the variables ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD. Additionally, if constant head boundaries are used at any of the cells, the water table or WT variable needs to be specified for those cells.

5.0 Initial Conditions

The head and concentrations at the start of the simulation period need to be specified in the BIOPLUME III input. The specific variables include: initial water table (WT), initial concentration of contaminants (CONC), oxygen (CONC1), nitrate (CONC2), ferrous iron (CONC3), ferric iron (CONC3A), sulfate (CONC4), and carbon dioxide (CONC5).

The initial water table (WT) may be developed by contouring water level data measurements and entering the resulting values into each cell in the model grid. This is however, time consuming and not entirely necessary since the model will recompute the water table anyway. The user can enter "0" for the initial water table elevation everywhere except where constant head nodes have been specified (the actual water level is entered for those).

The initial concentration of contaminants (CONC) and the initial concentrations for all the electron acceptors (CONC1 through CONC5) are determined from monitoring well data.

Note: The BIOPLUME III model does not require specific units for concentration. The user may select between mg/L and µg/L. The model does require that the user use a consistent set of units for all the concentration input. Therefore, if mg/L for example are to be used, then all the concentration data need to be entered in that systems of units. The output concentrations generated by the model will also reflect the same units as the input.

6.0 Sources and Sinks

The introduction of water or release of water from the aquifer (including contaminants and electron acceptors) is referred to as sources and sinks. These can be simulated using injection/ pumping wells, recharge/ discharge cells or constant head cells. The use of recharge and constant head nodes to represent sources and sinks has been illustrated in the previous section.

This section will focus on the use of injection wells to represent sources and/ or pumping and injection scenarios. The model parameters for injection/ pumping wells include: NREC, REC, CNRECH, CNRECO, CNRECN, CNRECF, CNRECS, and CNRECC.

NREC - defines the number of injection or pumping wells that will be used in the model input.

REC - specifies the injection (- ve) or pumping rate (+ ve) for each of the wells.

CNRECH - specifies the concentration of contaminant in injected water (parameter set to 0 for pumping wells).

CNRECO - specifies the concentration of oxygen in injected water (parameter set to 0 for pumping wells).

CNRECN - specifies the concentration of nitrate in injected water (parameter set to 0 for pumping wells).

CNRECF - specifies the concentration of ferrous iron in injected water (parameter set to 0 for pumping wells).

CNRECS - specifies the concentration of sulfate in injected water (parameter set to 0 for pumping wells).

CNRECC - specifies the concentration of carbon dioxide in injected water (parameter set to 0 for pumping wells).

7.0 Sorption, Source Decay, Radioactive Decay and Ion-Exchange Variables

A number of variables are used in the model to represent source decay, radioactive decay, sorption and ion-exchange reactions. The parameter IREACT is used to designate which of these reactions are to be used in the current simulation:

IREACT	**REACTION**	**PARAMETERS TO BE SPECIFIED**
-1	decay only	THALF
0	no reaction	None
1	linear sorption	DK, RHOB, THALF
2	Freundlich sorption	RHOB, EKF, XNF, THALF
3	Langmuir sorption	RHOB, EKL, CEC, THALF
4	monovalent exchange	RHOB, EK, CEC, CTOT, THALF
5	divalent exchange	RHOB, EK, CEC, CTOT, THALF
6	mono- divalent exchange	RHOB, EK, CEC, CTOT, THALF
7	di- monovalent exchange	RHOB, EK, CEC, CTOT, THALF

THALF is the decay half-life used for radioactive compounds. This half- life is applied both to the specified source concentration and to the dissolved concentrations in the model.

RHOB - is the aquifer bulk density.

DK - is the linear sorption distribution coefficient more typically referred to as K d. The distribution coefficient is generally computed using the following relationship:

$$K_d=K_{oc}*f_{oc}$$

where Koc is the normalized distribution coefficient and foc is the fraction of organic carbon found in uncontaminated soils at the site. The variable foc can be determined from laboratory analyses of the soils at the site or using the typical values.

EKF - is the Freundlich sorption coefficient.

XNF - is the Freundlich sorption exponent.

EKL - is the Langmuir sorption coefficient.

CEC - is the maximum sorption capacity or ion exchange capacity.

EK - is the Ion-exchange selectivity coefficient.

CTOT - is the total solution concentration of two exchanging ions.

THALFS - represents the source decay rate.

8.0 Biodegradation Variables

A number of variables are used in BIOPLUME III to simulate the aerobic and anaerobic biodegradation of contaminants. An overall first-order decay biodegradation rate (DEC1) can be designated to simulate the lumped effect of aerobic and anaerobic processes. Alternatively, detailed information about the electron acceptors may be provided to simulate their individual impacts. A biodegradation type specifier for each of the electron acceptors (IRECO, IRECN, IRECF, IRECS, IRECC) is used to select between the first- order, instantaneous, and Monod kinetic models. The electron acceptor data for oxygen, for example, depends on the selected kinetic model:

First-Order Decay Simulations:
DCO - is the first-order decay rate for oxygen.
FO - is the concentration of available oxygen in the groundwater. This value is needed to allow the model to decay hydrocarbons as long as oxygen is present in the aquifer. If oxygen concentrations reach their specified threshold concentrations (DOMIN), the biodegradation reaction is terminated. This ensures that the first-order decay model does not overestimate the amount of biodegradation that is likely to occur in the aquifer.
DOMIN - is the threshold oxygen concentration.

Instantaneous Reaction Simulations:
The variables **FO** and **DOMIN** (defined previously) are required.

Monod Kinetic Simulations:
In addition to **FO** and **DOMIN** (as in the case of the first-order model, these parameters are provided to ensure this model does not overestimate the amount of biodegradation that is likely to occur in the aquifer), the following parameters are required:

CMSO - is the concentration of microorganisms in the aquifer.
RMO - is the microbial retardation coefficient.
RKHO - is the half-saturation constant for the contaminant.
RKMAXO - is the maximum growth rate for the contaminant.
RKO - is the half-saturation constant for oxygen.

Similar variables are defined for all the electron acceptors.

9.0 Numerical Parameters

A number of variables used in BIOPLUME III define "numerical parameters" needed in the solution method used by the model. These include: **NPTPND**, **NPMAX**, **CELDIS**, **NITP**, **ITMAX**, **TOL**, **TIMX**, and **TINIT**.

NPTPND is the number of particles to be used in each cell in the model. The number of particles used in each cell will impact the runtime required for the model. A smaller number of particles will allow the model to run in a shorter period of time but may increase the mass balance errors in the simulation. In general, 9 particles provide adequate model accuracy without causing excessively long run times.

NPMAX is the maximum number of particles for the whole grid. In general, NPMAX should be set to a number greater than NX*NY*NPTPND.

CELDIS defines the maximum allowable distance within the cell that a particle is allowed to move in a time step. A CELDIS of 0.5 implies that a particle is not allowed to move more than half a cell length during the time step. This variable is needed in order to control the movement of the particles and the mass balance errors in the model. A smaller CELDIS causes lower numerical mass balance errors but may increase runtimes. In general, a CELDIS of 0.5 is recommended.

NITP is the number of iteration parameters used in solving the flow equation. A value of 7 is recommended for this variable.

ITMAX is the maximum number of iterations to be used in solving the flow equation. A value of 200 (the maximum) is recommended for this variable. If the model is unable to arrive at a solution of the flow equation using this value, an error message will be generated and the model run will be terminated. In this case it is recommended that the user review the input data for possible errors.

TOL is the convergence criterion that is used to iteratively solve the flow equation. A value £ 0.001 is recommended.

TIMX and **TINIT** define the time steps for transient simulations. TINIT is the size of the initial time step, and TIMX is the multiplier that will be used to generate subsequent time steps from TINIT. For example, if TINIT is set to 1000 seconds and TIMX is set to 10, the second time step will be 10 x 1000 = 10,000 seconds, the third time step will be 10,000 x 10 = 100,000 seconds, and so on.

10.0 Output Control Parameters

A number of variables in BIOPLUME III can be used to control the amount of output that is generated by the model. These include: **NPNT**, **NPNTMV**, **NPNTVL**, **NPNTD**, **NPDELC**, and **NPNCHV**. The majority of these parameters, except for **NPNT**, are typically set to "0. **NPNT** is usually set to "1" to allow viewing of the output at the end of the time step.

Other variables are used to control the type of output that can be generated by the model. These include variables that designate the number and location of observation points: **NUMOBS**, **IXOBS** and **IYOBS**.

NUMOBS is the number of observation or monitoring wells to be specified. A maximum of 5 is allowed.

IXOBS and **IYOBS** define the locations of the specified number of monitoring wells.

APPENDIX E –

Benzene Analytical Data and Isopleths

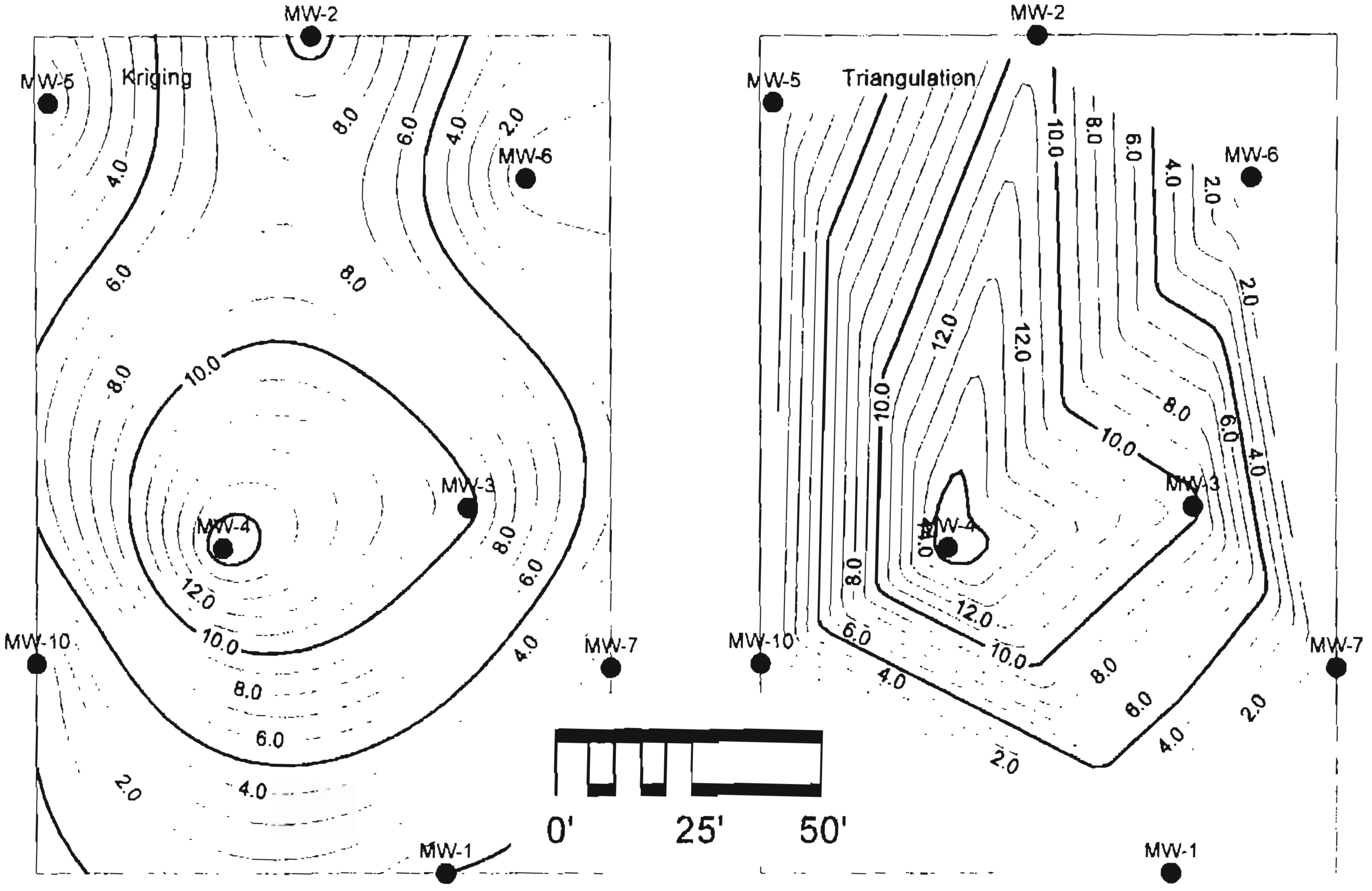
Benzene Concentrations In Groundwater (mg/L)

Well	7/25/94	10/10/94	4/6/95	10/26/95	11/13/95	12/21/95	2/20/96	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	<0.005	0.300	0.315	0.185			0.0576	<0.5	<0.5	<0.5	<0.5
MW-2	10.800	11.000	6.700	0.0108				<0.5	<0.5	<0.5	<0.5
MW-3	10.500	7.300	12.0	10.2			6.04	8.950	12.510	11.940	12.630
MW-4	16.100	8.200	6.920	6.250				7.850	16.030	40.260	25.530
MW-5	<0.005	<0.0002	0.002	0.0025				<0.5	<0.5	<0.5	<0.5
MW-6	<0.005	2.100	1.290	1.670				1.110	3.540	3.300	2.970
MW-7	0.071	0.520	0.004	0.161				1.650	2.600	2.800	2.970
MW-8		<0.0002	<0.001	0.0036				<0.5	<0.5	<0.5	<0.5
MW-9		0.0051		0.0668	0.0208		0.0182				
MW-10		0.0029		0.0014				<0.5	<0.5	<0.5	0.21
MW-11		<0.0002	<0.001	0.0258	0.0404		0.0258	<0.5	<0.5	<0.5	<0.5
MW-12		<0.0002	<0.001	0.0015			0.0048	<0.5	<0.5	<0.5	<0.5
MW-13		<0.0003	0.002	0.0018			0.0107	<0.5	<0.5	<0.5	<0.5
MW-14				0.0105				<0.5	<0.5	<0.5	<0.5
MW-15						<0.001	<0.001	<0.5	<0.5	<0.5	<0.5
MW-16						<0.001	<0.001	<0.5	<0.5	<0.5	<0.5

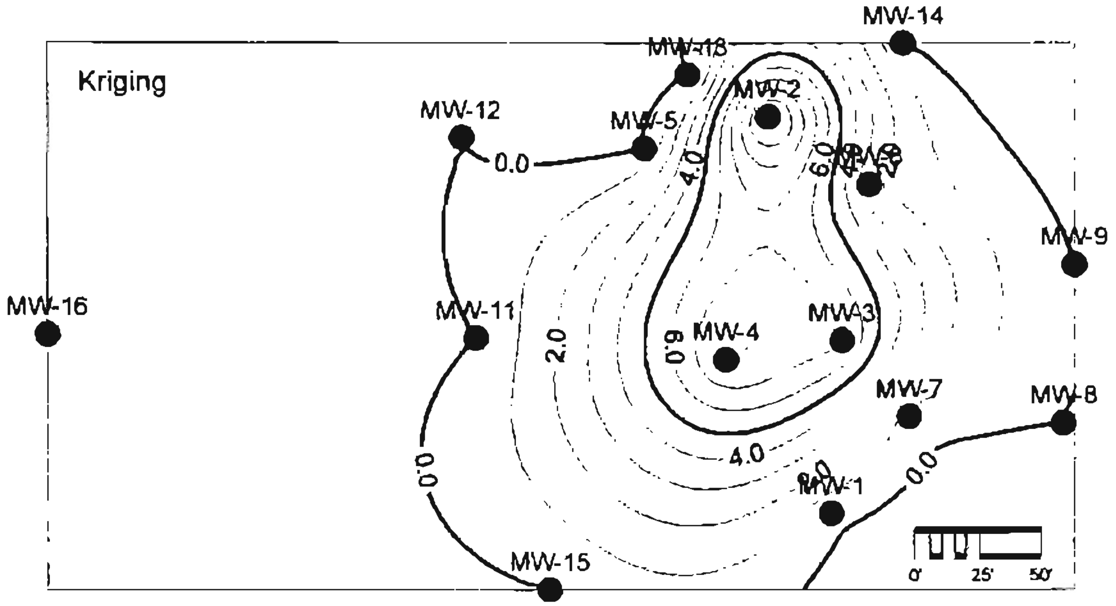
Notes:

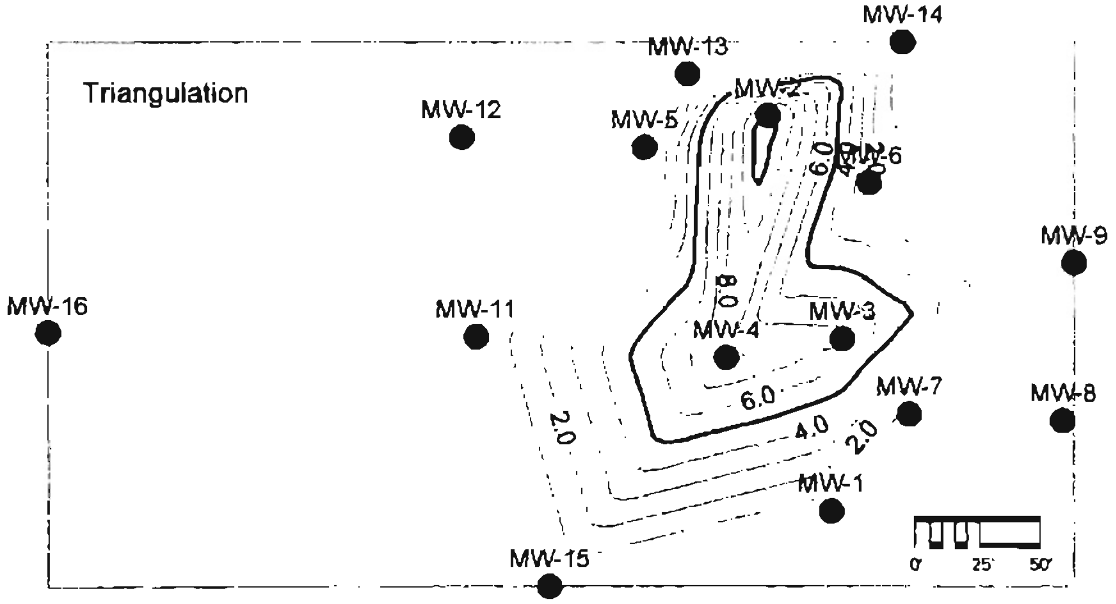
1. Less than signs (<) designate values below the detection limit.
2. 1994, 1995, and 1996 data is from Caldwell, 1995.
3. 1997 and 1998 data is from Akins, 1998.

BENZENE (mg/L) -- 7/25/94

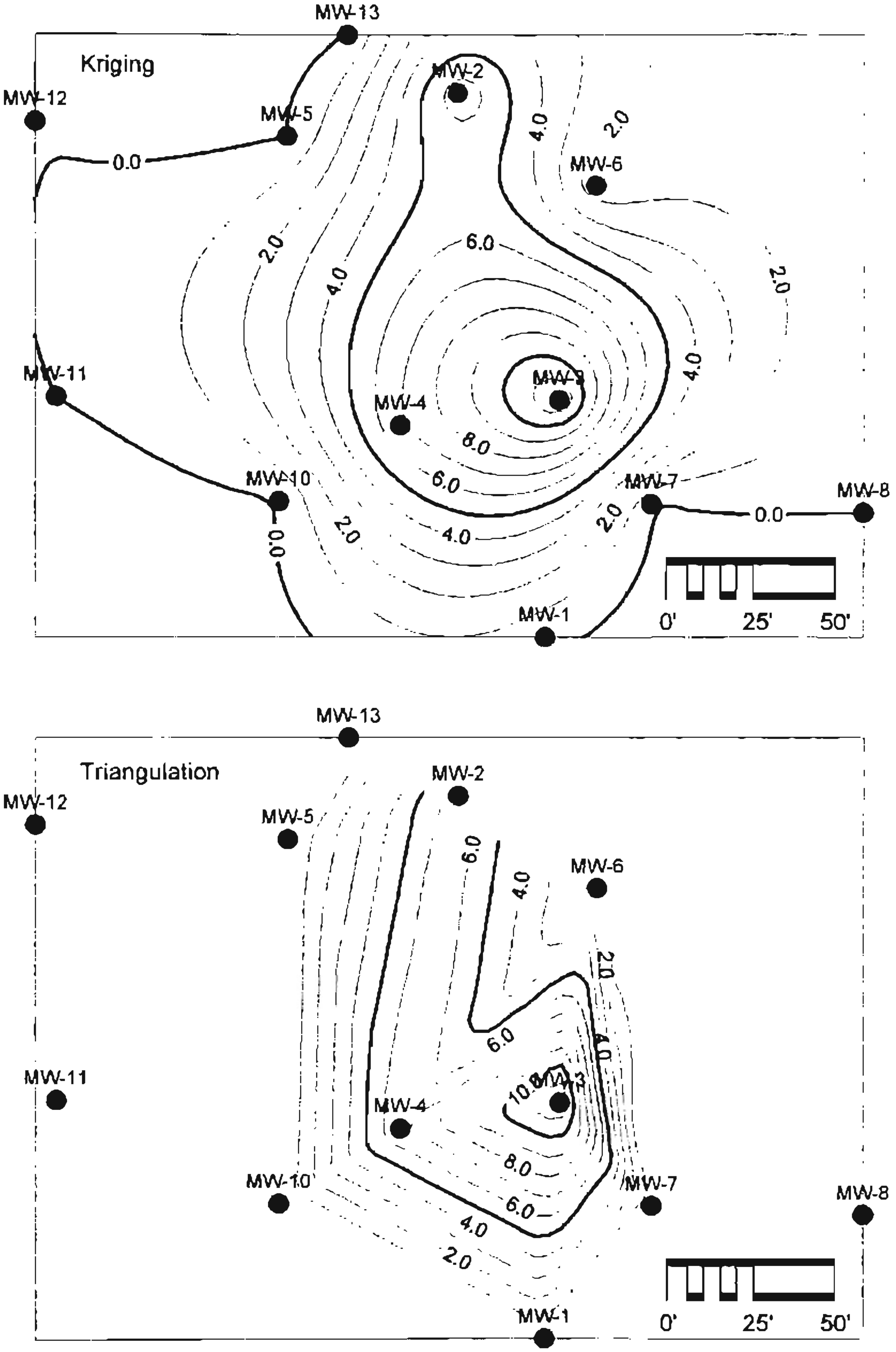


BENZENE (mg/L) -- 10/10/94





BENZENE (mg/L) -- 4/6/95



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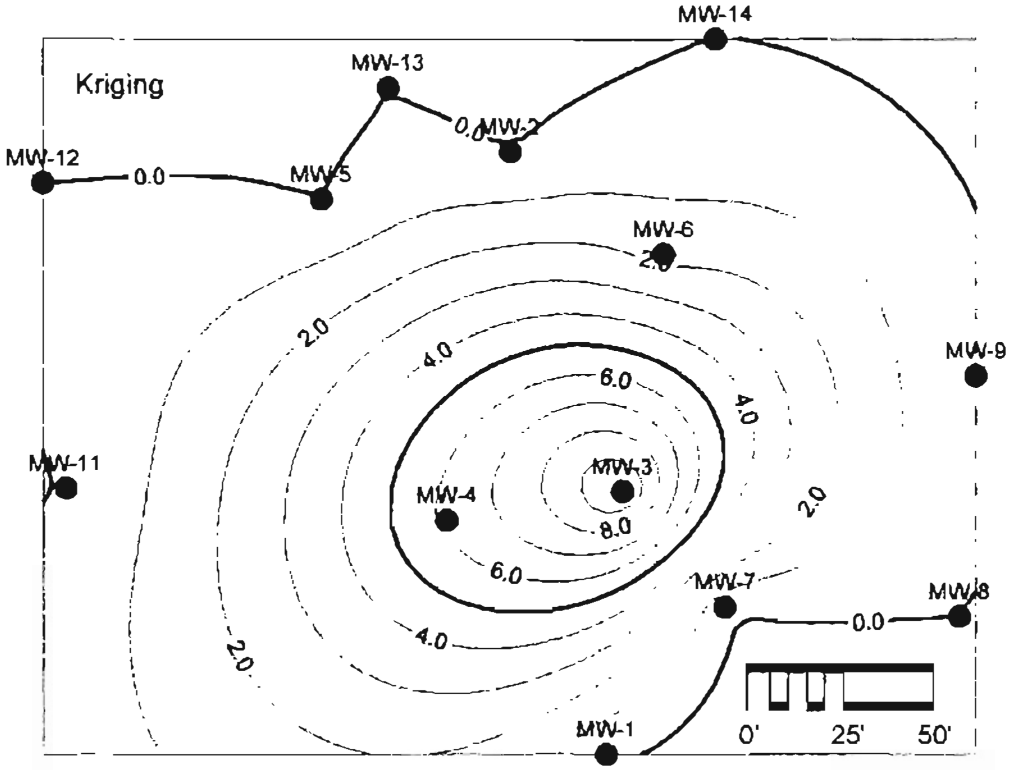

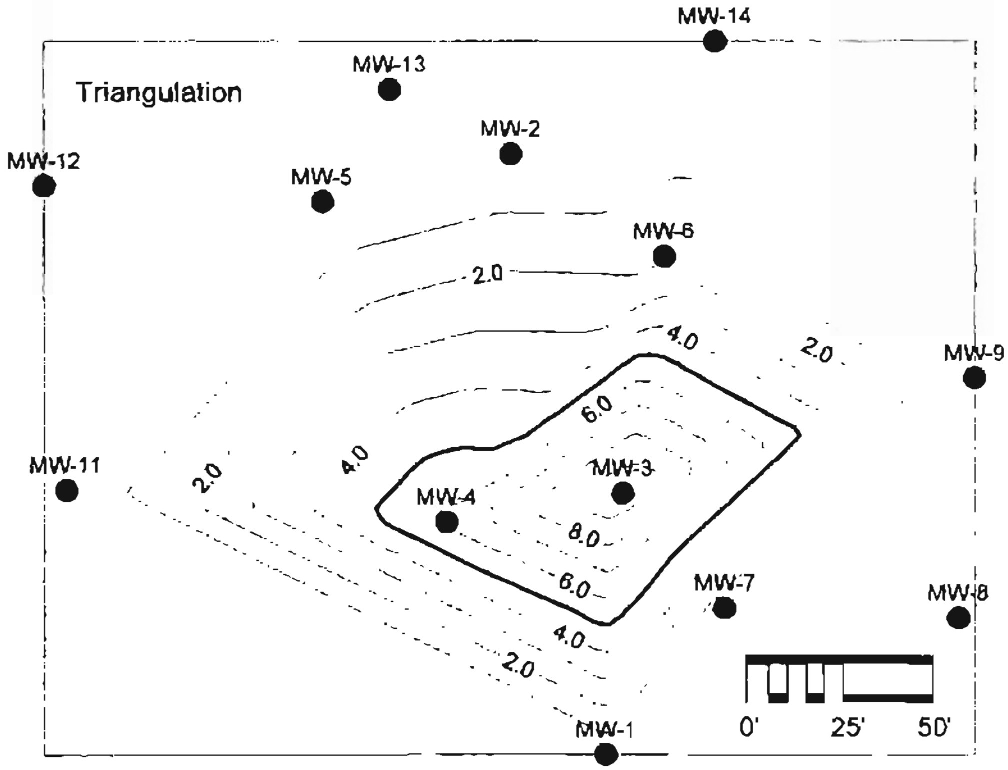

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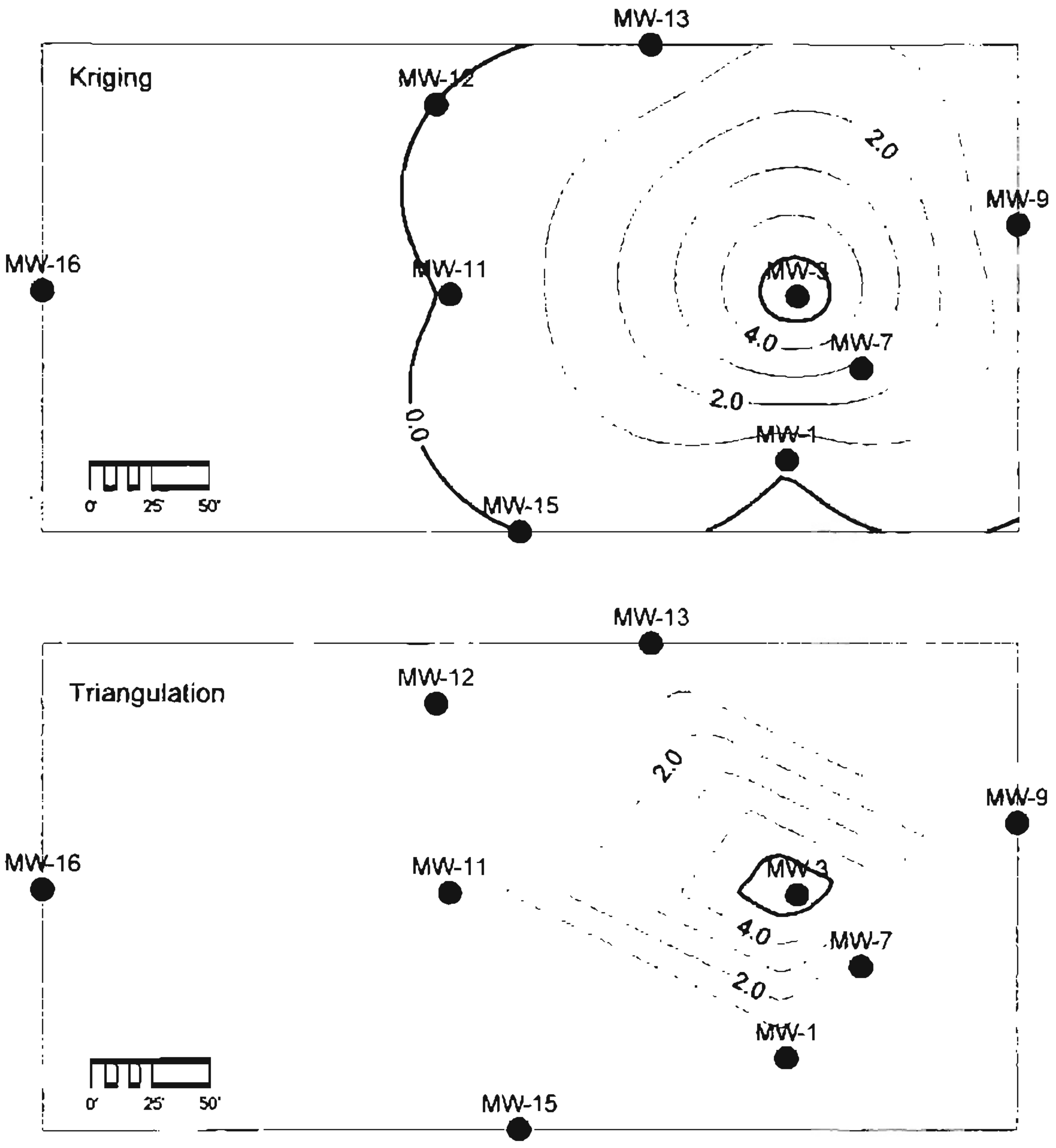
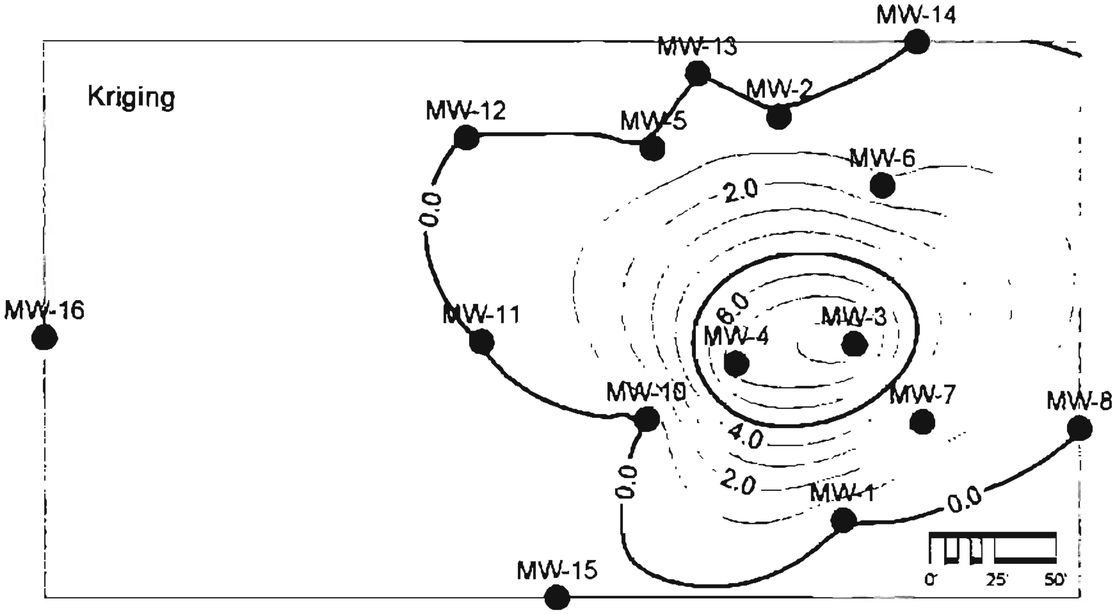
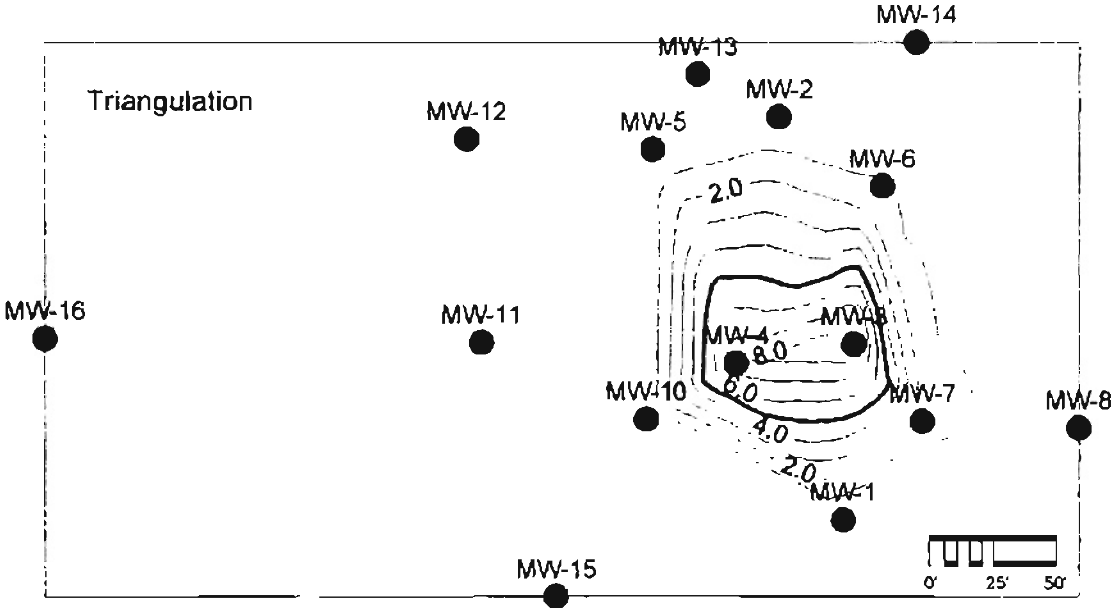
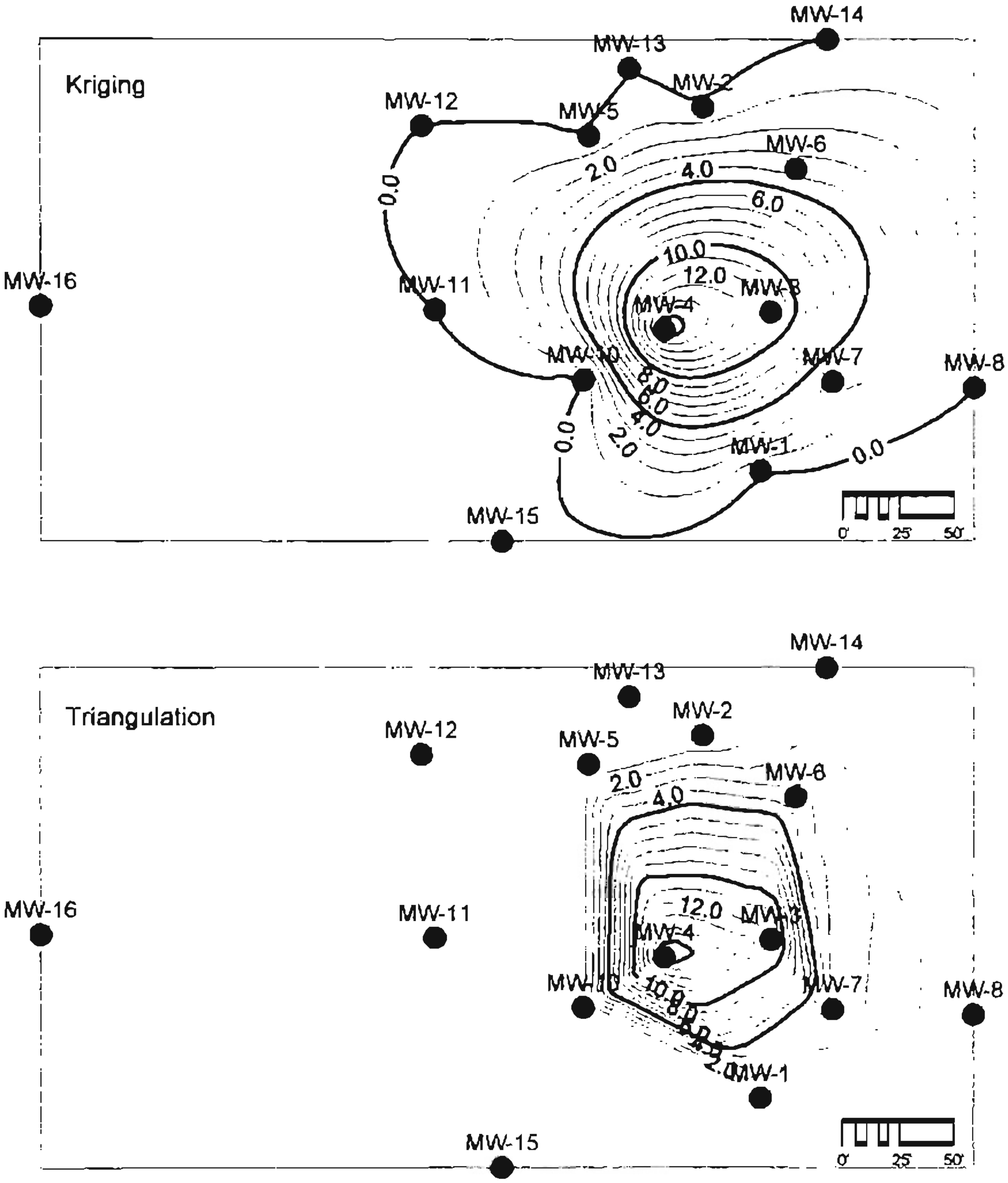


BENZENE (mg/L) -- 10/20/97

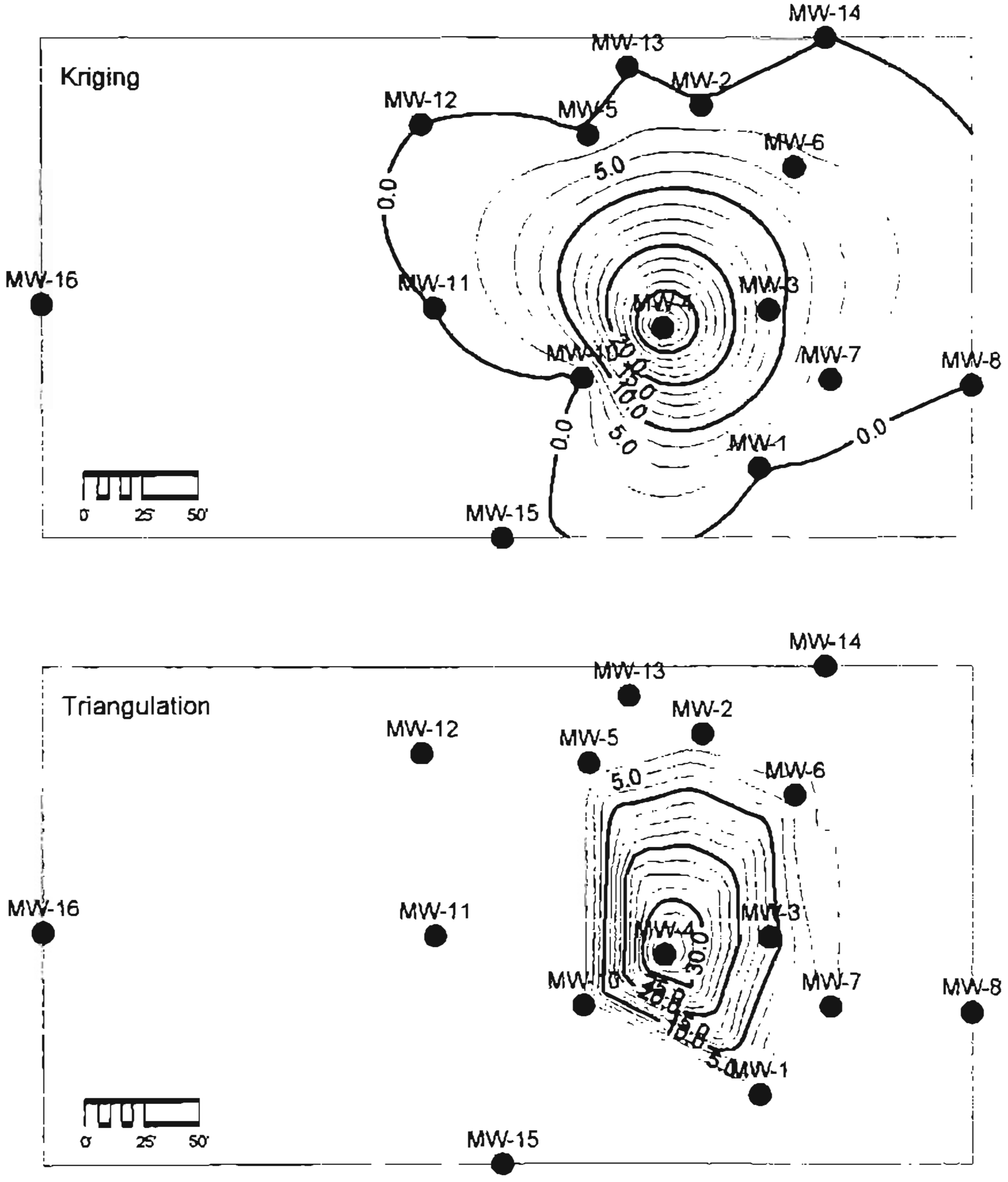




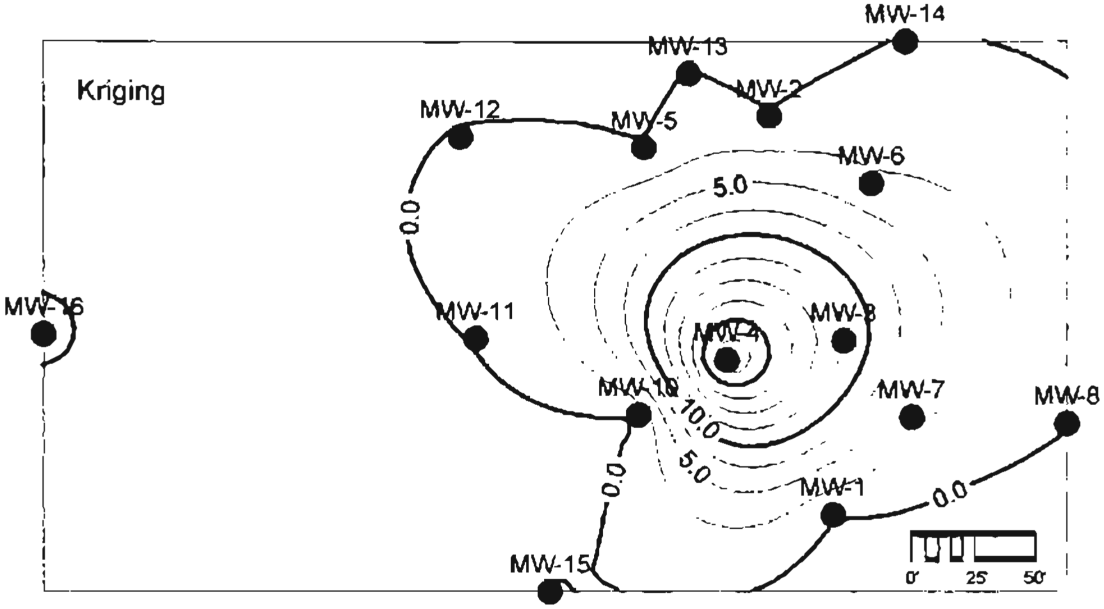
BENZENE (mg/L)-- 12/15/97

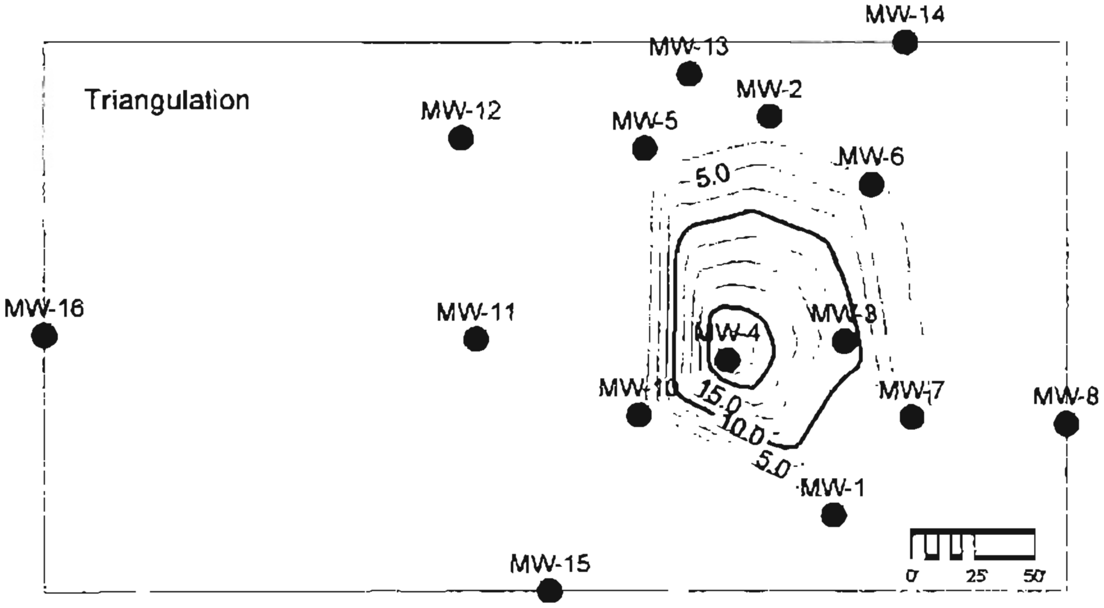


BENZENE (mg/L) -- 1/20/98



BENZENE (mg/L) -- 2/17/98





APPENDIX F –

Toluene Analytical Data and Isopleths

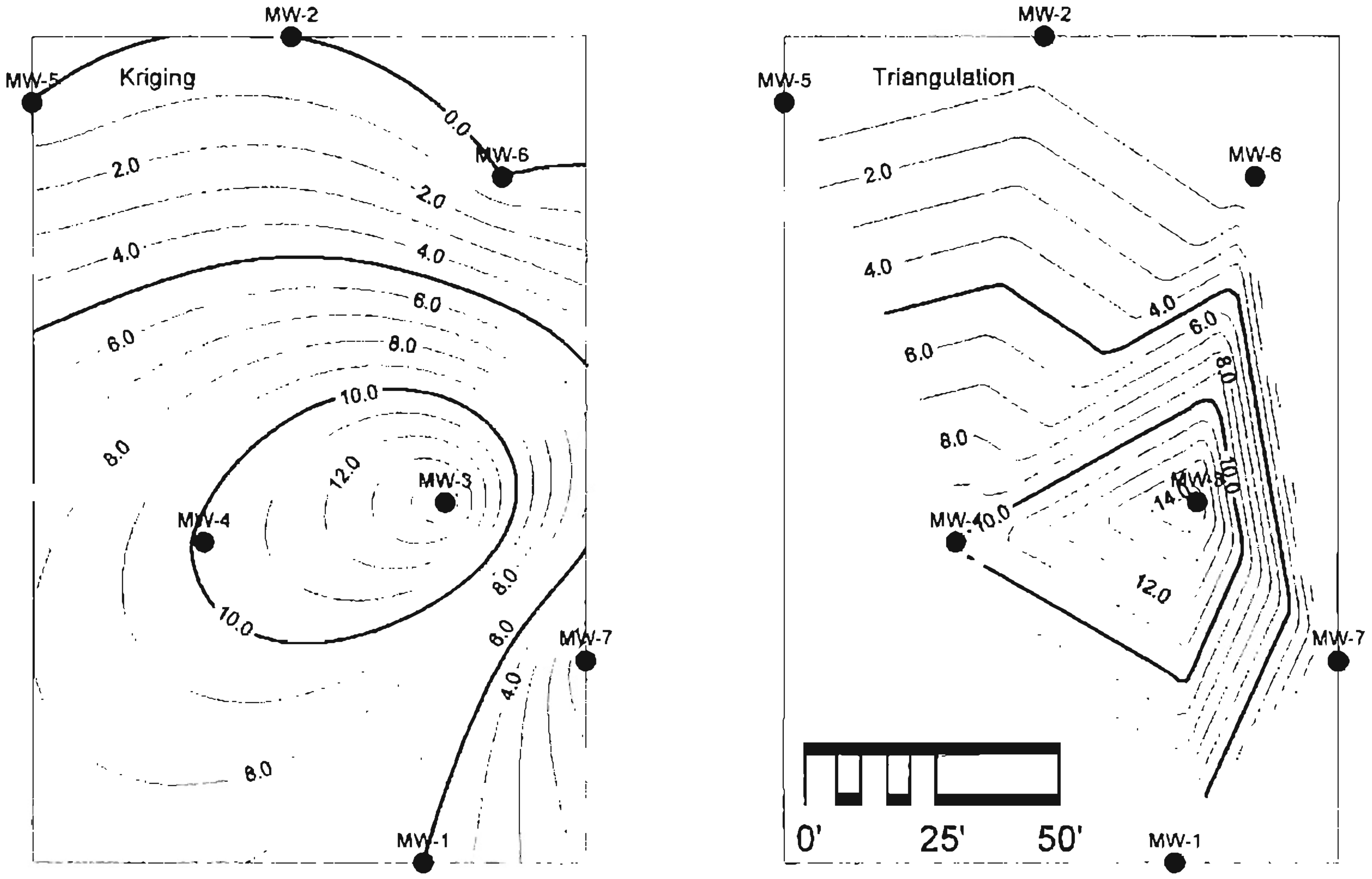
Toluene Concentrations in Groundwater (mg/L)

Well	7/25/94	10/10/94	4/6/95	10/26/95	11/13/95	12/21/95	2/20/96	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	<5	0.034	0.0115	0.0043			0.0022	0.129	0.129	0.129	0.172
MW-2	0.005	<0.0002	<1.0	<0.001				0.086	<0.005	<0.005	0.043
MW-3	15	11	18	15.1			8.8	11.435	19.877	18.470	24.116
MW-4	10.2	4.6	4.17	7				4.861	18.294	59.459	30.561
MW-5	<0.005	<0.0002	<0.001	<0.001				0.258	0.172	0.086	0.086
MW-6	<0.005	0.81	0.543	0.84				0.258	3.699	0.430	0.258
MW-7	0.0059	0.077	0.004	0.0098				1.914	3.183	3.355	2.495
MW-8		<0.0002	<0.001	<0.001				<0.005	<0.005	0.086	<0.005
MW-9		<0.0002	0.0081	0.0081	<0.001		<0.001				
MW-10		<0.0002		<0.001					<0.005	<0.005	0.602
MW-11		<0.0002	<0.001	0.0027	0.0038		0.0027	<0.005	0.086	0.086	0.172
MW-12		<0.0002	<0.001	<0.001			<0.001	0.172	<0.005	<0.005	<0.005
MW-13		<0.0002	<0.001	<0.001			<0.001	0.086	0.086	<0.005	<0.005
MW-14				<0.001				0.086	<0.005	<0.005	<0.005
MW-15						<0.001	<0.001	<0.005	<0.005	<0.005	<0.005
MW-16						<0.001	<0.001	<0.005	<0.005	<0.005	<0.005

Notes:

1. Less than signs (<) designate values below the detection limit.
2. 1994, 1995, and 1996 data is from Caldwell, 1995.
3. 1997 and 1998 data is from Akins, 1998.

