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**Modeling of a Jet Fuel Spill
in the Groundwater
at the Massachusetts Military Reservation**

by

Dimitris Triantopoulos

B.S.E. Civil Engineering And Operations Research
Princeton University, 1995

Submitted to the Department of Civil and Environmental Engineering in Partial Fulfillment of
the Requirements for the Degree of

Master of Engineering in Civil and Environmental Engineering

at the

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Abstract

This study uses a computer model to examine one of the jet fuel spills which occurred at the Massachusetts Military Reservation, in Cape Cod, Massachusetts. The spill studied is fuel spill 12 which contains JP-4 fuel and aviation gasoline. The main concern behind this study was the effects that the spill could have on Snake Pond, a kettle pond near the source area, used for recreational purposes. First, the natural flow of the groundwater was simulated. It was decided that benzene, because of its chemical characteristics, poses the greatest threat so the migration of benzene particles was then simulated. The benzene plume was at a higher elevation in the aquifer than measurements have shown. However, despite this unrealistic proximity to the surface, and to the pond, the pond was not significantly affected by the plume. The risk from the resulting concentration of benzene in the pond was below EPA's standards. It is believed that the uncertainty about the exact location of the groundwater divide of Cape Cod, as well as limited hydraulic conductivity data, are the reasons for the high vertical position of the plume.

Thesis Supervisor: E. Eric Adams

Title: Senior Research Engineer and Lecturer

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1. Introduction

The Massachusetts Military Reservation (MMR), located in Cape Cod, Massachusetts, has housed numerous branches of the military since 1911. Military activities on the reservation have been extensive, impacting the natural resources of Cape Cod. Because of the significant contamination, the MMR has been included in the Superfund sites' list. The site cleanup is being handled by the Installation Restoration Program (IRP) with offices located on the reservation. The current action to remediate the plumes on the reservation is deemed "interim"; only the source and leading edge of the plumes will be controlled. Remediation of the main portion of the plumes are not included within this plan.

Fuel Spill 12 (FS-12) is one of the plumes emanating from the MMR. It is located in the northeast section of the reservation. This plume is the result of a leak in a pipeline which carried JP-4 fuel to the MMR. It is estimated that 70,000 gallons was spilled. Two contaminants within the fuel which pose health hazards are EDB, a fuel additive, and benzene, a fuel component. These contaminants are known carcinogens. Currently, the FS-12 source is being controlled through air sparging and soil vapor extraction. However, the remainder of the plume continues to migrate off base. The nearby Snake Pond, which is used for recreational purposes, is potentially in the pathway of the plume. However, predictions say the plume will not affect the pond.

This thesis has been developed as part of group project which uses FS-12 as a case study to assess various remediation techniques and their applicability to a fuel-contaminated groundwater site. The project also examines water supply issues for the entire region. Specifically, the objectives are:

- To determine the movement of FS-12 and its potential effects on Snake Pond;
- To compare the “do nothing” alternative to treatment with three types of remediation schemes: extraction well fence, air sparging & soil vapor extraction, and permeable reactive wall technologies;
- To identify the water supply issues surrounding groundwater contamination including alternatives for water supply replacement and the public perception surrounding use of treated groundwater;
- To evaluate the decision to remediate at the MMR through a cost-benefit analysis.

This thesis will address the first of the above objectives; the movement of the plume and the pond’s safety.

2. Study Area Characterization

This section provides background information on the Massachusetts Military Reservation (MMR), as well as details on Fuel Spill 12 (FS-12). It covers physical and sociological features of the local region.

2.1 The Massachusetts Military Reservation Superfund Site

2.1.1 Physical Characteristics

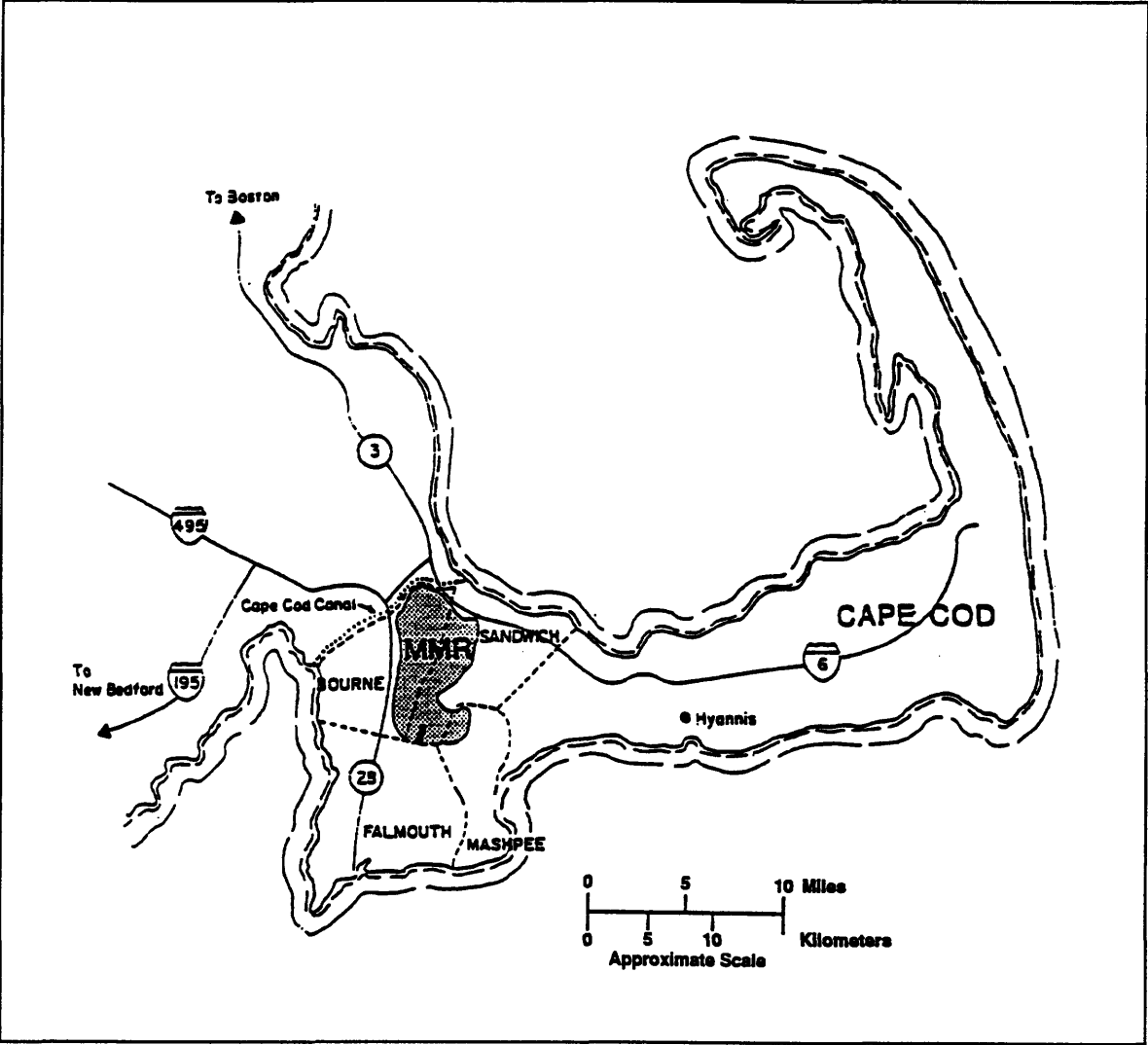
2.1.1.1 Location

The MMR is located in western Cape Cod, bordering the townships of Bourne, Falmouth, Mashpee, and Sandwich. The expanse of the MMR includes 22,000 acres located in Barnstable County (Figure 2-1).

2.1.1.2 Topography and Geology

The MMR is located on two distinct types of terrain on the Cape Cod Peninsula. The main Cantonment Area lies on a broad, southward-sloping glacial outwash plain. Elevation in the area ranges from 100 to 140 feet above sea level. To the north and west of the MMR, the terrain becomes hummocky with irregular hills and greater topographic relief, and lies in the

southward extent of Wisconsin Age terminal moraines. The highest elevation is 306 feet (Stone & Webster, 1995). The entire site is dotted with numerous kettle holes and depressions forming ponds and lakes.



[Stone & Webster, 1995]

Figure 2-1 Location of the MMR

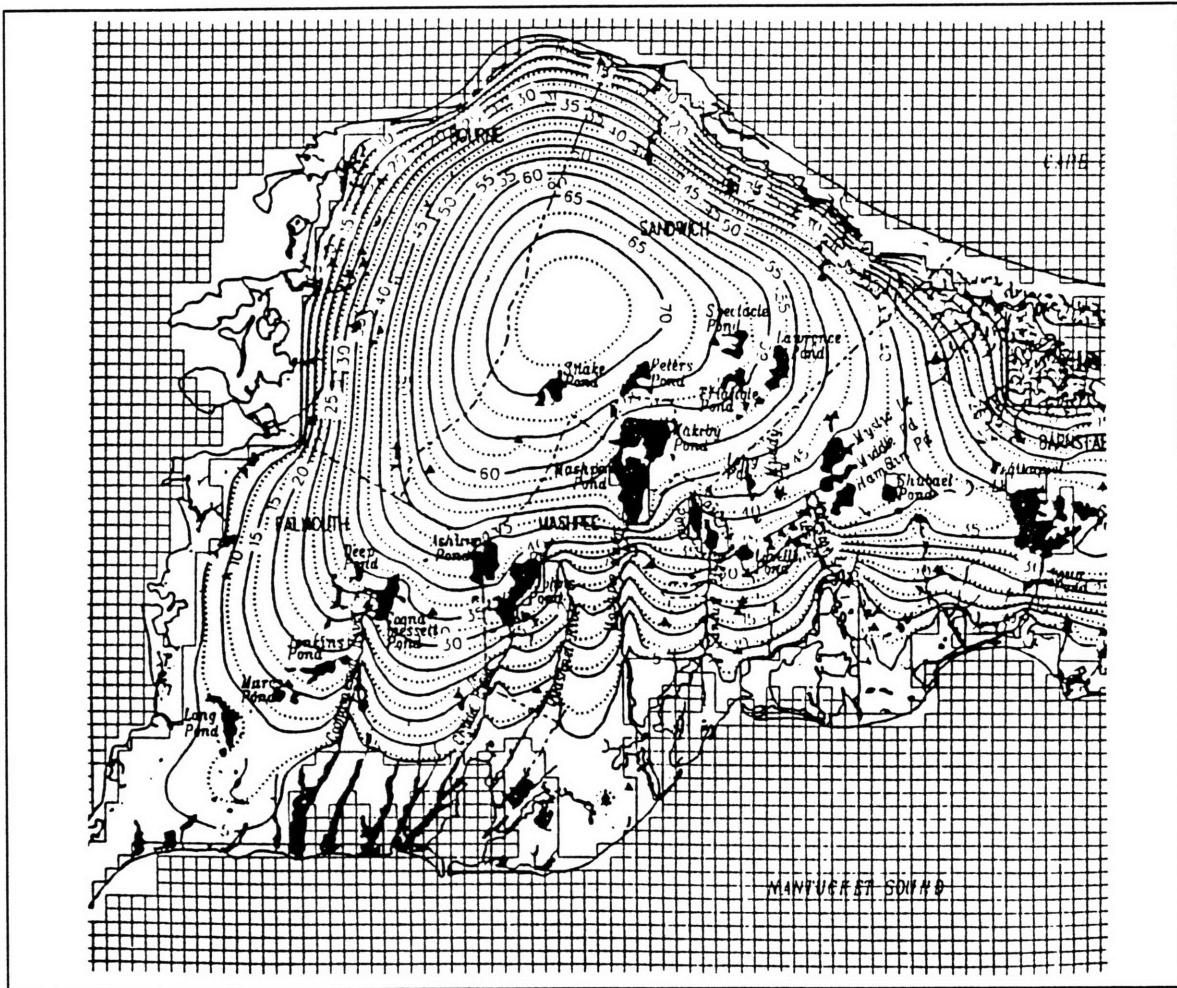
2.1.1.3 Geology and Hydrogeology

Geology

The area is categorized as a glacial outwash plain. Typically, the plain consists of highly permeable sand and gravel, as well as distinctly stratified layers of lower permeability silty sands and clays.

Hydrogeology

A single groundwater flow system underlies western Cape Cod, including the MMR. The aquifer system is described as unconfined and is recharged by infiltration from precipitation.



[Department of Environmental Management, 1994]

Figure 2-2 - Hydrogeology of the MMR

The aquifer has been characterized by the US Environmental Protection Agency (EPA) as a sole-source aquifer. The high point of the water table is located beneath the northern portion of the MMR [Figure 2-2]. Flow is generally radially outward from this mound. The ocean forms the lateral boundary of the aquifer on three sides.

2.1.1.4 Climate

Cape Cod has a temperate climate with precipitation distributed year round. The annual average precipitation is about 47 inches [Department of Environmental Management, 1994]. The highly permeable nature of the sands and gravel underlying the area allow for rapid infiltration of rainfall.

2.1.1.5 Ecosystems

The Massachusetts Division of Fisheries and Wildlife considers coastal plain ponds as unique, sensitive natural communities in the state. These ponds, found primarily in Cape Cod, occur in glacial kettles lacking surface water inlets. The specialized and rare ecosystem that develops on the shores of these ponds is highly sensitive to water level changes [Department of Environmental Management, 1994].

2.1.2 Socio-Economic Characteristics

The Upper Cape area consists of the townships of Falmouth, Sandwich, Mashpee and Bourne. This section discusses demographics, water use, and local economics pertaining to the MMR.

2.1.2.1 Demographics

The MMR has a year round population of approximately 2,000 people with an additional 800 nonresident employees. Both year round and seasonal residents live in the towns adjacent to the MMR - Falmouth, Mashpee, Sandwich, and Bourne. The populations of these towns fluctuate significantly between winter (29,000) and summer (70,000) due to the influx of vacationers. Between 1980 and 1990, the Upper Cape population grew 35%. However Mashpee

registered a 113% increase. During the same period, population growth throughout Massachusetts amounted to only 5% [Cape Cod Commission, 1996]. Due to the fact that the Upper Cape is sparsely inhabited, the population directly affected by the plumes is relatively small - 4,000 (current situation) to 6,500.

2.1.2.2 Water Use

Public water supply customers are the primary water users on Cape Cod, with a base off-season average demand of 8 million gallons per day (mgd) and 16 mgd in-season. In the Upper Cape, 80% of the population is on a central supply system; the remaining 20% of the population relies entirely on individual private wells [Department of Environmental Management, 1994].

2.1.2.3 Economy

The Upper Cape economy was valued at \$600 million in 1992; more than 60% was derived from tourists, seasonal residents, and retirement-based income. Hence, the economic base is believed to be highly sensitive to environmental contamination and associated perceived risk. The Upper Cape's overall valuation of real and personal property increased by 3 times in the past 10 years to \$8 billion in 1994 [Cape Cod Commission, 1996].

2.1.3 History

2.1.3.1 Activity History

Operational units over the MMR's history include the U.S. Air Force, U.S. Navy, U.S. Army, U.S. Marine Corps, U.S. Air National Guard, U.S. Army National Guard, and U.S. Coast Guard. The MMR has housed and served the U.S. military forces since 1911. Within the reservation, military activities included troop training and development, ordnance development, vehicle operation and maintenance, fire fighting, and fuel storage and transport. The MMR was particularly active during World War II (1940-1946). Between 1955-1970, the MMR operated a

number of surveillance missions and aircraft operations through the Air National Guard. Since 1970, the military activities have been scaled down [Advanced Sciences, Inc., 1993].

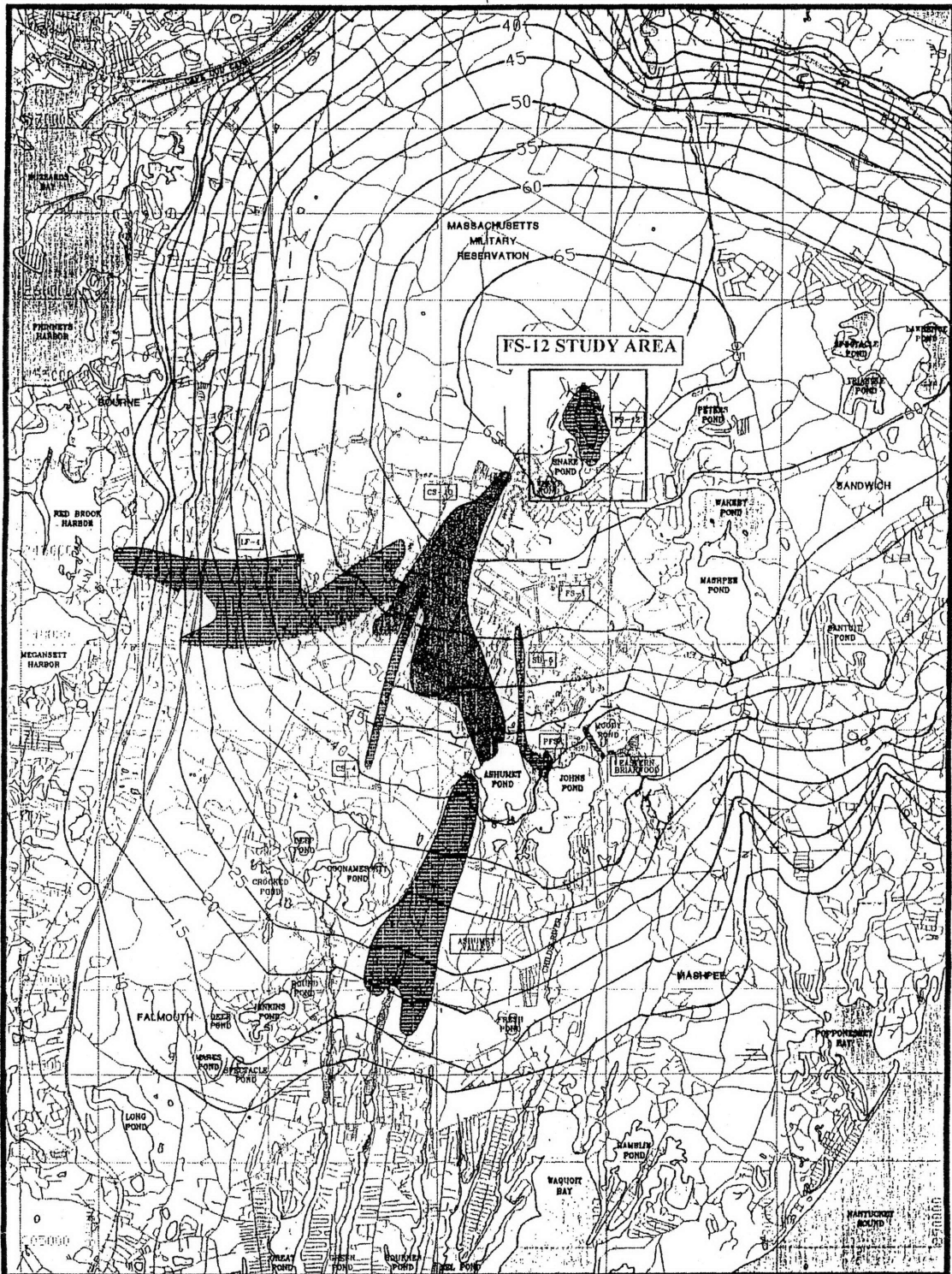
2.1.3.2 Regulatory History

On November 21, 1989, the MMR was listed on the National Priorities List as a Superfund site. As a result, the National Guard Bureau (NGB) and the U.S. Coast Guard entered into an Interagency Agreement (IAG) with the EPA in July 1991. As a result, the site investigations and remedial actions are subject to the requirements and regulations of the Comprehensive Environmental Response and Emergency and Liability Act (CERCLA). The Department of Defense (DOD) formulated and organized the Installation Restoration Program (IRP) to address investigations and remediation efforts as a result of hazardous waste sites at DOD facilities [Air National Guard, 1994]. Through the Air Force Engineering Services Center, the NGB entered into an IAG with the U.S. Department of Energy (DOE). The NGB, with the support of DOE, analyzed the extent of contamination and potential site contamination at the MMR facility [Air National Guard, 1994].

