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Developing Spatial Environmental Models For Risk-Based Decision Making

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Developing Spatial Environmental Modeling Systems For Risk-Based Decision Making

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Thesis

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Abstract

Developing Spatial Environmental Modeling Systems For Risk-Based Decision Making

Julie Kim, M.S.E

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Models developed in a Geographic Information System framework serve as useful analytical tools for assessing environmental risk and making corrective action decisions. In this research, three site-specific models were developed for a petroleum facility in Marcus Hook, Pennsylvania, to better understand subsurface conditions, groundwater movement and its groundwater interaction with surface water.

The first model is a contour map-based model that uses a procedure developed to analyze potential sources and source areas by overlaying maps of quantitative measurements of chemicals of concern with spatial features consisting of qualitative historical descriptions of environmental conditions. Despite limited underground pipeline information, the model identified the central region as a potential source area with various potential chemical sources.

The second model is a conservative screening-level groundwater/ surface water interaction model that calculates a target groundwater level for each chemical of concern,

so that its predicted surface water concentration meets state surface water quality standards. Benzene was the only chemical above its target groundwater concentration by a factor of forty. Since the interaction model depends on the accuracy of the groundwater flow model, the target level for each chemical changes for different groundwater flow values.

The third model is a comprehensive groundwater flow model that uses the subsurface description developed in ArcView, GMS, and MODFLOW. Two groundwater models were created based on different complexities, assumptions, and inputs. Both incorporated important subsurface features previously not included in the original model. The new models provided a more probable groundwater flow distribution than originally estimated; about 75% of groundwater flows into the minor tributary in the case study site, while the remainder flows to the major tributary.

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CHAPTER 1

INTRODUCTION

1.1 Objective

Researchers at The University of Texas at Austin are currently developing and integrating a methodology for Spatial Environmental Risk Assessment and Decision Analysis Framework for corrective action. This methodology is based on a Geographic Information System (GIS) framework and is applied to a case study site at the Marcus Hook Refinery (Marcus Hook) in Pennsylvania for remedial action. Eventually, the tools for environmental risk assessment and decision analysis may be applied to other large, complex industrial facilities.

This thesis focuses on the development of three environmental models that describe the subsurface environment at Marcus Hook. The first model uses a procedure to analyze potential sources and source areas based on a digital description of the facility, and provides qualitative descriptions of historical environmental conditions and quantitative measurements of chemicals of concern (COCs). The second model links a simple groundwater model with a surface water model to calculate a target groundwater concentration of a COC, so that its predicted surface water concentration meets Pennsylvania water quality standards. The third model is a groundwater flow model that uses the subsurface description developed in ArcView and Groundwater Modeling System (GMS) to understand and predict groundwater flow patterns. Understanding the

interactions between the surface and subsurface is a key to effectively assessing environmental risks associated with the fate and transport of COCs.

1.2 Spatial Environmental Risk Assessment using GIS

Risks are based on exposure pathways that describe the means by which a receptor is exposed to a COC. Figure 1.1 demonstrates an example of an exposure pathway. In general, exposure pathways include the source area (*COC in soil resulting from a release*), the transport mechanism (*groundwater*), the point of exposure (*a creek downgradient from the source area*), and the potential receptors (*worker and frog in the creek*) (Hay Wilson 1997).

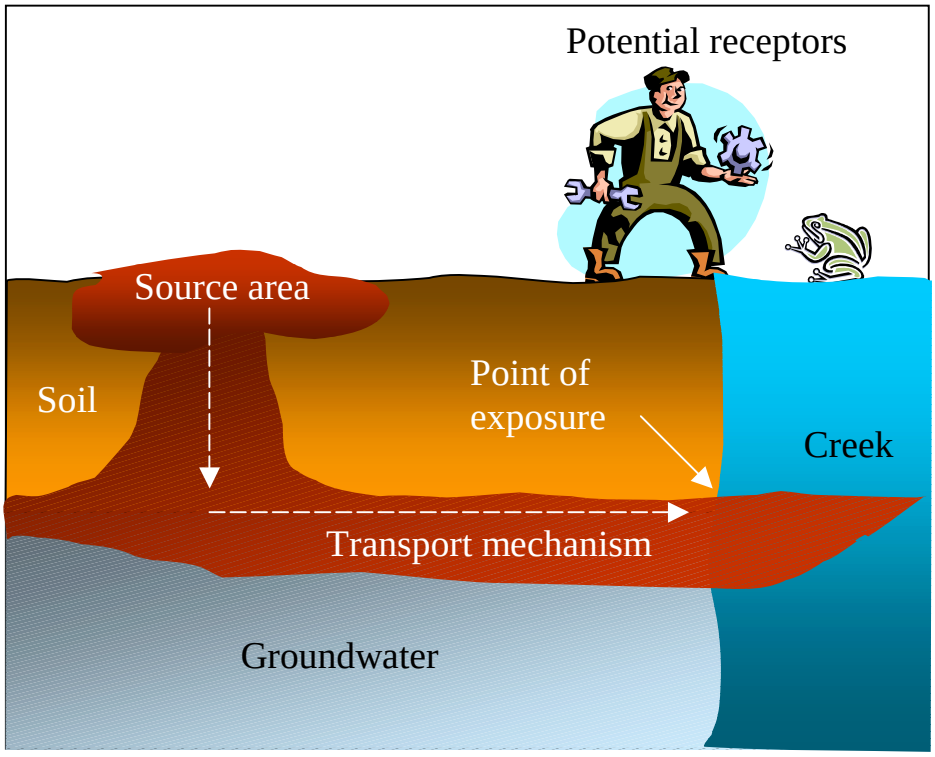


Figure 1.1: Example of an exposure pathway.

Environmental risk assessment helps develop an understanding of these exposure pathways. When a COC is discharged into the environment, there is a possibility for harmful effects to human and ecological receptors. Risk assessment is a process of estimating this potential for harmful effects.

Risk is a function of toxicity and exposure. Toxicity information can be obtained from the Environmental Protection Agency's (EPA) Integrated Risk Information System (IRIS) or from reference concentrations and slope factors. Exposure looks at where COCs in the environment could be and where receptors would come in contact with the COCs. Regulatory levels are based on risk, water quality protection, and environmental protection.

The risks vary based on the chemical properties of the particular substance released. COCs can have non-carcinogenic and carcinogenic effects on humans. For non-carcinogens, a threshold exists where, up to a certain dose, there is no observable adverse effect. Carcinogens do not have this threshold; instead, the dose of a carcinogen is proportional to an increased occurrence of cancer, based on the linear, no-threshold model for carcinogenic effect.

Once a chemical release is detected in the environment, the consequences must be assessed and corrective action decisions must be made. Risk-based decision-making is an iterative process that supports determining the best approach for protecting human health and the environment. The traditional approach has been to reduce COC concentrations to low levels regardless of cost and risk; however, in recent years, risk-

based corrective action accounts for health and ecological risks in addition to application costs (Hay Wilson et al. 1999a).

Figure 1.2 shows that risk assessment can be divided into three steps: exposure assessment, dose-response assessment, and risk characterization. The exposure assessment describes the transport of a COC from its source to a receptor. The dose-response assessment determines the toxicity of the COC. In addition, the magnitude of the dose is determined based on the exposure concentration. Risk characterization quantifies both the carcinogenic and non-carcinogenic effects associated with the receptor to a COC.

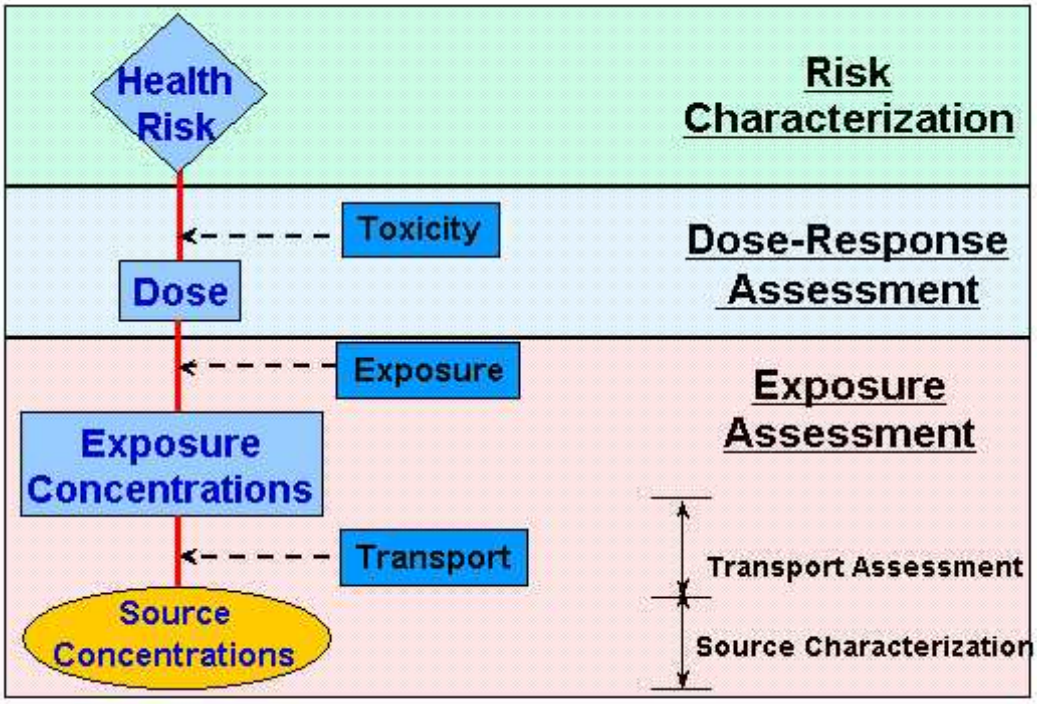


Figure 1.2: The general process of risk assessment
(*Source: Hay Wilson 1999*).

Implementing risk-based corrective action in practice is a challenge, particularly for larger sites like Marcus Hook (Hay Wilson et al. 1999b). Risk assessment at a large facility is a complex process because it requires managing and analyzing large quantities of temporal and spatial data. Thus, much of the current research was done within a GIS framework, with the aid of spreadsheets, relational databases, and computer models. The integration of these tools helps researchers evaluate risk and communicate risk to support risk-based decision-making.

Spatial environmental risk assessment can be viewed as an iterative process involving a digital facility description, a site conceptual model, and transport calculations (see Figure 1.3). The process begins with the development of a digital facility description, which contains the spatial and tabular databases for the refinery. The spatial database provides GIS shape files and coverages of the geographic and physical features in the refinery and its surrounding region. The tabular databases contain analytical, hydrological, and geological characteristics of the refinery.

Using the digital facility description, initial evaluations can be made to identify potential exposure pathways and estimate source concentrations, which become inputs for the site conceptual model. The site conceptual model describes the exposure pathways based on the chemical and physical characteristics of the facility. These calculation parameters are inputs to the transport calculations. The transport calculations involve the fate and transport of COCs. The outputs of these calculations are receptor concentrations, which are then input to update the site conceptual model.

Ultimately, all complete pathways are identified and represented in the digital facility description.

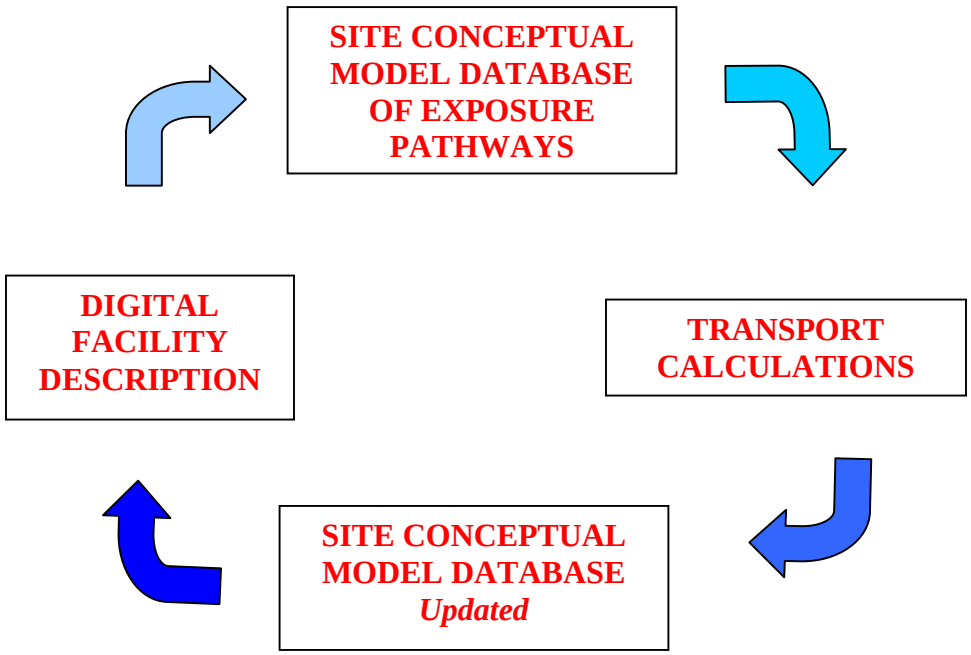


Figure 1.3: Spatial environmental risk assessment as an iterative process *(Source: Hay Wilson 1999).*

This thesis focuses on the digital facility description and the transport calculations shown in Figure 1.3. Lesley Hay Wilson has been developing the site conceptual model and running the iterations. Andrew Romanek developed the digital facility description, a facility surface water model, and a simple groundwater model. His thesis (Romanek 1999) discusses the digital facility description as the foundation

for risk assessment using GIS. The author's work builds on the existing digital facility description and groundwater model.

1.3 Study Area

Marcus Hook serves as the case study site because it has many potential sources, transport mechanisms, and receptors, which are typical of a large, complex industrial facility. Marcus Hook is a crude oil refinery and petroleum products storage facility (see Figure 1.4). This 350-acre facility is located in Marcus Hook, Pennsylvania, located in the southern part of Delaware County, along the west bank of the Delaware River. It was owned and operated by BP Oil Company (BP) from 1969 to 1996. In February 1996, BP sold the refinery and has taken responsibility for environmental conditions, such as chemical releases, that existed up to the time of sale. To satisfy the requirements of the Resource Conservation Recovery Act (RCRA) and the Pennsylvania Land Recycling and Environmental Remediation Standard Act (Act 2) (1997), a team of BP consultants, third party contractors, and researchers at The University of Texas at Austin (UT) has been developing a GIS-based application in risk-based approach for corrective action. Dr. David Maidment and Dr. Robert Gilbert head the UT research team.

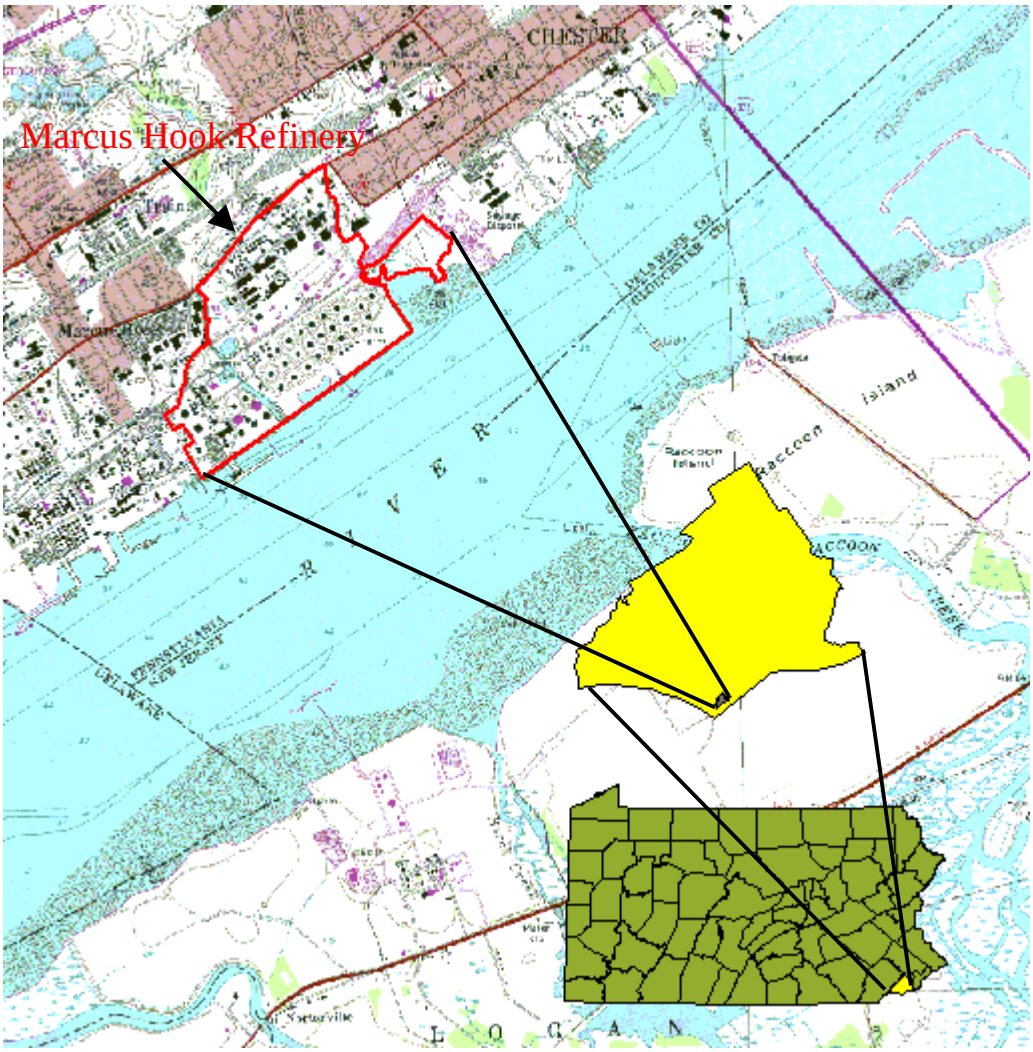


Figure 1.4: U.S. Geological Survey map of Marcus Hook Refinery (red) in Delaware County (yellow) in Pennsylvania (green)

(Source:http://www/topozone.com).

1.4. Thesis Layout

This thesis begins with a review of current research on integrating groundwater models and GIS and their applications for environmental risk assessment on a regional-

and facility-scale. The literature review (Chapter 2) demonstrates the growing interest in developing an integrated GIS-modeling system to assess risk and model groundwater. It also shows the uniqueness of this research and the overall project, because it specifically addresses a GIS-based integrated risk assessment.

Chapters 3 to 5 discuss the three environmental models developed for this research. Chapter 3 explains the procedure of developing and applying a contour map-based model to identify potential sources and source areas. Chapter 4 discusses the development and application of the simple groundwater/ surface water interaction model. This model is a screening-type model that calculates an acceptable target groundwater concentration. The development of the groundwater hydraulics model is detailed in Chapter 5. Several simulations were executed to obtain the best results. This chapter also includes the development of two groundwater models with different complexities, assumptions, and inputs. The results and challenges of each of the models are presented at the end of each chapter.

Chapter 6 provides a general overview and conclusions from this research. Despite some challenges encountered with modeling on a facility-scale, all three models may be practical tools to support environmental risk assessment and corrective action decisions at Marcus Hook.

CHAPTER 2

LITERATURE REVIEW

This chapter discusses recent applications of integrating a Geographic Information System (GIS) with groundwater models and other tools to assess environmental risk. There has been an increased interest and continuing effort to develop and use an integrated GIS-modeling system for risk assessment beyond what has been published. This research follows the general trend of recent works towards a more integrated GIS-modeling system. Like other facility-scale modeling, this research faced the common challenge of understanding and interpreting the natural environment with limited field data available. However, this research is rather unique; it is part of a larger project that uses GIS as the central tool for an integrated environmental risk assessment at a complex, industrial facility. In addition, new methods were used to overcome the obstacle of limited data for a site-specific facility and may be applied to other sites.

Human exposure assessment is one of the key factors in environmental risk assessment. It provides a qualitative and quantitative description of the exposure pathway by which a chemical of concern (COC) travels from source to receptor, and the interactions associated with the chemical and the transport media (Hay Wilson 1997). Determining exposure pathways is often difficult since they are dynamic, complex, and numerous (Harris 1997). GIS has the ability to spatially represent elements that have geometry and attributes. Since exposure pathways and the risks associated with them

are spatial in nature, they can be geo-referenced using GIS. Thus, GIS provides an ideal framework for human exposure assessment.

Integrating GIS with models can provide a more meaningful analysis. These models range from simple screening-level to complex multi-dimensional models. Therefore, not only can an integrated GIS-modeling system perform spatial analysis to facilitate exposure assessment, it can also analyze dynamic processes and interactions between the COC and the transport media.

An essential component of risk assessment is risk communication. The integration of GIS with models and other tools promotes communication among involved parties (*e.g., regulatory agencies, interest groups, the general public, and operators of the facilities*). Since the level of technical understanding varies with each stakeholder, GIS provides a common ground for communicating risk. The extent of the situation, the risks associated with it, and evaluation of remediation strategies can be easily explained and understood using the visual capabilities of GIS.

The following case studies demonstrate the use of an integrated GIS-modeling system for human exposure assessment and groundwater flow modeling on both a regional-scale and facility-scale. Although there were a number of studies reported in the literature that were devoted to groundwater modeling, there were very few concrete examples of using an integrated GIS-modeling system specifically for environmental risk assessment at large, complex industrial sites like Marcus Hook refinery.

2.1 Exposure Assessment and Groundwater Modeling on a Regional-Scale

The primary use of GIS has been in post-processing (i.e., generating and displaying results in the form of maps). However, the following case studies demonstrate the increased use of GIS as the central tool in an integrated risk assessment.

There are a number of existing integrated GIS-modeling systems that assess human exposure to COCs, such as XENVIS and GRIBS (Fedra 1998). XENVIS is an object-oriented system that integrates GIS and databases of hazardous chemicals with dynamic models. GRIBS integrates GIS with databases on industrial sites and hazardous and radioactive substances to support regulatory applications and provide a source of information for concerned residents and for fire fighters during emergency response situations.

An important part of exposure assessment is identifying potential source areas. Simple screening-level models provide a quick analysis of areas where COCs pose threats to groundwater. Tim (1996) developed an interactive modeling system to analyze groundwater vulnerability to pesticide leaching to an agricultural watershed. This modeling system incorporated GIS and three simple screening models with a windows-based interface to identify leaching potentials of pesticides under ideal conditions.

However, there were a few disadvantages to using simple screening-level models. They could not simulate all the processes leading to chemical concentrations in

groundwater and did not consider heterogeneity and variability of the natural environment (Tim 1996).

Because of the potential capabilities of combining GIS and groundwater models, there has been ongoing research to develop user-friendly interfaces. Watkins et al. (1996) presented three such interfacing methods: linked, integrated, and embedded GIS-groundwater models.

A linked GIS-groundwater model has an interface program that transfers data between the database for GIS and the database for the groundwater model, thus allowing the user to access each system separately. Although linked models do not require massive programming, they are not as efficient as the other models because the data must be stored in each of the databases, thus slowing down the processing time.

An integrated GIS-groundwater model has a "stronger" link than the linked model system. There is only one database that reads data for GIS and the groundwater model so that the user can work with either one. However, the programs that convert the data are "hidden" from the user and the model requires some advanced programming.

Finally, an embedded GIS-groundwater model does not require any data conversion; the user works with both GIS and groundwater model so all the input data can be characterized within GIS and easily transferred into the groundwater model. In addition, since the model is embedded within GIS, functions intrinsic to GIS such as statistical capabilities can be utilized. The programming level varies depending on how

complex the embedded model is and it cannot simulate large, heterogeneous, and anisotropic environments.

Watkins et al. (1996) demonstrated the use of a linked GIS-groundwater model called ARCMOD (Arc/Info-MODFLOW). The conclusion from this study was that in order to take advantage of a linked modeling system, data for modeling must be in a GIS format and the links between GIS and the groundwater model must be kept simple.

When using an integrated GIS-modeling system, the user must calibrate and verify the model, especially models used for regulatory applications (Bobba, Singh and Bengtsson 2000). Calibration is the process of adjusting model parameters so that the computed values match with observed data. Verification is the process of comparing the computed values with an independent data set without adjusting model parameters. The error values (i.e., computed minus observed values) reveal how closely the model simulated the natural environment.

Bobba, Singh and Bengtsson (2000) conducted a study using a numerical saturated-unsaturated transport (SUTRA) model to identify groundwater discharge areas into surface waters. After the model was calibrated and verified, areas with limited measured descriptions of the subsurface had greater error values, as expected. Theses error values could also be contributed by heterogeneities in those particular areas.

