IMPACT OF PHYTOREMEDIATION SYSTEM ON GROUNDWATER FLOW IN A SHALLOW AQUIFER SYSTEM

by

Edward J. Corack

Thesis submitted to the Faculty of the
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APPROVED:

(Signature on Electronic Thesis/Dissertation Approval Form)
Dr. Mark A. Widdowson, Chair

(Signature on Electronic Thesis/Dissertation Approval Form)
Dr. John T. Novak

(Signature on Electronic Thesis/Dissertation Approval Form)
Dr. David F. Kibler

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The Charles E. Via Department of Civil Engineering

(ABSTRACT)

There are many methods for cleaning up contaminated soil and groundwater. Phytoremediation is an engineered method that utilizes plants and trees to remove or immobilize inorganic and organic contaminants. The plants and trees can contain contaminant plumes, uptake the contaminants, or aid in the degradation of the contaminants through several poorly understood mechanisms.

Hybrid poplar trees were planted to contain a creosote contaminant plume at the study-site in Oneida, Tennessee. This research looks at how the trees will affect groundwater flow in the site. This is accomplished with the groundwater modeling program MODFLOW. The trees are simulated using the Evapotranspiration Package within MODFLOW, within the GMS modeling platform, to produce a two-dimensional unconfined aquifer viewpoint groundwater model.

Site characterization, setup, and rationale are provided. The modeling methodology including calibration, sensitivity analysis, non-unique solution check, and verification are also provided. The modeling methodology included steady-state model calibration at the study-site to match observed field data; precursory steady-state and subsequent practice transient calibrations at the site; and incorporation of the simulation of evapotranspiration in the final transient model calibrations at the site.

The results show that a phytoremediation system consisting of densely-planted hybrid poplar trees can indeed impact groundwater flow, although not to the extent that clearly would contain a creosote contaminant plume. Various input parameters including specific yield, transient recharge, starting heads, evapotranspiration rates, and evapotranspiration extinction depths impacted MODFLOW model sensitivity in transient calibrations. Varying the time steps in post-precipitation stress periods did not significantly impact the model output.

The interception trench conductance played a minimal role in the calibration, but trench groundwater collection data was lacking, and the trench was frequently in need of maintenance. Further suggested data requirements include more frequently collected rainfall and piezometer data, as well as the installation of more piezometers outside the model domain contained in this study.

Using the Evapotranspiration Package in MODFLOW provided more realistic and authentic results than using the Well Package (used in a previous study of the site by Panhorst in 2000) to simulate evapotranspiration. The Evapotranspiration Package in MODFLOW incorporates transpiration extinction depths that prevent transpiration when the water table drops below a certain depth. Further suggested program development includes incorporating an asymptotic function for transpiration rates and allowing the Evapotranspiration Package to import evapotranspiration rates, extinction depths, and elevations.

It may be deduced from this impact of flow that the tree system will aid in containment of a contaminant plume, but at the trees current growth stage, and with the coal layer present at the site, the containment is limited.
To the Corack’s and the Derbak’s
One should spend a lot of time considering the mood of a paper. I pondered about a few impressive political and academic quotes to precede this thesis. In the end, I decided to include both. The first is political; the second is very familiar to most:

“In practice, the majority of administrators have a rather ‘wait-and-see’ attitude toward models. They are not interested in their technical characteristics and they do not know how they work: the model is a kind of black box. What interests them are the models’ outcomes and, more than anything, their reliability. The drawback to simulation models is that they are always more or less accurate reflections of reality and therefore can never convey a completely reliable picture. And that is precisely what an administrator is after.”

L. Ginjaar
Chairman of the National Council for Environmental Protection, Rijswijk, The Netherlands, 1989.

“Rock n' Roll.”

Ed Corack et al.
Everywhere, Always.
Acknowledgements

I have accumulated a long list of people I need to thank after over 10 years and two degrees from Virginia Tech. The most important of all these people is Dr. Mark A. Widdowson. He provided me with guidance in and out of the classroom as an undergraduate advisor, thesis advisor, committee chair, mentor, and friend. His unrelenting drive with myself and other students at Virginia Tech truly makes the University a better place. It has been a pleasure, and I look forward to working with him in the future.

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If I could cry in this text, it would be right now. I want to thank my family — Mom, Dad, Cathy, Susan, Gregory (the Boogs), and Ryan (the Boogie-Boogies). They made me, encouraged me, inspired me, and are [me]. What can I say? Some things cannot be put into words.
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<td>Rearranged water budget equation to solve for ET</td>
<td>4-22</td>
</tr>
<tr>
<td>Equation 4-19</td>
<td>Mean Error</td>
<td>4-25</td>
</tr>
<tr>
<td>Equation 4-20</td>
<td>Mean Absolute Error</td>
<td>4-25</td>
</tr>
<tr>
<td>Equation 4-21</td>
<td>Root Mean Squared Error</td>
<td>4-25</td>
</tr>
<tr>
<td>Equation 4-22</td>
<td>Sensitivity Index</td>
<td>4-33</td>
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<tr>
<td>Equation</td>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>-------------</td>
<td>-------------------------------------------------</td>
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</tr>
<tr>
<td>Equation 4-23</td>
<td>Sensitivity Index in terms of RMSE</td>
<td>4-33</td>
</tr>
<tr>
<td>Equation 4-24</td>
<td>Sensitivity coefficient calculation</td>
<td>4-33</td>
</tr>
<tr>
<td>Equation 4-25</td>
<td>Maximum Transpiration Rate for ET Zone containing P-7</td>
<td>4-53</td>
</tr>
<tr>
<td>Equation 4-26</td>
<td>Maximum Transpiration Rate for ET Zone containing P-4</td>
<td>4-53</td>
</tr>
</tbody>
</table>
## List of Acronyms and Abbreviations

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>°F</td>
<td>degrees Fahrenheit</td>
</tr>
<tr>
<td>ARCADIS G&amp;M</td>
<td>ARCADIS Geraghty &amp; Miller, Inc.</td>
</tr>
<tr>
<td>BTEX</td>
<td>benzene, toluene, ethylbenzene, and total xylenes</td>
</tr>
<tr>
<td>cal/cm²</td>
<td>Langleys (calories per square centimeter)</td>
</tr>
<tr>
<td>DPT</td>
<td>Direct Push Technology</td>
</tr>
<tr>
<td>ET</td>
<td>Evapotranspiration</td>
</tr>
<tr>
<td>ft</td>
<td>Feet</td>
</tr>
<tr>
<td>gal/d/tree</td>
<td>Gallons per day per tree</td>
</tr>
<tr>
<td>GIS</td>
<td>Geographic Information Systems</td>
</tr>
<tr>
<td>GMS</td>
<td>Groundwater Modeling System</td>
</tr>
<tr>
<td>in/day</td>
<td>Inches per day</td>
</tr>
<tr>
<td>MJ/m²/d</td>
<td>Mega-joules per square meter per day</td>
</tr>
<tr>
<td>mm Hg</td>
<td>Millimeters of mercury</td>
</tr>
<tr>
<td>mm/day</td>
<td>Millimeters per day</td>
</tr>
<tr>
<td>MODFLOW</td>
<td>Computer program used to simulate 3-dimensional groundwater flow.</td>
</tr>
<tr>
<td>msl</td>
<td>Mean sea level</td>
</tr>
<tr>
<td>NAPL</td>
<td>Non-Aqueous Phase Liquid</td>
</tr>
<tr>
<td>PAH</td>
<td>polynuclear aromatic hydrocarbon</td>
</tr>
<tr>
<td>PCB</td>
<td>polychlorinated biphenyls</td>
</tr>
<tr>
<td>RCF</td>
<td>Root Concentration Factor</td>
</tr>
<tr>
<td>RDX</td>
<td>hexahydro-1,3,5-trinitro- 1,3,5triazine</td>
</tr>
<tr>
<td>TCE</td>
<td>Trichloroethene or trichloroethylene</td>
</tr>
<tr>
<td>TNT</td>
<td>2,4,6-trinitro-toluene</td>
</tr>
<tr>
<td>TOC</td>
<td>Top of casing</td>
</tr>
<tr>
<td>TSCF</td>
<td>Transpiration Stream Concentration Factor</td>
</tr>
<tr>
<td>UI</td>
<td>University of Iowa</td>
</tr>
<tr>
<td>USEPA</td>
<td>United States Environmental Protection Agency</td>
</tr>
<tr>
<td>USEPA TIO</td>
<td>USEPA Technology Innovation Office</td>
</tr>
<tr>
<td>USGS</td>
<td>United States Geological Survey</td>
</tr>
</tbody>
</table>
1.0 Project Introduction

1.1 Background

Among the many hazardous substances in groundwater that society must clean up is creosote. Creosote is commonly used as a wood preservative for telephone poles, fencing, and railroad crossties. It is composed of over 200 compounds, of which approximately 85 percent is composed of polynuclear aromatic hydrocarbons (PAHs), and is toxic and carcinogenic to humans (Arvin and Flyvbjerg 1992). Its variant composition makes creosote difficult to characterize and especially difficult to assign it physical properties (Mayfield 1996).

Creosote is typically found in three phases within the environment: water, sediments, and biota (Mayfield). It is not considered to be a significant air contaminant since the high molecular weight PAH’s do not volatilize readily (Godsy et al. 1992). The transport of creosote contaminants in groundwater is dependent on the chemical and physical properties of each compound in its makeup (Mayfield).

The Oneida Tie Yard Site (Figure 1-1), in Oneida, Tennessee (Figure 1-2), is a 100-year-old facility that was used intermittently over 25 years for creosote treatment operations until 1973. The crosstie treatment operation process required a crosstie treatment facility, creosote holding tank (aboveground storage tank), treatment unit, holding pond, and rail-spur track (ARCADIS G&M 1).

The U.S. Army Corps of Engineers rerouted a nearby creek (Pine Creek) and discovered creosote seepage in 1990. The creosote holding pond for treating the railroad ties is the probable origin of the contamination. After testing by the Tennessee Department of Health and Environment confirmed the site contamination and seepage, Environmental Technology, Inc., installed an interception trench in 1991 (refer to Figure 1-3). The trench is approximately 330 feet long, 20 feet wide at the top, and 3 feet wide at the bottom. A four-inch slotted drain tile lies along the bottom of the trench and is tied into a 24-inch vertical standpipe. A submersible pump sits at the bottom of this vertical culvert and allows drainage to be pumped to an oil/water separator on the surface.

In addition to avoiding potential exposure of contaminants to human and environmental receptors, the railroad company would like to completely remediate the site to return it to full and productive use.
A phytoremediation system was approved and then installed in May 1997 by Ecolotree, Inc. The system consists of hybrid poplar trees strategically planted on the site between the railroad tracks and the property boundaries. The phytoremediation system is designed to alter the plume migration towards the creek back towards the site, and also promote biodegradation of the creosote compounds.
1.0 PROJECT INTRODUCTION

1.2 Problem Statement
The capability of MODFLOW to simulate the evapotranspiration of vegetation at various study sites will be investigated. This will allow for predictive capabilities of resulting calibrated models that may be applied at other phytoremediation study sites. Limited research has been performed to explore the aspects of evapotranspiration in groundwater models. The model will also demonstrate the impact of the poplar trees and/or the groundwater interception trench on the Oneida Tie Yard site groundwater flow system.

1.2 Objectives
The objective of this research is to determine the hydrologic impact of the installed phytoremediation system in addition to the upgraded trench system. Subsequent to this will be an evaluation of current model capabilities for evapotranspiration coupled to groundwater flow. Evaluation of the current site design as well as recommendations for future site design will be provided.

1.3 Approach
Development and calibration of numerical groundwater flow model using MODFLOW are detailed. This model builds on previous research and modeling efforts by Loftis (1999) and Panhorst (2000), who developed single layer models. This thesis will examine a more complex single-layer aquifer viewpoint groundwater model, incorporating multifaceted input data and calibration.

Figure 1-3: Trench System (from ARCADIS G&M 1)
1.0 PROJECT INTRODUCTION

The GMS platform program will be used to utilize the Conceptual Model Approach in MODFLOW to model the site. For calibration, the site will be modeled without the phytoremediation system (that is, poplar trees) in place or the trench system in operation under steady-state conditions. Boundary conditions will consist of Pine Creek, modeled as a drain, and two streamline (that is, no-flow) boundaries. After calibration is complete, a sensitivity analysis and a check for a non-unique solution will be performed. The model will then be run under transient conditions, simulating the poplar trees with the Evapotranspiration (ET) Package and simulating the trench with the Drain Package. Once this model is calibrated, a sensitivity analysis and a non-unique solution will be performed once again. The final model will be verified with more recent data and conclusions will be drawn.