TOLUENE (mg/L) -- 7/25/94



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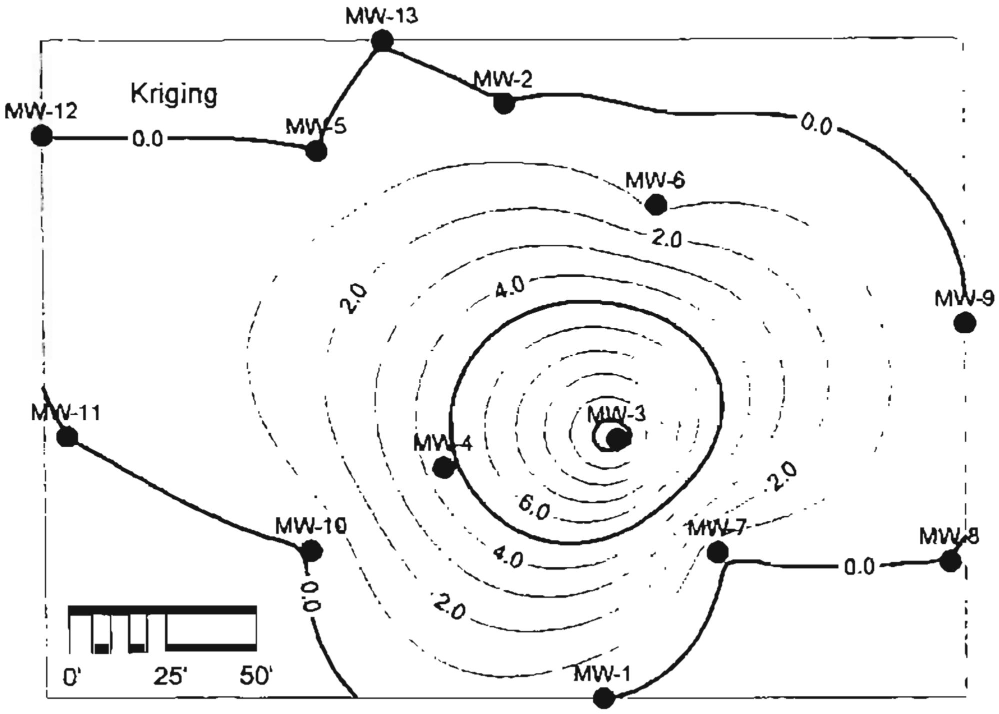
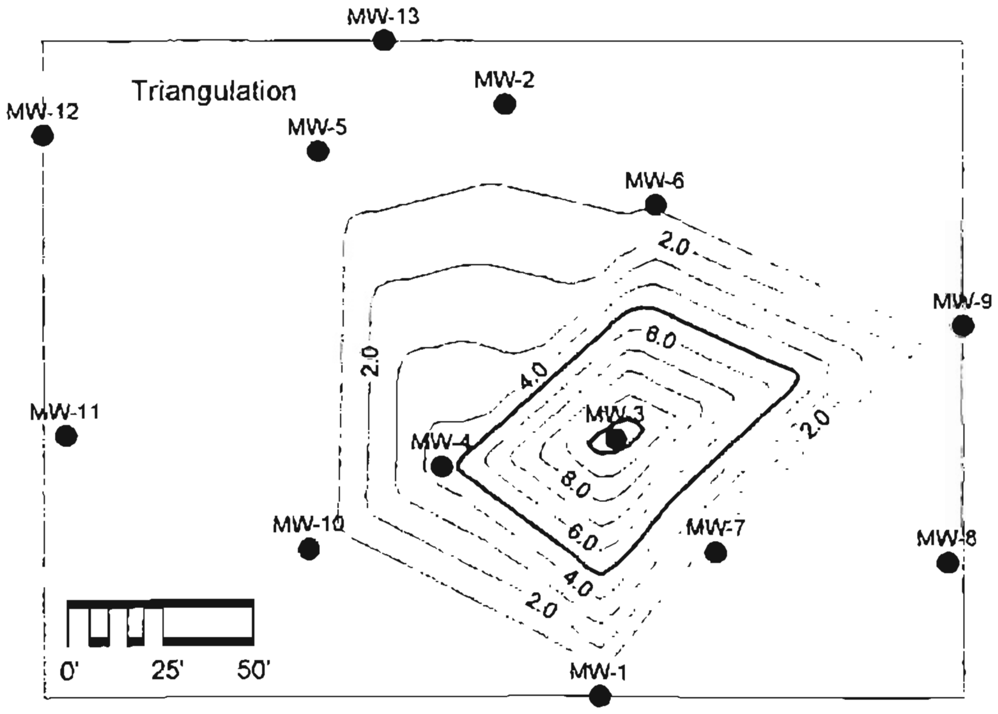
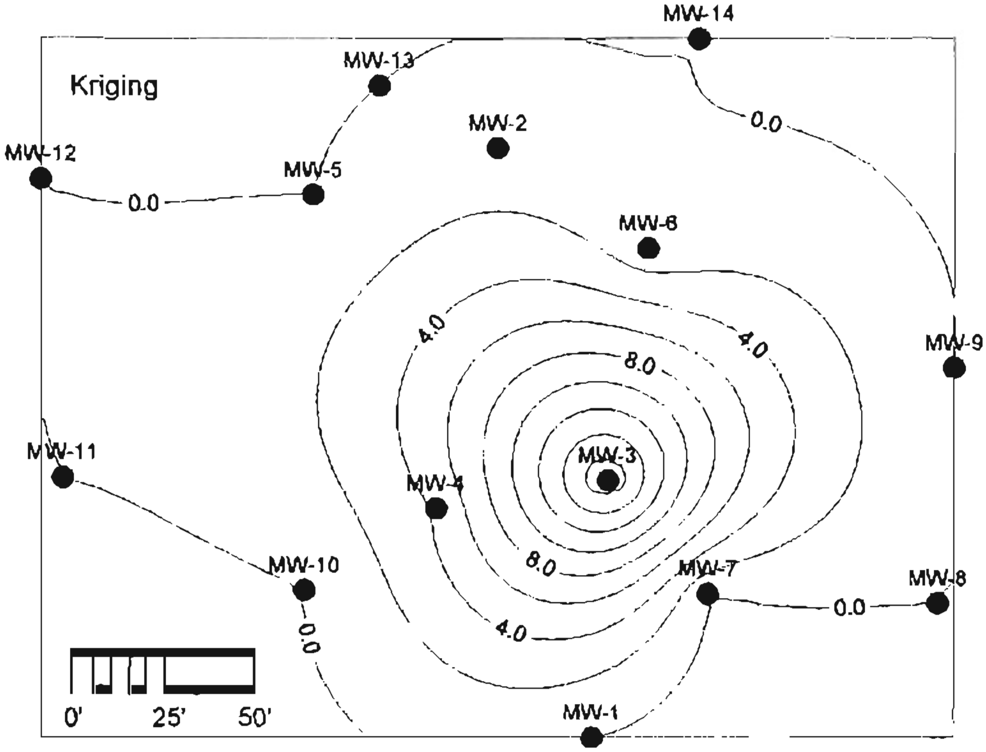
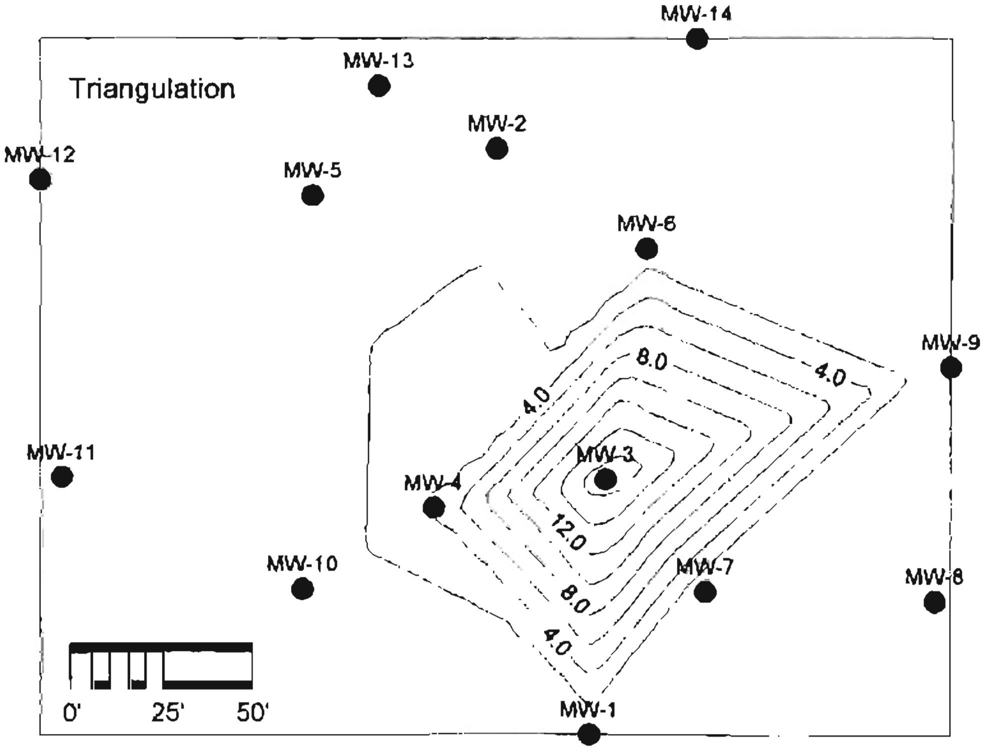


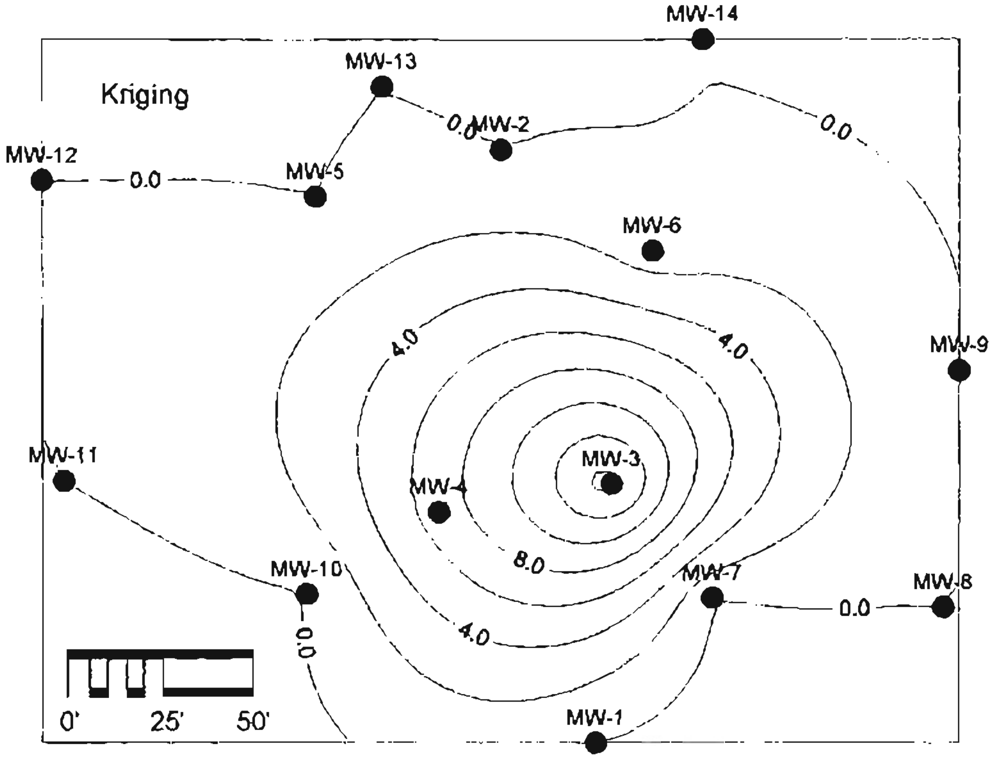


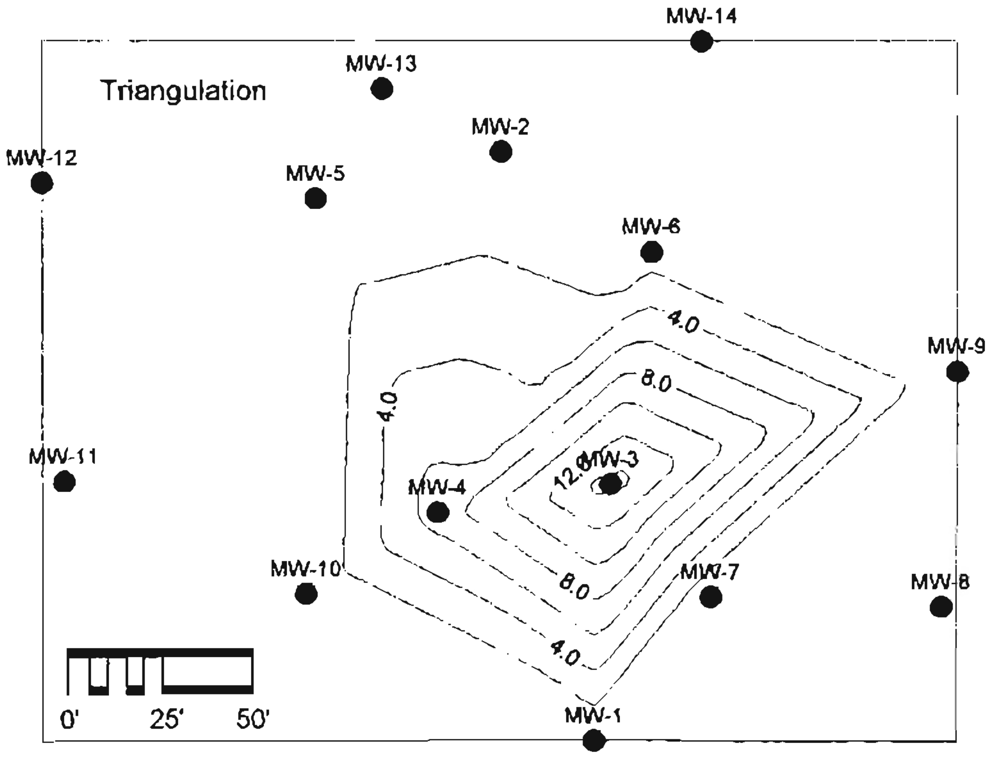
TOLUENE (mg/L) -- 4/6/95



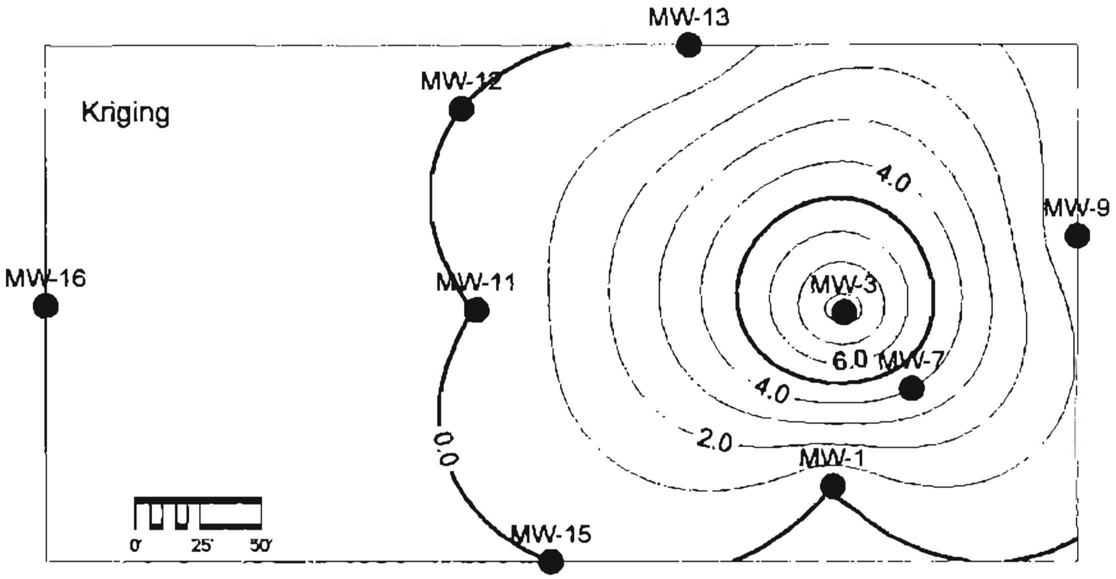


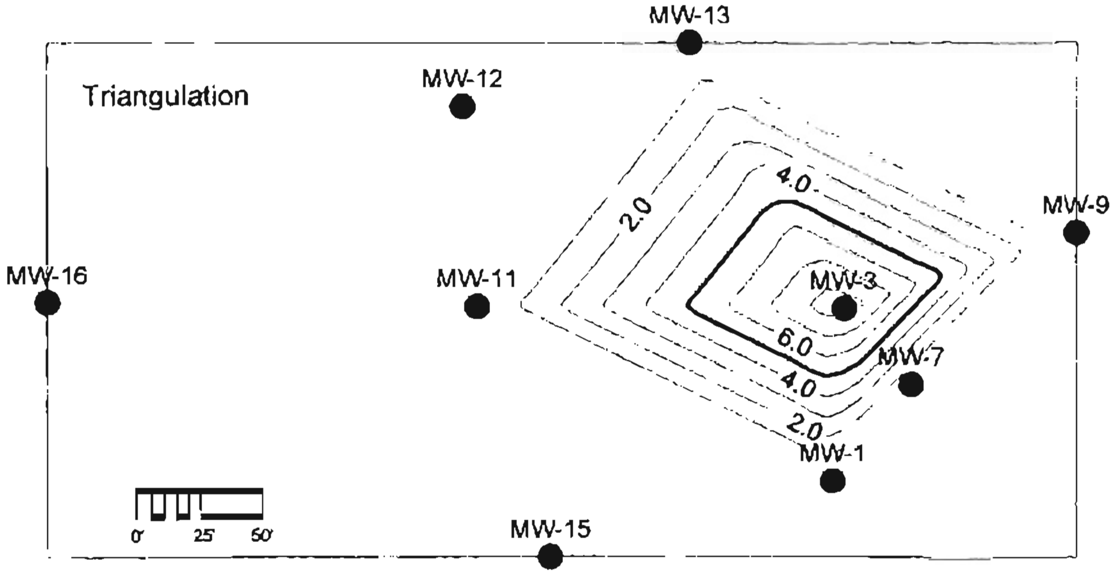
TOLUENE (mg/L) -- 10/26/95



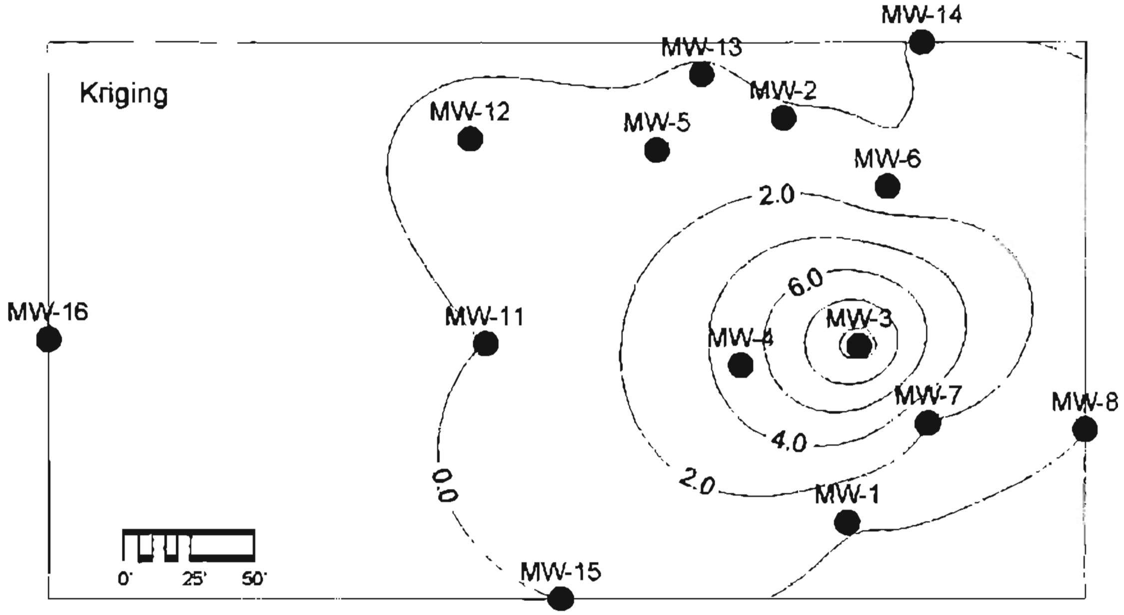


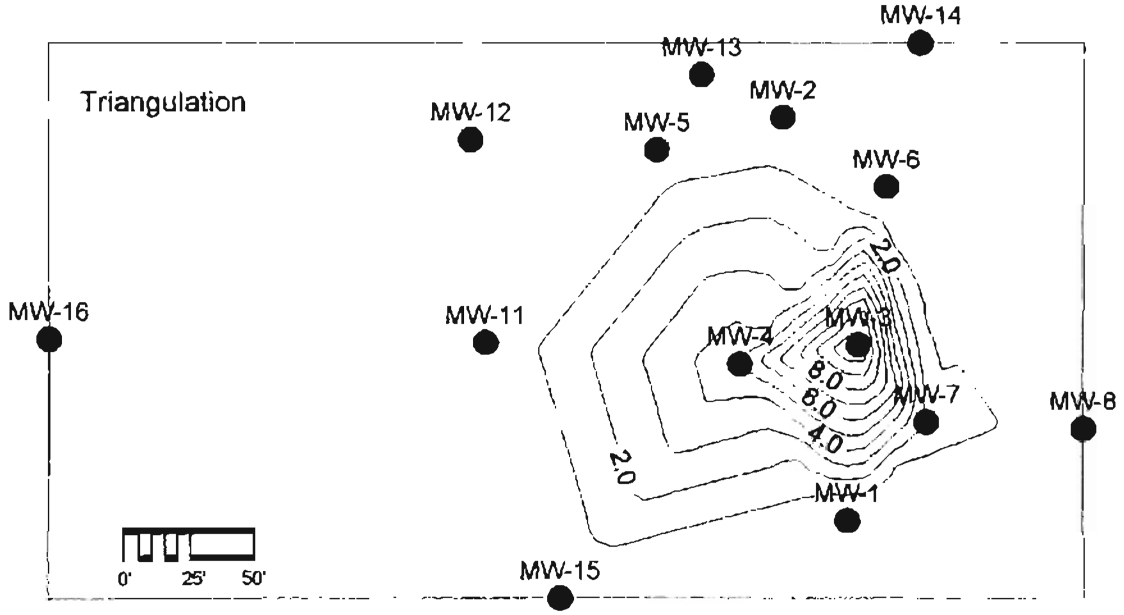
TOLUENE (mg/L) -- 2/20/96



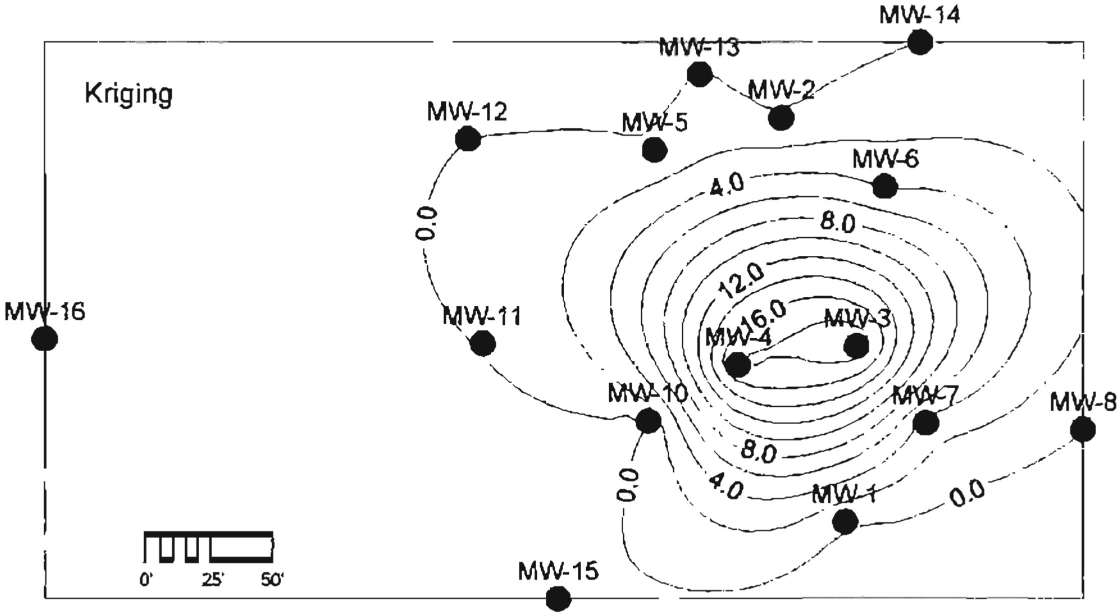


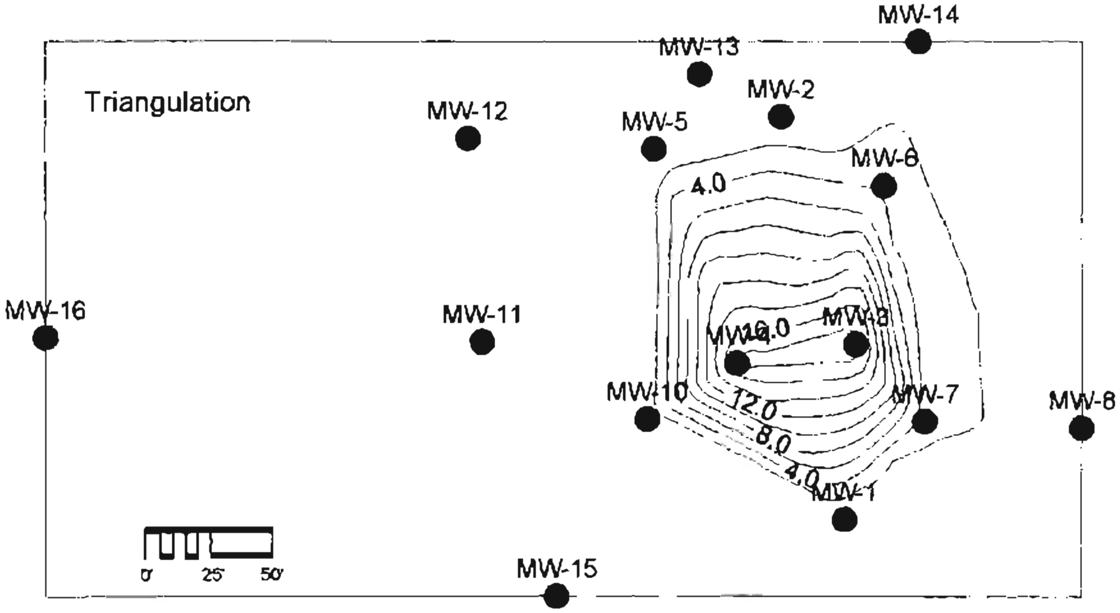
TOLUENE (mg/L) -- 10/20/97



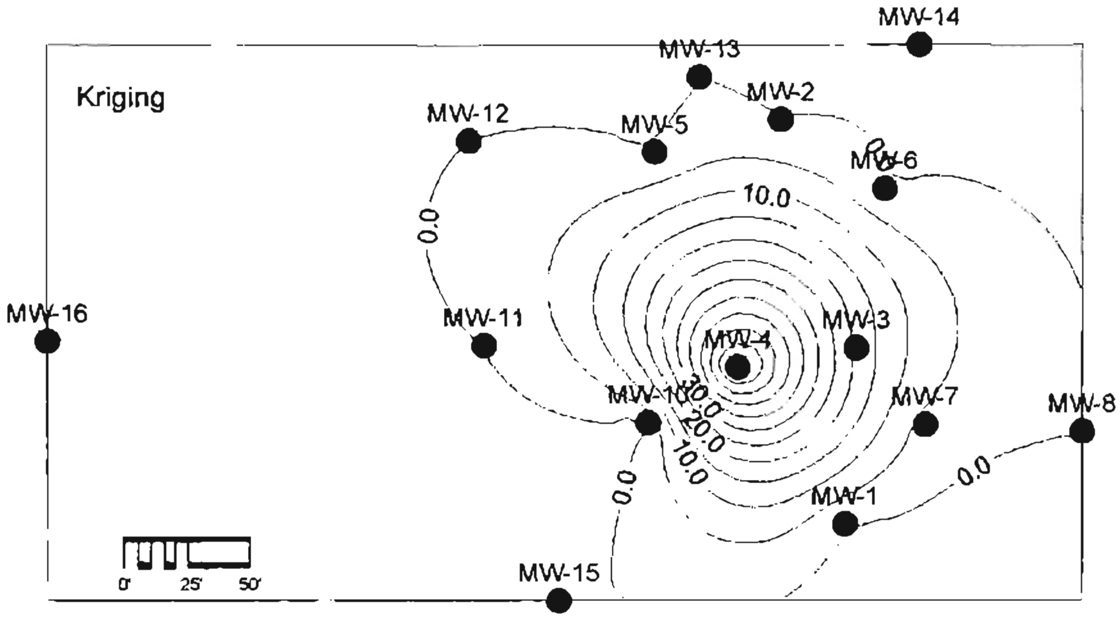


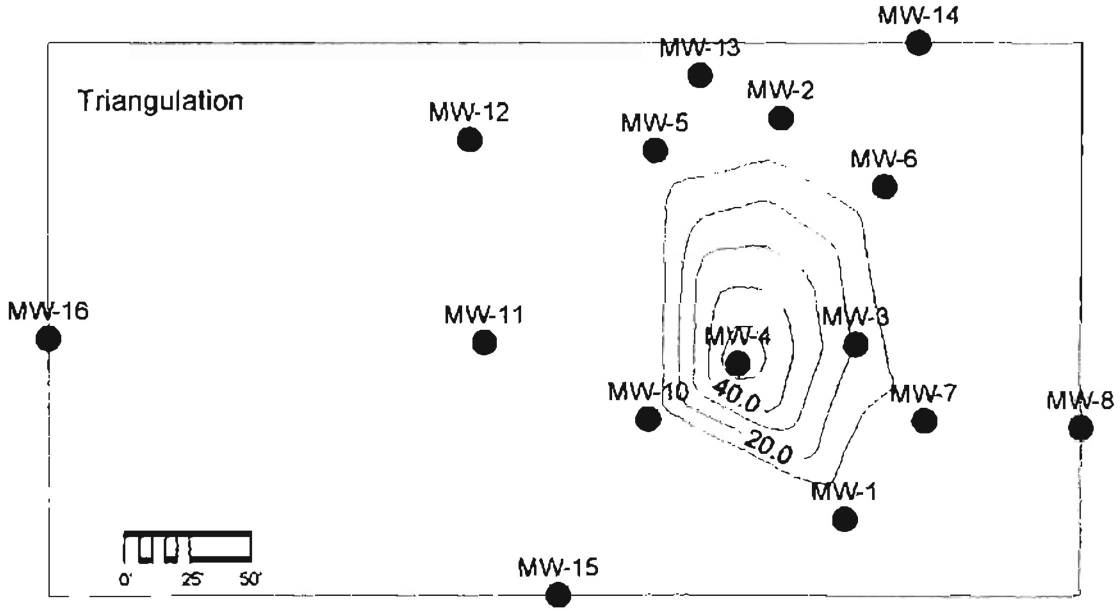
TOLUENE (mg/L) -- 12/15/97



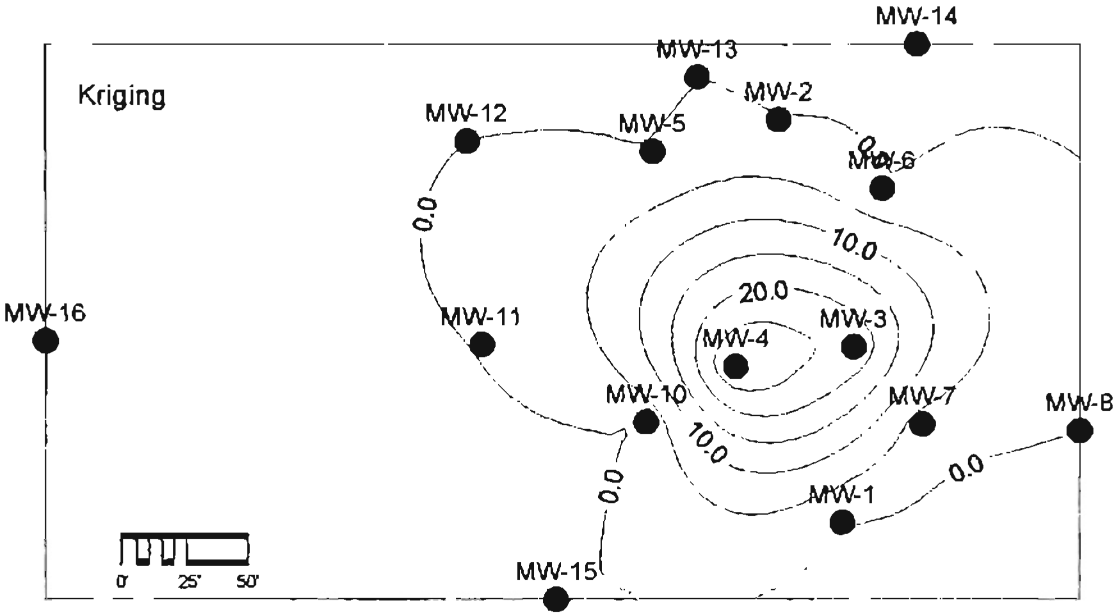


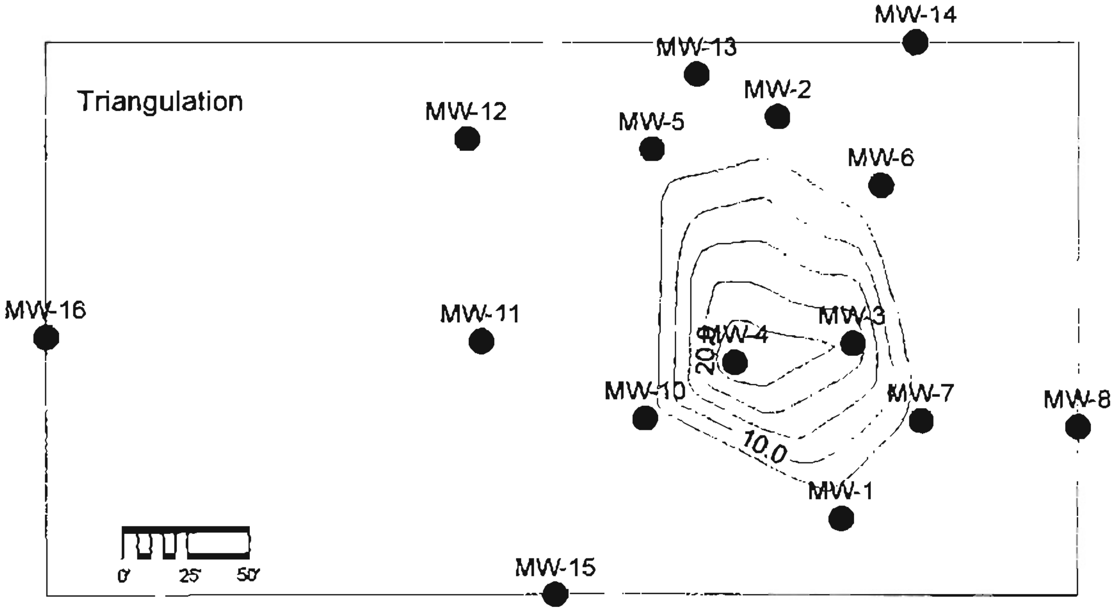
TOLUENE (mg/L) -- 1/20/98





TOLUENE (mg/L) -- 2/17/98





APPENDIX G –

Ethylbenzene Analytical Data and Isopleths

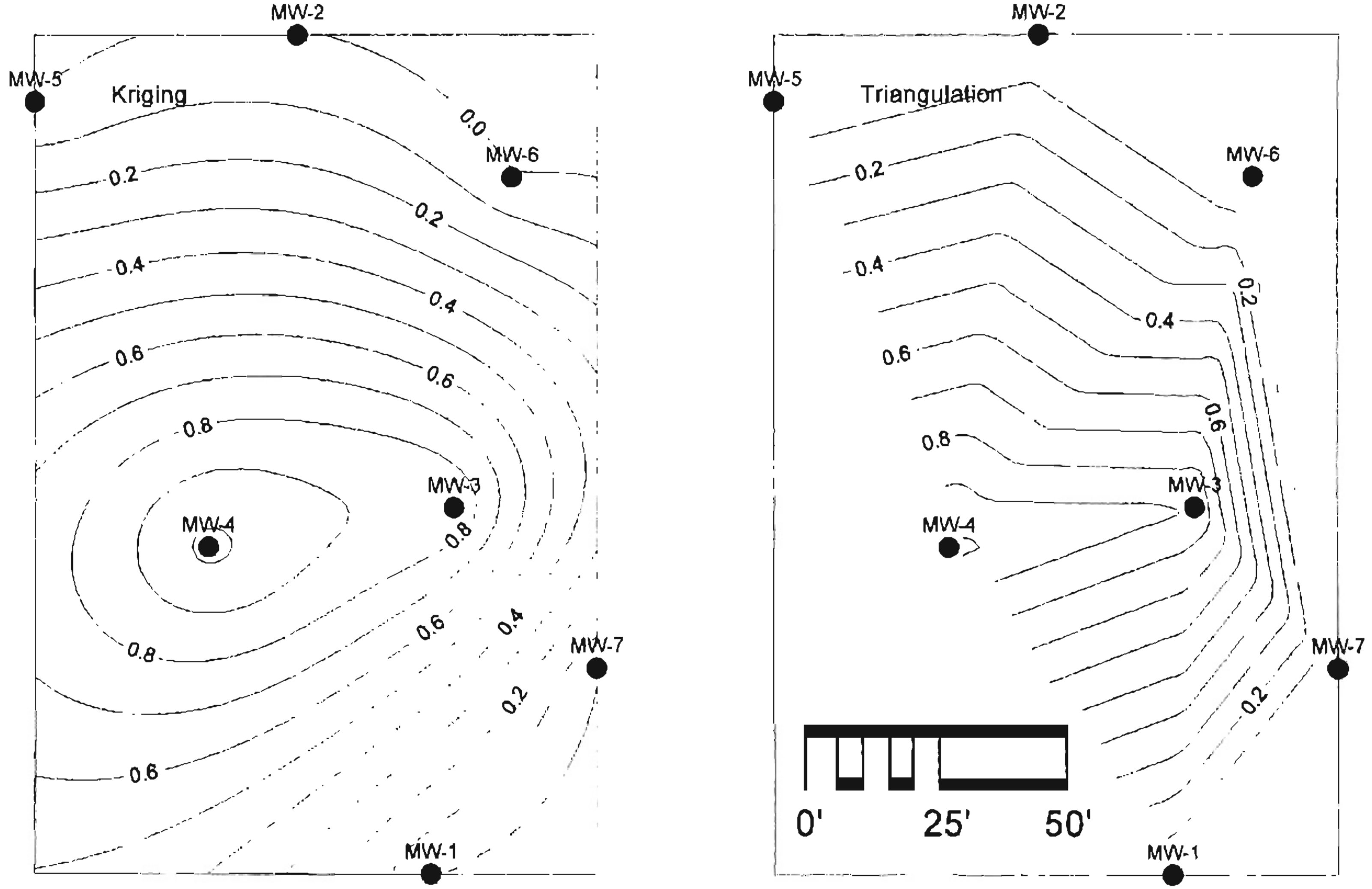
Ethylbenzene Concentrations in Groundwater (mg/L)

Well	7/25/94	10/10/94	4/6/95	10/26/95	11/13/95	12/21/95	2/20/96	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	<0.005	<0.0002	<0.001	<0.001			<0.001	0.070	<0.005	<0.005	<0.005
MW-2	<0.005	<0.0002	<0.001	<0.001				0.046	<0.005	<0.005	<0.005
MW-3	0.901	0.57	0.73	0.892			<0.100	0.325	1.320	1.467	0.839
MW-4	1.03	0.64	0.625	0.497				0.418	3.815	4.529	2.180
MW-5	<0.005	<0.0002	<0.001	<0.001				0.093	0.186	<0.005	<0.005
MW-6	<0.005	0.016	<0.025	<0.05				0.046	0.046	0.093	0.093
MW-7	<0.005	<0.0002	<0.001	<0.001				0.186	0.279	0.325	0.279
MW-8		<0.0002	<0.001	<0.001				<0.005	<0.005	<0.005	<0.005
MW-9		<0.0002		<0.001	<0.001		<0.001				
MW-10		<0.0002		<0.001					<0.005	<0.005	0.046
MW-11		<0.0002	<0.001	0.0033	0.0012		0.0021	<0.005	0.028	0.093	0.093
MW-12		<0.0002	<0.001	<0.001			<0.001	<0.005	<0.005	<0.005	<0.005
MW-13		<0.0002	<0.001	<0.001			<0.001	<0.005	<0.005	<0.005	<0.005
MW-14				<0.001				<0.005	<0.005	<0.005	<0.005
MW-15						<0.001	<0.001	<0.005	<0.005	<0.005	<0.005
MW-16						<0.001	<0.001	<0.005	<0.005	<0.005	<0.005

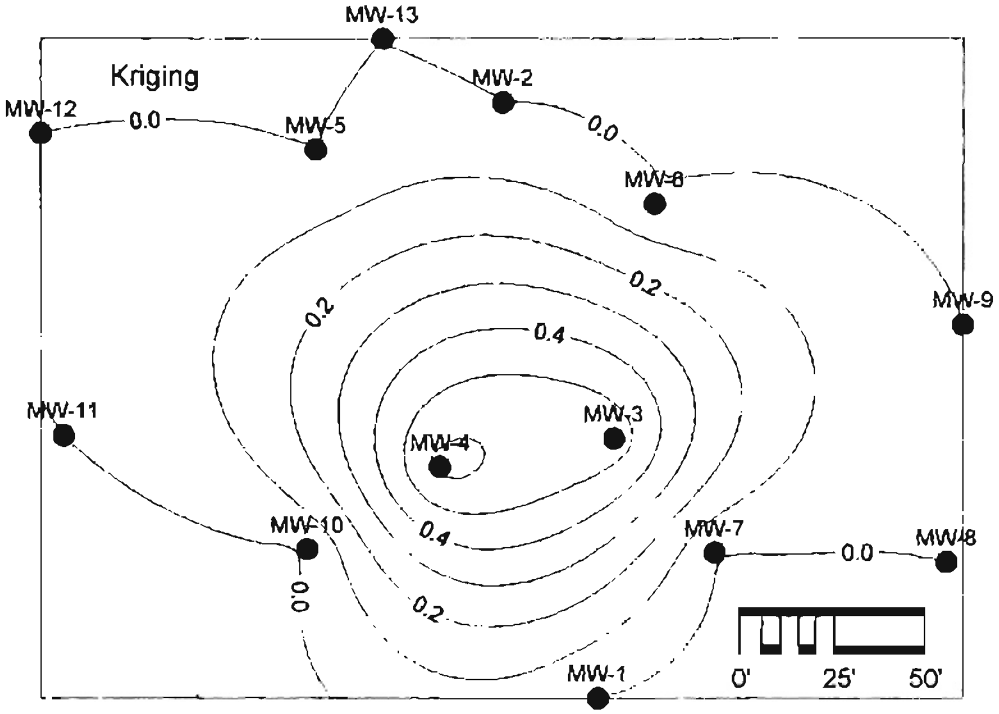
Notes:

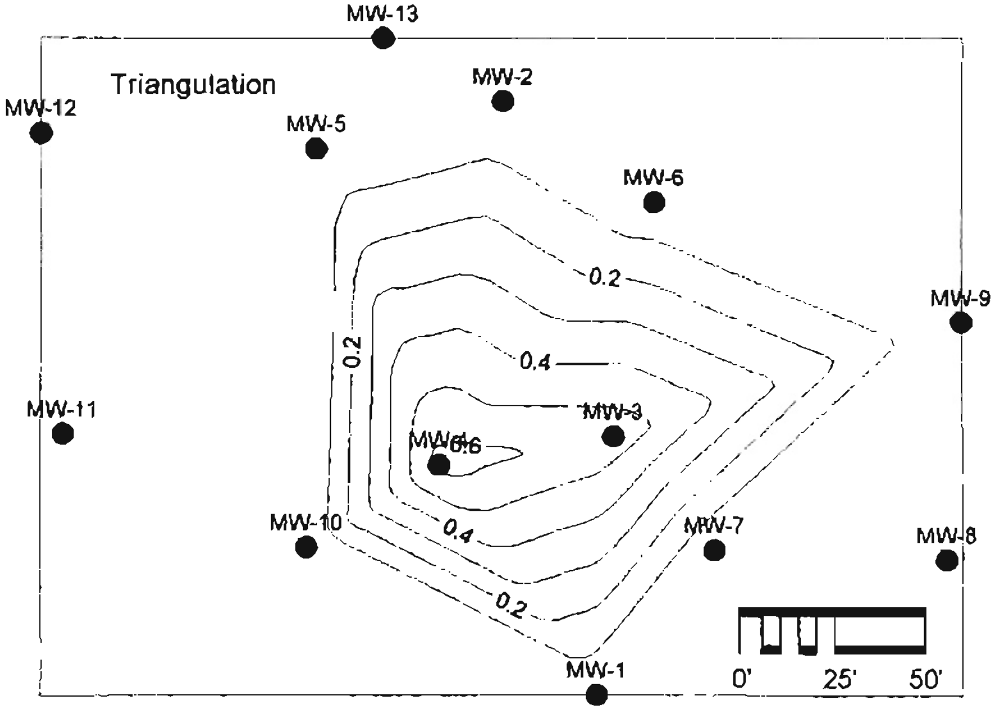
1. Less than signs (<) designate values below the detection limit.
2. 1994, 1995, and 1996 data is from Caldwell, 1995.
3. 1997 and 1998 data is from Akins, 1998.