2.2 Exposure Assessment and Groundwater Modeling on a Facility-Scale

Models have provided a more cost-effective method of simulating the environment, since sampling data can be rather costly. How a model simulates actual conditions depends heavily on the amount of field data available. One of the common challenges facing case studies conducted on a facility-scale is limited field data on the natural environment, particularly the subsurface environment. In addition, many facility-scale models do not incorporate aquifer boundary conditions (Leake et al. 1998). Thus groundwater modeling and exposure assessment of COCs in groundwater can be complex tasks.

For groundwater modeling, well-log data have been useful for understanding the subsurface environment. Camp and Brown (1993) presented a case study of a well field to demonstrate the use of well-log data in developing a three-dimensional subsurface profile in GIS. To interpolate the entire extent of the analysis, wells were created along the extent of analysis and were assumed to have the same subsurface descriptions as their nearest neighbors.

If economically possible, more sampling is recommended to pinpoint the sources of releases (Harris 1997). Sampling data is important for determining the transport media as well as the extent of concentrations of COCs in soil and groundwater. In a human exposure study by Harris (1997), sampling COCs in groundwater was conducted after a release from an underground storage tank to help predict potential points of exposure in the impacted area. In addition, toxicology evaluations helped identify exposure routes and potential receptors. Thus, an integrated

GIS-modeling system was successfully used to predict exposure pathways near the underground storage tank site.

Another application of interpolating well data was for a study conducted by Lantzy, Cichy and Leitzinger (1998), in which the groundwater was impacted with volatile organic compounds (VOCs) from a chemical plant. With sufficient spatial and temporal environmental data, the integrated GIS-modeling system proved to be a powerful tool to evaluate data, develop a conceptual model of the subsurface and extent of COC impacts, evaluate remedial alternatives, inform the public of the risks, and reach a plan for mitigating the effects of exposure.

In recent years, incorporating spatial and temporal environmental data with epidemiologic and demographic data have provided a more meaningful assessment of human exposure to chemicals in the environment (Maslia et al. 1994). In a site-specific case study by Maslia et al. (1994), COC transport scenarios were simulated to provide an estimate of the population exposure to tricholorethene (TCE) in groundwater and help evaluate remediation plans. Spatial queries revealed the extent of TCE in groundwater and which part of the population might be exposed to groundwater containing TCE.

Another benefit of integrating GIS with models is that the user can take advantage of functionalities intrinsic to GIS. Chen, Huang and Chakma (1998) applied SIMRA, a GIS-facilitated simulation and risk analysis, to a petroleum-impacted site in order to identify and manage site remediation actions. The system was used to perform statistical analysis.

Interfaces between the GIS and groundwater models are often developed to facilitate pre- and post-processing data. In the pre-processing, interfaces help create layers for input and output data (El-Kadi 1994). In the well field study by Camp and Brown (1993), a GIS-MODFLOW interface was created to update the input well-log data. The interface had capabilities of computing parameters based on the well-log data such as vertical conductivity and hydraulic parameters.

In the post-processing, the GIS interface was primarily used to spatially interpret output data. In the well field case, the GIS-MODFLOW interface displayed MODFLOW results. In the TCE case study by Maslia et al. (1994), a GIS interface was used to reference spatial features with model coordinates, rather than referencing them with a specific geographic location, as many other models do.

One of the drawbacks of developing interfaces is that the interfaces may not be compatible with external models. For example, in a site-specific case study by El-Kadi (1994), the interface MapInfo was unable to contour groundwater heads and COC concentrations; any contour plots created externally could not be superimposed onto the output layers that were created in the pre-processing.

There are other challenges of integrating GIS with groundwater models. First, it can be rather programming intensive, especially when developing an interface that facilitates the pre- and post-processing. In the pre-processing, input files have to be built and modified using various programming languages, which is often difficult and time consuming (El-Kadi 1994; Inbau and Rindahl 1997). In the post-processing,

additional programming is also often required to translate and display groundwater model results into GIS (Inbau and Rindahl 1997; Lee et al. 1999).

Understandably, since the pre- and post-processing can be time consuming, many efforts have been taken to automate these processes. However, even if only minimum programming is required, a fully automated GIS-modeling system may not be realistic for every site case especially if there is limited information about the site (El-Kadi 1994). Field data is not as readily available for facility-scale modeling as they are for regional-scale modeling.

Another challenge is interpreting available data. An interesting issue in the case study by Talbot and Kolm (1996) was the interpretation and interpolation of sampled hydraulic conductivity data. Hydraulic conductivity is a crucial parameter for simulating groundwater flow and COC transport. When measurements of hydraulic conductivity are not available, their values must often be estimated from various analyses. However, these parameters are particularly sensitive to data errors; a minor head observation error may result in greater conductivity error (Yeh 1986). Thus, to minimize instability, all available field data should be used.

Talbot and Kolm (1996) created five models, each with different methods of interpolating conductivity. The interpolation schemes were manual interpretation (i.e., trial and error), statistical trend-surface analysis, nearest-neighbor method, inverse distance weighted method, and the Kriging method. They concluded that the manual interpretation of conductivity values were better suited for facility-scale studies that had limited data and the models developed should consist of a few layers with just several

hundred cells. However, it is important to emphasize that there is no "best method" to interpolate conductivity values, because it varies from case to case (EMS-I, personal communication 2000).

As in the previous section, models must be calibrated with observed data and verified with an independent data set. There have been several studies that have focused on the inverse problem, which is basically the problem of selecting parameter values (Brooks, Lerner and Tobias 1994; Freyberg 1988). The inverse problem was used to obtain a single best model with a set of ideal parameters (Brooks, Lerner and Tobias 1994).

Calibrating models with one set of observed data may not be the best method since groundwater heads vary; thus, for sites with limited field data, a set of acceptable calibrations may be able to predict conditions more effectively than just using one set of good calibrations (Brooks, Lerner and Tobias 1994). Another way to minimize uncertainty in predicting parameter values is to reduce the number of parameters to be calibrated, such as hydraulic conductivity, by subdividing the study area into smaller homogeneous areas (Yeh 1986). Still, one of the most crucial data source for calibration are groundwater flow measurements; unfortunately, many facilities have no or very limited groundwater discharge data (Brooks, Lerner and Tobias 1994).

CHAPTER 3

MODELING HISTORICAL SOURCES AND SOURCE AREAS USING CONTOUR MAP-BASED MODELS

This chapter discusses the first of three models developed for the Marcus Hook Refinery (Marcus Hook). This model uses contour map-based modeling to develop a procedure to spatially analyze potential sources and source areas based on descriptions of historical releases and field environmental measurements. Initial evaluations were made to attempt to distinguish between areas that need to be studied further and areas that do not need to be investigated. This chapter also provides an application of how incorporating a Geographic Information System (GIS) and Microsoft Access (Access) is effective in compiling, displaying, and analyzing data to support risk-based decision-making.

3.1 Study Area

The model was developed using the Lubricant Production Plant (Lube Plant) as the specific study area. The Lube Plant comprises of 63 acres of the refinery and is located on the southwest corner of the refinery, bordered by Marcus Hook Creek to the east, the Delaware River to the south, and the northern and western facility boundaries (see Figure 3.1). Historical processes and operations include producing and storing blended lubrication oils and solvents (Langan 1999). The Lube Plant has a lengthy history of industrial activity (Remediation Technologies, Inc. 1992). Most of the

processes and operations have ceased and many units, such as tanks, are no longer present or no longer in use.

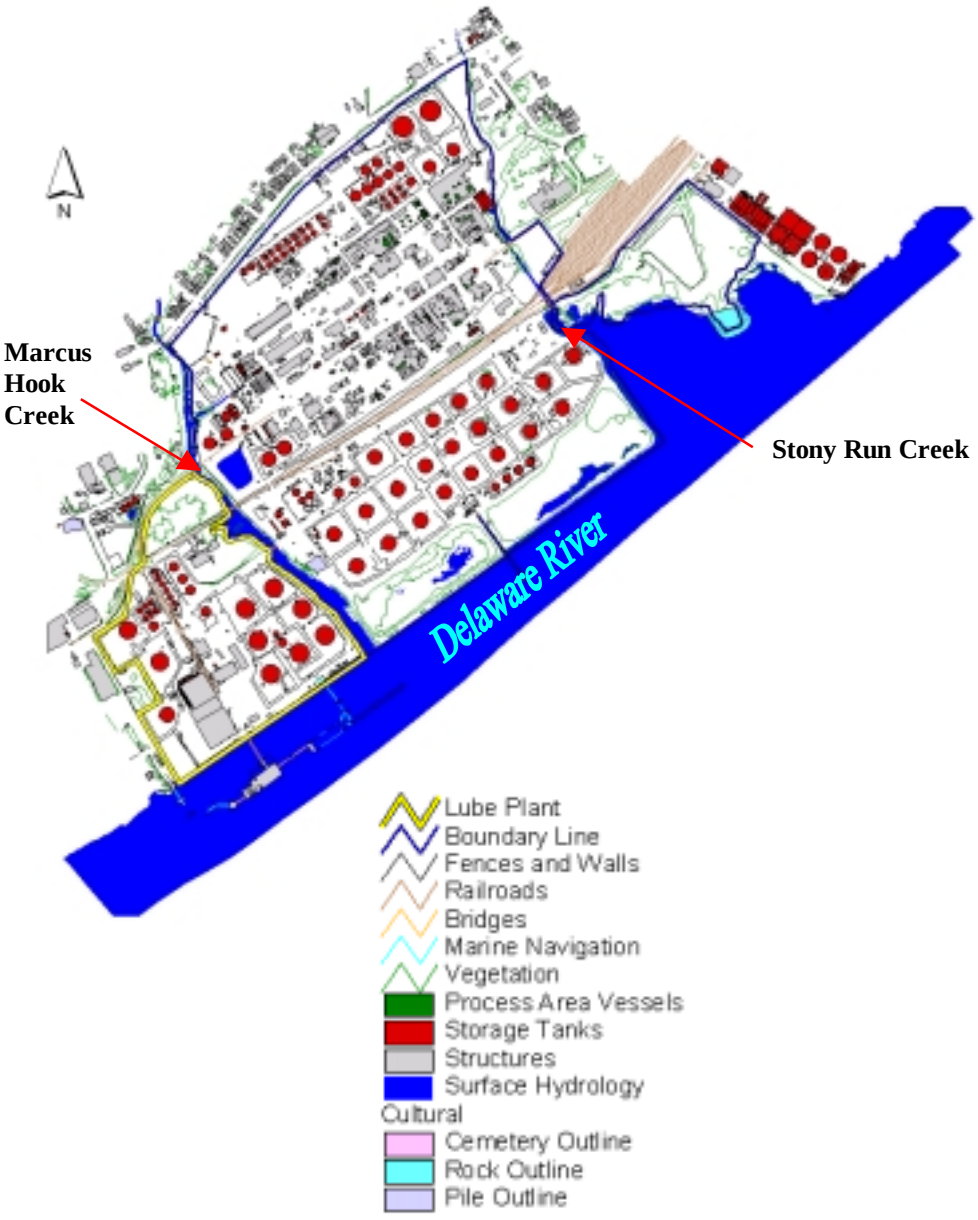


Figure 3.1: Digital facility description of the refinery with the Lube Plant (yellow) *(Source: Romanek 1999).*

3.2 Objective

The objective of the contour map-based modeling was to develop a procedure to correlate measured environmental data to historical and current spatial features, so that the potential sources and source areas could be determined. Based on the contents of the digital facility description, contour maps of chemicals of concern (COCs) were developed in GIS ArcView. After overlaying the historical source area themes and COC data contours, areas requiring further study and investigation were identified.

3.3 Digital Facility Description

The digital facility description (Figure 3.1) was developed and compiled in GIS by Andrew Romanek (1999). It serves as the primary source of information for conducting many of the analyses in this research. The digital facility description contains two types of data for Marcus Hook: spatial and tabular data. The spatial database provides GIS shape files and coverages of the geographic and physical features in the refinery and its surrounding region. The tabular databases are Access files that contain analytical, hydrological and geological characteristics of the refinery. Further details of the development of the digital facility description can be found in Romanek's thesis (1999).

3.4 Incorporating Spatial and Tabular Databases for the Lube Plant

A map for the Lube Plant was compiled using the **Spatial Analyst** extension and the digital facility description. Figure 3.2 shows a map of the Lube Plant and the

associated shape files: the Lube Plant boundary, historical features, former Resource Conservation Recovery Act (RCRA) units, and tank coverages.

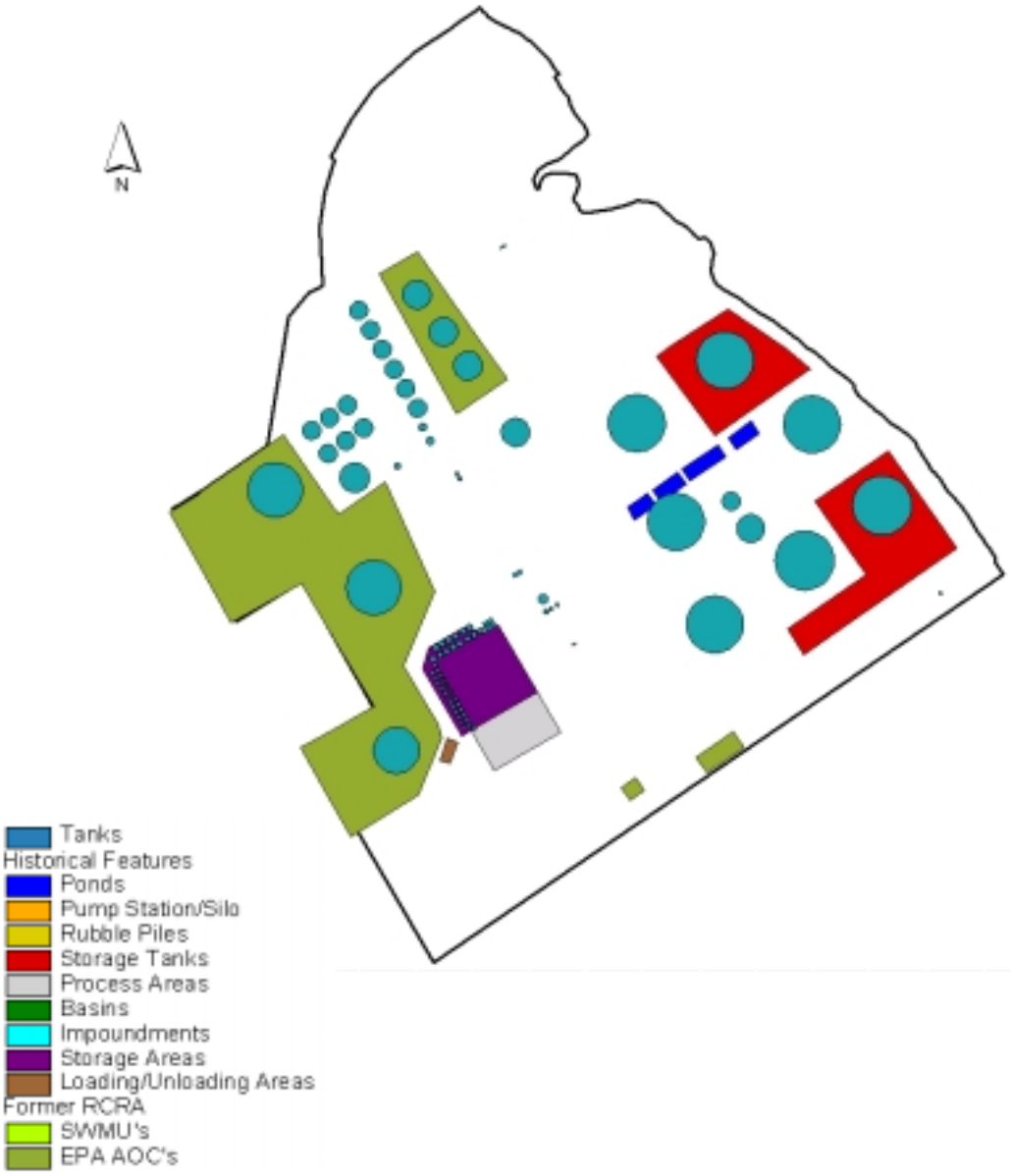


Figure 3.2: Map of the Lube Plant containing coverages of the tanks, historical features, and former RCRA units in ArcView.

Previously, no record of the environmental conditions was associated with the spatial features. With this information added to the attribute table, the user is able to click on any feature and get information about environmental conditions associated with it. The environmental conditions descriptions were available from information compiled from historical reports by the current owner and operator of Marcus Hook. This information contained descriptions of the environmental conditions that existed up to the time of sale of the refinery, and was available in a table format.

The information table was imported into and edited in Microsoft Excel. Based on the descriptions of the environmental conditions, the following five new fields were created in the Excel table:

- materials stored
- volume stored
- time period of operation
- release descriptions
- data classification number

The spreadsheet was then saved as a text file and imported into ArcView. The new attribute tables for the spatial features now contain environmental conditions descriptions.

A data classification system, shown in Table 3.1, was developed to rate the environmental conditions descriptions in hopes of better analyzing historical sources and source areas. The data classification number describes the relative specificity of the description. In this classification system, the ideal data are entries that describe a release with a volume and date or time, i.e., Data Classification #1. After assigning a

data classification number to each environmental conditions description in the Excel table, data with a volume and time (i.e., *Data Classification #1*) were not found for the Lube Plant. Thus, for the analysis, the next best available data were used, i.e., Data Classification #2.

Table 3.1: Data quality classification system for releases.

Data Classification Number	Type of Data
1	Specific release with specified volume and date or time
2	Anecdotal evidence describing release but no time and date specified; visual observation of standing oil or stained soils
3	Oily stains or discoloration or other evidence from historical photographs or reports
4	No releases identified; not a source feature

Figure 3.3 is a map of the Lube Plant with all features and their associated classification number. Figure 3.4 is a map of the features with only Data Classification #2. There were 54 tanks with Classification #2 data, in which 15 of them had records of the types of materials stored. There were four historical features with Data Classification #2 that were former wastewater storage, lubricant production, and truck loading/ unloading areas. There were also seven former RCRA units with Classification #2 data.

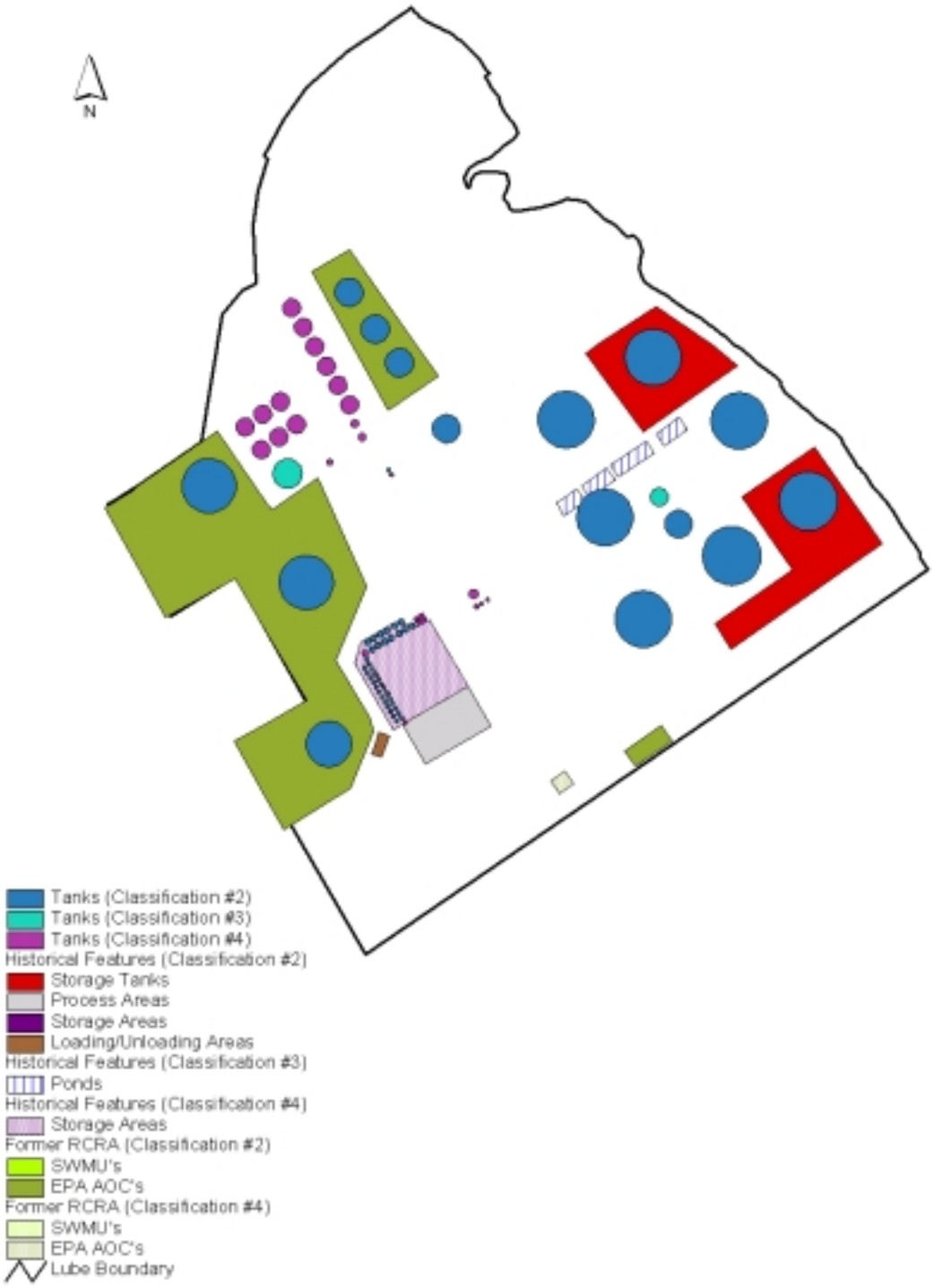


Figure 3.3. Map of the Lube Plant containing features from all data classifications in ArcView.

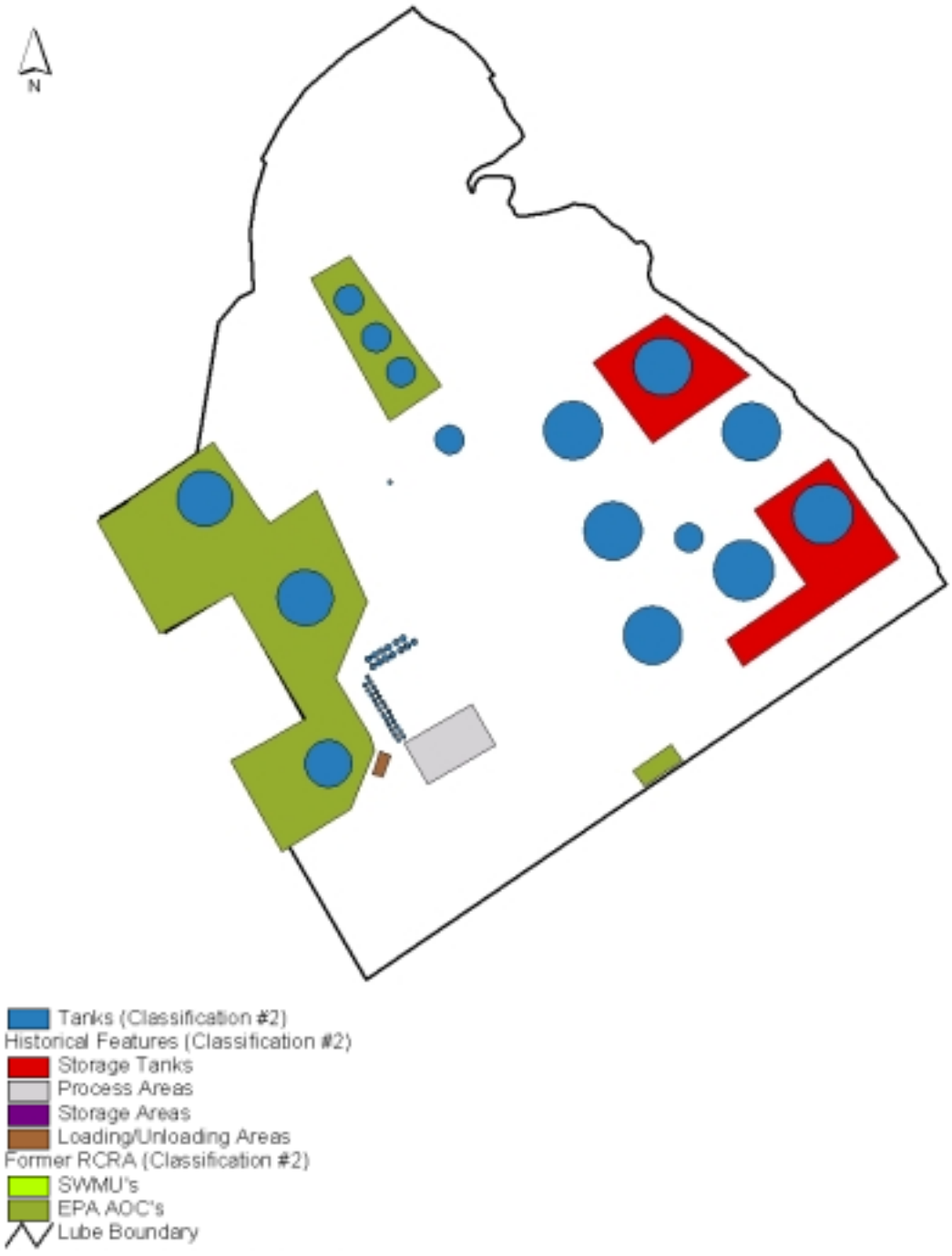


Figure 3.4. Map of Lube Plant containing features with Data Classification #2 in ArcView.