1.4 Overview of Thesis

The following sections are provided to accomplish the above. Section 2.0 serves as a literature review on all areas that this research deals with. A review of poplar trees, phytoremediation, and evapotranspiration makes up the bulk of this section. Section 3.0 details the site setup and rationale. Section 4.0 begins with a review of groundwater theory and transitions to MODFLOW theory. Section 4.0 then transitions to developing the model, presenting the result of the modeling study, and discussing the different modeling runs. Section 5.0 provides a summary of findings, conclusions, and future research suggestions. References may be found in Section 6.0, the Epilogue is Section 7.0, and the Appendices appear at the end of this thesis.
2.0 Literature Review

2.1 Poplar Trees

2.1.1 Introduction

“[The genus *Populus* is comprised of] about 30 species of poplars, cottonwoods, and aspens widely distributed over the northern hemisphere and planted in many parts of the world (Stettler *et al.* 1996).” Poplars are of concern to this research because they are the trees used in the phytoremediation system at the Oneida Tie Yard Site (as well as many other phytoremediation systems). The *Populus* genus is researched often by botanists, too, due to the fact that it is “…replete with genetic variation at many different levels: among sections within the genus, as well as among species, provenances, populations, individuals, and genes (Stettler).”

Species of the genus *Populus* are all single-trunked, deciduous, or semi-evergreen, trees and most spread clonally by means of root-borne sucker shoots, a feature uncommon among trees (Stettler). Zsuffa *et al.* (1996) provide an excellent overview of poplar trees:

Poplars (*Populus* L.) grow naturally on a variety of sites from boreal to subtropical and from mountainous to riparian. At times they form large stands, as still nowadays in boreal forests and along major river valleys, and at other times small stands, lines, and groups of trees.

Poplars have been useful to humans and cultivated since historical times. Poplars grow fast, are easy to propagate, and can be grown on many types of sites in the forest, as well as in the open landscape. They serve as an excellent source of a wide range of wood products, especially in temperate zones. Poplars also play a significant role in environmental protection and improvement, especially in protecting land from wind and flood erosion, in remedying contaminated groundwater, in the safe disposal of sewage sludge, and in improving the carbon balance of the atmosphere. These fast-growing trees can augment forest diversity and enrich the open landscape, providing it with aesthetic appeal through a variety of forms.

2.1.2 Hybrids

The poplar trees planted at the Oneida Tie Yard Site are x *euramericana* (*P. deltoides* x *P. nigra*), hybrid DN34 and hybrid OP367. There are many motives for hybridization of trees. Stettler reports that the three main reasons are: (1) to combine desirable traits from different species; (2) to capture heterosis, or hybrid vigor; and (3) to obtain increased developmental homeostasis. Desirable traits include, but are not limited to rootability, stem growth, branching, leaf traits, phenology, and disease resistance. Braatne *et al.* (1992) demonstrate the importance of hybridization.
Braatne et al. looked at water deficit stresses on three kinds of poplar trees: *Populus trichocarpa*, *Populus deltoides*, and their hybrid, *Populus trichocarpa* x *deltoides*. They exposed the trees to three stages of water availability: Stage I had soil moisture at its maximum; Stage II simulated the beginning of a water deficit to the trees; and Stage III had the soil moisture at its lowest. They found that only the hybrid trees prepared for the water shortage by “…[initiating] a water conservation response at higher soil water content than either parent [tree].” They then stated that the hybrids “…were more drought resistant than either parental species…”

### 2.1.3 Root System

Hybrid poplars are famous for their lateral root development. Up to seven orders of lateral roots may be developed by each poplar tree extending more than 30 meters from the stem (Stettler). Little is known about these root structures, however, and is the focus of current research. It is known that “…the majority of roots grow radially away from the taproot… at angles between 0 (horizontal) to 30 degrees… and lie between 5 to 20 cm from the soil surface (Stettler).”

The College of Forest resources at the University of Washington has been doing extensive research with poplar trees. They report that the absorption surface of roots in a stand of poplars can approach 300,000 kilometers per hectare (Gordon et al. 1997). Poplar roots (*Populus deltoides* x *nigra*) have proven to enhance the viability of degrading microorganisms in the rhizosphere (Jordahl et al. 1997). Jordahl et al. state that “The proliferation of desirable phenotypes in the root zone is conducive to enhanced contaminant removal capabilities and rates, and thus, reduced duration and cost of site remediation.”

![Figure 2-1: Sketches of *Populus* Root Systems](image)

…depicting the structural (woody) roots (from Stettler et al. 1996). (A) The general appearance of the root system of an Euramerican *Populus* clone. (B) The vertical and partial horizontal root system of *Populus tremuloides*.
2.1.4 Tree Growth

Rapid tree growth is associated directly with the tree’s rapid root growth (Stettler). This rapid growth also correlates with poplars known affinity for transpiring considerable amounts of groundwater. Lockhart (1965) analyzed cell growth in plants and found that the relative growth rate of plant cells (dV/V dt) is a function of the amount that the osmotic potential gradient from outside to inside of the cell, dπ, exceeds the yield threshold of the cell walls, Y or dπ - Y. Also included in the equation are wall extensibility, m, and hydraulic conductance, Lp, (from Stettler):

\[
\frac{dV}{V dt} = \frac{mLp (d\pi - Y)}{m + Lp}
\]  

(2-1)

This research does not lend to examining tree growth at this level, though. Instead, parameters set forth by Ecolotree, Inc., as well as research performed by Lawrence (2000), are utilized for modeling the poplar trees’ stem and root growth rates (that is, for inputting information into the ET Package in MODFLOW; see Section 4.0). For instance, Ecolotree reports that the poplars in this study grow three to five meters each year. Suthersan (1997) reports that poplar trees grow six to eight feet per year, far less. Lawrence (2000) developed a relationship between the poplar tree height and root depth for the Oneida Tie Yard Site. Lawrence’s research showed that the root depth of the hybrid poplars was approximately one-third of the total height of the trees. Tree growth data (collected by ARCADIS G&M) collected in November 2000 suggested that most of the trees at the study site had reached their maximum height.

Figure 2-2: Development of the Root Zone and Tree Over Time (from Suthersan 1997).
2.1.5 Water Use

The ability to produce wide-spreading and prolific root systems gives poplars their ability to resist water stresses. They are phreatophytic, capable of extending their roots into aerobic water tables (Suthersan). “The degree to which poplar roots [will] penetrate the saturated zone cannot be easily estimated…” However, if their access to soil moisture from precipitation is limited, poplars will draw large amounts of water from the top of the saturated aquifer (Suthersan).” Evapotranspiration draws down the water table below the poplars “…similar to a pump and treat system (Suthersan).” Hybrid poplars occupying 4 square-meters of ground can cycle 100 liters of groundwater per day under optimal conditions (Stomp et al. 1993). This is equivalent to about 27,000 gallons per day per acre. Ecolotree reports that each hybrid poplar in this study will transpire the same, about 100 liters each day after five years of growth. Ari Ferro of Phytokinetics reports that poplar trees in Ogden, Utah, for hydraulic control at a site, will transpire 150 liters each day after five years of growth [USEPA (United States Environmental Protection Agency) Technology Innovation Office (USEPA TIO) 1996]. A study by the University of Washington and Occidental Chemical Co. (Dallas) reports their poplar trees using up to 200 liters each day (Kim 1996).

Loftis (1999) modeled the Oneida Tie Yard Site using the Evapotranspiration Package. Loftis determined transpiration rates by calibrating his MODFLOW model of the study site (using the ET Package for the poplar trees). Loftis found that 0.3 inches per day (in/day), or 4.6 gallons per day per tree (gal/d/tree), was the minimum transpiration rate that would calibrate to the site data.

Panhorst (2000) investigated the transpiration rates of the hybrid poplars at the Oneida Tie Yard Site in three ways, below, and determined the following:

- Using White’s Equation (refer to Section 2.3), the transpiration rate was approximately 0.030 inches per day, or 0.62 gallons per day per tree;
- Using the Groundwater Recession Method, the transpiration rate was approximately 0.030 inches per day, or 0.62 gallons per day per tree;
- Using the groundwater flow model he developed (using wells/sinks for the poplar trees), the transpiration rate was approximately 0.65 inches per day, or 1.34 gallons per day per tree.

Panhorst found that all three methods provided reasonable results, and that the groundwater flow model “can be a powerful tool when looking at [groundwater consumption by the poplar trees]…[and] can be used as a predictor for how the aquifer will respond as the trees consume more water.” Note that Panhorst modeled the ET of the poplar trees by simulating the trees with individual wells. Panhorst stated that “a disadvantage of using the Well Package is that it only models water withdrawn from the water table and not water that is taken from the vadose zone.”
2.1.6 Nutrient Use

“Populus species are generally reported to be rapid accumulators of nutrients compared with other tree species… (Bargali and Singh 1991).” The large amount of water and nutrient uptake makes poplars an obvious candidate for phytoremediation. “Rapid nutrient accumulation in Populus is accounted for by a combination of high growth-induced demand, high root length densities, and/or high rates of ion uptake (Hui-jun and Ingestad 1984).” Little is known about ion uptake kinetics with these trees other than work done by Chapin et al. (1986) and Lajtha (1994).

2.2 Phytoremediation

2.2.1 Introduction

Phytoremediation is a word from the Greek prefix “phyto” meaning plant while the Latin suffix “remedium” means to cure or restore. The term and the study of its mechanisms are relatively new. “Phytoremediation is defined as a set of processes that use plants to clean contamination in soil, groundwater, surface water, sediment, and air (USEPA TIO 1996).”

Any remediation process starts with a site assessment, followed by containment of the identified problem, and theoretically ends with the cleanup of the area of concern (Cunningham et al. 1997). Yet the term “remediation” can have more of a legal connotation rather than a technical one (Cunningham):

(a) “cleanup,” where either the contaminant is removed from the matrix (leaching, bioremediation, and so on) or the entire contaminated matrix is removed from the site (excavation and landfilling at a second site); or

(b) “stabilization,” where the physical or chemical form of the matrix or contaminant is transformed to a more inert condition.

Whichever implication, the intended solution must be accomplished in a certain time frame at a feasible cost, while being technically and logistically possible and in compliance with all legal requirements.

2.2.2 History

In the early 1980’s, researchers started to scrutinize others work in plant-based bioremediation. After the Chernobyl nuclear accident in 1986, a company named Phytotech developed a plan to use plants to decontaminate the radioactive water and soil. In 1994, Phytotech researchers from Monmouth Junction, New Jersey, and their colleagues installed floating rafts in a 75 square-meter pond located 1 kilometer from the Chernobyl reactor (Adler 1996). The rafts held 24 sunflowers. Sunflowers are known to preferentially
absorb cesium and strontium from a mixture of metals (Adler). “The plants don’t metabolize the radionuclides, but the cesium stays in the roots and most of the strontium moves to the shoots (Adler).” The sunflowers are disposed of as radioactive waste after three weeks on the pond. The following years found Phytotech using more sunflowers until the pond was completely remediated. They had to clean the surrounding soil to prevent recontamination of the pond, though, by growing Indian mustard (Adler).

After Phytotech published their results in 1989, Iowa City started to use tree farms to clean landfill areas (Dempsey). 1990 saw New Jersey using phytoremediation to control nitrogen contamination in an aquifer (Dempsey). These were the earliest days of phytoremediation research.

Although phytoremediation is still mostly in the research and development phase, the pace of the research and development is quickening. After only ten years of directional research, companies with names like Ecolotree, Phytokinetics, Phytotech, and PhytoWorks are already reaping the financial benefits of employing phytoremediation.

### 2.2.3 Mechanisms of Phytoremediation

Phytoremediation is a general term for many processes and/or mechanisms that any kind of vegetation uses to “clean” contaminants. A workshop hosted by the USEPA TIO in December 1996 congregated virtually all of the phytoremediation researching community. In this conference, Steve Rock from USEPA’s National Risk Management Research Laboratory in Cincinnati, Ohio, reviewed the mechanisms of phytoremediation:

Mechanisms of phytoremediation include enhanced rhizosphere biodegradation, phytoextraction, phytodegradation, and volatilization. Enhanced rhizosphere biodegradation takes place in the soil surrounding plant roots. Natural substances released by plant roots supply nutrients to microorganisms, which enhances their ability to biodegrade hazardous materials. Plant roots also loosen the soil and then die, leaving paths for transport of water and aeration. This process tends to pull water to the surface zone and dry the lower saturated zones.