ETHYLBENZENE (mg/L) -- 7/25/94

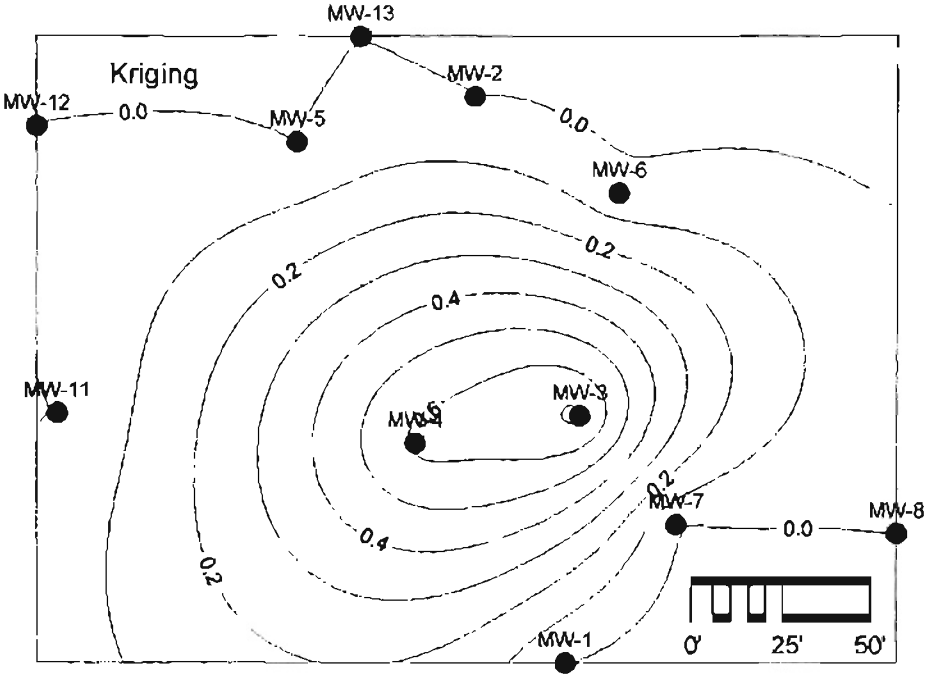


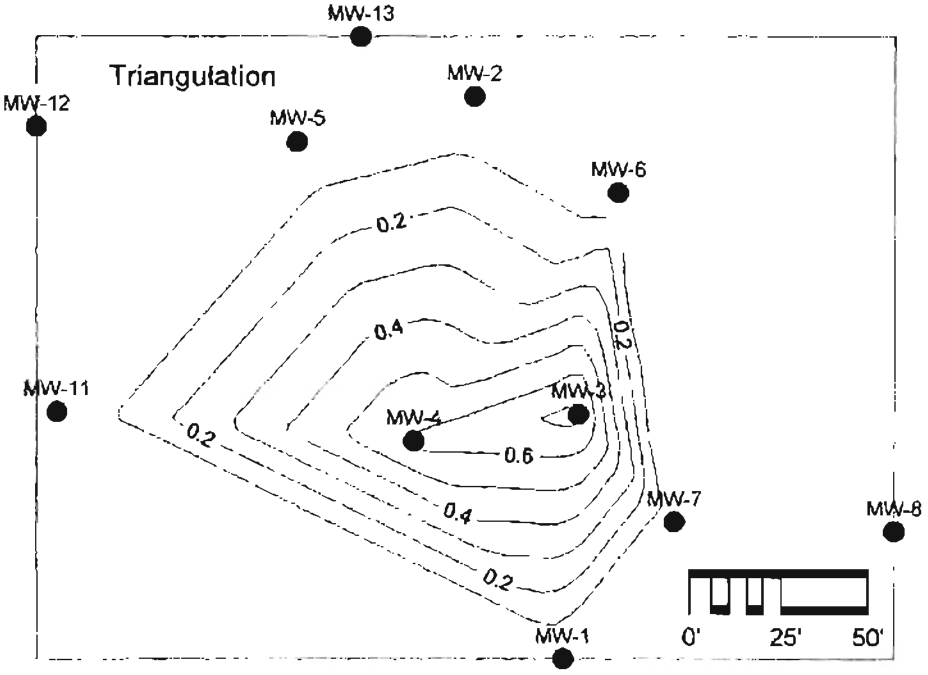
ETHYLBENZENE (mg/L) -- 10/10/94



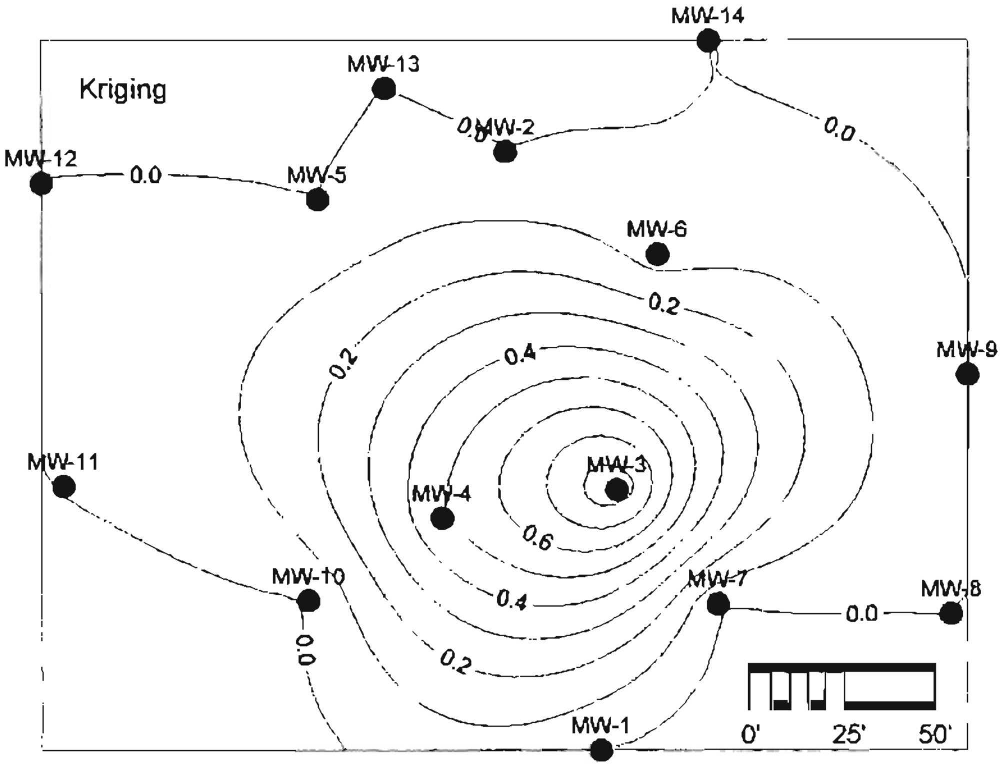


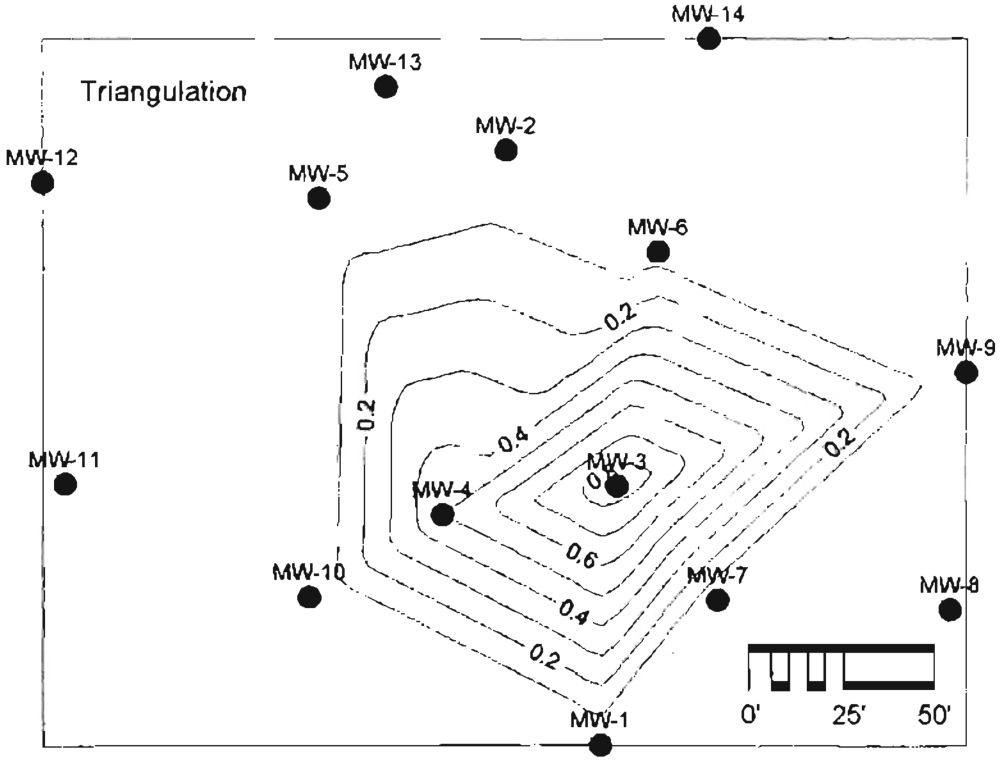
ETHYLBENZENE (mg/L) -- 4/6/95



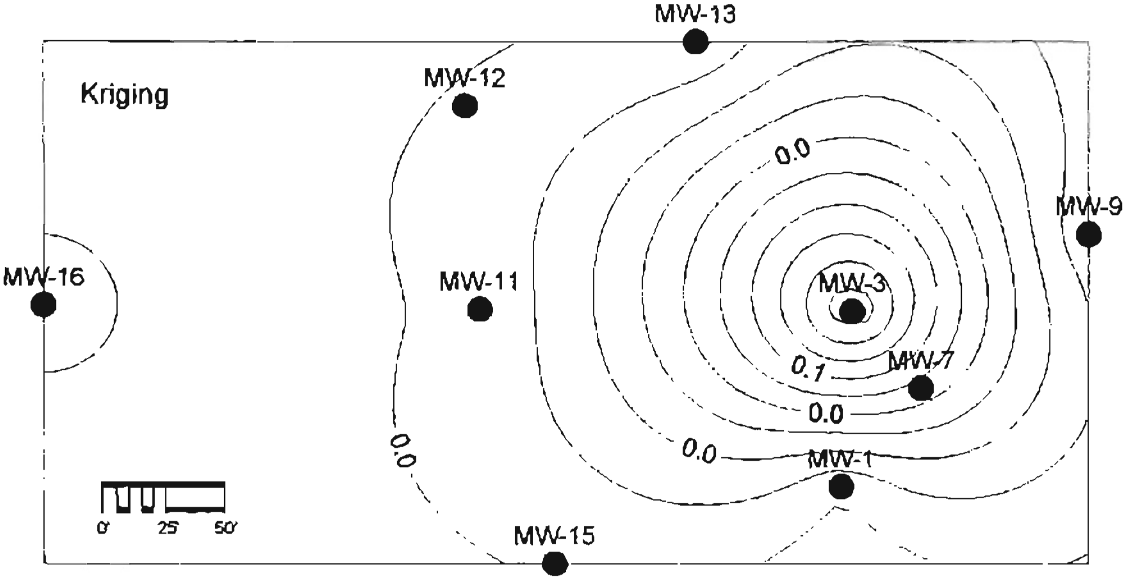


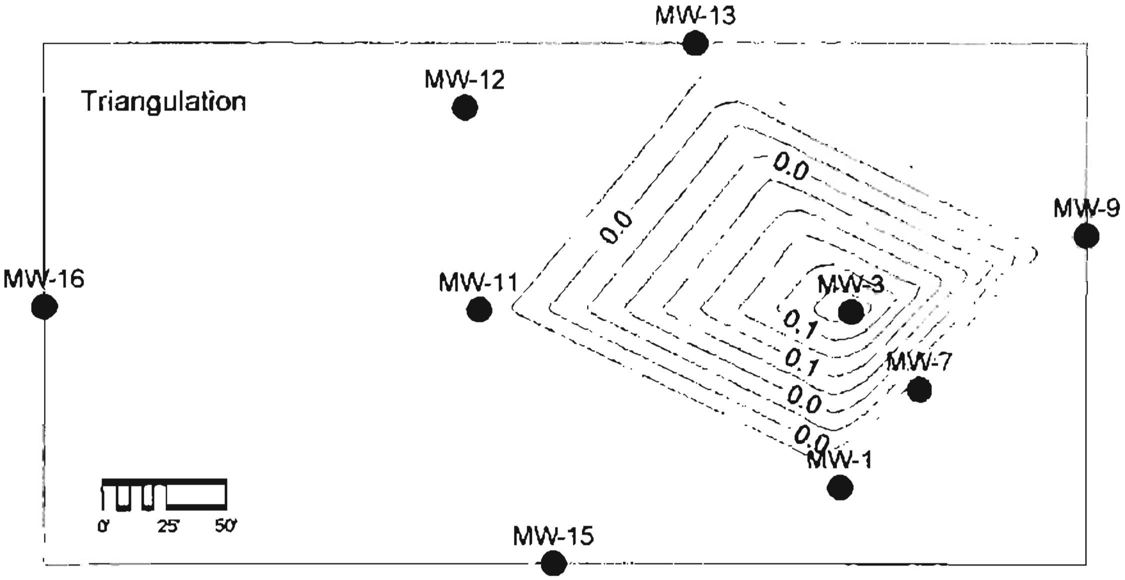
ETHYLBENZENE (mg/L) -- 10/26/95



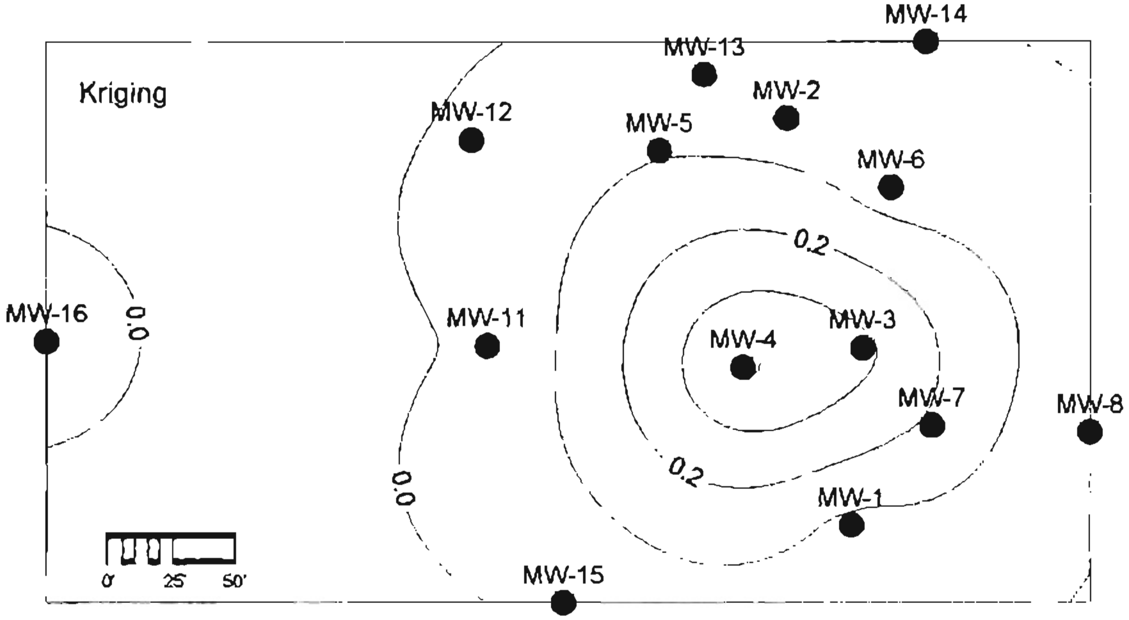


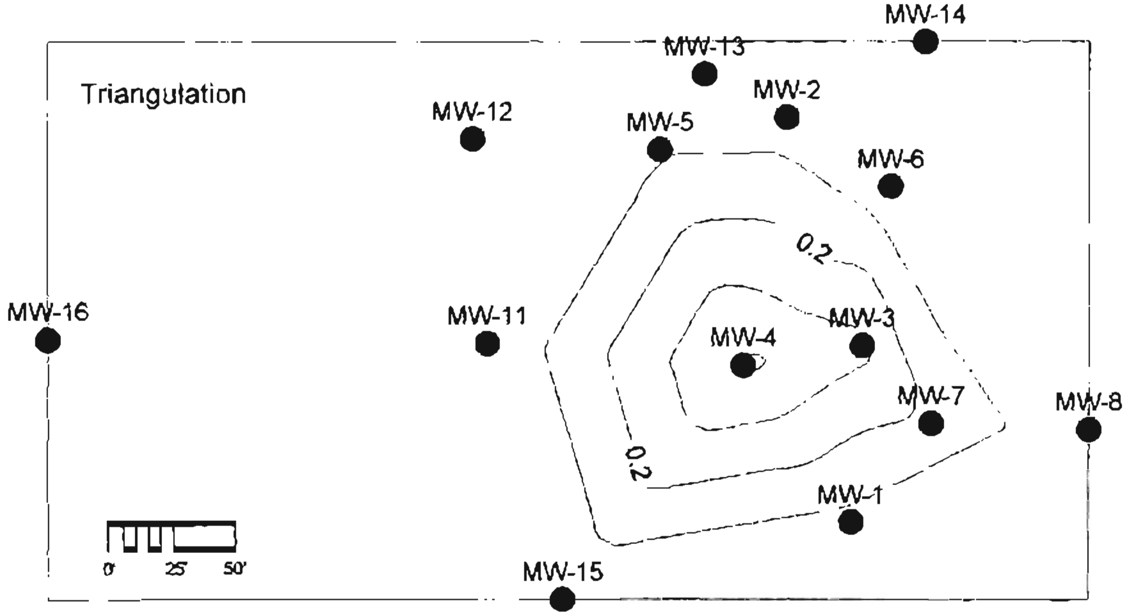
ETHYLBENZENE (mg/L) -- 2/20/96



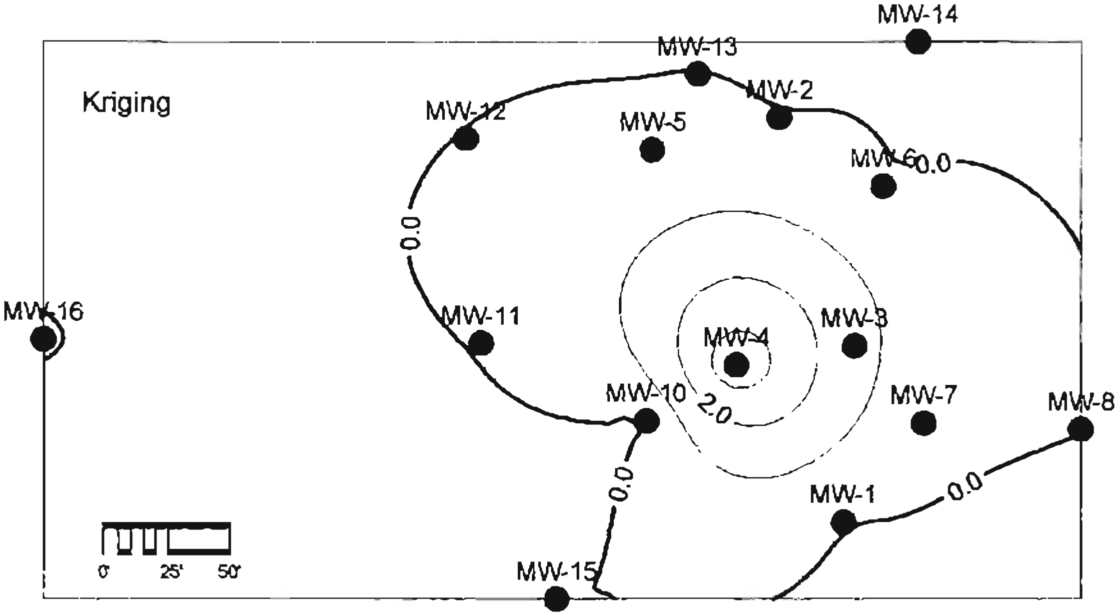


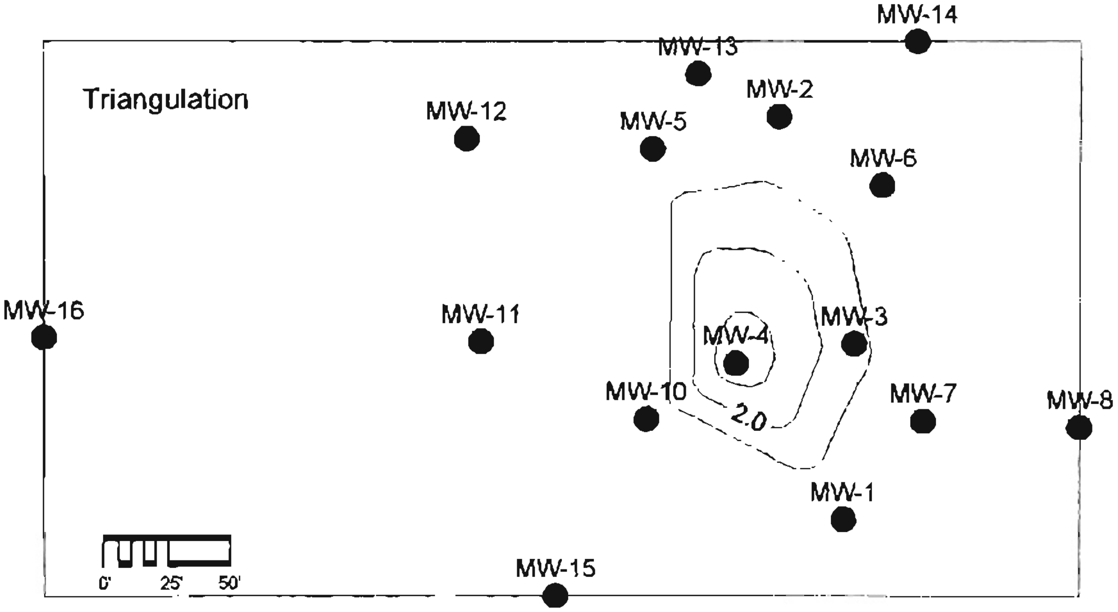
ETHYLBENZENE (mg/L) -- 10/20/97



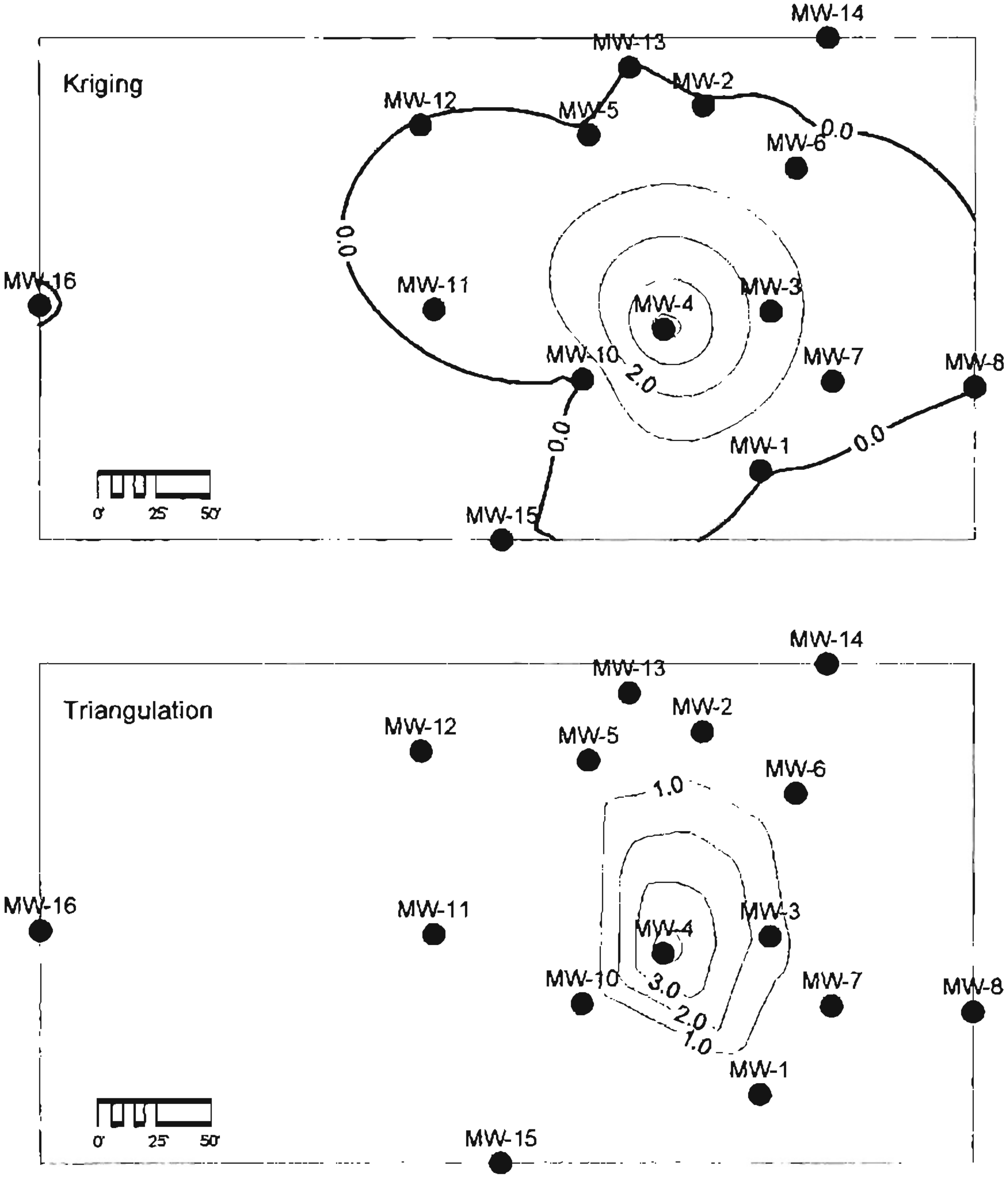


ETHYLBENZENE (mg/L)-- 12/15/97

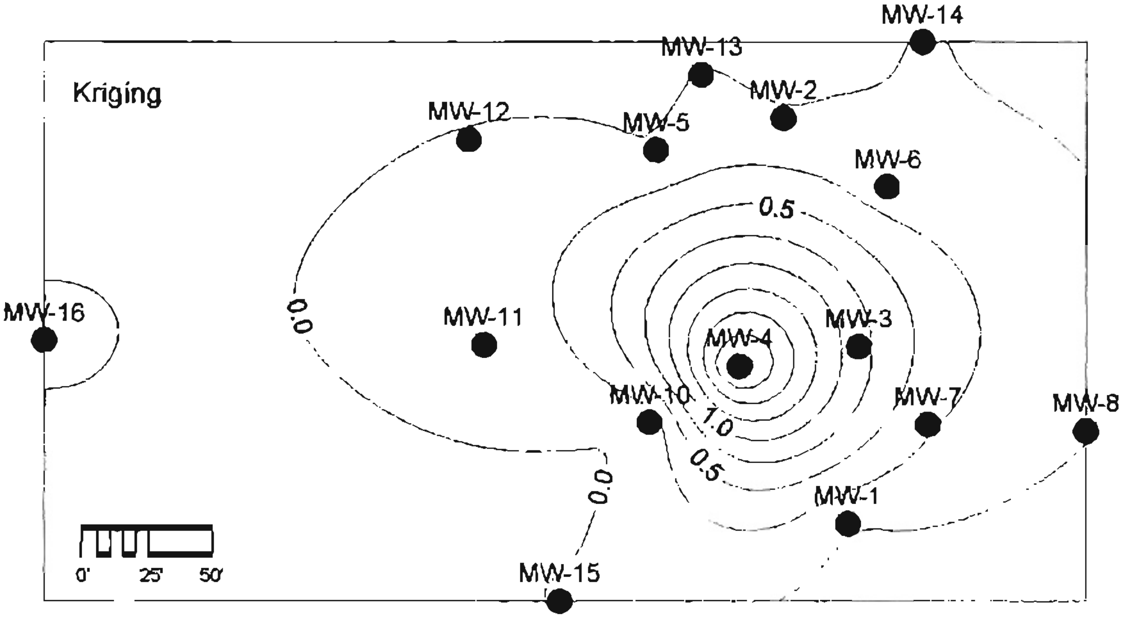


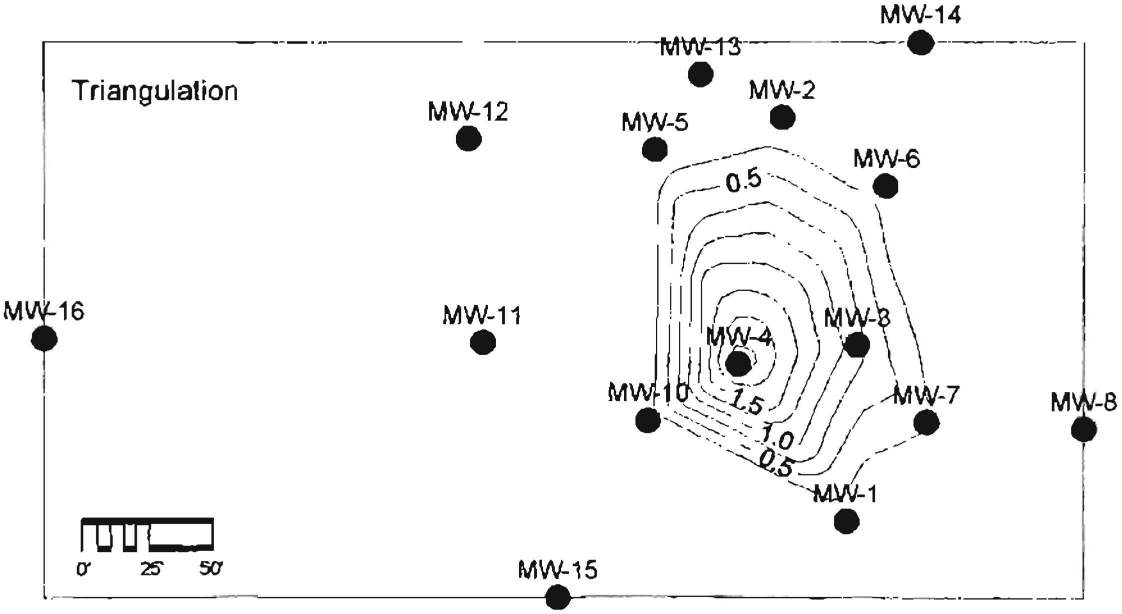


ETHYLBENZENE (mg/L) -- 1/20/98



ETHYLBENZENE (mg/L) -- 2/17/98





APPENDIX H –

Xylene Analytical Data and Isopleths

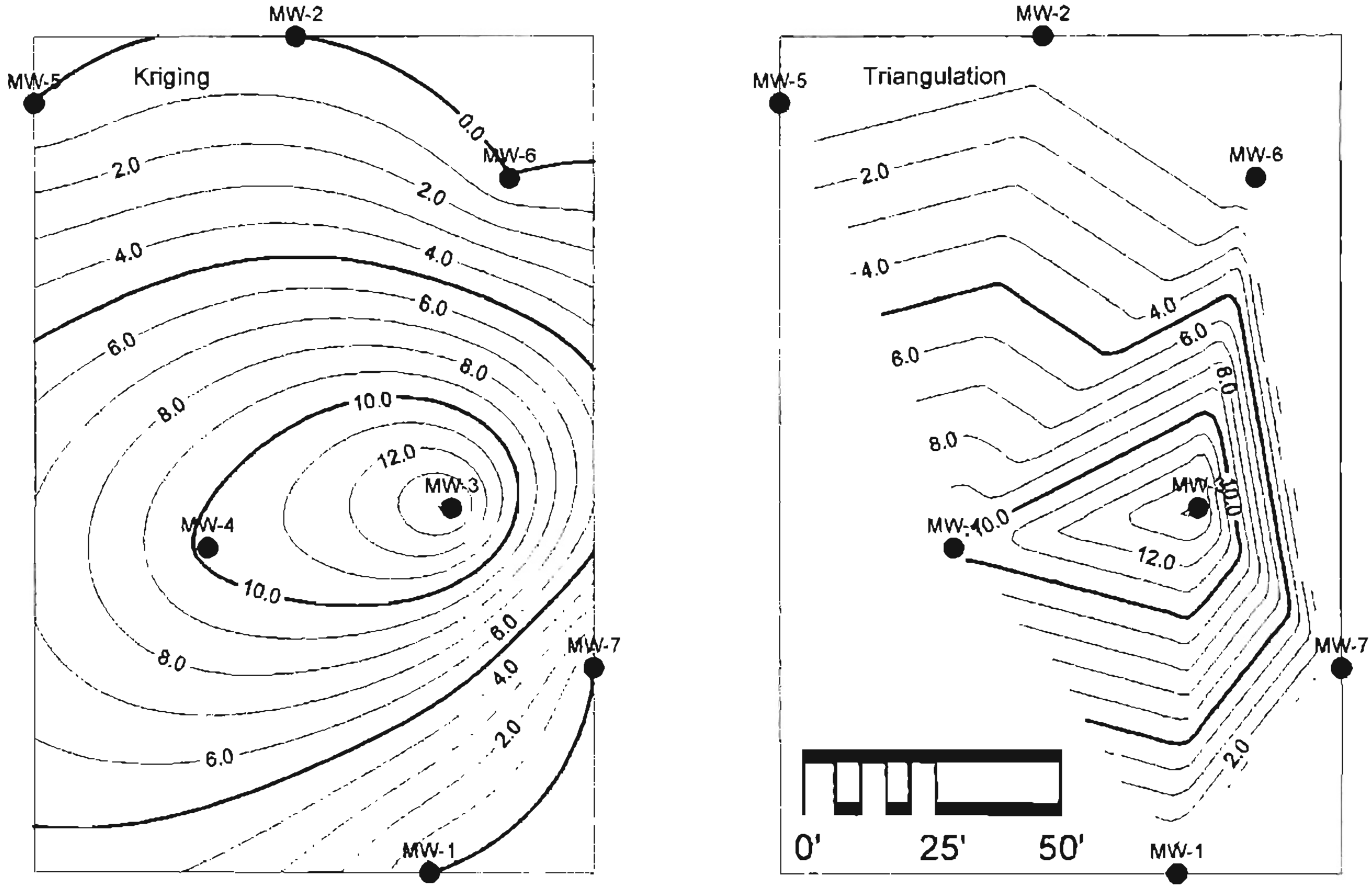
Xylene Concentrations in Groundwater (mg/L)

Well	7/25/94	10/10/94	4/6/95	10/26/95	11/13/95	12/21/95	2/20/96	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	0.0058	0.016	0.0085	0.0068			0.0022	0.075	<0.005	<0.005	<0.005
MW-2	<0.005	<0.0002	<0.001	<0.001				0.100	<0.005	<0.005	<0.005
MW-3	14.40	7.800	10.20	9.45			5.15	1.295	4.913	4.082	7.380
MW-4	10.300	5.800	4.040	2.720				0.299	3.477	10.902	6.374
MW-5	<0.005	<0.0002	<0.001	<0.001				0.100	0.921	0.049808	<0.005
MW-6	0.0445	1.000	0.534	0.85				0.087	0.249	0.324	0.174
MW-7	0.008	0.054	0.021	0.0194				0.349	0.648	0.797	0.548
MW-8		<0.0002	<0.001	<0.001	<0.001			<0.005	<0.005	<0.005	<0.005
MW-9		<0.0002		0.0239	<0.001		0.001				
MW-10		<0.0002		<0.001					<0.005	<0.005	0.100
MW-11		<0.0002	<0.001	0.0125	0.0168		0.0089	<0.005	0.100	0.050	<0.005
MW-12		<0.0002	<0.001	<0.001			<0.001	<0.005	<0.005	<0.005	<0.005
MW-13		<0.0002	<0.001	<0.001			<0.001	<0.005	<0.005	<0.005	<0.005
MW-14				<0.001				<0.005	0.049808	<0.005	<0.005
MW-15						<0.001	<0.001	<0.005	<0.005	<0.005	<0.005
MW-16						<0.001	<0.001	<0.005	<0.005	<0.005	<0.005

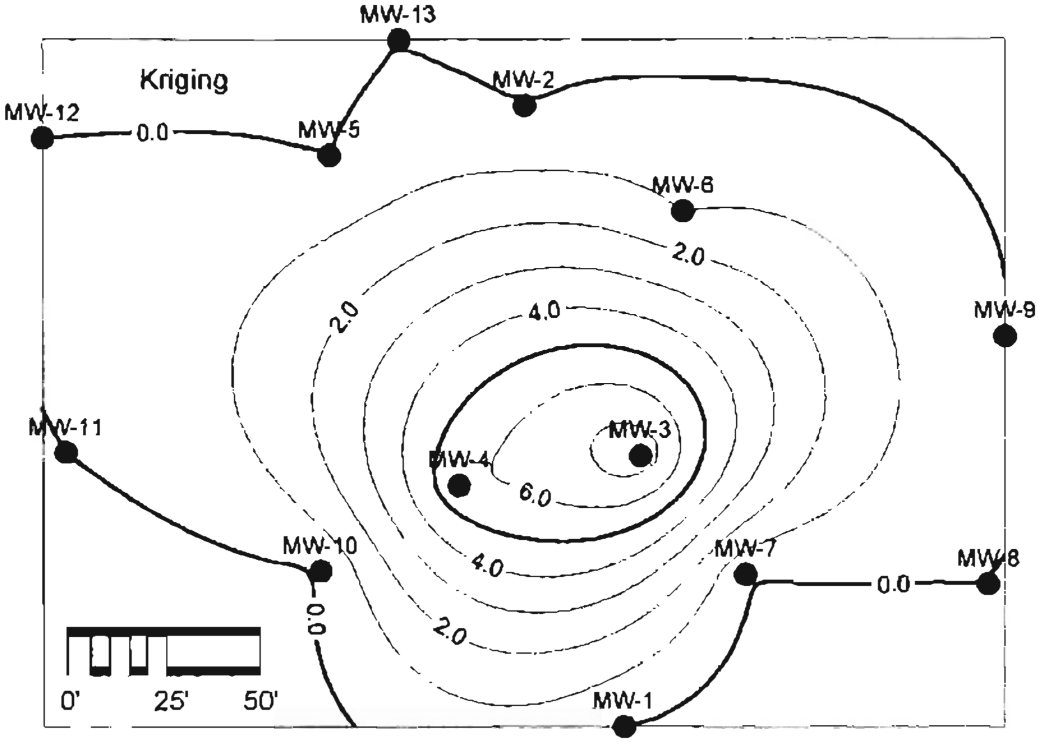
Notes:

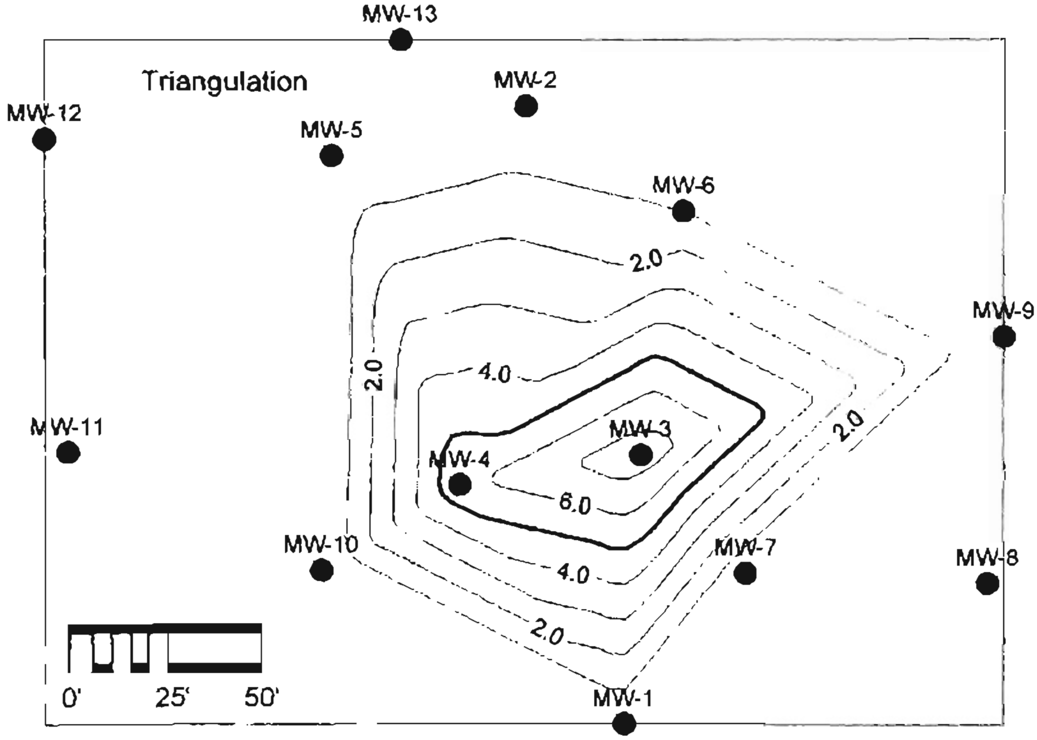
1. Less than signs (<) designate values below the detection limit.
2. 1994, 1995, and 1996 data is from Caldwell, 1995.
3. 1997 and 1998 data is from Akins, 1998.