3.5 Environmental Field Data

For the field environmental data, a separate environmental database compiled by BP was used. Databases can be imported from Access to ArcView by establishing an **Open DataBase Connectivity** connection and by adding an Access driver. The database can then be joined with an attribute table in ArcView using a Structured Query Language (SQL) Connect.

Several queries were created using the environmental database. Queries are used to view, change, and analyze data by bringing together data from multiple tables and establishing relationships with each table, using a common field. Figure 3.5 shows the relationships among the tables in the database. Each table is linked to another table by the common field name using a common field ***LOC_ID***.

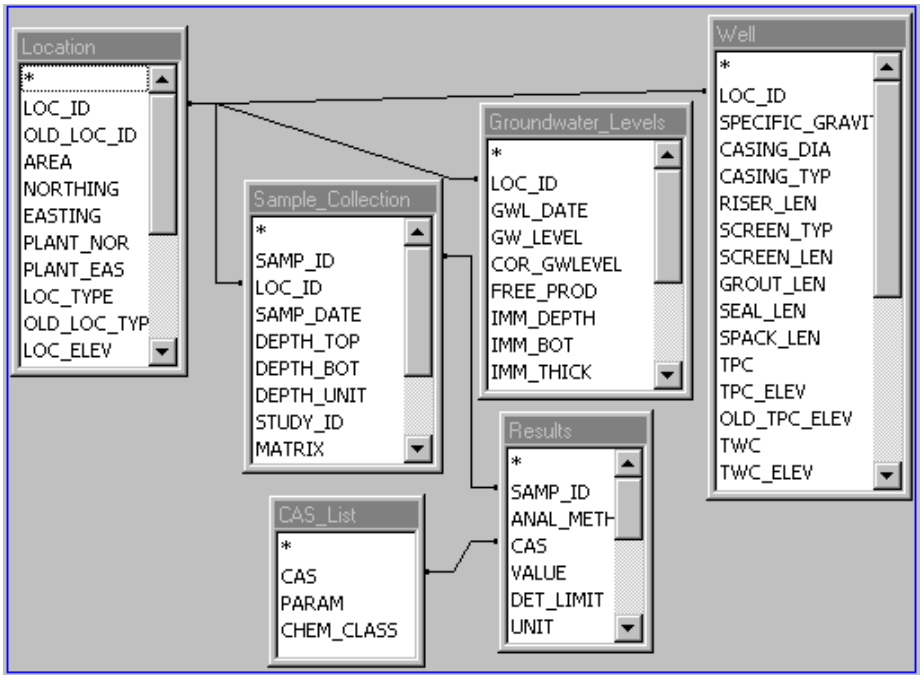


Figure 3.5: Design view of the query for the COCs, groundwater elevations, and thickness for the light non-aqueous phase liquid (LNAPL) detections in Access.

Based on the queries for all chemicals within the Lube Plant, 147 detections of chemicals were found in the groundwater for all sample dates. These detections represent chemical concentrations in groundwater samples that the laboratory was able to quantify. Thus, the detection limit is a function of the laboratory methods used in the sample analysis. Table 3.2 lists the detection limits reported in the environmental database for the eight COCs chosen for this study, which are typically found in petroleum mixtures. It should be noted that the detection limits are not related to risks posed by exposure to the COCs at these concentrations; they are a function of the laboratory's ability to quantify the COC in the environmental sample.

Table 3.2: Detection limits for the eight COCs.

Chemical	Detection Limit (µg/L)
Benzene	5
Ethylbenzene	5
MTBE	1
Naphthalene	10
TCE	5
Toluene	5
Total Xylenes	5
Lead	100

Data were queried to determine whether the groundwater flow direction indicated a potential upgradient source area. Such a source area may cause the concentrations of COCs in the groundwater to be increased in a region that has no direct source located within in. However, such a direct comparison could not be made, since in the available data set, the sampling for COCs was done much earlier than the

measuring of the groundwater elevation. The sampling dates for the COCs were between May 2 and 6, 1996, while the groundwater elevation measurements were taken on August 17, 1998. For a better comparison, the sampling date for the COC and groundwater elevation data should have been the same (Alley, Reilly and Franke 1999). In addition, COCs trapped in soil that are above or below the water table cause the concentrations in groundwater to vary with the rise and fall of the water table. A more useful comparison could have been made if the COC and groundwater elevation data were sampled over a longer period of time, with both data sets measured at the same dates.

No definitive conclusions were made from this model about upgradient sources that contributed COCs to the groundwater, nor could the potential migration pathways of COCs in groundwater be determined. Such analyses could be accomplished with a better understanding of the groundwater movement. Chapter 5 discusses the development of a comprehensive groundwater flow model.

3.6 Contours of Corrected Groundwater Elevations and LNAPL Distribution

Queries were also created for the groundwater elevations and the light non-aqueous phase liquid (LNAPL) thickness. LNAPL is an immiscible layer that sits on top of the water table and causes the water table to depress. LNAPL is an oil phase, also known as free product, which contains hydrocarbons and other COCs. LNAPL can be a long-term source of COCs to groundwater.

To account for the presence of LNAPL, the field groundwater elevations were corrected using the Equation 3.1:

$$h_C = h + t_L * SG \qquad \text{(Equation 3.1)}$$

where:

- h_C = corrected groundwater elevation (feet)
- h = groundwater elevation (feet)
- t_L = LNAPL thickness (feet)
- SG = specific gravity (gram/cm^3 LNAPL per gram/cm^3 water)

The specific gravity varied by monitoring well location. Specific gravity data was collected from laboratory analysis of LNAPL samples. A script called ***Correct_GWElev.ave*** (Appendix A.1) was developed to automate the calculations of the corrected groundwater elevations. If there were no free product, i.e., no LNAPL present, the corrected groundwater elevation would simply equal its measured value. Similarly, if there were free product, the script would calculate the corrected groundwater elevation given a specific gravity. Figure 3.6 lists the LNAPL thickness and corrected groundwater elevations for each monitoring well.

Analytical measurements for COCs in the LNAPL were also available. The analytical results showed that benzene and lead were found in the LNAPL.

Attributes of GW Elevations and LNAPL Thicknesses 8/17/98 (ft)

LOC_ID	NORTHING	EASTING	GW_ELEV	SPECGRC_GRAVI	MM_THICK	FREE_PROD	CorrectGWE
MW-32	184489.243880	2625975.026910	-2.497000	0.902500	5.250000	Yes	2.24
MW-33	184216.409780	2625947.067650	-0.209000	0.849600	2.920000	Yes	2.27
MW-9	183972.056600	2626290.200160	1.661000	0.892400	0.450000	Yes	2.06
MW-28	183920.977300	2626530.055330	2.755000	0.890800	0.330000	Yes	3.05
MW-25	183582.073780	2626234.498180	2.893000	0.810000	0.040000	Yes	2.93
MW-11	183460.427040	2626078.947310	6.507000	0.810000	0.020000	Yes	6.52
MW-34	184944.479190	2625642.199490	3.169000	0.849600	0.010000	Yes	3.18
MW-26	183329.469300	2625870.440510	4.157000		0.000000	No	4.16
MW-10	183794.166530	2625885.174730	2.298000		0.000000	No	2.30
MW-27	183649.747530	2626015.450060	5.911000		0.000000	No	5.91
MW-12	184369.837950	2627263.265800	5.383000		0.000000	No	5.38
MW-7	184645.975850	2626779.710340	5.110000		0.000000	No	5.11
MW-8	184401.245370	2626241.548690	2.479000	0.832800	0.000000	No	2.48
MW-29	183931.164290	2626704.877810	5.501000		0.000000	No	5.50

Figure 3.6: Attribute table of corrected groundwater elevations and LNAPL thickness in ArcView.

The queries of LNAPL thickness and groundwater elevations were imported into ArcView and point coverages were created. Contours of the elevations were generated using the Inverse Distance Weighting (IDW) interpolation method. The IDW method gives more weight to cells closer to measurement points and less for more distant points (BYU 1999). The IDW method is better suited for groundwater elevation data, because it does not "smooth" over pits and peaks like other interpolation methods do (Romanek 1999).

The LNAPL thickness point coverage and the corrected groundwater elevation contours were then overlaid on the historical features with Data Classification #2 for preliminary analysis of potential sources and source areas, shown in Figure 3.7. Since LNAPL depresses the groundwater table, the area with the greatest LNAPL thickness corresponds to the area with the lowest groundwater elevation. Thus, the central part of the Lube Plant, which had the greatest LNAPL thicknesses, corresponding to the lowest range of groundwater elevations.

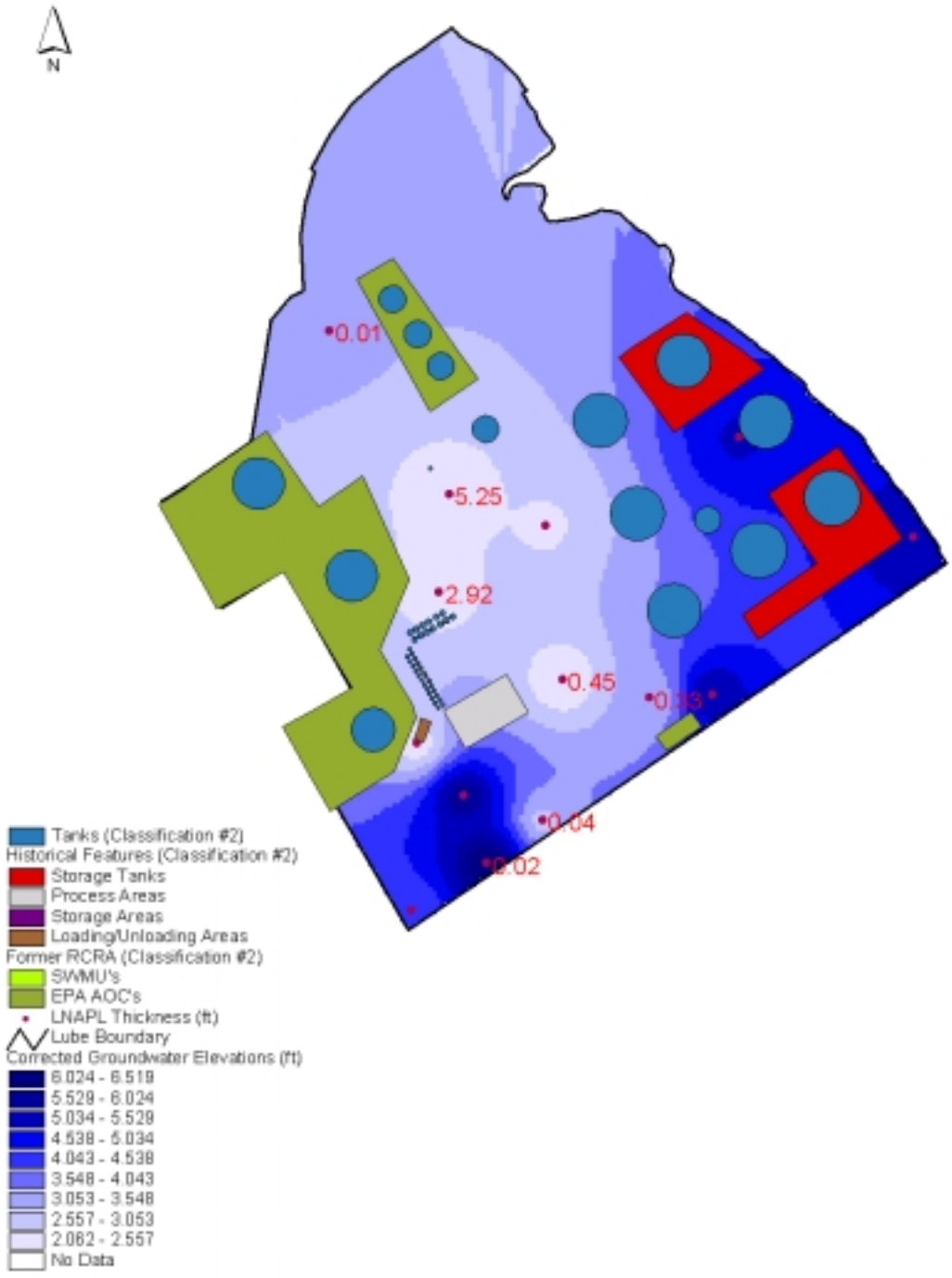


Figure 3.7. Map of LNAPL thickness points and corrected groundwater elevation contours overlaid on historical features with Data Classification #2.

3.7 Contours for Concentrations of Chemicals of Concern

After the queries for the eight COCs were imported into ArcView, point coverages were created for each COC. Some of the samples did not have measured concentration data in the ***Value*** field, indicating that the concentration of the chemical was below its detection limit. Thus, to be able to use the below-detection results in the contouring, values had to be assigned to these no-data cells.

A script developed by Romanek (1999) called ***Newfield.ave*** was used to fill these blank cells with a concentration equal to one-half of the detection limit. ***Newfield*** inserts a new column and fills each cell with either zero, one half of the detection limit, or a custom value.

Once the point coverages were created in ArcView, contours of COC concentrations were created using the IDW method for those COCs whose concentrations were above their respective detection limits: benzene, ethylbenzene, MTBE, lead, and total xylenes. These contours were overlaid on the feature coverage with Classification #2 data shown in Figures 3.8a to 3.8e. No contour maps were created for naphthalene, TCE, and toluene, because these samples had concentrations below their respective detection limits.

Benzene, ethylbenzene, MTBE, and total xylenes are typical constituents of gasoline so as expected, these COCs were detected together. With the exception of lead, the highest concentrations were located in the central part of the Lube Plant, as seen in Figure 3.8.

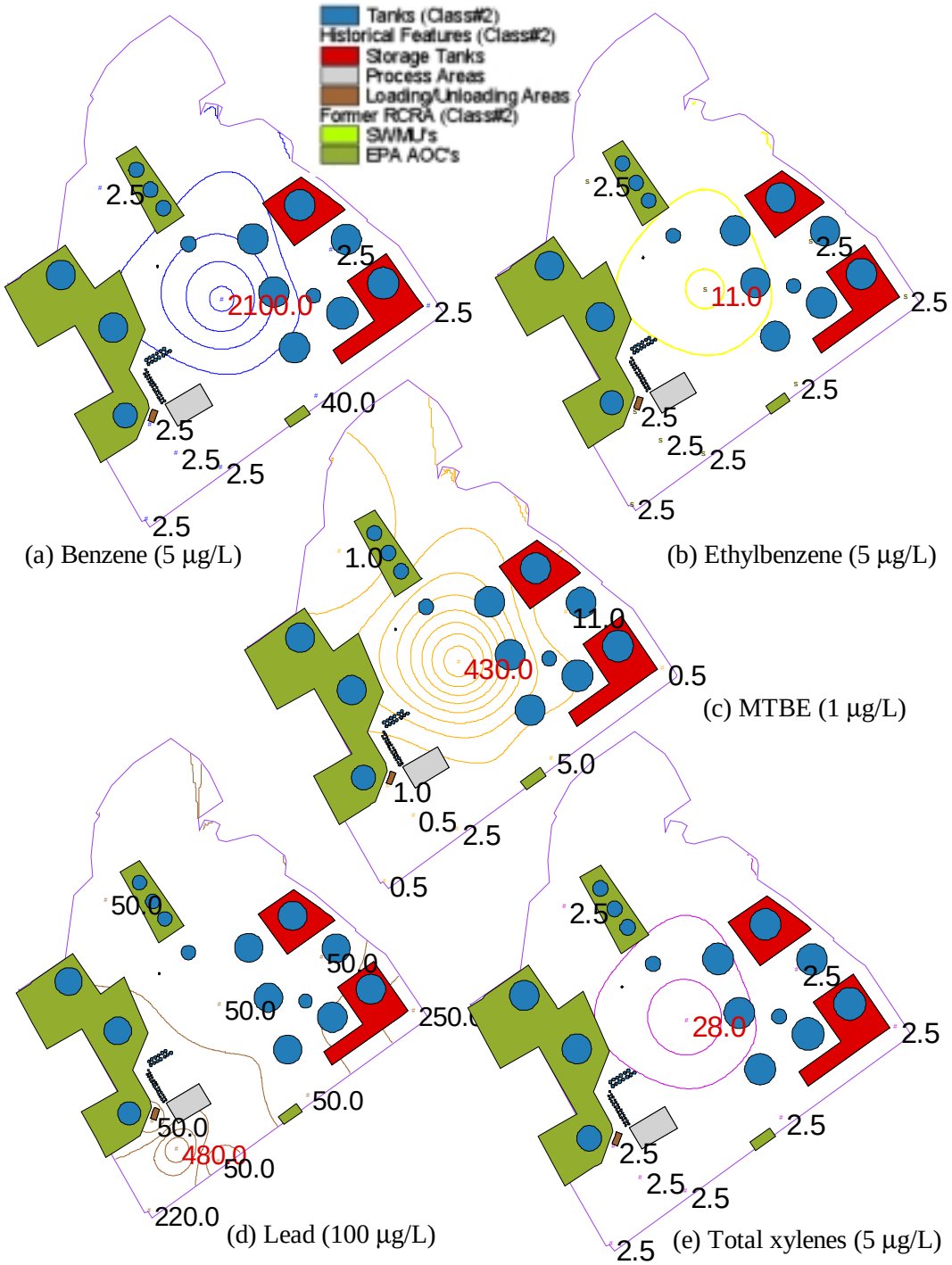


Figure 3.8. Contours of concentrations for COCs above their respective detection limits in parentheses.

3.8 Data Analysis and Discussion

The purpose of the contour map-based model was to develop a procedure to help locate potential sources and source areas using both quantitative concentration data and qualitative historical environmental conditions data. After creating concentration contours for each COC, the contours were overlaid on the three coverages with Classification #2 data to see if any correlation could be made between the COC measurements and historical information.

The Total Petroleum Hydrocarbon Criteria Working Group (TPHCW) is a consortium of experts from industry, government, and academia who have conducted studies on petroleum mixture composition (Potter and Simmons 1998). According to these composition studies, there are general characteristics for each petroleum fuel mixture typically found in a refinery. Commonly used acronyms are BTEX and PAH. BTEX stands for benzene, toluene, ethylbenzene, and total xylenes, which are four aromatic hydrocarbons found in petroleum mixtures. PAH stands for polynuclear aromatic hydrocarbons, which have more than two fused benzene rings as a structural characteristic.

The following data analysis refers to the contour maps and petroleum mixture characteristics. The analysis was simplified by dividing the Lube Plant into nine sections. According to the data analysis, there were no COCs whose concentrations were above their respective detection limits for the east, north, northwest, west, and southwest sections of the Lube Plant. Figure 3.9 shows the areas in the Lube Plant that had COCs whose concentrations were above their respective detection limits.

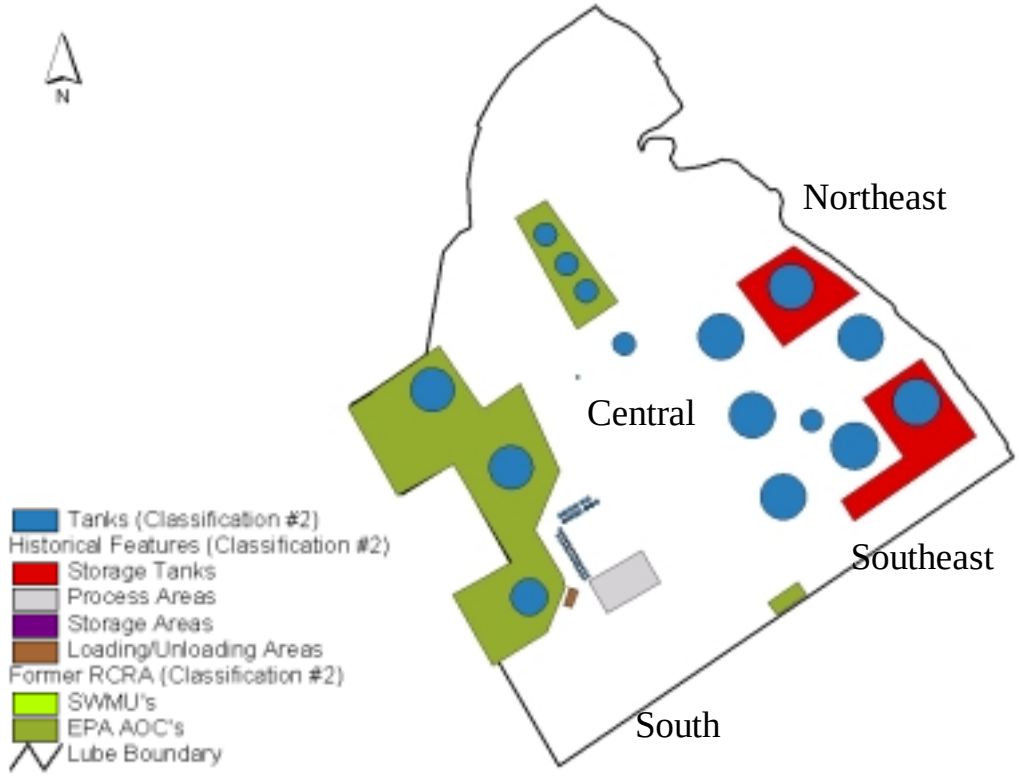


Figure 3.9: Area designation of the Lube Plant.

The central part of the Lube Plant had the most COCs with concentrations above their respective detection limits. These COCs and their concentrations were as follows:

- benzene, with a concentration of 2100 µg/L
- ethylbenzene, with a concentration of 11 µg /L
- total xylenes, with a concentration of 28 µg /L
- MTBE, with a concentration of 430 µg /L

The units closest to the detections contained crude and fuel no.6 oils, which typically do not contain high concentrations of BTEX (Potter and Simmons 1998). Information was not available about the underground piping that runs through the central part of the Lube Plant. Information about historical piping and the products carried in that piping may have assisted in the evaluation of concentrations detected in the central part of the Lube Plant.

In the south region, there were two lead detections, with measurements of 480 and 220 μg/L. MTBE was also detected, with a concentration of 1 μg/L. This area stored and processed lubricating oils, which might explain the concentrations of lead in this area (Potter and Simmons 1998). However, lubricating oils do not contain MTBE; MTBE is an additive that is put into gasoline when it is a finished product (Potter and Simmons 1998). The detected MTBE concentration is so low in this region as to not be relevant to a study of sources and source areas.

There was 40 μg/L of benzene and 5 μg/L of MTBE measured in the southeastern part of the Lube Plant. The unit closest to the detections was the filter changing/ product metering area, which might explain the benzene detection. Again, the concentrations detected in this area are so low as to not be relevant to a study of sources and source areas.

The northeast corner of the refinery had a detection of MTBE, with a measurement of 1 μg/L. This area processed and stored crude oil, which does not contain MTBE. The concentration detected is so low as to not be relevant to a study of sources and source areas.

Source areas could not be defined based only on the groundwater data. Patterns in the soil data were studied using the same procedures described in the sections above, in hopes of providing a more complete analysis. Because of limited soil sampling, the soil analysis did not provide any new information about potential sources and source areas.