Phytoextraction is the uptake of contaminants by plant roots and the translocation of contaminants into plant shoots and leaves. Where contaminants are stored in plant shoots and leaves, the plants can be harvested and disposed of. Some plant species have demonstrated the ability to store metals in roots. Although roots generally cannot be harvested in a natural environment, a process called rhizofiltration can be used where plants are raised in greenhouses and transplanted to sites to filter metals from wastewaters. As the roots become saturated with metal contaminants, they then can be harvested and disposed of. Plants also have been used to concentrate radionuclides in the Ukraine and Ashtabula, Ohio.

Phytodegradation is the metabolism of contaminants within plant tissues. Plants produce enzymes, such as dehalogenase and oxygenase, [which] help catalyze degradation.
Physical effects include volatilization, which occurs as plants take up water containing organic contaminants and release the contaminants into the air through plant leaves. Researchers are not sure how much contamination is being transpired into the air. Data on transpiration is still at a preliminary stage. The Cincinnati laboratory is building chambers to monitor the amount of organic contaminants released into the air.

Not quite a mechanism, but another physical effect of phytoremediation is the hydraulic control of contaminated plumes that can be exerted by trees (USEPA TIO 1996). “Poplars, cottonwoods, and willows can use up to 200 gallons of water per day and prevent contaminated plumes from flowing past tree roots (USEPA TIO 1996).” This hydraulic control is the focus of the modeling efforts of this research.

The rhizosphere mechanism seems the most important for mineralization and degradation of contaminants. Root exudates contain a variety of compounds providing carbon and energy sources for the microbial population (Erickson et al. 1995). “Decaying plant organic matter and root exudates sustain a diverse microbial population with genetic capability for the mineralization and transformation of many contaminants (Erickson).” Jordahl et al. (1997) found “increased populations of heterotrophic and denitrifying organisms relative to the surrounding soil…” in the rhizosphere of hybrid poplar trees. This was part of a study using poplar trees to buffer a nitrate rich watershed that was mentioned earlier.

![Figure 2-3: Conceptual model of Plant and Soil Influences](image)

... on bioavailability and biodegradation of xenobiotic soil contaminants by microbial communities in the rhizosphere (Crowley et al. 1997).

Although it is clear that many contaminants are mineralized in the root zone, “...the full extent of involvement of plant enzymes is often not clear (Schnoor).” Dehalogenase, laccase, nitrilase, nitroreductase, and peroxidase are among the enzyme systems that have been identified and found to be active in degradation of contaminants (Schnoor).
### 2.2.4 Phytoremediation with Plants and Grasses

There are many plants, grasses, aquatic plants, and so forth that have been used for phytoremediation. The list is constantly growing as researchers try virtually every kind of vegetation. Although this thesis focuses on a poplar tree phytoremediation system, a selection of plants and grasses used for phytoremediation is provided in Table 2-1:

<table>
<thead>
<tr>
<th>Plant</th>
<th>Function</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Aeollanthus subcaulis</em> var. <em>lineris</em></td>
<td>Accumulates copper</td>
<td>s</td>
</tr>
<tr>
<td><em>Medicago sativa</em> (Alfalfa)</td>
<td>Symbolic with hydrocarbon-degrading bacteria, degradation of deicing agents</td>
<td>g, r</td>
</tr>
<tr>
<td><em>Apocynum</em> sp. (hemp dogbone) and <em>Ambrosia</em> sp. (common ragweed)</td>
<td>Accumulates lead</td>
<td>d</td>
</tr>
<tr>
<td><em>Arabidopsis thaliana</em></td>
<td><strong>Carries a bacterial gene that transforms mercury into a gaseous state, accumulates lead</strong></td>
<td>e, g</td>
</tr>
<tr>
<td><em>Arriplx prostrata</em> and <em>Suaeda calceoliformis</em></td>
<td>Remediation of brine impacted soil</td>
<td>m</td>
</tr>
<tr>
<td><em>Bladder campion</em></td>
<td>Accumulates zinc and copper</td>
<td>c</td>
</tr>
<tr>
<td><em>Brassica juncea</em> (Indian mustard)</td>
<td>Accumulates selenium, sulfur, lead, chromium, cadmium, nickel, zinc, and copper</td>
<td>c, g, f</td>
</tr>
<tr>
<td><em>Buxaceae</em> (boxwood)</td>
<td>Accumulates nickel</td>
<td>g</td>
</tr>
<tr>
<td><em>Compositae</em> family</td>
<td>Symbolic with Arthrobacteria, accumulates cesium and strontium</td>
<td>g</td>
</tr>
<tr>
<td>Corn</td>
<td>Reducing nitrate</td>
<td>p</td>
</tr>
<tr>
<td>Crested wheatgrass</td>
<td>Degradation of pentachlorophenol</td>
<td>j</td>
</tr>
<tr>
<td><em>Euphorbiaceae</em></td>
<td>Accumulates nickel</td>
<td>d</td>
</tr>
<tr>
<td><em>Poa pratensis</em> (Kentucky bluegras)</td>
<td>Biodegradation of deicing agents</td>
<td>r</td>
</tr>
<tr>
<td>Maize plant</td>
<td>Degrades atrazine and TNT</td>
<td>o</td>
</tr>
<tr>
<td>Ordinary Tomato</td>
<td>Accumulates lead, zinc, and copper</td>
<td>g</td>
</tr>
<tr>
<td><em>Paspalum notatum</em></td>
<td>Accumulates Cs</td>
<td>s</td>
</tr>
<tr>
<td><em>Phormidium</em> blue green algae and <em>Myriophyllum spicatum</em> (water milfoil)</td>
<td>Adsorption of cadmium, zinc, nickel, and copper</td>
<td>u</td>
</tr>
<tr>
<td>Prairie grasses</td>
<td>Degrade PAHs</td>
<td>b</td>
</tr>
<tr>
<td>Soybeans</td>
<td>Stimulate mineralization of trichloroethene (TCE)</td>
<td>l</td>
</tr>
<tr>
<td><em>Sphagnum peat moss in BIO-FIX porous beads</em></td>
<td>Adsorption of cadmium and lead</td>
<td>k</td>
</tr>
<tr>
<td><em>Thlaspi caerulescens</em></td>
<td>Accumulates zinc</td>
<td>d</td>
</tr>
<tr>
<td><em>Panicum coloratum</em> var. ‘Verde’ (Kleingrass)</td>
<td>Degradation of PAHs</td>
<td>q</td>
</tr>
<tr>
<td><em>Lemna gibba</em> (duckweed)</td>
<td>Reductive dechlorination</td>
<td>i</td>
</tr>
</tbody>
</table>
Table 2-1: A Selection of Plants and Grasses for Phytoremediation (continued)

<table>
<thead>
<tr>
<th>Plant</th>
<th>Function</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Typha latifolia (common cattail)</td>
<td>Accumulates acid drainage: aluminum, iron, and manganese</td>
<td>v</td>
</tr>
<tr>
<td>Sunflowers</td>
<td>Accumulates radionuclides</td>
<td>f, h</td>
</tr>
<tr>
<td>Tobacco with ice plant gene</td>
<td>Accumulates copper</td>
<td>n</td>
</tr>
<tr>
<td>Thlaspi alpestre (white-flowered European alpine pennycress)</td>
<td>Accumulates zinc and cadmium</td>
<td>a</td>
</tr>
<tr>
<td>White sweet clover</td>
<td>Mineralization of fluoranthene, phenanthrene, and naphthalene</td>
<td>t</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a Adams 1998</td>
<td></td>
<td></td>
</tr>
<tr>
<td>b Aprill and Sims 1990</td>
<td></td>
<td></td>
</tr>
<tr>
<td>c Blaylock et al. 1996</td>
<td></td>
<td></td>
</tr>
<tr>
<td>d Brown et al. 1995</td>
<td></td>
<td></td>
</tr>
<tr>
<td>e Chen et al. 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>f Cooney 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>g Cunningham and Berti 1993</td>
<td></td>
<td></td>
</tr>
<tr>
<td>h Dempsey 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>i Ensley et al. 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>j Ferro et al. 1994</td>
<td></td>
<td></td>
</tr>
<tr>
<td>k Jeffers et al. 1993</td>
<td></td>
<td></td>
</tr>
<tr>
<td>l Kansas 1995</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m Keiffer et al. 1997</td>
<td></td>
<td></td>
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<tr>
<td>n Kim 1996</td>
<td></td>
<td></td>
</tr>
<tr>
<td>o Mueller et al. 1993</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p Paterson and Schnoor 1993</td>
<td></td>
<td></td>
</tr>
<tr>
<td>q Qiu et al. 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>r Rice et al. 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>s Sutheran 1997</td>
<td></td>
<td></td>
</tr>
<tr>
<td>t Walton et al. 1994</td>
<td></td>
<td></td>
</tr>
<tr>
<td>u Wang et al. 1995</td>
<td></td>
<td></td>
</tr>
<tr>
<td>v Wiley 1997</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.2.5 Phytoremediation with Poplar Trees

Gordon et al. (1997) found that a hybrid poplar breed, *Populus trichocarpa x deltoides*, metabolized $^{14}$C-labeled TCE to produce trichloroethanol, di- and trichloroacetic acid. Some of the TCE was incorporated into insoluble, non-extractable cell residue, and small amounts were mineralized to $^{14}$C-CO$_2$. Mass balance studies done by Gordon found that the poplar hybrids actually transpired TCE, but only a small fraction (that is, 0.8 percent).

Newman et al. (1996) used a hybrid poplar breed, *Populus trichocarpa x P. deltoides*, H-11-11, to metabolize and transpire TCE and carbon tetrachloride. The poplars were capable of removing 95 percent of the carbon tetrachloride from the soil after one year, and 97 percent of TCE after two years. They report that the trees had somewhat of a high susceptibility to the toxicity of carbon tetrachloride.

Aitchison et al. (1996) found that poplars metabolized 1,4-dioxane. 1,4-dioxane is a suspected carcinogen that is found as a solvent in paints, varnishes, and cosmetics. They used the same DN34 hybrids that are planted at the Oneida site.
Burken (1996) and Burken and Schnoor (1997) found that a hybrid poplar breed, *Populus deltoides x nigra*, could uptake, hydrolyze, and dealkylate $^{14}$C-labeled atrazine. Interestingly, they showed that metabolism occurred in the roots, stems, and leaves of the poplar cuttings. Additionally, they found unidentified metabolites.
In another study, Schnoor et al. (1995) found that poplars may be used to: metabolize or uptake many hydrophobic compounds, such as benzene, toluene, ethylbenzene, and total xylenes (BTEX), chlorinated solvents; and excess nutrients such as nitrate, ammonium, and phosphate. They provided an excellent table that is adapted below summarizing poplar applications and the respective phytoremediation project location.