XYLENE (mg/L) -- 7/25/94

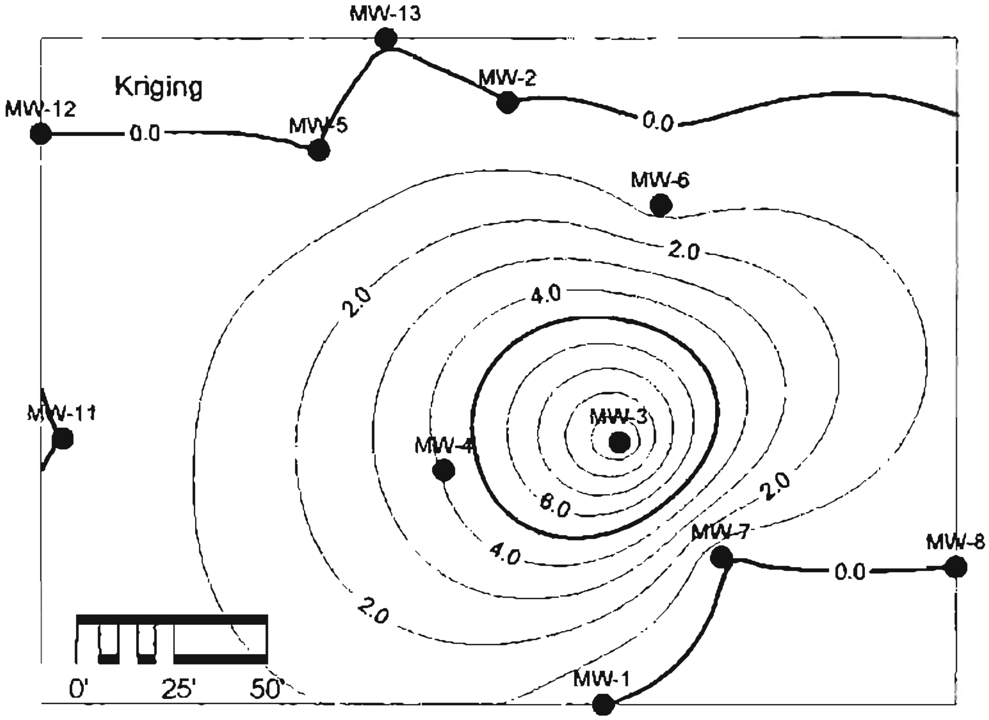


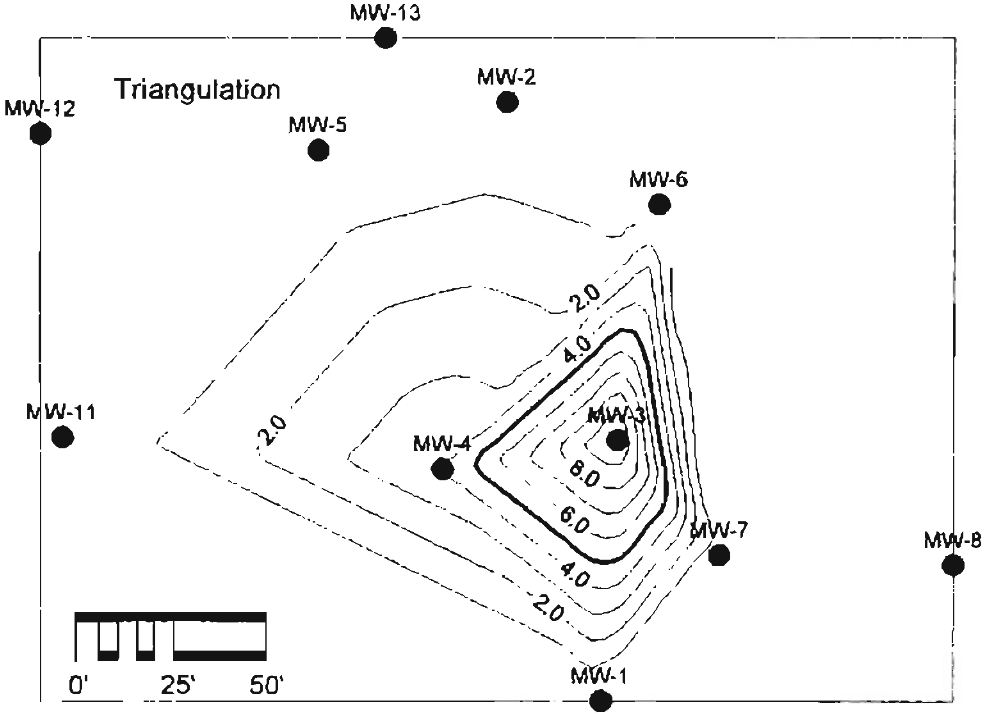
XYLENE (mg/L) -- 10/10/94



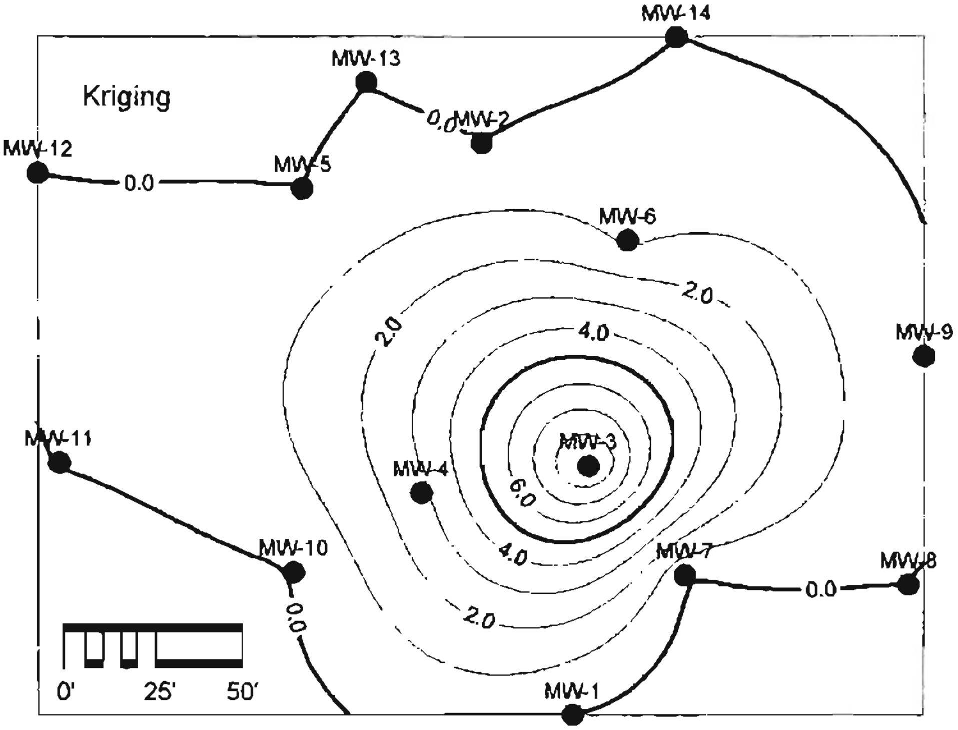


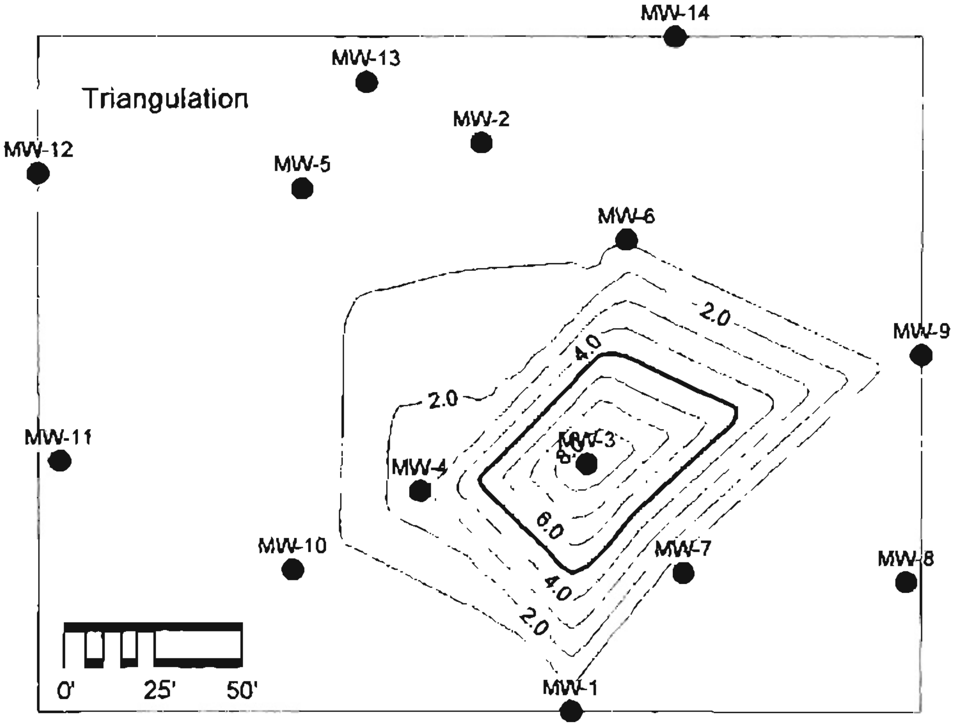
XYLENE (mg/L) -- 4/6/95



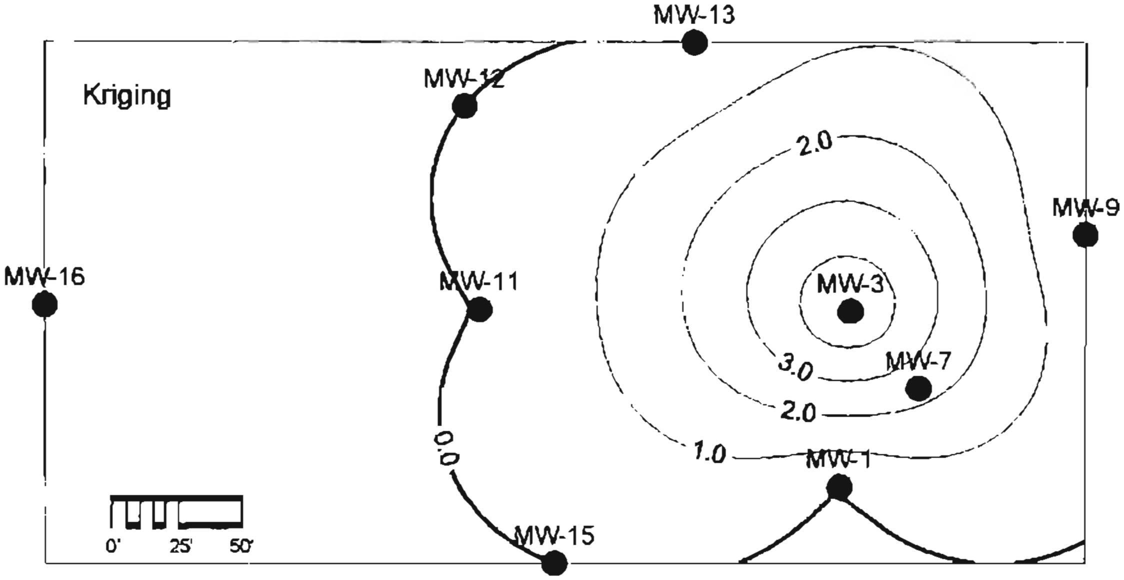


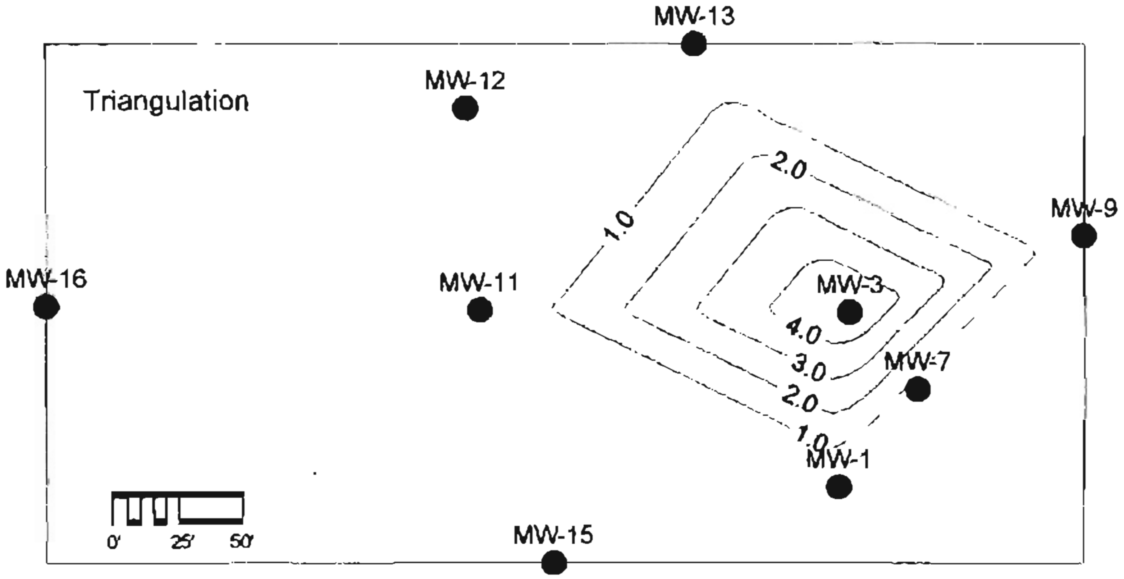
XYLENE (mg/L) -- 10/26/95



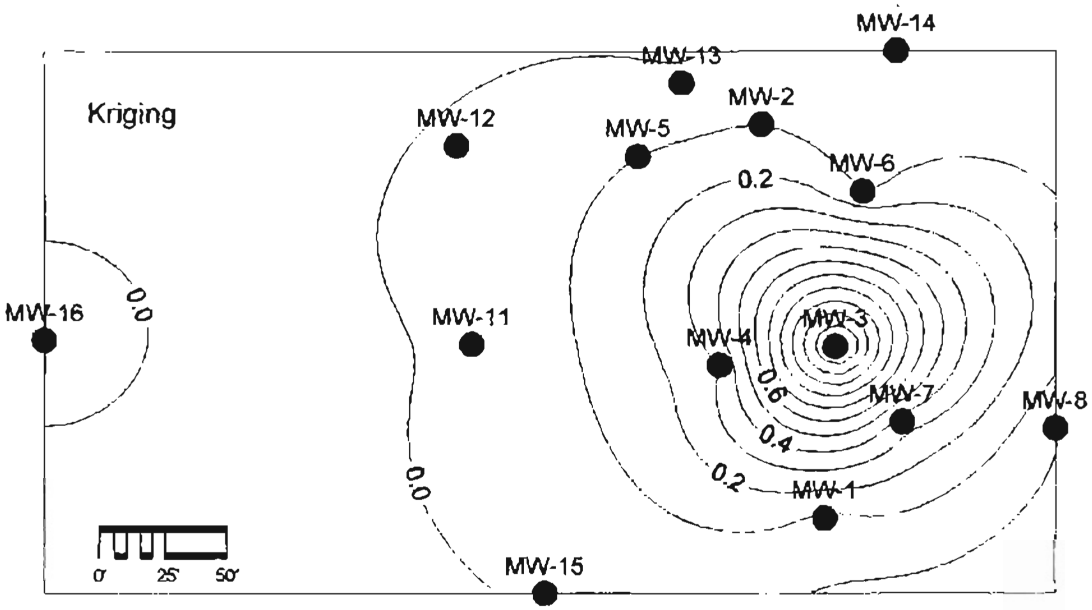


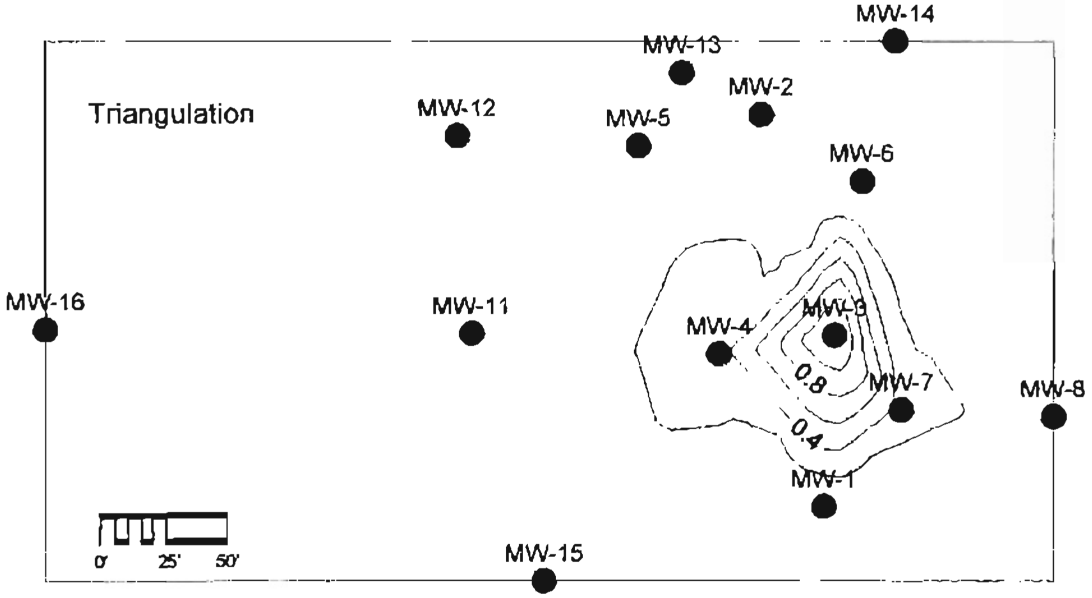
XYLENE (mg/L) -- 2/20/96



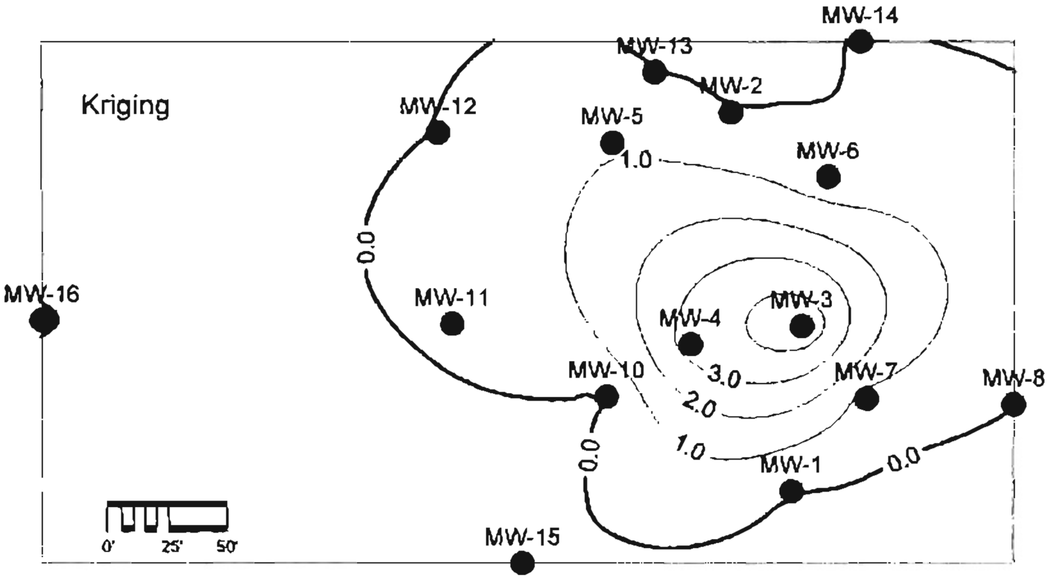


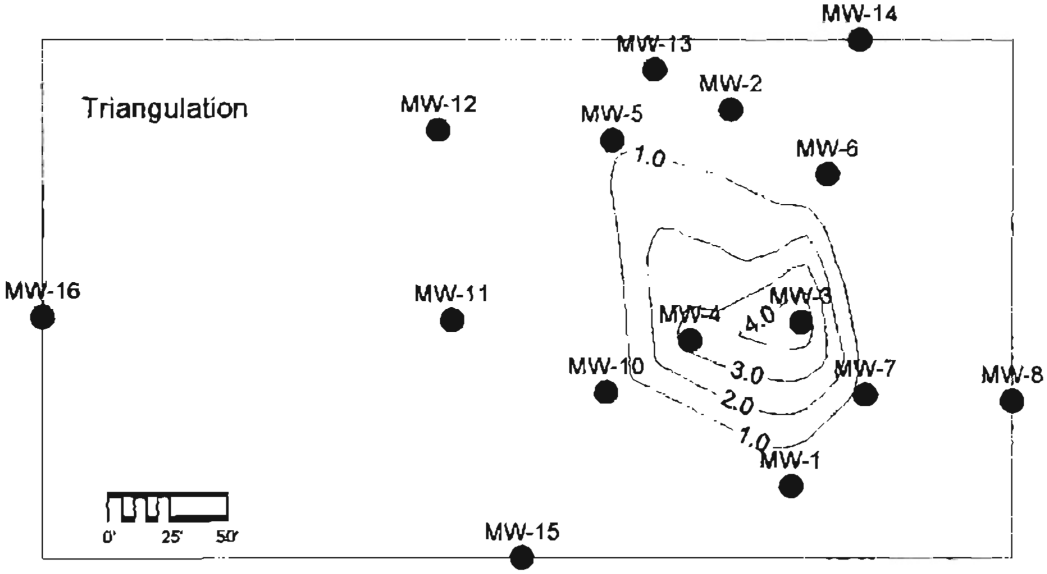
XYLENE (mg/L) -- 10/20/97



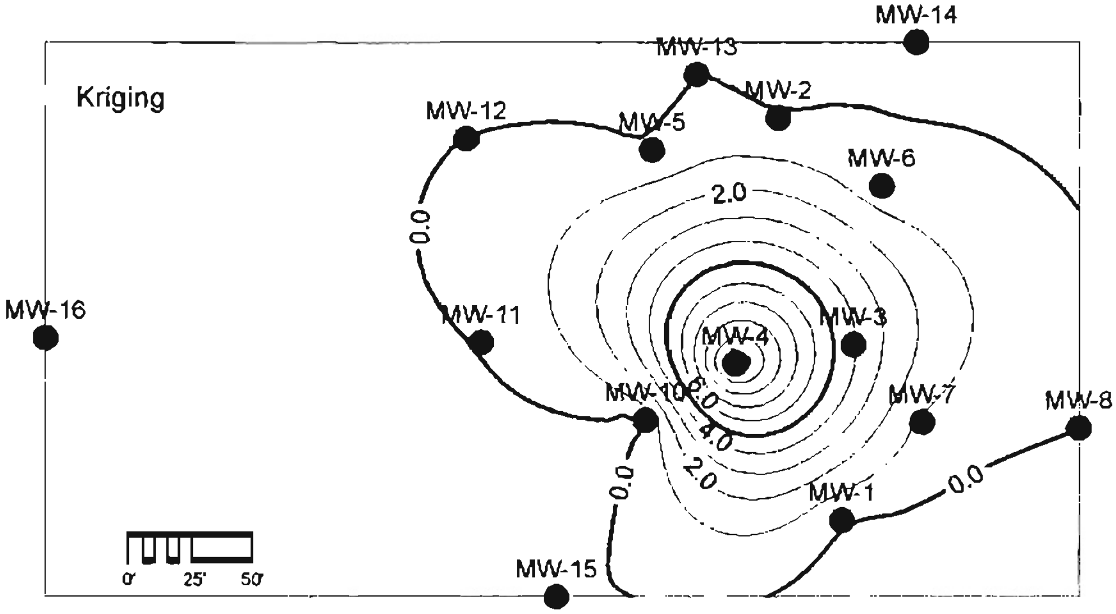


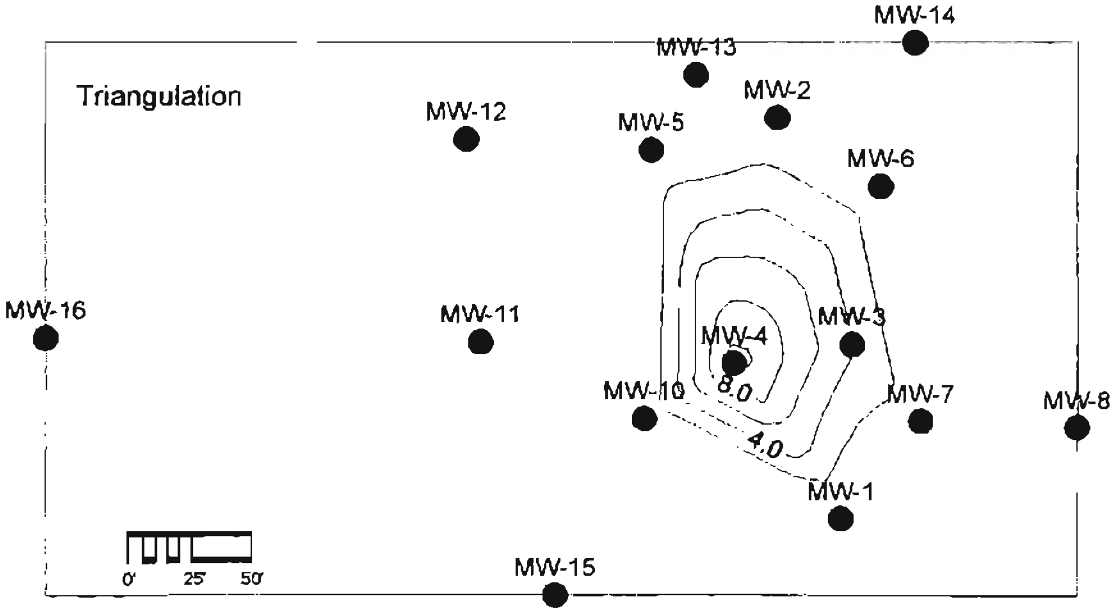
XYLENE (mg/L) -- 12/15/97



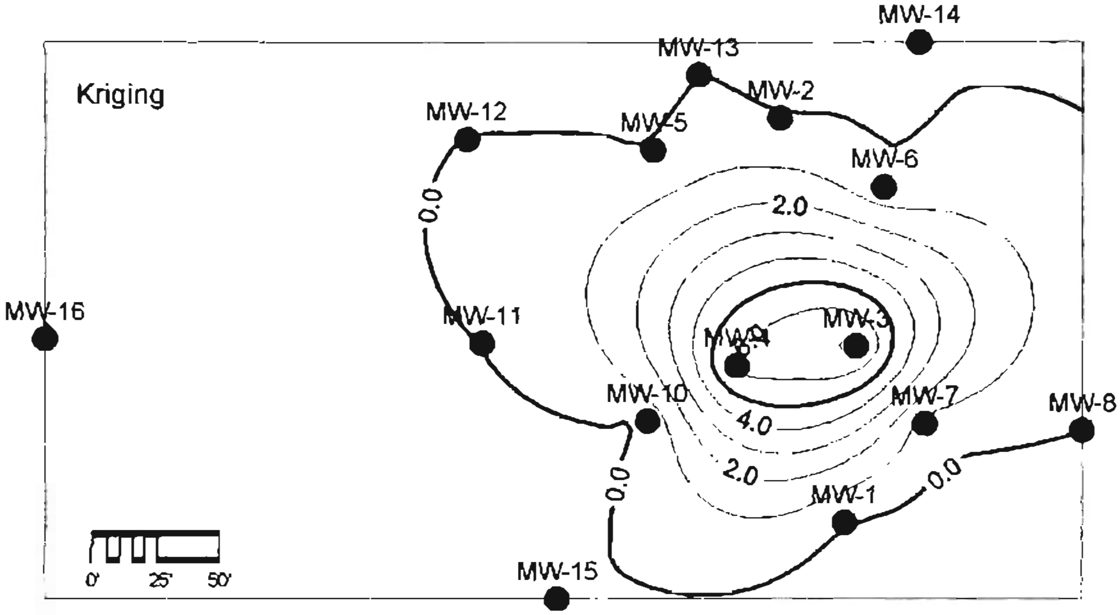


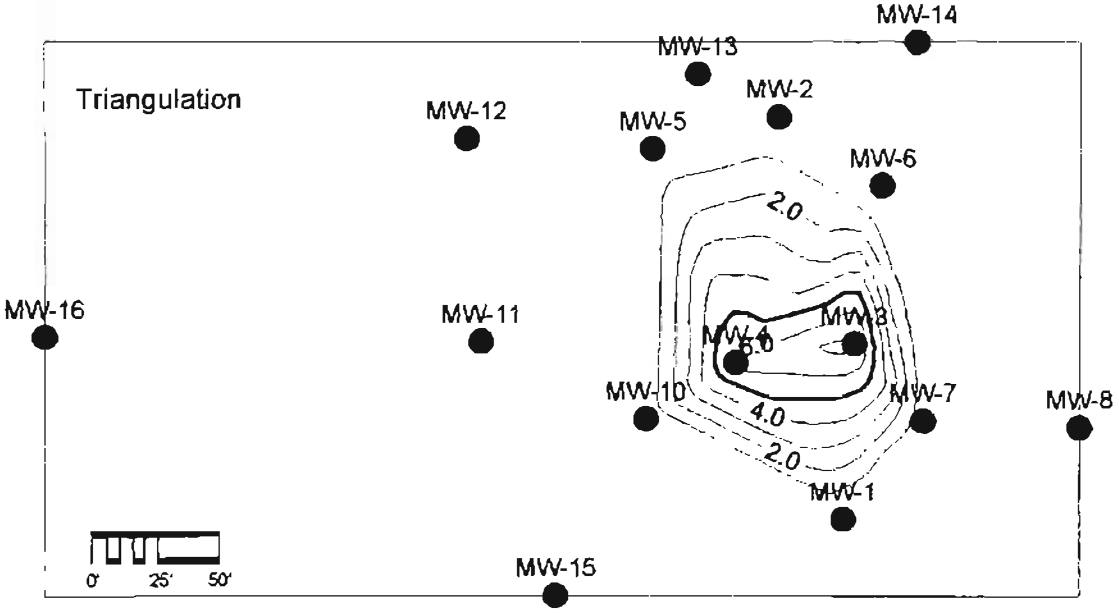
XYLENE (mg/L) -- 1/20/98





XYLENE (mg/L) -- 2/17/98





APPENDIX I --

Dissolved Oxygen Analytical Data and Isopleths

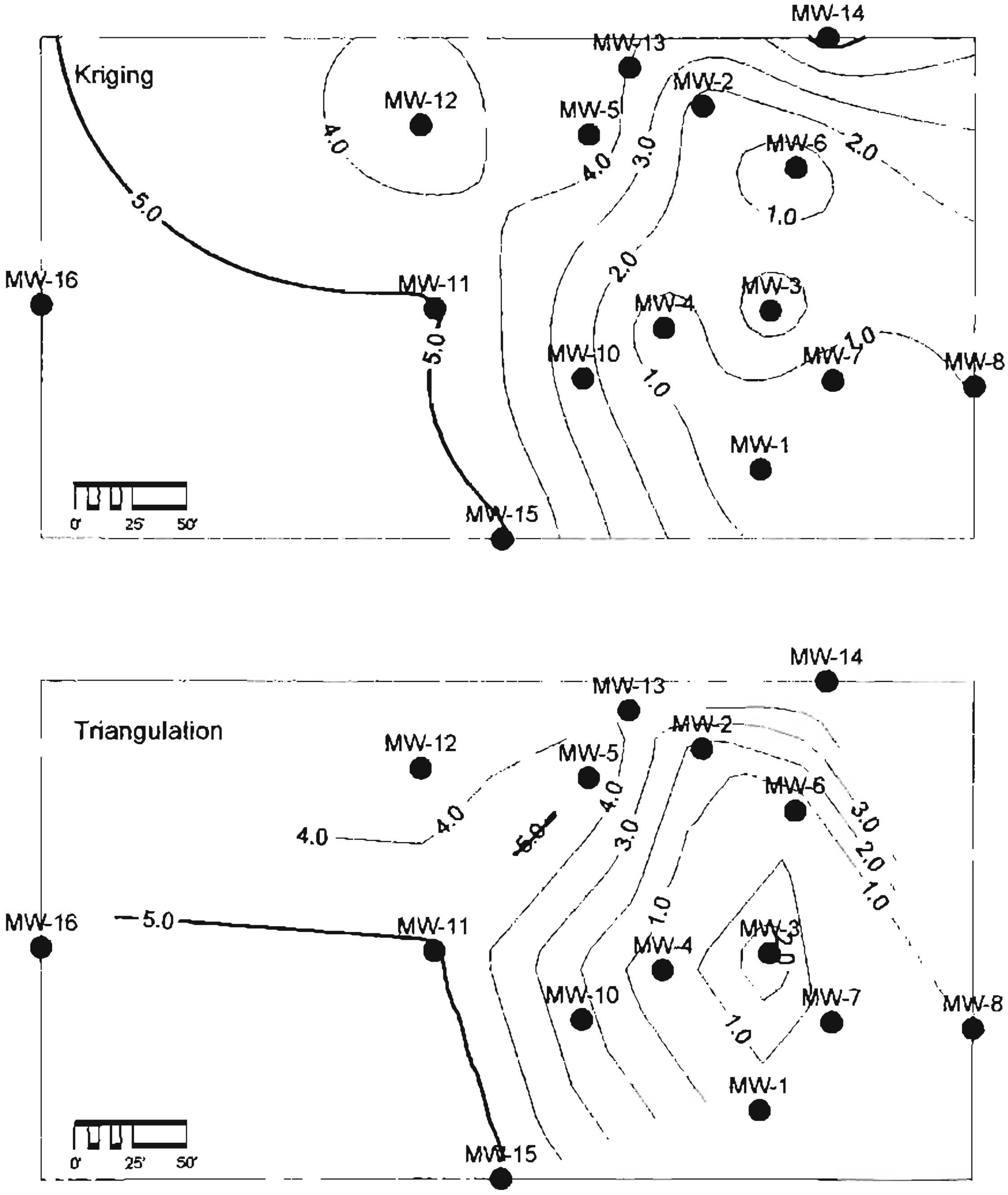
Dissolved Oxygen Concentrations in Groundwater (mg/L)

Well	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	0.21	0.21	0.63	0.77
MW-2	1.45	2.58	1.98	1.82
MW-3	2.90	4.40	3.10	0.99
MW-4	0.19	0.22	0.08	0.20
MW-5	5.01	5.48	4.67	4.07
MW-6	0.18	0.23	0.25	0.52
MW-7	0.23	0.18	2.33	0.62
MW-8	1.06	0.22	0.33	0.71
MW-9				
MW-10		7.77	6.99	
MW-11	5.11	0.85	0.57	1.13
MW-12	3.20	2.90	3.11	3.02
MW-13	4.00	6.03	5.15	4.58
MW-14	5.50	5.36	5.39	5.30
MW-15	5.21	4.55	4.80	4.90
MW-16	5.37	6.23	5.37	5.23

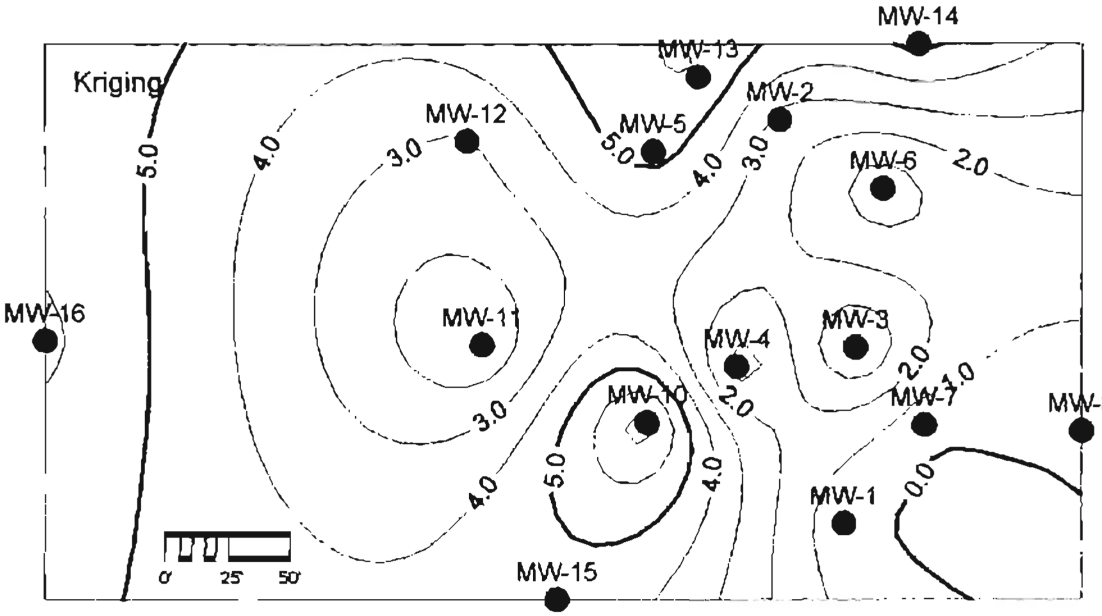
Notes:

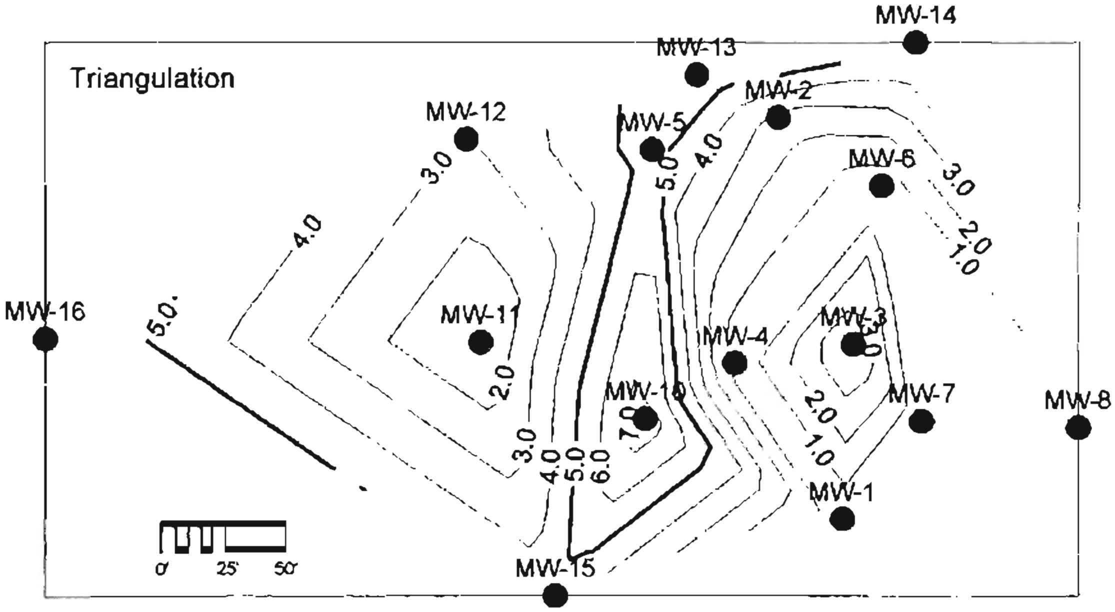
1. Less than signs (<) designate values below the detection limit.
2. 1994, 1995, and 1996 data is from Caldwell, 1995.
3. 1997 and 1998 data is from Akins, 1998.

DISSOLVED OXYGEN (mg/L) -- 10/20/97

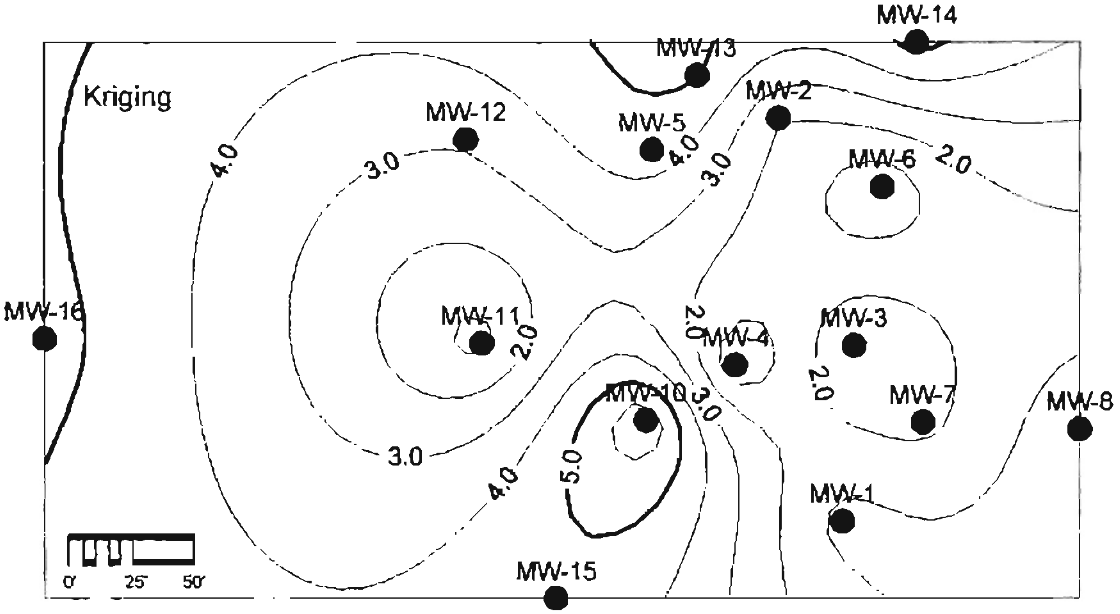


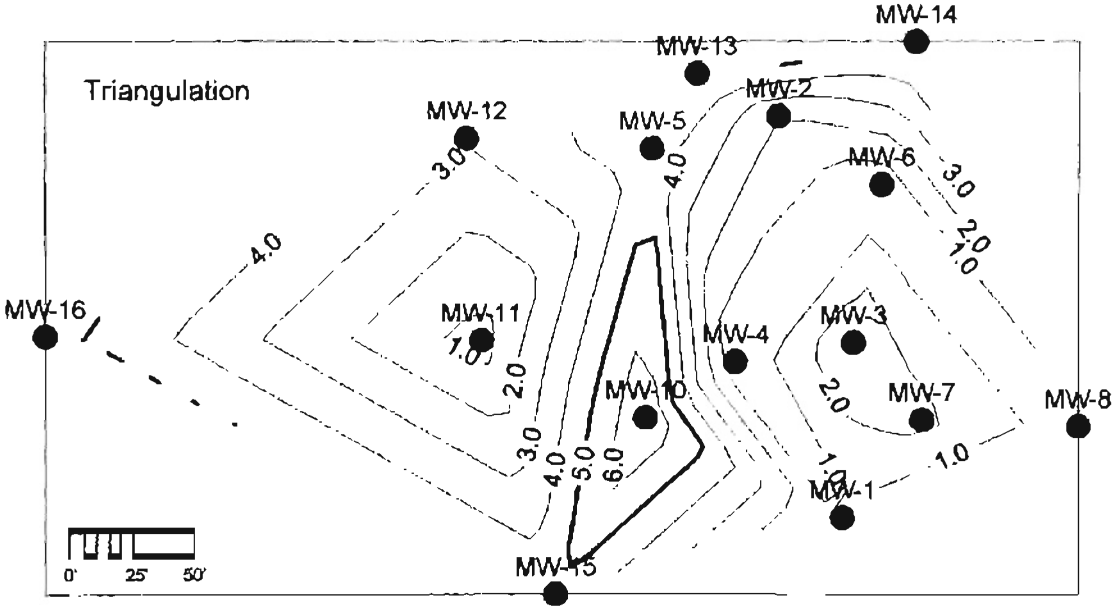
DISSOLVED OXYGEN (mg/L) -- 12/15/97



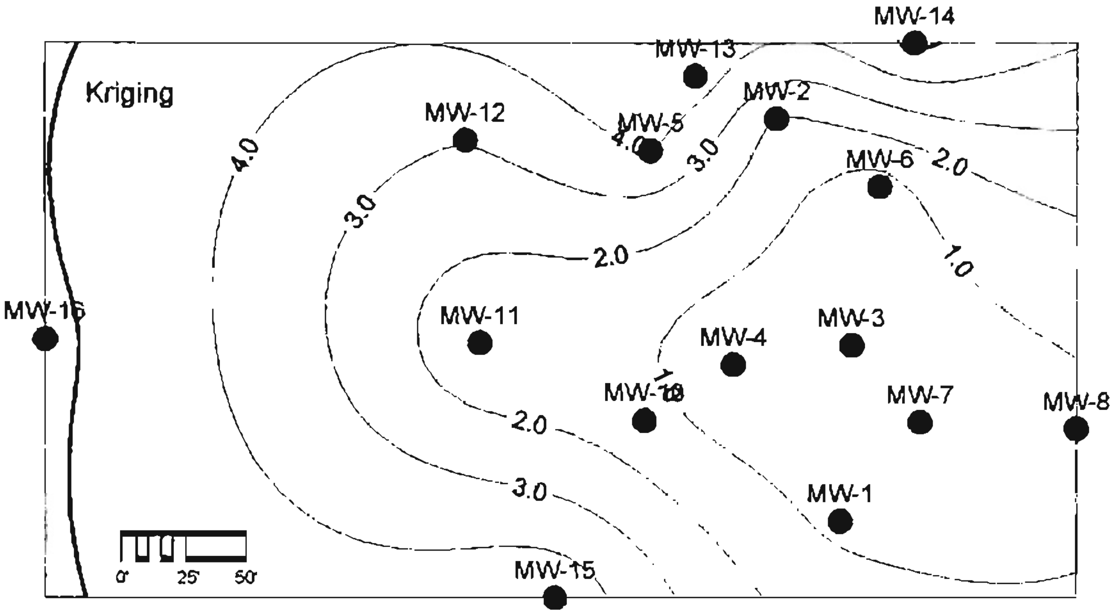


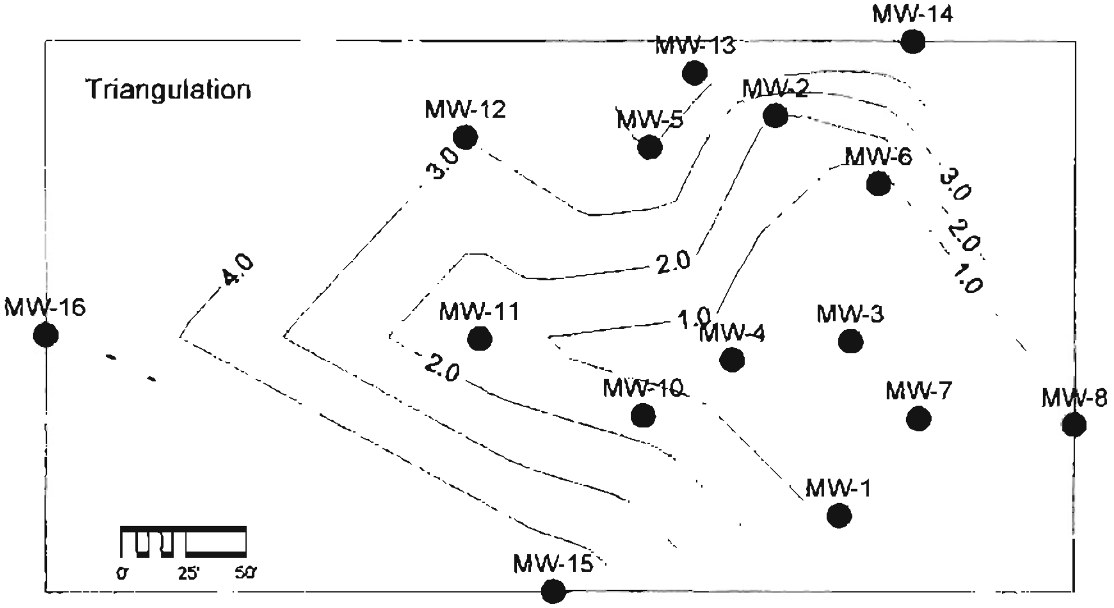
DISSOLVED OXYGEN (mg/L) -- 1/20/98





DISSOLVED OXYGEN (mg/L) -- 2/17/98





APPENDIX J –

Nitrate Analytical Data and Isopleths

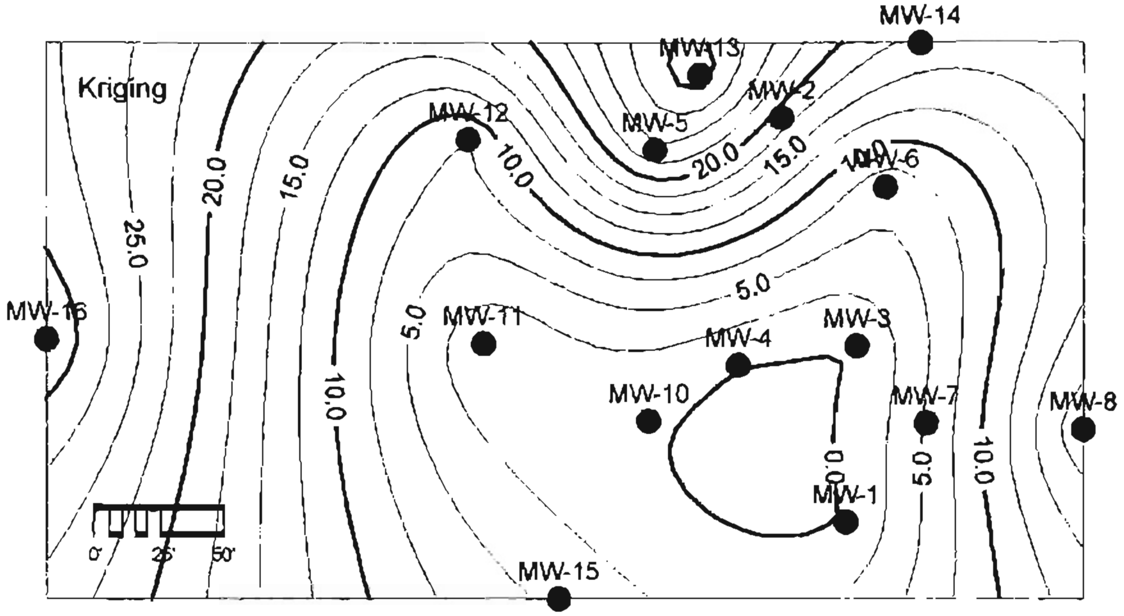
Nitrate Concentrations in Groundwater (mg/L)

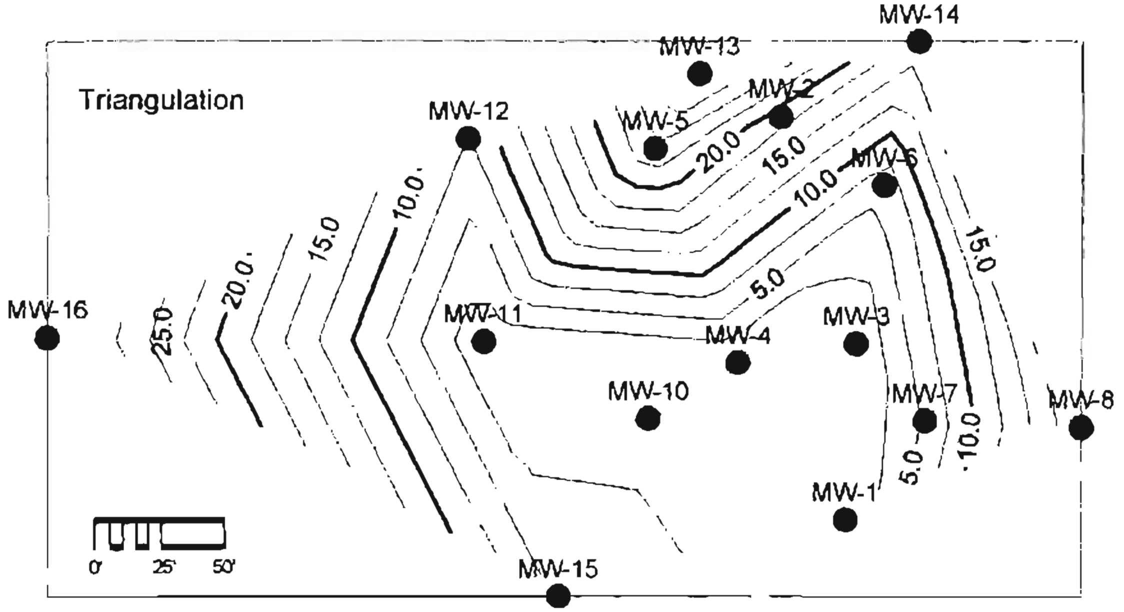
Well	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	0.04	0.08	0.40	1.19
MW-2	18.53	14.21	25.39	13.57
MW-3	0.04	0.17	0.79	0.04
MW-4	0.07	0.13	0.05	0.12
MW-5	24.75	18.39	22.54	21.94
MW-6	5.66	1.46	3.05	0.93
MW-7	5.29	6.89	5.55	4.30
MW-8	19.71	13.44	13.71	6.98
MW-9				
MW-10		0.95	1.06	0.79
MW-11	0.35	0.42	0.11	0.19
MW-12	7.32	5.18	5.72	6.05
MW-13	31.72	25.44	34.64	34.37
MW-14	16.74	11.78	13.84	10.74
MW-15	4.52	3.02	3.69	3.40
MW-16	32.48	26.61	19.42	14.77

Notes:

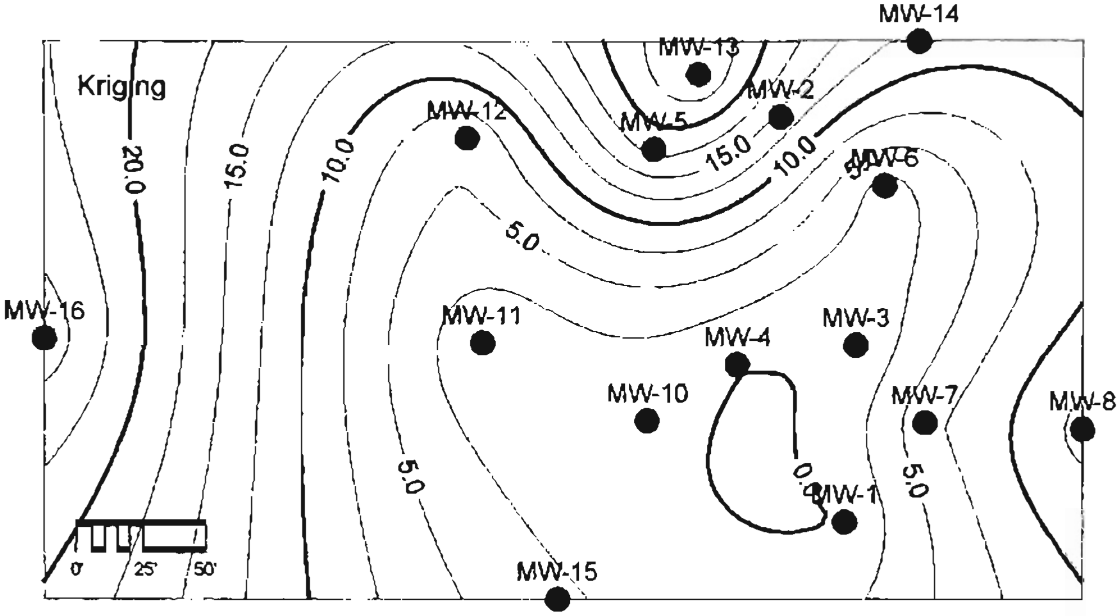
1. Less than signs (<) designate values below the detection limit.
2. 1994, 1995, and 1996 data is from Caldwell, 1995.
3. 1997 and 1998 data is from Akins, 1998.