2.1.3.3 Contamination History

Past releases of hazardous materials at the MMR have resulted in groundwater contamination in a number of areas. Documented sources of contamination include former motor pools, landfills, fire training areas and drainage structures such as dry wells. Nine major plumes of groundwater contamination [Figure 2-3] have been found to be migrating from these sources areas and have been defined during extensive groundwater investigations. Seven of the nine plumes have migrated beyond the MMR facility boundary. Extraction and treatment of groundwater have already been initiated for the purpose of containing one plume, the CS-4 plume, to manage the migration of contaminants and prevent further pollution of downgradient areas. The interim action planned by the IRP proposes to extend plume containment schemes to six other plumes [Stone & Webster, 1995].

Figure 2-3 - Plume Area Map



FS-12 STUDY AREA

- LEGEND**
- - - - - BASE BOUNDARY
 - RIVER/POND/STREAM
 - 5 LINE OF EQUAL GROUNDWATER ELEVATION (FEET MSL)
 - [Stippled pattern] COMPOSITE MCL EXCEEDANCE SOLVENT GROUNDWATER CONTAMINATION
 - [Cross-hatched pattern] COMPOSITE MCL EXCEEDANCE FUEL GROUNDWATER CONTAMINATION
 - [Diagonal lines pattern] COMPOSITE MCL EXCEEDANCE EDB CONTAMINATION
 - [Blue pattern] WATER

- NOTES:**
1. GROUNDWATER ELEVATION INFORMATION IS BASED ON DATA COLLECTED IN NOVEMBER 1995 AND USGS WATER TABLE MAPS
 2. PLUME PRESENTATIONS BASED ON COMBINATION OF DATA GAP AND REMEDIAL INVESTIGATION REPORTS
 3. LOW LEVEL SPORADIC DETECTIONS OF EDB AT LOCATIONS OTHER THAN FS-12 ARE NOT SHOWN
 4. PFSA PLUME DETERMINATION IS BASED ONLY ON RI DATA
 5. CS-4 PLUME IS REPRESENTED AS A SUM OF THE VOCs PRESENT BASED ON 1989 DATA



Figure 3 - Plume Area Map

Massachusetts Military Reservation
Cape Cod, Massachusetts

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SOURCE: HIAZWRAP, MODIFIED BY OPTECH 1996

2.2 The Fuel Spill 12

2.2.1 Physical Site Data

The FS-12 area is located within the Mashpee pitted plain, with a substrata consisting of outwash sands and gravel. The subsurface contains discontinuous lenses of low and high permeability that extend down to 130 feet below the water table. On average, the unconfined Cape Cod aquifer lies 90 feet below ground level on average. It surfaces at Snake Pond which is located south-southwest of the source. The velocity of the plume is less than characteristic rates for other plumes on the MMR. This area is located near the crest of the water table mound where the hydraulic gradient is small. Horizontal hydraulic conductivities range from 150 to 400 feet/day.

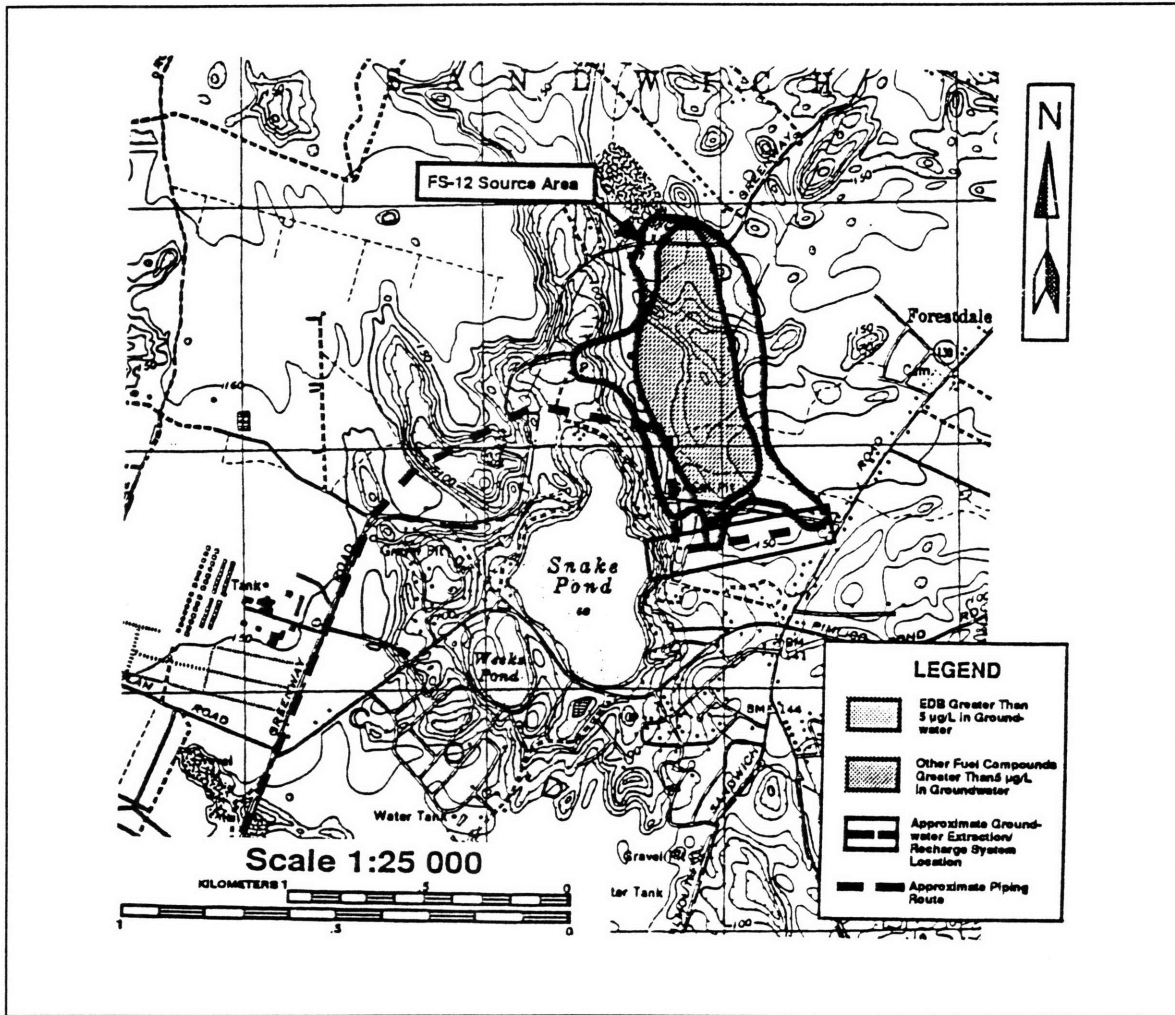
The topography consists of low relief and rolling hills. Elevations range from approximately 200 feet mean sea level (MSL) to 50 feet MSL. Generally, the north-northwestern portion is characterized by higher relief. Topographical elevation decreases in a southeastern direction. Several water bodies are present in the area surrounding the zone of contamination.

The case study site area, FS-12, is sparsely populated, although a summer camp is located off-base directly south of the source. Most of the contamination flows beneath Camp Good News, as can be seen on Figure 2-4.

2.2.1.1 Geology of FS-12

FS-12 is located within the Mashpee pitted plain. The Mashpee pitted plain is characterized by coarse grained materials, mostly sands and gravel. The sand and gravel grains become finer with depth. Throughout the entire depth of the outwash there exists discontinuous lenses of fine sands, clays and silts left from ice and glacial sediments. The sand and gravel materials are underlain by the bedrock. In the FS-12 area, the bedrock elevation ranges between 82 to 328 feet below MSL. Observations suggest the existence of fine sands and clay deposits at depths of 130 to 215 feet below MSL [Advanced Sciences, Inc., 1993]. It is possible that these sediments are part of a continuous layer of finer materials within the sandy aquifer. However,

there is not enough data to verify the existence of a continuous layer of finer sediments [HydroGeoLogic, Inc., 1994].



[Stone & Webster, 1995]

Figure 2-4 FS-12 Area Map

2.2.1.2 Hydrology

FS-12 is located above the Cape Cod aquifer. The aquifer is unconfined and its water table is located on average 80 feet below ground surface. The water table intersects the ground surface creating the following ponds in the area: Snake Pond, Peter's Pond, Mashpee Pond, and Wakeby pond. The groundwater flows in the south-southeastern direction. From the Feasibility Study [Advanced Sciences, Inc., 1993], it was determined that the horizontal

hydraulic gradient varies between 0.0003 and 0.00067. The aquifer test indicates the horizontal conductivity to vary between 237 and 368 feet/day [HydroGeoLogic, Inc., 1994]. From the aquifer test other properties were found as shown by Table 2-1.

Table 2-1 Aquifer properties

Kr	Kz / Kr	Ss	Sy
horizontal conductivity (ft/day)	vertical/horizontal conductivity ratio	Specific Storage	Specific Yield
237 - 368	0.05 - 0.55	0.000001 - 0.00058	0.008 - 0.184

[HydroGeoLogic, Inc., 1994]

The runoff from the site can be assumed to be insignificant due to the high permeability of the soils. The only significant form of recharge to the aquifer is rainfall. Recharge averages approximately 23 inches/year [Masterson and Barlow, 1994].

2.2.2 Site History

The current FS-12 contamination area is the result of an extended leak in a fuel line discovered in 1972. The location of the leak is at the intersection of Greenway Road and the western entrance to the L-firing range. The pipeline was constructed in the early 1960's. Its main purpose was to transport aviation fuel from Cape Cod Canal to the Air National Guard flight line area. Both aviation gasoline and JP-4 jet fuel were carried in the pipeline. In order to stop the leak, it underwent repairs in 1972. Part of the repairs included the use of contaminated soil as backfill for the excavation. Thus, even after the 1972 repairs, JP-4 fuel entered the subsurface soil and groundwater. The line was later closed in 1973. The IRP has estimated a spill volume of approximately 70,000 gallons, which currently contaminates 11 acres of soil. The plume originating from the FS-12 source area extends 5400 feet in length south-southeast from the spill; 1,100 feet wide; 50 feet thick.

2.2.3 Extent of Contamination

As estimated from evaluations of organic soil vapor concentrations, benzene and ethylene dibromide (EDB) are the primary contaminants of concern at FS-12. [Figure 2-4] maps out the extent of soil contamination from an areal view. EDB, a significant organic contaminant at this site, is not a component of jet fuel and was added to the aviation gas as a lead gas scavenger. It is present throughout the dissolved plume, though the free product does not constitute a continual source, as with benzene. When contaminants are not absorbed by soil particles or dissolved into the groundwater, they remain in the free phase form, also known as free product. Being less dense than water, the free product tends to float on top of the groundwater. The free product 'source' of the plume covers five acres ranging in thickness up to 0.7 feet. Near the spill, higher concentrations of benzene and EDB were measured at 1600 ppb and 600 ppb, respectively. The plume extends in an elliptical shape, approximately 5000 feet downgradient [Advanced Sciences, Inc., 1993].

During the remedial investigation of FS-12, it was determined that EDB and benzene posed the largest threat to human health. Their distributions are similar, with the EDB plume located at a slightly deeper depth in the aquifer than the benzene plume [HAZWRAP, 1994]. Risk values were determined for the contaminants of concern based on groundwater exposure and future land use. Most probable carcinogenic risks far exceeded the EPA's upper limit for cleanup guidelines. Therefore, cleanup processes were promptly initiated [Advanced Sciences, Inc., 1993].

2.2.4 Current Situation

After surveying applicable treatment schemes, the IRP selected a combined Air Sparging/Soil Vapor Extraction system to control the source and a well fence to contain the plume movement. The air sparging pilot study was deemed a success for two reasons: (1) the pressure differentials were conclusive enough to predict an adequate extraction well radius of influence and (2) field measurements are indicative of productive vapor extraction in the outwash sands and gravel [HAZWRAP, 1994].

Consequently, an air sparging/soil vapor extraction system was designed and quickly implemented to control the source area at FS-12. The air stripping action of the sparging will transfer contamination from the aqueous phase into the vapor phase and carry it to the

unsaturated zone. There it can be captured by the soil vapor extraction wells, and treated with catalytic oxidation and activated carbon in a vapor control unit. The combined system has been running since November 1995, though the first 100 days utilized only the vapor extraction wells. At the March 1996 FS-12 Sandwich Subcommittee Meeting, Ed Pesce of the IRP reported that clean-up of the source area is expected to take two years (HAZWRAP, 1994).

The Plume Containment committee meets regularly, and is involved in design analysis for site remediation. Preliminary designs indicate proposed locations for the five pump and treat wells that will capture and extract a total of 300-330 gallons/minute of contaminated groundwater. This will be treated and reinjected nearby. With an estimated start-up in September 1996, this process is not a final solution, but meets the immediate goals of the MMR in "source control and plume containment." The MMR is not currently planning to reuse any of the treated water, which means that 100% of it will be reinjected. Public perception of water reuse issues indicate a current unwillingness to drink any treated water [Installation Restoration Program, July 1995].

3. Contamination Assessment

Two major types of fuel were released at the FS-12 source area: aviation gasoline (also referred to as AVGAS in the literature,) and JP-4 Jet Fuel. The compositions of the two types of fuel are similar [Hutchings, 1995]. Table 3-1 lists the most important components of a JP-4 sample. The addition of tetraethyl lead distinguishes AVGAS from JP-4 [Hutchings, 1995]. It will be assumed that the composition of the mixture of the two fuels is the same as the composition of JP-4. Each one of the components listed in Table 3-1 exists in concentration of 0.1% by weight, or more [Hutchings, 1995].

The 75 compounds listed in Table 3-1 are affected differently by various processes such as volatilization, sorption, degradation, and solubility [Hutchings, 1995]. As these compounds move from their source down to the groundwater table, and then follow the groundwater flow, their relative concentrations change. This happens due to the four aforementioned processes which are spatially variable. For example, volatilization is much more effective in the vadose zone (where an air phase exists in the pores) than in the saturated zone. The primary concern, for this study, is the solubility of chemicals in the groundwater, and the subsequent transport of the contaminated water. As Snake Pond is a surface representation of the groundwater table, chemicals transported with the groundwater could possibly discharge in the pond. Snake Pond is used for recreational activities by the occupants of Camp Good News, a local Christian youth camp. Chemicals such as benzene, when in dermal contact (or ingested) in critical quantities, could pose serious threat to human health.

Partitioning in the liquid phase, therefore, is the most important process in terms of human health hazard, and the chemicals with highest solubilities, as can be seen in Table 3-1, are: benzene, toluene, ethylbenzene, and xylene [Hutchings, 1995]. These chemicals are

therefore most likely to be encountered in relatively high concentrations. Furthermore, by looking at the octanol-water partition coefficients, (which are a way of estimating the retardation, due to sorption, of a chemical) we can deduce that isobutane and benzene are the least retarded of the compounds found in JP-4 and AVGAS. Low retardation translates to higher relative mobility, and as a result the most mobile chemicals could reach Snake Pond (if the flow field directs them to it) faster than the other compounds. Isobutane, though, has a high volatilization rate so it is not as threatening as benzene [Hutchings, 1995]. Finally, biodegradation is a factor which needs to be considered. Aromatic hydrocarbons display a variety of biodegradation rates with benzene having one of the lowest values [Hutchings, 1995]. Low biodegradation translates to higher relative concentrations. Finally, benzene is a compound of average abundance. It constitutes 0.5% of the mass of JP-4, so there was 350 gallons (0.5% of 70,000 gallons) of benzene spilled.

The combination of the above information, for the different compounds found in JP-4, shows that benzene, because of its high solubility, persistence against biodegradation, and abundance, is the chemical of greatest concern [Hutchings, 1995]. Hence, this study will concentrate on the modeling of benzene.