The procedure used in this modeling effort proved to be sound in its implementation. Historical qualitative data was made more accessible by associating the data with the spatial objects to which they relate. Overlays of the spatial features and the environmental measurements data allow patterns to be identified and potentially for correlations to be recognized. This procedure may be a useful tool in the analysis of other parts of the refinery, or for other facilities.

In the specific case used here, there were several challenges to defining potential sources and source areas. Limited sampling points made it difficult to definitively state the location of a source area. The highest concentration at a sampling point did not necessarily mean that it was a source area. Also, lead concentrations in groundwater may be deceiving. It is uncertain whether the detections are actually lead in the groundwater or on fine soil particles in the water sample; the analytical results do not contain filtered and unfiltered data. Furthermore, there was insufficient information about the underground piping system and the materials that were transported in it.

Based on the existing measurements and historical records, the following are *possible* source areas within the Lube Plant: benzene, ethylbenzene, total xylenes, and

MTBE in the central area. These COCs and the central area could be studied further, including additional data and information gathering.

In conclusion, the contour map-based model may be a useful tool to analyze the spatial distribution of the chemicals relative to the potential source features. However, due to the limitations discussed in this section, the contour map-based model was not able to provide great insights at the Lube Plant.

CHAPTER 4

MODELING THE GROUNDWATER/ SURFACE WATER INTERACTION

This chapter discusses the second of three models developed for the Marcus Hook Refinery (Marcus Hook). This model incorporates the results from a preliminary groundwater model into an existing surface water model. Details on the development of the groundwater and surface water models can be found in Romanek's thesis (1999). The purpose of developing a groundwater/ surface water interaction model is to calculate a groundwater target level for each chemical of concern (COC) and check whether predicted surface water concentrations are below the Pennsylvania water quality standards. Because there are several different transport mechanisms that can move a chemical from a source to a point of exposure, it is important to study the fate and transport of these chemicals in order to develop solutions for corrective action. In one scenario, the spilled chemical may leach from the soil into the groundwater and travel into the surface water. If the concentration in the groundwater is high enough, the chemical can be detected in the surface water (*Marcus Hook Creek or the Delaware River*). The water quality standards are determined by the state to be protective of the surface water and its designated uses. Initial evaluations were made to identify the COCs whose measured concentrations were above their calculated target groundwater concentrations.

4.1 Study Area

The Lube Plant was chosen as the study area for the development of the interaction model. Along the east boundary of the Lube Plant is Marcus Hook Creek, as shown in Figure 4.1. Table 4.1 lists the properties of Marcus Hook Creek, a relatively small stream with a drainage area of 5.22 square miles.

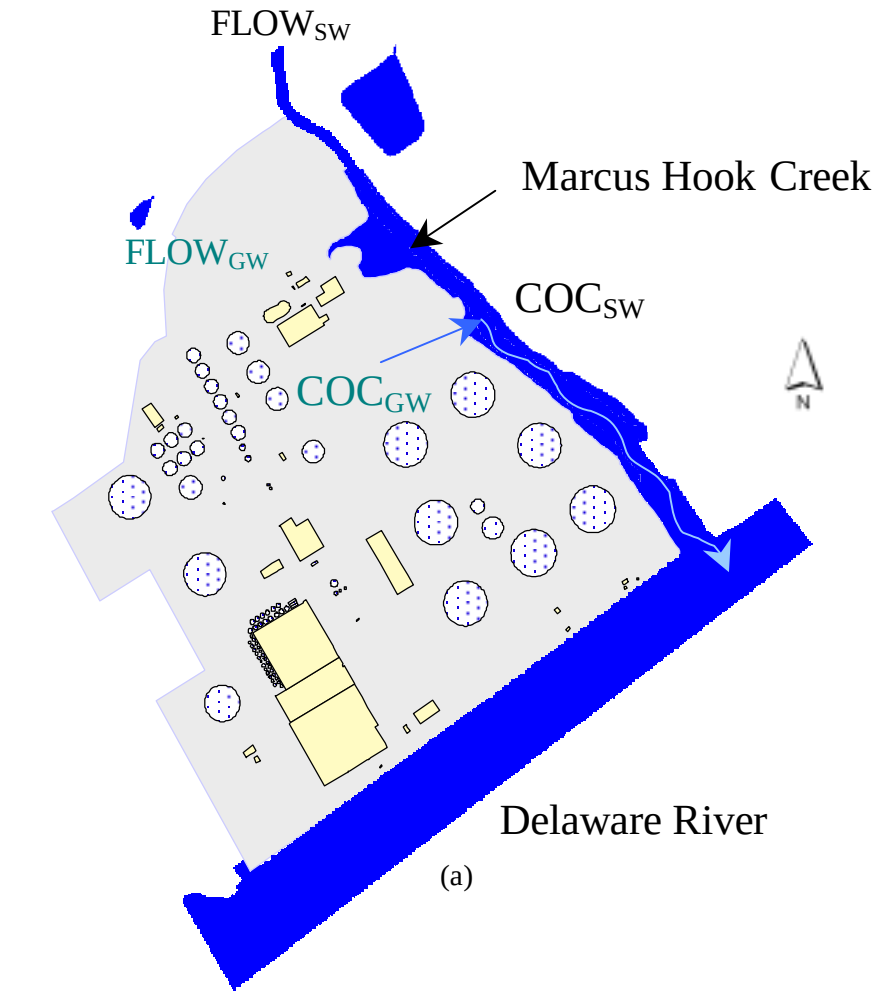
Table 4.1: Characteristics of Marcus Hook Creek.

County	Delaware
Basin	Lower Delaware
USGS Stream Code Number	00511
Latitude (ddmmss)	394855
Longitude (dddmmss)	0752417
Drainage Area (square miles)	5.22

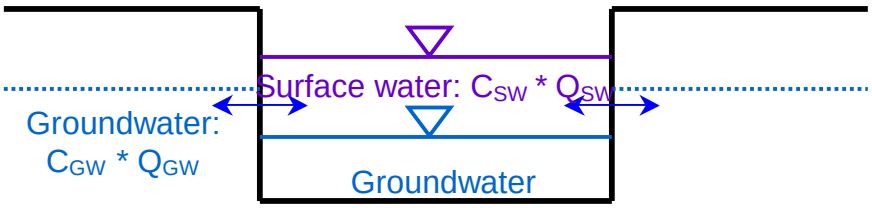
Source of data: Pennsylvania Department of Environmental Protection (1989), Courtesy of John M. Nantz, U.S. Geological Survey

4.2 Objective

The primary objective of the groundwater/ surface water interaction model was to calculate a groundwater target level for each COC, so that its predicted concentration in the surface water was not above the applicable surface water standard concentrations, as outlined by the Pennsylvania Department of Environmental Protection (PaDEP). The model incorporated the output from a preliminary groundwater model into an existing surface water model.



(a)



(b)

Figure 4.1. (a) Plan view and (b) cross sectional view of groundwater and surface water interaction for the Lube Plant.

In addition to calculating the groundwater target levels, predictions for stream flow from the surface water model were compared with actual stream gauging results from United States Geological Survey (USGS) to establish the accuracy of the surface water model.

4.3 Mass Balance

A simple mass balance, shown in Equation 4.1, was used to estimate the relationship between the flows of and concentrations in the groundwater and surface water.

$$C_{GW} * Q_{GW} = C_{SW} * Q_{SW} \qquad \text{(Equation 4.1)}$$

where:

- C_{GW} = concentration in groundwater
- C_{SW} = concentration in surface water
- Q_{GW} = groundwater flow
- Q_{SW} = surface water flow

The simple mass balance (Equation 4.1) can be rearranged to obtain either a forward surface water calculation or a target level calculation, as shown in Figure 4.2. Since the objective is to calculate target groundwater levels, a target level calculation is used, as outlined in Sections 250.309 and 250.406 of the Pennsylvania Land Recycling and Environmental Remediation Standard Act (Act 2) (1997).

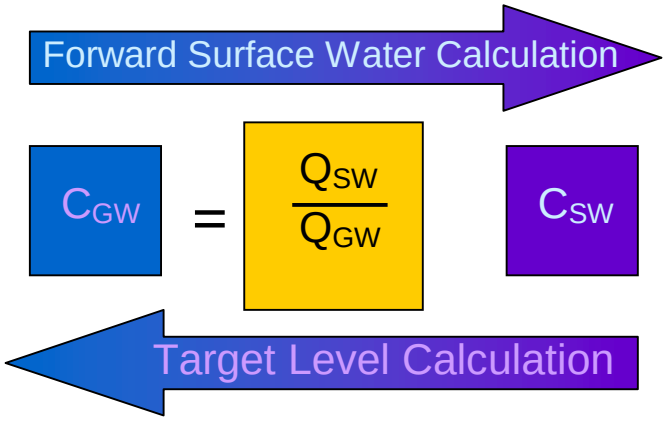


Figure 4.2. Forward surface water calculation and target level calculation.

The concentration and flow values in Figure 4.2 represent the following:

- C_{GW} = target level concentration of COC in groundwater (µg/L)
- C_{SW} = surface water quality standard concentration (µg/L)
- Q_{GW} = groundwater flow from cross-sectional area of plume into stream (cfs)
- Q_{SW} = surface water quantity upstream of the site at design flow conditions (cfs)

Equation 4.1 and Figure 4.2 are used with the assumptions that there is no COC concentration in the surface water upstream of Marcus Hook Creek, and that the total COC mass load into the stream is constant over time. In addition, the surface water flow is assumed to be much greater than the groundwater flow, and the diffuse groundwater flow into the cross-sectional area of the stream is uniformly mixed. The model does not consider any attenuation or degradation of the chemical in the

movement from groundwater to surface water. The only concentration reduction mechanism is the mixing in the creek flow volume. Thus, the actual concentrations are likely to be lower than the predicted concentrations in the surface water. This is part of what makes this a conservative, screening-level calculation.

Figure 4.2 shows that the diffuse groundwater flow directly impacts the quality of surface water. Thus, for a given COC, it is necessary to determine its groundwater concentration that results in a predicted surface water concentration that is below its surface water quality standard. Using the equation in Figure 4.2, a target level groundwater concentration for each COC can be calculated given three input values: the surface water quality standards (C_{SW}), the surface water flow (Q_{SW}), and the groundwater flow (Q_{GW}).

4.4 Surface Water Quality Standard Concentrations

PaDEP has developed and established guidelines for surface water quality standards for numerous chemicals and other substances. As long as the predicted surface water concentrations are below water criteria, both human health and aquatic life are protected. The COCs and their Pennsylvania surface water quality criteria are listed in Table 4.2. These values were input values for C_{SW}, the surface water concentration, in the mass balance equation in Figure 4.2.

Table 4.2: Surface water quality standard concentrations.

Chemical of Concern	Surface Water Quality Criteria (µg/L)
Benzene	1
Ethylbenzene	580
Lead	2.5
Naphthalene	10
Trichloroethene	3
Toluene	330
Total Xylenes	211

Source of data: Pennsylvania Surface Water Quality Standards (1998)

4.5 Surface Water Flow Calculations

The surface water flow, Q_{SW}, was the next value to calculate. The surface water in consideration is Marcus Hook Creek. Daily stream flow data for Marcus Hook Creek was needed to conduct time analyses to obtain Q_{SW}. However, historical stream flows for Marcus Hook Creek were not available from USGS. An alternative method was used to obtain *hypothetical* stream flow data for the creek, illustrated in Figure 4.3.

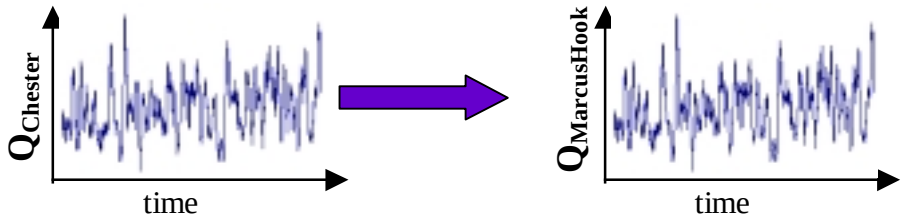


Figure 4.3. Time series analysis using flow data from Chester Creek to obtain hypothetical flow data for Marcus Hook Creek.

A simple drainage area ratio, shown in Equation 4.2, was performed to correlate a creek with unknown stream flow data (*Marcus Hook Creek*) to a creek with known stream flow data (*Chester Creek*).

$$\frac{Q_1}{Q_2} = \frac{A_1}{A_2} \qquad \text{(Equation 4.2)}$$

where:

- Q_1 = unknown stream flow
- Q_2 = known stream flow
- A_1 = drainage area of known stream flow
- A_2 = drainage area of unknown stream flow

Chester Creek was used to estimate the hypothetical stream data for Marcus Hook Creek, because it is located in the same basin and county as Marcus Hook Creek and its historical discharge record spanned 66 years from October 1, 1931 to September 30, 1997. Table 4.3 shows information about Chester Creek. Figure 4.4 is a map of the location and drainage area for Chester Creek.

Table 4.3: Characteristics of Chester Creek.

Station Name	Chester Creek
Station Number	01477000
County	Delaware
Basin	Lower Delaware
Latitude (ddmmss)	395203
Longitude (dddmmss)	0752431
Drainage Area (square miles)	61.1

Source of data: Pennsylvania U.S. Geological Survey

Figure 4.4. Map of the location (blue line) and drainage area (red dot) of Chester Creek relative to Marcus Hook Creek (*http://www.topozone.com*).

Equation 4.2 was rearranged to generate hypothetical stream flow data for Marcus Hook Creek, given information on Chester Creek in the following equation:

$$Q_{MarcusHook} = Q_{Chester} * \frac{A_{MarcusHook}}{A_{Chester}} \qquad \text{(Equation 4.3)}$$

where:

- $Q_{MarcusHook}$ = stream flow for Marcus Hook (cfs)
- $Q_{Chester}$ = stream flow for Chester Creek (cfs)
- $A_{MarcusHook}$ = drainage area of Marcus Hook Creek (square miles)
- $A_{Chester}$ = drainage area of Chester Creek (square miles)

The stream flows for Marcus Hook and Chester Creeks were analyzed using a frequency analysis (Chow, Maidment and Mays 1988); the stream flows and steps used to generate these values can be found in Appendix B.1.

The hypothetical stream flow data for Marcus Hook Creek were calculated and the mean daily flow was 7.74 cfs. However, this flow was not used as the input value for the surface water flow, Q_{SW}, in the mass balance equation in Figure 4.2.

According to the Act 2 guidance, the appropriate surface water stream flow characterization should be different for carcinogenic chemicals than for non-carcinogenic chemicals. For carcinogens, the recommended flow value is a mean value, because exposure to the chemical is modeled over a lifetime. Act 2 guidance states that the mean harmonic flow, $Q_{HARMONIC}$, should be used for carcinogens. The mean harmonic is defined as the reciprocal of the arithmetic mean of reciprocals.

For non-carcinogens, the recommended flow value is a low flow value, because exposure to the chemical is modeled over a shorter time frame. According to the Act 2 guidance, the 7-day/ 10-year low flow, $Q_{7\text{-}10}$, should be used for non-carcinogens. The $Q_{7\text{-}10}$ is defined as the lowest mean stream flow over seven consecutive days, which on average occurs at least once every ten years (Schreffler 1998).

Of the COCs in this study, EPA classifies benzene and trichloroethene (TCE) as carcinogens and classifies ethylbenzene, lead, naphthalene, toluene, and total xylenes as non-carcinogens (EPA IRIS). Thus, depending on the chemical, the value of $Q_{HARMONIC}$ or $Q_{7\text{-}10}$ was used as the input value for the surface water flow, Q_{SW}. Using the adjusted stream flow data for Marcus Hook Creek from Chester Creek, the mean

harmonic flow used for the carcinogens was 9.75 cfs and the $Q_{7\text{-}10}$ used for the non-carcinogens was 7.51 cfs.

4.6 Groundwater Flow

The groundwater discharge (Q_{GW} in the mass balance in Figure 4.2) is 0.028 cfs for Marcus Hook Creek, which is the result of groundwater calculations by Romanek (1999). This value accounts for groundwater flow from both sides of the creek. After a more comprehensive groundwater flow model is developed, calibrated, and verified, an updated groundwater discharge value, Q_{GW}, can be used. However, this groundwater flow is suitable for the purpose of this analysis.

4.7 Target Groundwater Concentrations

Once the values for the surface water concentration (C_{SW}), surface water flow (Q_{SW}), and groundwater flow (Q_{GW}) are known, the groundwater target level (C_{GW}) can determined for each COC. The target groundwater concentrations are listed in Table 4.4.

Table 4.4: Target groundwater concentrations for each COC.

Chemical of Concern	Target Groundwater Concentration (µg/L)
Benzene	348
Ethylbenzene	155,589
Lead	671
Naphthalene	2683
Trichloroethene	1044
Toluene	88,525
Total Xylenes	56,602

4.8 Data Analysis and Discussion

It is important to stress that the above analyses are simple, conservative screening-type calculations. Once the target groundwater concentrations were calculated for each COC, comparisons were made with field groundwater measurements; maximum groundwater measurements from December 1998 were used to compare with the target levels. Table 4.5 illustrates such comparisons for the COCs in the Lube Plant.

Table 4.5: Comparison of target groundwater concentrations with field peak values.

Chemical of Concern	Target Groundwater Concentration (µg/L)	Measured Peak Groundwater Concentration (µg/L)
Benzene	348	14,000
Ethylbenzene	155,589	6800
Lead	671	370
Naphthalene	2683	81
Trichloroethene	1044	250
Toluene	88,525	250
Total Xylenes	56,602	25,000

If the field concentrations are less than the target levels, then those COCs may be eliminated from further consideration of the groundwater-to-surface water exposure pathway, since conservative inputs are used. The analysis and elimination of chemicals from consideration would be based on the demonstration that the maximum values from the historical measurements are representative of maximum concentrations in the groundwater that is discharging to Marcus Hook Creek at the Lube Plant. As stated in Section 4.6, this analysis would need to be updated based on the final groundwater flow model results.

According to sections 250.309 and 250.406 of Act 2:

- "If the results indicate that surface water quality standards are being achieved, no action is required
- If the results of the sampling indicate surface water quality standards are not being achieved, additional sampling may be performed to help evaluate whether surface water quality standards are being achieved
- If the results of the sampling indicate surface water quality standards are being met, no further action is required
- If the results of the modeling, and sampling if any, indicate that surface water quality standards are not being met, the person shall perform further remedial action"

Of the seven COCs in Table 4.5, benzene is the only COC above its target groundwater concentration of 348 μg/L. The concentration of benzene is above the target groundwater concentration by a factor of forty. Thus, according to Act 2 statements, additional analyses or remediation of benzene should be conducted to meet the surface water quality criteria of 1 μg/L. Although no further action is warranted for the other COCs that met their target levels, additional analyses may be warranted for lead, TCE, and total xylenes, since the magnitudes of their peak groundwater concentrations were within the magnitudes of their respective target levels. As stated earlier, additional evaluations may be appropriate to determine if the concentration and groundwater flow data used in this analysis properly represent the conditions in the Lube Plant.

Having a working interaction model requires that the surface water and groundwater models correctly simulate the surface and subsurface environments,

respectively. Validating and calibrating the models are means of obtaining working models. The surface water model developed by Romanek (1999) was validated by comparing its flow to the flow obtained from the time series analyses discussed above. The mean annual flow for Marcus Hook Creek was 7.76 cfs. The surface water model predicted a regional daily flow of 7.74 cfs, which was estimated using an annual runoff value; this runoff value was obtained by converting a USGS annual runoff coverage of the United States into a point coverage and then interpolating it into a surface. The difference between the flow generated from stream gauging data and the value obtained from the surface water model is 0.3%. Thus, the surface water model could be a useful and accurate tool to predict stream flows for the refinery.

However, there is concern about the accuracy of the groundwater flow value. Since the interaction model will produce different groundwater target levels based on different groundwater flows (see Appendix B.2), a more comprehensive groundwater flow model needs to be developed. The next chapter discusses the development and modification of a groundwater flow model.

In conclusion, the groundwater/ surface water interaction model is a potentially useful tool in the corrective action analyses at Marcus Hook. Unlike the contour map-based model, the interaction model was not limited to the spatial distribution of COCs relative to source features; it also focused on the magnitude of COCs in the groundwater. However, one limitation of the interaction model was that it did not actually address the fate and transport of COCs. The next chapter discusses the development of a groundwater flow model that could help in determining the fate and

transport of COCs in groundwater. Once this groundwater model has been calibrated and verified, it can be linked to the facility surface water model developed by Romanek (1999) to produce a more sophisticated groundwater/ surface water interaction model.

CHAPTER 5

MODELING GROUNDWATER FLOW

This chapter discusses the last of the three models developed for the Marcus Hook Refinery (Marcus Hook). A more comprehensive groundwater hydraulics model was developed using GIS ArcView, Groundwater Modeling System (GMS), and MODFLOW, a modular three-dimensional finite difference groundwater flow model. The purpose of developing a more sophisticated model is to better understand groundwater movement under the Lube Plant, particularly how much groundwater discharges into Marcus Hook Creek and the Delaware River. The model can approximate groundwater flows based on boundary conditions and subsurface structures and properties. Knowing these flow values helps determine the fate and transport of a chemical of concern (COC) in the groundwater. After the groundwater model has been calibrated and verified, it can then be connected to a COC transport model to determine scenarios of the fate and transport of a COC in groundwater.

5.1 Study Area

The Lube Plant was chosen as an initial area to study in detail. Modeling groundwater becomes increasingly difficult for larger areas with complex natural and man-made subsurface features.

5.2 Objective

The main objective of developing a more sophisticated groundwater model was to better estimate the groundwater heads and flows in the Lube Plant. The groundwater model is a long-term, steady state description of the groundwater flow in the Lube Plant. Spatial data describing the relevant surface and subsurface features were developed in ArcView and exported into GMS. The subsurface description for the model was then defined in GMS. GMS is one of the most comprehensive groundwater modeling systems available. The Environmental Research Laboratory at Brigham Young University developed GMS in conjunction with The Department of Defense.

Once the conceptual model of the subsurface was built, it was converted into a numerical solution using MODFLOW. MODFLOW is one of the numerical modeling packages supported by GMS. The version used for this research was MODFLOW-88, which is the U.S. Geological Survey version with a few minor changes (e.g., MODFLOW in GMS has a graphical user interface) (BYU 1999). Simulations were executed to obtain estimated groundwater elevations and flows, and after calibrating and verifying the model output with observed measurements, these data were imported back into ArcView.

Lastly, the groundwater flows into Marcus Hook Creek were incorporated into the facility surface water model developed by Romanek (1999) in order to estimate the creek's overall flow at the outlet. Once a strong link has been established between the two models, fate and transport of a chemical of concern (COC) in groundwater discharging to surface water can be addressed.

5.3 Three Groundwater Flow Models

Three steady state, unconfined, one-layer groundwater models are discussed in this chapter: Model 1, Model 2, and Model 3. Model 1 is a simple groundwater flow model developed by Romanek (1999). The author developed Models 2 and 3 as additional subsurface information became available. The assumptions for each model varied depending on the field data available at the time of the work:

- Model 1: assumes a single horizontal hydraulic conductivity value for the Lube Plant
- Model 2: assumes a single horizontal hydraulic conductivity value for the Lube Plant and includes horizontal flow barriers (e.g., mud fences and bulkheads)
- Model 3: assumes different horizontal hydraulic conductivity values for different areas of the Lube Plant based on new stratigraphy data, includes horizontal flow barriers (e.g., mud fences and bulkheads), incorporates staff gauge data in Marcus Hook Creek and the Delaware River and additional groundwater elevation data

The purpose of developing Model 2 and Model 3 was to find out the degree of complexity needed for groundwater modeling in the Lube Plant and whether a more complex groundwater model resulted in better modeling results. Sections 5.4 and 5.5 discuss the digital description and geology of the Lube Plant for both Models 2 and 3, respectively. Sections 5.6 and 5.7 focus specifically on the development of Models 2 and 3, respectively. Details on Model 1 can be found in Romanek's thesis (1999).