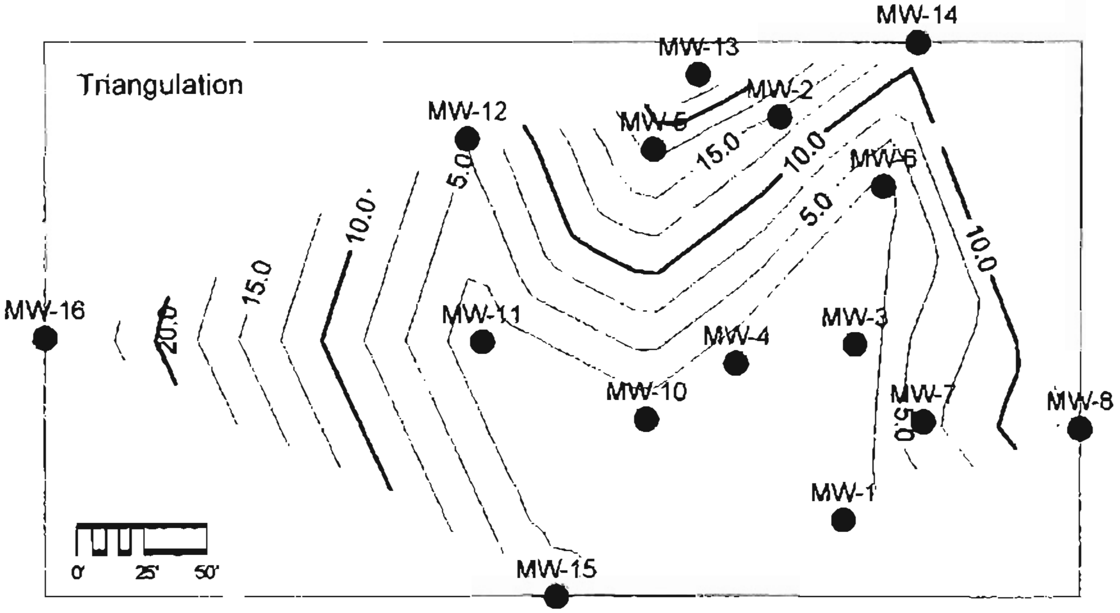
NITRATE (mg/L) -- 10/20/97



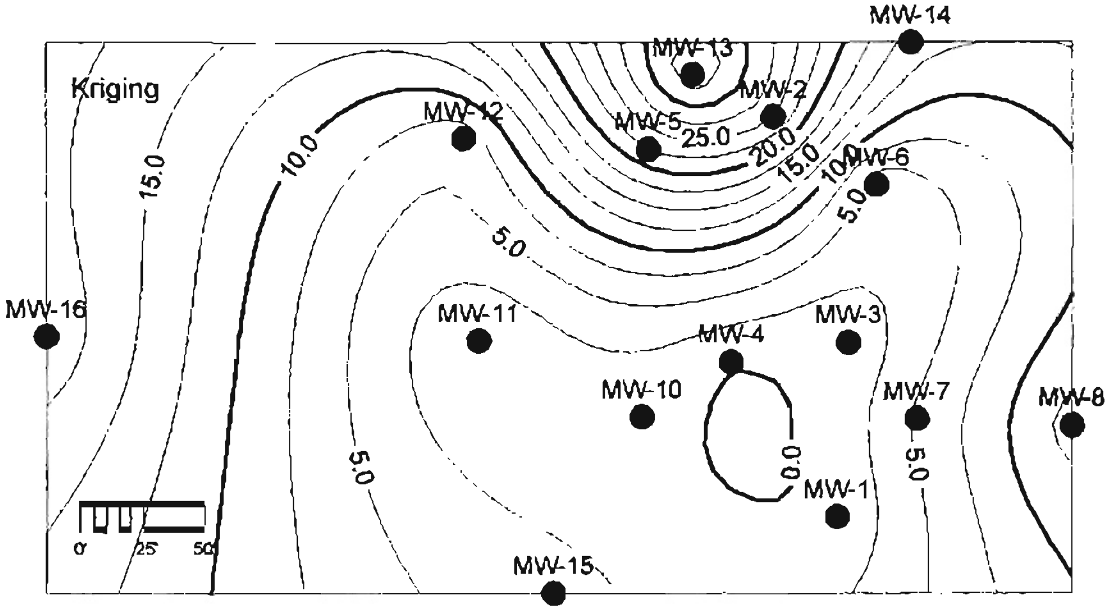


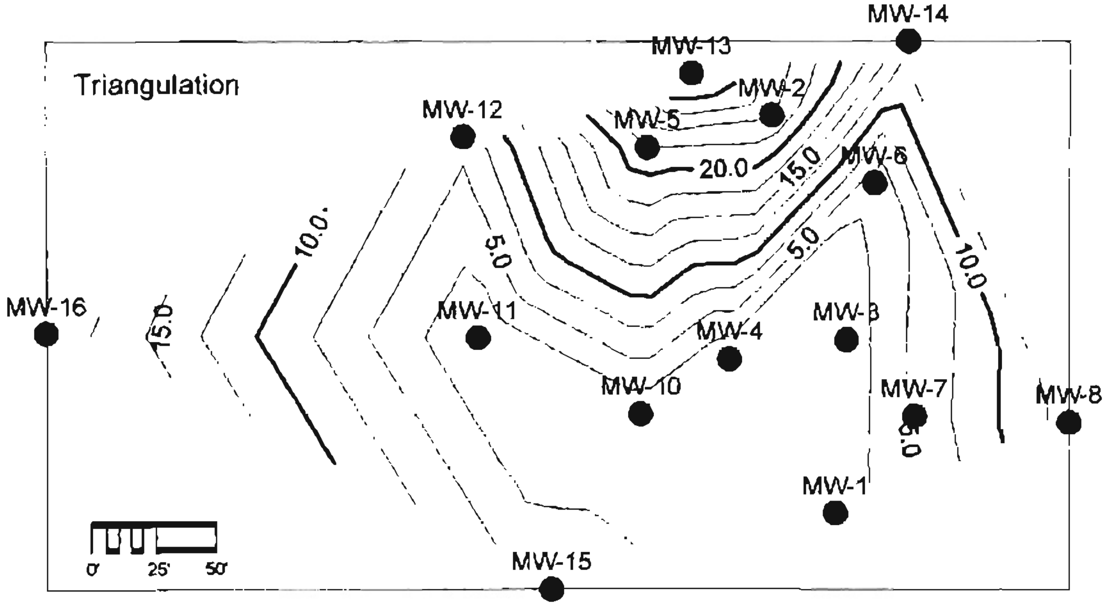
NITRATE (mg/L) -- 12/15/97



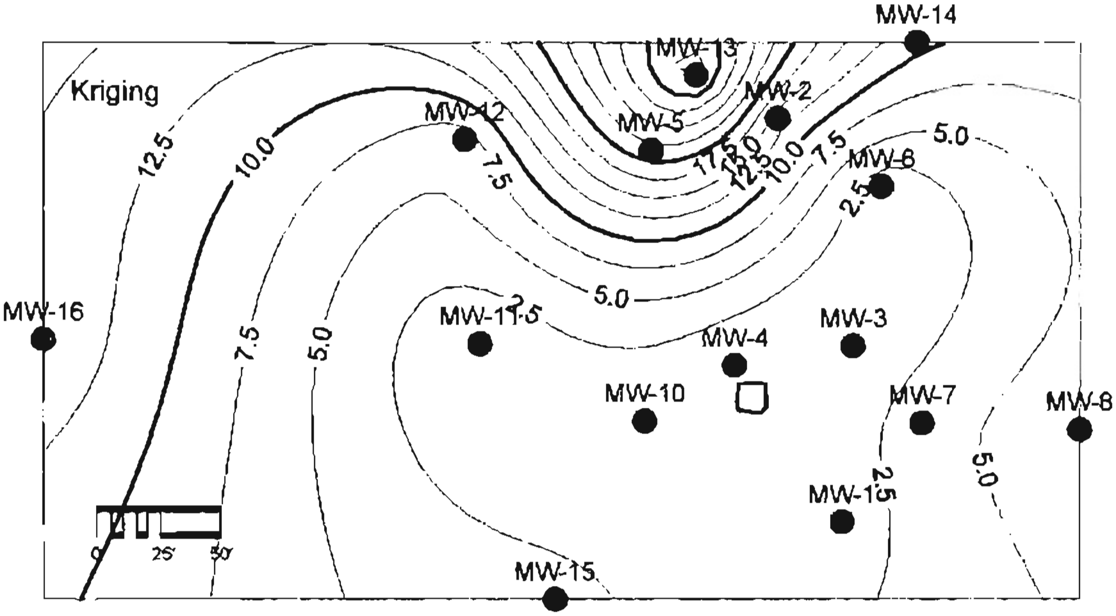


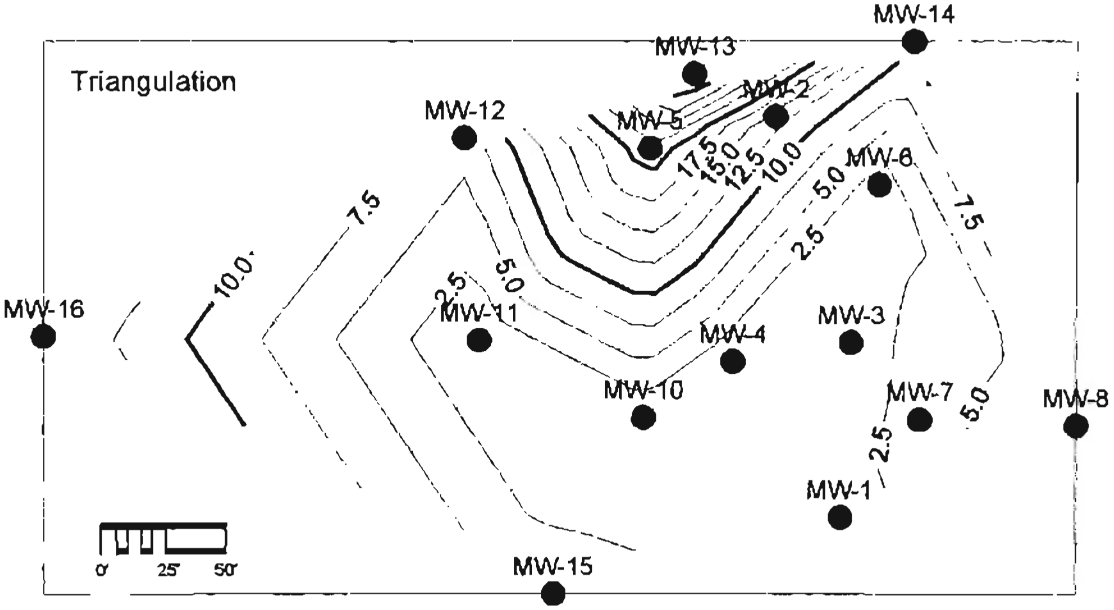
NITRATE (mg/L) -- 1/20/98





NITRATE (mg/L) -- 2/17/98





APPENDIX K --

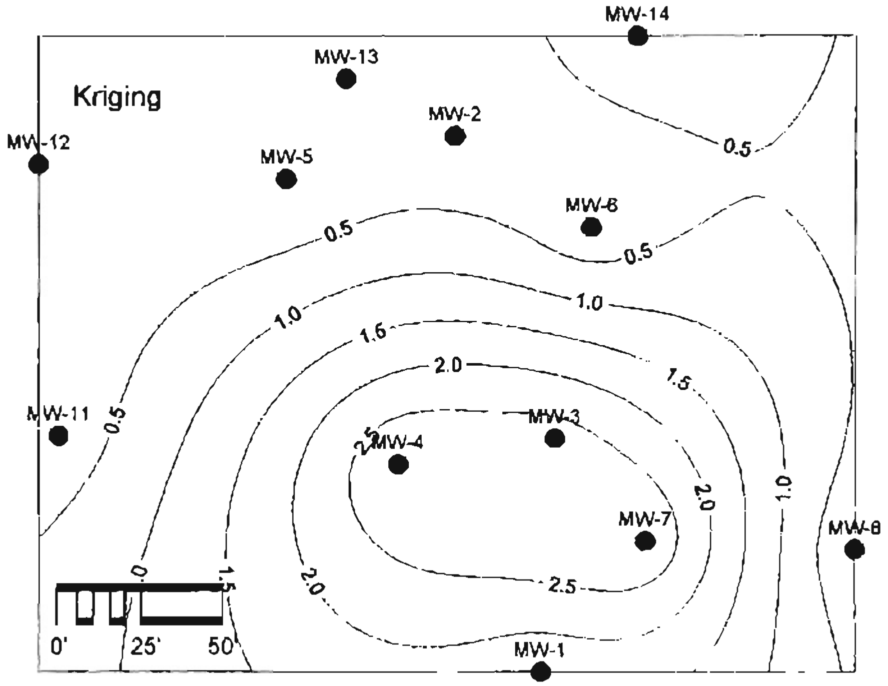
Ferrous Iron Analytical Data and Isopleths

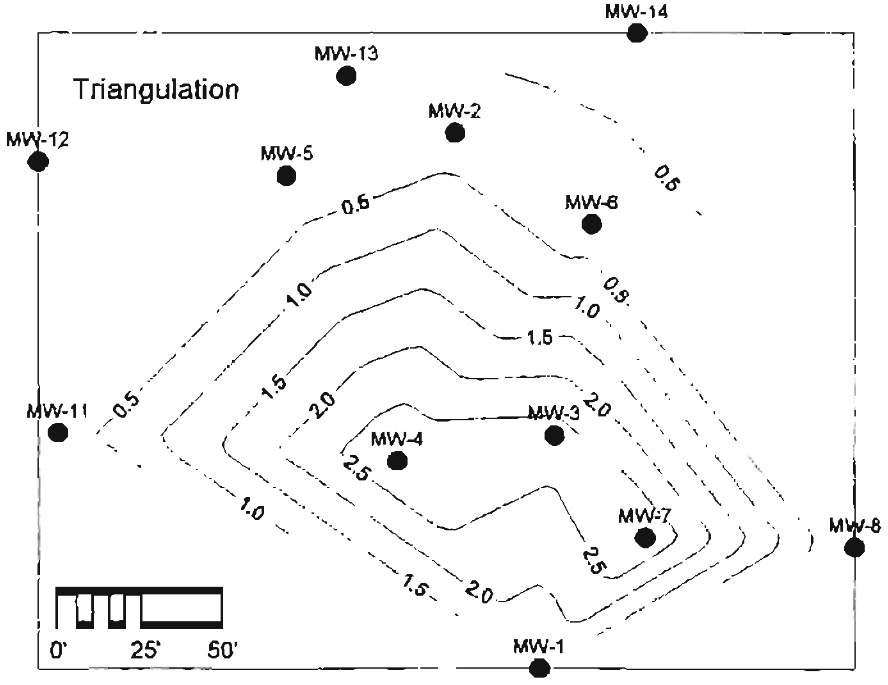
Ferrous Iron Concentrations in Groundwater (mg/L)	
Well	**4/14/98**
MW-1	1.56
MW-2	0.18
MW-3	2.74
MW-4	>3
MW-5	0.00
MW-6	0.09
MW-7	>3
MW-8	0.00
MW-9	
MW-10	0.15
MW-11	0.19
MW-12	0.07
MW-13	0.28
MW-14	0.85
MW-15	
MW-16	

Notes:

1. Greater than signs (>) designate values above the detection limit.
2. Data were obtained in the field. Laboratory total iron analyses were inconclusive.
3. Data is from Akins, 1998.

FERROUS IRON (mg/L) - 4/14/98





APPENDIX L --

Sulfate Analytical Data and Isopleths

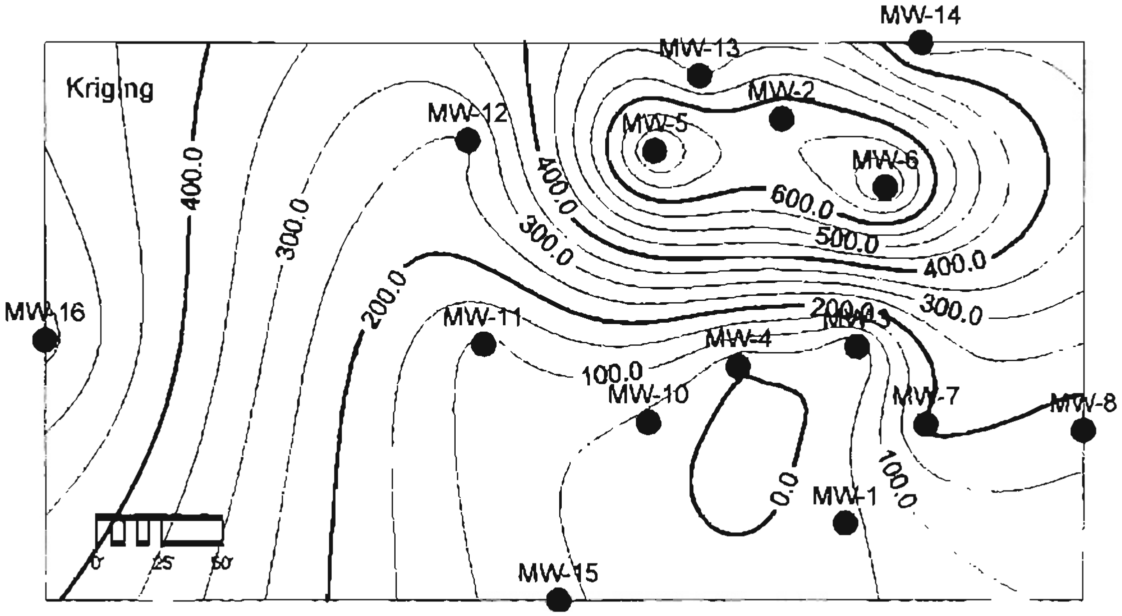
Sulfate Concentrations in Groundwater (mg/L)

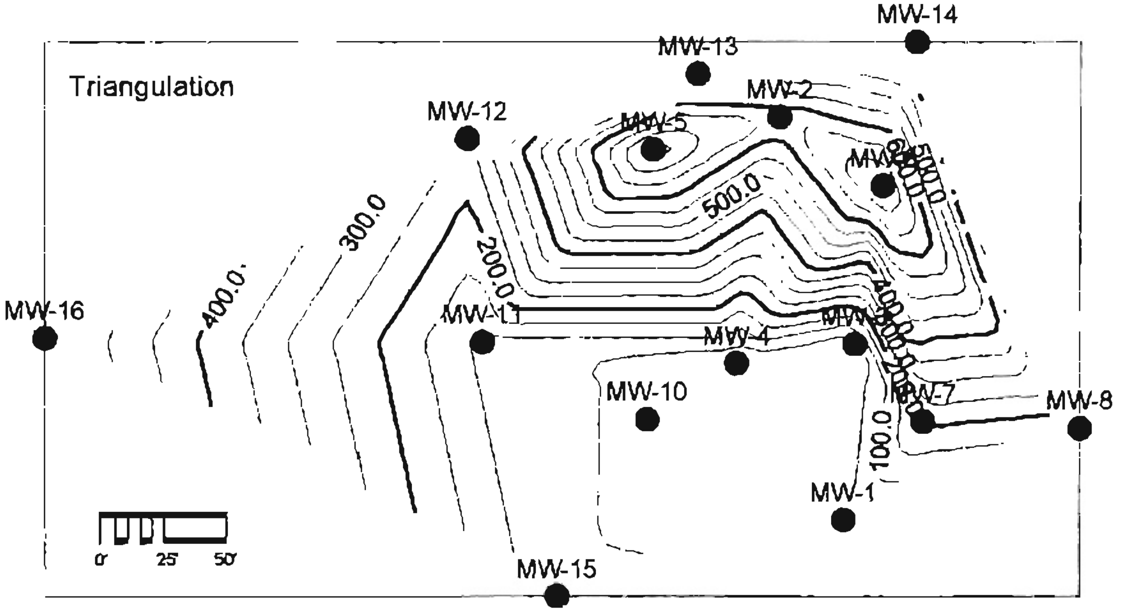
Well	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	33.65	26.72	28.23	25.16
MW-2	639.33	537.51	565.99	562.24
MW-3	8.56	7.34	24.56	4.14
MW-4	7.71	2.88	1.11	1.36
MW-5	776.06	637.61	787.47	756.88
MW-6	764.64	543.29	743.51	704.41
MW-7	212.40	229.50	248.62	208.01
MW-8	163.58	131.30	123.06	70.86
MW-9				
MW-10		35.75	38.07	163.64
MW-11	86.37	62.57	51.65	41.33
MW-12	244.45	171.91	187.03	199.41
MW-13	483.87	402.87	455.12	448.34
MW-14	313.42	185.45	179.88	158.51
MW-15	62.65	47.16	54.74	51.31
MW-16	569.48	455.25	273.60	181.03

Notes:

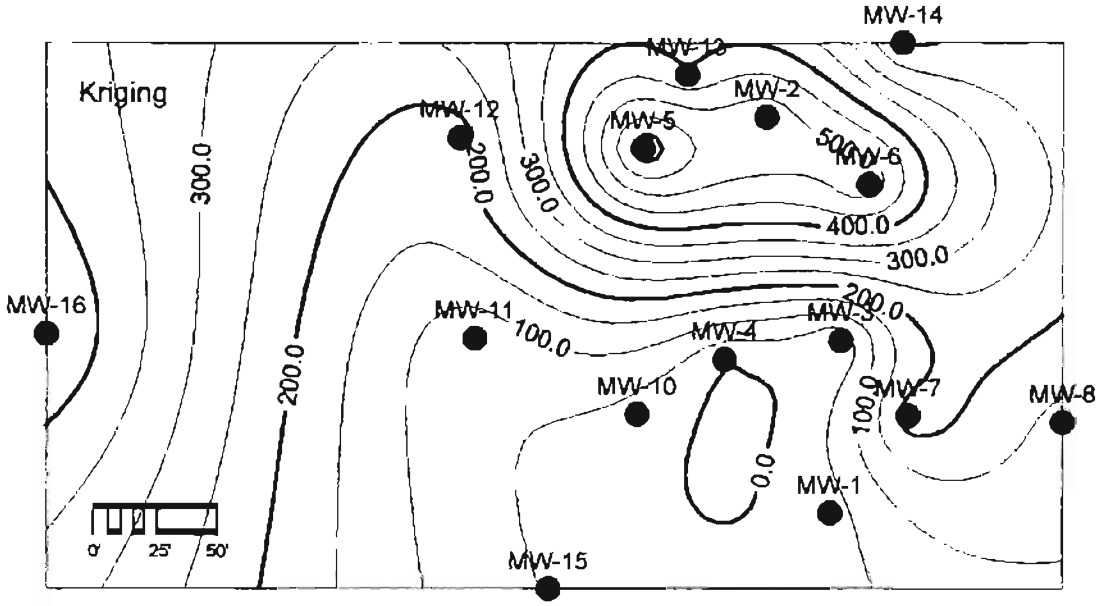
1. Less than signs (<) designate values below the detection limit.
2. 1994, 1995, and 1996 data is from Caldwell, 1995.
3. 1997 and 1998 data is from Akins, 1998.

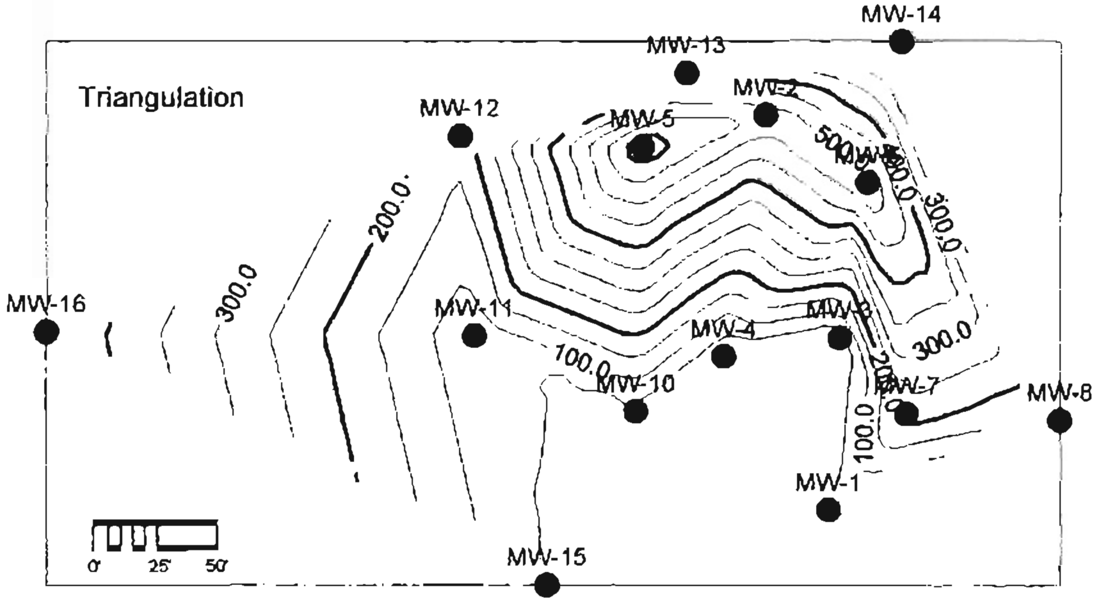
SULFATE (mg/L) -- 10/20/97



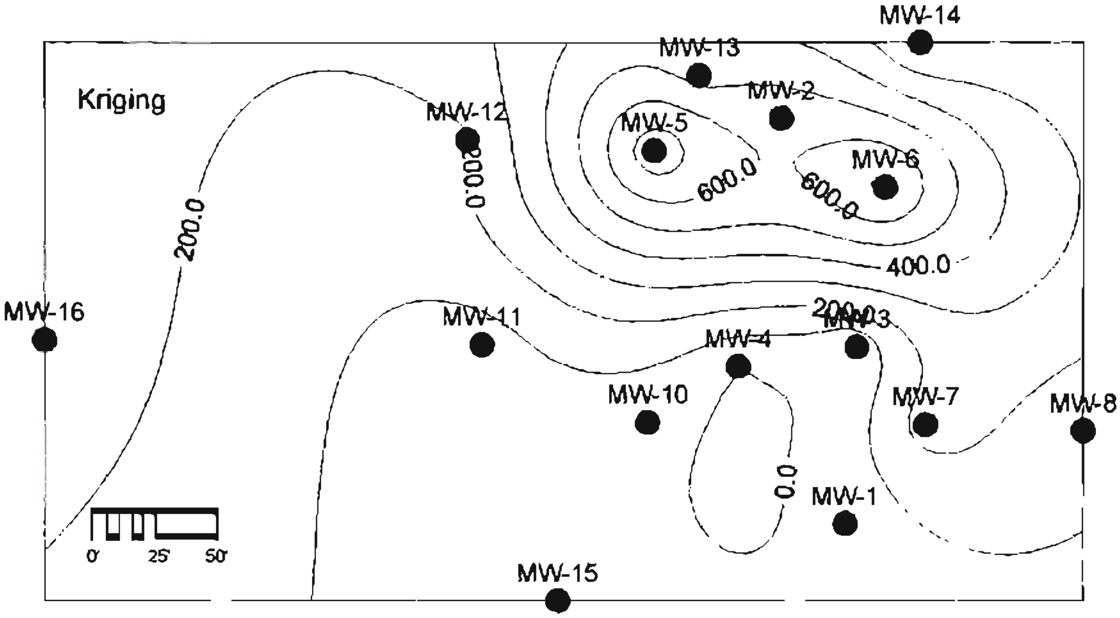


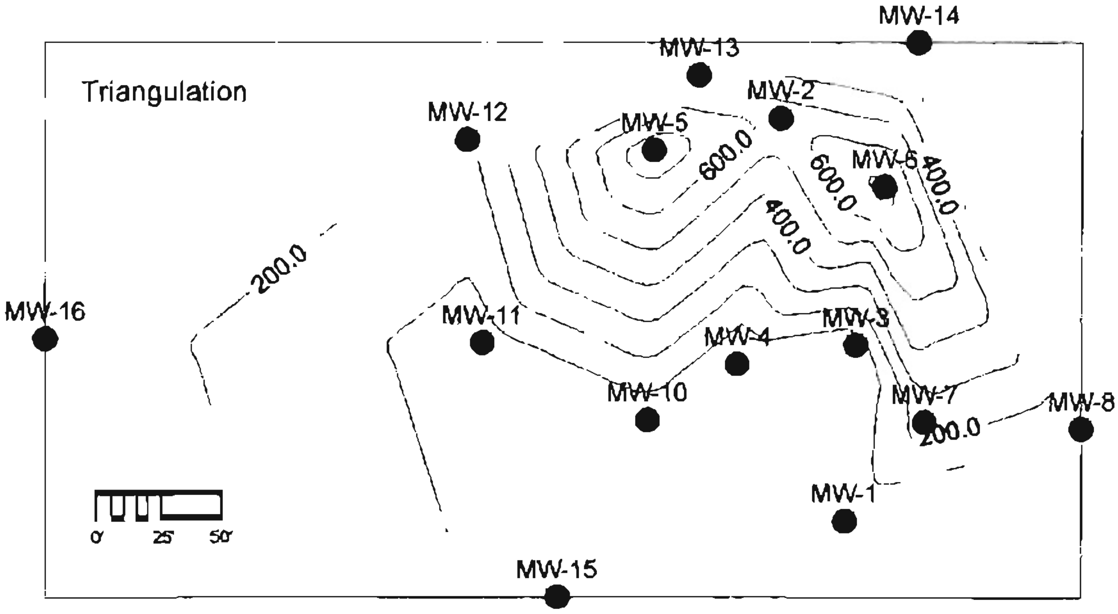
SULFATE (mg/L) -- 12/15/97



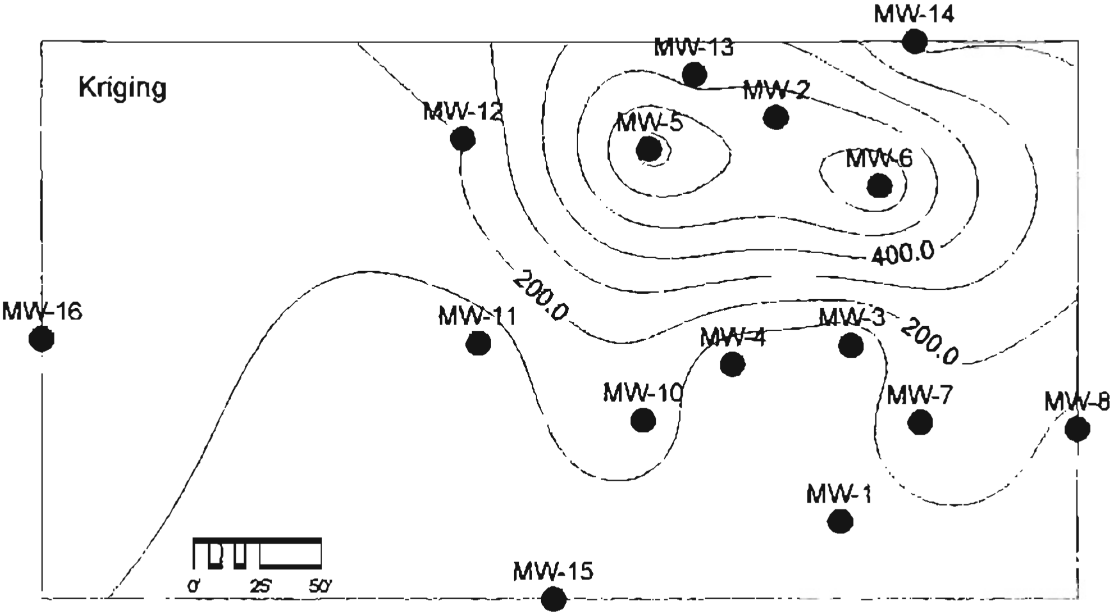


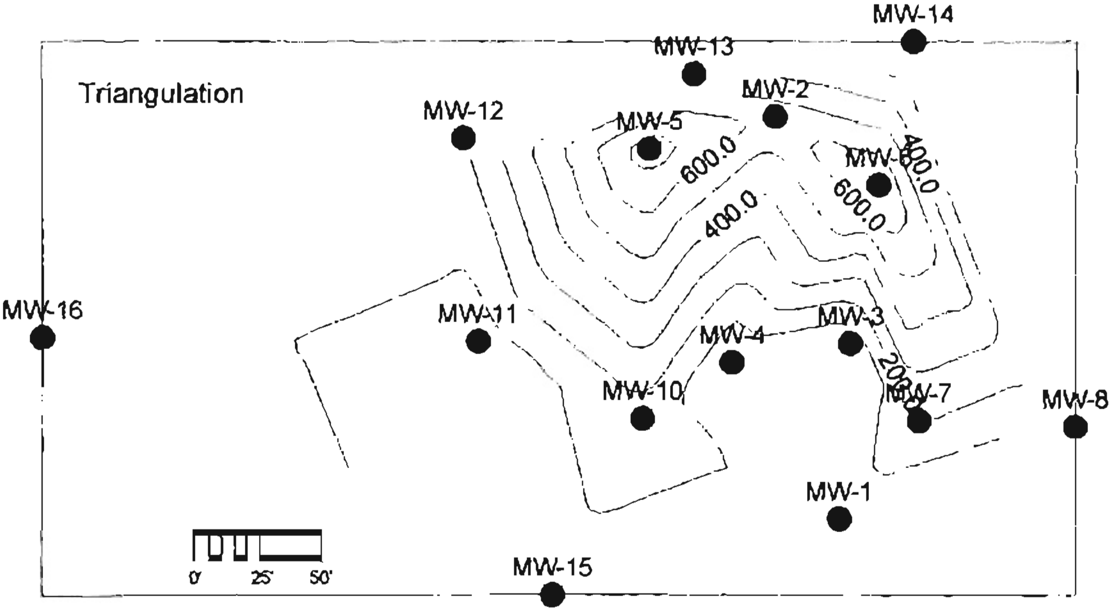
SULFATE (mg/L) -- 1/20/98





SULFATE (mg/L) -- 2/17/98





APPENDIX M --

Total Organic Carbon Analytical Data and Isopleths

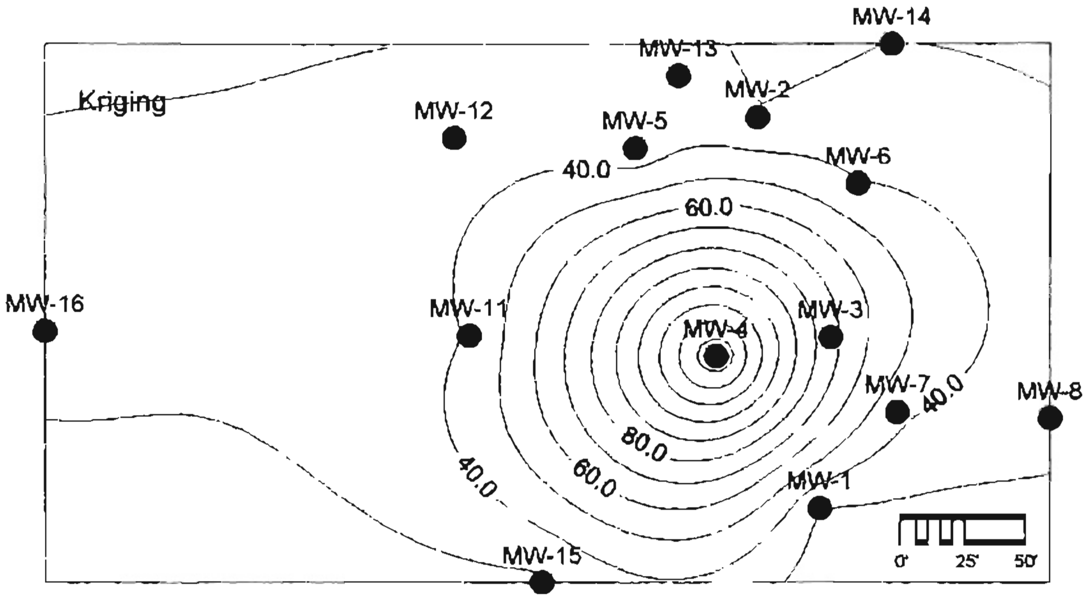
Total Organic Carbon Concentrations in Groundwater (mg/L)

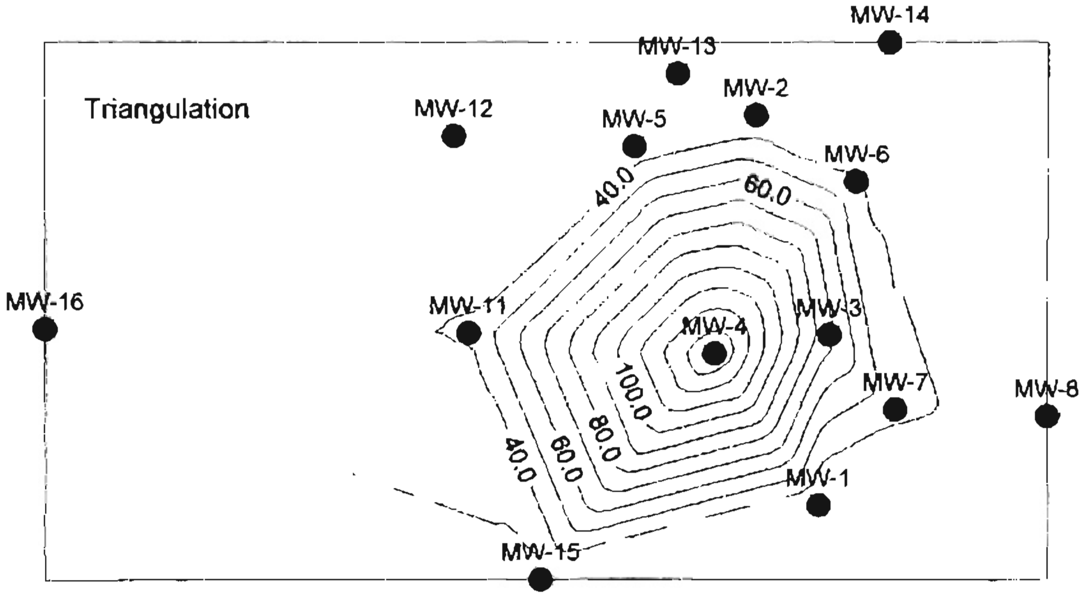
Well	10/20/97	12/15/97	1/20/98	2/17/98
MW-1	29.54	56.72	2.45	24.14
MW-2	30.46	43.16	-4.15	29.42
MW-3	72.90	93.17	47.65	81.72
MW-4	140.96	151.70	68.85	72.05
MW-5	32.68	40.02	18.88	38.97
MW-6	40.47	62.50	13.95	45.09
MW-7	42.52	37.66	21.78	39.49
MW-8	34.27	37.92	16.45	24.82
MW-9				
MW-10		47.31	0.00	27.61
MW-11	40.72	82.14	25.30	39.17
MW-12	34.24	56.09	17.27	29.77
MW-13	34.53	55.02	17.82	26.54
MW-14	30.20	52.59	17.30	29.51
MW-15	27.71	29.35	13.21	24.86
MW-16	32.14	64.02	16.29	27.01

Notes:

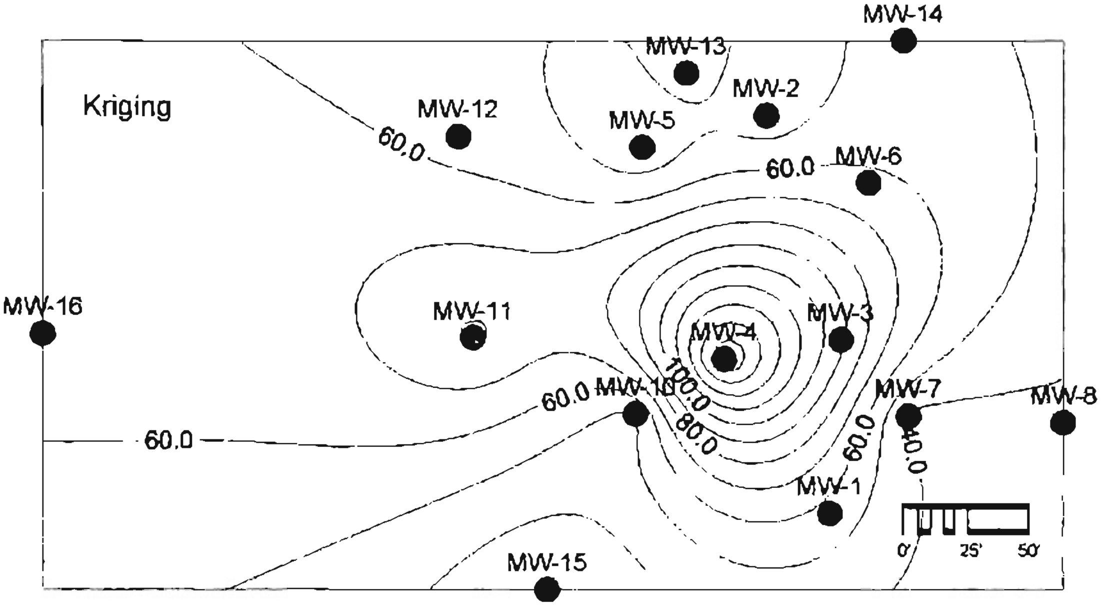
1. Less than signs (<) designate values below the detection limit.
2. Data is from Akins, 1998.