Table 3-1 Major Components of JP-4

Fuel Component	Molecular Formula	Percent by Weight	Molecular Weight (g/mol)	T _{melt} °C	T _{boil} °C	Vapour Pressure at 25°C (mm) -log ₁₀ P ^o	Aqueous Solubility at 25°C (mol/L) -log ₁₀ C _{sat}	Hewy's Law Constant at 25°C (litat/mol) log ₁₀ K _H	Octanol-Water Partition Coefficient at 25°C (l/mol octanol)/(mol/L water) log ₁₀ K _{ow}	NOTES
n-Butane	C ₄ H ₁₀	0.12	58.10	-138.40	-0.50	-0.39	2.69	2.98	2.89	
Isobutane	(CH ₃) ₂ CHCH ₃	0.66	58.12	-155.40	-1.10	-0.47	3.07	3.54	3.54	sol. mass & v.p. estimated at 20C
n-Pentane	C ₅ H ₁₂	1.06	72.20	-129.70	36.10	0.16	3.25	3.09	3.02	
2,2-Dimethylbutane	CH ₃ C(CH ₃) ₂ CH ₂ CH ₃	0.10	86.18	-98.90	60.30	0.39	4.79	4.40	4.86	
2-Methylpentane	C ₅ H ₁₂	1.28	86.18	-153.70	49.30	0.56	4.95	4.39	3.81	
3-Methylpentane	(CH ₂) ₂ CH(CH ₃) ₂	0.89	86.18	63.30	63.30	0.61	4.95	4.34	3.81	
n-Hexane	C ₆ H ₁₄	2.21	86.20	-95.00	69.00	0.69	3.83	3.71	4.11	
Methylcyclopentane	CH ₃ C ₅ H ₁₀	1.16	84.16	-142.40	71.80	0.76	5.63	3.77	3.47	
2,2-Dimethylpentane	C ₆ H ₁₄	0.25	100.20	-123.80	79.20	0.88	5.46	4.22	4.22	
Benzene	C ₆ H ₆	0.60	78.10	5.50	80.10	0.90	1.64	0.74	2.13	
Cyclohexane	C ₆ H ₁₂	1.24	84.20	6.60	80.70	0.90	3.15	2.25	3.44	
2-Methylhexane	C ₇ H ₁₆	2.35	100.20	-118.30	90.00	1.02	5.62	4.55	4.35	
3-Methylhexane	CH ₃ (CH ₂) ₃ CH ₂ CH ₃	1.97	100.20	-114.00	92.00	1.11	5.62	4.51	4.35	
trans-2,3-Dimethylcyclopentane	2,3-ICH ₃ 2C ₅ H ₈	0.36	98.19	-120.00	91.80	1.10	5.19	4.08	4.00	
cis-1,3-Dimethylcyclopentane	1,3-ICH ₃ 2C ₅ H ₈	0.34	98.19	-120.00	91.80	1.10	5.19	4.00	4.00	
cis-1,2-Dimethylcyclopentane	1,2-ICH ₃ 2C ₅ H ₈	0.64	98.19	-82.00	99.25	1.24	5.19	3.95	4.00	
n-Heptane	C ₇ H ₁₆	3.67	100.20	-90.60	98.40	1.21	4.51	3.30	4.66	
Methylcyclohexane	CH ₃ C ₆ H ₁₁	2.27	98.19	-126.60	100.90	0.72	3.85	3.12	4.04	v.p. & sol. measured at 20C
2,2,3,3-Tetramethylbutane	CH ₃ C(CH ₃) ₂ C(CH ₃) ₂ CH ₃	0.24	114.23	100.70	106.50	1.37	5.51	4.14	4.26	
Ethylcyclopentane	C ₂ H ₅ C ₅ H ₉	0.26	98.19	-138.40	103.50	1.31	3.89	3.21	4.01	
2,5-Dimethylhexane	(CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ CH ₃	0.37	114.23	-91.20	109.00	1.41	6.12	4.78	4.78	
2,4-Dimethylhexane	C ₂ H ₅ CH(CH ₃)CH ₂ CH ₂ CH ₃	0.68	114.23	-91.20	109.00	1.45	5.84	4.68	4.76	
1,2,4-Trimethylcyclopentane	1,2,4-ICH ₃ 3C ₅ H ₇	0.25	112.22	-128.10	112.00	1.46	6.12	4.78	4.76	
3,3-Dimethylhexane	1,2,3-ICH ₃ 3C ₆ H ₁₁	0.26	112.22	-128.10	112.00	1.46	5.84	4.78	4.76	
1,2,3-Trimethylcyclopentane	1,2,3-ICH ₃ 3C ₅ H ₇	0.25	112.22	-128.10	112.00	1.46	5.84	4.78	4.76	
Toluene	C ₇ H ₈	1.33	92.10	-95.00	110.60	1.42	2.75	0.83	2.69	
2,2-Dimethylheptane	(CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ CH ₃	0.71	114.23	-121.00	108.80	1.37	6.12	4.76	4.76	
2-Methylheptane	C ₈ H ₁₈	2.70	114.23	-109.00	117.60	1.52	6.28	4.72	4.89	
4-Methylheptane	(CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ CH ₃	0.92	114.23	-121.00	117.60	1.57	6.28	4.72	4.89	
cis-1,3-Dimethylcyclohexane	1,3-ICH ₃ 2C ₆ H ₁₀	0.42	112.22	-75.60	120.10	1.61	5.80	4.19	4.50	
3-Methylheptane	C ₈ H ₁₈	3.04	114.23	-120.60	119.00	1.59	6.28	4.69	4.89	
1-Methyl-3-ethylcyclohexane	C ₂ H ₅ CH(CH ₃)C ₆ H ₁₁	0.17	126.24	-113.20	126.24	1.81	6.47	5.04	5.04	
1-Methyl-2-ethylcyclohexane	1,1-ICH ₃ 2C ₆ H ₁₀	0.39	126.24	-113.20	126.24	1.81	6.47	5.04	5.04	
Dimethylcyclohexane	C ₈ H ₁₈	0.43	114.23	-33.60	119.50	1.60	5.80	4.20	4.50	
n-Octane	C ₈ H ₁₈	3.80	114.20	-56.80	125.70	1.73	5.20	3.47	5.16	
1,3,5-Trimethylcyclohexane	1,3,5-ICH ₃ 3C ₆ H ₉	0.99	126.24	-49.70	138.50	1.95	5.64	3.69	4.37	
1,1,3-Trimethylcyclohexane	1,1,3-ICH ₃ 3C ₆ H ₉	0.48	126.24	-49.70	138.50	1.95	5.64	3.69	4.37	
2,6-Dimethylheptane	C ₂ H ₅ CH(CH ₃)CH ₂ CH ₂ CH ₂ CH ₃	0.62	128.26	-128.26	136.00	1.81	5.95	5.02	5.42	
Ethylbenzene	C ₈ H ₁₀	0.37	106.20	-95.00	136.00	1.90	2.80	0.90	3.16	
m-Xylene	1,3-ICH ₃ 2C ₆ H ₄	0.96	106.20	-48.00	139.10	1.95	3.82	1.87	3.20	v.p. calc. by interpolating bet. 20C and 30C
p-Xylene	1,4-ICH ₃ 2C ₆ H ₄	0.35	106.20	-48.00	139.10	1.95	3.82	1.87	3.18	v.p. calc. by interpolating bet. 20C and 30C
3,4-Dimethylheptane	CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₂ CH ₃	0.43	128.26	-113.20	140.10	1.98	6.94	4.96	5.42	
4-Ethylheptane	(CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ CH ₃	0.18	128.26	-113.20	140.10	1.98	6.94	4.96	5.42	
4-Methylheptane	C ₈ H ₁₈	0.86	128.26	-80.10	142.80	2.03	6.95	4.95	5.43	
2-Methylheptane	CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₂ CH ₃	0.86	128.26	-80.10	142.80	2.03	6.95	4.95	5.43	
2-Methylheptane	CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₂ CH ₃	0.79	128.26	-107.60	143.00	2.04	6.95	4.91	5.43	
o-Xylene	1,2-ICH ₃ 2C ₆ H ₄	1.01	106.20	-25.35	144.40	2.03	2.68	0.65	3.13	v.p. calc. by interpolating bet. 20C and 30C
1-Methyl-4-ethylcyclohexane	4-C ₂ H ₅ (CH ₃)C ₆ H ₁₀	0.48	128.24	-51.00	150.80	2.12	6.47	4.30	5.04	
n-Nonane	C ₉ H ₂₀	2.25	128.20	-60.00	150.80	2.12	5.94	3.70	5.04	
Isopropylbenzene	(CH ₃) ₂ CHC ₆ H ₅	0.30	120.20	-96.60	164.20	2.37	3.38	1.01	3.74	v.p. & sol. measured at 20C
n-Propylbenzene	C ₉ H ₁₂	0.71	120.20	-101.60	169.20	2.37	3.38	1.01	3.63	
1-Methyl-3-ethylbenzene	3-C ₂ H ₅ C ₆ H ₄ CH ₃	0.49	120.19	-95.50	181.30	2.38	3.72	1.38	3.89	
1-Methyl-4-ethylbenzene	4-C ₂ H ₅ C ₆ H ₄ CH ₃	0.43	120.19	-87.30	182.00	2.40	3.72	1.37	3.89	
1,3,5-Trimethylbenzene	C ₉ H ₁₂	0.42	120.20	-44.70	184.70	2.48	3.40	0.92	3.42	
1-Methyl-2-ethylbenzene	2-C ₂ H ₅ C ₆ H ₄ CH ₃	0.23	120.20	-80.95	185.20	2.46	3.21	0.75	3.53	
1,2,4-Trimethylbenzene	C ₉ H ₁₂	1.01	120.20	-43.80	189.40	2.57	3.33	0.76	3.65	
n-Decane	C ₁₀ H ₂₂	2.16	142.30	-29.70	174.10	2.78	6.57	3.81	6.10	

Table 3-1 (cont'd)

Fuel Component	Molecular Formula	Percent by Weight	Molecular Weight (g/mol)	T melt °C	T boil °C	Vapour Pressure at 25°C (atm) $-\log_{10} p^0$	Aqueous Solubility at 25°C (mol/l) $-\log_{10} C_{sat}$	Henry's Law Constant at 25°C (atm/mol) $\log K_H$	Octanol-Water Partition Coefficient at 25°C (mol/l octanol)/(mol/l water) $\log K_{ow}$	NOTES
n-Butylcyclohexane	C ₁₄ H ₂₆	0.70	140.27	-74.70	181.00	2.77	7.15	4.38	5.59	
1,3-Diethylbenzene	1,3-(C ₂ H ₅) ₂ C ₆ H ₄	0.46	134.22	-83.90	181.00	2.77	4.40	1.63	4.53	
1-Methyl-4-propylbenzene	4-C ₃ H ₇ C ₆ H ₄ CH ₃	0.40	134.24				4.40		4.53	
1,3-Dimethyl-5-ethylbenzene	1,3-(CH ₃) ₂ -5-C ₂ H ₅ C ₆ H ₃	0.61	134.24				4.53		4.85	
1-Methyl-2-isopropylbenzene	2-(CH ₃)C ₆ H ₄ CH(CH ₃) ₂	0.29	134.24	-71.50	178.10	2.71	4.24	1.53	4.40	
1,4-Dimethyl-2-ethylbenzene	1,4-(CH ₃) ₂ -2-C ₂ H ₅ C ₆ H ₃	0.70	134.24				4.53		4.85	
1,2-Dimethyl-4-ethylbenzene	1,2-(CH ₃) ₂ -4-C ₂ H ₅ C ₆ H ₃	0.77	134.24				4.53		4.85	
n-Undecane	C ₁₁ H ₂₄	2.32	156.24	-25.60	196.00	3.06	8.44	5.38	8.64	
1,2,3,4-Tetramethylbenzene	1,2,3,4-(CH ₃) ₄ C ₆ H ₂	0.75	134.22	-6.20	205.00	3.24	4.67	1.43	4.72	
Naphthalene	C ₁₀ H ₈	0.50	128.20	80.60	217.90	3.43	3.06	-0.37	3.36	
2-Methylundecane	C ₉ H ₁₈ CH ₂ CH ₃	0.64	170.30				8.95		7.05	
n-Dodecane	C ₁₂ H ₂₆	2.00	170.30	-9.60	216.30	3.80	7.52	3.72	7.18	
2,6-Dimethylundecane	C ₅ H ₁₁ CH(CH ₃)C ₃ H ₆ CH(CH ₃) ₂	0.71	184.41				9.46		7.46	
1-Methylnaphthalene	2-CH ₃ C ₁₀ H ₇	0.58	142.20	34.45	241.00	3.87	3.74	3.86	4.02	
n-Tridecane	C ₁₃ H ₂₈	1.52	184.30	-22.15	244.60	4.04	3.70	3.87	4.02	
2,6-Dimethylnaphthalene	2,6-(CH ₃) ₂ C ₁₀ H ₆	0.25	156.20	-5.50	235.40	3.86	9.78	5.92	7.72	
n-Tetradecane	C ₁₄ H ₃₀	0.73	198.30	107.85	253.70	4.23	4.89	3.72	4.31	
				5.90			7.95		8.38	

[From Hutchings, 1995]

Explanatory Notes:
 1. Experimental data used where available. Sources: [19][20][21]
 2. Underlined figures are estimated values. Estimation methods are detailed in Appendix B

4. Modeling of the FS-12 Plume

4.1 CONCEPTUAL MODEL

4.1.1 Introduction

An essential step prior to the actual implementation of a model, is the development of a conceptual model of the area and the compounds to be modeled. Consideration of all the available information, such as the history of the spill, the hydrogeologic characteristics of the aquifer, and the topography of the area, is needed for the conceptualization of the model. The modeling consists of two major parts: the simulation of the natural flow field and the simulation of the contaminant transport. It is, therefore, logical to implement a two-part conceptual model.

4.1.2 The natural flow field

The whole of Cape Cod receives its recharge from precipitation, and the groundwater flows radially outward from the groundwater divide. This is the point with the highest value of hydraulic head on the Cape, and it is located to the north of the contamination source of FS-12. Its exact position, however, has not been precisely defined. Two major mapping projects, have addressed the groundwater flow field [LeBlanc et al., 1986; Savoie, 1995]. Neither of the two provides conclusive information on the position of the groundwater divide. As will be

shown in a subsequent section, this could be crucial in determining the transport rate of the contaminants, and the potential threat to Snake Pond.

Both of the above maps as well as the one in Figure 4-1 (from the Remedial Investigation) show the north-to-south decrease in hydraulic head in the vicinity of FS-12 and thus necessitate a more detailed study of the flow (such as a modeling effort) to determine the proximity of the plume to Snake Pond. The presence of the divide (north of the source area) and of Mashpee and Wakeby Ponds (to the southeast,) immediately gave a general idea for the boundaries of the study area; all flowlines start from the divide, and the hydraulic heads at the Ponds can be considered constant.

By looking at the geologic cross-sections constructed during the RI/FS [Figures 4-2 to 4-6] one can get an idea of the stratigraphy of the area between the source and Snake Pond. It is obvious from these sections that sand and gravel is the predominant soil type at FS-12. Groundwater 'prefers' to travel horizontally in the areas of higher hydraulic conductivity [Domenico and Schwartz, 1990], therefore, we could also have an initial estimate of the travel time of groundwater. Using the map by Savoie, the distance between the source and the area just to the east of the northern tip of Snake Pond is approximately 3200 ft. The hydraulic gradient (estimated from the same map,) is 0.0005 and the porosity of the area has been estimated to be 0.39 [Garabedian et al., 1988]. The horizontal hydraulic conductivity, as mentioned in Section 2.2.1.2, is approximately 330 ft/day. From this information, a quick calculation using Darcy's Law gives a velocity of 0.42 ft/day. The time required to travel 3200 ft, would be approximately 20 years. It has been a little over 20 years since the spill occurred, and measurements show that the plume is near the Pond, which is consistent with these calculations.

All the above information was useful in conceptualizing the model and having a general idea of the expected outcome of the model. Moreover it was useful in defining the area to be modeled and its boundaries.

4.1.3 Contaminant Transport

As explained previously, the model will focus on the transport and dispersion of benzene, as it is one of the most hazardous chemicals (in terms of human health effects) and it has high solubility and low retardation.

The process by which benzene reached the groundwater needs consideration. The fuel spill occurred through a hole in a transfer pipe. The pipe was a few feet below the

ground surface. The fuel is, consequently, released in the unsaturated zone. In order to reach the groundwater, it has to travel vertically (gravity-driven movement) in the unsaturated zone until it reaches the groundwater table. The travel time in the unsaturated zone could potentially affect our estimates of the total time needed for benzene to travel from the pipe hole, to the area of concern (near or in Snake Pond.) Another study of a similar spill at the Massachusetts Military Reservation (JP-4 and AVGAS were, again, the fuels spilled) showed that the scale of the travel time of benzene from the ground surface to the water table, is much smaller than that of the travel time in the groundwater. In the first case, the travel time is in the order of days, whereas we are interested in the movement of benzene over several years [Hutchings, 1995]. It is, therefore, logical to ignore the effects of the unsaturated zone travel.

Another characteristic of the FS-12 spill, which is important in terms of modeling, is the shape of the contaminants once they reach the groundwater table. During the Remedial Investigation phase it was discovered that the source of the contamination (at the water table surface) was pancake-shaped, with a thickness of a few inches [Advanced Sciences, vol. I, 1993]. It is suspected that the various components of the fuels traveled through the unsaturated zone, then stopped at the water table, where they accumulated, thus creating the free product volume. The estimate of the area of the free product is depicted in Figure 4-7. These fuels constitute a separate phase (a NAPL or nonaqueous phase liquid) which is in contact with the water phase. As water moves through the soil, in contact with the NAPL, the compounds of the fuel slowly dissolve in the water phase and thus get carried away. Because of the abundance of the compounds, it was assumed that the compounds' concentrations right at the water interface are equal to the compounds' solubilities. Consequently, the free product can be thought of as a constant concentration source (the concentration being equal to the solubility of the modeled compound, benzene in our case.) It is believed that this is a conservative estimation for the concentration of compounds right at the source. Fluctuations of the elevation of the water table may result in the distancing of the free product from the flowing groundwater which will decrease the contact between the water and the fuel.

4.2 THE DYN SYSTEM

The modeling system used in this study, the DYN system, consists of three programs: Dynflow, Dyntrack, and Dynplot. Dynflow simulates the natural groundwater flow field of the area, Dyntrack is used for the tracking of contaminant particles and Dynplot is a plotting program used for the visualization of the results from the other two programs. The DYN System was developed by Camp, Dresser & McKee, Inc. [Camp, Dresser & McKee, 1984a, 1984b, 1992].

Dynflow discretizes the area of study by dividing it into many smaller discrete triangular areas, called elements. The size of these elements is variable. All the elements form a grid over the study area. The grid is usually much denser in the region where detailed information is needed and sparse in the remaining region. A dense grid implies a high number of elements per unit of modeled area. The grid also has a vertical dimension and can be divided to several horizontal layers. The corners of the triangular elements are called nodes. A value of hydraulic head is defined at each node. Dynflow solves numerically the groundwater flow equation and the advection-dispersion-reaction equation using a finite element method. Hydraulic head is the variable for which Dynflow solves these equations. Linear variation in head, between adjacent nodes, is assumed. Furthermore, after solving for the values of hydraulic head, Dynflow assigns a velocity vector at the center of each element. Once the area of study has been divided to its layers, and hydraulic properties have been assigned to them, Dynflow solves for the heads, assigns the velocity vectors, and thus the flow field is fully represented.