Table 2-2: Applications of Poplar Trees at Contaminated Sites

<table>
<thead>
<tr>
<th>Location</th>
<th>Application</th>
<th>Contaminants</th>
<th>Site Results</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amana, IA</td>
<td>Non-point source control, 1-mi stream with poplars</td>
<td>NO$_3^-$, atrazine, alachlor, soil erosion</td>
<td>NO3- and 0.10-20 percent atrazine were removed</td>
<td>a, b, c, d, e</td>
</tr>
<tr>
<td>Amana, IA</td>
<td>Municipal solid waste compost land application on poplars, corn, fescue</td>
<td>Chlordane</td>
<td>Organics were immobilized</td>
<td>f</td>
</tr>
<tr>
<td>Beaverton, OR</td>
<td>Municipal landfill cap with hybrid poplars</td>
<td>Organics, metals, BOD</td>
<td>Landfill cap successful, full scale</td>
<td>g</td>
</tr>
<tr>
<td>Slovenia</td>
<td>Landfill cap, closure with hybrid poplars</td>
<td>Organics, metals, BOD</td>
<td>Two years of growth</td>
<td>h</td>
</tr>
<tr>
<td>Iowa City, IA</td>
<td>Landfill leachate abatement with poplars</td>
<td>Chlorinated solvents, metals, BOD, NH$_3$</td>
<td>Poplars survived in lab 1200 mg/L</td>
<td>i</td>
</tr>
<tr>
<td>Prince George’s County, MD</td>
<td>Sewage sludge in trenches, poplars on degraded lands</td>
<td>Nitrogen in sludge</td>
<td>170 tons/acre of sludge treated full scale, 6-yr plantation</td>
<td>j</td>
</tr>
<tr>
<td>Corvallis, OR</td>
<td>Organics in hydroponic system with poplars, Russian olive, soybean, green ash</td>
<td>Nitrobenzene and others</td>
<td>Essentially complete uptake in the lab</td>
<td>k</td>
</tr>
</tbody>
</table>

* Shimp et al. 1993  
* Briggs et al. 1982  
* Moser and Haselwandter 1983  
* Licht 1990  
* Nair et al. 1993  
* Hsu et al. 1993  
* Madison 1991  
* Licht et al. 1994  
* Kull 1995  
* Gouin and Flamino 1988  
* McFarlane et al. 1990

Jordahl (1997) looked at using hybrid poplar trees for land application of saline wastewater. Jordahl found that the trees “…proved surprisingly tolerant to a high salinity, high chloride wastewater.” Jordahl listed the most tolerant hybrids as *Populus deltoides* x *P. nigra* and *Populus trichocarpa* x *P. deltoides*. Salts were generally retained near the soil surface, with the most tolerant clones having a threshold level of seven decisiemens per meter. The production of munitions containing the explosives RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine) and TNT (2,4,6-trinitro-toluene) has led to the contamination of numerous areas in the United States and worldwide. Thompson and Schnoor (1996) looked at using poplar trees to remediate these soils:
The results of this research indicate that RDX and TNT behave quite differently in terms of rate of uptake, translocation, and chemical fate. The concentration of RDX in hydroponic solutions increases whereas TNT concentrations decrease quickly. Once the explosives are in the plant, over 60 percent of the RDX-related radioactivity is translocated to the leaves in as little as 48 hours while the majority of the TNT-related label is immobilized in the roots during this same period.

They project that the differences in translocation between the two are related to the chemical fate of the parent compounds within the plant.

Deep-rooted poplars can be used for phytoextraction of heavy metals even at depths up to ten feet (Suthersan). Rakin et al. (1997) report “…phytoextraction and phytofiltration are the best-developed subsets of toxic metal phytoremediation nearing commercialization.” They state that phytostabilization is not quite developed, but will be once researchers focus on it. Rakin et al. go further by stating that “short-term advances in phytoextraction are likely to come from the development of effective chemical soil amendments and the efficient ways of applying them.” They add that enhancement of plant shoot accumulation of toxic metals will be provided by metal-chelating agents.

Poplar trees are also used as a capping technology. The Ecolotree™ cap is marketed as such. 10,000 poplar trees per hectare were planted as a final cap on a landfill in Oregon (Schnoor et al. 1995). Ecolotree has also used its proprietary procedure successfully in Baltimore, Maryland, and in Slovenia (RDTF 1997).

Similarly, poplar trees are used for stabilization and erosion control. Pierzynski et al. (1994) used hybrid poplars to stabilize zinc smelter wastes in Kansas and to immobilize the co-contaminant lead. Schnoor et al. (1995) used a similar approach to control wind-blown dust and soil erosion from cadmium- and arsenic-rich mine tailings at Whitewood Creek in South Dakota. Cadmium and arsenic were not found to accumulate at high levels in the aboveground biota.

2.2.6 Limitations of Phytoremediation

There are known limitations of phytoremediation just like any other remediation technology. Based on past and current research, problems with phytoremediation include (USEPA TIO 1996):

- It is limited to shallow soils, streams, and groundwater;
- High concentrations of hazardous materials can be toxic to plants;
- It involves the same mass transfer limitations as other biotreatments;
- It is slower than other treatments, particularly in cold weather;
- It can transfer contamination across media;
- It is not effective for strongly sorbed [for example, polychlorinated biphenyls (PCBs)] and weakly sorbed contaminants;
- The toxicity and bioavailability of biodegradation products is not always known; and
- Products may be mobilized into groundwater or bioaccumulated in animals.
At the University of Iowa (UI), researchers from UI have teamed up with consultants from companies with experience in design, irrigation techniques, and tree planting to propagate their phytoremediation research. Dr. Jerald Schnoor, of the University of Iowa, is considered one of the top researchers in this field. He set forth a list of research needs to insure the success of phytoremediation as a technology (USEPA TIO 1996):

- Long-term field studies to show the presumed efficacy of phytoremediation (some historical sites “remediated” with phytoremediation could be candidate sites for post audits);
- Screening test methods for determining the optimum plant species for each site;
- Models for fate and transport of soil and groundwater contaminants under the influence of phytoremediation (the HELP, PRZM, and EPIC models have been utilized but were not developed for phytoremediation applications so new models developed specifically for phytoremediation would be helpful);
- A better understanding of the ecology of the system, such as mycorrhizae, bacteria, and plant interrelationships and functions;
- Transgenic plants for potential future applications;
- The ability to degrade common contaminants, such as TCE and BTEX; and
- More feeding studies to determine the bioavailability and toxicity of contaminant metabolites in the soil following phytoremediation.

2.2.7 Role of Phytoremediation

Civil Engineering magazine interviewed Edward Gatiff, the founder of Applied Natural Sciences in Hamilton, Ohio, about phytoremediation (Matso 1995). He is an acknowledged expert in the phytoremediation field. He conveyed that phytoremediation would not replace current mechanical or biological systems, but serve as their counterpart. Gatiff said, “There’s definitely a synergistic benefit to using both systems together... The vegetation is a polishing step.” He added that after mechanical systems finish, as much as 70 percent of the soil content is still contaminated due to micropores in the soil. “And the plants, although it does take time, access those micropores.”

2.2.8 Cost of Phytoremediation

“Phytoremediation experts say the growth of interest in the field is driven by its relative cost-efficiency compared to standard remediation methods for government-mandated site cleanup (Watanabe 1997).” Cunningham et al. (1997) estimated cost ranges for in situ and ex situ remediation projects. In situ remediation of a contaminated site costs from $10 to $100 per cubic meter, while ex situ remediation costs as much as $30 to $300 per cubic meter. They also figured that land farming phytoremediation, “…in which plants are cultivated the same way a farmer plants a field or orchard, may cost as little as $0.05 per cubic meter.” Gatiff (1994) reports that the cost to remediate a one-acre site with vegetation was $250,000 compared to $660,000 using conventional pump-and-treat.
2.3 Evapotranspiration

“Evaporation is the process by which water is transferred from the land and water masses of the earth to the atmosphere,” while “transpiration is the evaporation counterpart for plants (Viessman and Lewis 1996).” The term ‘evapotranspiration’ first appeared in a paper written by Warren Thornthwaite in 1948 entitled, “An Approach Towards a Rational Classification of Climate” (Monteith 1985). He defined it as “the combined evaporation from the soil surface and transpiration from plants.”

There are many methods for measuring, calculating, or approximating ET rates. Three major approaches are suggested by Viessman and Lewis (1996):

1. Theoretical, based on physics of the process
2. Analytical, based on energy or water budgets
3. Empirical

Regardless of the approach, a method must be chosen that considers availability of data and practicality to the researcher.

Equation 2-2 and Figure 2-5 help to explain the basic hydrologic equation (Viessman and Lewis 1996):

\[
P = R + G + E + T + \Delta S
\]  \hfill (2-2)

where:  
P = precipitation;  
R = surface runoff;  
G = groundwater baseflow;  
E = Evaporation;  
T = Transpiration; and  
\Delta S = change in water storage.

![Figure 2-5: The Hydrologic Cycle (from Viessman and Lewis 1996)](image_url)
Total ET can be found by solving this most basic hydrologic equation for \( E + T \); however, sometimes the other variables in the equation are not known. In such cases lysimeters may be utilized.

Lysimeters are “devices for measuring percolation of water through soils and sampling soil water for chemical analyses (Howell et al. 1991).” Although precision lysimetry for the purpose of measuring ET has been developed in the last 50 years, lysimeters have been utilized for over 330 years to determine water use by vegetation (Howell).

Usually, the hydrologist has to calculate ET rates based on assumptions using equations and models developed over the years. Perhaps the simplest, yet not always the less costly, are the hydrological methods based on water budgets, just as with using Equation 2-2. Still, another form of equations stems from a mass transfer approach. The Thornthwaite-Holzman equation assumes that “…the atmosphere is adiabatic and the wind speed and moisture are distributed logarithmically in a vertical direction (Viessman and Lewis)”:

\[
E = \frac{833\kappa^2 (e_1 - e_2)(V_1 - V_2)}{(T + 459.4) \ln \left( \frac{z_2}{z_1} \right)^2}
\]  

where:  
\( E = \) evaporation (inches per hour);  
\( \kappa = \) von Kármán’s constant (0.4);  
\( e_1, e_2 = \) vapor pressures (inches of mercury);  
\( V_1, V_2 = \) wind speeds (miles per hour);  
\( T = \) the mean temperature [degrees Fahrenheit (°F)] of the layers \( z_1 \) and \( z_2 \); and  
\( z_1, z_2 = \) lower level, upper level, respectively.

Additional assumptions include that eddy shear stress is constant with height and that eddy diffusivity for water vapor is equal to that for momentum (Parmel and Jocoby 1975).

An energy balance method that is widely accepted is known as the Bowen ratio method (Bowen 1926). This method was validated by Tanner (1960) in a humid region and Fritschen (1965) in a warm arid region. The Bowen ratio method calculates the evaporative flux (Jones 1992):
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\[ \text{LE} = \frac{-(R_n + S)}{1 + (C_p/P)(K_h/K_w)(\Delta T/\Delta e)} \]  \hspace{1cm} (2-4)

where:  
LE = evaporative flux in langleys (cal/cm²);  
\( R_n \) = net radiation in langleys;  
S = soil heat flux in langleys;  
\( C_p \) = specific heat of dry air at constant pressure;  
P = atmospheric pressure;  
L = atmospheric pressure;  
\( \varepsilon \) = ratio of the molecular weight of water vapor to that of dry air;  
\( K_h, K_w \) = transfer coefficients of sensible heat and water vapor, respectively; and  
\( \Delta T, \Delta e \) = average air temperature and water vapor pressure differences, respectively, between two heights above crops.

Thornthwaite defined potential ET as “the water loss that will occur if at no time there is a deficiency of water in the soil for the use of vegetation (Viessman and Lewis).” Penman developed an equation that combines mass transport and energy budget theories to express this potential ET:

\[ \text{ET} = \frac{\Delta H + (0.27)E}{\Delta + 0.27} \]  \hspace{1cm} (2-5)

where:  
ET = the evapotranspiration for a given period (mm/day);  
\( \Delta \) = the slope of the saturated pressure curve of air at absolute temperature (mm Hg/°F);  
H = the daily heat budget at the surface (mm/day); and  
E = daily evaporation (mm).

Many variations of this equation exist in the literature (Brutsaert 1965, Van Bavel 1966, Kohler and Parmele 1967).

Hanks et al. (1973) evaluated several ET calculation methods. They compared use of a lysimeter to the Penman equation, van Bavel’s modification of the Penman equation, the Bowen ratio, and a modification of the Thornthwaite-Holzman equation. The experiment site was a relatively small test plot in Utah during the summer months, and they did not find that soil water limited ET. They ultimately found that the Bowen ratio method “…more closely approximated actual evapotranspiration than any of the other methods tested, but gave values which were about 17 percent too low.” They also reported on the other methods:

During this period actual evapotranspiration was 1.33 times that estimated by the Penman equation, 0.73 times that estimated by the van Bavel modification of Penman’s equation, and 2.86 times that estimated by the [modified Thornthwaite-Holzman] equation.
They noted that when they examined the data using daily averages of hourly computations, the Bowen ratio and the van Bavel modification “…yielded improved estimates of actual evapotranspiration values… [but] the Penman and [Thorntwaite-Holzman modification] gave estimates [even more] in error…”

As mentioned in Section 2.1.5, Panhorst (2000) used both the White Equation and the Groundwater Recession Method to determine transpiration rates at the Oneida Tie Yard Site. W.N. White (1932) developed an equation to estimate transpiration based on water table fluctuations and the specific yield:

\[ q = y(24r \pm s) \]  

where:  
- \( q \) = the transpiration rate (that is, the depth of water withdrawn over 24 hours in inches);  
- \( y \) = specific yield;  
- \( r \) = hourly rate of water table rise from 12:00 a.m. to 4:00 a.m. (inches); and  
- \( s \) = net fall or rise of water table over 24 hours (inches).