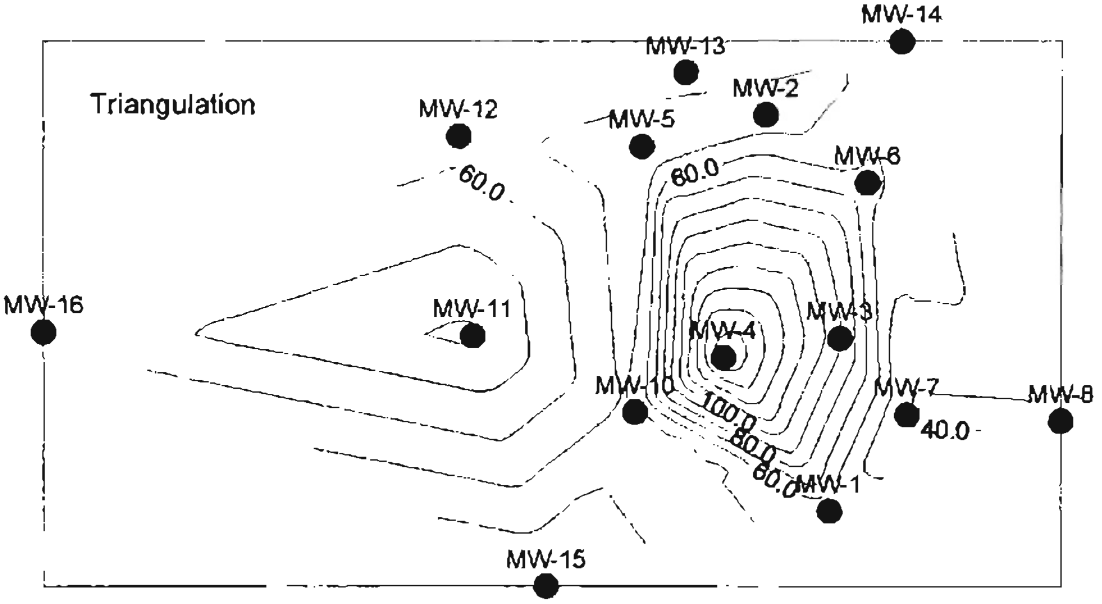
TOTAL ORGANIC CARBON (mg/L) -- 10/20/97



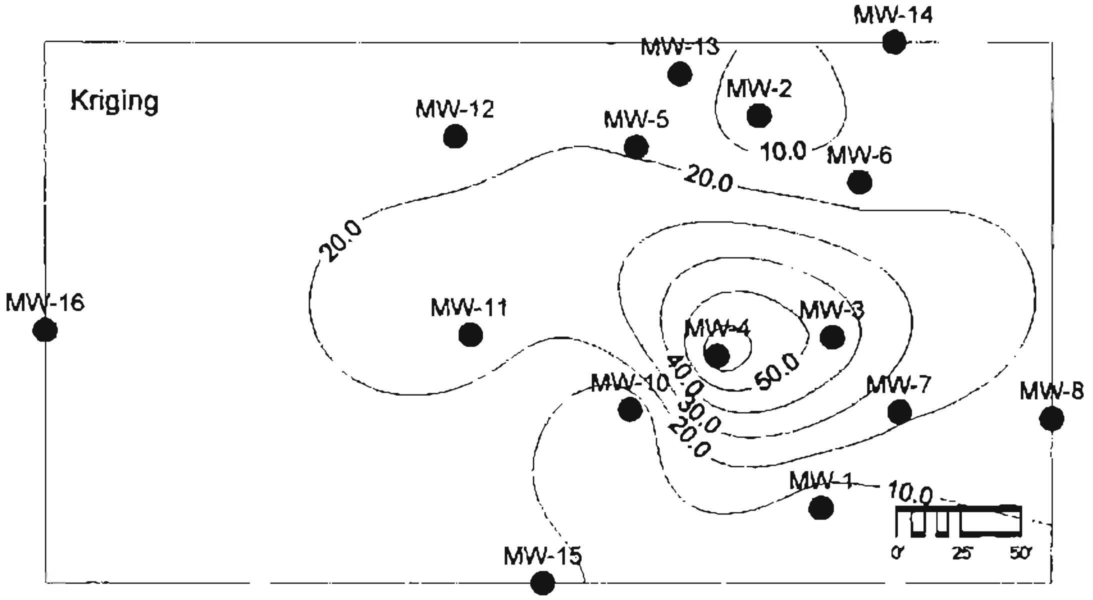


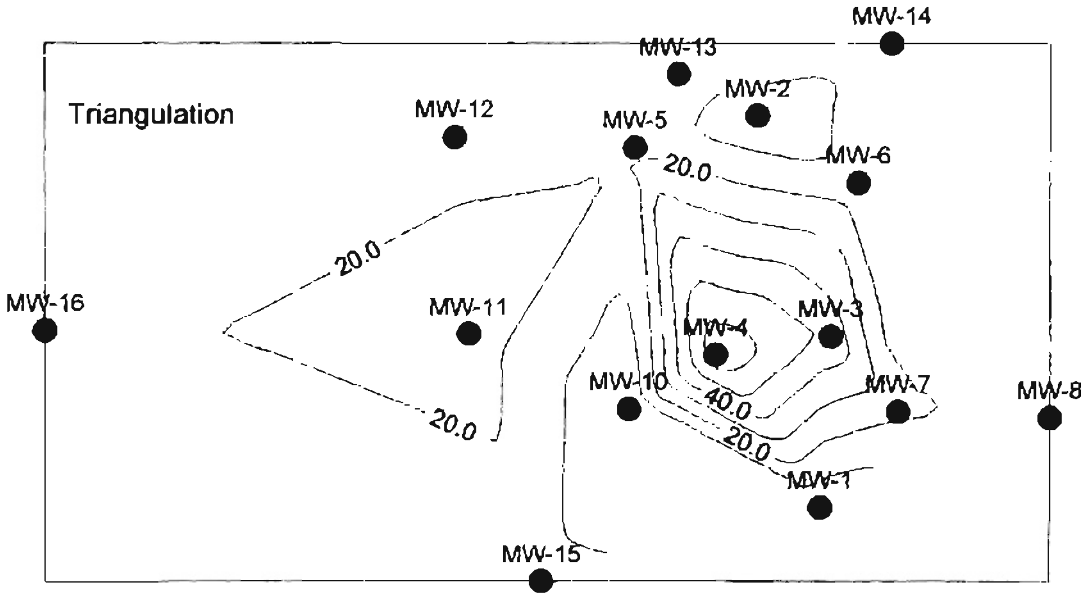
TOTAL ORGANIC CARBON (mg/L) -- 12/15/97



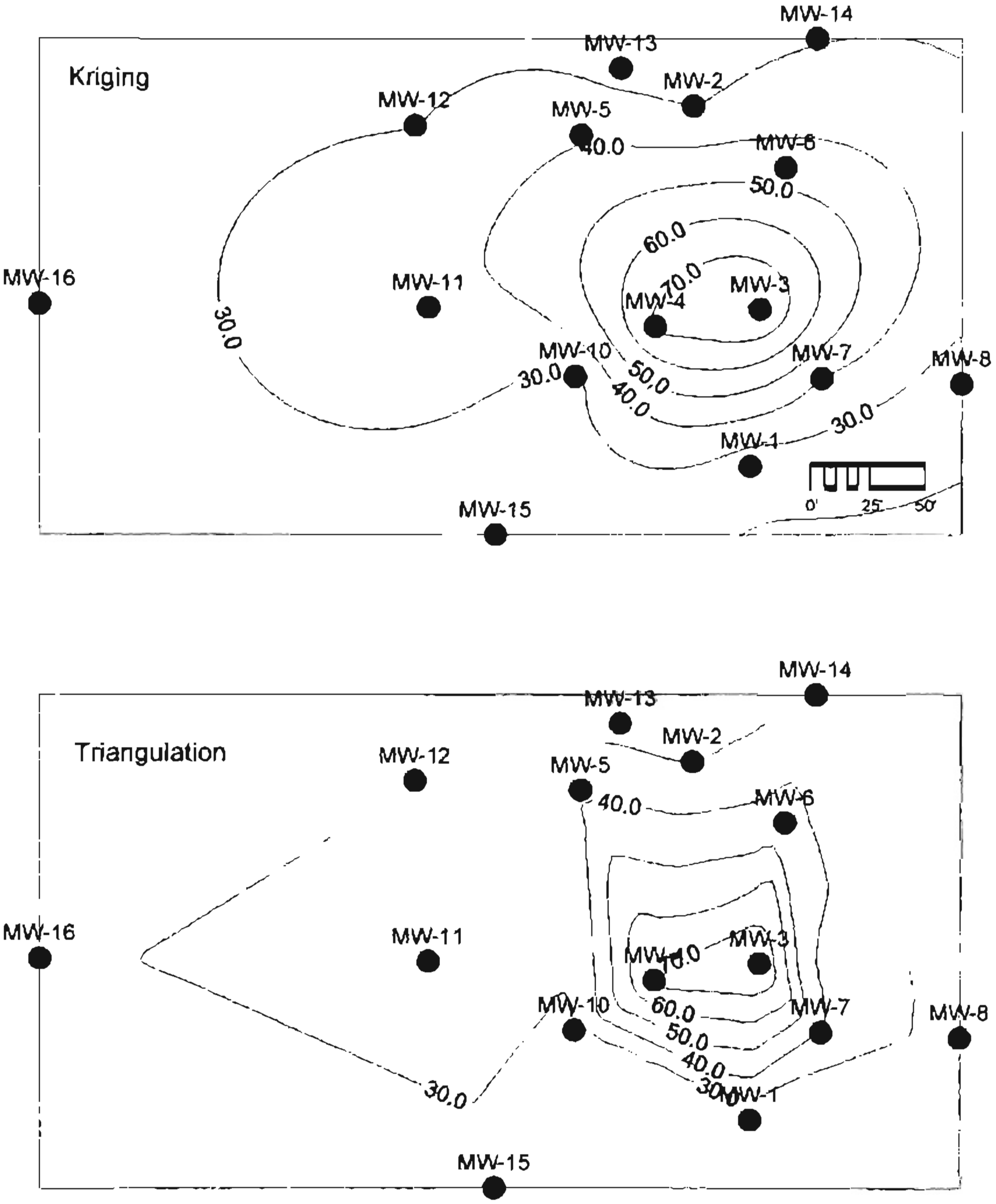


TOTAL ORGANIC CARBON (mg/L) -- 1/20/98





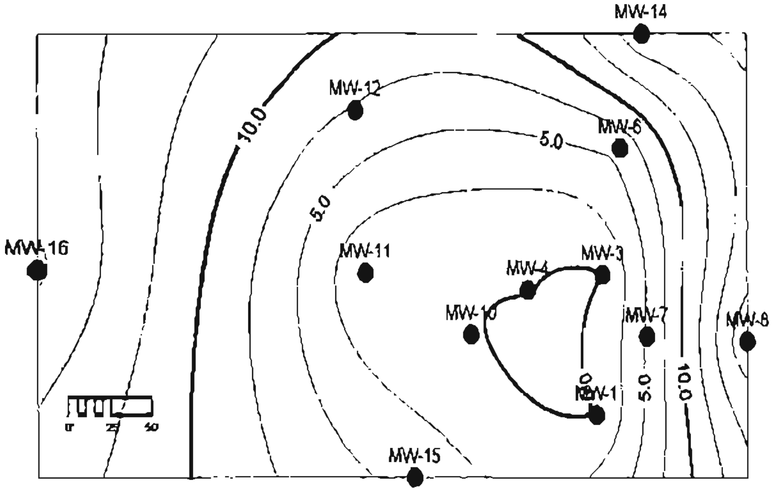
TOTAL ORGANIC CARBON (mg/L) -- 2/17/98



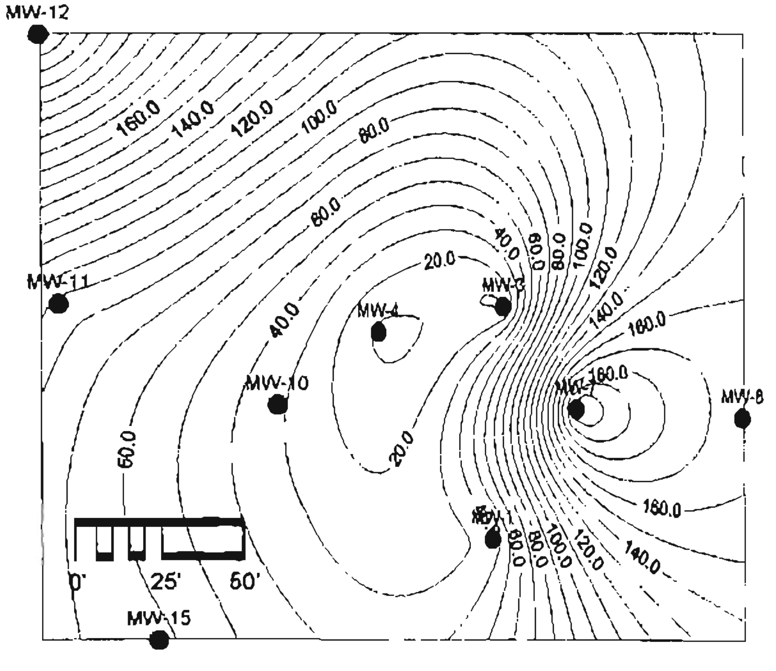
APPENDIX N –

Nitrate and Sulfate Isopleths, Selected Data

Nitrate (mg/L) - 10/20/97 - Selected data

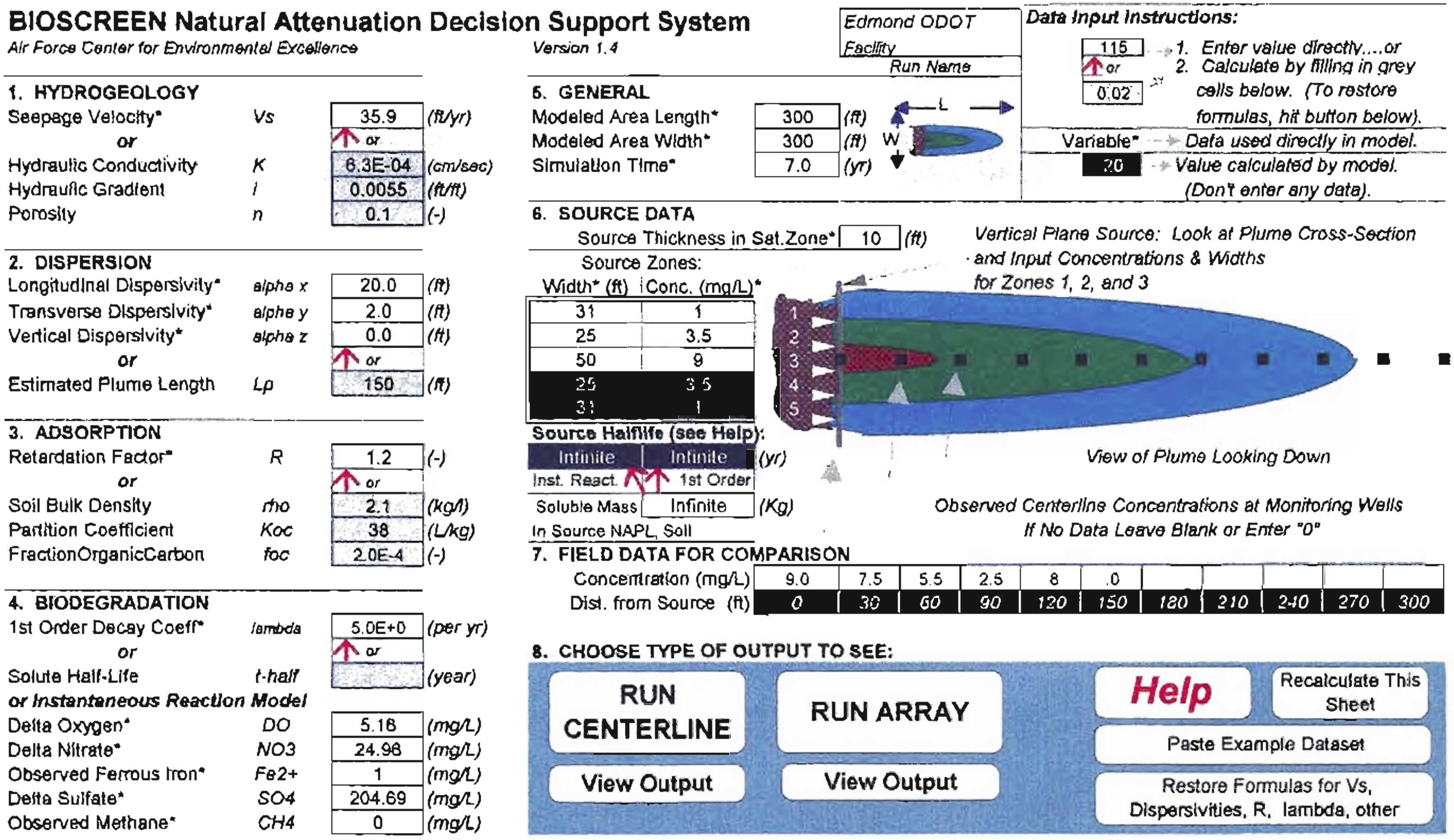


Sulfate (mg/L) - 10/20/97 - Selected data



APPENDIX O --

BIOSCREEN Simulation #1 Input Data and Output



BIOSCREEN Natural Attenuation Decision Support System
Air Force Center for Environmental Excellence
Version 1.4

Edmond ODOT
Facility
Run Name

Data Input Instructions:
115 → 1. Enter value directly....or
or 2. Calculate by filling in grey cells below. (To restore formulas, hit button below).
0.02
Variable* → Data used directly in model.
20 → Value calculated by model. (Don't enter any data).

1. HYDROGEOLOGY

Seepage Velocity*	Vs	35.9	(ft/yr)
or		or	
Hydraulic Conductivity	K	6.3E-04	(cm/sec)
Hydraulic Gradient	i	0.0055	(ft/ft)
Porosity	n	0.1	(-)

2. DISPERSION

Longitudinal Dispersivity*	alpha x	20.0	(ft)
Transverse Dispersivity*	alpha y	2.0	(ft)
Vertical Dispersivity*	alpha z	0.0	(ft)
or		or	
Estimated Plume Length	Lp	150	(ft)

3. ADSORPTION

Retardation Factor*	R	1.2	(-)
or		or	
Soil Bulk Density	rho	2.1	(kg/l)
Partition Coefficient	Koc	38	(L/kg)
FractionOrganicCarbon	foc	2.0E-4	(-)

4. BIODEGRADATION

1st Order Decay Coeff*	lambda	5.0E+0	(per yr)
or		or	
Solute Half-Life	t-half		(year)
or Instantaneous Reaction Model			
Delta Oxygen*	DO	5.18	(mg/L)
Delta Nitrate*	NO3	24.98	(mg/L)
Observed Ferrous Iron*	Fe2+	1	(mg/L)
Delta Sulfate*	SO4	204.69	(mg/L)
Observed Methane*	CH4	0	(mg/L)

5. GENERAL

Modeled Area Length*	300	(ft)
Modeled Area Width*	300	(ft)
Simulation Time*	7.0	(yr)

6. SOURCE DATA

Source Thickness in Sat.Zone* 10 (ft)

Source Zones:

Width* (ft)	Conc. (mg/L)*
31	1
25	3.5
50	9
25	3.5
31	1

Source Halflife (see Help):

Infinite	Infinite	(yr)
Inst. React.	1st Order	

Soluble Mass Infinite (Kg)
In Source NAPL, Soil

Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3

View of Plume Looking Down

Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"

7. FIELD DATA FOR COMPARISON

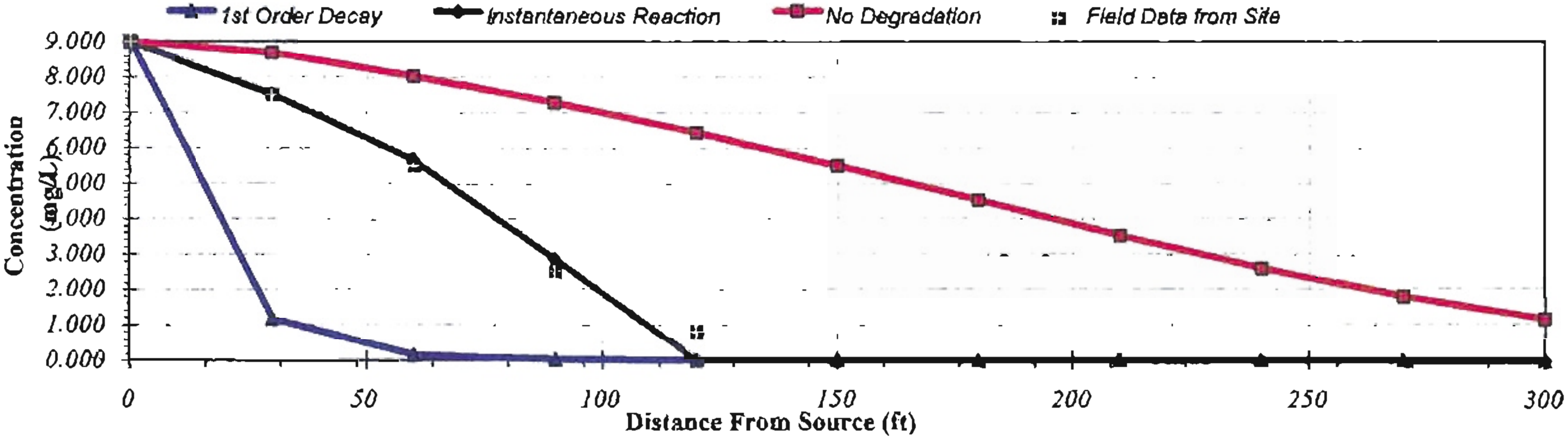
Concentration (mg/L)	9.0	7.5	5.5	2.5	8	.0					
Dist. from Source (ft)	0	30	60	90	120	150	180	210	240	270	300

8. CHOOSE TYPE OF OUTPUT TO SEE:

BIOSCREEN Simulation #1 Input Data - Calibrated to 10/20/97

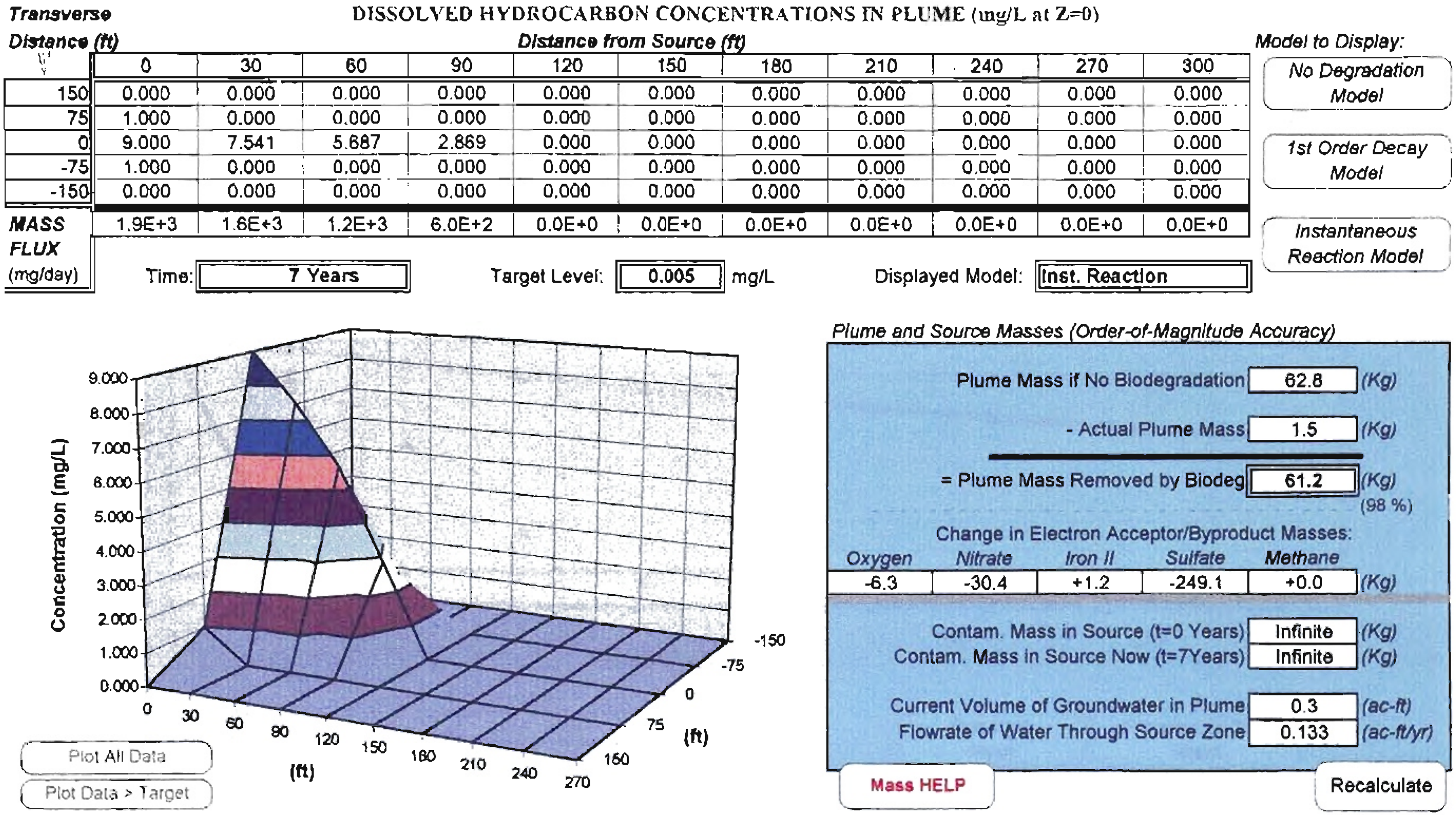
DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

	Distance from Source (ft)										
TYPE OF MODEL	0	30	60	90	120	150	180	210	240	270	300
No Degradation	9.000	8.676	8.021	7.255	6.415	5.493	4.506	3.506	2.566	1.753	1.111
1st Order Decay	9.000	1.143	0.139	0.017	0.002	0.000	0.000	0.000	0.000	0.000	0.000
Inst. Reaction	9.000	7.541	5.687	2.869	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Field Data from Site	9.000	7.500	5.500	2.500	0.800						



Time: 7.0 Years

BIOSCREEN Simulation #1 Plume Centerline - Calibrated to 10/20/97



DISSOLVED HYDROCARBON CONCENTRATIONS IN PLUME (mg/L at Z=0)

Transverse Distance (ft)	0	30	60	90	120	150	180	210	240	270	300
150	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
75	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0	9.000	7.541	5.687	2.869	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-75	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-150	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MASS FLUX (mg/day)	1.9E+3	1.6E+3	1.2E+3	6.0E+2	0.0E+0	0.0E+0	0.0E+0	0.0E+0	0.0E+0	0.0E+0	0.0E+0

Distance from Source (ft)

Time: 7 Years

Target Level: 0.005 mg/L

Displayed Model: Inst. Reaction

Plume and Source Masses (Order-of-Magnitude Accuracy)

Plume Mass if No Biodegradation: 62.8 (Kg)

- Actual Plume Mass: 1.5 (Kg)

= Plume Mass Removed by Biodeg: 61.2 (Kg) (98 %)

Change in Electron Acceptor/Byproduct Masses:

Oxygen	*Nitrate*	*Iron II*	*Sulfate*	*Methane*	
-6.3	-30.4	+1.2	-249.1	+0.0	(Kg)

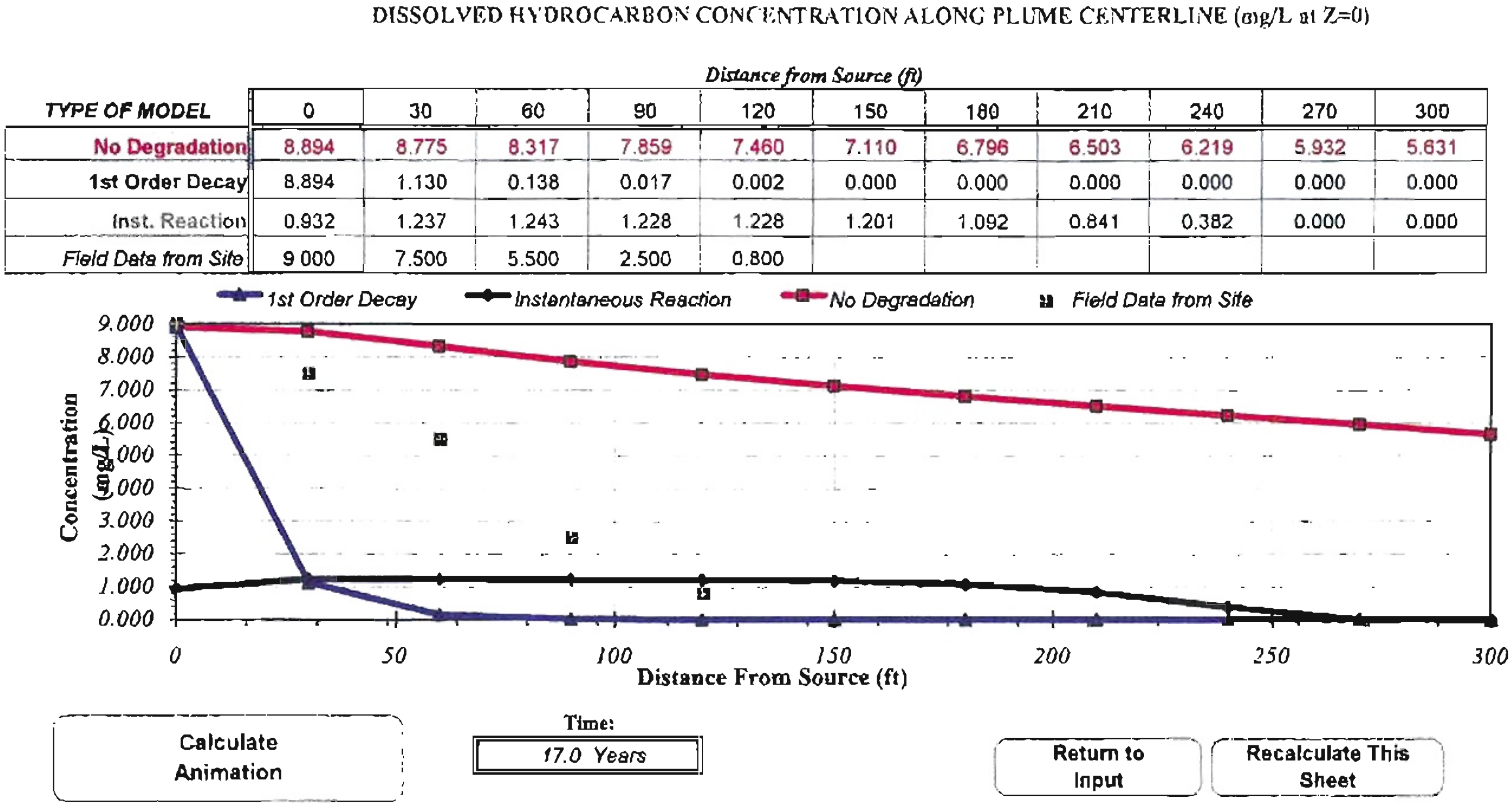
Contam. Mass in Source (t=0 Years): Infinite (Kg)

Contam. Mass in Source Now (t=7Years): Infinite (Kg)

Current Volume of Groundwater in Plume: 0.3 (ac-ft)

Flowrate of Water Through Source Zone: 0.133 (ac-ft/yr)

BIOSCREEN Simulation #1 3D Plume - Calibrated to 10/20/97



DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

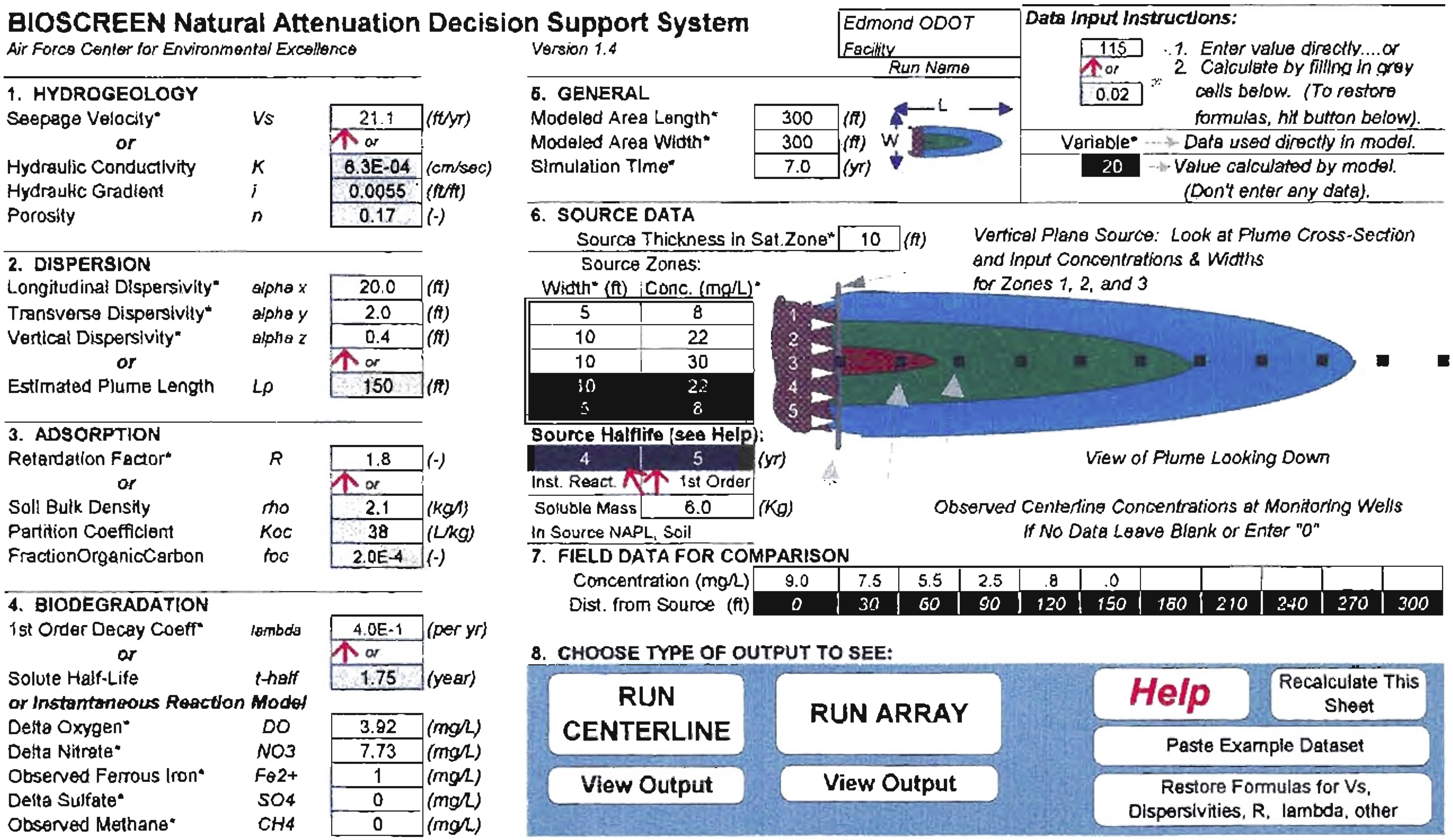
Distance from Source (ft)

TYPE OF MODEL	0	30	60	90	120	150	180	210	240	270	300
No Degradation	8.894	8.775	8.317	7.859	7.460	7.110	6.796	6.503	6.219	5.932	5.631
1st Order Decay	8.894	1.130	0.138	0.017	0.002	0.000	0.000	0.000	0.000	0.000	0.000
Inst. Reaction	0.932	1.237	1.243	1.228	1.228	1.201	1.092	0.841	0.382	0.000	0.000
Field Data from Site	9.000	7.500	5.500	2.500	0.800						

BIOSCREEN Simulation #1 Plume Centerline - 17 year simulation, assuming 1000 kg source

APPENDIX P --

BIOSCREEN Simulation #2 Input Data and Output



BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence

Version 1.4

Edmond ODOT Facility

Run Name

1. HYDROGEOLOGY

Seepage Velocity*	Vs	21.1	(ft/yr)
or		↑ or	
Hydraulic Conductivity	K	6.3E-04	(cm/sec)
Hydraulic Gradient	i	0.0055	(ft/ft)
Porosity	n	0.17	(-)

2. DISPERSION

Longitudinal Dispersivity*	alpha x	20.0	(ft)
Transverse Dispersivity*	alpha y	2.0	(ft)
Vertical Dispersivity*	alpha z	0.4	(ft)
or		↑ or	
Estimated Plume Length	Lp	150	(ft)

3. ADSORPTION

Retardation Factor*	R	1.8	(-)
or		↑ or	
Soil Bulk Density	rho	2.1	(kg/l)
Partition Coefficient	Koc	38	(L/kg)
FractionOrganicCarbon	foc	2.0E-4	(-)

4. BIODEGRADATION

1st Order Decay Coeff*	lambda	4.0E-1	(per yr)
or		↑ or	
Solute Half-Life	t-half	1.75	(year)
or Instantaneous Reaction Model			
Delta Oxygen*	DO	3.92	(mg/L)
Delta Nitrate*	NO3	7.73	(mg/L)
Observed Ferrous Iron*	Fe2+	1	(mg/L)
Delta Sulfate*	SO4	0	(mg/L)
Observed Methane*	CH4	0	(mg/L)

5. GENERAL

Modeled Area Length*	300	(ft)
Modeled Area Width*	300	(ft)
Simulation Time*	7.0	(yr)

Data Input Instructions:

115 ↑ or 0.02	1. *Enter value directly....or* 2. *Calculate by filling in grey cells below. (To restore formulas, hit button below).*
Variable*	→ *Data used directly in model.*
20	→ *Value calculated by model. (Don't enter any data).*

6. SOURCE DATA

Source Thickness in Sat.Zone* 10 (ft)

Source Zones:

Width* (ft)	Conc. (mg/L)*
5	8
10	22
10	30
10	22
5	8

Source Halflife (see Help):

4	5	(yr)
Inst. React.	1st Order	
Soluble Mass	6.0	(Kg)

In Source NAPL, Soil

Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3

View of Plume Looking Down

Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"

7. FIELD DATA FOR COMPARISON

Concentration (mg/L)	9.0	7.5	5.5	2.5	.8	.0					
Dist. from Source (ft)	0	30	60	90	120	150	180	210	240	270	300

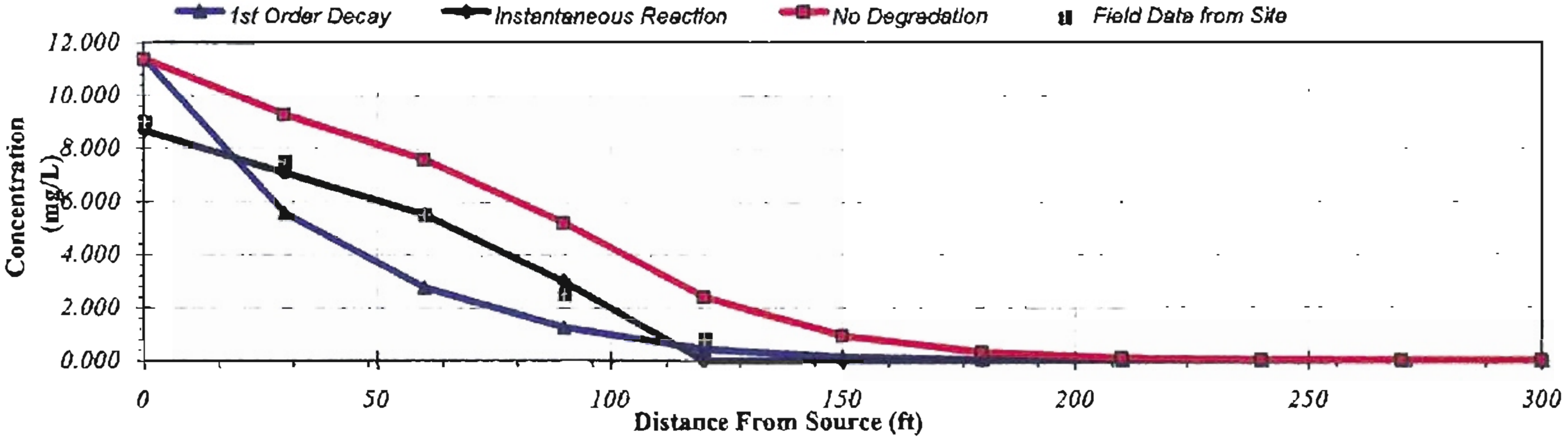
8. CHOOSE TYPE OF OUTPUT TO SEE:

BIOSCREEN Simulation #2 Input Data - Calibrated to 10/20/97

DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

Distance from Source (ft)

TYPE OF MODEL	0	30	60	90	120	150	180	210	240	270	300
No Degradation	11.366	9.273	7.580	5.185	2.396	0.933	0.297	0.076	0.016	0.002	0.000
1st Order Decay	11.366	5.566	2.761	1.267	0.432	0.135	0.036	0.008	0.002	0.000	0.000
Inst. Reaction	8.673	7.082	5.527	3.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Field Data from Site	9.000	7.500	5.500	2.500	0.800						



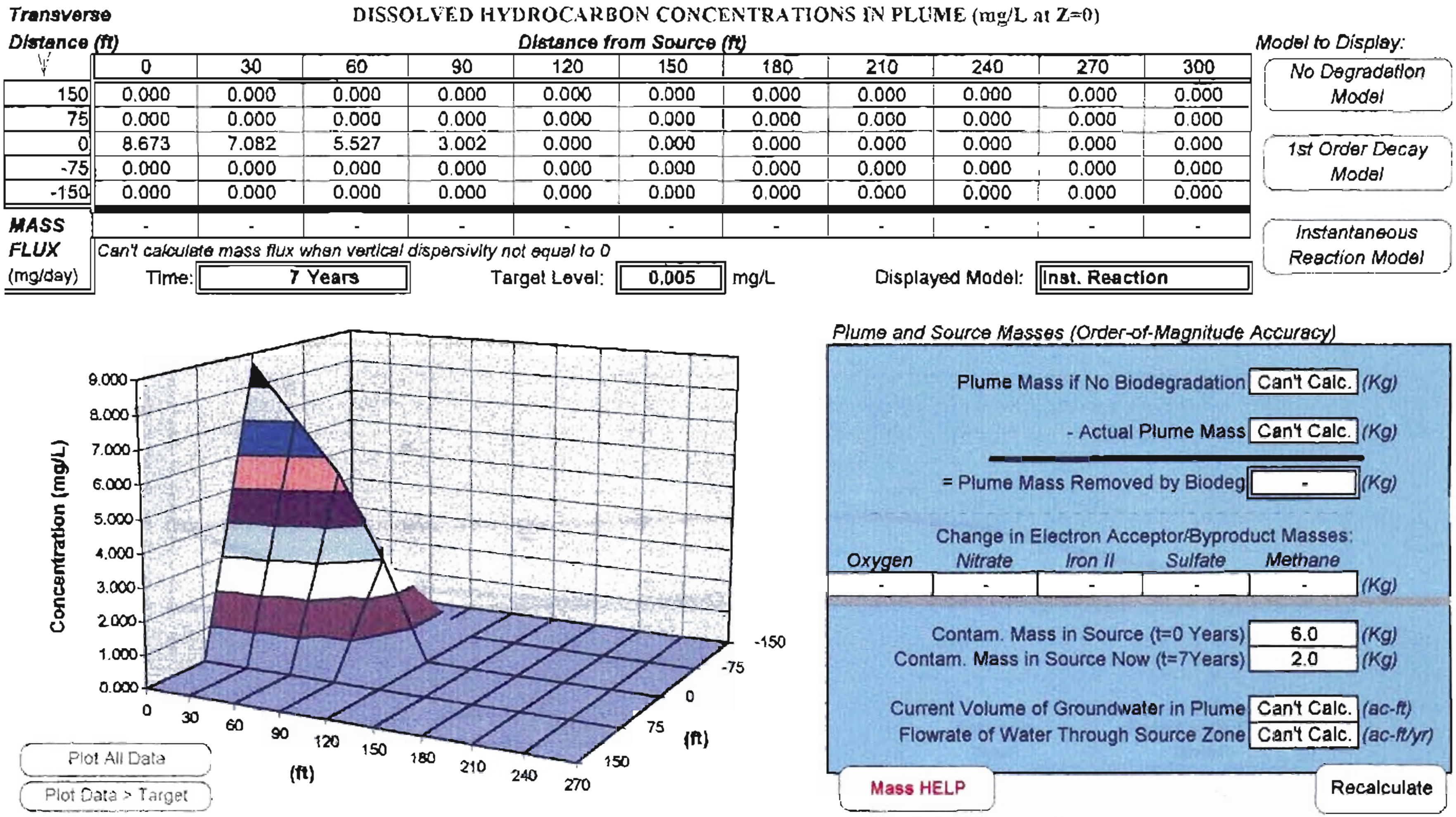
Calculate Animation

Time:
7.0 Years

Return to Input

Recalculate This Sheet

BIOSCREEN Simulation #2 Plume Centerline - Calibrated to 10/20/97



Transverse Distance (ft)

DISSOLVED HYDROCARBON CONCENTRATIONS IN PLUME (mg/L at Z=0)

Distance from Source (ft)

	0	30	60	90	120	150	180	210	240	270	300
150	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
75	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0	8.673	7.082	5.527	3.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-75	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-150	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MASS FLUX (mg/day)	-	-	-	-	-	-	-	-	-	-	-

Can't calculate mass flux when vertical dispersivity not equal to 0

Time: 7 Years   Target Level: 0.005 mg/L   Displayed Model: Inst. Reaction

Plume and Source Masses (Order-of-Magnitude Accuracy)

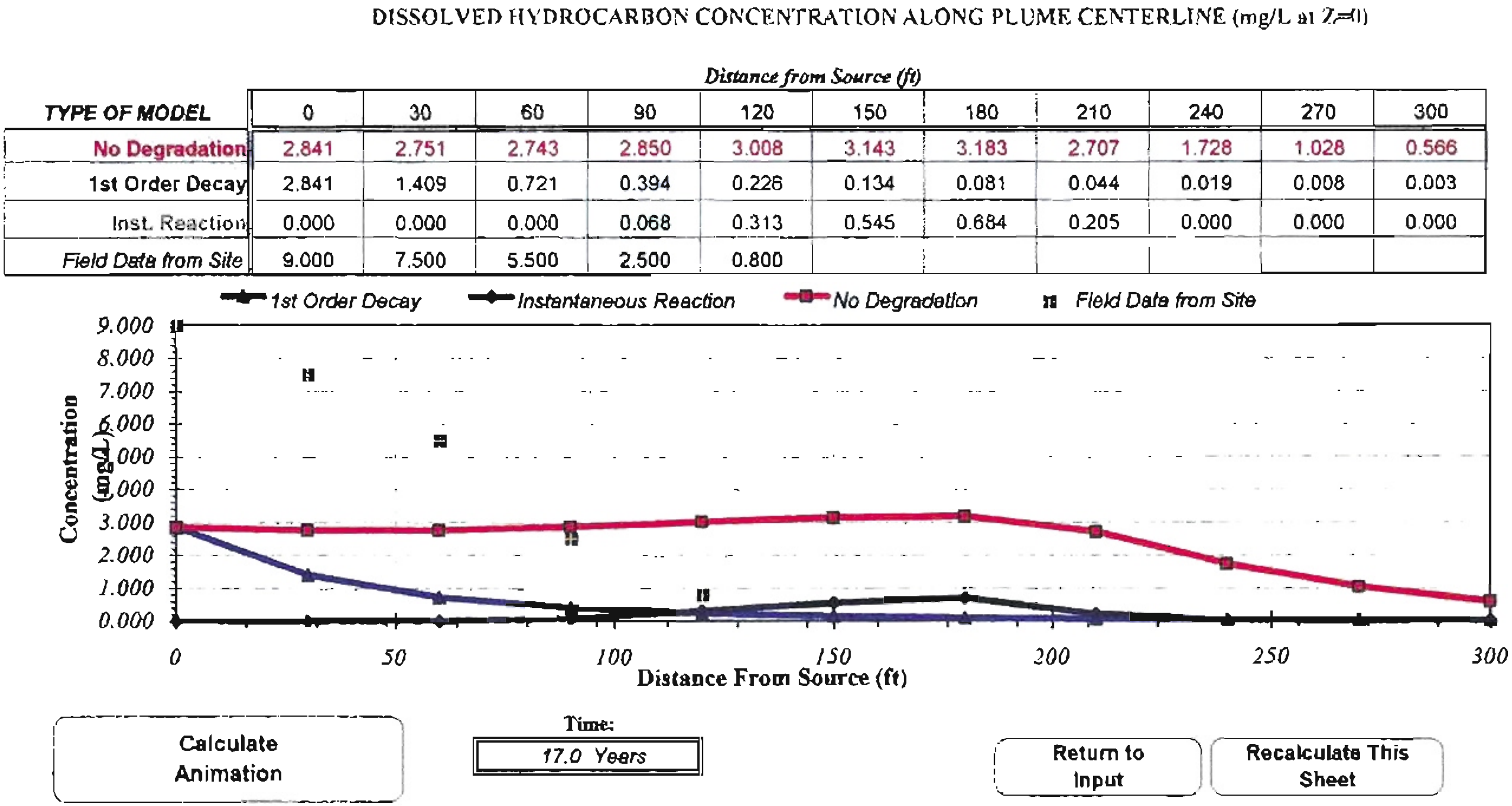
Plume Mass if No Biodegradation	Can't Calc.	*(Kg)*
- Actual Plume Mass	Can't Calc.	*(Kg)*
= Plume Mass Removed by Biodeg	-	*(Kg)*

Change in Electron Acceptor/Byproduct Masses:

Oxygen	*Nitrate*	*Iron II*	*Sulfate*	*Methane*	
-	-	-	-	-	*(Kg)*

Contam. Mass in Source (t=0 Years)	6.0	*(Kg)*
Contam. Mass in Source Now (t=7Years)	2.0	*(Kg)*
Current Volume of Groundwater in Plume	Can't Calc.	*(ac-ft)*
Flowrate of Water Through Source Zone	Can't Calc.	*(ac-ft/yr)*

BIOSCREEN Simulation #2 3D Plume - Calibrated to 10/20/97



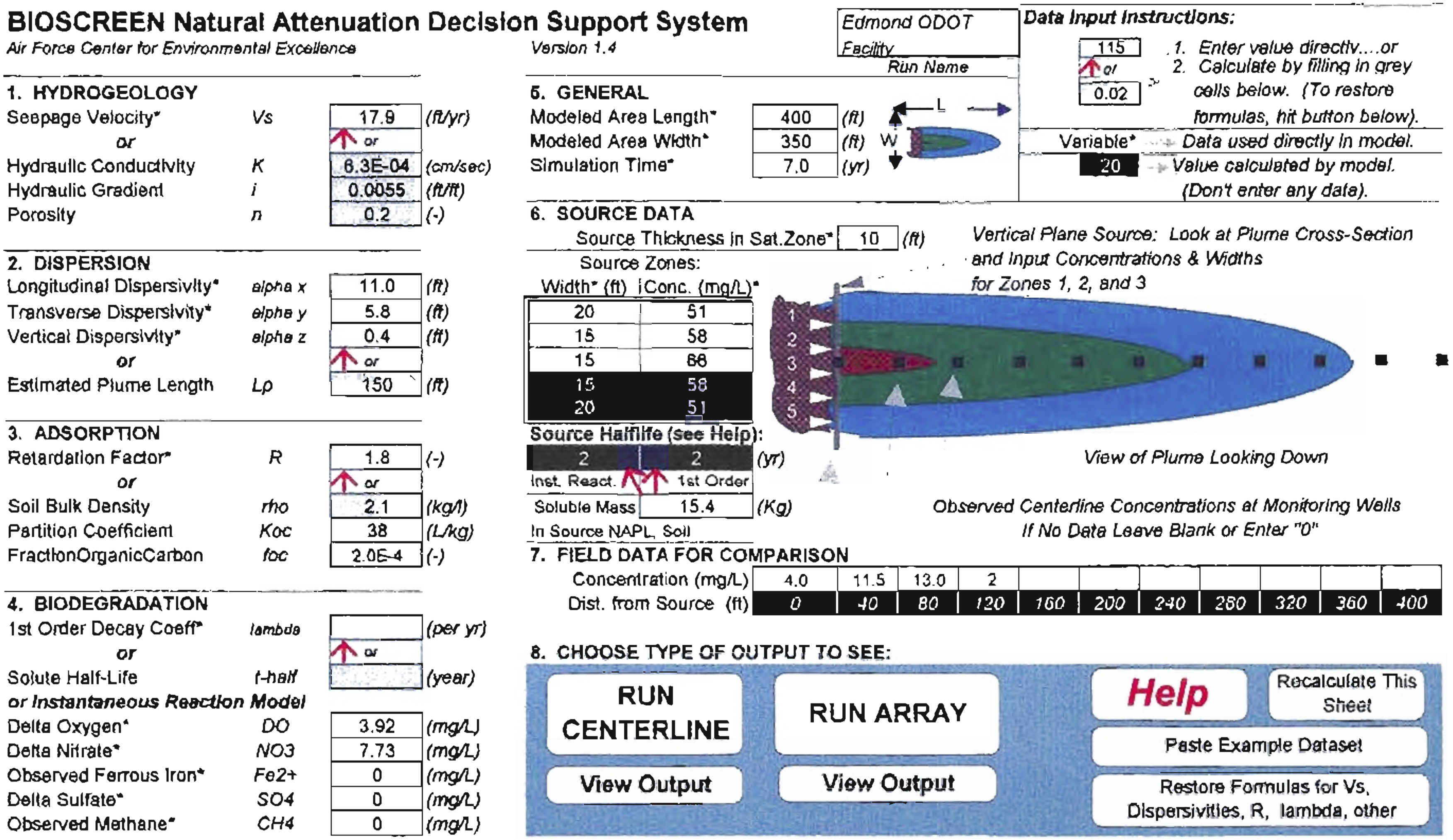
DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