5.4. Digital Description of the Lube Plant in ArcView

The first step to developing the groundwater model was to spatially represent the important facility features in GIS, as shown in Figure 5.1. As with Model 1, Models 2 and 3 consisted of the Lube Plant boundary, tanks, monitoring wells and piezometers, buildings, and concrete slabs. In addition, several modifications were included in these models. First, three new coverages of important subsurface features, previously unavailable, were included in Models 2 and 3 as shown in Figure 5.1 (Langan 1999):

- Wooden bulkhead: unreinforced seawall situated on a wooden decking structure that allows flow between the Lube Plant and Delaware River
- Steel bulkhead: steel sheet pilings driven to the bedrock, joined to the wooden bulkhead and mud fences; impedes lateral groundwater flow between the Lube Plant and the Delaware River, and a portion of Marcus Hook Creek
- Mud fences: lower permeability sediments placed perpendicular to the river that provide lateral support for soil behind the wooden bulkhead

Second, Models 2 and 3 included the West Tank Farm area, located in the southeastern part of the Lube Plant as shown in Figure 5.2. The West Tank Farm area, also known as the crude tank farm area, is considered to be a significant impervious cover to infiltration, covering 24% of the Lube Plant. It contains a network of dikes around the above storage tanks that collects storm water and drains it into the sewer system, thereby reducing recharge into the groundwater. Recharge calculations for Model 2 and Model 3 are discussed in Sections 5.6.2 and 5.7.2, respectively.

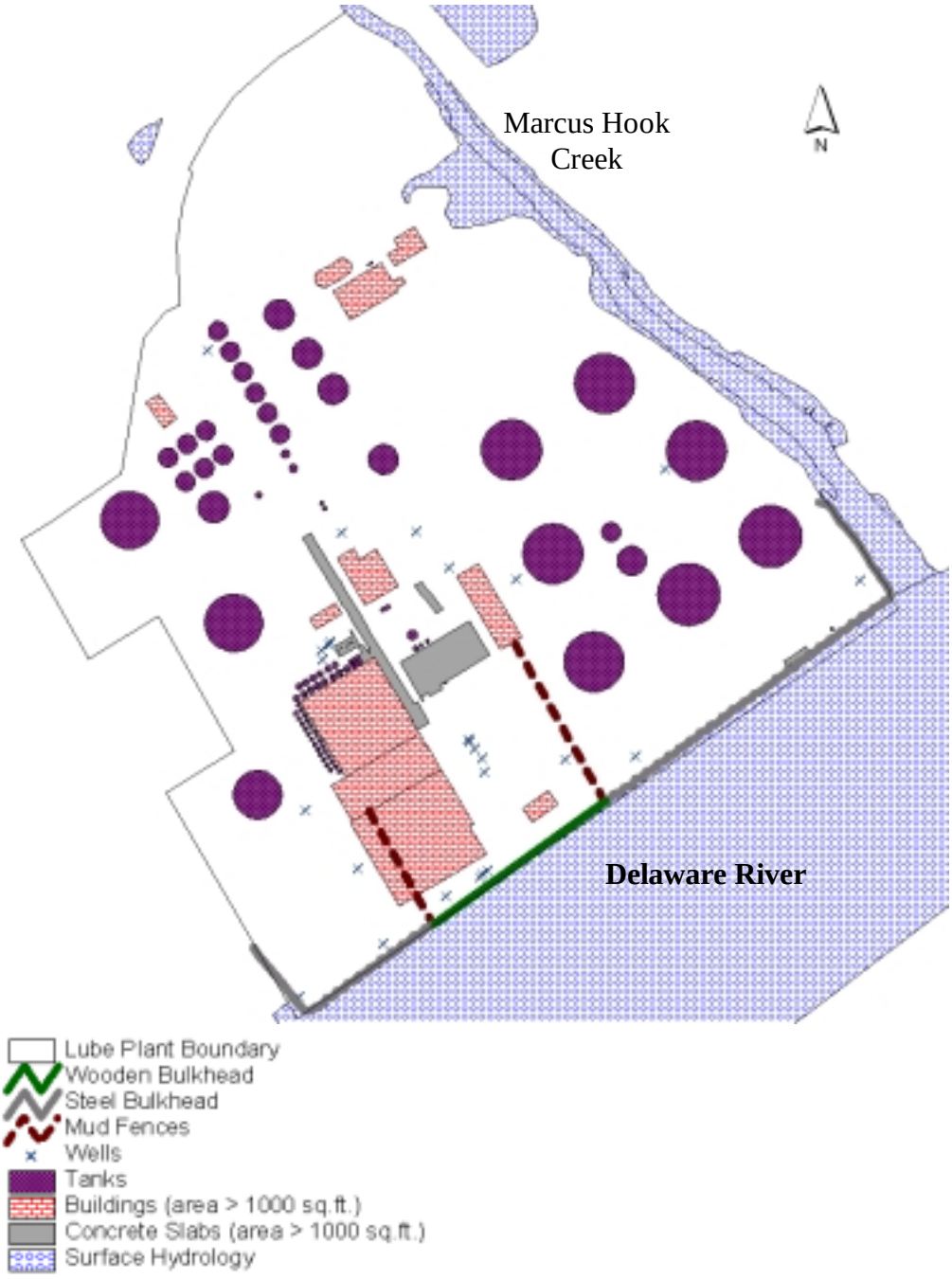


Figure 5.1. Lube Plant with the wooden bulkhead, steel bulkhead, and mud fences in ArcView.

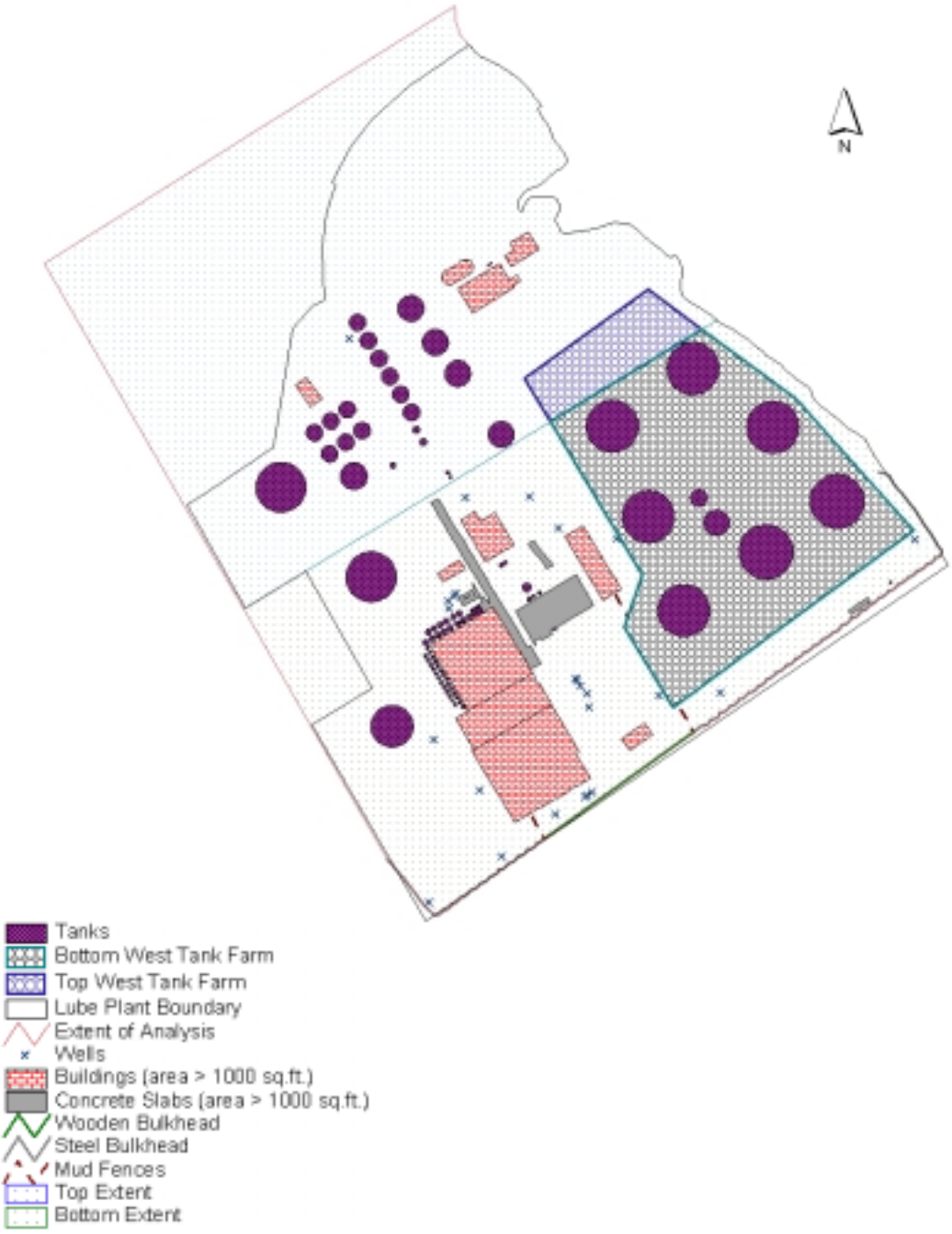


Figure 5.2. Lube Plant represented in ArcView.

Third, a new boundary called the extent of analysis was created to include the Lube Plant boundary and the area northwest of it. This helps minimize the computed errors along the northern and northwestern boundaries of the Lube Plant when running simulations in MODFLOW.

Lastly, the extent of analysis was split into two polygons, the top extent and bottom extent. This was done because of problems encountered when building the model and its shapefiles in GMS. Subsequently, dividing the study area into two also split the northern portion of the West Tank Farm. Figure 5.2 shows all the spatial data in the Lube Plant in ArcView.

Other spatial data needed to build the conceptual model of the subsurface in GMS were surface water elevations around the boundary. Elevations were taken directly from the digital elevation model (DEM) developed from the aerial photography (Romanek 1999). It uses NAVD88 as its vertical datum; all elevations are measured from sea level.

5.5 Lube Plant Geology

According to the boring logs, the Lube Plant is locally heterogeneous. The site's geology can be grouped into four vertical layers descending from the ground surface (see Figure 5.3) (Langan 1999):

- Fill: includes native and man-made debris, predominantly in the area behind the wooden bulkhead
- Silty clay: organic-rich layer, usually the thickest layer in the Lube Plant except for the southwestern part of the site
- Sand and gravel: discontinuous layer
- Bedrock: includes weathered and competent rock

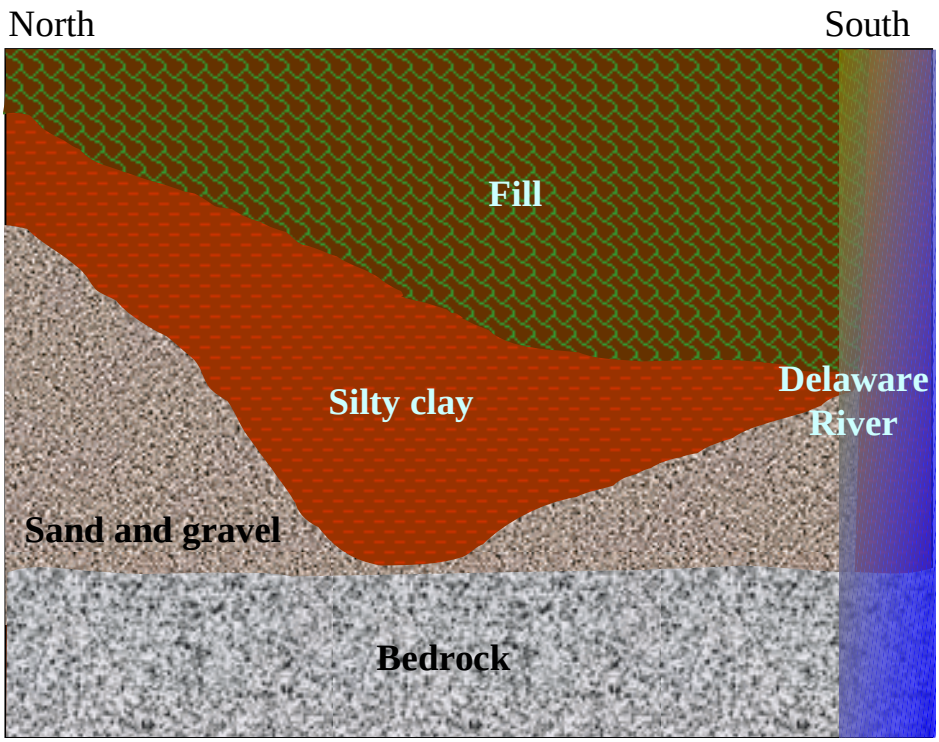


Figure 5.3. Conceptualized cross-section of the stratigraphy from the northern to southern part of the Lube Plant.

5.6 Development of Model 2 in GMS and MODFLOW

5.6.1 Coverage Types in GMS for Model 2

The conceptual model of the subsurface utilized five coverage types:

- Sources and sinks
- Hydraulic conductivity zones
- Recharge Zones
- Groundwater observations for August 1998 (*used for calibration*)
- Groundwater observations for June 1999 (*used for verification*)

Each of these coverage types contains shapefiles that were imported from ArcView. In addition, various assumptions are made about the subsurface description.

The sources and sinks coverage type defines the boundary of the study area being modeled, as well as the local sources and sinks. In this case study, the extent of analysis served as the principle boundary (the Lube Plant boundary was visible but remained inactive in the model). The local sources and sinks included the surface waters (*Marcus Hook Creek and the Delaware River*), general head boundaries (*the northwestern and western boundaries*), and horizontal flow barriers (*mud fences and bulkheads*). The wells in the Lube Plant were not considered to be sources or sinks since they were monitoring wells; thus, they remained inactive but visible in the model. Figure 5.4 illustrates the sources and sinks coverage type in GMS.

In the sources and sinks coverage type, the boundaries along Marcus Hook Creek and a portion of the Delaware River (where the wooden bulkhead lies) were defined as specified head arcs. Although the elevation of the surface water is not static, it rises and falls throughout the day; it can be considered a constant head boundary for

the long-term steady state groundwater model. The specified head boundaries are represented in red in Figure 5.4. Using the information from the DEM, four points along the creek and two along the wooden bulkhead were assigned head values (see Figure 5.4). These heads remained constant during the MODFLOW simulation.

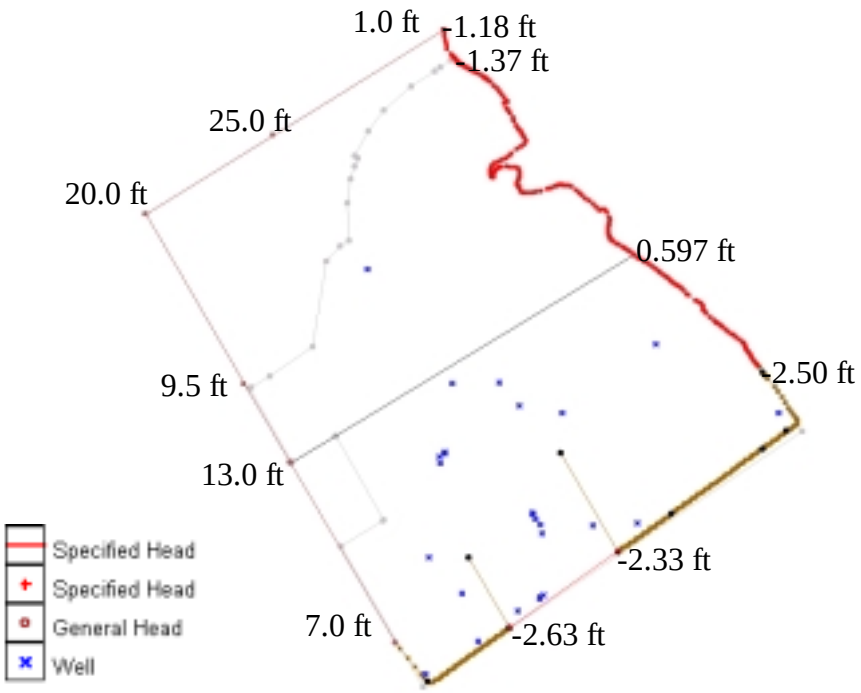


Figure 5.4. Sources and sinks coverage type in GMS with initial head boundary elevations for Model 2.

The northwestern and western boundaries were defined as general head boundaries; general head boundaries are used to incorporate groundwater movement from the region beyond the study site (BYU 1999). The general head boundaries are represented in brick red in Figure 5.4. General heads based on the DEM were assigned

at various points along these boundaries. The conductance values also had to be assigned to the general head arcs. Conductance along a general head arc is equal to the hydraulic conductivity times the width of the material along the length of the arc (BYU 1999). The conductance of the general head arcs was estimated to be 0.113 ft^2/d, assuming that the hydraulic conductivity of the "material" was that of silty clay or clay (1E-7 cm/s) and that the width was a unit width. A more accurate conductance value of the general head arcs could not be obtained because of limited stratigraphy data in the northern and northwestern parts of the Lube Plant.

The final features in the sources and sinks coverage type were the mud fences and the steel bulkhead. These spatial features were defined as horizontal flow barriers, because they limit or prevent groundwater movement through their structures. The horizontal flow barriers are represented in brown in Figure 5.4.

In GMS, the hydraulic characteristics must be assigned to each horizontal flow barrier. The hydraulic characteristic for an unconfined layer is equal to the hydraulic conductivity of the barrier divided by the thickness of the barrier (BYU 1999). Since the steel bulkhead was considered to be a no-flow barrier, its hydraulic characteristic was assigned to be 1E-14 ft/d per ft, which is close to zero. The mud fences do allow some flow; assuming a hydraulic conductivity of clay (1E-7 cm/s = 0.0002835 ft/d) and the thickness to be no greater than one foot in the direction of flow, the hydraulic characteristic was estimated to be 0.0002835 ft/d per day.

The second coverage type was the hydraulic conductivity zones. A hydraulic conductivity of 0.0018 cm/s (5.10 ft/d) was assigned for the study area. This value is

the average of twenty-five measurements from the environmental database that were taken across the entire refinery, not just within the Lube Plant. The variance for the data set is 9.7E-6.

The third coverage type was the recharge zones. The polygon shapefiles of all impervious cover features could have been imported into GMS from ArcView to define the recharge zones in the study area. However, as mentioned in Section 5.4, because of problems with the GMS software, the model had to be simplified and only two polygons were imported into the recharge zones coverage type: the top extent and bottom extent. The recharges were calculated separately for each area based on how much of the surface area is open to precipitation. Section 5.6.2 discusses the recharge calculations for the two areas.

The final two coverage types were the well measurements from August 17, 1998 and June 1, 1999. The 1998 and 1999 observation coverages were used to calibrate and verify the model, respectively. Discussions of calibrating and verifying Model 2 are found in Sections 5.6.5 and 5.6.6. All groundwater measurements were corrected to account for the presence of light non-aqueous phase liquid (LNAPL) (see Section 3.6). For each groundwater data point, the standard deviation was needed as input and was calculated based on all of the sampling data.

5.6.2 Recharge Calculations for Model 2

The recharge for the top and bottom extents of the Lube Plant were calculated as a percentage of the total recharge, based on how much of the surface area was subject

to infiltration. To calculate the recharge for each section, the areas of impervious cover were needed.

The buildings, concrete slabs, tanks, and the West Tank Farm shapefiles were overlaid on the top and bottom extent polygons. The total areas of impervious covers were then calculated for each polygon. A simple equation (Equation 5.1) was used to calculated the recharge for the top and bottom extents:

$$R = R_T * A_O \qquad \text{(Equation 5.1)}$$

where:

- R = recharge (length per time)
- R_T = total recharge (length per time)
- A_O = percent of pervious area (%)

As Section 5.6.5 explains, recharge is one of the parameters that was used to calibrate the model so that the computed groundwater heads matched observed head data. For Model 2, a total recharge of 5 in/yr (0.00114 ft/d) was used for the Lube Plant, because it yielded the best modeling results, that is, the difference between the computed and observed groundwater head measurements were minimized. Table 5.1 shows that the recharge values for the top half and bottom half were calculated to be 4.5 in/yr (0.0013 ft/d) and 2.5 in/yr (0.00059 ft/d), respectively. Appendix C.1 includes all recharge calculations.

Table 5.1. Recharge calculations for top and bottom extents for Model 2.

Total recharge = 5 in/yr	Area (sq. ft)
Lube Plant	2711480.75
Top extent	1668517.00
Buildings	23576.52
Concrete Slabs	0.00
West Tank Farm	76265.90
Tanks	61598.08
Sum	161440.49
% covered	9.7%
% open	90.3%
Top recharge (in/yr)	4.5
Bottom extent	1700957.13
Buildings	165961.83
Concrete Slabs	41349.78
West Tank Farm	580330.48
Tanks	71485.02
Sum	859127.11
% covered	50.5%
% open	49.5%
Bottom recharge (in/yr)	2.5

5.6.3 MODFLOW Inputs for Model 2

Before converting the object-based model into a grid-based numerical model, several assumptions were made. The updated model was assumed to be steady state, one-layer, unconfined, and homogeneous. The starting heads for the interior model cells were assumed to be 7 feet. This is the initial condition for heads for the steady state simulations. The horizontal hydraulic conductivity was 5.10 ft/d for the Lube Plant and the recharges were 4.5 in/yr and 2.5 in/yr for the top and bottom extents of the Lube Plant, respectively. The final inputs needed before running MODFLOW were the top and bottom elevations of the aquifer for the study area.

5.6.3.1. Stratigraphy Data for Model 2

The top and bottom elevations were based on the stratigraphy table in the environmental database. Because the model was assumed to be one-layer, the soil boring data had to be aggregated over the whole soil column. Each boring was assigned an ID number and the top and bottom elevations were calculated. A bottom elevation of –25 feet was assigned for boring locations that were terminated at shallow depths, since –25 feet represented the mean bedrock elevation.

In addition, nine phantom borings were placed around the boundary of the study site to obtain better interpolation results (see Figure 5.5). Their elevations were approximated using adjacent measured boring data; -35 feet below ground surface (bgs) was assigned for phantom borings closer to surface waters and -25 feet bgs was assigned for borings further inland.

Once imported into GMS, the soil boring data were interpolated using the linear method. Figure 5.5 illustrates bottom elevation contours. The red circles represent soil borings. It is interesting to see the wide range of bottom elevation data from -20 feet to -45 feet and how such variations influence groundwater movement.

Figure 5.5. Bottom elevation contours for Model 2 based on stratigraphy data in GMS.

5.6.4 MODFLOW Outputs in Model 2

Based on the assumptions and inputs for Model 2, MODFLOW generated computed groundwater heads and flow rates. Data from the simulation were copied and formatted in Excel using macros. Figure 5.6 illustrates groundwater head contours for the Lube Plant.

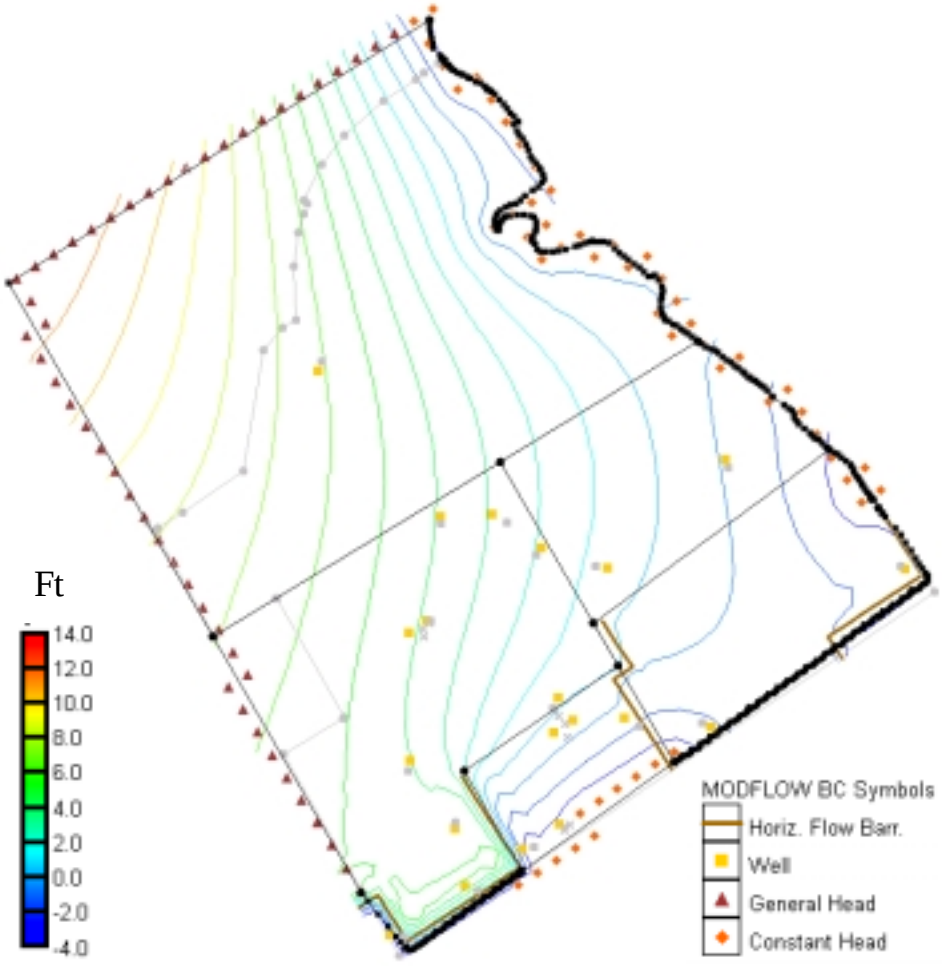


Figure 5.6. Groundwater contours for Model 2 generated in MODFLOW.