The Groundwater Recession Method that Panhorst used involved comparing summer and winter groundwater recession curves for the Oneida Tie Yard Site. The method suggests that ET does not occur during the winter months since the poplar trees are dormant during this time. This recession method assumes that the difference between aquifer outflows in the winter and summer months is due to the absence of ET in the winter.

### 2.4 Modeling Evapotranspiration and Phytoremediation

“A model is any device that represents an approximation of a field situation (Anderson and Woessner 1992).” Physical models simulate groundwater flow directly while mathematical models simulate groundwater flow indirectly by means of governing equations. These equations are thought to represent physical processes, heads or flows, initial conditions, etc. These mathematical models can be solved analytically or numerically, either of which may require a digital computer.

The study of groundwater hydrology is complemented by the study of ET. Many ET models have been developed over the years, especially with the new digital computer age. Many of these models are targeted towards crop development rather than modeling phytoremediation. They are still very germane to this section, and will be mentioned, but may not be detailed. Full references are cited at the end of this work for further research.

Some soil and water resource models that incorporate ET as a major component include (Arnold and Williams 1985): CREAMS — Chemicals, Runoff, and Erosion from Agricultural Management Systems (Knisel 1980); EPIC — Erosion-Productivity Impact Calculator (Williams et al. 1984); SPUR —
Simulation of Production and Utilization of Rangelands (Wight 1983); SWRRB — Simulator for Water Resources in Rural Basins (Williams et al. 1985); SPAW — soil-plant-air-water model was developed to estimate daily ET considering daily potential ET, plant growth characteristics, and soil moisture availability (Saxton et al. 1974); and GLERL LBRM — Great Lakes Environmental Research Laboratory Large Basin Runoff Model (Croley 1983).

Makkink and Heemst (1974) modeled the water budget for hypothetical crops. They only used approximate functions for ET, though, rather than including separate functions for the radiation and evaporation shares. Afshar and Marino (1976) attempted to model transpiration by single roots and root groups. They did not include hysteresis, but utilized a root density function as well as rooting zones for calculation of ET.

Davis et al. (1995) developed a model for plant-based bioremediation which “…visualized the root-soil environment with transpiring plants as a porous medium comprised of soil particles and soils which may be partially or fully saturated.” Their model provides for both water and gas phases in the vadose zone. This model looks mainly at the transpiration of the contaminants into the vegetation utilizing what is known as a Root Concentration Factor (RCF) and a Transpiration Stream Concentration Factor (TSCF). The RCF and TSCF coefficients are determined using octanol-water partition coefficients (logKow) of each contaminant. The RCF, TSCF, and their relation to logKow are presented below as developed by Briggs et al. (1982):

\[
RCF = 0.82 + 10^{0.77 \log K_{ow} - 1.52} 
\]

\[
TSCF = 0.784 \exp \left( -\frac{(\log K_{ow} - 1.78)^2}{2.44} \right) 
\]

They modeled the rate of soil-water uptake by the vegetation, q, as:

\[
q = S_n R_R \Gamma (\Psi_s - \Psi_r) 
\]

where:  \( S_n = \frac{\theta}{n} \); where \( \theta \) is water content and \( n \) is porosity;

\( R_R \) = Root density factor;

\( \Gamma \) = parameter describing permeability of the plants’ root system [L/T];

\( \Psi_s \) = water pressure head in the soil [L]; and

\( \Psi_r \) = water pressure head in the roots [L].

Their model was applied to alfalfa plants degrading toluene in a laboratory chamber. Model results were promising with measured concentrations almost matching simulated concentrations. Davis et al. concluded that their model supports the theory that the rhizosphere effect of vegetation promotes microbial decay of contaminants.
Tracy et al. (1994) used a similar model called BIORoot to examine precipitation and ET, as well as their affect on “…a nonvolatile compound with all other properties being those of benzene.” They modeled the fate of the “benzene” using alfalfa for eleven years using known precipitation and potential evaporation data. It was determined that the model should account for additional nutrient requirements “…that may arise when high amounts of carbon substrate allow production of high microbial biomass which in turn drives the oxygen or other limiting nutrient level very low (Davis).”

Trapp (1995) developed a model called PlantX which considers the following processes: diffusive exchange between soil and roots in water and air pores; transfer into roots with the transpiration stream; translocation in the plant with the transpiration stream; partitioning into the stem; transport with the assimilation stream; diffusive exchange between air and leaf via stomata and cuticle; metabolism; and dilution by growth. The roots, stems, leaves, and fruits of the plant are assumed to be homogeneously mixed. Trapp validated the model by using Phaseolus vulgaris var. Prozessor (beans) to uptake a systemic pesticide, carbofuran (2,3-dihydro-2,2-methylbenzofuranyl-N-methyl-phenylcarbamate). Plant growth patterns almost matched exactly while there were slight discrepancies in the uptake data. Trapp also validated the model with nitrobenzene, which he notes is a volatile organic compound; showing that his model predicts leaf/air interaction.

Paterson and Mackay (1995) developed a model based on the fugacity concept. Fugacity can be described as the “escaping tendency” of a chemical to migrate from one compartment of the environment to another (Goldsborough). Goldsborough also states that chemicals move from high to low fugacity (measured in Pascals) and that fugacity is to mass diffusion as temperature is to heat diffusion. Paterson and Mackay used this concept to make a model that “…treats chemical migration into three plant compartments — root, stem, and foliage — from two environmental compartments, soil and atmosphere.” The model includes chemical transport between air and soil and can “…treat chemical emissions into any or all of the five compartments.” The model calculates rates of transport between, and transformation in, the various plant and environmental compartments. Metabolism and plant growth will be included in future versions of the model. Experimental data is still needed for “…a number of chemicals of known properties, gathered with a view to fitting the results to a model such as this [(that is, they have not validated the model)].”

Matthies and Behrendt (1995) developed a model called SNAPS to combine fate models for chemicals in soil and plants and their exchange with the atmosphere. The model deals with transport, uptake, and translocation of contaminants. They tested the model with three water-soluble pesticides in two scenarios. The pesticides included carbofuran, isoproturon, and terbutylazine. They found that the model simulated the field results satisfactorily.
Chang (1996) developed a mathematical model to investigate the effect of plant roots on bioremediation of hydrocarbons. A sink term was incorporated into an advection-dispersion transport equation to model the root interactions with soil-water and the hydrocarbons. Rather than maintaining ET, the model determines what the saturation level of the soil is in combination with root location and density. Empirical equations detailing a time-specific distribution of root quantity were utilized. These equations show dynamic changes in the soil environment due to root behavior. Chang found that the mean daily root water uptake rate per unit volume of soil, $S_w$, was:

$$S_w = L_d \times q_{av} = L_d \times \frac{q_{max}}{2}$$  \hspace{1cm} (2-10)

where: $q_{av} =$ mean daily root water uptake $[L^3 T^{-1}]$; and
$L_d =$ rooting density (length of roots per unit volume) $[L L^{-3}]$.

Chang then integrated $S_w$ to the rooting depth, $z_m$, to get the transpiration rate, $E$:

$$E = \int_0^{z_m} S_w \, dz$$  
$$= \frac{q_{max}}{2} \int_0^{z_m} L_d \, dz$$  \hspace{1cm} (2-11)
$$= \frac{q_{max} L_d (1-e^{-fn})}{2f}$$

where: $f =$ constant $[L^{-1}]$.

Microbial transport as well as microbial population changes in the root-soil zone were not incorporated. The model was tested on a TCE contaminated site using seeded cotton as the vegetation. The simulation results were compared to the results of unplanted soil remediation.

Chang found that “degradation of the volatile hydrocarbon was greater in the presence of the plant than in its absence.” He noted significant model sensitivity to diffusion in the gas phase, and that the model “…needs more information on microbial behavior such as microbial transport and microbial population changes in the root-soil, as well as on the volatilization affects of plants.”

Burken (1996) and Burken and Schnoor (1997) developed a mathematical model to model the metabolization of atrazine within the plant tissues of the hybrid poplar trees. This study was described earlier in this thesis. They created the model specifically for their experiment rather than for general conditions, but it could be adapted to other contaminants:
The model considers the following specific processes: metabolism in the bulk solution, transfer into roots with the transpiration stream, translocation within the plant via the transpiration stream, metabolism in the root and leaf tissues. The resulting model then describes the uptake, distribution, metabolism, and accumulation of atrazine and its metabolites in plant compartments.

They set forth that their model “…demonstrates that hybrid poplar, a plant shown to offer other distinct advantages for treatment of organic contaminants, has the capability to remove, hydrolyze, and dealkylate atrazine from contaminated soils.”

Jinquan (1996) developed a computer model to examine chemical transport in soil and groundwater systems. This model incorporated “…rainfall-recharge relationships, infiltration recharge processes, plant root uptake, biologically-induced hydraulic conductivity reduction, and contaminant transport of a nonaqueous phase liquid (NAPL).” Jinquan found that the “simulated cumulative actual evapotranspiration matched that calculated from the measured soil water content and soil water potential with an average deviation of 8.3 percent.” The model was ultimately used to simulate the movement of NAPL contaminants.

As mentioned earlier, Loftis (1999) and Panhorst (2000) employed various methods of estimating and/or modeling the transpiration rate of the phytoremediation system at the Oneida Tie Yard Site. Loftis used the ET Package in MODFLOW to simulate the direct transpiration of groundwater by poplar trees. He assumed an ET elevation of 1430 feet and an extinction depth of 1427 feet for the entire ET/poplar tree area. He calibrated his model, varying the one ET rate until the model produced “…dry cells over the majority of the site.” Panhorst calculated the transpiration rates with the White Equation and the Groundwater Recession Method for comparison. He modeled the impact of the poplar trees by using wells to simulate the transpiration of the poplar trees. For the 10 feet by 10 feet model cells, 3.3 poplar trees were assigned to each well, one well per cell. The well pumping rates varied, depending on the well locations (that is, based on tree height and probable access to groundwater), and were determined by calibrating the model. Both Loftis (1999) and Panhorst (2000) used single layer models.

Najjar (1999) monitored and modeled ET from constructed wetlands dominated by cattail (*Typha* spp.). Cattails were monitored in microlysimeters and in the field in the constructed wetlands for the study. Two models were developed, calibrated, and validated for predicting ET from constructed wetlands:

1. Crop coefficient model – ET = $K_c^\ast PET$, where ET is evapotranspiration (mm/d), $K_c$ is a dimensional cattail crop coefficient, and PET is a potential ET (mm/d); and

2. Parametric model – ET = $k_1R_s + k_2VPD$, where $R_s$ is solar radiation (MJ/m$^2$/d), VPD is vapor pressure deficit in kPa, and $k_1$ and $k_2$ are dimensionless empirical model coefficients.

Najjar found that the crop coefficient model was best for predicting ET for the cattails.
Garatuza-Payan (1999) hypothesized that “…remotely sensed information from climatological satellites [could] be used to estimate the actual evapotranspiration from agricultural crops to improve irrigation scheduling and water use efficiency.” The study region was the Yaqui Valley in Sonora, Mexico. After measuring and modeling the evapotranspiration and crop factors for wheat and cotton (indigenous crops), a “…high-resolution (4 kilometers x 4 kilometers) method for determining cloud cover and solar radiation from GOES satellite data…” was developed and tested. Garatuza-Payan demonstrated the application of satellite data “…to calculate the actual evaporation for sample crops… by combining potential rate with relevant crop factors and information on crop measurement.”

Buyuktas (2000) developed an “integrated three-dimensional model” by modifying the SWMS_3D model. Buyuktas incorporated “irrigation practices, evaporation, transpiration, and soil water extraction by roots (with vadose zone and groundwater flow and transport) to simulate and predict changes in water table elevations and groundwater quality due to agricultural management strategies.” The modified SWMS_3D model was verified, underwent a sensitivity analysis, calibrated, and validated. Buyuktas specifically investigated the effect of using averaged soil hydraulic parameters under homogeneous and heterogeneous crop conditions. The research concluded that “…the effective soil hydraulic properties can be used to represent the heterogeneous porous media in numerical simulations.”
3.0 Site Description and Data Collection Strategy

3.1 Hydrogeology of the Oneida Site

ARCADIS Geraghty & Miller (ARCADIS G&M) are the consultants in charge of the remediation project at the Oneida Tie Yard Site. They provided Virginia Tech with data and reports of past and current site characterizations. Section 3.1 provides an overview of these findings. All figures in this section are provided at the end of the section.