Once the flow field has been established with Dynflow, the next step is the simulation of the path followed by individual particles containing a chemical of concern. A number of particles is chosen, as well as a source of contamination, from which the particles begin their path. Each particle carries a specified mass of contaminant. The transport of the contaminants is governed by the flow field obtained from Dynflow. Dyntrack tracks the path of each particle by following two processes, advection and dispersion. Furthermore, again at each time step, Dyntrack changes the amount of mass carried by each particle according to the decay rate input. The concentration values are stored in each node. However, since the area corresponding to each node is not known, in order to compute the concentration in a larger area (such as Snake Pond) the mass of all the particles in the area's elements is added, and then divided by its volume (which can be calculated since the area of each element is known).

4.3 FS-12 MODEL DEVELOPMENT

The following paragraphs describe the essential ‘building blocks’ of the developed model for the FS-12 plume. The combination of choices for the boundary locations and conditions, stratigraphy, and input parameters (such as conductivities, porosities, etc.) is significant in interpreting the final results of the flow and transport simulations.

4.3.1 Discretization

First of all, the area of concern was identified from the information compiled in the Remedial Investigation/Feasibility Study [Advanced Sciences, vol. I, 1993.] A map of the area was digitized and incorporated into the Dynplot program [Figure 4-8]. In order to be more effective in the study of the FS-12 plume, the modeling area was chosen to be much larger than that defined by the observed distribution of data near the source and Snake Pond. This way, the boundaries were more easily defined, as the next section will show.

As mentioned earlier, Dynflow is a finite element modeling program. A horizontal grid, consisting of triangular elements, is generated over the specified area. Dynflow program solves the groundwater flow equations (as described in previous section) assuming a linear variation in hydraulic head between adjacent nodes. The area of concern, located at the center of the grid bounded to the north by the source of the contamination, and to the east by Snake Pond, needs a much finer grid (more elements per area) because we need more detailed information on the movement of the contaminant plume. Figure 4-9 depicts the grid and an outline of the three ponds in the general study area. Near Snake Pond, because of the fine resolution, velocities are calculated between points which are very close to each other, thus providing a finer resolution of the groundwater flow. The grid was also divided vertically, into nine layers. The description of the materials assigned in these layers can be found in Section 4.3.3

4.3.2 Boundaries

The boundaries of the study area were selected to match (as much as possible) observed [Savoie, 1995] constant head lines. Fixed head conditions were considered on the south

and the southeast boundary of the study area [Figure 4-10]. The greatest part of the southern boundary matches an observed constant head line from Savoie, 1995. Most of the nodes on it were fixed at a hydraulic head value of 45m. However, since the line defining the south boundary of the grid does not exactly follow the constant 45m head line, some of the nodes were set at different values, depending on their position with respect to the 45m line. The area near the ponds in the southeast part of the study area, Mashpee and Wakeby, also had fixed head boundaries. These values were the observed water elevations of the ponds. The remaining boundaries were chosen so as to represent flow lines (by following lines perpendicular to the isopotentials) [Figure 4-10].

4.3.3 Geology-Stratigraphy

The geologic data input to the model were based on the well information (boring logs) from the drilling and sampling during the Remedial Investigation and Feasibility Study [Advanced Sciences, vols. II & III, 1993]. As was mentioned, the horizontal grid can have a number of layers. Nine layers were input to the grid of the modeled area. Although less than nine types of geologic materials were input, the division of the vertical dimension in nine layers was done in order to describe discontinuities (such as clay/silty-sand layers) or special features such as the ponds. The following types of geologic material were input: three types of sand and gravel, labeled *Upper Sand*, *Medium Sand*, and *Lower Sand* [Figures 4-7 and 4-8]. The distinction was made because it has been determined [Advanced Sciences, vol. I, 1993] that hydrologic characteristics such as hydraulic conductivity change with depth. The boring logs from the Remedial Investigation, proved the existence of some localized clay and/or silty sand layers. These layers are characterized by low values of hydraulic conductivity, and could, potentially, affect the groundwater flow. These are labeled as *clay* [Figure 4-8]. Another type of geologic material is the *pond sediment* which is located beneath every pond. Finally the *water* in the ponds was represented as a distinct type of material (with very high hydraulic conductivity) [Figure 4-9].

The elevations of each layer were taken from the same boring logs [Advanced Sciences, vols. II & III, 1993]. Finally, the elevations of the bedrock were interpolated from seismic investigations done in the area by Oldale [1969].

4.3.4 Hydraulic parameters

The development of the first phase (the natural flow simulation) of the modeling required the input of certain hydraulic properties, such as hydraulic conductivity and porosity, to each of the elements described above. There was a significant lack of such data. Although most of the area of the Massachusetts Military Reservation has had a lot of slug and aquifer tests, the FS-12 area has been relatively neglected. Only one aquifer test (conducted at the area just east of Snake Pond) was available [HydroGeoLogic, 1994]. A general idea of the values of the hydraulic conductivity was gained, but some educated guessing was required to successfully represent the flow field. Apart from the information given in the one pumping test, other information more information was gained from general geologic data found in groundwater hydrology textbooks [Freeze and Cherry, 1979; Domenico and Schwartz, 1990]. Generally, because of the lack of data on these parameters, during the calibration of the model, the hydraulic conductivities were changed many times until the natural flow field was successfully calibrated. The final values used are given in the following table:

Table 4-1 Hydraulic Parameters Of Different Materials

Material	Hydraulic Conductivities (ft/day)			Specific Yield
	K _x	K _y	K _z	
Water	10000	10000	100	1
Pond Sediment	355	355	118	0.2
Upper Sand	355	355	118	0.2
Medium Sand	275	275	92	0.2
Clay/Silty-Sand	19	19	6	0.1
Lower Sand	50	50	17	0.2

As Table 4-1 illustrates, the hydraulic conductivity of the water was assigned an arbitrary high value of 10,000 ft/day. The sediments below the pond were represented as a distinct geologic layer. It is suspected that the conductivity of the sediments is generally low (lower than that of sand and gravel). Due to lack of data, though, it was assumed that the

conductivities were equal. This way, a conservative case was represented. Thus, the horizontal and transverse conductivities were set at 355 ft/day and the vertical was set at 118 ft/day. The vertical conductivities, for all the layers, were calculated by assuming a horizontal to vertical ratio of 3:1 as shown in Section 2.2.1.2. Table 4-1 also shows the decreasing-with-depth trend for the sand's conductivity. Finally, the values for the *clay* material were based on general geologic data [Freeze & Cherry, 1979]. The specific yield values were also a combination of data from the aquifer test and general reference books. As is described in the next chapter, these values produced a good calibration.

During the particle tracking phase, another set of input parameters was compiled. It included the longitudinal, transverse, and vertical dispersivities of the aquifer, the effective porosities of the different materials, and the retardation coefficient and half-life of benzene. These parameters were used by Dyntrack for the simulation of the benzene plume movement. The following table shows these values:

Table 4-2 Particle Tracking Input Parameters

Material	Dispersivities (ft)		Vertical Dispersion Anisotropy	Effective Porosity	Half-life (days)	Retardation
	longitudinal	transverse	Ratio			
Water	40	10	0.06	0.39	13	1.0
Pond Sed.	40	10	0.06	0.39	720	1.0
Upper Sand	40	10	0.06	0.39	720	1.0
Medium Sand	40	10	0.06	0.39	720	1.0
Cl./Silt.-Sand	40	10	0.06	0.39	720	1.0
Lower Sand	40	10	0.06	0.39	720	1.0

The values for the longitudinal dispersivities were estimated considering that dispersivities have been shown to be dependent to the scale of the plume [Gelhar et al., 1992]. A tracer test conducted in Ashumet Valley was of similar scale. Dispersivity values of the same magnitude, as documented in Gelhar et al., 1992, were used. The vertical dispersion anisotropy ratio shown in Table 4-2, is the square root of the vertical over the longitudinal dispersivity. The value for the porosity came from the same source [Gelhar et al., 1992]. Although benzene is believed to be retarded, even though very little, it was decided to model its transport using a

conservative estimate of no retardation. Finally, from the range of values found in the literature [MacKay et al., 1992] for the half-life of benzene, both the one used for the groundwater (720 days) and the one used for surface waters (13 days) were among the highest values, again aiming for a conservative simulation. The associated decay rates are $9.6 \times 10^{-4} \text{ days}^{-1}$ (for groundwater) and $5.33 \times 10^{-2} \text{ days}^{-1}$ (for surface waters).

What's more, since the half-life of 13 years was measured in a pond different from Snake Pond, an estimate for the volatilization rate of benzene, was also done, for more accuracy, using the film theory for reaeration in lakes [Harleman, 1990]. An average wind speed was assumed to be 5 m/sec. Yu & Hamrick, 1984, give a value of approximately 10^{-5} m/sec for K_L , the overall liquid film coefficient. Assuming that the behavior of benzene is not very different from that of oxygen, the volatilization rate (another assumption is that decay in surface waters is caused entirely by volatilization) is equal to K_L divided by the depth. The average depth of the pond is assumed to be 25ft (since the maximum depth is 35 ft [Advanced Sciences, 1993]). The resulting volatilization rate, therefore, is 0.113 days^{-1} . This rate correspond to a half-life of 6.1 days. Although this is probably a more accurate calculation because it takes into account the depth of the pond, a half-life of 13 days will be used in order to be conservative.

4.3.5 Contaminant Source

The source of the contamination is a pancake-shaped volume of free product on top of the water table. The area of the extent of the free product is shown in Figure 4-7. Because of the abundance of the free product, 70,000 gallons [Advanced Sciences, Inc., vol. I, 1993], the source was modeled as a 'fixed concentration source'. This means that at every time step, at the specified nodes (the nodes in the area of the free product), particles are added, so that the resulting concentration in the elements of the area equals the specified (fixed) concentration. When, at the next time step, particles are carried away due to advection, Dyntrack 'replenishes' the nodes at the source area. The fixed concentration was set at benzene's solubility, 1780 mg/L [MacKay et al., 1992]. This assumption is also based on the abundance of free product and it also gives a conservative estimate. Dissolution occurs as the water table surface moves in contact with the free product surface. A relatively small amount of water, therefore, comes to contact with the fuel. Moreover, the water table elevation fluctuates throughout the year, so it is not always in contact with the free product. That is why the assumption of 1780 mg/L is conservative.

Figure 4-1 Head Contours at the FS-12 Area

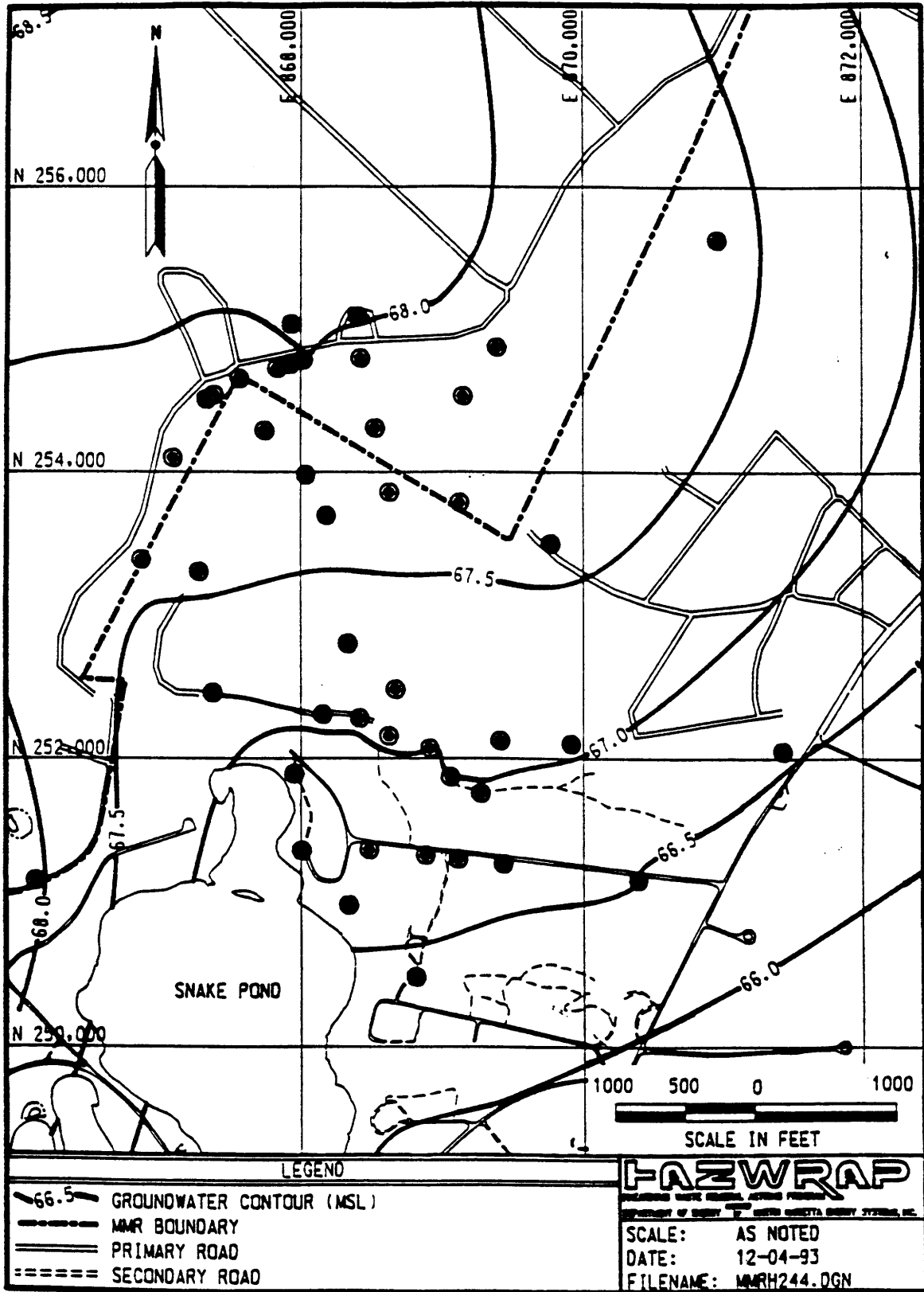


Figure 4-2 FS-12 Study Area Cross-Sections

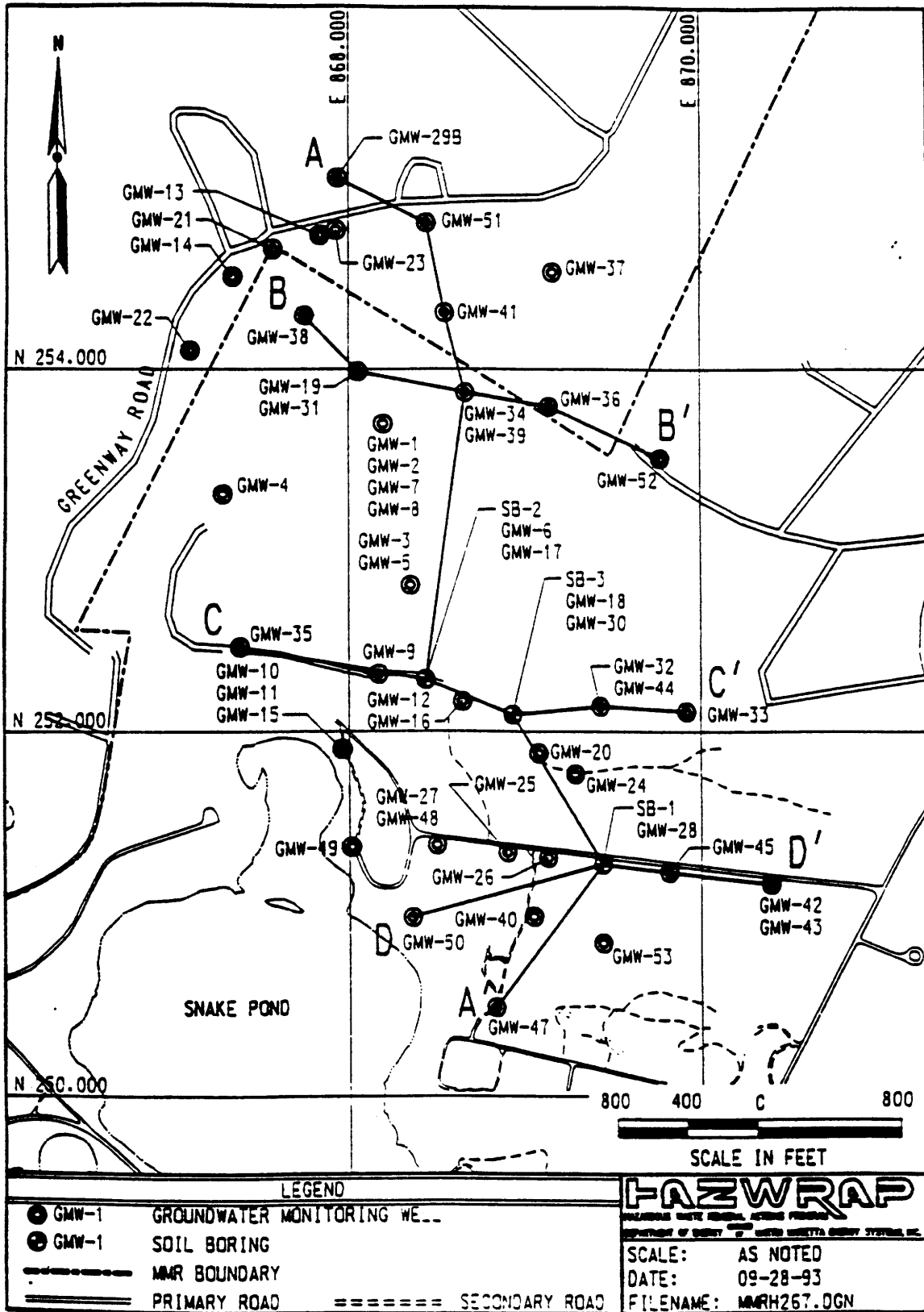


Figure 4-3 Cross Section AA'