As expected, the groundwater flows from the northwest and discharges into the creek and river. There is limited flow through the mud fences and no flow through the steel bulkhead.

5.6.5 Calibration for Model 2

Three parameters were varied in order to calibrate the model's groundwater output: the general head conditions, the starting heads, and the recharge values. Each of these inputs affected the groundwater levels.

The groundwater observations coverage type was used to plot calibration error, which represents the difference between the computed and observed data from August 1998. Table 5.2 lists statistical information about how the computed outputs matched with observed data. Figure 5.7 shows the error at each observed well.

Figure 5.7 and Table 5.2 show that MODFLOW generally underpredicted groundwater heads. One approach to obtaining closer groundwater heads especially in the southern and southeastern parts of the Lube Plant was to look at a more complex stratigraphy and vary hydraulic conductivity in the model. Section 5.7 discusses the development of such a groundwater model, Model 3.

Table 5.2. Calibration errors for Model 2.

Mean error (ft)	-1.43
Mean absolute error (ft)	3.45
Root mean square error (ft)	3.91

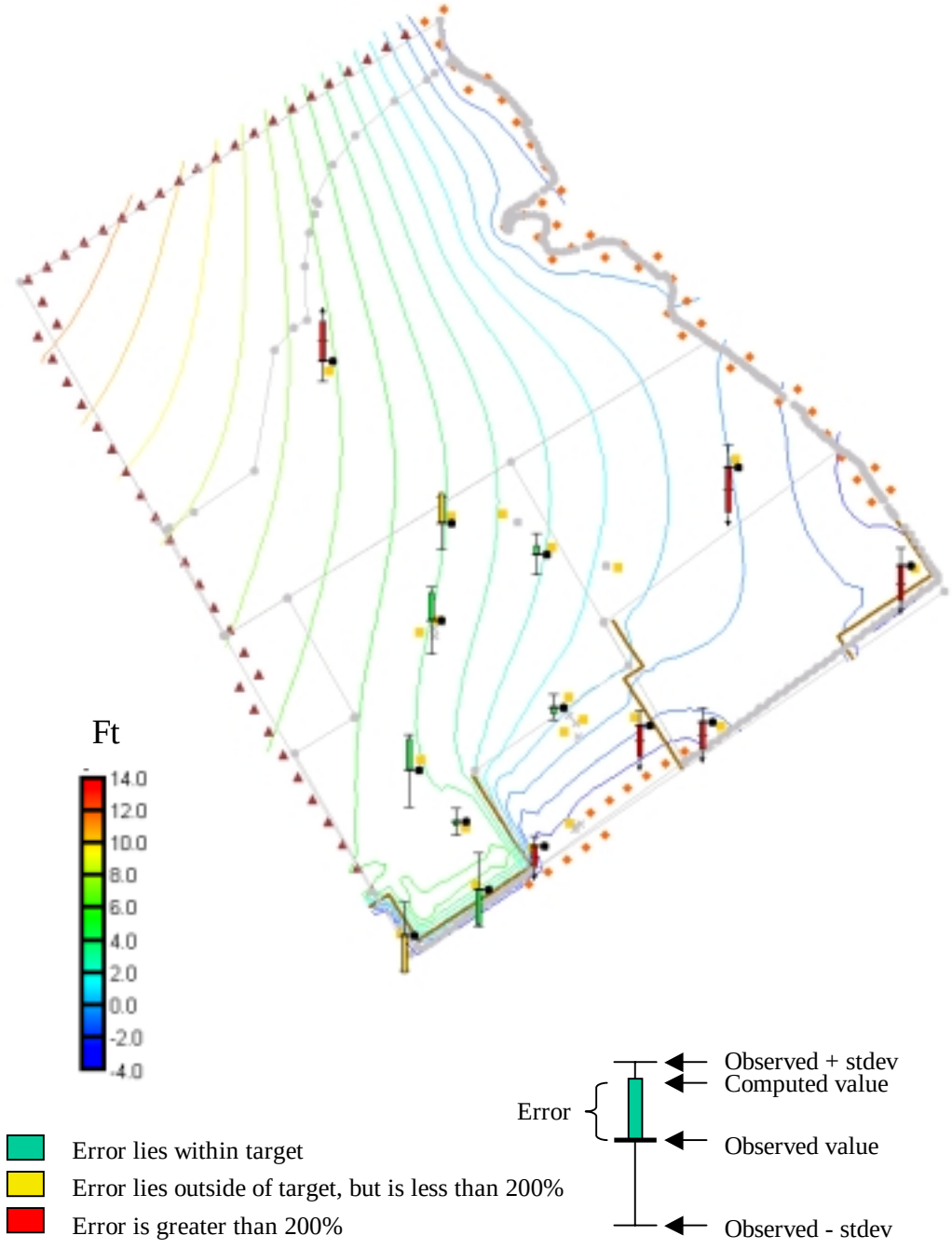


Figure 5.7. Groundwater heads for Model 2 calibrated with August 1998 data.

5.6.6 Verification of Model 2

After Model 2 was calibrated, it was verified using groundwater data from June 1, 1999, an independent data set. Without changing any of the parameters, the model's outputs were compared to the 1999-groundwater heads, shown in Figure 5.8.

The errors during the calibration and verification were compared with one another in Table 5.3. The mean absolute error and root mean square error for the verification were slightly lower compared to the errors for calibration. This meant that the model performed better with the 1999 data set than with the 1998 data set.

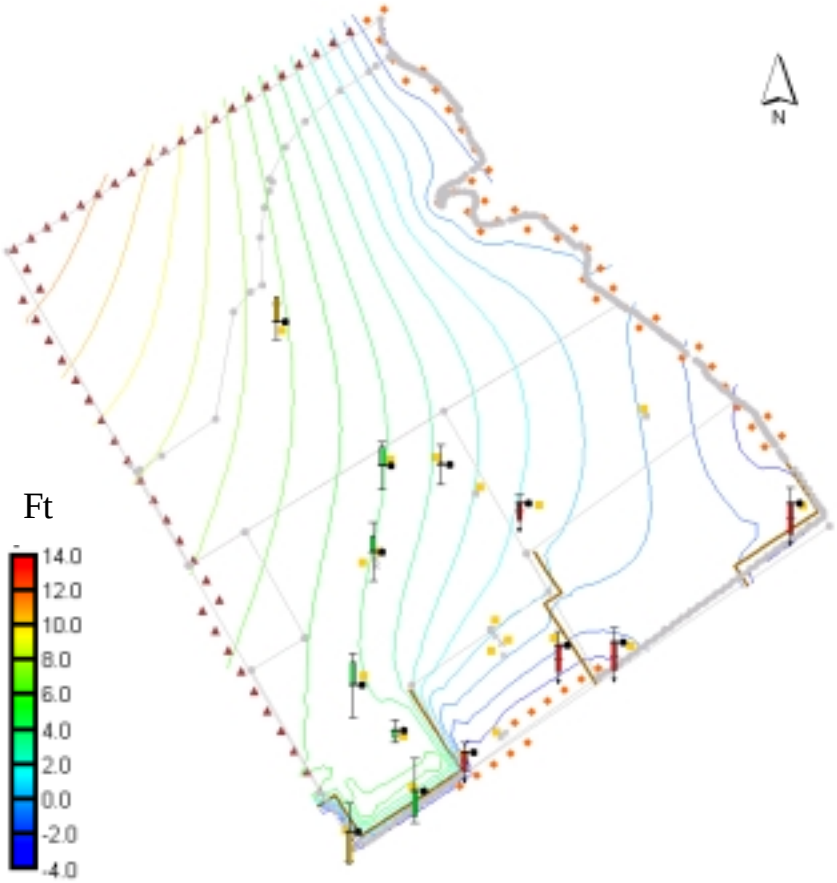


Figure 5.8. Groundwater heads for Model 2 verified with June 1999 data.

Table 5.3. Comparison of errors between calibration and verification for Model 2.

Error (ft)	Calibration (8/98)	Verification (6/99)
Mean error	-1.43	-1.71
Mean absolute error	3.45	3.15
Root mean square error	3.91	3.63

5.7 Development of Model 3 in GMS and MODFLOW

Model 3 was developed to incorporate the new soil boring data, groundwater elevation data, and staff gauge data that were recently collected. The purpose of developing this model was to see whether a more complex model would generate better modeling results (i.e., computed MODFLOW output more closely matches observed data).

The surface elevations based on the DEM were used in combination with staff gauge measurements taken on November 1, 1999 in order to develop elevation data along the length of the surface water boundaries (see Figure 5.9). These staff gauges had been recently installed in Marcus Hook Creek and the Delaware River to measure the surface water elevations. The elevation differences between the DEM and staff gauges were calculated and applied along the surface water boundaries. These new surface water elevations were then incorporated into the sinks and sources coverage type in GMS, as discussed in Section 5.7.1.

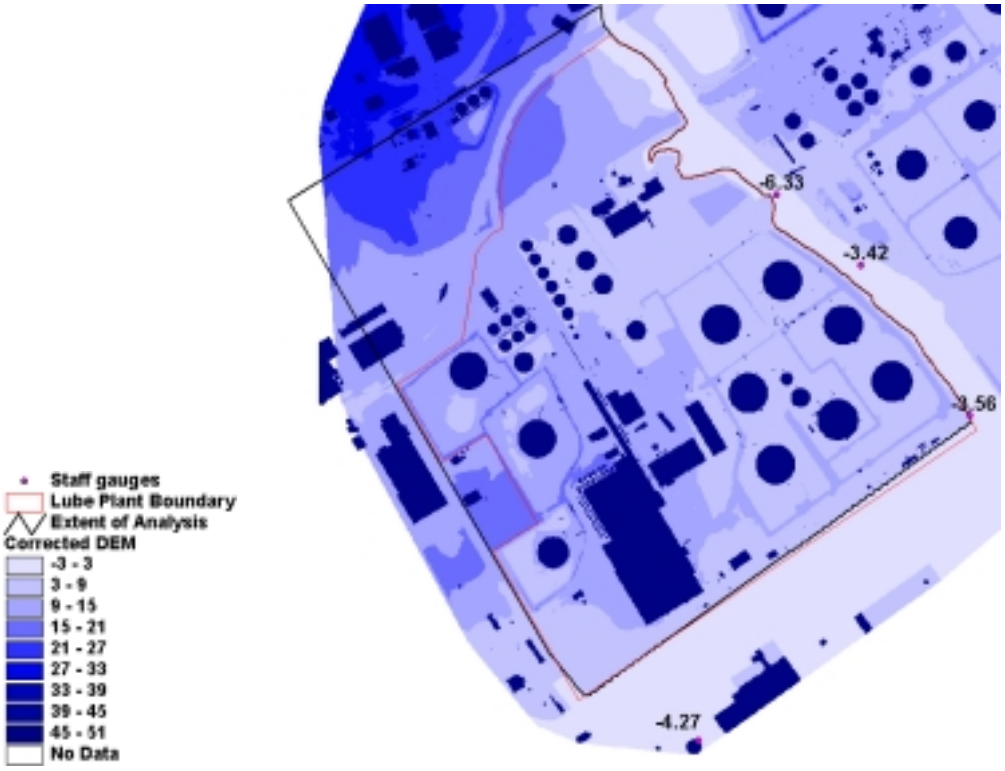


Figure 5.9. Map of staff gauges (November 1, 1999) with DEM in ArcView.

5.7.1 Coverage Types in GMS for Model 3

In the sources and sinks coverage type, all of the boundary conditions remained the same. However, the points along the specified head boundaries (Marcus Hook Creek and Delaware River) now reflected the new surface water elevations based on the DEM and staff gauges, as shown in Figure 5.10.

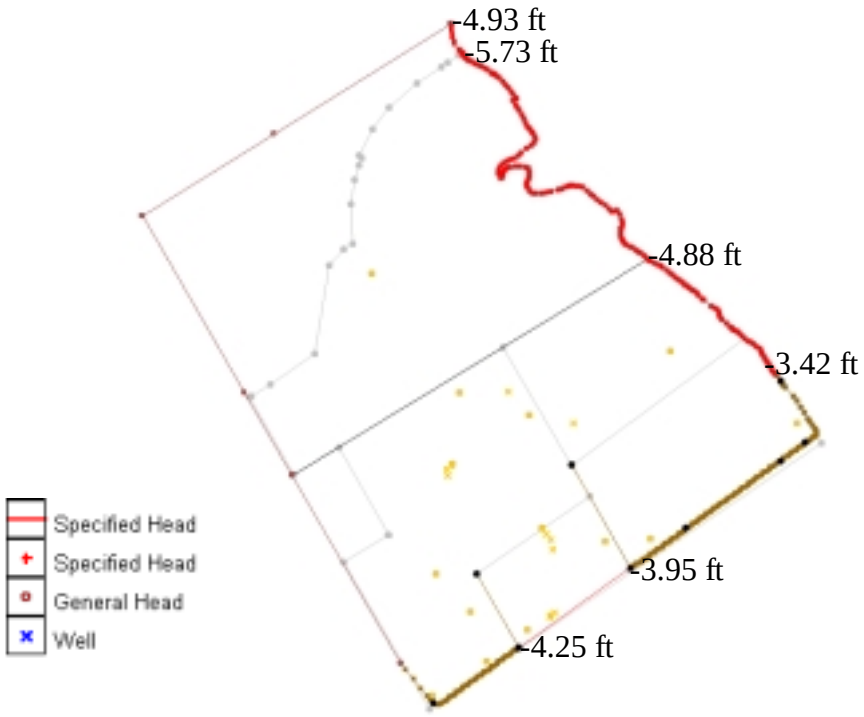


Figure 5.10. Sources and sinks coverage type in GMS with initial head boundary elevations for Model 3.

Since the previous model had difficulty matching the output heads with observed data, particularly in the southern and southeastern areas of the Lube Plant (refer to Figure 5.7), the new soil boring data from September 30, 1999 was used to obtain better results. Based on the soil stratigraphy data from the new soil borings, varied hydraulic conductivity values were assigned to the different areas of the study site to see if the errors could be minimized. Thus, the Lube Plant was divided into five sections, as shown in Figure 5.11:

- top extent: top half of the Lube Plant
- region 1: area between the mud fences
- region 2: area east of the region 1
- region 3 : area north of region 1
- bottom extent 2: remainder of the bottom half of the Lube Plant

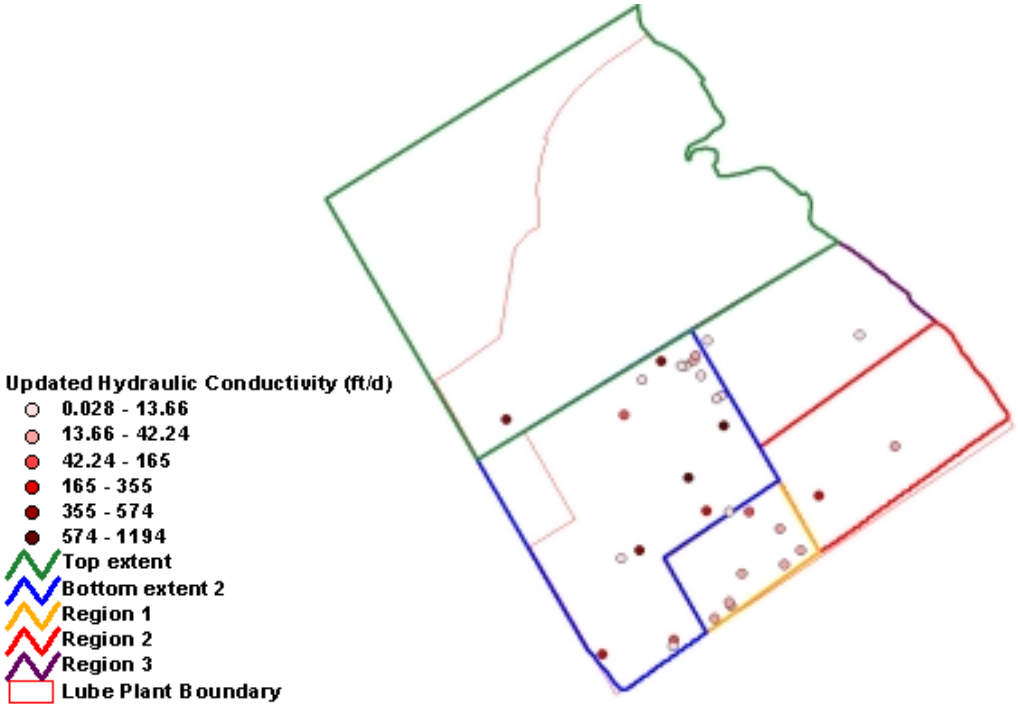


Figure 5.11. New sections of the Lube Plant for Model 3 with hydraulic conductivity points in ArcView.

Although the new soil boring data did not have actual conductivity measurements, they were estimated based on the grain size analytical results. The Hazen equation was used to provide a rough estimate of the hydraulic conductivity,

based on an empirical correlation that depends on effective grain size and predicts the power-law relation with conductivity (Freeze and Cherry 1979):

$$K = Ad_{10} \qquad \text{(Equation 5.2)}$$

where:

- K = hydraulic conductivity (cm/s)
- d_{10} = effective diameter of grain in which 10% of particles are finer (mm)
- A = coefficient = 1 (when using the above units for K and d_{10})

The Hazen approximation may be useful for most soils within the fine sand and gravel range, although it was originally for uniformly graded sands. This equation can still provide a good rough estimate of hydraulic conductivity of soil (Freeze and Cherry 1979).

To estimate the parameter d_{10}, grain size distribution curves were created for each soil (see Appendix C.2). Equation 5.2 was then used to determine hydraulic conductivity values.

The estimated values and measured values were spatially distributed in ArcView to determine which sampling points were in each section (see Figure 5.11). Some of the sampling points had multiple hydraulic conductivity values, because multiple soil samples were taken at different elevations within the soil boring. Thus, an equivalent hydraulic conductivity value was calculated for sampling points with more than one conductivity value using the following equation (Charbeneau 2000):

$$K_{eq} = \sum_{1}^{i} \frac{K_i d_i}{d} \qquad \text{(Equation 5.3)}$$

where:

- K_i = hydraulic conductivity in the i^{th} layer
- d_i = depth of the i^{th} layer
- d = total depth
- K_{eq} = equivalent hydraulic conductivity

Figure 5.12 is a conceptual diagram of how the equivalent hydraulic conductivity was calculated based on each layer's conductivity values

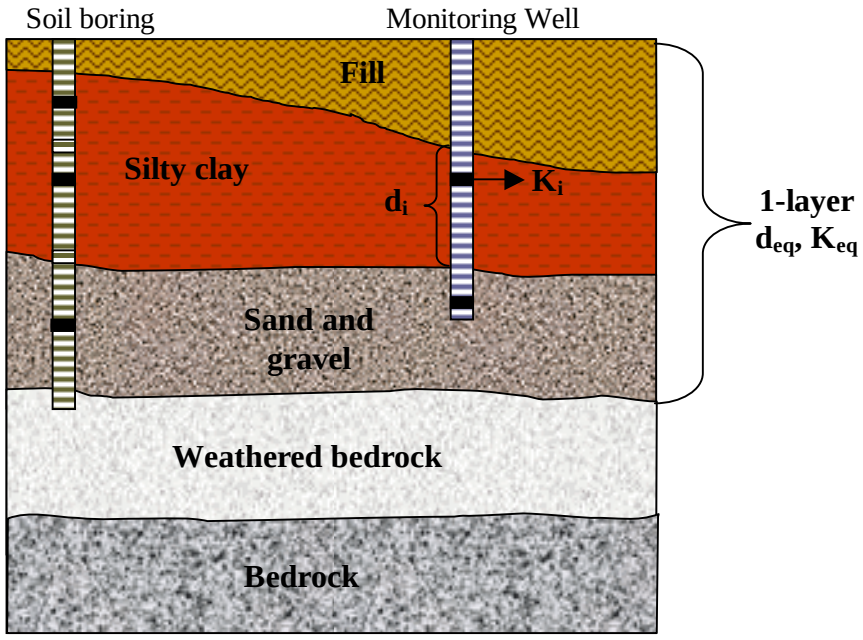


Figure 5.12. Conceptualized cross-section of stratigraphy and approximation for estimating equivalent hydraulic conductivity.

Once the equivalent hydraulic conductivities were determined, a mean hydraulic conductivity and the standard deviation were calculated for regions 1,2, and 3, as shown in Table 5.4. The hydraulic conductivity values listed in region 1 and region 2 represent values estimated from the grain size distribution. The hydraulic conductivity values assigned for the top extent, bottom extent 2, and region 3 represent actual field values. The hydraulic conductivity value for the top extent was 9.01 ft/d, based on the Lube Plant mean value (standard deviation of 11.2 ft/d) and the bottom extent was 5.10 ft/d, based on the facility mean value (standard deviation of 8.8 ft/d). These values were chosen because they yielded the best modeling results.

Table 5.4. Hydraulic conductivity values (ft/d) for Model 3.

Location		K
Top extent	Mean	9.01
	Std Dev	11.2
Bottom extent 2	Mean	5.10
	Std Dev	8.8
Region 1	BH-99-1	23
	BH-99-4	23
	BH-99-5	23
	BH-99-7	23
	MW-41	23
	MW-44	23
	MW-47	34
	BH-99-8	68
	Mean	30
	Std Dev	16
Region 2	MW-61	23
	Mean	23
Region 3	MW-7	9.64
	CPT-6	3.63
	Mean	6.63
	Std Dev	4.25

A t-test was conducted to determine the difference in conductivity means between the entire data set (includes both estimated and measured conductivities) and the estimated conductivity data set. The t value was –1.1, which meant that statistically, the two data sets could not be distinguished from one another.

5.7.2 Recharge Calculations for Model 3

The same method described in Section 5.6.2 was used to calculate the recharge values for the top and bottom extents of the Lube Plant. For Model 3, a total recharge of 20 in/yr (0.00457 ft/d) produced the best modeling results (see Appendix C.1). Although this value is four times greater than the recharge used for Model 2 (5 in/yr), it is a reasonable assumption since the mean annual precipitation is 43.2 inches in this particular part of Pennsylvania (Romanek 1999).

5.7.3 MODFLOW Inputs for Model 3

As with Model 2, Model 3 was assumed to be steady state, one-layer, and unconfined. The starting heads were also 7 feet and the recharge values were defined in the previous section. The hydraulic conductivity values for each area (see Figure 5.11) based on the estimated mean values are listed in Table 5.4.

5.7.3.1. Stratigraphy Data for Model 3

With the addition of new stratigraphy data, the top and bottom elevations were reinterpolated using the basic method described in Section 5.6.3.1. Figure 5.13

illustrates contours of the bottom elevations. For bottom elevations that were less than –20 feet bgs or greater than zero, an elevation of –28 ft was assigned (mean bottom elevation). The same phantom borings were also used. For phantom borings in contact with surface water, the top elevation was assigned to be –9 ft and the bottom elevation was assigned to be –44 ft (maximum depth to bedrock based on the new soil borings). For phantom borings further away from the surface water, the top and bottom elevations were 9 ft (mean top elevation) and –28 ft (mean bottom elevation), respectively.