TYPE OF MODEL	*Distance from Source (ft)* 0	30	60	90	120	150	180	210	240	270	300
No Degradation	2.841	2.751	2.743	2.850	3.008	3.143	3.183	2.707	1.728	1.028	0.566
1st Order Decay	2.841	1.409	0.721	0.394	0.226	0.134	0.081	0.044	0.019	0.008	0.003
Inst. Reaction	0.000	0.000	0.000	0.068	0.313	0.545	0.684	0.205	0.000	0.000	0.000
Field Data from Site	9.000	7.500	5.500	2.500	0.800						

BIOSCREEN Simulation #2 Plume Centerline - 17 Year Simulation

APPENDIX Q --

BIOSCREEN Simulation #3 Input Data and Output



BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence

Version 1.4

Edmond ODOT Facility

Run Name

Data Input Instructions:

115 or 0.02

1. *Enter value directly....or*
2. *Calculate by filling in grey cells below. (To restore formulas, hit button below).*

Variable* → *Data used directly in model.*

20 → *Value calculated by model. (Don't enter any data).*

1. HYDROGEOLOGY

Seepage Velocity*	*Vs*	17.9	*(ft/yr)*
or		or	
Hydraulic Conductivity	*K*	6.3E-04	*(cm/sec)*
Hydraulic Gradient	*i*	0.0055	*(ft/ft)*
Porosity	*n*	0.2	*(-)*

2. DISPERSION

Longitudinal Dispersivity*	*alpha x*	11.0	*(ft)*
Transverse Dispersivity*	*alpha y*	5.8	*(ft)*
Vertical Dispersivity*	*alpha z*	0.4	*(ft)*
or		or	
Estimated Plume Length	*Lp*	150	*(ft)*

3. ADSORPTION

Retardation Factor*	*R*	1.8	*(-)*
or		or	
Soil Bulk Density	*rho*	2.1	*(kg/l)*
Partition Coefficient	*Koc*	38	*(L/kg)*
FractionOrganicCarbon	*foc*	2.0E-4	*(-)*

4. BIODEGRADATION

1st Order Decay Coeff*	*lambda*		*(per yr)*
or		or	
Solute Half-Life	*t-half*		*(year)*
or Instantaneous Reaction Model			
Delta Oxygen*	*DO*	3.92	*(mg/L)*
Delta Nitrate*	*NO3*	7.73	*(mg/L)*
Observed Ferrous Iron*	*Fe2+*	0	*(mg/L)*
Delta Sulfate*	*SO4*	0	*(mg/L)*
Observed Methane*	*CH4*	0	*(mg/L)*

5. GENERAL

Modeled Area Length*	400	*(ft)*
Modeled Area Width*	350	*(ft)*
Simulation Time*	7.0	*(yr)*

6. SOURCE DATA

Source Thickness in Sat.Zone* 10 *(ft)*

Source Zones:

Width* (ft)	Conc. (mg/L)*
20	51
15	58
15	68
15	58
20	51

Source Halflife (see Help):

Inst. React.	1st Order	
2	2	*(yr)*

Soluble Mass In Source NAPL, Soil 15.4 *(Kg)*

Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3

View of Plume Looking Down

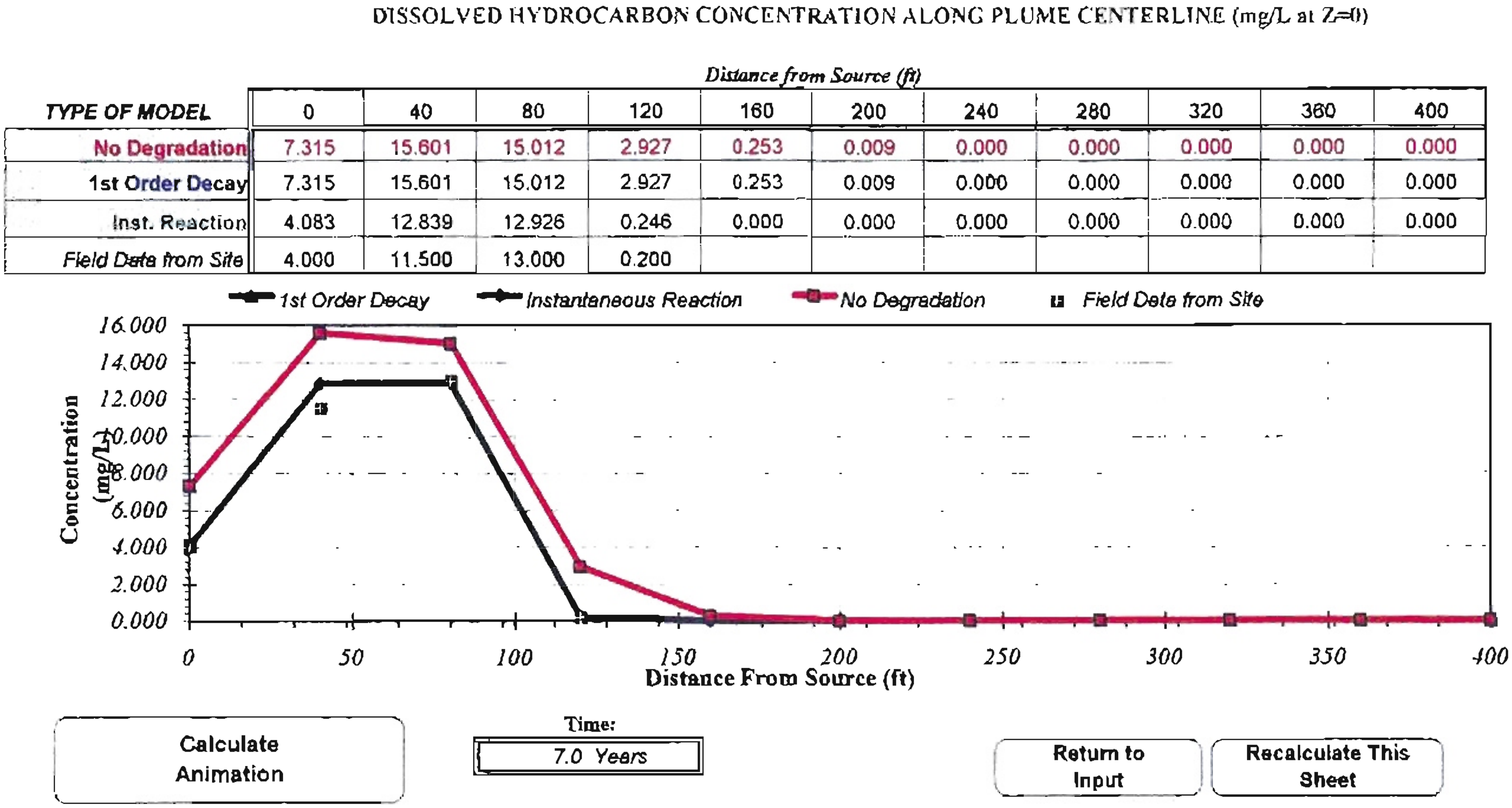
Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"

7. FIELD DATA FOR COMPARISON

Concentration (mg/L)	4.0	11.5	13.0	2							
Dist. from Source (ft)	0	40	80	120	160	200	240	280	320	360	400

8. CHOOSE TYPE OF OUTPUT TO SEE:

BIOSCREEN Simulation #3 Input Data - Calibrated to 7/25/94



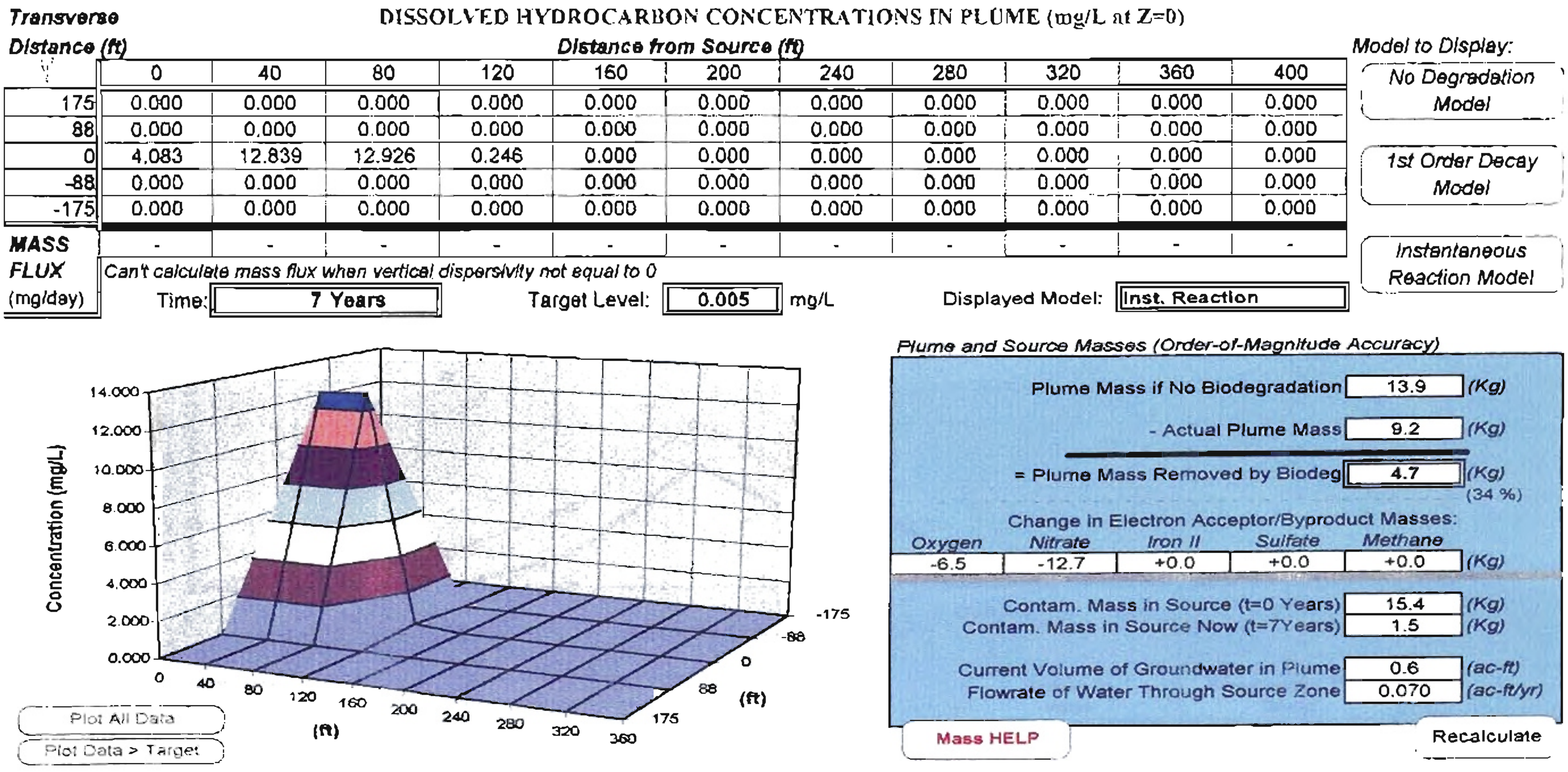
DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

Distance from Source (ft)

TYPE OF MODEL	0	40	80	120	160	200	240	280	320	360	400
No Degradation	7.315	15.601	15.012	2.927	0.253	0.009	0.000	0.000	0.000	0.000	0.000
1st Order Decay	7.315	15.601	15.012	2.927	0.253	0.009	0.000	0.000	0.000	0.000	0.000
Inst. Reaction	4.083	12.839	12.926	0.246	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Field Data from Site	4.000	11.500	13.000	0.200							

Time: 7.0 Years

BIOSCREEN Simulation #3 Plume Centerline - Calibrated to 7/25/94



DISSOLVED HYDROCARBON CONCENTRATIONS IN PLUME (mg/L at Z=0)

Transverse Distance (ft)	*Distance from Source (ft)* 0	40	80	120	160	200	240	280	320	360	400
175	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
88	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0	4.083	12.839	12.926	0.246	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-88	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
-175	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MASS FLUX (mg/day)	-	-	-	-	-	-	-	-	-	-	-

Can't calculate mass flux when vertical dispersivity not equal to 0

Time: 7 Years

Target Level: 0.005 mg/L

Displayed Model: Inst. Reaction

Plume and Source Masses (Order-of-Magnitude Accuracy)

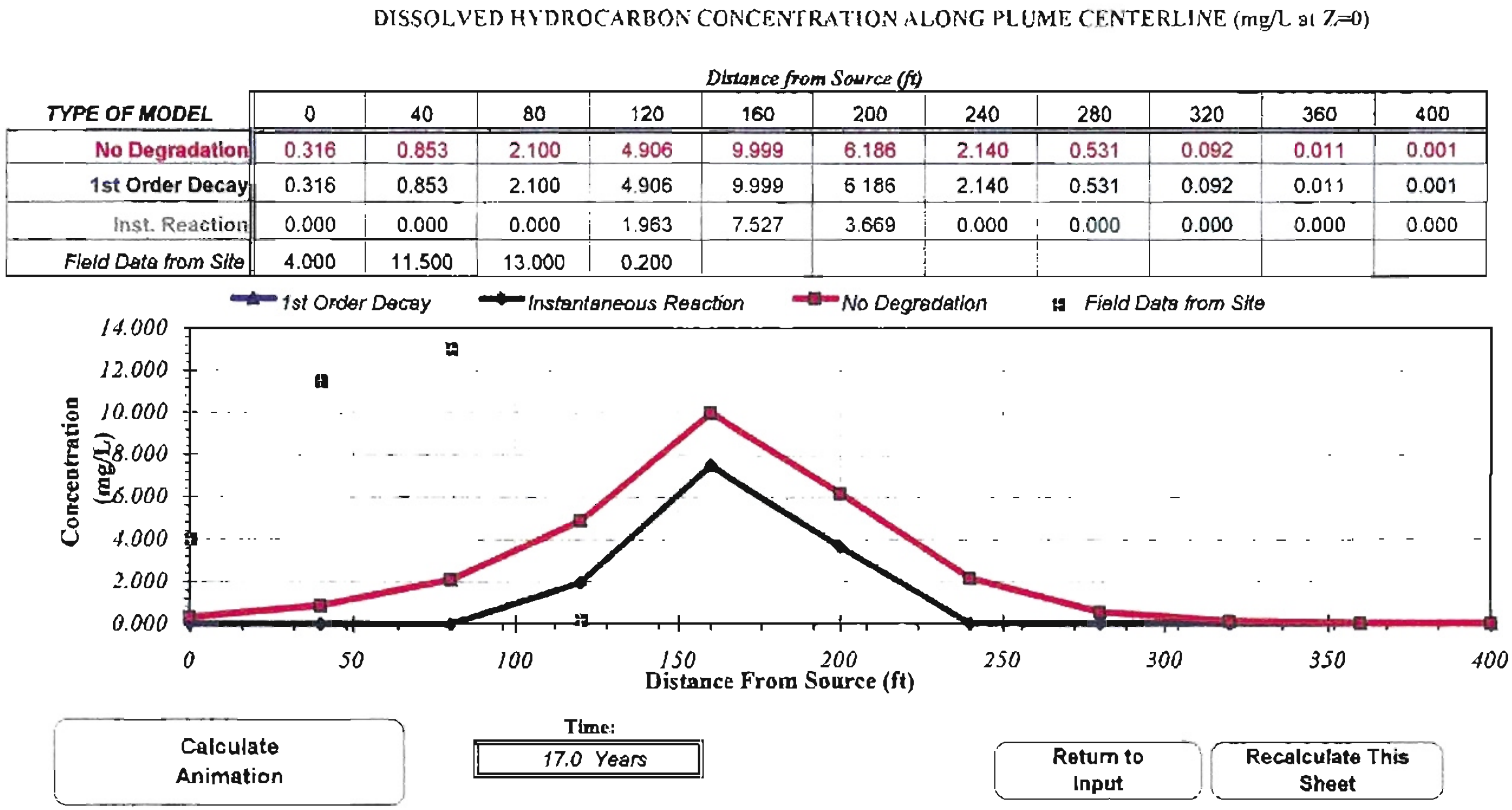
Plume Mass if No Biodegradation	13.9	*(Kg)*
- Actual Plume Mass	9.2	*(Kg)*
= Plume Mass Removed by Biodeg	4.7	*(Kg)* (34 %)

Change in Electron Acceptor/Byproduct Masses:

Oxygen	*Nitrate*	*Iron II*	*Sulfate*	*Methane*	
-6.5	-12.7	+0.0	+0.0	+0.0	*(Kg)*

Contam. Mass in Source (t=0 Years)	15.4	*(Kg)*
Contam. Mass in Source Now (t=7Years)	1.5	*(Kg)*
Current Volume of Groundwater in Plume	0.6	*(ac-ft)*
Flowrate of Water Through Source Zone	0.070	*(ac-ft/yr)*

BIOSCREEN Simulation #3 3D Plume - Calibrated to 7/25/94



DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

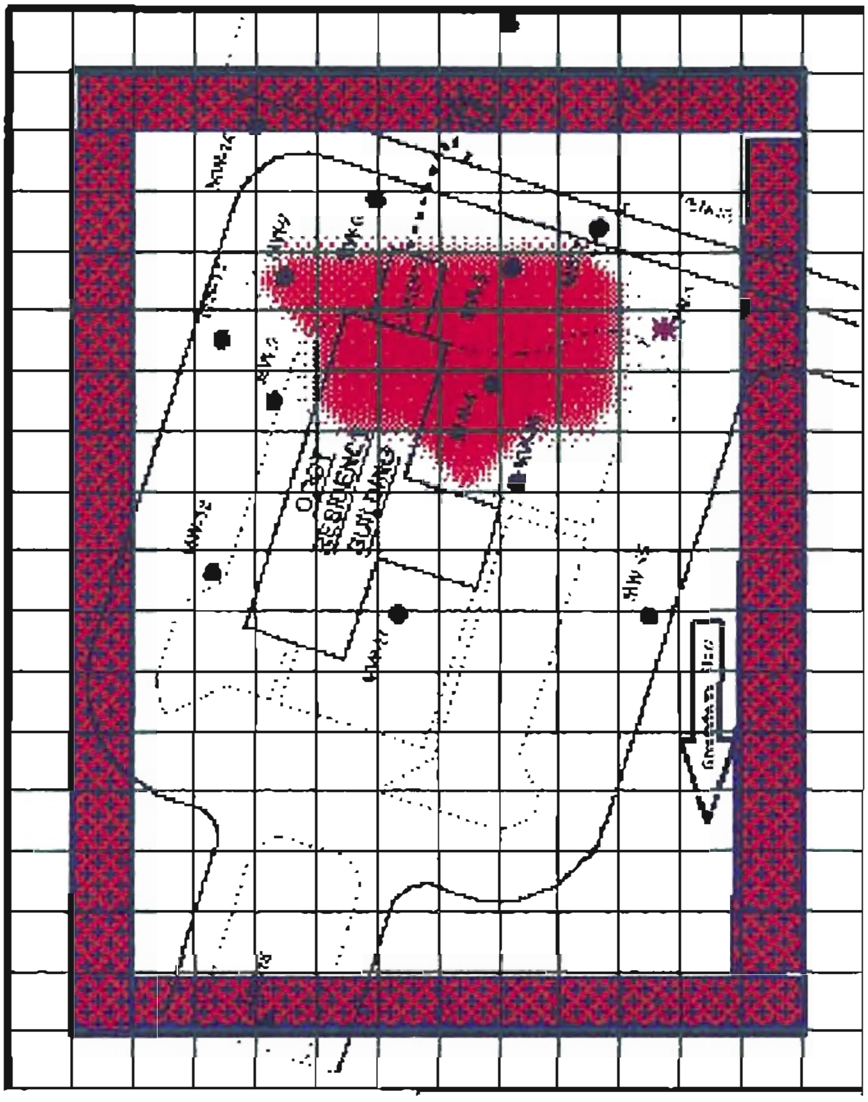
	Distance from Source (ft)										
TYPE OF MODEL	0	40	80	120	160	200	240	280	320	360	400
No Degradation	0.316	0.853	2.100	4.906	9.999	6.186	2.140	0.531	0.092	0.011	0.001
1st Order Decay	0.316	0.853	2.100	4.906	9.999	6.186	2.140	0.531	0.092	0.011	0.001
Inst. Reaction	0.000	0.000	0.000	1.963	7.527	3.669	0.000	0.000	0.000	0.000	0.000
Field Data from Site	4.000	11.500	13.000	0.200							

Time: 17.0 Years

BIOSCREEN Simulation #3 Plume Centerline - 17 Year Simulation

APPENDIX R --

BIOPLUME III Simulation #1 Source Definition and Results

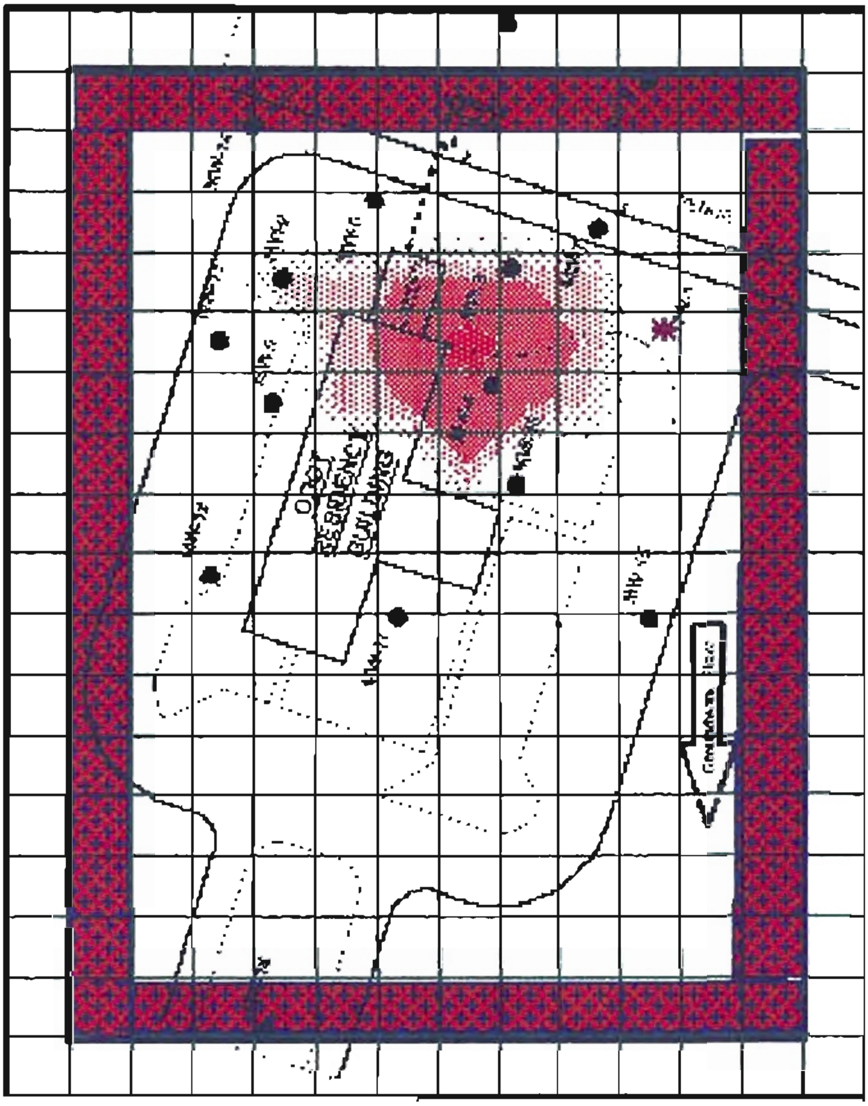


Results of BIOPLUME III Simulation #1 - Source Definition, January 1992

BIOPLUME Simulation #1 - Source Definition, January 1992

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	26.3	25.3	28.7	29.3	28.1	27.5	0	0	0	0
0	0	0	0	0	27.1	29.8	32.9	30.8	27.6	0	0	0	0
0	0	0	0	0	26.3	28.3	31	30.2	24	0	0	0	0
0	0	0	0	0	0	0	29.2	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

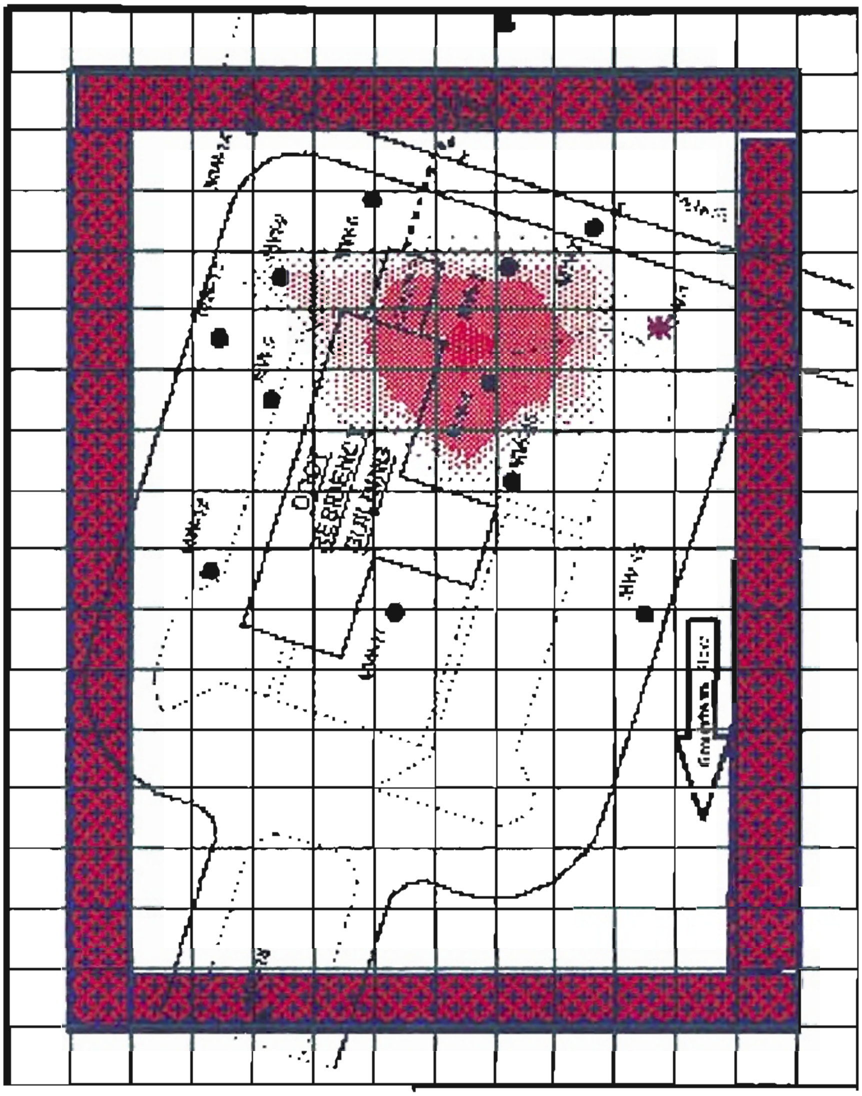


Results of BIOPLUME III Simulation #1 - Hydrocarbon Plume, July 1994

BIOPLUME Simulation #1 - Hydrocarbon Plume, July 1994

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	12.8	11.9	15.3	15.9	14.7	14	0	0	0	0
0	0	0	0	0	13.7	16.3	19.5	17.4	14.2	0	0	0	0
0	0	0	0	0	12.9	14.9	17.5	16.8	10.6	0	0	0	0
0	0	0	0	0	0	0	15.7	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

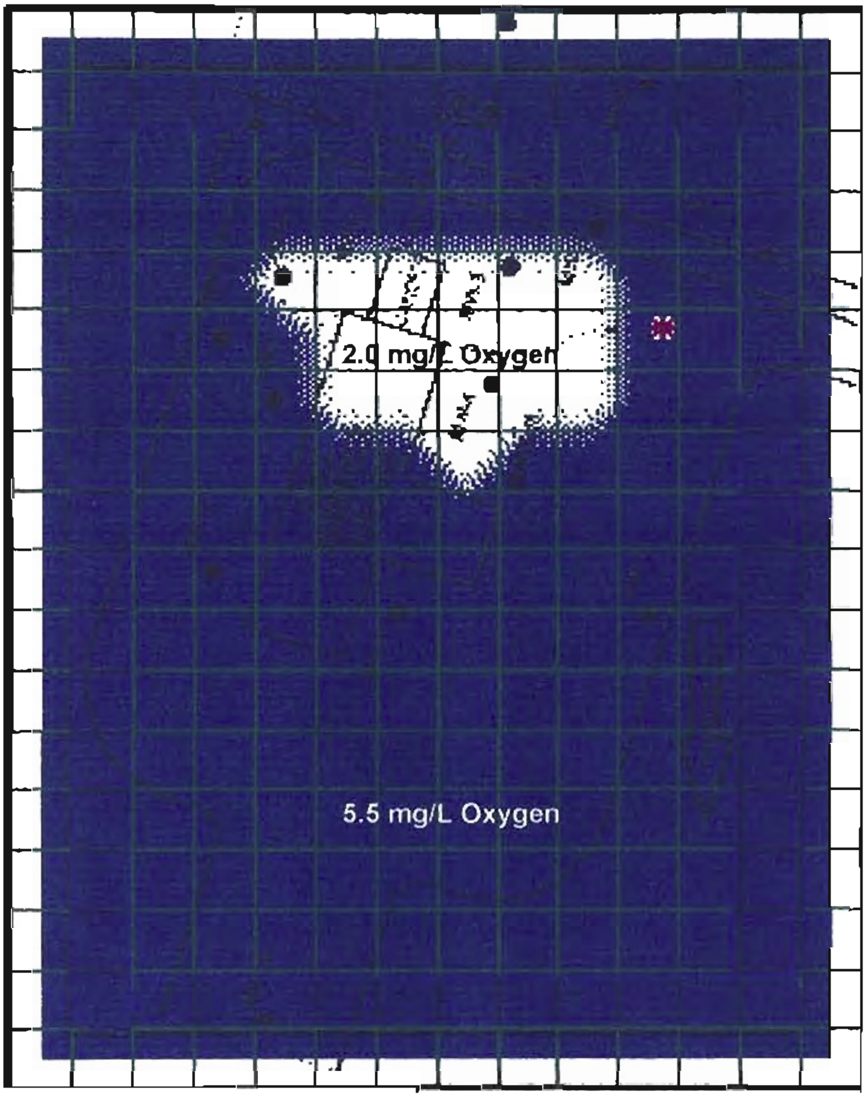


Results of BIOPLUME III Simulation #1- Hydrocarbon Plume, October 1997

BIOPLUME Simulation #1 - Hydrocarbon Plume, October 1997

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	12.8	11.9	15.3	15.9	14.7	14	0	0	0	0
0	0	0	0	0	13.7	16.3	19.5	17.4	14.2	0	0	0	0
0	0	0	0	0	12.9	14.9	17.5	16.8	10.6	0	0	0	0
0	0	0	0	0	0	0	15.7	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

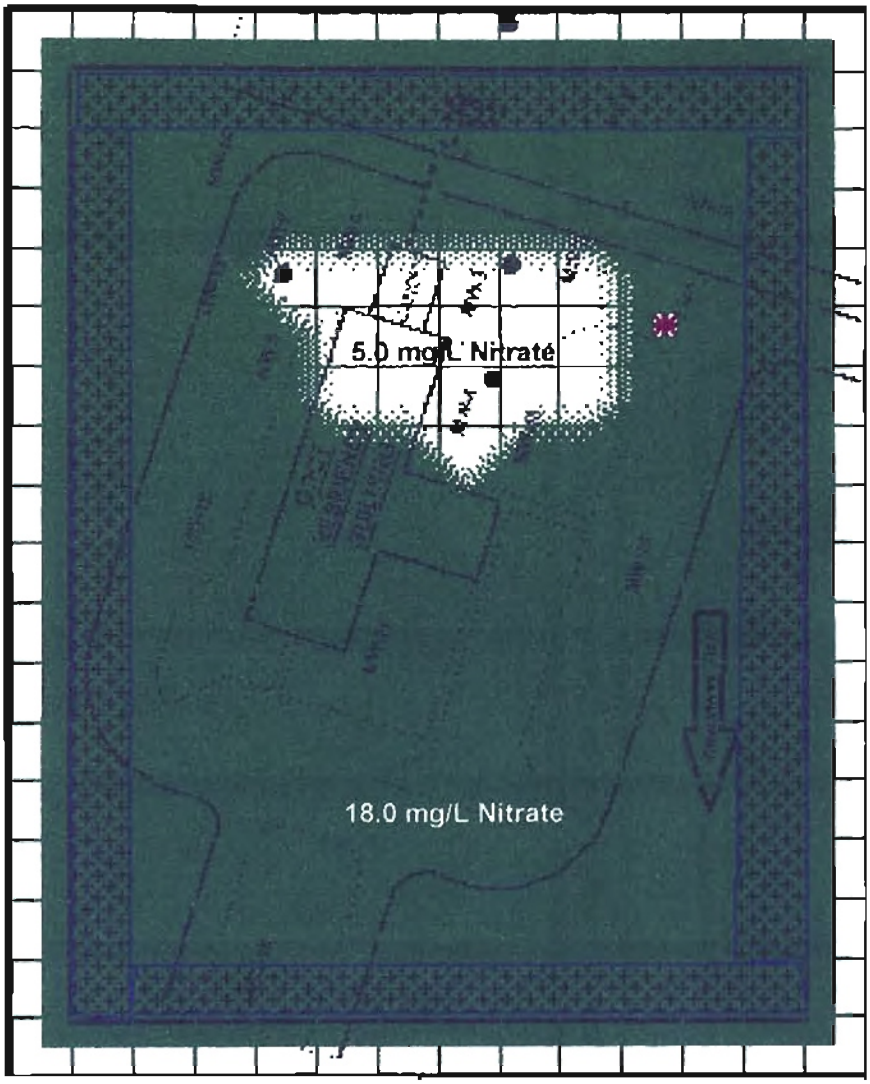


Results of BIOPLUME III Simulation #1- Dissolved Oxygen, October 1997

BIOPLUME Simulation #1 - Dissolved Oxygen, October 1997

Average Grid Cell Concentrations (mg/L)

5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.49	5.48	5.48	5.49	5.48	5.49	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.47	2	2	2	2	2	2	5.48	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.44	2	2	2	2	2	5.49	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.49	2	2	2	2	2	5.49	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.47	5.46	2	5.47	5.48	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.48	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5

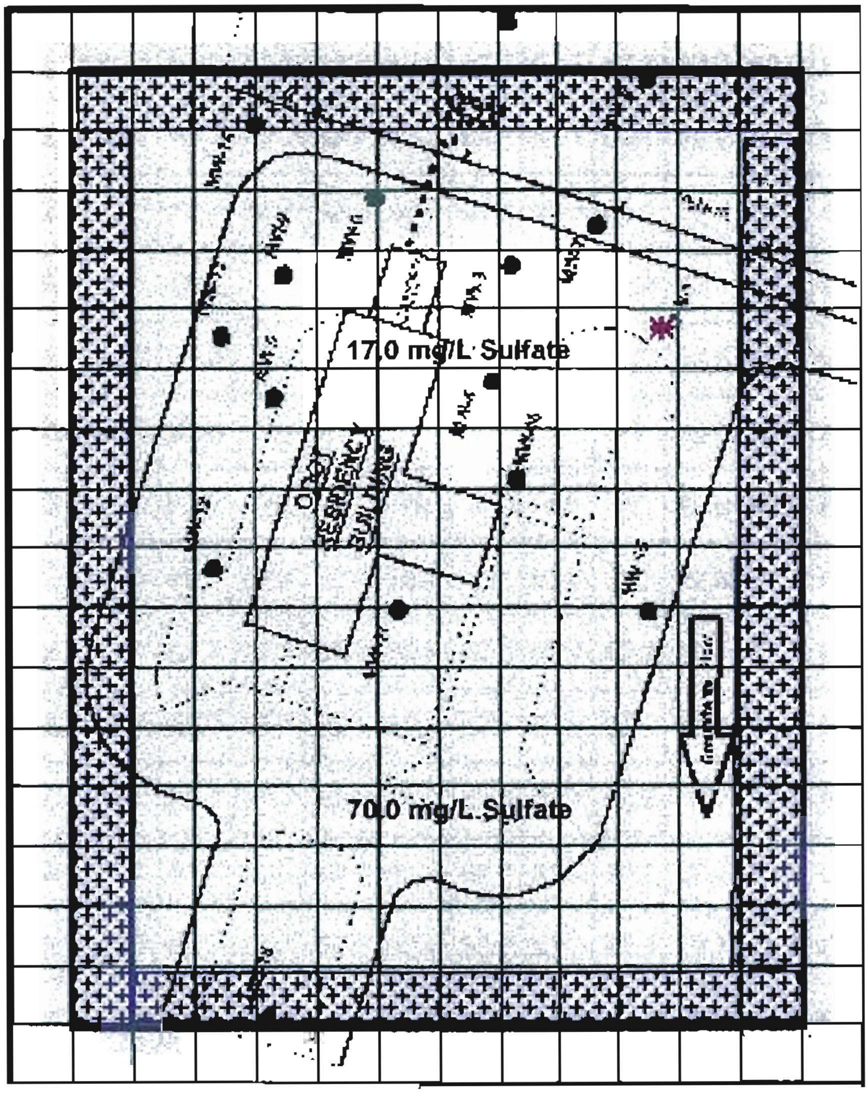


Results of BIOPLUME III Simulation #1- Nitrate, October 1997

BIOPLUME Simulation #1 - Nitrate, October 1997

Average Grid Cell Concentrations (mg/L)

18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	5	5	5	5	5	5	18	18	18	18
18	18	18	18	18	5	5	5	5	5	18	18	18	18
18	18	18	18	18	5	5	5	5	5	18	18	18	18
18	18	18	18	18	18	18	5	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18

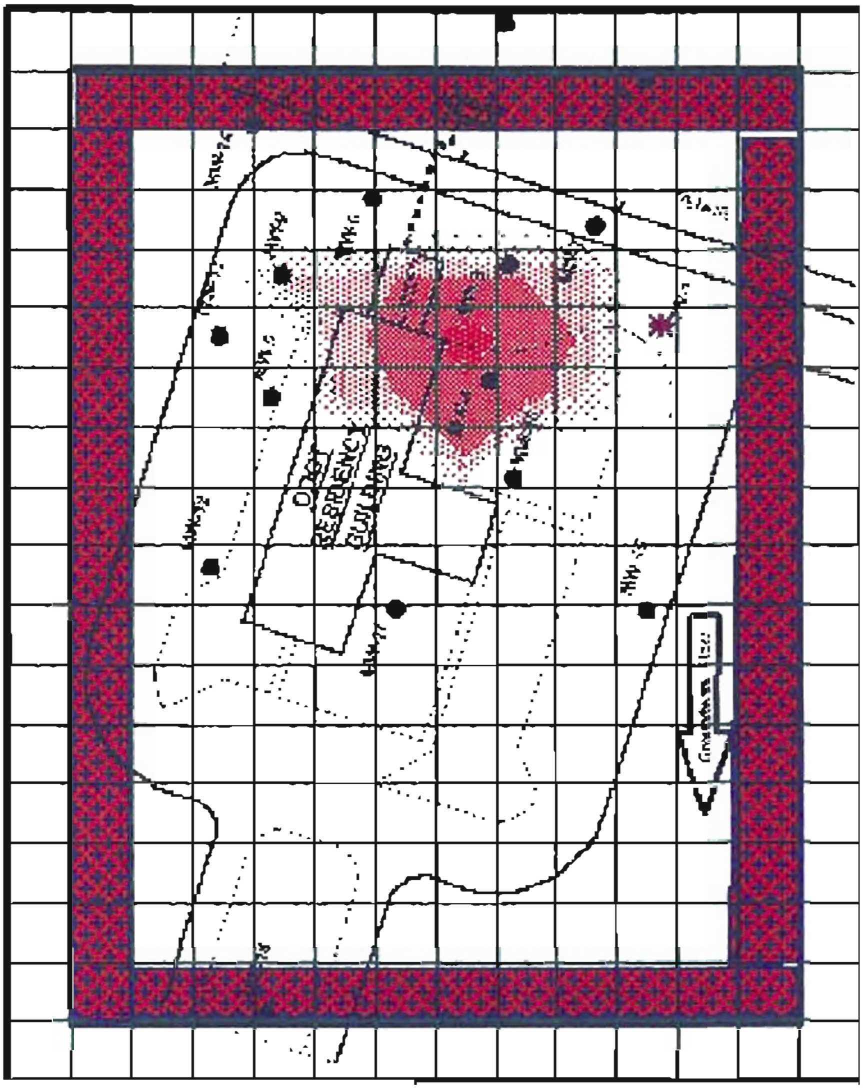


Results of BIOPLUME III Simulation #1- Sulfate, October 1997

BIOPLUME Simulation #1 - Sulfate, October 1997

Average Grid Cell Concentrations (mg/L)

62.7	62.7	62.7	62.7	63.2	62.7	62.7	62.7	62.7	62.7	62.7	62.9	62.7	62.7
62.7	62.7	62.7	62.7	63.2	62.7	62.7	62.7	62.7	62.7	62.7	62.9	62.7	62.7
62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.6	62.6	62.6	62.6	62.6	62.6	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.6	17	17	17	17	17	17	62.6	62.7	62.7	62.7
62.7	62.7	62.7	62.6	62.6	17	17	17	17	17	62.6	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.6	17	17	17	17	17	62.6	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.6	62.6	62.6	17	62.6	62.6	62.6	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.7	62.7	62.6	62.6	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.8	62.8	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.8	62.8	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.8	62.8	62.8	62.8	62.8	62.7	62.7	62.7	62.7	62.7	62.7
62.7	62.7	62.7	62.8	62.8	62.8	62.8	62.8	62.7	62.7	62.7	62.7	62.7	62.7



Results of BIOPLUME III Simulation #1- Hydrocarbon Plume, January 2072 (80 years)

BIOPLUME Simulation #1 - Hydrocarbon Plume, January 2072

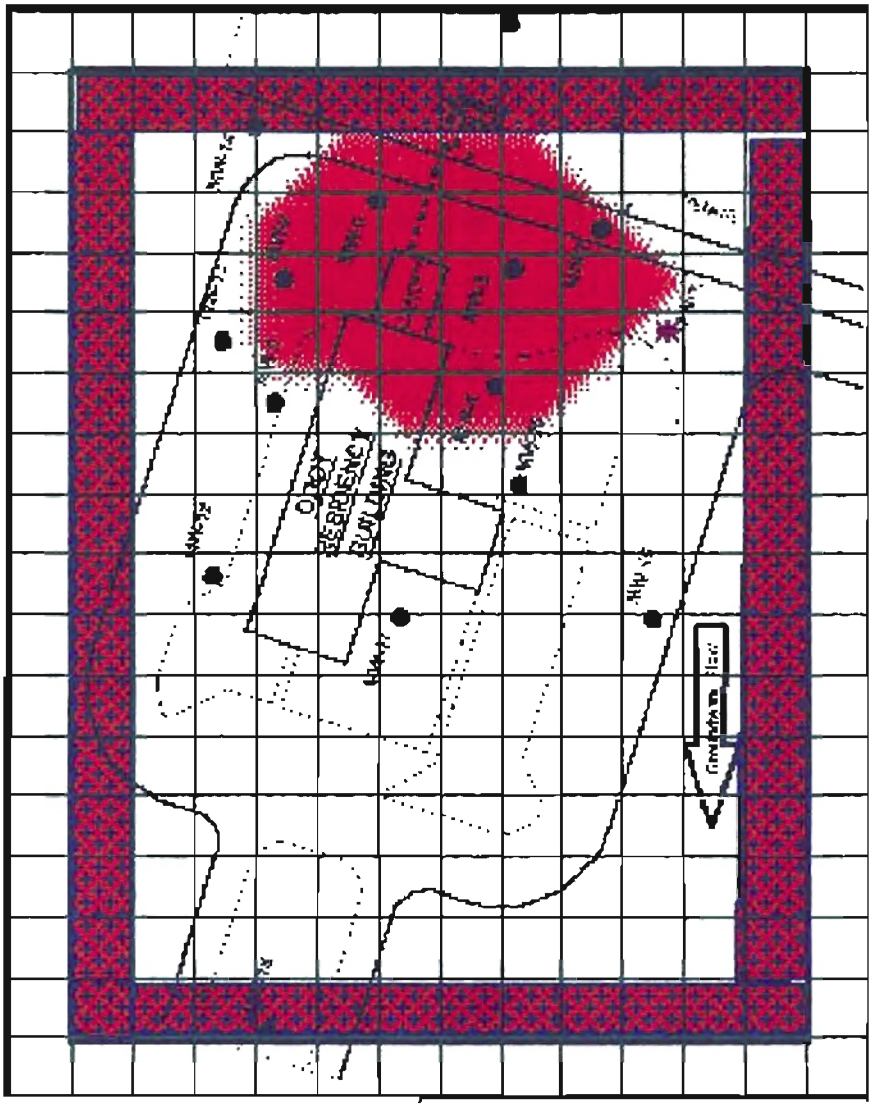
(80 years)

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	12.6	11.8	15.2	15.8	14.6	13.9	0	0	0	0
0	0	0	0	0	13.6	16.3	19.5	17.4	14.1	0	0	0	0
0	0	0	0	0	12.8	14.8	17.5	16.7	10.5	0	0	0	0
0	0	0	0	0	0	0	15.5	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

APPENDIX S –

BIOPLUME III Simulation #2 Source Definition and Results

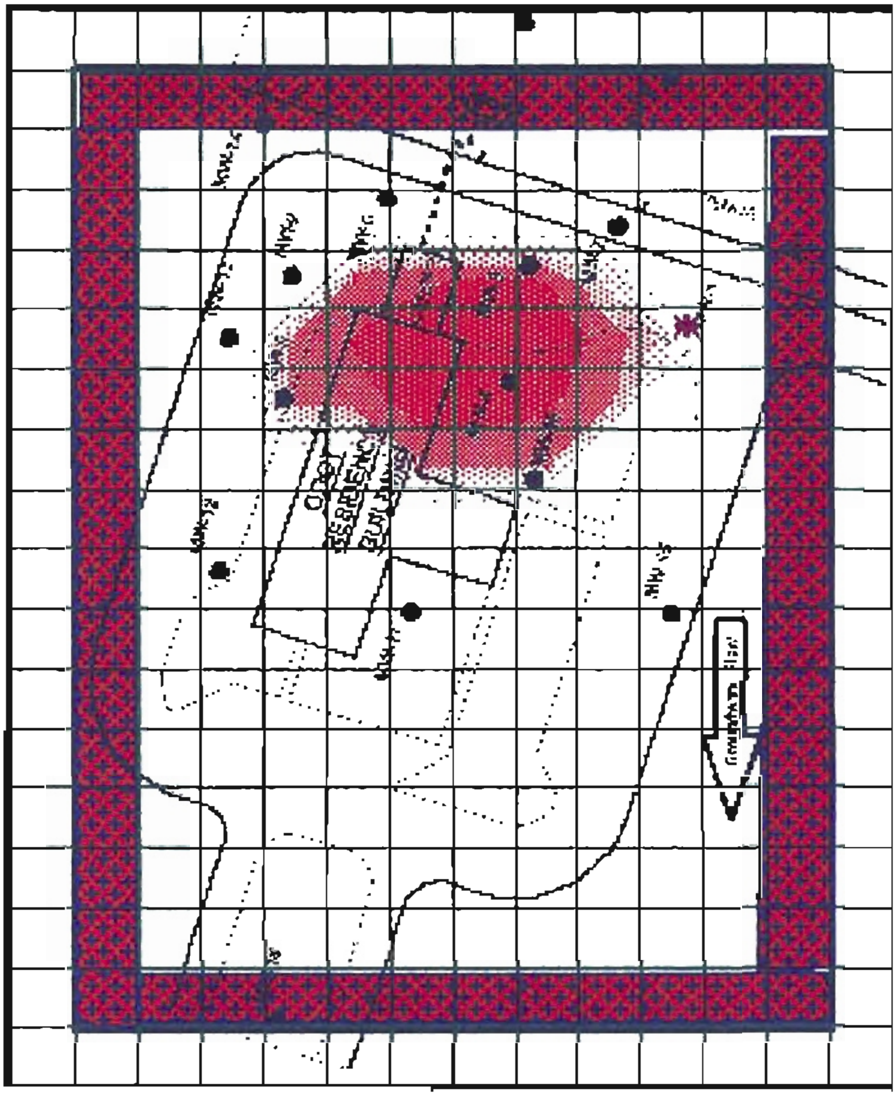


Results of BIOPLUME III Simulation #2 - Source Definition, January 1992

BIOPLUME Simulation #2 - Source Definition, January 1992

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	33.5	34.4	34.8	34.2	0	0	0	0	0
0	0	0	0	31.8	34.4	35.6	36.3	35.7	33.5	0	0	0	0
0	0	0	0	31.7	34.3	35.6	36.1	35.1	33.7	32.4	0	0	0
0	0	0	0	32.8	33.7	34.1	34.1	33.8	32.9	0	0	0	0
0	0	0	0	0	0	33.7	33.7	33.6	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0