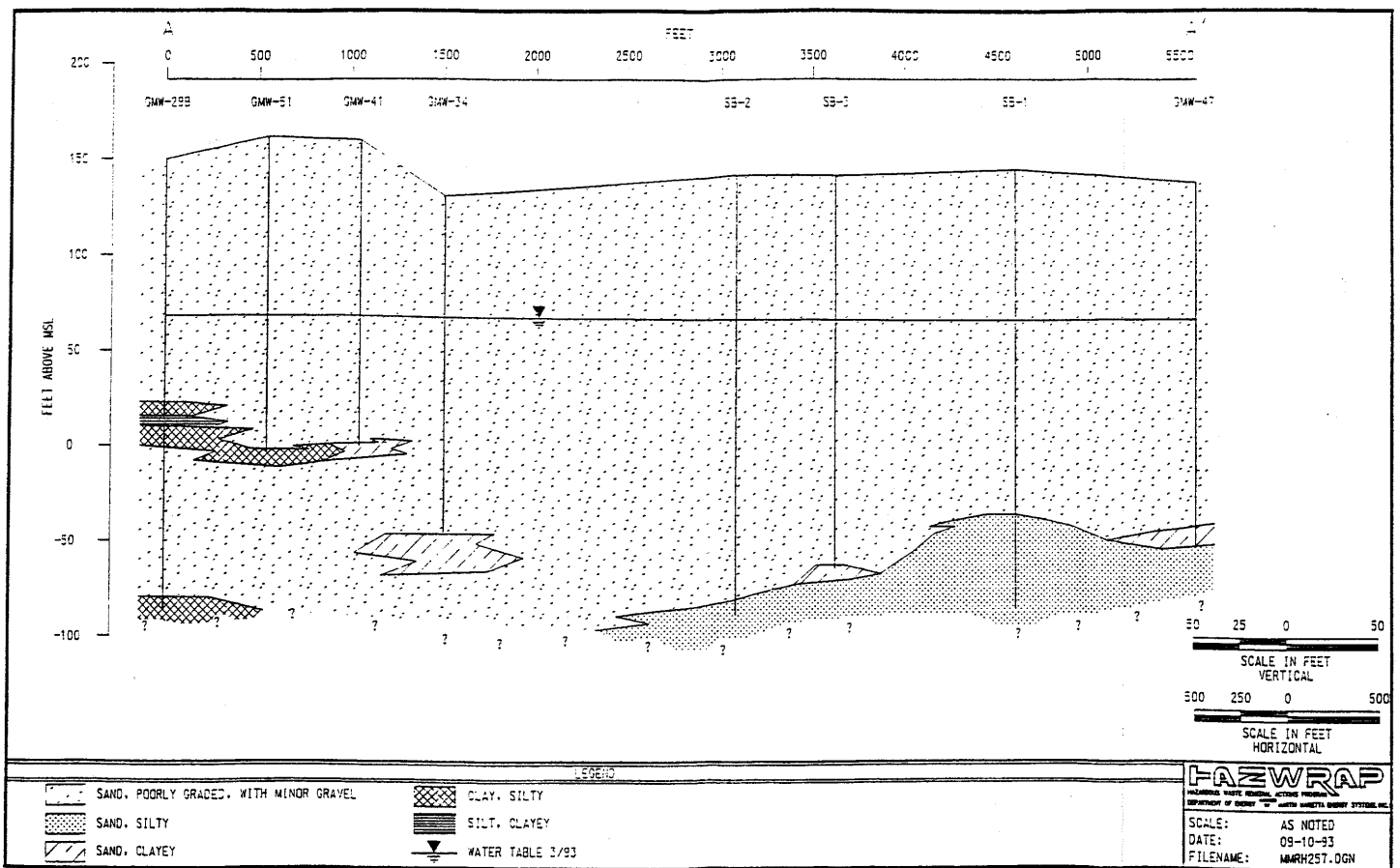


Figure 4-4 Cross Section BB'

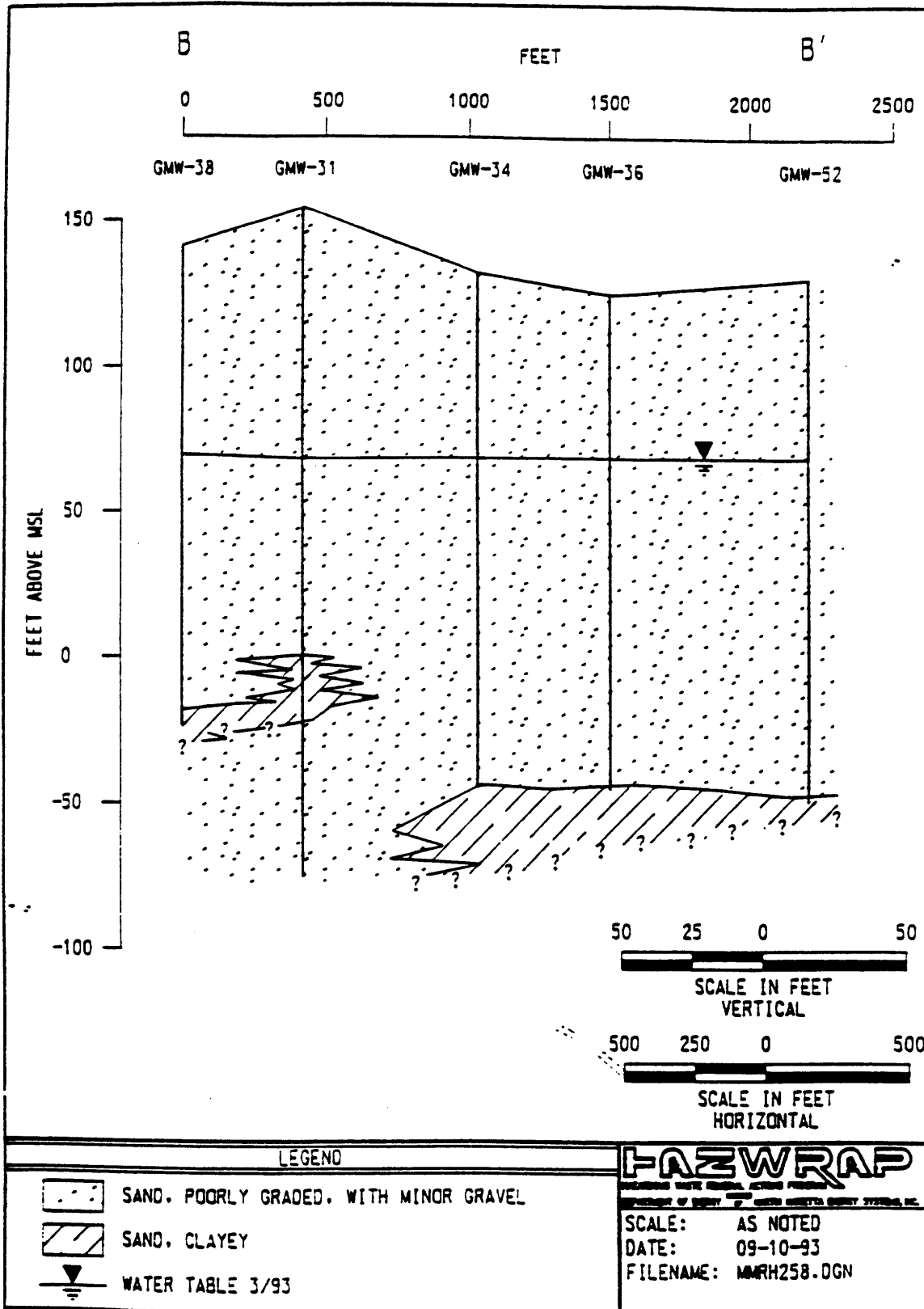


Figure 4-5 Cross Section CC'

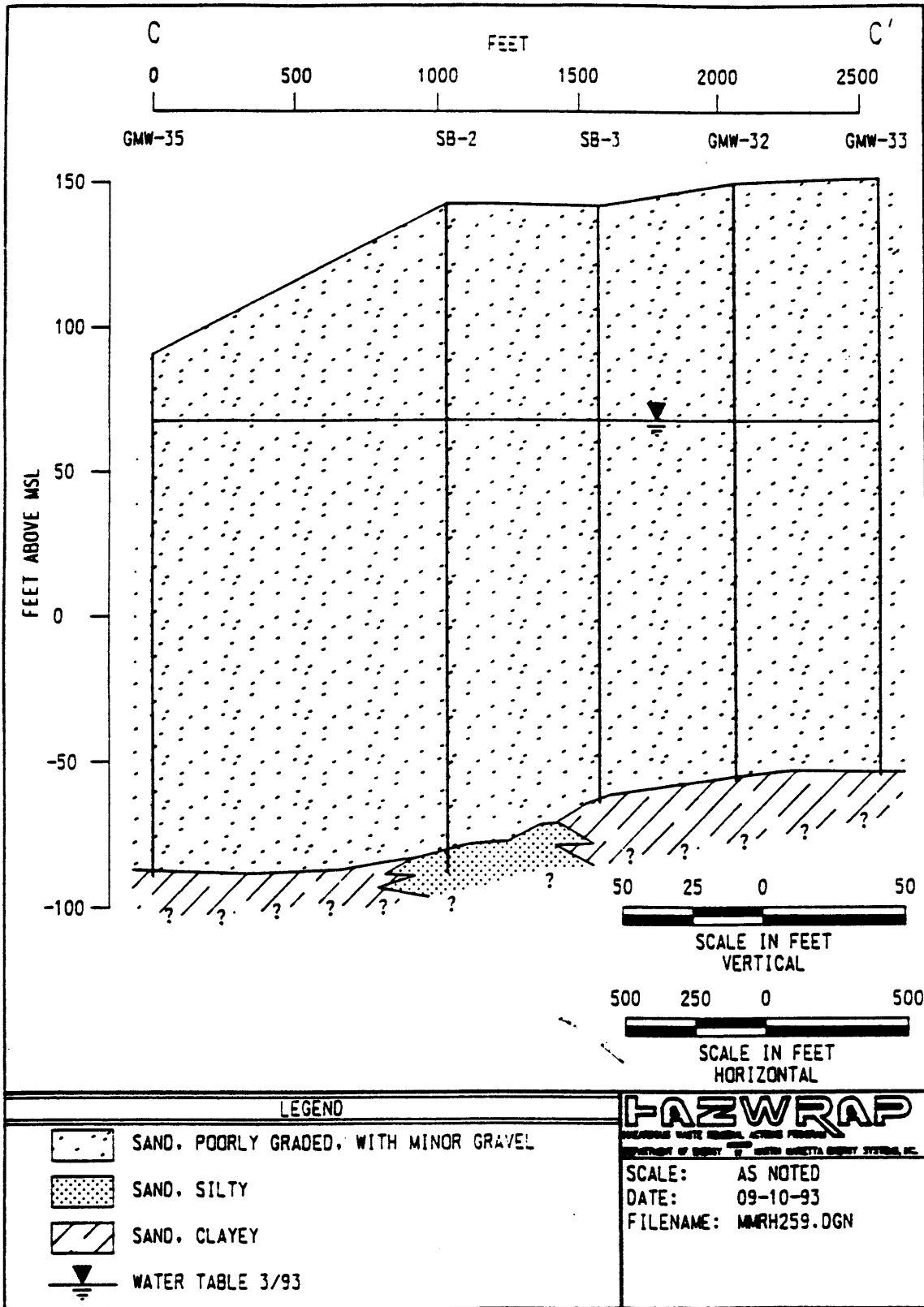


Figure 4-6 Cross Section DD'