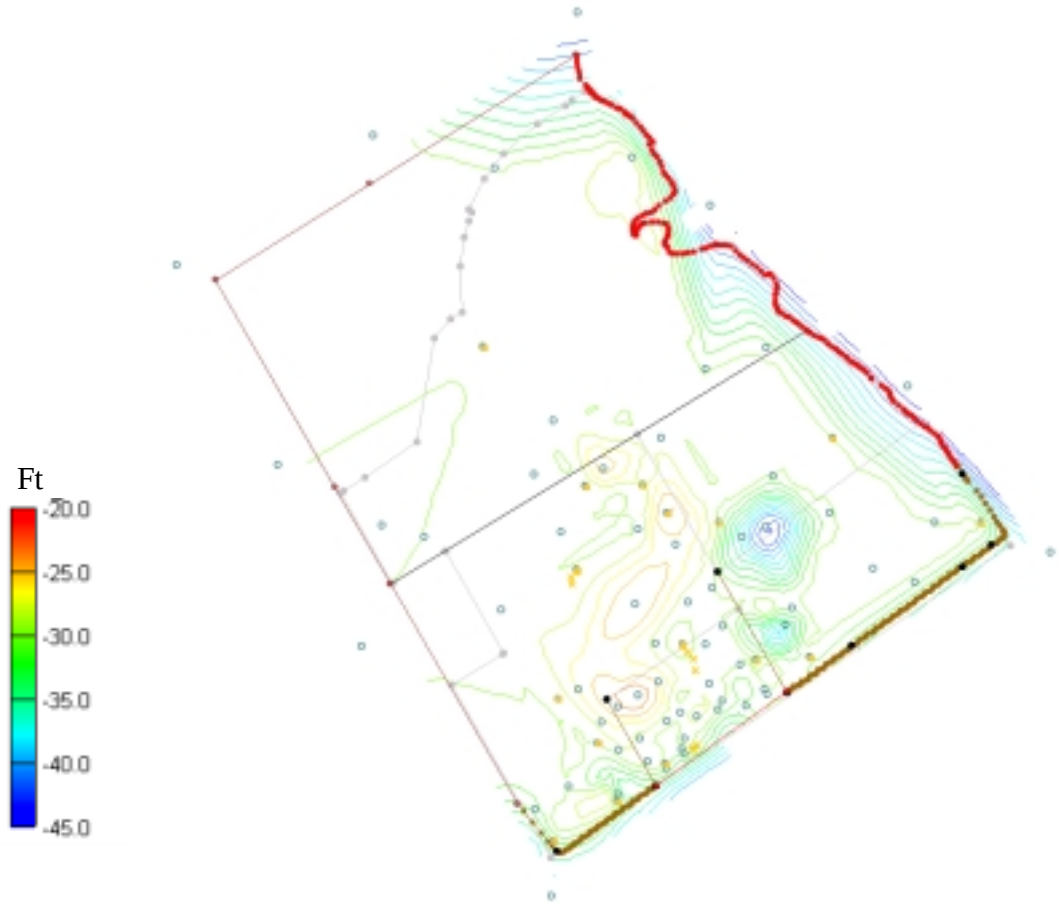


Figure 5.13. Bottom elevation contours for Model 3 based on additional stratigraphy data in GMS.

5.7.4 MODFLOW Outputs for Model 3

Based on the assumptions and inputs for Model 3, MODFLOW simulations were executed to obtain groundwater heads and flow rates. Figure 5.14 illustrates groundwater head contours for the Lube Plant.

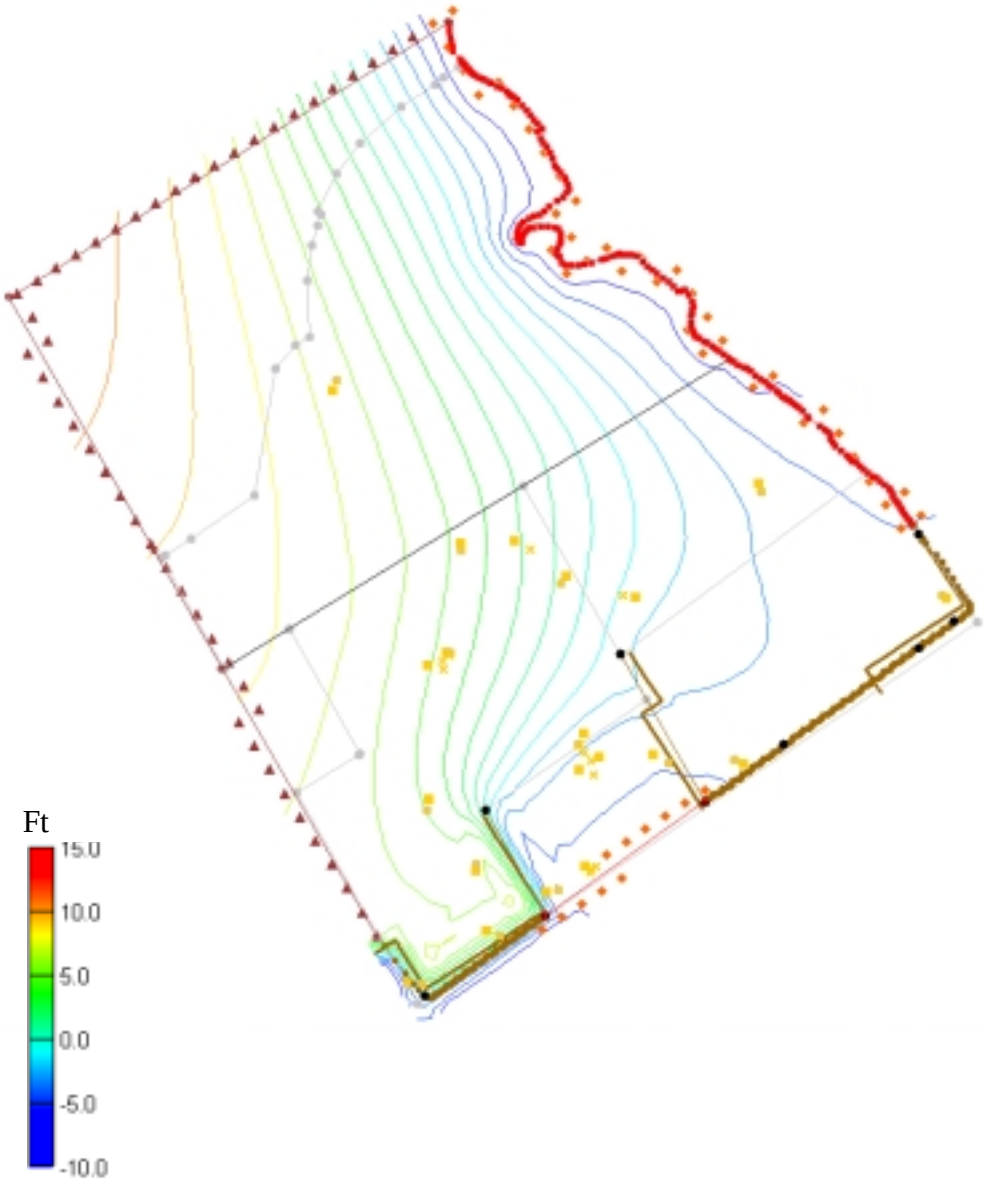


Figure 5.14. Groundwater head contours for Model 3 generated in MODFLOW.

5.7.5 Calibration for Model 3

The two main parameters that were varied in order to yield results that matched observed data were the recharge values and hydraulic conductivities. The main difficulty was assigning the hydraulic conductivity values for each section. Since conductivity varies over several magnitudes, representing one value for an entire layer can lead to greater errors. In addition, the estimated conductivity values were based on the Hazen approximation (Equation 5.2), which was originally used for uniformly graded sands (Freeze and Cherry 1979). The final hydraulic conductivity values used are detailed in Table 5.4.

Table 5.5 lists the various errors between the computed and observed groundwater data (August 1998). On average, MODFLOW still underpredicted the groundwater heads. In addition, the errors in the southern and southeastern parts of the Lube Plant did not decrease with a more complex stratigraphy. It is possible that the additional data may not have improved the modeling results. This is further discussed in Section 5.8. Figure 5.15 illustrates the error at each observed monitoring well for Model 3.

Table 5.5. Calibration errors for Model 3.

Mean error (ft)	-2.49
Mean absolute error (ft)	4.48
Root mean square error (ft)	5.16

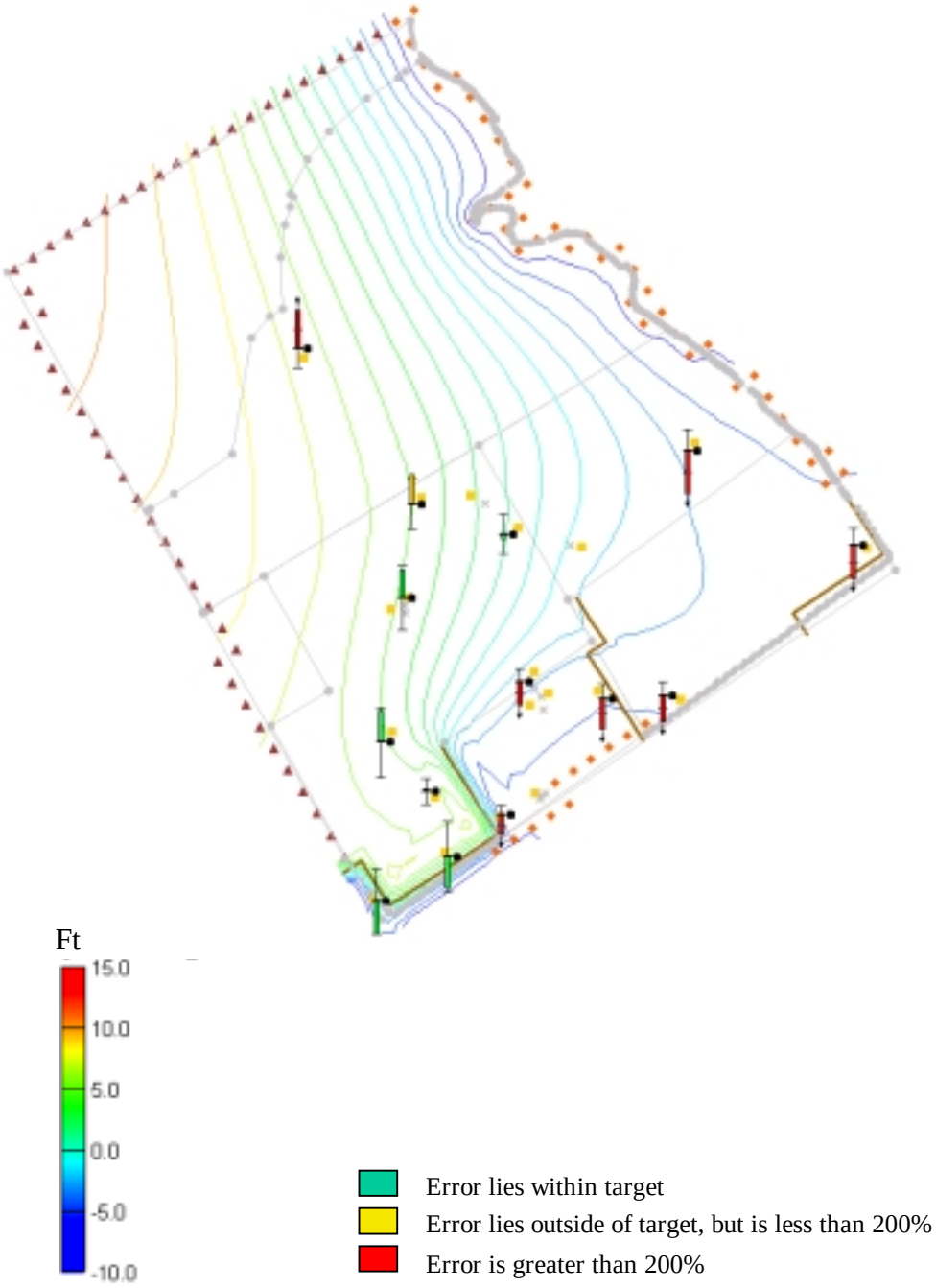


Figure 5.15. Computed groundwater heads from Model 3 calibrated with August 1998 data.

5.7.6 Verification of Model 3

As in Section 5.6.6, Model 3 was verified with groundwater data from June 1, 1999. Figure 5.16 illustrates the errors at each monitoring well and Table 5.6 compares the errors calibration and verification of this model.

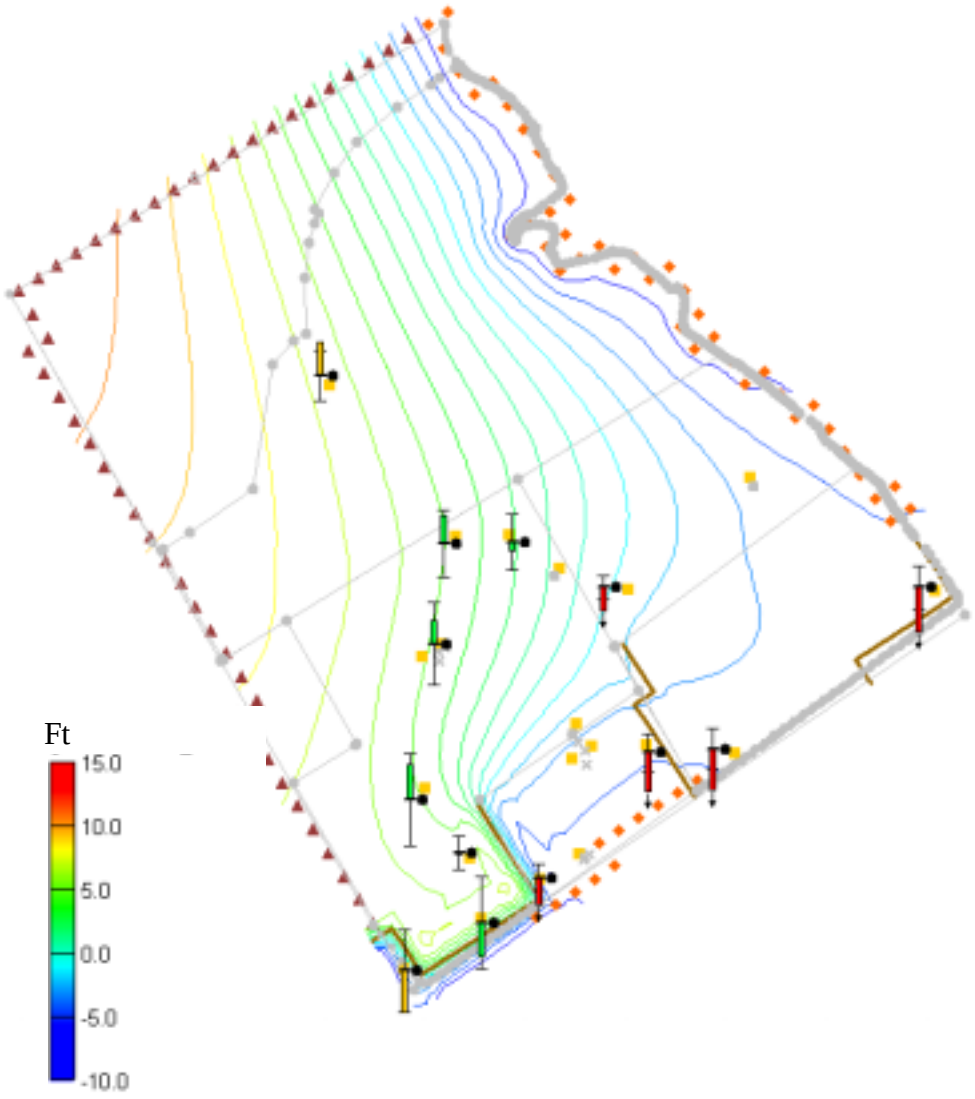


Figure 5.16. Groundwater heads from Model 3 verified with June 1999 data.

Table 5.6. Comparison of errors between calibration and verification of Model 3.

Error (ft)	Calibration (8/98)	Verification (6/99)
Mean error	-2.49	-2.51
Mean absolute error	4.48	3.97
Root mean square error	5.16	4.78

Table 5.6 shows that the root mean square error using the independent data set (June 1999) was less than the root mean square error using the calibration data set (August 1998). Thus, the groundwater head output from Model 3 matched more closely to the independent data set than the observation data set.

5.8 Results and Discussion of Models 2 and 3

The errors from the calibration and verification of Models 2 and 3 are summarized and compared in Table 5.7. Table 5.7 shows that the root mean square error for Model 3 was greater than the error for Model 2. The more complex groundwater model (Model 3) did not minimize the errors in the Lube Plant. One reason for this greater error may be attributed to hydraulic conductivity values estimated from the Hazen equation (Equation 5.2). As discussed in Section 5.7.1, this relationship is primarily used for uniformly graded sands and not for fill or clays, which make up the majority of the bottom extent of the Lube Plant (Freeze and Cherry 1979).

Furthermore, calculating an equivalent hydraulic conductivity value for multiple samples taken within the same soil boring could have increased the error. In spite of making the model more complex (Model 3), the results from Model 2 yielded

better modeling results. More soil stratigraphy data in the southeastern part of the Lube Plant may have provided better modeling results for Model 3.

The errors may also be reduced if the recharge were spatially distributed instead of being constant for the Lube Plant (as discussed in Sections 5.6.2 and 5.7.2), which was the assumption in all three groundwater models. In particular, the West Tank Farm in the southwestern part of the Lube Plant may not be entirely impervious; spatially varying recharge could affect the computed groundwater head elevations in this part of the Lube Plant.

Table 5.7. Comparison of calibration and verification errors between Models 2 and 3.

	Calibration error (ft)		Verification error (ft)	
	Model 2	Model 3	Model 2	Model 3
Mean error	-1.43	-2.49	-1.71	-2.51
Mean absolute error	3.45	4.48	3.15	3.97
Root mean square error	3.91	5.16	3.63	4.78

After Models 2 and 3 were calibrated and verified, the final groundwater discharges into Marcus Hook Creek and the Delaware River (at the wooden bulkhead) were determined. Table 5.8 shows a comparison among the groundwater flow results for Models 1, 2, and 3.

As Table 5.8 shows, Model 2 produced the least amount of total groundwater discharge into surface water and Model 3 produced less total groundwater flow than Model 1, developed by Romanek (1999). The predicted groundwater flows are still

very small relative to the flow in the creek and are within one order of magnitude of one another. Section 5.9.2 discusses the groundwater contribution to surface water.

Table 5.8. Groundwater flows for all three models.

	Groundwater flow (cfs)			Percent of total groundwater flow		
	Model 1	Model 2	Model 3	Model 1	Model 2	Model 3
To Marcus Hook Creek	0.11	0.040	0.12	36.4%	72.7%	74.6%
To Delaware River	0.18	0.015	0.039	63.6%	27.3%	25.3%
Total Flow	0.29	0.056	0.15			

Calculating the percent of total groundwater flowing into the creek and river provided an interesting analysis of groundwater flow in the Lube Plant. In Model 1, over a third of the groundwater discharged into Marcus Hook Creek while a little less than two thirds discharged into the Delaware River through the wooden bulkhead. However, the percentage of groundwater discharging into the creek and river were very close for the Models 2 and 3, even though the total flows were different.

Both Models 2 and 3 showed a more probable division of groundwater discharge between Marcus Hook Creek (25%) and the Delaware River (75%), as estimated by the groundwater flow direction and the creek and river boundary lengths. The groundwater contours in Figures 5.6 and 5.14 show that the groundwater generally flows from the northwest. The river and creek boundary lengths were measured using

the ruler tool in ArcView and were 525 feet and 2330 feet, respectively. The ratio of river to creek lengths was 1 to 4.4 (22.5%); Models 2 and 3 more closely approximate that ratio than does Model 1.

The groundwater models developed in this research (Model 2 and Model 3) may be useful for an integrated GIS-modeling system, provided there is sufficient sampling data available throughout the Lube Plant. Based on the errors, the model with the more complex subsurface conditions (Model 3) did not yield better results than the model with less complex subsurface conditions (Model 2). However, Models 2 and 3 reflected more probable percentages of groundwater flows into Marcus Hook Creek and the Delaware River, as compared with Model 1. Incorporating the horizontal flow barriers (mud fences and bulkheads) seemed to make a significant difference to the groundwater movement than previously thought, particularly the percentage of groundwater flowing to the creek and to the river. In addition, since the percent of flows into the tributaries were about the same for Models 2 and 3, the output groundwater heads were more influenced by the horizontal flow barriers than adjusting the input parameters.

5.9 Groundwater Flow from MODFLOW into ArcView

After the groundwater flows were estimated from MODFLOW, the next step was to export the creek and river shapefiles and their attributes (e.g., groundwater heads and flows) from MODFLOW into ArcView. The groundwater flow in particular may be used as a source input to the facility surface water model (Romanek 1999). Once the

contribution of flow from groundwater is incorporated with the surface water flow, the fate and transport of COCs can be addressed.

5.9.1 Challenge with Importing MODFLOW Data into ArcView

The major challenge of linking the groundwater and surface water models was not being able to import the creek and river shapefiles with the associated groundwater heads and flows directly from MODFLOW into GIS. Although all spatial features can be exported as GIS shapefiles, only certain attributes can be exported, and they are based on the type of feature. Recall from Section 5.6.1 that the creek and river shapefiles were assigned as specified head arcs and these cannot be exported into GIS. Currently, there is a beta version of GMS v3.1 that has the capability to export GIS shapefiles with MODFLOW attributes, regardless of the type of spatial feature. Until GMS v3.1 is available, an alternative approach was used to input the ground water data to the surface water model.

First, the shapefiles of the creek and river were imported into GIS and the segments were converted into a single shape. A simple program could then automate the steps to format the new shapefiles in ArcView, so that they contain the appropriate field headings for the surface water model, and input MODFLOW results. Specifically, a field heading for the groundwater flow would be created. Due to time constraints, a program to facilitate this post-processing was not developed at the time of this thesis. Instead, after the shapefiles were modified in ArcView, the groundwater flow was manually put into the attribute table. The groundwater flow is the total flow into the

creek and the river. The shapefiles with their groundwater flows were then added to the surface water model and the accumulated flow grids were generated.

5.9.2 Groundwater Contribution to Surface Water Flow

The facility surface water model contains an ArcView extension developed by Romanek (1999) that calculates downstream COC concentrations from known inputs, called **COC Transport**. **COC Transport** is based on relationships shown between flow, concentration, and load. The initial calculations estimate flow at the downstream outlet.

Using the flow component of the **COC Transport**, flows for Marcus Hook Creek were generated. As Table 5.9 shows, the groundwater flows based on the Models 2 and 3 did not contribute significantly to the flow in Marcus Hook Creek; the groundwater contribution to the creek was 0.5% with a groundwater flow of 0.04 cfs, and 1.5% with a groundwater flow of 0.12 cfs. Therefore, flow grids were not generated. Figure 5.17 illustrates a map with the input water sources in the Lube Plant.

Table 5.9. Flows generated from the surface water models[1] and groundwater models.

Regional runoff from regional surface water[2] (cfs)	7.74
Facility runoff from facility surface water[2] (cfs)	0.21
Groundwater flow from Model 2 (cfs)	0.04
Groundwater flow from Model 3 (cfs)	0.12

[1]developed by Andrew Romanek (1999)
[2]includes wastewater treatment plant outfall

In the case where the groundwater model and surface water model need to be connected in order to generate flow, concentration, and load grids, the steps are simple to execute with the user-friendly menu. Further detail on the development of **COC Transport**, the steps, and an example application can be found in Romanek's thesis (1999).

Figure 5.17. Map of the Lube Plant in ArcView with the point and area water sources.

5.10 Discussion of the Contribution of Groundwater to Surface Water

Based on the results of the groundwater models presented in this chapter, the preliminary conclusion is that a COC released from a source area into the groundwater would not have a significant impact on potential receptors at the creek and the river, because of the small contribution of groundwater flow to surface water. The groundwater model should continue to be developed into a COC fate and transport model.

Importing MODFLOW shapefiles and attributes did present some setbacks, but the preliminary link between the groundwater and surface water has been established and can be further developed to include COC fate and transport calculations. The major challenge was the post-processing of MODFLOW results. A simple program could be developed to automate some of the post-processing steps, which includes importing the shapefiles and flow data from MODFLOW into ArcView and modifying them so that they can be used with **COC Transport** extension.

CHAPTER 6

CONCLUSIONS

The focus of this research was to develop site-specific models in a Geographic Information System (GIS) framework that could contribute towards integrated environmental risk assessment and corrective action decision support at a large, complex industrial facility. These models help provide insight on the groundwater flux and its interaction with the surface water. Furthermore, they can be integrated with other decision support systems to assess risk more effectively, particularly at industrial sites.

The first of three models was a contour map-based model. The purpose of this model was to develop and apply a procedure to identify potential sources and source areas based on qualitative historical information about environmental conditions and quantitative measurements of concentrations of various chemicals of concern (COCs). The descriptions of environmental conditions were attributes of potential source features such as tanks and process units. Both the potential source features and COC concentrations were represented in GIS ArcView. GIS facilitated the spatial analysis of sources and source areas by providing the means to visualize the distribution of COCs relative to the potential source features.