3.1.1 Geology

Oneida, Tennessee (Figure 1-2), is located in the central portion of the northern edge of the Cumberland Plateau. This part of the Cumberland Plateau is known to have “gently dipping strata to the east” with varying “anomalous structural features.” This physiographic province is underlain by rocks of the Pennsylvanian System, consisting almost entirely of clastic material which include: shale, siltstone, sandstone, conglomerate, coal, and thin discontinuous beds of impure limestone.

Direct Push Technology (DPT) tests around the Oneida Tie Yard Site detail the substrata. The soil at the site ranges from 8 feet to 12 feet in thickness, and is comprised of interbedded yellow-brown to orange-brown silty clays, with an underlying unconsolidate sand that is gray and orange in color. The clays measure as much as 8 feet in thickness while the sand overlying the shale bedrock is generally less than 5 feet thick (Figure 3-1). It is believed that these soils originated from alluvial deposits from Pine Creek and from weathering of the underlying bedrock. The northern part of the site where the abandoned coal hopper was located has a surficial layer of coal and gravel ranging up to four feet thick (Figure 3-2).

The ground surface of the site is at an elevation of approximately 1,430 feet above mean sea level. The top 8 to 10 inches of soil originates from the soil piles that were on the site. The former locations of the soil piles may be seen in Figure 3-2.

Soil borings from previous site investigations detailed the bedrock contours for part of the site. Depth to bedrock ranges from 8 feet to 12 feet. Figures 3-3, 3-4, and 3-5 show bedrock cross-sections and Figure 3-6 presents the bedrock contours.
3.0 SITE SETUP AND RATIONALE

Figure 3-1: Soil Distribution at Oneida Tie Yard Site (ARCADIS G&M 1)

Figure 3-2: Oneida Tie Yard Site Map Showing Old Hopper and Soil Piles (from ARCADIS G&M 1)
Figure 3-3: Location of Geologic Cross Sections (ARCADIS G&M 1)
Figure 3-4: Geologic Cross Section A – A' (ARCADIS G&M 1)

Figure 3-5: Geologic Cross Section B – B' (ARCADIS G&M 1)
3.1.2 Groundwater Hydrology

Table 3-1 shows the water level data collected by ARCADIS Geraghty & Miller through April 1997, just before the submittal of their Supplemental Investigation Report to Norfolk Southern Corporation in June 1997.

When compared to the previous data, the water levels recorded on April 3, 1997, prove to be the lowest recorded except for at monitoring well MW-2. A comparison also reveals that levels varied the least in MW-1 and the most in MW-4. The fluctuation of MW-1 was only 0.18 feet while MW-4 showed changes of 2.68 feet. Their location near Pine Creek demonstrates how bank storage influences the water table inconsistently. Additional water level data is located in Table A-1 in Appendix A.

The unconsolidated residuum and fluvial deposits from Pine Creek greatly affect the flow of groundwater through the site. Additionally, the bedrock plays a role. ARCADIS Geraghty & Miller reports:

In a typical hydrogeologic setting in this part of Tennessee, the Pennsylvanian bedrock units are generally hydraulically connected to the overlying unconsolidated saturated interval. However, shale bedrock at the site influences groundwater flow by directing it horizontally toward local discharge points. Groundwater flow typically mimics land topographic features on the Cumberland Plateau with flow towards key surface-water drainage features.
Table 3-1: Summary of Water-Level Elevations at the Oneida Tie Yard Site (adapted from ARCADIS G&M 1)

<table>
<thead>
<tr>
<th>Well Number</th>
<th>Date Measured</th>
<th>Measuring Point Elevation (TOC) (ft, msl)</th>
<th>Depth to Water (ft)</th>
<th>Water-Level Elevation (ft, msl)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MW-1</td>
<td>4/28/94</td>
<td>1433.64</td>
<td>8.91</td>
<td>1424.73</td>
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<tr>
<td></td>
<td>6/2/94</td>
<td></td>
<td>8.97</td>
<td>1424.67</td>
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<td></td>
<td>2/23/95</td>
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<td>8.92</td>
<td>1424.72</td>
</tr>
<tr>
<td></td>
<td>4/3/97</td>
<td></td>
<td>9.09</td>
<td>1424.55</td>
</tr>
<tr>
<td>MW-2</td>
<td>4/28/94</td>
<td>1436.11</td>
<td>8.20</td>
<td>1427.91</td>
</tr>
<tr>
<td></td>
<td>6/2/94</td>
<td></td>
<td>7.84</td>
<td>1428.27</td>
</tr>
<tr>
<td></td>
<td>2/23/95</td>
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<td>8.92</td>
<td>1427.19</td>
</tr>
<tr>
<td></td>
<td>4/3/97</td>
<td></td>
<td>8.50</td>
<td>1427.61</td>
</tr>
<tr>
<td>MW-3</td>
<td>4/28/94</td>
<td>1437.15</td>
<td>6.17</td>
<td>1430.98</td>
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<tr>
<td></td>
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<td>1430.16</td>
</tr>
<tr>
<td>MW-4</td>
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<td>5.67</td>
<td>1428.55</td>
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</tr>
<tr>
<td>MW-5</td>
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<td>3.97</td>
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<td>4.06</td>
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<tr>
<td></td>
<td>4/3/97</td>
<td></td>
<td>4.98</td>
<td>1430.54</td>
</tr>
</tbody>
</table>

Note: ft = feet, msl = mean sea level, and TOC = top of casing

Water level measurements from April 3, 1997, were used to delineate the water table (Figure 3-7). The ARCADIS G&M figure shows that the phreatic surface varies up to 6 ft across the southern part of the site, and that groundwater flow is to the south and southeast, toward Pine Creek, as expected. The rail lines west of the site may affect groundwater flow and associated recharge, although this was not obvious during the previous study (ARCADIS G&M 1).

The collected field data combined with several assumptions allow for calculation of the groundwater flow rate. The lack of a homogeneous medium is not conducive to such calculations without guesswork. Based on the soil composition of the site, unconsolidated intervals of clay, silt, and sand, the approximate site-wide hydraulic conductivity and effective porosity are estimated by ARCADIS G&M to be $3.28 \times 10^{-2}$ feet per day and 0.15, respectively (ARCADIS G&M 1). Loftis (1999) found the average hydraulic conductivity to be 4 feet per day through his model calibration. Panhorst (2000) found the site hydraulic conductivity to range from 1 foot per day to 25 feet per day through his model calibration.
3.0 SITE SETUP AND RATIONALE

Figure 3-7: Water Table Contours at Oneida Tie Yard Site (April 3, 1997) (ARCADIS G&M 1)

The hydraulic gradient is determined from Figure 3-7 to be 0.04 by dividing the change in hydraulic head between two points by the distance between those points. The values of these parameters are used to calculate the range of horizontal seepage velocities at the site with Freeze and Cherry’s (1979) average linear velocity equation:

\[
\frac{V}{nA} = \frac{v}{n} = -\frac{K}{nA} \frac{\partial h}{\partial l}
\]

\[
= -\frac{(4\% \text{ to } 20\%)}{0.15} \times (-0.04\%)
\]

\[
= 1.1\% \text{ to } 5.3\%
\]

where:  
- \(Q\) = groundwater flow rate \([L^3/T]\)  
- \(n\) = porosity (\(n_e\) is effective porosity, and is used here)  
- \(A\) = area of perpendicular to flow \([L^2]\)  
- \(V\) = velocity of groundwater \([L/T]\)  
- \(K\) = hydraulic conductivity of medium \([L/T]\)  
- \(\frac{\partial h}{\partial l}\) = hydraulic gradient (negative in the direction of flow) \([L/L]\)

1.1 feet per day and 5.3 feet per day are better evaluated over the span of a year as 402 to feet per year and 1,935 feet per year.
3.1.3 Groundwater Interception System

From March 1991 through July 1991 ETI performed initial abatement and preliminary site assessment activities that included excavating 11 test pits in the southeastern portion of the site. These pits served to characterize the area down gradient from the former creosote treatment area. After collection of the necessary data, the test pits were connected to create a groundwater collection trench. This collection trench should prove to prevent further migration of free product and impacted groundwater to Pine Creek. Figures 3-1, Figure 3-2, and Figure 3-3 show the location of the trench on the site as black triangles connected by a red line parallel to Pine Creek.

Figure 3-8 shows a profile view of the trench system. The trench, itself, is approximately 330 feet long, 20 feet wide at the top, and 3 feet wide at the bottom. Its depth is approximately 10 to 12 feet. A four-inch slotted drain tile lies along the bottom of the trench and is tied into a 24-inch vertical standpipe. A submersible pump sits at the bottom of this vertical culvert, two feet into the shale, and pumps drainage to an oil/water separator on the surface. The groundwater interception trench has recovered more than one million gallons of groundwater since it was first put into service in 1991 (Panhorst, 2000). The trench had not been operational for some time, but was fixed and turned back on in February 1998. Monthly trench data appear in Table A-2 in Appendix A.

Figure 3-8: Groundwater Interception System (adapted from ARCADIS G&M 1)
3.1.4 Phytoremediation System

A phytoremediation system with hybrid poplar trees was chosen for the Oneida Tie Yard Site for a number of reasons:

- Hardwoods, especially poplars, grow well in and are native to Tennessee;
- The small site allows for ease of monitoring and maintenance;
- PAH concentrations are within poplar tolerance;
- The site has a shallow aquifer; and
- The trees, themselves, are aesthetically pleasing and provide a sound barrier to the noise from railroad operations (ARCADIS G&M 2).

The reasons for using ‘hybrid’ poplars are explained in Section 2.1.2. The hybrid poplar varieties, DN34 and OP367, were chosen for their demonstrated growth in the laboratory (ARCADIS G&M 2).

The system was designed to manage water on the site in addition to the trench system. That is, the hybrid poplars, chosen for their increased growth rate, were also subsequently chosen for their demonstrated use of groundwater (refer to Section 2.1.5). By using more groundwater at the site, the trees effectively would hydraulically demobilize the creosote contaminate plume at the site. In May 1997, 960 poplar trees were planted. Although the planting area of the trees is only about 50 percent of the 1.25-acre site (Figure 3-9), the poplars should be able to transpire the 55 inches of average annual rainfall by their third year of growth (ARCADIS G&M 2). Additionally, the tree canopy will reduce percolation into the groundwater from precipitation.

The trees are planted in rows with 2.5 feet between trees and 10 feet between rows (Figure 3-9). Zone A, consisting of coal residue covered by ‘soil pile’ soil, has 320 poplars that aid in hydraulic control and act as a visual barrier to the adjacent property. Zone B, consisting of coal residue covered by ‘soil pile’ soil, has 350 poplars. This zone also aids in hydraulic control of the groundwater and acts as a visual barrier between the tie yard and the adjacent property. It also serves as the location of the Virginia Tech grass testing plots. Zone C has the largest soil pile incorporated into it. This zone has the worst impacted soil and groundwater. It provides hydraulic control in a joint effort with the groundwater interception system.

Additional trees were added to the southeast end of the site, between the trench and Pine Creek, after the trench system was upgraded during summer 1999. Upgrading consisted of unclogging the drain tile and cleaning out the ‘cleanout’ ports.
Figure 3-9: Tree Planting Schematic (by Ecolotree, Inc., in ARCADIS G&M 1)
3.2 Virginia Tech Site Investigation

Researchers from Virginia Tech (VT) installed groundwater-monitoring devices at the site in order to aid in several research objectives. The hydrology of the site, which is the emphasis of this thesis, is examined using data collected from piezometers and a weather station. Groundwater quality is analyzed using samples collected from multilevel sampling devices that were installed along with the piezometers. The locations of the piezometers and multilevel samplers are displayed in Figure 3-10. The locations of the soil borings appear in Figure 3-11. Previously published VT theses have presented the details of the soil and groundwater sampling data collected from this site.