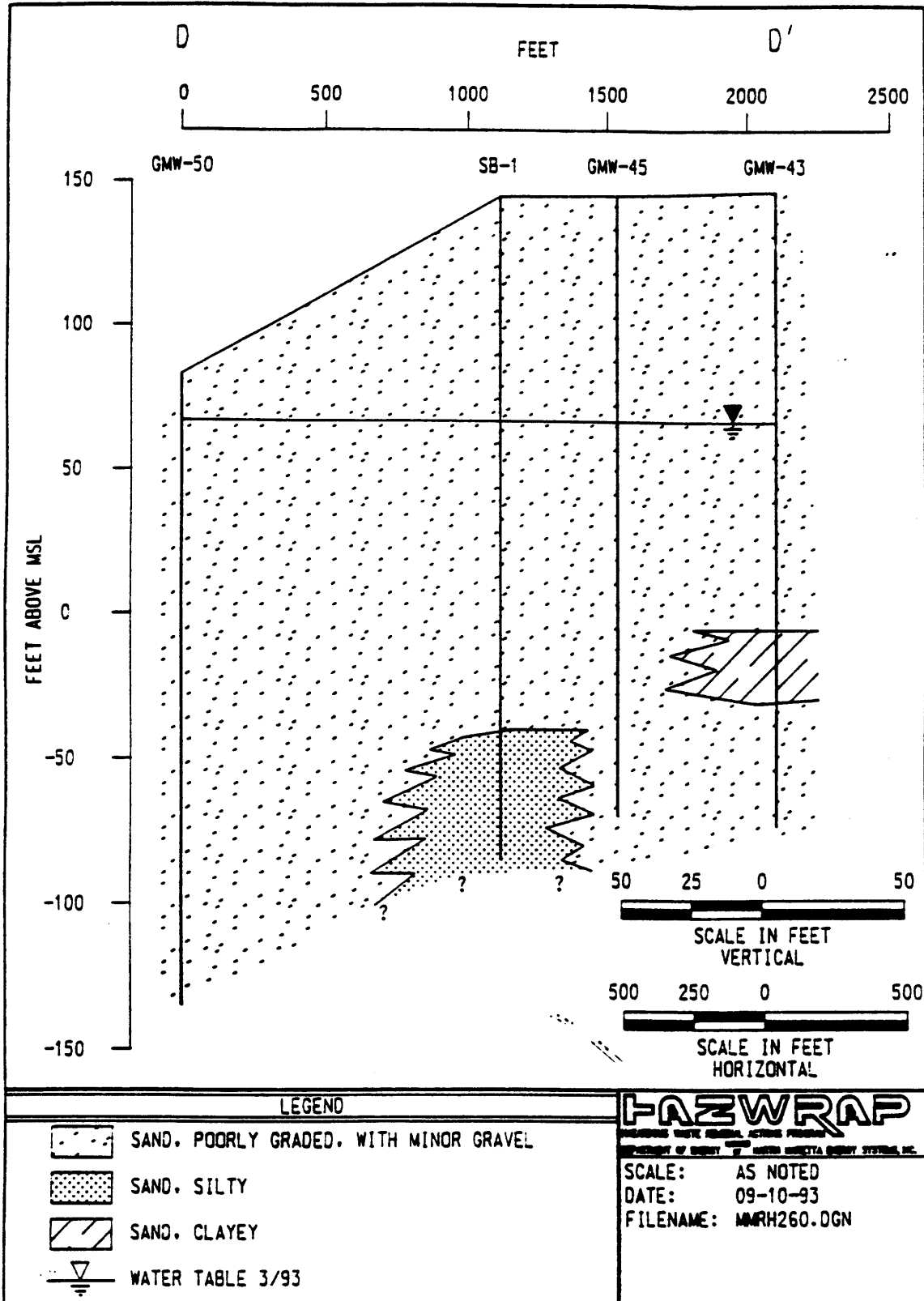


Figure 4-7 Source Area

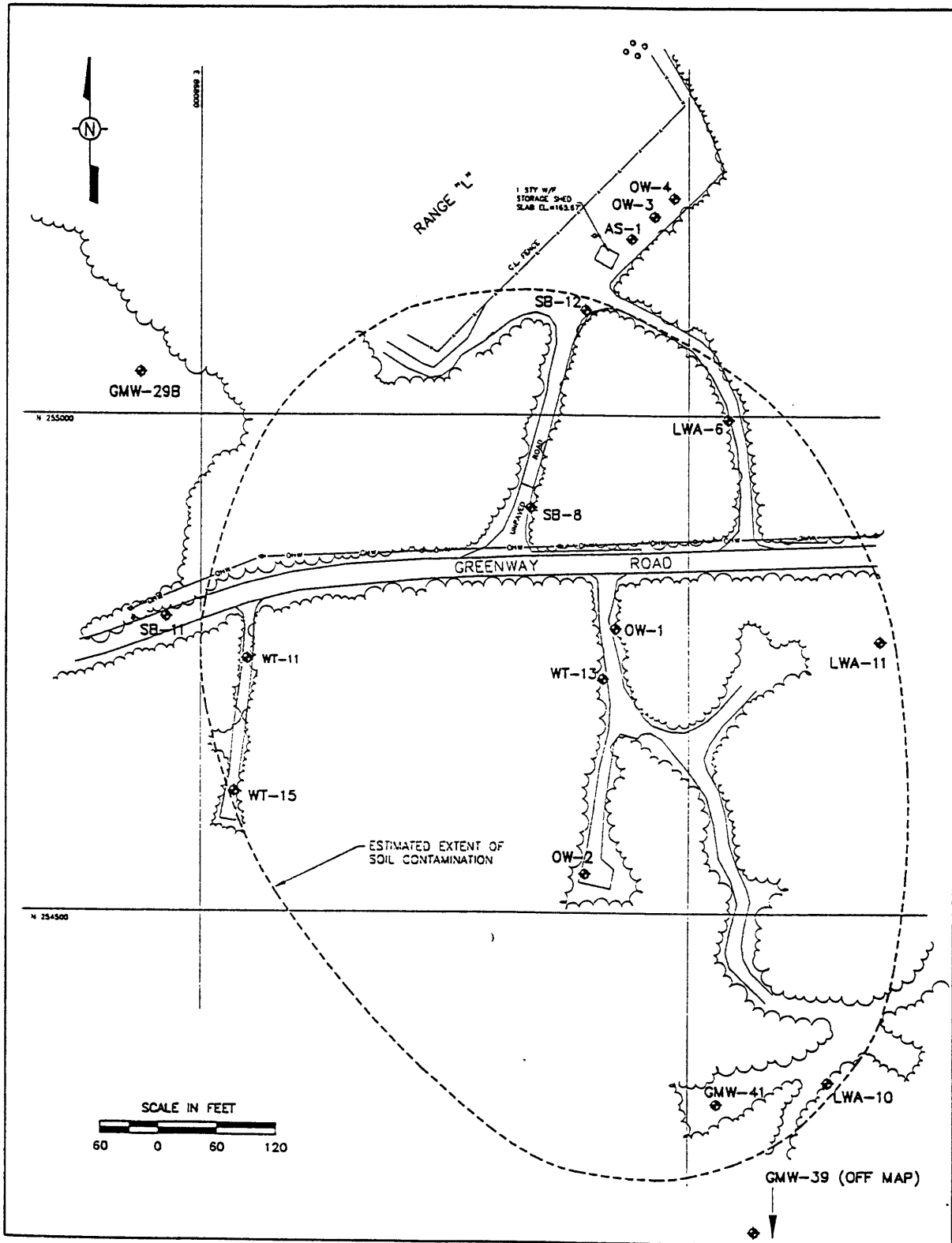


Figure 4-8 Digitized Map of the FS-12 Area

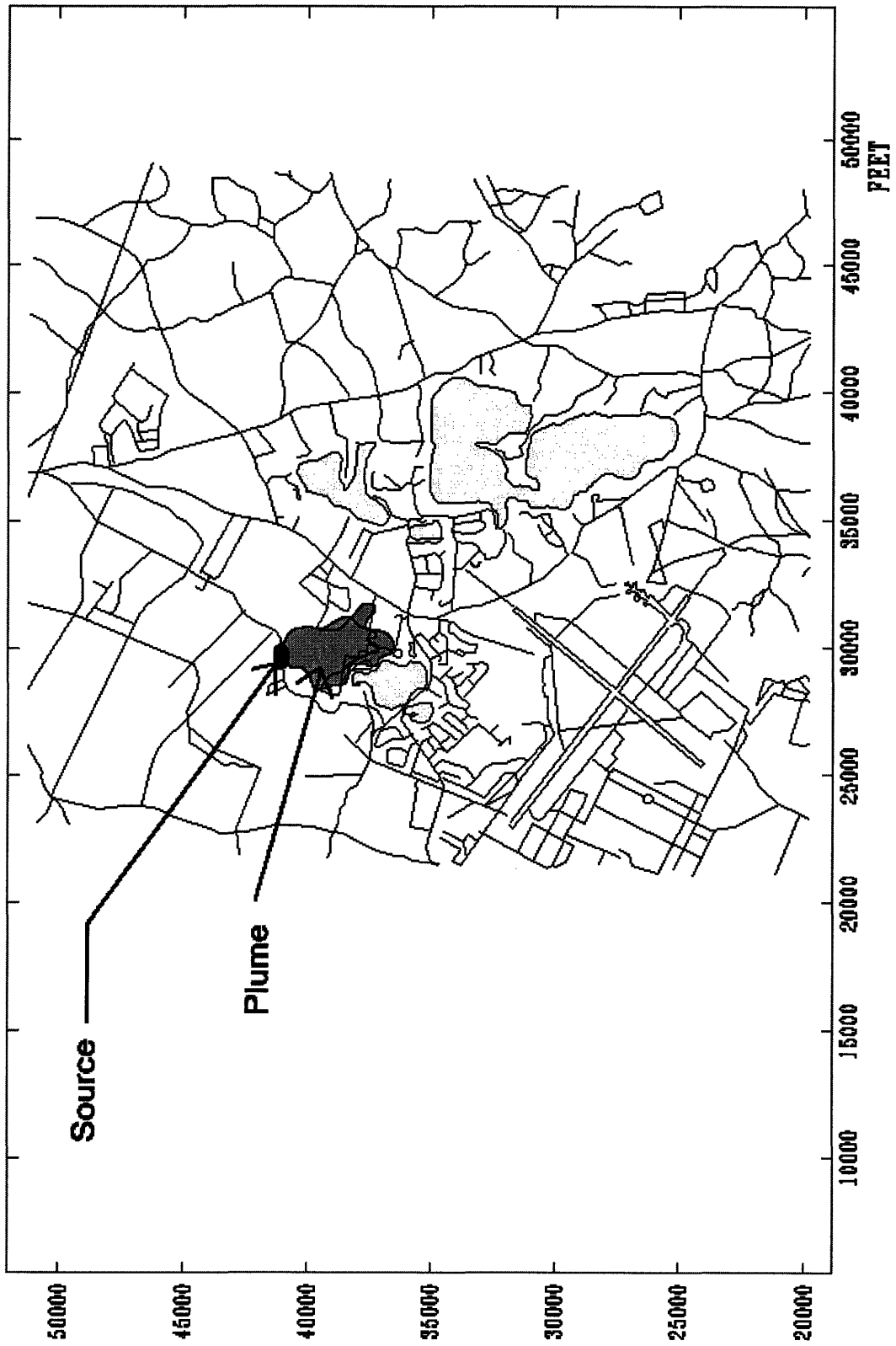


Figure 4-9 Generated Grid With Outline of Ponds

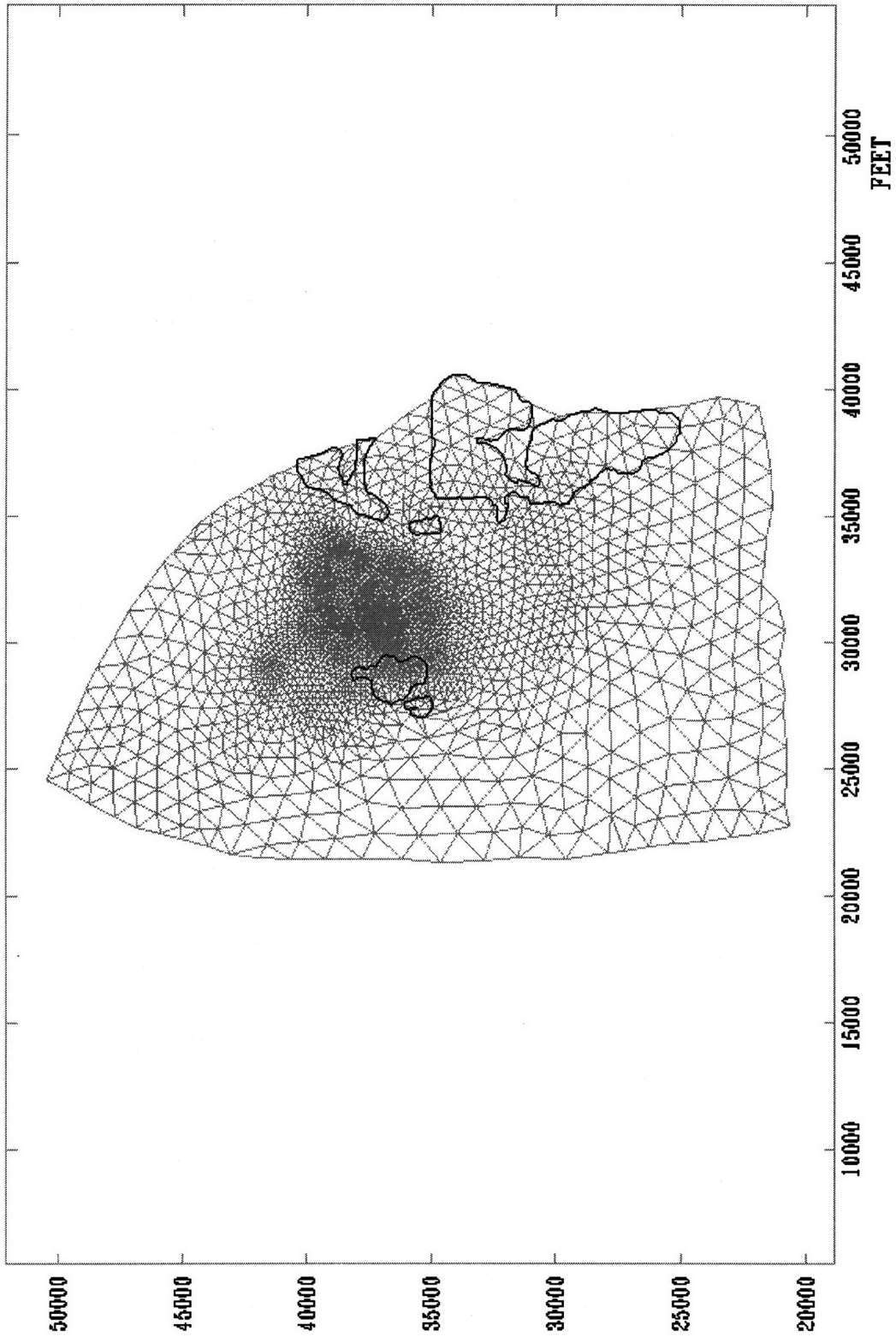


Figure 4-10 Grid and Boundary Conditions

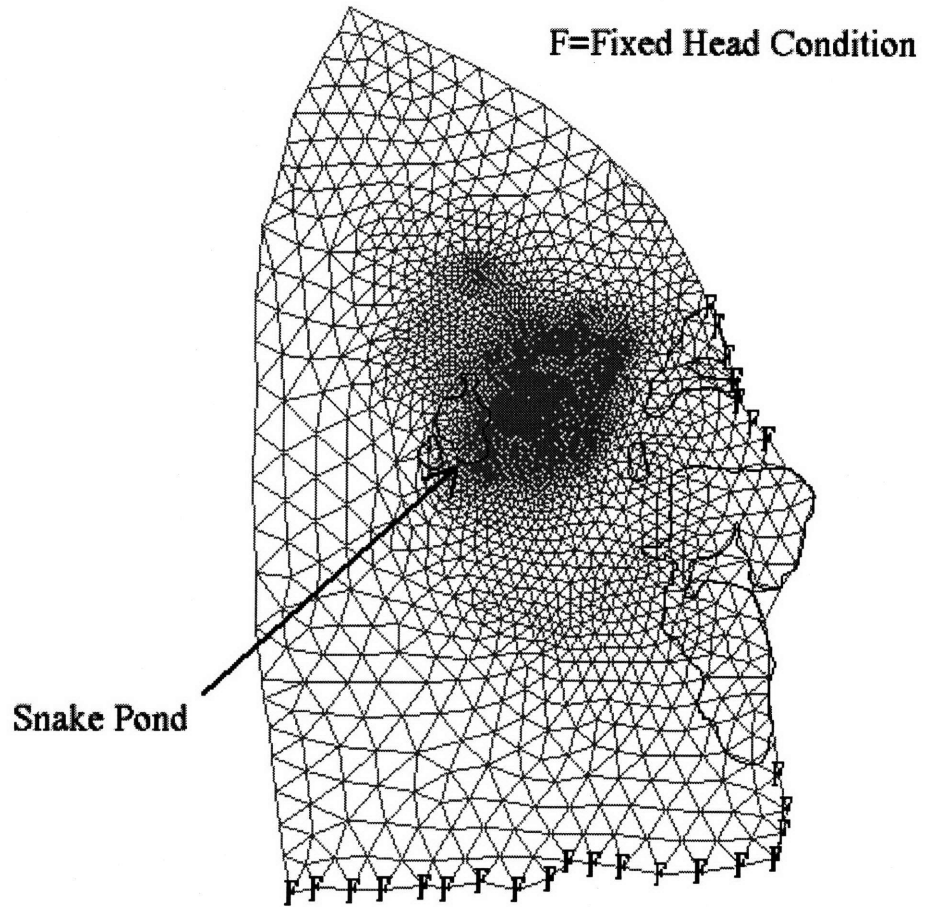


Figure 4-11 Location of Cross Sections



Figure 4-12 Modeled Stratigraphy (AA')

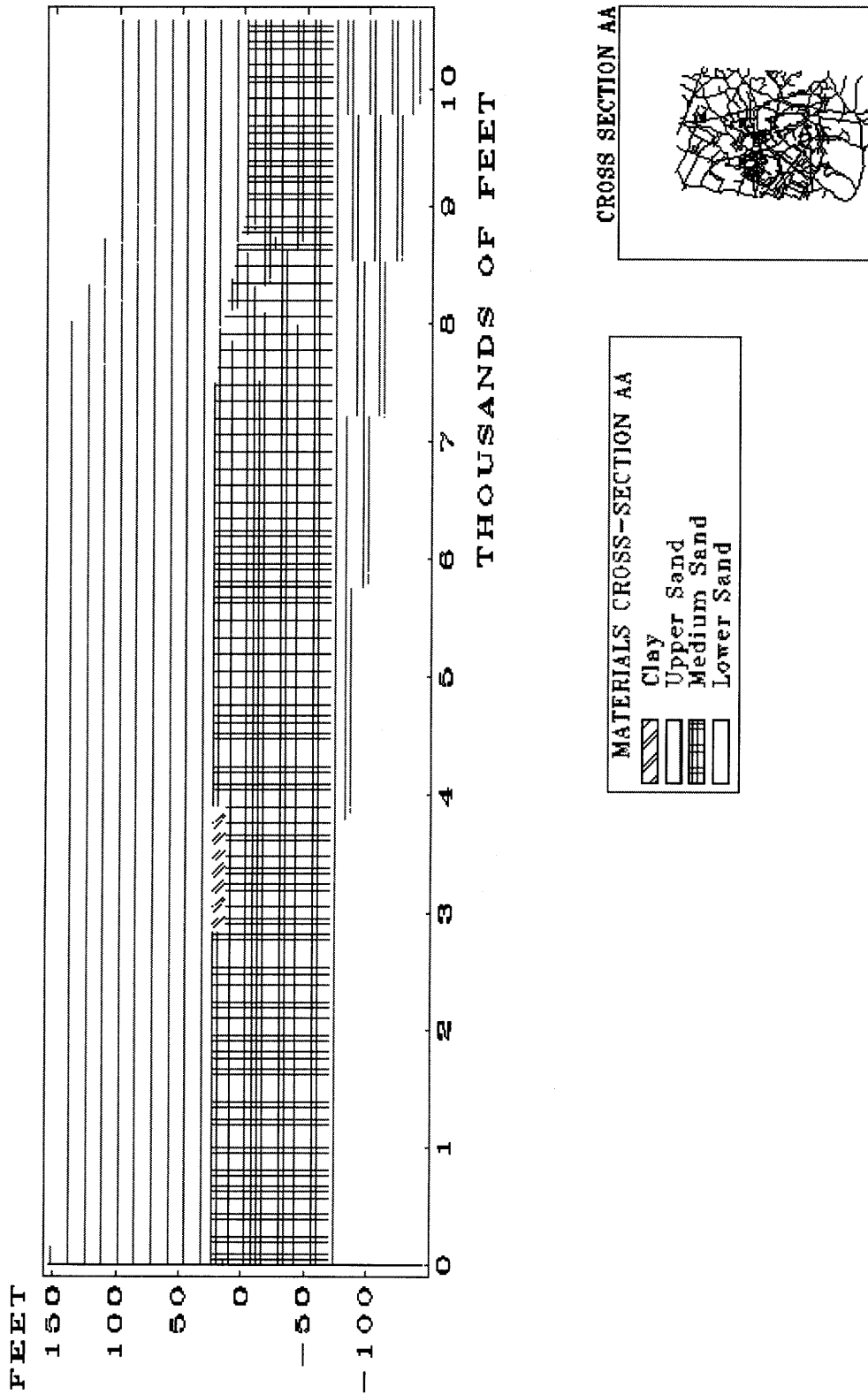
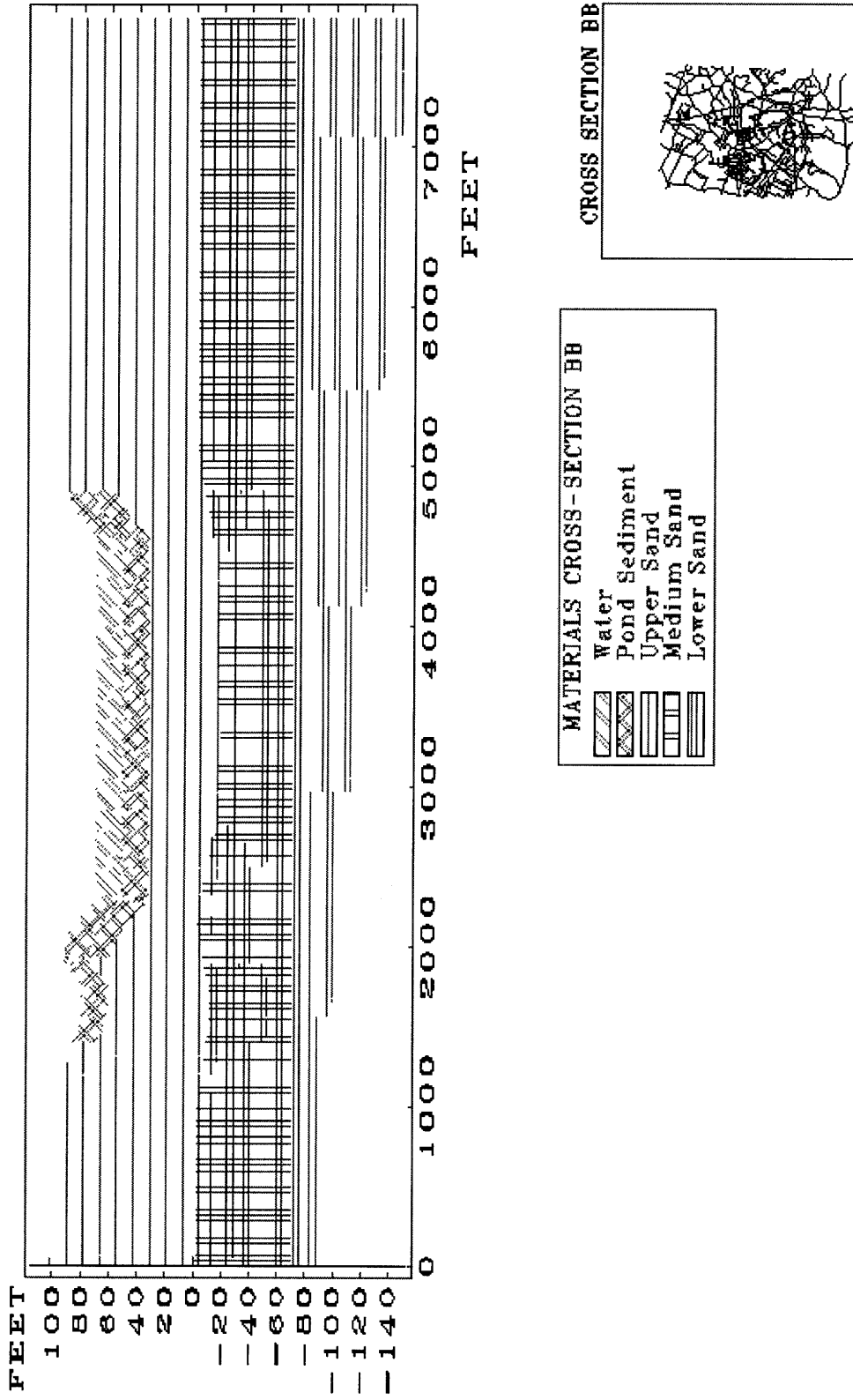


Figure 4-13 Modeled Stratigraphy (BB')



5. Model Results And Assessment

The development of the model provided a lot of information regarding the FS-12 area and the migration of the contaminants. It also identified certain questions which need to be answered, or studies which need to be conducted, in order to get a more accurate representation of the subsurface and its groundwater flow. In the following paragraphs, the model results are described and analyzed.