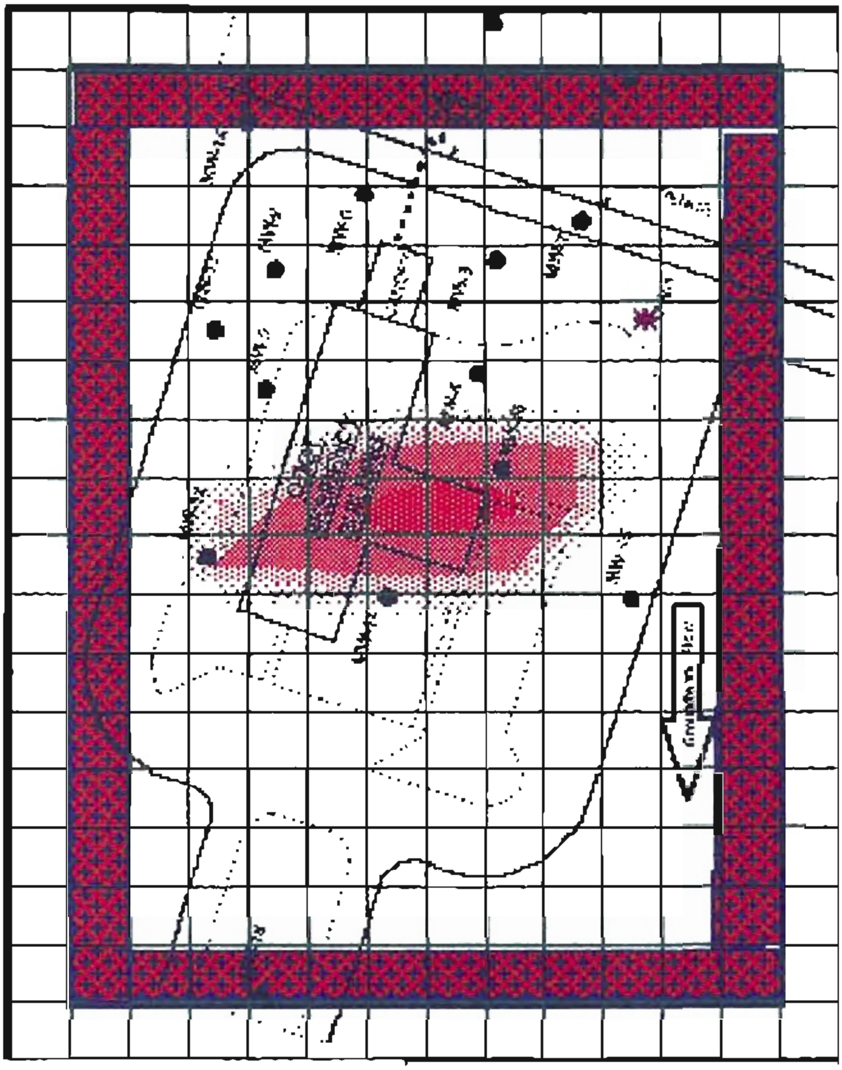
Results of BIOPLUME III Simulation #2 - Hydrocarbon Plume, July 1994 (Longitudinal Dispersivity = 1.0 ft)

BIOPLUME Simulation #2 - Hydrocarbon Plume, July 1994

(Longitudinal Dispersivity = 1.0 ft)

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	17.6	19.6	20.7	20	10.7	0	0	0	0
0	0	0	0	17.7	20.4	21.9	22.6	21.8	19.3	9.68	0	0	0
0	0	0	0	18	19.4	21	21.3	20.7	18.4	0	0	0	0
0	0	0	0	0	1.53	19.1	19.4	19	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

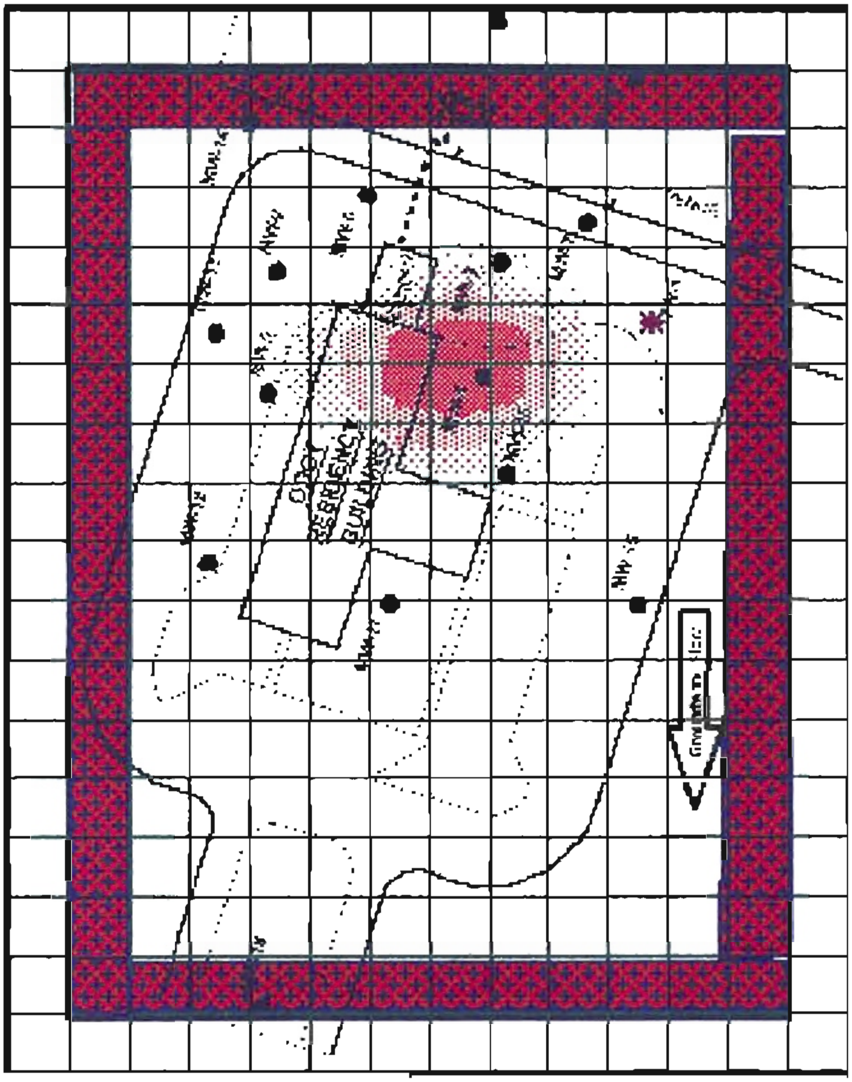


Results of BIOPLUME III Simulation #2 - Hydrocarbon Plume, February 1998 (Longitudinal Dispersivity = 1.0 ft)

BIOPLUME Simulation #2 - Hydrocarbon Plume, February 1998
(Longitudinal Dispersivity = 1.0 ft)

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	14.2	16.2	18.3	17.7	16.4	7.45	0	0	0
0	0	0	12.9	16.5	20	21.5	21.7	20.8	17.7	4.73	0	0	0
0	0	0	16.3	17.5	18.5	18.9	18.6	17.8	1.73	0	0	0	0
0	0	0	0	0	3.3	3.18	6.28	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0



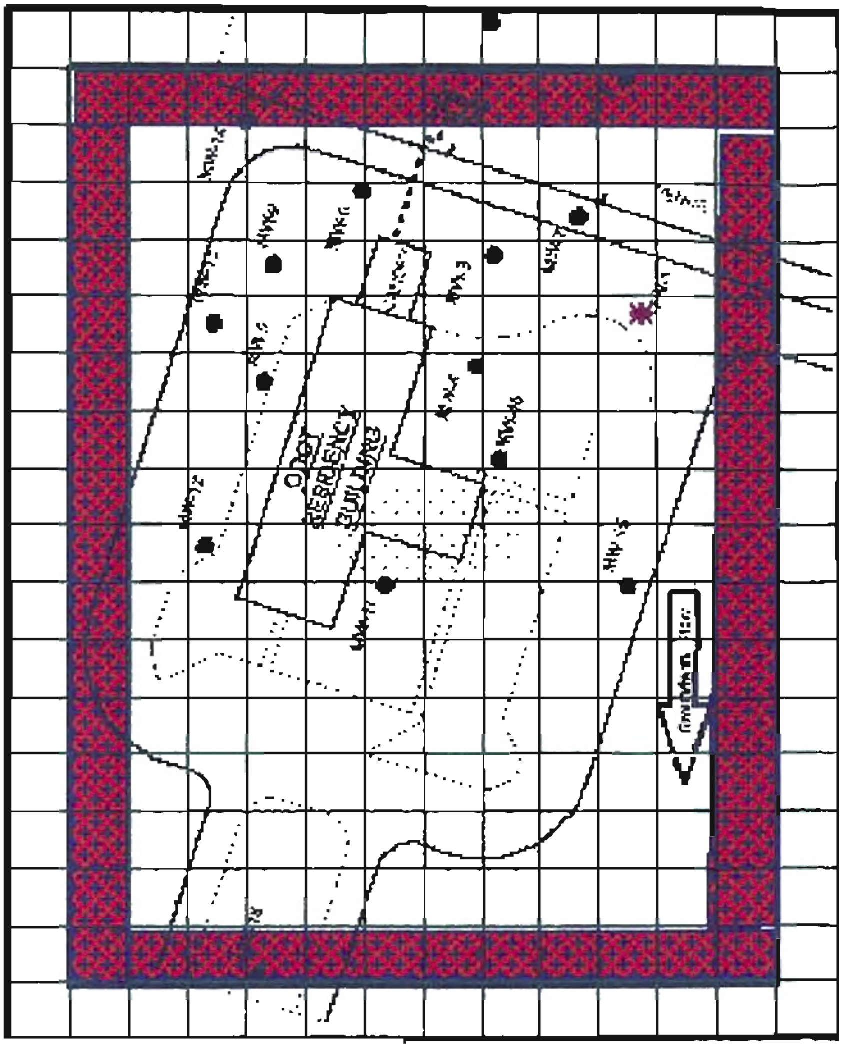
Results of BIOPLUME III Simulation #2 -
Hydrocarbon Plume, July 1994
(Longitudinal Dispersivity = 12.1 ft)

BIOPLUME Simulation #2 - Hydrocarbon Plume, July 1994

(Longitudinal Dispersivity = 12.1 ft)

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	6.36	9.98	7.53	1.45	0	0	0	0
0	0	0	0	4.86	12.3	17.1	18.5	17.3	10.5	0.16	0	0	0
0	0	0	0	7.45	11.6	17.4	18.6	17.3	9.13	0	0	0	0
0	0	0	0	0	4.01	10.8	12.1	10.2	0.98	0	0	0	0
0	0	0	0	0	0	0.07	1.41	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0



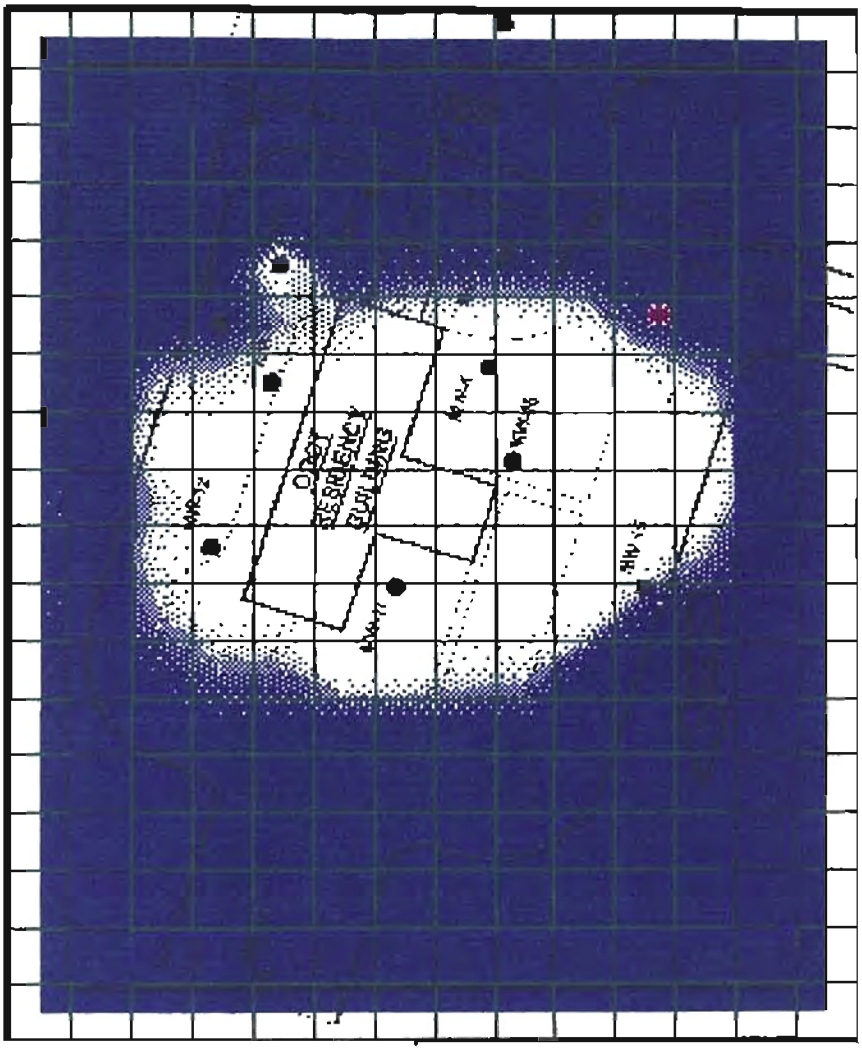
Results of BIOPLUME III Simulation #2 -
Hydrocarbon Plume, February 1998
(Longitudinal Dispersivity = 12.1 ft)

BIOPLUME Simulation #2 - Hydrocarbon Plume, February 1998

(Longitudinal Dispersivity = 12.1 ft)

Average Grid Cell Concentrations (mg/L)

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1.74	4.53	5.82	4.82	0.46	0	0	0	0
0	0	0	0	0.91	4.35	6.3	6.4	4.44	0	0	0	0	0
0	0	0	0	0	0.48	1.06	2.31	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

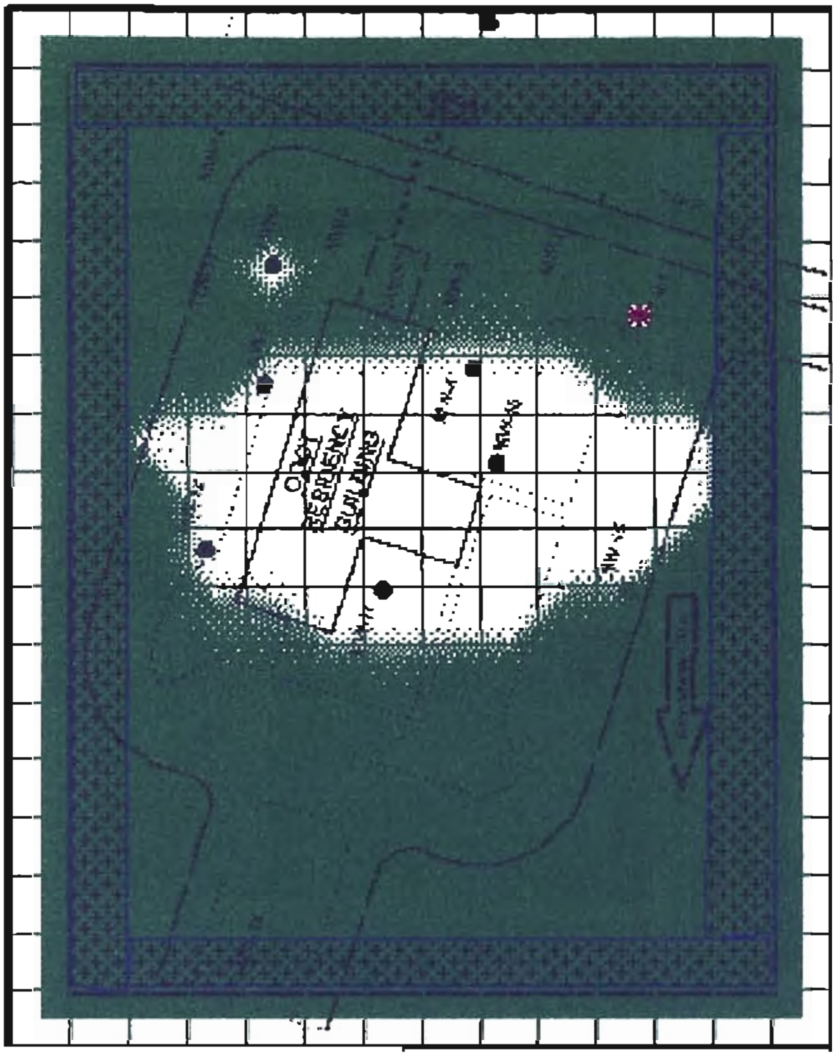


Results of BIOPLUME III Simulation #2 -
Dissolved Oxygen, February 1998
(Longitudinal Dispersivity = 1.0 ft)

BIOPLUME Simulation #2 - Dissolved Oxygen, February 1998
(Longitudinal Dispersivity = 1.0 ft)

Average Grid Cell Concentrations (mg/L)

5.5	5.5	5.5	5.5	5.5	5.5	5.48	5.48	5.49	5.48	5.45	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.48	5.48	5.49	5.48	5.45	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.46	5.45	5.47	5.49	5.45	5.5	5.5	5.5
5.5	5.5	5.5	5.49	5.48	5.48	5.38	5.36	5.41	5.43	5.42	5.5	5.5	5.5
5.5	5.5	5.5	5.45	2.4	5.3	5.01	4.93	4.97	5.12	5.28	5.54	5.5	5.5
5.49	5.49	5.44	5.24	3.72	3.32	2	2	2	2.48	4.65	5.34	5.49	5.49
5.44	5.44	3.44	3.06	2	2	2	2	2	2	2	3.34	5.4	5.4
5.4	5.4	2	2	2	2	2	2	2	2	2	2	5.19	5.19
5.1	5.1	3.37	2	2	2	2	2	2	2	2	2	5.24	5.24
5.24	5.24	2.82	2	2	2	2	2	2	2	2	3.82	5.32	5.32
5.09	5.09	3.5	2	2	2	2	2	2	2	4.92	5.38	5.45	5.45
5.41	5.41	4.93	3.85	3.92	2.03	2	2.76	2.95	5.35	5.47	5.49	5.52	5.52
5.45	5.45	5.41	5.36	5.26	5.22	5.22	5.3	5.41	5.49	5.5	5.5	5.46	5.46
5.49	5.49	5.49	5.49	5.48	5.46	5.47	5.48	5.49	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5
5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5	5.5

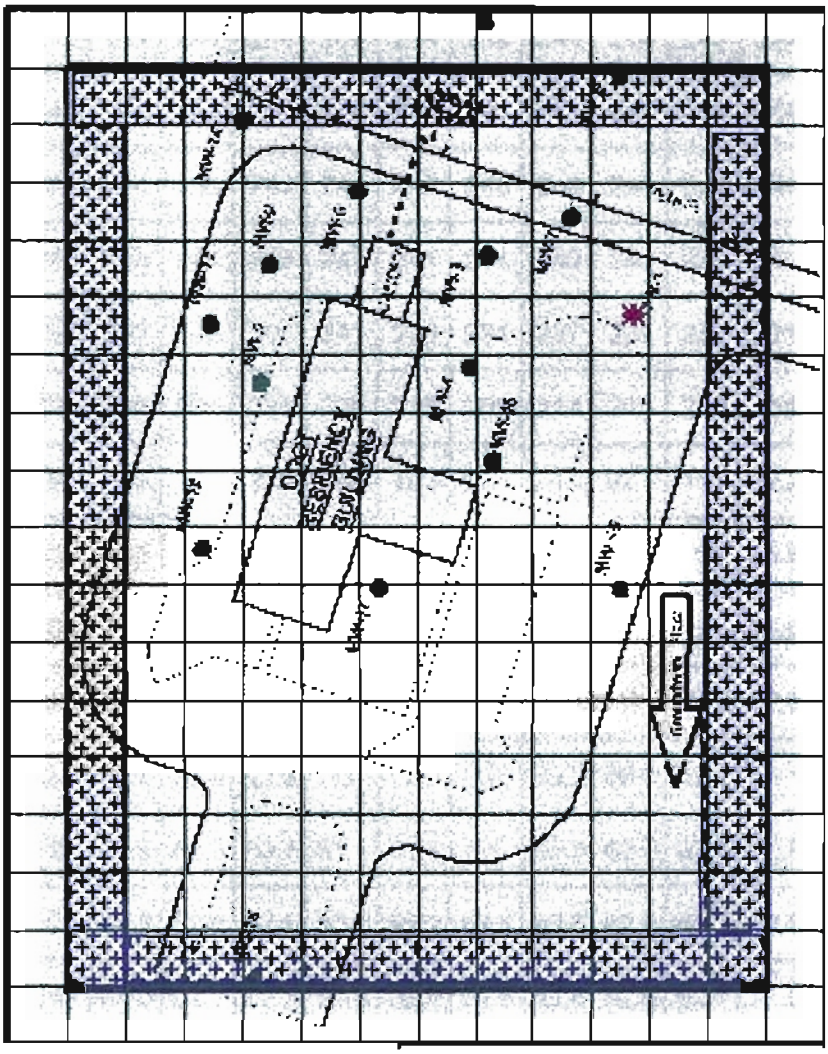


Results of BIOPLUME III Simulation #2 -
Nitrate, February 1998
(Longitudinal Dispersivity = 1.0 ft)

BIOPLUME Simulation #2 - Nitrate, February 1998
(Longitudinal Dispersivity = 1.0 ft)

Average Grid Cell Concentrations (mg/L)

18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	17.9	18	18	18	18	18	18	18	18	18
18	18	18	17.8	7.53	17.9	17.9	17.9	17.9	17.9	18	18	18	18
18	18	18	17.7	17.3	17.5	15.9	14.8	14.7	17.5	17.7	18	18	18
18	18	17.6	17.3	5	5	5	5	5	5	15.8	17.5	18	18
18	18	7.4	5	5	5	5	5	5	5	5	5	17.9	17.9
17.9	17.9	18.3	5	5	5	5	5	5	5	5	5	17.9	17.9
17.9	17.9	18.1	5	5	5	5	5	5	5	5	17.6	17.9	17.9
17.9	17.9	18	14.3	12.7	5	5	5	5	16.3	17.7	17.9	17.9	17.9
18	18	17.6	17.5	17.5	17.6	15.9	17.5	17.7	17.9	18	18	18	18
18	18	18	18	17.9	17.8	17.9	17.9	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18
18	18	18	18	18	18	18	18	18	18	18	18	18	18



**Results of BIOPLUME III Simulation #2 -
Sulfate, February 1998
(Longitudinal Dispersivity = 1.0 ft)**

BIOPLUME Simulation #2 - Sulfate, February 1998

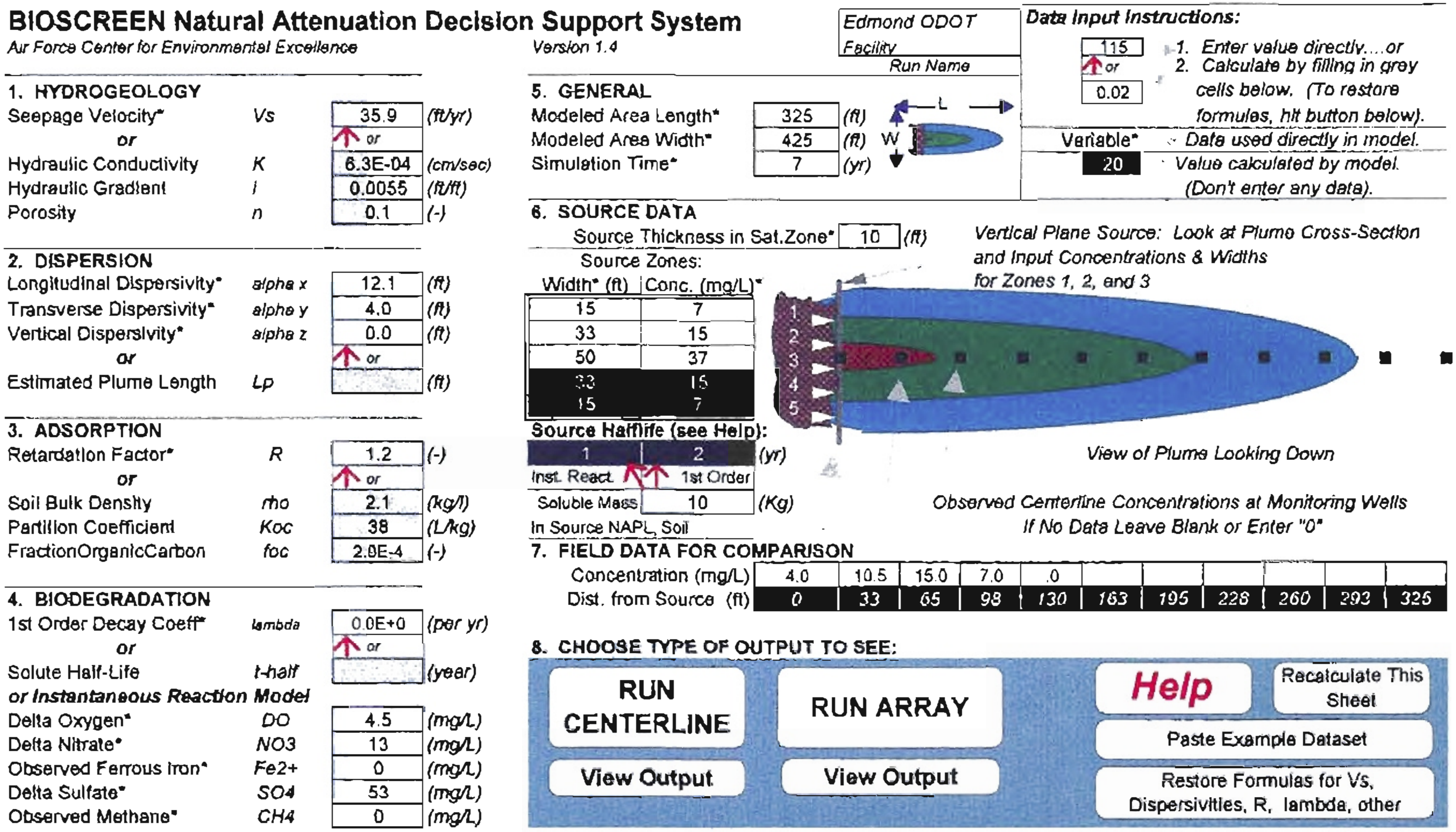
(Longitudinal Dispersivity = 1.0 ft)

Average Grid Cell Concentrations (mg/L)

243	243	244	244	244	244	244	243	244	244	243	244	244	244
243	243	244	244	244	244	244	243	244	244	243	244	244	244
242	242	244	244	244	244	243	243	244	244	242	244	223	223
242	242	244	244	243	243	241	241	242	243	239	242	238	238
231	231	243	242	106	241	236	234	237	237	232	221	239	239
204	204	236	239	233	228	213	209	214	213	209	182	232	232
191	191	219	225	216	144	102	81.1	74.2	92.1	111	82.2	216	216
157	157	121	33.3	63	17	17	17	17	17	17	54.6	197	197
104	104	71.2	17	17	17	17	17	17	17	17	28.8	169	169
79.5	79.5	63.4	17	17	17	17	17	17	17	58.3	62.6	141	141
73.6	73.6	61.7	62.4	61.9	17	17	17	39.2	60.3	62.1	63.1	109	109
128	128	62.9	61.3	60.7	61.1	61.1	61	61.5	62.5	62.6	62.8	84.9	84.9
120	120	63.9	62.6	62.5	62.2	62.3	62.5	62.6	62.6	62.7	62.9	69.7	69.7
149	149	64.5	62.7	62.6	62.6	62.6	62.6	62.6	62.6	62.7	77.5	113	113
167	167	64.1	62.7	62.7	62.6	62.6	62.7	62.6	62.8	65.2	121	141	141
199	199	66.1	62.9	62.7	62.7	62.7	62.9	63.5	64.8	101	165	192	192
239	239	151	64.5	62.8	63.6	66.1	75.6	109	133	181	213	226	226
239	239	151	64.5	62.8	63.6	66.1	75.6	109	133	181	213	226	226

APPENDIX T –

BIOSCREEN Simulation #4 Input Data and Output



BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence

Version 1.4

Edmond ODOT Facility	
Run Name	

Data Input Instructions:

115 — 1. *Enter value directly....or*

or — 2. *Calculate by filling in grey cells below. (To restore formulas, hit button below).*

0.02

Variable* — *Data used directly in model.*

20 — *Value calculated by model. (Don't enter any data).*

1. HYDROGEOLOGY

Seepage Velocity*	*Vs*	35.9	*(ft/yr)*
or		or	
Hydraulic Conductivity	*K*	6.3E-04	*(cm/sec)*
Hydraulic Gradient	*i*	0.0055	*(ft/ft)*
Porosity	*n*	0.1	*(-)*

2. DISPERSION

Longitudinal Dispersivity*	*alpha x*	12.1	*(ft)*
Transverse Dispersivity*	*alpha y*	4.0	*(ft)*
Vertical Dispersivity*	*alpha z*	0.0	*(ft)*
or		or	
Estimated Plume Length	*Lp*		*(ft)*

3. ADSORPTION

Retardation Factor*	*R*	1.2	*(-)*
or		or	
Soil Bulk Density	*rho*	2.1	*(kg/l)*
Partition Coefficient	*Koc*	38	*(L/kg)*
FractionOrganicCarbon	*foc*	2.0E-4	*(-)*

4. BIODEGRADATION

1st Order Decay Coeff*	*lambda*	0.0E+0	*(per yr)*
or		or	
Solute Half-Life	*t-half*		*(year)*
or Instantaneous Reaction Model			
Delta Oxygen*	*DO*	4.5	*(mg/L)*
Delta Nitrate*	*NO3*	13	*(mg/L)*
Observed Ferrous Iron*	*Fe2+*	0	*(mg/L)*
Delta Sulfate*	*SO4*	53	*(mg/L)*
Observed Methane*	*CH4*	0	*(mg/L)*

5. GENERAL

Modeled Area Length*	325	*(ft)*
Modeled Area Width*	425	*(ft)*
Simulation Time*	7	*(yr)*

6. SOURCE DATA

Source Thickness in Sat.Zone* 10 *(ft)*

Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3

Source Zones:

Width* (ft)	Conc. (mg/L)*
15	7
33	15
50	37
33	15
15	7

Source Halflife (see Help):

1	2	*(yr)*
Inst. React.	1st Order	
Soluble Mass	10	*(Kg)*

In Source NAPL, Soil

View of Plume Looking Down

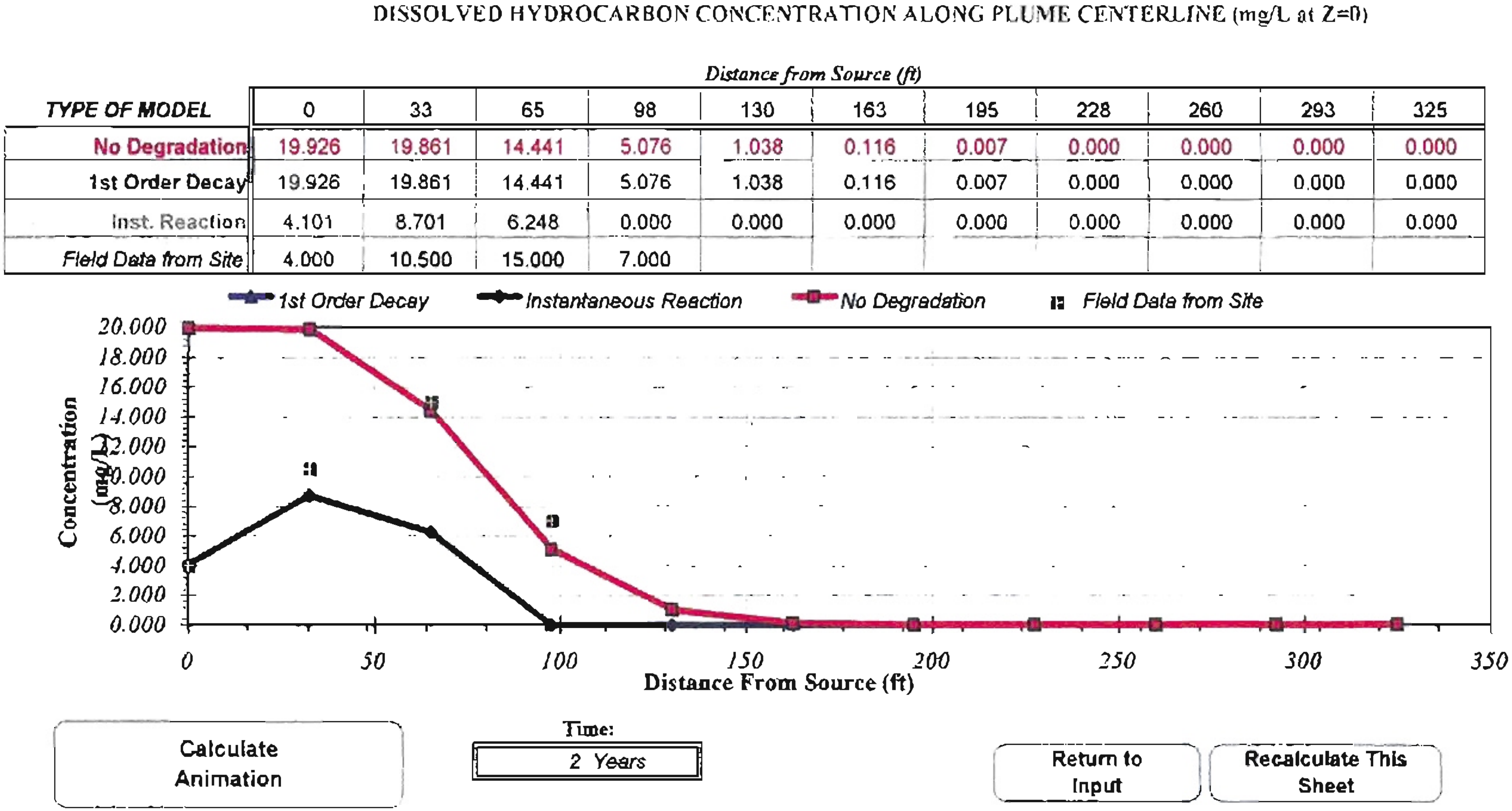
Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"

7. FIELD DATA FOR COMPARISON

Concentration (mg/L)	4.0	10.5	15.0	7.0	.0						
Dist. from Source (ft)	*0*	*33*	*65*	*98*	*130*	*163*	*195*	*228*	*260*	*293*	*325*

8. CHOOSE TYPE OF OUTPUT TO SEE:

BIOSCREEN Simulation #4 Input Data - 7/25/94

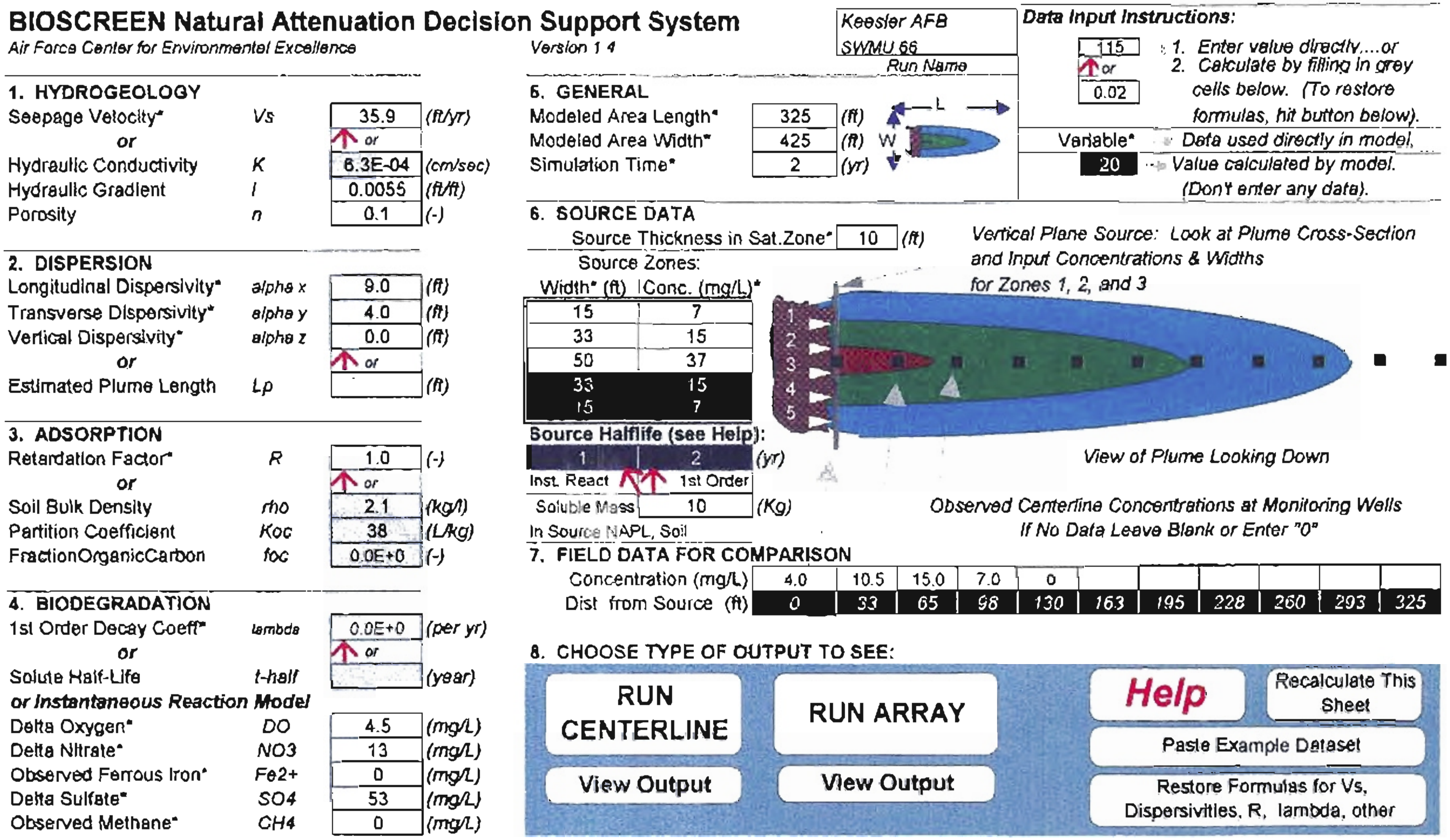


DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

	Distance from Source (ft)										
TYPE OF MODEL	0	33	65	98	130	163	195	228	260	293	325
No Degradation	19.926	19.861	14.441	5.076	1.038	0.116	0.007	0.000	0.000	0.000	0.000
1st Order Decay	19.926	19.861	14.441	5.076	1.038	0.116	0.007	0.000	0.000	0.000	0.000
Inst. Reaction	4.101	8.701	6.248	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Field Data from Site	4.000	10.500	15.000	7.000							

Time: 2 Years

BIOSCREEN #4 Plume Centerline - 7 Year Simulation



BIOSCREEN Natural Attenuation Decision Support System
Air Force Center for Environmental Excellence
Version 1.4

Keesler AFB
SWMU 66
Run Name

Data Input Instructions:

115 ↑ or 0.02
1. Enter value directly....or
2. Calculate by filling in grey cells below. (To restore formulas, hit button below).

Variable* → Data used directly in model.
20 → Value calculated by model. (Don't enter any data).

1. HYDROGEOLOGY

Seepage Velocity*	Vs	35.9	(ft/yr)
or		↑ or	
Hydraulic Conductivity	K	6.3E-04	(cm/sec)
Hydraulic Gradient	i	0.0055	(ft/ft)
Porosity	n	0.1	(-)

2. DISPERSION

Longitudinal Dispersivity*	alpha x	9.0	(ft)
Transverse Dispersivity*	alpha y	4.0	(ft)
Vertical Dispersivity*	alpha z	0.0	(ft)
or		↑ or	
Estimated Plume Length	Lp		(ft)

3. ADSORPTION

Retardation Factor*	R	1.0	(-)
or		↑ or	
Soil Bulk Density	rho	2.1	(kg/l)
Partition Coefficient	Koc	38	(L/kg)
FractionOrganicCarbon	foc	0.0E+0	(-)

4. BIODEGRADATION

1st Order Decay Coeff*	lambda	0.0E+0	(per yr)
or		↑ or	
Solute Half-Life	t-half		(year)
or Instantaneous Reaction Model			
Delta Oxygen*	DO	4.5	(mg/L)
Delta Nitrate*	NO3	13	(mg/L)
Observed Ferrous Iron*	Fe2+	0	(mg/L)
Delta Sulfate*	SO4	53	(mg/L)
Observed Methane*	CH4	0	(mg/L)

5. GENERAL

Modeled Area Length*	325	(ft)
Modeled Area Width*	425	(ft)
Simulation Time*	2	(yr)

6. SOURCE DATA

Source Thickness in Sat.Zone* 10 (ft)

Source Zones:

Width* (ft)	Conc. (mg/L)*
15	7
33	15
50	37
33	15
15	7

Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3

View of Plume Looking Down

Source Halflife (see Help): 1 | 2 (yr)
Inst. React ↑ ↑ 1st Order

Soluble Mass 10 (Kg)
In Source NAPL, Soil

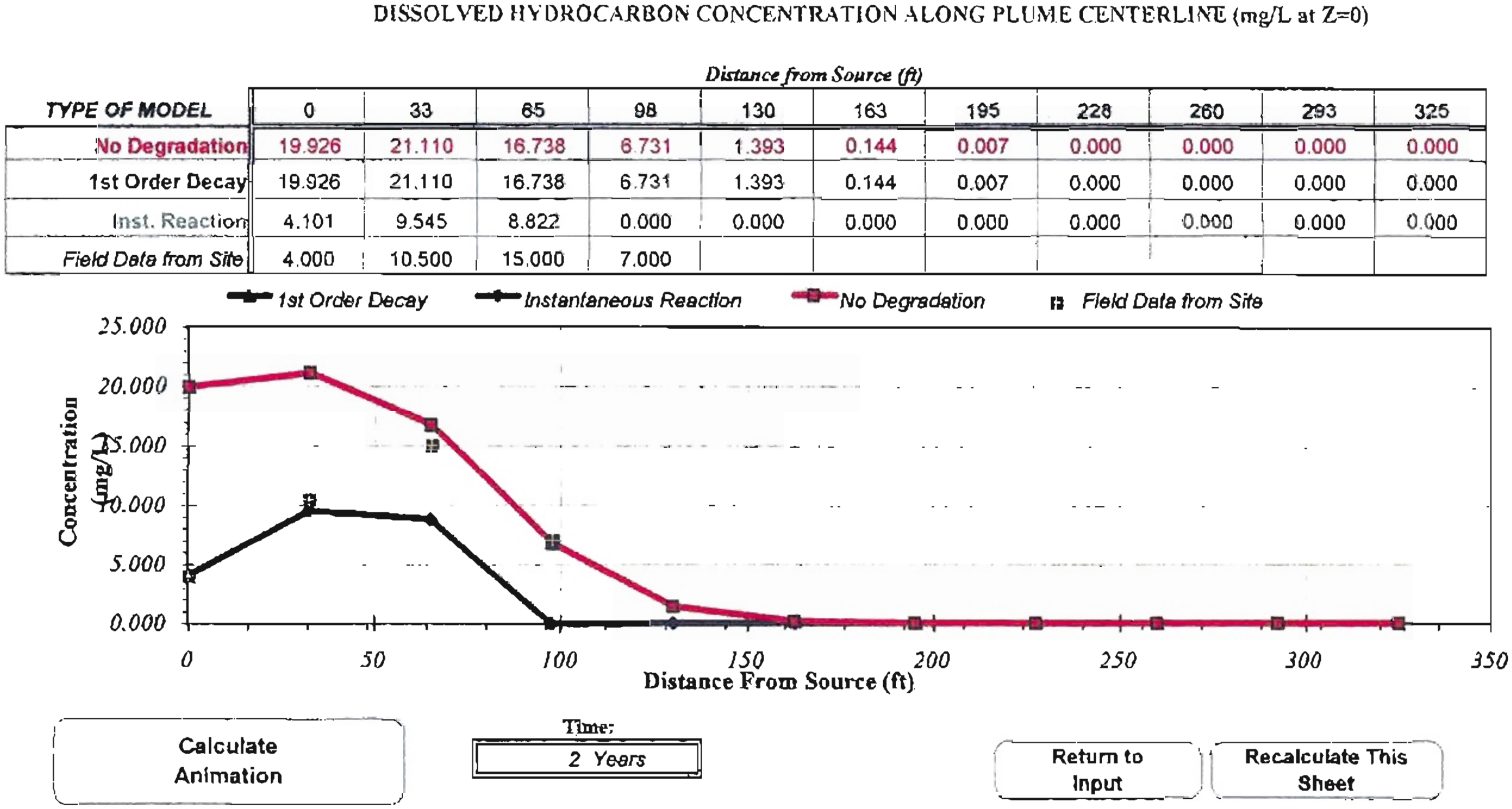
Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"

7. FIELD DATA FOR COMPARISON

Concentration (mg/L)	4.0	10.5	15.0	7.0	0						
Dist from Source (ft)	0	33	65	98	130	163	195	228	260	293	325

8. CHOOSE TYPE OF OUTPUT TO SEE:

BIOSCREEN Simulation #4 Input Data - Attempted Calibration



DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

Distance from Source (ft)

TYPE OF MODEL	0	33	65	98	130	163	195	228	260	293	325
No Degradation	19.926	21.110	16.738	6.731	1.393	0.144	0.007	0.000	0.000	0.000	0.000
1st Order Decay	19.926	21.110	16.738	6.731	1.393	0.144	0.007	0.000	0.000	0.000	0.000
Inst. Reaction	4.101	9.545	8.822	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Field Data from Site	4.000	10.500	15.000	7.000							

Time: 2 Years

BIOSCREEN Simulation #4 Plume Centerline - Attempted Calibration

VITA

Jami Alison Striegel

Candidate for the Degree of

Master of Science

Thesis: MODELING NATURAL ATTENUATION OF PETROLEUM HYDROCARBON CONTAMINATION IN GROUNDWATER USING ALTERNATE ELECTRON ACCEPTORS

Major Field: Environmental Engineering

Biographical:

Education: Graduated from Guthrie High School, Guthrie, Oklahoma in May 1990 as a National Merit Finalist; received Bachelor of Science degree with Honors in Civil Engineering from Oklahoma State University, Stillwater, Oklahoma in December 1996. Completed the requirements for the Master of Science degree with a major in Environmental Engineering at Oklahoma State University in May, 1998.

Experience: Previously employed as a Civil Engineering Aide by the Tennessee Valley Authority Engineering Laboratory in Norris, Tennessee during a one-year cooperative education term; previously performed scholarship-supported undergraduate research for the Department of Civil and Environmental Engineering at Oklahoma State University; previously employed by Roberts/Schornick & Associates, Inc. (RSA) in the Norman, Oklahoma office as a summer intern; currently employed by RSA in the Tulsa, Oklahoma office as a staff professional since December, 1996.

Professional Memberships: Chi Epsilon, Tau Beta Pi, Phi Kappa Phi, Oklahoma Society of Professional Engineers, National Society of Professional Engineers.