The map-based model is a tool to identify areas that needed further investigation. The central part of the Lube Plant showed the highest COC concentrations. One potential source feature that was not included in the model was the

network of underground piping, because at the time of this research, there was very limited locational information about these features and the products transported by them.

Overall, the map-based model provided a rapid analysis of potential sources and source areas, which may be practical in determining areas that need further sampling. This procedure of characterizing potential sources using a map-based model may also be extended to other parts of the refinery or other facilities.

The second model was a simple groundwater/ surface water interaction model. This model provided a conservative screening-level analysis by calculating a target groundwater concentration. Usually, a forward risk calculation is done to determine the surface water concentration and this concentration is compared to surface water quality standards. However, in this project, a "backward" calculation was performed to determine the groundwater target level for each COC. These COC concentrations were then compared to peak field data to see which COCs were above their target groundwater concentrations.

The inputs necessary for the simple interaction model were the groundwater flow from the groundwater model, the surface water quality standards for Pennsylvania for each COC, and the surface water flows for Marcus Hook Creek. One of the challenges of developing this model was the unavailability of actual surface water flow measurements. An alternative approach was used to overcome this obstacle; "hypothetical" flows for Marcus Hook Creek were generated from U.S. Geological Survey stream gauge data of a nearby creek, based on a simple drainage area ratio.

Frequency analyses were then conducted to obtain the necessary creek flows. This alternative method was compared to the results of the surface water model developed by Romanek (1999); the difference in flows between the two were less than 1%, thus validating the surface water model and the frequency analysis used to generate "hypothetical" flows for Marcus Hook Creek. Once the inputs were calculated, the target groundwater concentration for each COC was determined.

Benzene was the only COC above its target groundwater concentration based on a groundwater discharge of 0.028 cfs into Marcus Hook Creek. Therefore, according to the Pennsylvania Land Recycling and Environmental Remediation Standard Act (Act 2), no further investigation for surface water is warranted for the other COCs that met their target levels. However, it is important to note that this target level changes with varying groundwater flow, even though the groundwater flow is much smaller than the surface water flow. The interaction model depends on the accuracy of the groundwater flow. Therefore, it is crucial to have a reliable groundwater flow model.

Overall, the groundwater/ interaction model determined a conservative estimate of target groundwater levels for COCs, which may be incorporated in a Tier 1/ Tier 2 risk-based corrective action approach; maximum COC concentration measurements were compared with these target groundwater levels. In addition, the estimation of flows using the time series analysis may be useful for other sites that do not have stream flow data.

The final model was a groundwater hydraulics model developed in ArcView, Groundwater Modeling System (GMS), and the modular finite-difference groundwater flow model (MODFLOW). Two models (Model 2 and Model 3) were developed based on different assumptions and inputs. Efforts to build a groundwater model originally began with Romanek (1999) (Model 1). Models 2 and 3 differed from Model 1 in that they incorporated additional important subsurface features, such as the mudfences and the bulkheads. The mudfences and steel bulkhead serve as flow-limiting and no-flow barriers, respectively. Since these features are located along the southern boundary of the Lube Plant, most of the groundwater in Models 2 and 3 flowed into Marcus Hook Creek, approximately 75%. In Model 1, more groundwater flowed through the wooden bulkhead and into the Delaware River. Thus, Models 2 and 3 provided more probable pictures of groundwater movement.

Model 2 may have yielded better flow results with additional sampling data. One of the challenges of developing groundwater models for complex subsurface environments is the practical limitation on sampling data. Many assumptions were made and some parameters had to be estimated. Towards the end of this research, new sampling data were obtained and Model 2 was altered to reflect the new data. The new groundwater model (Model 3) was divided into five areas with different hydraulic conductivity values in each area. In addition, new groundwater data and surface water elevation data were incorporated into this model (Model 3).

The hydraulic conductivity values for the southwestern and southern parts of the Lube Plant were estimated based on new grain-size analysis data. Using the Hazen equation and particle-size distribution graphs, an estimated conductivity value was calculated for those areas in Model 3. In addition, for some soil borings, an equivalent hydraulic conductivity value was determined.

The purpose of running more simulations was to see if additional data could yield better modeling results for Model 3, a more complex model. However, based on the calibration, Model 3 did not yield better results; there were relatively large calibration errors with this model. Model 3 was still underpredicting groundwater heads along the southern and southeastern parts of the Lube Plant.

One reason for these errors could be that in those areas that yielded greater errors (specifically the southeastern and northern part of the Lube Plant), there were only one or two new sampling points. With more field data in these areas, these errors may be minimized. Another reason could be that the 1998 groundwater data that was used for calibration may not have been representative of the historical groundwater heads. In addition, the recharge was assumed to be spatially uniform across the Lube Plant. The West Tank Farm in the southwestern part of the Lube Plant may not be as impervious as previously assumed. Spatially varying recharge may reduce the errors, particularly in the south and southeastern parts of the Lube Plant. Still, after verifying both models, the errors were less with the 1999 verification data set than compared with the 1998 calibration set.

With each model, several challenges and obstacles had to be overcome before continuing the research. One of the common problems faced in most facility-scale modeling is limited field data. It can be rather costly to collect additional sample data; hence, models are used as a cost-effective alternative. A general challenge when developing models deals with the input data. Building, modifying, and adding input data for the models can be time consuming and difficult at times, even with minimum programming. A more automated method to build, modify, or add input data could be developed, but the programming may be rather intensive.

One of the advantages of formatting input data in GIS is that it is user-friendly. However, importing these data into GMS was difficult, particularly if the GIS shapefiles are complex in geometry. With the upcoming release of the most recent version of GMS, transferring data between GMS and GIS is expected to be smoother. Thus, attributes such as groundwater flows and heads may be more easily imported into GIS and these attributes would not be limited to certain shape file types.

Since the basic foundation of developing a more complex groundwater model in GIS, GMS, and MODFLOW has been set, further work can be done to yield more accurate modeling results. Attempts have been made to modify the groundwater model into a 2-layer model, consisting of fill and silty clay (top layer), and sand and gravel (bottom layer). With more field data becoming available, a more accurate groundwater model could be developed. In addition, developing a groundwater model with spatially varying recharge could be investigated.

Although the results presented in this research were site-specific to Marcus Hook Refinery, the basic methods and procedures developed and used at this case study may be applied to other industrial sites. All of the models presented in this research can contribute to the overall goal of a GIS-based, integrated risk assessment at a large, complex industrial facility.

APPENDIX A

CONTOUR MAP-BASED MODEL

APPENDIX A.1

CORRECTED GROUNDWATER ELEVATION AVENUE SCRIPT

```
'----------------------------
'--- Creation Information ---
'----------------------------
'
'Name: corrected_gwelev.ave
'Version: 1.0
'Date: July 12, 1999
'Author: Julie Kim
'            Center for Research in Water Resources
'            University of Texas at Austin
'             juki@mail.utexas.edu
'
'--------------------------
'--- Purpose/Description ---
'--------------------------
'
'Adds a new field to an existing theme table that will calculate
'the corrected groundwater elevations for measured LNAPL thicknesses
'based on the specific gravities at various monitoring wells.
'Requirements: The view must be active, and there must be a theme
'table with GW_Elev, Imm_Thick, and Specific_Gravity fields.

'Find the table
theProject = av.GetProject
theView = av.GetActiveDoc
theThemeList = theView.GetThemes
theTheme = MsgBox.Choice(theThemeList,"Choose the Theme Table to
Modify","Theme Table Selection")

'Set the editing properties
theftab = theTheme.GetFTab
if (theftab.CanEdit) then
  theftab.SetEditable(true)
else
  MsgBox.Info("Can't edit the theme table","Error")
  exit
end
```

```
'Add the new field
outfields=List.Make
outfields.Add(Field.Make("Corrected_GWElev",#FIELD_DECIMAL,18,2))
outfieldsc=outfields.DeepClone
theftab.addfields(outfieldsc)

'Define fields
gwelevfield = theftab.findfield("GW_ELEV")
immthickfield = theftab.findfield("IMM_THICK")
specgravfield = theftab.findfield("SPECIFIC_GRAVITY")
newfield = theftab.findfield("Corrected_GWElev")

'Return values
 for each rec in theftab
  GWelev = theftab.returnvalue (gwelevfield,rec)
  Immthick = theftab.returnvalue (immthickfield,rec)
  Specgrav = theftab.returnvalue (specgravfield,rec)

  if (Specgrav.IsNull) then
    theftab.setvalue(newfield,rec,GWelev)
  else
    Correctgw = GWelev + (Immthick * Specgrav)
    theftab.setvalue(newfield,rec,Correctgw)
  end
end

theftab.SetEditable(false)
```

APPENDIX B

GROUNDWATER/ SURFACE WATER INTERACTION MODEL

APPENDIX B.1

TIME SERIES ANALYSIS OF MARCUS HOOK CREEK

There are 66 years of stream flow data for Chester Creek from October 1, 1931 to September 30, 1997 (columns A and B). The "hypothetical" discharge for Marcus Hook Creek (column C) was calculated using the simple drainage area ratio (Equation 4.2) for each date. The mean flow was then calculated to be 7.74 cfs.

This arithmetic mean flow value was not used for the surface water flows in the interaction model (Chapter 4). The waste water discharge to the creek contributes significantly to the overall flow. Thus, the mean daily waste water flow of 4.46 cfs was added to the hypothetical flow data. Column D lists the adjusted flow values for Marcus Hook Creek.

According to Act 2 guidance, the mean harmonic flow should be used for carcinogens and the $Q_{7\text{-}10}$ should be used for non-carcinogens in surface water. The mean harmonic flow is the reciprocal of the arithmetic mean of reciprocals; using the statistics function in Microsoft Excel, a mean harmonic flow of 9.75 cfs was obtained.

The $Q_{7\text{-}10}$ was determined using a frequency analysis. The $Q_{7\text{-}10}$ is the minimum mean yearly flow whose return period is 10 years or whose probability of occurring is 10%. Using the adjusted creek flows, the mean flow for a 7-consecutive-day window was calculated for all dates (column E). An additional column (F) was inserted to represent each year. The minimum flow (column G) was selected from the 7-consecutive-day mean flows (column E) for each year. These minimum flows and their corresponding years were then ranked from highest to lowest minimum mean yearly flow (columns I and J).

The exceedance probability (column K) was calculated for each minimum mean yearly flow (column J) using Gringorton's formula (Chow, Maidment and Mayes, 1988):

$$P(X \geq x_m) = \frac{m - b}{n + 1 - 2b}$$

where:

- P = exceedance probability of the m^{th} largest value
- m = rank of a value in a list from descending order of magnitude
- n = number of years in the record
- b = 0.44 for Gringorten's formula

The return period (column L) is the inverse of the exceedance probability. Since the return period is approximately 10 years, the corresponding $Q_{7\text{-}10}$ for non-carcinogens was 7.51 cfs.

	A	B	C	D	E	F	G	H	I	J	K	L
1	Date	Chester Creek Discharge (cfs)	Marcus Hook Creek Discharge w/o waste water (cfs)	Marcus Hook Creek Discharge w/ waste water (cfs)	Mean 7-consecutive day Flow (cfs)	Year	Minimum Mean Yearly Flow (cfs)	Rank	Year	Minimum Mean Yearly Flow (cfs)	Exceedance Probability (%)	Return Period (yr)
2	10/1/1931	16	1.37	5.83	5.78	1931	5.17	1	1970	6.57	0.0%	118.1
3	10/2/1931	17	1.45	5.91	5.86	1932	5.64	2	1989	7.73	2.4%	42.4
4	10/3/1931	16	1.37	5.83	6.08	1933	6.56	3	1983	7.65	3.9%	25.8
5	10/4/1931	14	1.20	5.66	6.14	1934	6.66	4	1988	7.60	5.4%	18.6
6	10/5/1931	15	1.28	5.74	6.21	1935	5.94	5	1993	7.56	6.9%	14.5
7	10/6/1931	15	1.28	5.74	6.27	1936	6.21	6	1971	7.55	8.4%	11.9
8	10/7/1931	15	1.28	5.74	6.38	1937	6.51	7	1987	**7.51**	**9.9%**	**10.1**
9	10/8/1931	23	1.96	6.42	6.28	1938	6.74	8	1995	7.49	11.4%	8.7
10	10/9/1931	35	2.99	7.45	6.19	1939	6.63	9	1982	7.33	12.9%	7.7
11	10/10/1931	21	1.79	6.25	6.02	1940	5.19	10	1977	7.18	14.5%	6.9
12	10/11/1931	19	1.62	6.08	6.02	1941	5.28	11	1974	7.17	16.0%	6.3
13	10/12/1931	20	1.71	6.17	6.00	1942	5.72	12	1986	7.16	17.5%	5.7
14	10/13/1931	16	1.37	5.83	5.94	1943	5.49	13	1984	7.15	19.0%	5.3
15	10/14/1931	15	1.28	5.74	5.95	1944	6.49	14	1973	7.13	20.5%	4.9
16	10/15/1931	16	1.37	5.83	5.95	1945	7.00	15	1992	7.10	22.0%	4.5
24094	9/16/1997	35	2.99	7.45	7.15							
24095	9/17/1997	33	2.82	7.28	7.10							
24096	9/18/1997	32	2.73	7.19	7.05							
24097	9/19/1997	30	2.56	7.02	7.02							
24098	9/20/1997	31	2.65	7.11	7.02							
24099	9/21/1997	31	2.65	7.11	6.99							
24100	9/22/1997	28	2.39	6.85	6.96							
24101	9/23/1997	31	2.65	7.11	7.23							
24102	9/24/1997	29	2.48	6.94	7.36							
24103	9/25/1997	30	2.56	7.02								
24104	9/26/1997	30	2.56	7.02								
24105	9/27/1997	28	2.39	6.85								
24106	9/28/1997	29	2.48	6.94								
24107	9/29/1997	50	4.27	8.73								
24108	9/30/1997	42	3.59	8.05								
24109	mean		7.76									
24110	harmean			9.75								

APPENDIX B.2

CALCULATION OF TARGET GROUNDWATER LEVELS

In Section 4.7, the target groundwater levels represent values using a groundwater flow of 0.028 cfs. Using the output flows from the groundwater models developed in Chapter 5 (Model 2 and Model 3), new target groundwater levels were obtained to see how varying groundwater flows affect the groundwater target levels. Because the interaction model is a conservative, screening-type model, the target levels obtained using Models 2 and 3 were also compared with measured peak groundwater concentrations from December 1998.

The groundwater flow inputs to the interaction model were doubled to account for flow discharging from the eastern part of the facility. The groundwater flow values determined from Models 2 and 3 represented groundwater flow under the Lube Plant. For the purpose of the procedure, these flow values were doubled so that the groundwater inputs into the interaction model represents groundwater flow from both sides of the creek.

For Model 2: Groundwater flow = 0.04 cfs x 2 = 0.08 cfs

COC	Surface water concentration, C_{SW} (µg/L)	Target groundwater concentration, C_{GW} (µg/L)	Measured peak groundwater concentration (µg/L)
Benzene*	1	122	14,000
Ethylbenzene	580	54,456	6,800
Lead	2.5	235	370
Methyl-tert-butyl-ether	n/a	n/a	not detected
Naphthalene	10	939	81
Trichloroethene*	3	365	250
Toluene	330	30,984	250
Total Xylenes	211	19,811	25,000

**Carcinogen*

For Model 3: Groundwater flow = 0.12 cfs x 2 = 0.24 cfs

COC	Surface water concentration, C_{SW} (µg/L)	Target groundwater concentration, C_{GW} (µg/L)	Measured peak groundwater concentration (µg/L)
Benzene*	1	41	14,000
Ethylbenzene	580	18,152	6,800
Lead	2.5	78	370
Methyl-tert-butyl-ether	n/a	n/a	not detected
Naphthalene	10	313	81
Trichloroethene*	3	122	250
Toluene	330	10,328	250
Total Xylenes	211	6,604	25,000

**Carcinogen*

According to the interaction model results for Model 2, benzene, lead, and total xylenes were above their respective target groundwater levels. For Model 3, benzene, lead, trichloroethene, and total xylenes were above their respective target groundwater levels. According to Act 2, further investigation is warranted for these COCs. However, as the interaction modeling results show, the target levels vary with different groundwater flow inputs. Therefore, developing a more accurate groundwater model may provide a better estimate of the target groundwater levels.

APPENDIX C

GROUNDWATER FLOW MODEL

APPENDIX C.1

RECHARGE CALCULATIONS

Recharge is one of the parameters used to calibrate the groundwater models in Chapter 5. As discussed in Section 5.6.2, the recharges for the top and bottom extents of the Lube Plant were determined based on the percent of pervious cover, shown in Table 5.1. Below are the recharge calculations ranging from a recharge value of 2.5 in/yr to 25 in/yr. The final recharge selected for Model 2 was 5 in/yr and for Model 3 was 20 in/yr.

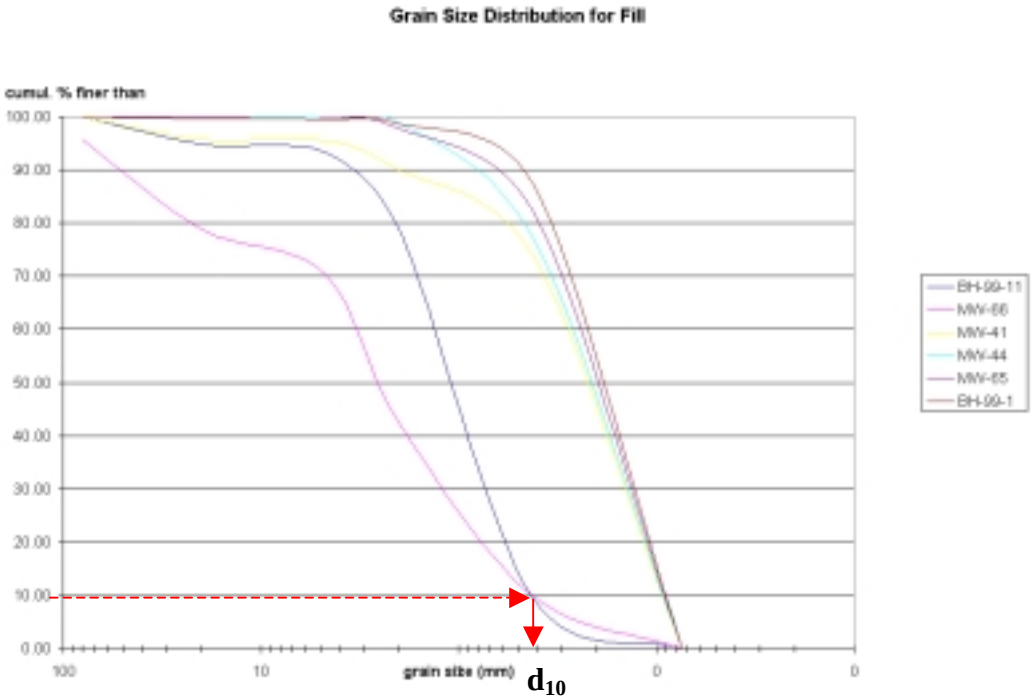
Trial	Recharge (in/yr)	Recharge (ft/d)	Top (ft/d)	Top (in/yr)	Bot (ft/d)	Bot (in/yr)
0	25	0.00571	0.00516	22.58	0.00295	12.92
1	20	0.00457	0.00412	18.06	0.00236	10.33
2	15	0.00342	0.00309	13.55	0.00177	7.75
3	10	0.00228	0.00206	9.03	0.00118	5.17
4	5	0.00114	0.00103	4.52	0.00059	2.58
5	2.5	0.00057	0.00052	2.26	0.00029	1.29

APPENDIX C.2

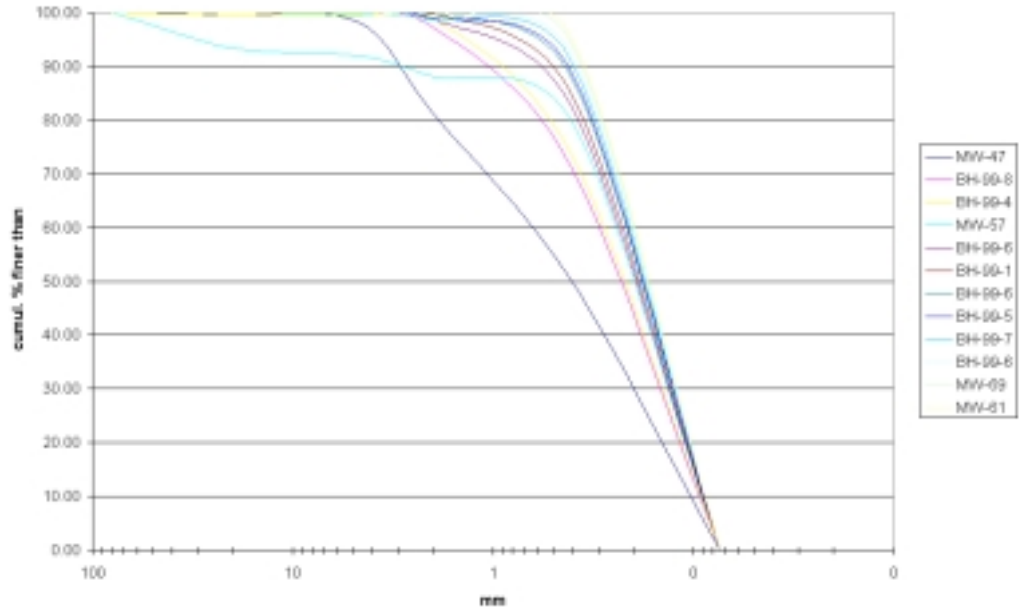
GRAIN SIZE DISTRIBUTION GRAPHS

New soil borings from September 30, 1999 were incorporated into Model 3. As discussed in Section 5.7.1, the hydraulic conductivities were estimated based on the grain size analytical results (raw data). According to the Hazen approximation (Equation 5.2), the hydraulic conductivity depends on the effective grain size, d10, in which 10% of particles are finer than the effective diameter. Grain size distribution graphs help estimate the effective grain size.

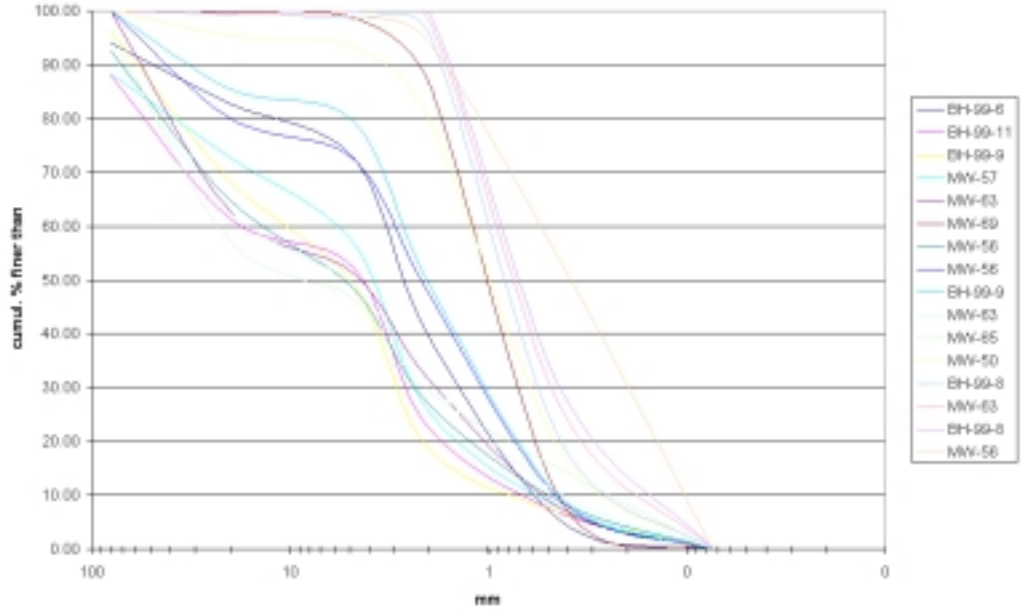
Grain size distribution graphs were generated for each layer type (fill, silty clay, and sand and gravel) based on the grain size analytical data. After the effective grain size was determined from these graphs, an estimated hydraulic conductivity was obtained from the Hazen approximation.



Grain Size Distribution for Silty Clay



Grain Size Distribution for Sand & Gravel



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