5.1 Groundwater Flow Field

5.1.1 Calibration

The final values of the input parameters shown in Table 4-1, were chosen so as to produce a groundwater flow field which matches observed data. The data used for the calibration, was the observations in Savoie, 1995. The head distribution simulated by Dynflow was compared to the data from the observation wells in Savoie, 1995 and the results are shown in Figure 5-1. The average difference between observed and calculated head values was 0.348 ft with a standard deviation of 1.687 ft. Considering that the overall head difference in the area of concern is approximately 20 ft, the calibration was successful. The equipotentials from Savoie, 1995 are also shown in Figure 4-14. It should be noted that these are interpolations from the well observations as well. The equipotentials from the calibration and Savoie, 1995 are in satisfactory agreement.

5.1.2 Calibration Uncertainties

As was pointed out in Section 4.3.4 one of the obstacles in the development of the model was the lack of data about the hydraulic conductivity of the geologic layers of the area. The values of the hydraulic conductivities were based on just one aquifer test [HydroGeoLogic, 1994] which is not adequate information. Therefore despite the agreement between observation and simulation, the simulation is uncertain because the conductivities are uncertain.

What's more, a second critical uncertainty concerns the location of the groundwater divide, which is the point with the highest hydraulic conductivity. It is located to the north of the FS-12 source. However, that area lacks observation wells and, consequently, hydraulic head data. Two groundwater resources maps used as a reference during this study [LeBlanc et al., 1986; Savoie, 1995] showed the locations of different observation wells and in both of them, the lack of data from the area where the groundwater divide seems to be was apparent. Since the grid was constructed so that its northernmost tip is at the groundwater divide [Figure 5-2] this results to one more source uncertainty about the flow calibration.

5.2 Benzene Transport

The second part of the modeling, consisted of particle tracking. Despite the well-calibrated flow field, two kinds of inconsistencies with observed measurements were indicated. The travel time of the modeled plume was higher than that observed, for same distances, and more important, the vertical position of the plume was higher than the concentration data distribution showed. These two inconsistencies are illustrated below.

The results from the benzene particle tracking are shown in Figures 5-3, 5-4, and 5-5. Figure 5-3 displays a particle tracking run conducted for a period of ten years. In the simulation the plume is shown to have traveled a distance of approximately 3000 ft (the center of mass has traveled a little less, approximately 2500 ft [see the cross-section in Figure 5-5]). The observed horizontal extent of the plume [Figure 5-6] is similar; however, the real travel time of the contaminants has been approximately twenty years, which means that there is a difference of a factor of two between observation and simulation.

The second -and more important- difference between observation and simulation is the vertical position of the contaminant plume. Figure 5-7 displays a vertical cross-section of the subsurface along the longitudinal axis of the plume. The vertical position of the simulated

plume is displayed as well as observed benzene concentrations. It is obvious that the observed data are lower than the modeled data by approximately 25 feet. It should also be mentioned that the modeled concentrations were greater than the observed ones by one to two orders of magnitude.

The above deviation from the real situation is attributed to the uncertainty of the position of the groundwater divide. As was mentioned, the position of the modeled divide was estimated from the groundwater contours in Savoie, 1995. It is believed (as a result of the model-data difference) that the modeled position is inaccurate. It is suspected that the location of the divide is closer to the source of the FS-12 spill, thus located further south than the topmost tip of the grid shows [Figure 5-2]. Closer proximity of the divide to the source would result in more pronounced vertical movement of the plume which would align the modeled plume with the observed data. The difference in travel time is attributed to the lack of hydraulic conductivity data. A difference of a factor of two between the input and the real values is possible, and it would explain the travel time difference.

5.3 Surface Water Impacts

One of the primary intentions of this study is to predict potential impacts on Snake Pond from the migration of contaminants from the fuel spill. Despite the departures from the actual plume characteristics described above, the modeled plume provides significant information about the safety of Snake Pond. First of all, it is assumed that the higher velocity of the contaminants, as shown in the modeled plume, does not alter the path they follow. A change in the position of the groundwater divide would possibly alter the vertical velocity and a lower value of hydraulic conductivity would alter the horizontal velocity, but the horizontal path would not change since the hydrogeologic characteristics would stay the same. The horizontal extent of the plume is believed to be an accurate representation of the contaminants' path.

The vertical location, although not accurate, can be considered a 'worst case scenario' for the pond. The plume's high vertical position can only be a greater threat to the pond, as the contaminant particles' likelihood of being discharged in the pond is increased.

The simulation in Figure 5-3 (and the blown-up in Figure 5-4) depicts a ten year run with the input parameters shown in Table 4-2. It is obvious that there exists a small number of particles (therefore a certain mass of benzene) which are discharged into Snake Pond [Figure 5-8]. The estimate of the concentration resulting from adding the mass of the particles in the

pond was suspected to be inaccurate because Dyntrack deletes particles which contain mass below a threshold. It was, therefore, decided to estimate the resulting concentration in the pond by using a box model approach.

The pond was considered to have the following inflows and outflows:

Q_{in} , the groundwater flow entering Snake Pond,

Q_{out} , water coming out of the pond and entering the groundwater.

The following concentrations are associated with these flows:

C_{in} , benzene concentration of water entering the pond,

C_{pond} , the steady-state concentration in the pond.

Finally, volatilization was also considered as a process of removal of benzene from the pond. The surface water decay rate of 0.0533 (half-life of 13 days), mentioned in Section 4.3.4, was assumed to be attributed to volatilization.

A steady-state mass balance was conducted:

$$Q_{in} * C_{in} = Q_{out} * C_{pond} + k * C_{pond} * V$$

where Q's are the flows expressed in ft³/day, C's are the concentrations expressed in mg/L, k is the decay/volatilization rate expressed in days⁻¹, and V is the volume of the pond (ft³). (The necessary unit adjustments were done during calculations).

The decay rate is $5.33 * 10^{-2}$ days⁻¹.

The discharge in the pond was calculated by programming Dynflow to compute the hydraulic head gradients at the horizontal and vertical boundaries of the pond, and then applying Darcy's law. Since there is no accumulation or depletion of water from the pond, the outflow was equated to the inflow. The value obtained by Dynflow was 262,000 ft³/day. However, since the modeled travel velocity was double the observed velocity, a flow of 131,000 ft³/day was considered.

The concentration of benzene going into the pond was considered to be equal to the modeled benzene concentration of the groundwater at the location right before it enters the pond. This concentration was shown to be 10 mg/L. It should be mentioned that this concentration is a conservative estimate. The modeled concentrations were significantly higher than the observed ones (probably because of the conservative assumption of benzene solubility being the source concentration).

The volume of the pond was estimated by superimposing a square grid over the pond, thus calculating its area and then multiplying with the average depth of 25 ft. Thus, the volume is modeled to be 89,000,000 ft³.

Solving the above equation for C_{pond} , the resulting concentration is 0.27 mg/L. Before analyzing the risk associated with such a concentration in a water body like Snake Pond, it should be restated that the above concentration is a *very* conservative estimate. This is due to the following factors: 1) the modeled plume is higher than what the observed concentration distribution shows, therefore closer to the pond 2) the concentration at the source is assumed to be equal to benzene's solubility, which in turn increases the concentration entering the pond (by one to two orders of magnitude), 3) lowest observed decay rates for benzene in water were used (for groundwater and surface waters).

Even with the above assumptions which, probably, give a high prediction for the concentration in the pond, the resulting concentration does not pose significant risk. The associated carcinogenic risk, assuming that the exposure pathway is dermal contact, was calculated with the equation shown in Table 5-1. It is the standard equation used by the Environmental Protection Agency [Automated Sciences Group, Inc., 1994].

The resulting risk for a 0.27 mg/L concentration is 1.26×10^{-6} . The target risk level according to the Massachusetts Contingency Plan is 1×10^{-5} [Automated Sciences Group, Inc., 1994]. The calculated risk is, therefore, well below the legislated standard. Actually, the concentration which would result in the threshold risk is 2.136 mg/L, 8 times higher than the expected one.

The above calculations show that the risk associated with the possible discharge of chemicals to Snake Pond is low and there is no threat to humans.

Table 5-1 Risk Assessment Parameters and Methods

DERMAL RISK/EXPOSURE Parameters	Dermal Risk/ppm	Dermal CSF (mg/kg/day) ⁻¹	Exp. Dur. years	Exp. Freq. days/yr.	Surface Area cm ²	Dermal Perm. cm/hour	Unit Adj. l/cm ³	Unit Adj. hours/day	Body Wt. kilograms	Avg. Time years	Unit Adj. days/yr
<i>Volatile Organic Compounds</i>											
Benzene	4.6807E-06	0.0280	5	5	19,400	0.0248	0.001	24	70	70	365
DERMAL RISK/EXPOSURE = (Exposure Duration x Exposure Frequency x Dermal CSF x Surface Area x Dermal Permeation) x (Unit Adjustments)											
Notes Assumed frequency of exposure: 5 days per year Assumed duration of exposure: 5 years (remediation will have occurred by then) Other data are EPA standards [from Automated Sciences Group, Inc., 1994]											

Figure 5-1 Modeled Hydraulic Head Contours

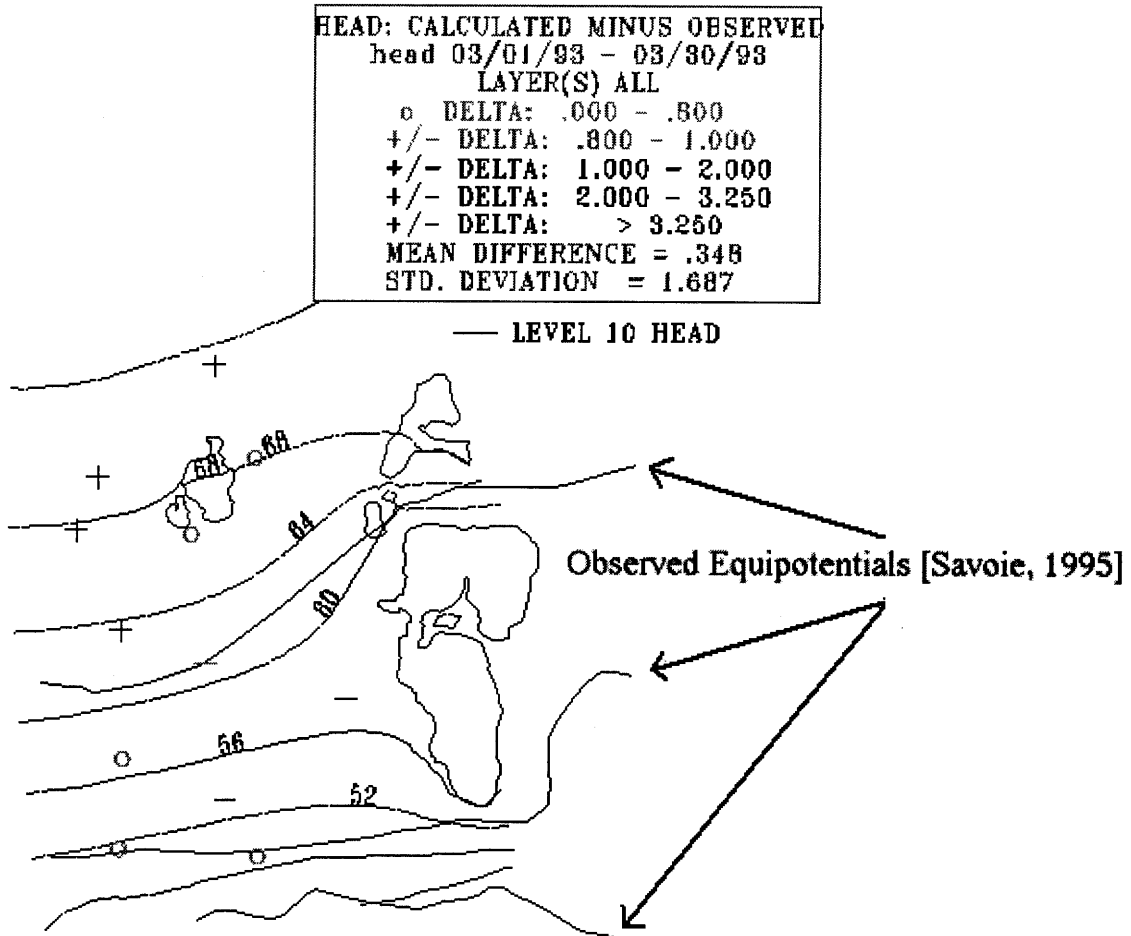


Figure 5-2 Groundwater Divide Position

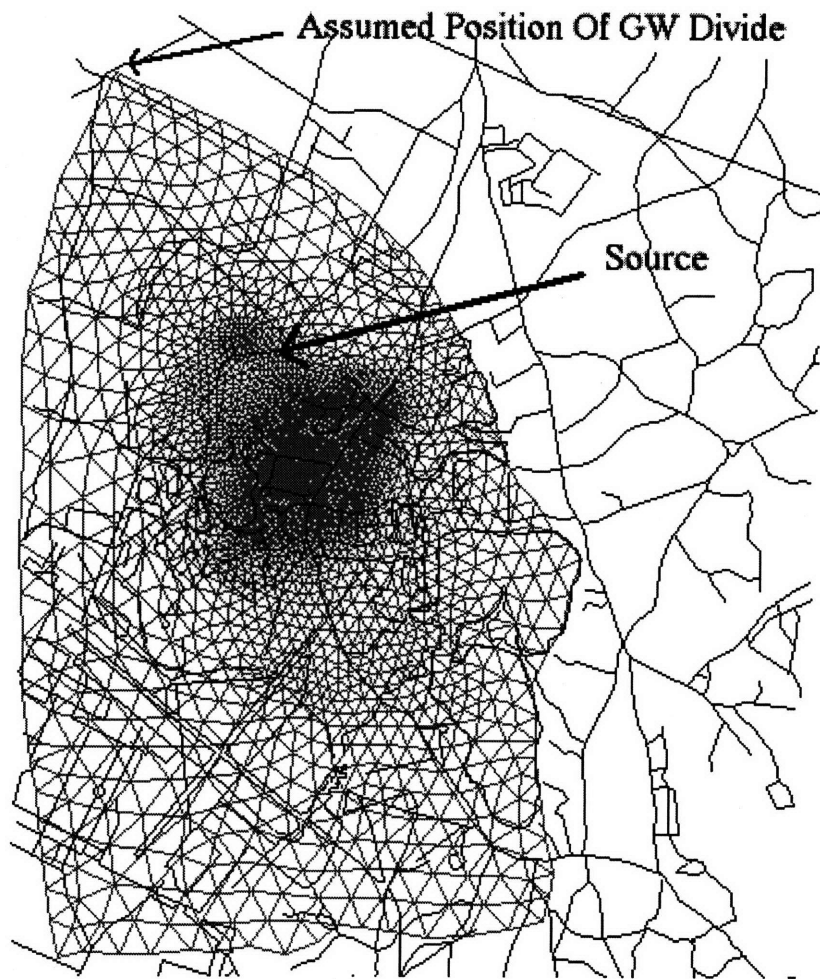


Figure 5-3 Plan View of the Plume



Figure 5-4 Plan View of the Plume (Blow-Up)