The piezometers are constructed with 1-inch diameter schedule-40 polyvinyl chloride (PVC) pipe (Figure 3-12). Each piezometer consists of a five-foot PVC slotted segment and a riser PVC segment. The risers were originally 5 feet in length, but where the depths of the borehole were less than 10 feet, the riser pipe was cut in order to maintain clearance for vehicles traversing the site. The top of casing (TOC) is the location on the top of the riser segment where depth-to-water is measured from with a water level indicator. This point at the TOC is marked so that future water level measurements may be made from the same point. This mark is the point that a contracted surveyor used to survey the locations and elevations of the site. An inventory of the piezometers is provided in Table 3-2.

<table>
<thead>
<tr>
<th>Piezometer</th>
<th>Height Above Ground (inches)</th>
<th>Height Above Ground (feet)</th>
<th>Depth to Top of Bentonite Seal (feet)</th>
<th>Depth to Top of Sand (feet)</th>
<th>Total Depth of Well (feet)</th>
<th>Total Depth of Borehole (feet)</th>
<th>Screened Interval (feet)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12</td>
<td>1.00</td>
<td>1.50</td>
<td>2.50</td>
<td>8</td>
<td>8.8</td>
<td>3-8</td>
</tr>
<tr>
<td>2</td>
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<td>1.92</td>
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</tr>
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<td>1.50</td>
<td>3.50</td>
<td>4.50</td>
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<td>3.50</td>
<td>9</td>
<td>9.8</td>
<td>4 – 9</td>
</tr>
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</table>
To install the piezometers in the ground researchers hand-augured 4- to 5- inch diameter boreholes to bedrock, except for some that were installed by contracted drillers. In all, 20 piezometers were installed from June 1997 to October 1997. Nine of the piezometers were paired with multilevel samplers in the same boreholes for convenience. Researchers used a variation of ASTM procedure number D5092-90 to fill in the filter sand pack, bentonite seal, and concrete pad for each piezometer.

The multilevel samplers are constructed with 2.5-inch diameter schedule-50 PVC pipe (Figure 3-13 and Figure 3-14). The multilevel samplers’ lengths vary individually due to varying bedrock depths. The ports on each sampler, eight or ten depending on the length of the sampler, are 0.25-inch color coated plastic tubing spaced at 1-foot intervals. Nylon material serves to filter the end of each sample port.
Figure 3-11: Oneida Tie Yard Site Map Showing Soil Borings Used For Soil Sampling
3.0 SITE SETUP AND RATIONALE

Figure 3-12: Piezometer Schematic

Note: TOC = Top of Casing
Elevations surveyed at TOC
Valid for Piezometers 1-20
Figure 3-13: Eight-Port Multilevel Sampler

Figure 3-14: Ten-Port Multilevel Sample
Each multilevel sampler is topped with an extension of PVC to house the free lengths of sample port tubes. All multilevel samplers were installed to bedrock. An inventory of the multilevel samplers appears is presented in Table 3-3.

<table>
<thead>
<tr>
<th>Multilevel Sampler</th>
<th>Type of MLS (8 or 10 ports)</th>
<th>Elevation of Bedrock (feet)</th>
</tr>
</thead>
<tbody>
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<td>8</td>
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</tr>
<tr>
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<td>11</td>
<td>10</td>
<td>1418.34</td>
</tr>
<tr>
<td>12</td>
<td>10</td>
<td>1419.54</td>
</tr>
<tr>
<td>13</td>
<td>10</td>
<td>1419.19</td>
</tr>
<tr>
<td>14</td>
<td>8</td>
<td>1421.77</td>
</tr>
<tr>
<td>15</td>
<td>8</td>
<td>1421.16</td>
</tr>
<tr>
<td>16</td>
<td>10</td>
<td>1420.66</td>
</tr>
</tbody>
</table>

Sixteen multilevel samplers were installed from July 1997 to October 1997 in the same fashion as the piezometers. In some instances, a multilevel sampler shares the same borehole with a piezometer; if this is the case, the sampler and piezometer are designated with the same number. Again, researchers used a variation of ASTM procedure number D5092-90 for monitoring well construction to fill in the filter sand pack, bentonite seal, and concrete pad for each multilevel sampler.

Researchers installed the Davis GroWeather Systems™ weather station in April 1998. The location of the weather station may be seen in Figure 3-10 and Figure 3-11. Pictures of the assembled weather station are presented in Section 5. The weather station is marketed by Davis Weather Systems and is comprised of a central console and controller with specific peripherals: humidity and temperature sensor, leaf wetness sensor, anemometer, solar radiation sensor, rain collector, an optional soil thermometer probe, and a data logger. The data logger is set to record data at two-hour intervals so as to allow eighty days of storage. This data must be downloaded on a monthly to bimonthly basis to assure continuous data throughout the year.
4.0 Modeling the Site

4.1 Groundwater Flow Equations

There are two conceptual viewpoints for modeling groundwater systems: the aquifer viewpoint and the flow system viewpoint. “The aquifer viewpoint is based on the concept of confined and unconfined aquifers… [where] a confined aquifer is overlain by a confining bed… and an unconfined aquifer has a water table as its upper boundary (Anderson and Woessner).” The aquifer viewpoint is only used to simulate two-dimensional horizontal flow in confined and unconfined aquifers. A quasi three-dimensional approach may be used to simulate leaky confined aquifers with this viewpoint. The governing equation for the aquifer viewpoint can be put in its general form (Anderson):

\[
\frac{\partial}{\partial x} \left( T_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( T_y \frac{\partial h}{\partial y} \right) = S \frac{\partial h}{\partial t} - R - L
\]

(4-1)

where:
- \( h \) = head [L];
- \( T_x, T_y \) = transmissivities in the x- and y-directions (allows for anisotropy) [L²/T];
- \( S \) = storage coefficient;
- \( R \) = source or sinks where recharge is intrinsically positive [L/T]; and
- \( L = -K_z \left( \frac{h_{\text{source}} - h}{b'} \right) \), the leakage term for a leaky confined aquifer [L/T].

The left-hand side of this equation corresponds to horizontal flow through the aquifer. The transmissivities are included in the partial derivatives in order to provide for heterogeneity. The leakage term provides for the net rate of inflow from an adjacent aquifer through a confining layer of thickness, \( b' \), and vertical hydraulic conductivity, \( K_z' \).

When Equation 4-1 is applied to an unconfined aquifer, the well-known Dupuit assumptions are utilized (Anderson): (1) flow lines are horizontal and equipotential lines are vertical, and (2) the horizontal hydraulic gradient is equal to the slope of the free surface and is does not change with depth.

The flow system viewpoint concerns the three-dimensional distribution of heads, hydraulic conductivities, and storage properties everywhere in the system (Anderson). A flow system viewpoint is used for vertical profile models and fully three-dimensional models. Both vertical and horizontal flow components are accounted for in the general form of the governing equation (Anderson):
\[
\frac{\partial}{\partial t} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) = S_s \frac{\partial h}{\partial t} - R
\] (4-2)

where: \( K_x, K_y, K_z \) = components of the hydraulic conductivity in three dimensions [L/T]; \( S_s \) = specific storage [L^{-1}]; and \( R \) = source or sink term in which outflow is negative [T^{-1}].

Figure 4-1 shows the differences between the aquifer and flow system viewpoints.

Figure 4-1: Conceptual viewpoints

(a) The geologic system.

(b) The aquifer viewpoint. In this example, the aquifer viewpoint focuses on the confined aquifer. The vertical hydraulic conductivity and thickness of the confining bed and the assigned head in the overlying unconfined source bed are used to calculate the leakage of water into or out of the confined aquifer. The head distribution is calculated only for the confined aquifer.

(c) The flow system viewpoint. In this viewpoint, hydraulic properties are assigned to each geologic unit and heads are calculated in all three layers.

Anderson and Woessner (1992)

Based on site conditions, a fully three dimensional flow model is not explored in this study. The presence of a low permeability coal layer is the only feature that could suggest a low permeability layer, and the average depth to bedrock (shale) at the site is just over 10 feet. Therefore, the model for this thesis will be a two-dimensional model (aquifer viewpoint), using intricate input data simulating varying parameters across the site model due to the desire to model the intricate geology of the site (that is, there will be multiple hydraulic conductivities, ET extinction depths and rates, and recharge areas). The modeler wants to evaluate a groundwater modeling program’s ability to model evapotranspiration (that is, the rate at which the poplar trees transpire the groundwater flow). Evaporation aspects are not supported in MODFLOW.
4.2 Infiltration Models

Interception is the part of precipitation “...which wets and adheres to aboveground objects until it is returned to the atmosphere through evaporation (Viessman and Lewis 1996).” Viessman and Lewis report that the amount of water intercepted is a function of: (1) storm character; (2) the species, age, and density of prevailing plants and trees; and (3) the season of the year. They also state that “usually about 10-20 percent of the precipitation that falls during the growing season is intercepted and returned to the hydrologic cycle by evaporation.” With the necessary parameters, interception can be estimated with the following equation (Viessman):

\[ L_i = S(1 - e^{-Kt}) + KEt \]  \hspace{1cm} (4-3)

where:
- \( L_i \) = the volume of water intercepted (inches);
- \( S \) = the interception storage on foliage that resists wind and gravity (varies between 0.01 and 0.05 inches);
- \( P \) = the amount of rainfall (inches);
- \( K \) = ratio of surface area of intercepting leaves to horizontal projection;
- \( E \) = amount of water evaporated per hour during the precipitation period (inches); and
- \( t \) = time (hours).

Precipitation that does reach the ground will either “…infiltrate, flow over the surface, or become trapped in numerous small depressions from which the only escape is evaporation or infiltration (Viessman).” All depression storage will eventually evaporate or infiltrate into the groundwater. A generalized parametric equation for depression storage is virtually impossible due to the extreme variability of land surfaces from site to site. Linsley and others (1949) developed the following to approximate the volume of water stored by surface depressions at any given time:

\[ V = S_d\left(1 - e^{-\frac{P_e}{S_d}}\right) \]  \hspace{1cm} (4-4)

where:
- \( V \) = the volume actually in storage at some time of interest [L];
- \( S_d \) = the maximum storage capacity of the depressions; and
- \( P_e \) = rainfall excess (gross rainfall after evaporation, interception, and infiltration).

Mein and Larson (1971) describe three general cases of infiltration associated with rainfall events: (1) the rainfall rate is less than the saturated conductivity of the soil; (2) the rainfall rate exceeds the saturated conductivity but is less than the infiltration capacity; and (3) the rainfall intensity exceeds the infiltration capacity. In case (1), all rainfall infiltrates the soil and runoff never occurs. Case (2) describes heavy
rainfall that affects infiltration rates yet still does not produce. Case (3) is the condition that produces runoff. Infiltration and overland flow may be examined with many infiltration models such as Horton’s, Green-Ampt’s, Huggins-Monke’s, and Holtan’s models.

Horton’s infiltration model came about in the 1930’s. Appearing below, it shows that if the rainfall supply exceeds the infiltration capacity, infiltration tends to decrease in an exponential manner (Horton 1935):

\[
f_p = f_c + (f_0 - f_c)e^{-kt}
\]  

where: 
- \( f_p \) = the infiltration capacity [L/T] at some time, \( t \);  
- \( f_c \) = final or equilibrium capacity [L/T];  
- \( f_0 \) = the initial infiltration capacity [L/T]; and  
- \( k \) = a constant representing the rate of decrease in \( f \) capacity.

Equation 4-5 is shown graphically in Figure 4-2. The difficulty in determining useful values for \( f_0 \) and \( k \) restrict the use of Horton’s infiltration equation (Viessman).

The Green-Ampt infiltration model was originally proposed in 1911 and has been modified over the years to more useful forms (Viessman). The original form assumed that the soil surface was submerged at all times under a negligible depth and that the water infiltrated a homogeneous soil with a uniform water content (Green and Ampt 1911):
where: \( f_p \) = the infiltration capacity \([L/T]\); 
\( K_s \) = the saturated hydraulic conductivity of soil \([L/T]\); 
\( L \) = the distance from the ground surface to the wetting front \([L]\); and 
\( S \) = the capillary suction at the wetting front \([L]\).