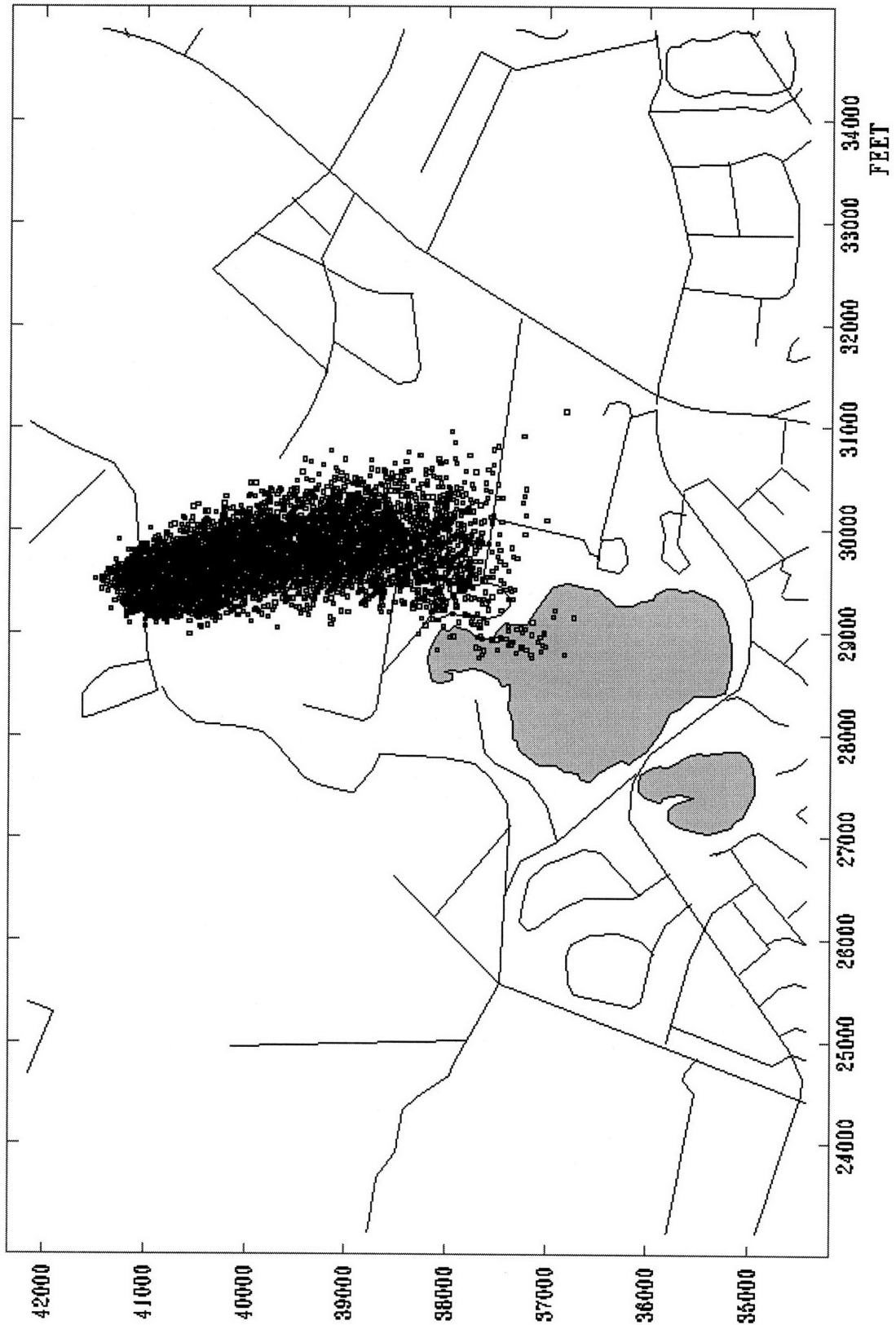


Figure 5-5 Cross Section Across Plume

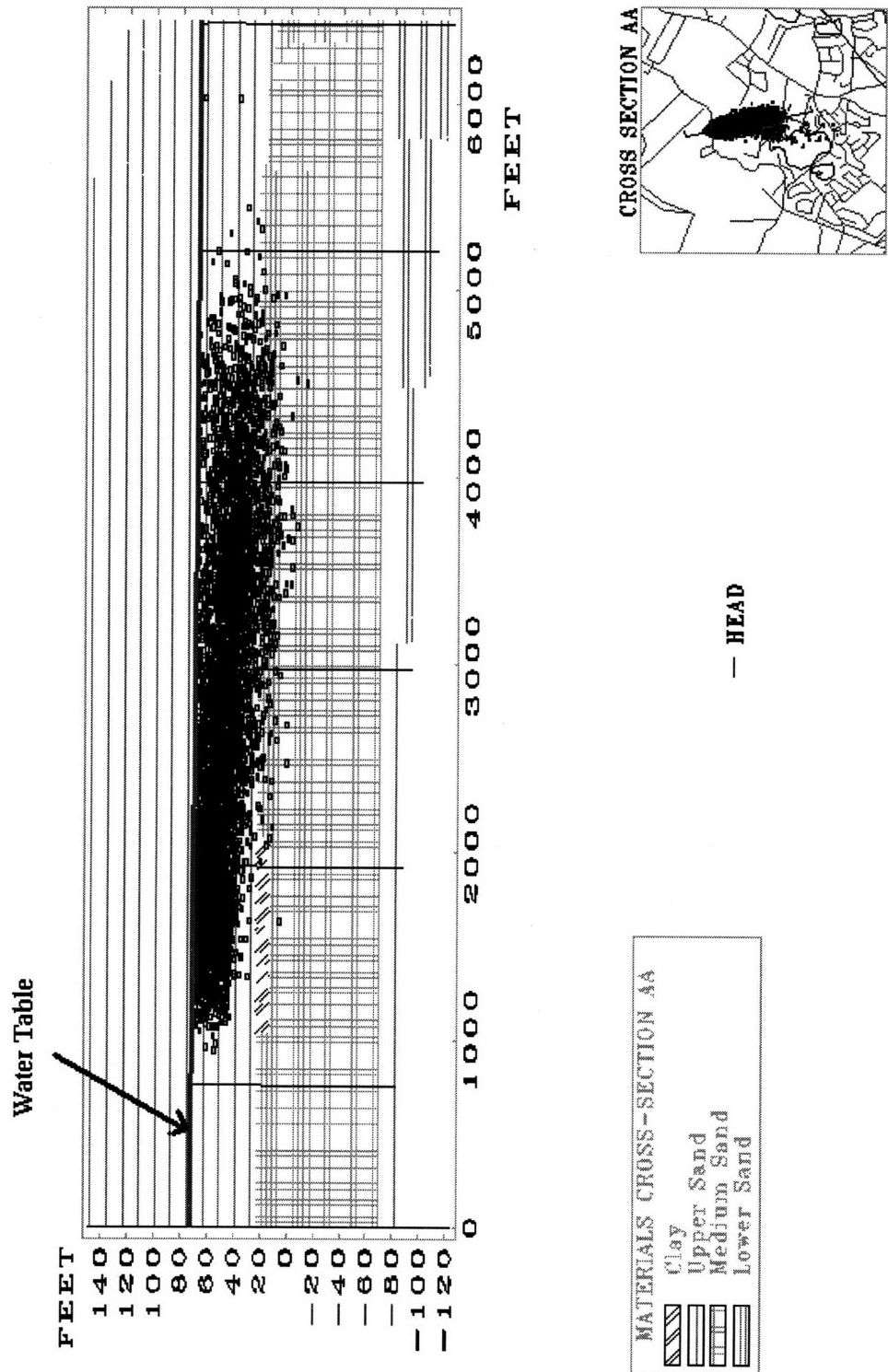


Figure 5-6 Observed Benzene Concentrations

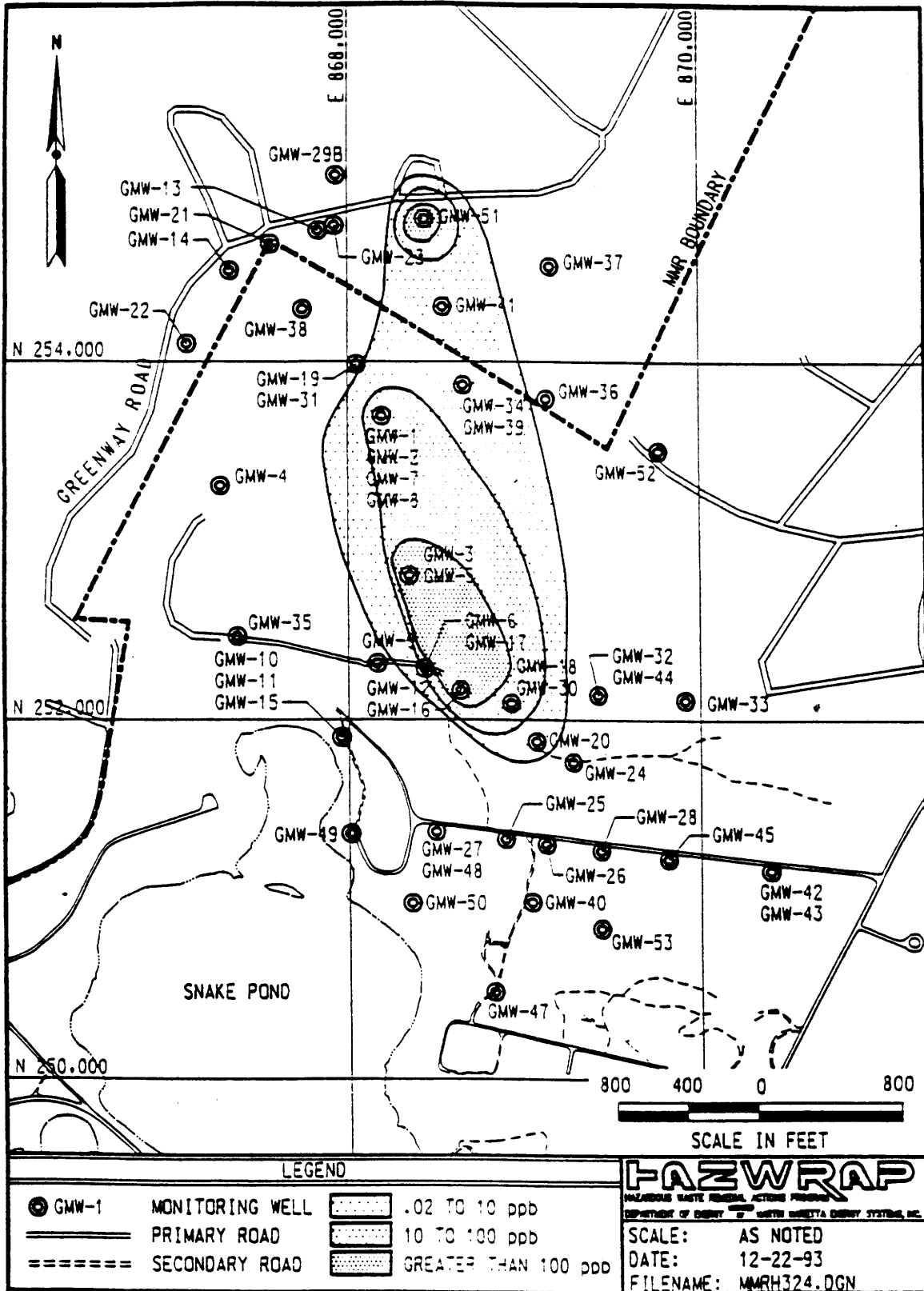


Figure 5-7 Vertical Location of Observed Benzene Concentrations

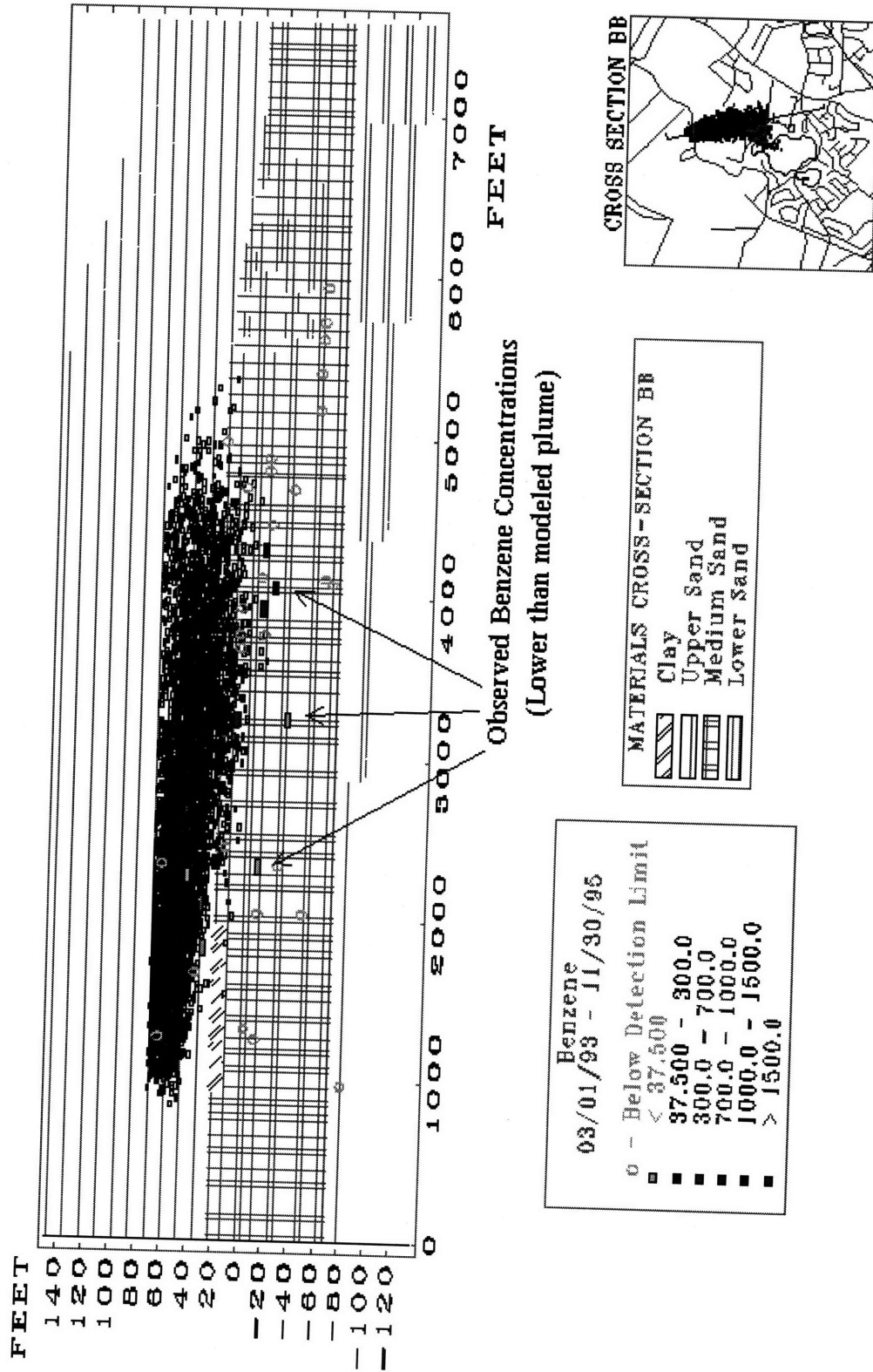
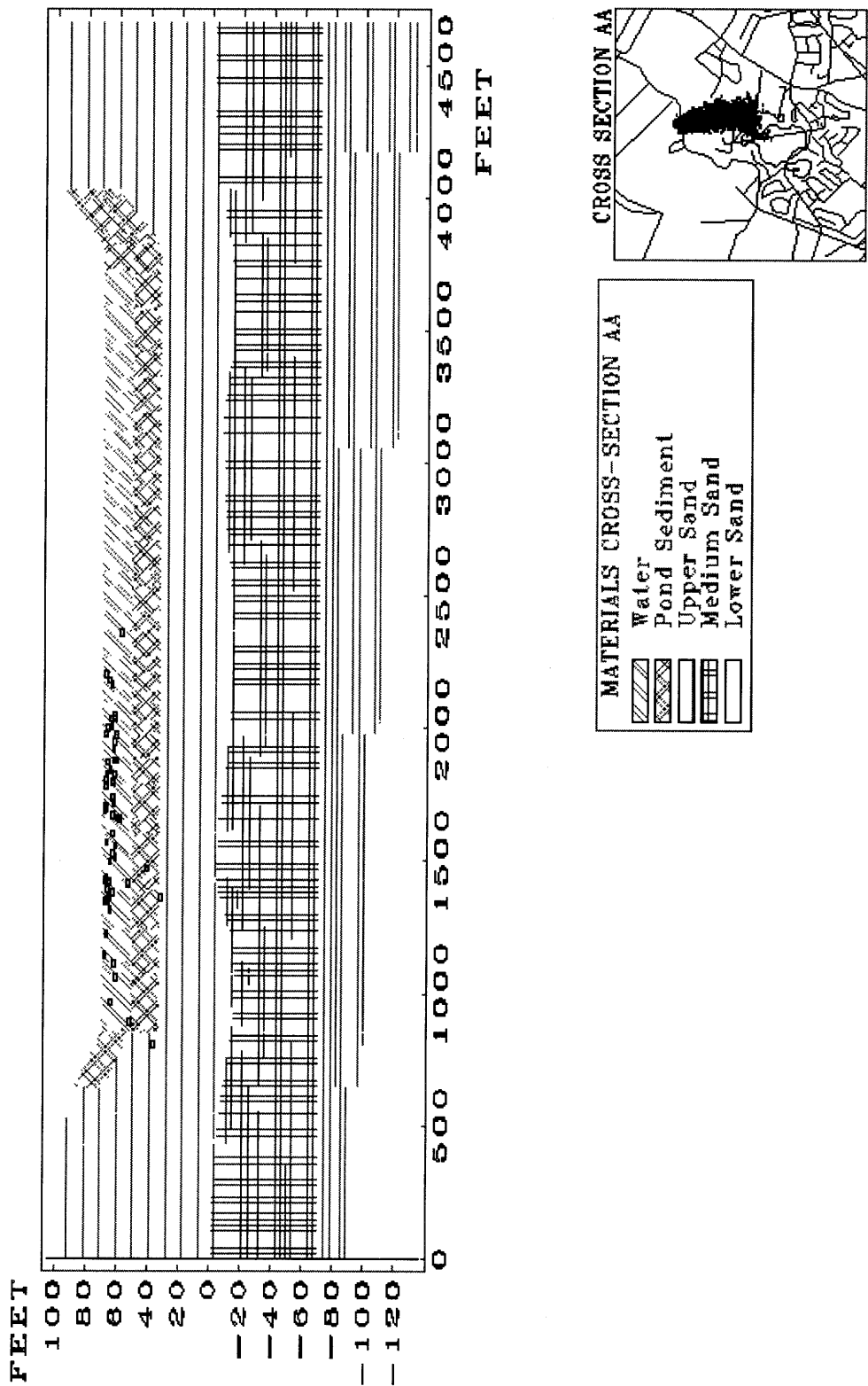


Figure 5-8 Cross Section Across Snake Pond



6. Summary, Conclusions, and Future Work

6.1 Summary and Conclusions

The transport and fate of the spilled jet fuel at FS-12 were examined using a finite element computer model, in order to assess the potential danger of contamination for Snake Pond, the closest surface water body used by humans. Benzene was simulated because it was determined to pose the greatest threat to humans.

Although the modeled plume did not match the observed data perfectly, it gave a 'worst-case scenario' as far as discharge into Snake Pond is concerned. The results show that even in this 'worst-case scenario,' the concentration of benzene in the pond was negligible, showing a very conservative estimate of 0.3 mg/L. The risk associated with such a concentration was below State standards. Furthermore, it should be noted that the modeling did not take into account any of the current efforts to control the source or the leading edge of the plume. Since these efforts are also decreasing the amount of contaminants in the subsurface, the safety of the pond is certain.

6.2 Future Work

Although this study reached a conclusion in regard to the safety of the pond, it did not accurately depict the movement of the plume. As was discussed, a probable cause to the encountered difficulties was the uncertainty of the groundwater divide location. Therefore a future modeling effort should concentrate on this issue.

Concurrent with this study, were two other modeling efforts for two other plumes at the Massachusetts Military Reservation. It is the belief of the author as well as of the authors of the other two reports (Personal Communication with Kishan Amarasekera and Enrique

Lopez-Calva) that a complete modeling effort at Cape Cod should include all the Cape, and not just sections of it. Because the aquifer in Cape Cod is a sole source aquifer, many local characteristics, such as the location of the divide, possibly affect the flow of the water on a regional scale. By dividing the Cape in smaller modeling areas, it may be impossible to account for such effects which, in turn, result in uncertain predictions. Data are especially limited in the north part of the Cape, which is a substantial part of the area's flow system. As far modeling with the intention to assess remediation schemes for the MMR is concerned, then, a model including all the contaminated sites (even though not the entire Cape) would be more efficient.

Hence, although in this case a local model answered questions regarding the safety of the pond, a regional model will be better suited for simulating Cape Cod's groundwater resources.

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