Mein and Larson (1973) suggest manipulation of Equation 4-6 to allow for use in watershed modeling by relating the cumulative infiltration to the time at which infiltration began (from Viessman):

\[
F - S \times IMD \times \ln \left( \frac{F + IMD \times S}{IMD \times S} \right) = K_s \cdot t
\]  

where: 
\( f \) = actual infiltration rate (feet per second); 
\( f_p \) = infiltration capacity (feet per second); 
\( i \) = rainfall intensity (feet per second); 
\( F \) = cumulative infiltration volume in the event (feet); 
\( F_i \) = cumulative infiltration volume required to cause surface saturation (feet); 
\( S \) = average capillary suction at the wetting front (feet of water); 
\( IMD = \theta_s - \theta_i \) = initial moisture deficit for the event (feet per foot); and 
\( K_s \) = saturated hydraulic conductivity of soil (feet per second).

A modified form of the Green-Ampt infiltration model is employed in the storm water simulation model SWMM (Huber et al. 1981).
Huggins and Monke (1966) approached the infiltration ordeal with soil moisture as the dependant variable rather than time (from Viessman):

\[ f = f_c + A \left( \frac{S - F}{T_p} \right)^p \]  

(4-8)

where:  
- \( A \) and \( P \) = coefficients determined from sprinkling infiltrometer studies;  
- \( S \) = the storage potential of a soil overlying the impeding layer (\( T_p \) minus antecedent moisture);  
- \( F \) = the total volume of water that infiltrates; and  
- \( T_p \) = the total porosity of soil lying over the impeding stratum.

Holton (1965) also developed an infiltration capacity equation (from Viessman):

\[ f = aS_a^{1.4} + f_c \]  

(4-9)

where:  
- \( f \) = the infiltration capacity (inches per hour);  
- \( a \) = the infiltration capacity of the available storage [(inches per hour per inch)^{1.4}];  
- \( S_a \) = available storage in the surface layer (inches of water); and  
- \( f_c \) = the constant rate of infiltration after long wetting (inches per hour).

The aforementioned models and modified versions are used in many hydrologic modeling programs such as SWMM and USDAHL, (Holtan et al. 1975). The necessary parameters for calculating interception, depression storage, and infiltration are not known for the study site and need to be experimentally determined. The presumptions required for calculating these pieces of the water balance is outweighed by the triviality of their use in a small study area. Although they are ignored in this study, they are important aspect of the modeling effort and should show purpose in future studies of this type.

The initial importance of these infiltration models was to calculate the recharge as a function of time on an annual basis (as the tree cover increased or decreased). This will be reserved for future study. Instead, recharge rate will be determined with rain data from the site and model calibration.

### 4.3 Modeling

#### 4.3.1 MODFLOW and GMS Fundamentals

##### 4.3.1.1 Finite Difference Analysis

When modified for unconfined flow, Equation 4-1 describes the two-dimensional movement of ground water of constant density:
\[
\frac{\partial}{\partial x} \left( K_x h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y h \frac{\partial h}{\partial y} \right) = S_y \frac{\partial h}{\partial t} - R - Q \tag{4-10}
\]

where:  
- \( K_x, K_y \) = components of the hydraulic conductivity in two dimensions [\( L/T \)];  
- \( S_y \) = specific yield;  
- \( R \) = recharge rate [\( L/T \)]; and  
- \( Q \) = source or sink term [\( L/T \)].

Provided that the principal axes of hydraulic conductivity are aligned with the coordinate directions,  
Equation 4-10 describes groundwater flow under non-equilibrium conditions in a heterogeneous and  
anisotropic medium (McDonald and Harbaugh). Combining this equation with flow and/or head boundary  
conditions as well as initial head conditions allows a mathematical representation of a groundwater flow  
system to be developed.

Analytical solutions of this equation would prove too difficult to derive and simplify for this study, and  
may require enormous assumptions. Instead, the modeler employs the use of a numerical method to obtain  
approximate solutions to the groundwater flow equation. The familiar numerical finite-difference method  
replaces the difficult continuous equation with “…a finite set of discrete points in space and time [while]  
the partial derivatives are replaced by terms calculated from the differences in head values at these points  
(McDonald and Harbaugh).” The finite-difference method allows for the simultaneous solution of linear  
algebraic difference equations, yielding the values of head at specific points and times (McDonald and  
Harbaugh). Finite element analyses exist but are not used in this study.

The groundwater modeling program, MODFLOW, utilizes this finite-difference approach to give solutions  
to groundwater modeling scenarios. MODFLOW’s finite difference form of the groundwater flow  
equation “…follows from the application of the continuity equation [in which] the sum of all flows into and  
out of the cell must be equal to the rate of change in storage within the cell (McDonald and Harbaugh).”

\subsection*{4.3.1.2 Grid Types}

When creating a numerical model “…the continuous problem domain is replaced by a discretized domain  
consisting of an array of nodes and associated finite difference blocks (cells) or finite elements (Anderson  
and Woessner).” The two types of finite difference grids are block-centered and point- or mesh-centered  
grids (Figure 4-4). Block centered grids have nodes at the center of the cells or blocks. Point- or mesh-  
centered grids nodes are at the intersection of points of the sets of parallel lines defining the cells or blocks;  
the “…cells are drawn around the nodes with faces halfway between nodes (McDonald and Harbaugh).”  
The main difference between the two types of grids is how they handle flux boundary conditions. "In the  
block-centered approach flux boundaries always are located at the edge of the block… [whereas] in a  
mesh-centered grid, the boundary coincides with a node (Anderson and Woessner).” MODFLOW uses the  
block-centered approach because “large general computer codes” can handle the finite difference  
mathematics for boundaries more easily with the block-centered approach (Anderson and Woessner).
4.2.1.3 MODFLOW Key Features

MODFLOW simulates groundwater flow in three dimensions within an aquifer using a block-centered finite-difference approach (McDonald and Harbaugh):

The modular structure consists of a Main Program and a series of highly independent subroutines called "modules." The modules are grouped into "packages." Each package deals with a specific feature of the hydrologic system which is to be simulated, such as flow from rivers or flow into drains, or with a specific method of solving linear equations which describe the flow system, such as the Strongly Implicit Procedure or Slice-Successive Overrelaxation…

…[Model] layers can be simulated as confined, unconfined, or a combination of confined and unconfined. Flow associated with external stresses, such as wells, areal recharge, evapotranspiration, drains, and
4.0 Model The Site

streams, can also be simulated. The finite-difference equations can be solved using either the Strongly Implicit Procedure, Preconditioned Conjugate Gradient, or Slice-Successive Overrelaxation Packages.

Boundary conditions are set by grouping cells (the boundary cells) into two categories: “constant-head” cells and “no-flow” cells (McDonald and Harbaugh).

Constant-head cells are those for which the head is specified in advance, and is held at this specified value through all time steps of the simulation… No-flow cells are those for which no flow into or out of the cell is permitted, in any time step of the simulation… [Both of these types] are used to represent conditions along various hydrologic boundaries.

The interior cells are termed “variable-head” cells. These are “…characterized by heads which are unspecified and free to vary with time (McDonald and Harbaugh).

GMS includes a comprehensive graphical interface to MODFLOW (BYU GMS v3.0 Reference Manual):

[This] special version of MODFLOW is …the same as the version distributed by the USGS except for a few minor changes primarily related to file input…

Table 4-1 shows that certain packages are required in order for MODFLOW to run, and that one of three iterative solver techniques must be chosen. The modeler will use the PCG2 solver package for all models in this thesis, as it uses the popular preconditioned conjugate gradient technique.

MODFLOW checks its iterative solutions with a volumetric water budget. A continuity check on the total flows into and out of the model, accounting for change in storage, is “…calculated independently of the equation solution process, and in this sense may provide independent evidence of a valid solution (McDonald and Harbaugh).”

Table 4-1: MODFLOW Packages Supported By GMS

<table>
<thead>
<tr>
<th>Package Name</th>
<th>Abbreviated Name</th>
<th>DESCRIPTION</th>
<th>Always Required?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basic Package</td>
<td>BAS1</td>
<td>Used to specify the grid dimensions, the computational time steps, and an array identifying which packages are to be used.</td>
<td>Y</td>
</tr>
<tr>
<td>Output Control</td>
<td>OUT1</td>
<td>Controls what information is to be output from MODFLOW and when it is to be output.</td>
<td>N</td>
</tr>
<tr>
<td>Block Center Flow Package, Version 1</td>
<td>BCF1</td>
<td>Performs the cell by cell flow calculations. The input to this package includes layer types and cell attributes such as storage coefficients and transmissivity</td>
<td>Y†</td>
</tr>
<tr>
<td>Block Center Flow Package, Version 2</td>
<td>BCF2</td>
<td>Similar to BCF1 except that the capability to rewet dry cells has been added.</td>
<td>Y†</td>
</tr>
<tr>
<td>Block Center Flow Package, Version 3</td>
<td>BCF3</td>
<td>Similar to BCF2 except that a more sophisticated technique for computing cell to cell conductances is supported.</td>
<td>Y†</td>
</tr>
</tbody>
</table>
### Table 4-1: MODFLOW Packages Supported By GMS (continued)

<table>
<thead>
<tr>
<th>Package Name</th>
<th>Abbreviated Name</th>
<th>DESCRIPTION</th>
<th>Always Required?</th>
</tr>
</thead>
<tbody>
<tr>
<td>River Package</td>
<td>RIV1</td>
<td>Simulates river type boundary conditions.</td>
<td>N</td>
</tr>
<tr>
<td>Recharge Package</td>
<td>RCH1</td>
<td>Simulates recharge to the groundwater from precipitation.</td>
<td>N</td>
</tr>
<tr>
<td>Well Package</td>
<td>WEL1</td>
<td>Simulates injection/extraction wells.</td>
<td>N</td>
</tr>
<tr>
<td>Drain Package</td>
<td>DRN1</td>
<td>Simulates drain type boundary conditions.</td>
<td>N</td>
</tr>
<tr>
<td>Evapotranspiration Package</td>
<td>EVT1</td>
<td>Simulates the effect of evapotranspiration in the vadose zone.</td>
<td>N</td>
</tr>
<tr>
<td>General Head Boundary Package</td>
<td>GHB1</td>
<td>Simulates a general purpose head-dependent source/sink. Commonly used to simulate lakes.</td>
<td>N</td>
</tr>
<tr>
<td>Stream/Aquifer Interaction Package</td>
<td>STR1</td>
<td>Simulates the exchange of water between the aquifer and surficial streams. Includes routing and automatic computation of stage.</td>
<td>N</td>
</tr>
<tr>
<td>Horizontal Flow Barrier Package</td>
<td>HFB1</td>
<td>Simulates the effect of horizontal flow barriers such as sheet piles and slurry trenches.</td>
<td>N</td>
</tr>
<tr>
<td>Time Variant Specified Head Package</td>
<td>CHD1</td>
<td>Simulates specified head boundary conditions where the head is allowed to vary with time.</td>
<td>N</td>
</tr>
<tr>
<td>Strongly Implicit Procedure Package</td>
<td>SIP1</td>
<td>An iterative solver based on the strongly implicit procedure.</td>
<td>Y*</td>
</tr>
<tr>
<td>Preconditioned Conjugate Gradient Package, Version 2</td>
<td>PCG2</td>
<td>An iterative solver based on the preconditioned conjugate gradient technique.</td>
<td>Y*</td>
</tr>
<tr>
<td>Slice Successive Overrelaxation Package</td>
<td>SOR1</td>
<td>An iterative solver based on the slice successive overrelaxation technique.</td>
<td>Y*</td>
</tr>
</tbody>
</table>

† One of the BCF packages must be used.
* One of the solver packages must be used.

Note: Table taken directly from BYU GMS v3.0 Reference Manual.

### 4.2.1.4 GMS Key Features

The GMS platform provides a number of analysis code interfaces for groundwater and contaminant modeling, including: MODFLOW, MT3D, RT3D, MODPATH, SEAP2D, and FEMWATER. For the purposes of this thesis, only the MODFLOW interface will be utilized.

GMS supports MODFLOW as a pre- and post-processor. The input data for MODFLOW are generated by GMS and saved to a set of files. These files are then read by MODFLOW when MODFLOW is executed. MODFLOW can be executed with a GMS menu command… The output from MODFLOW is then imported to GMS for post-processing (BYU GMS v3.0 Reference Manual).

In order to construct a MODFLOW simulation in GMS, one of two approaches can be used: the grid approach or the conceptual model approach (BYU GMS v3.1 Tutorials).
The grid approach involves working directly with the three dimensional grid and applying sources/sinks and other model parameters on a cell by cell basis [in the 3D Grid module]… The conceptual model approach involves using the GIS tools in the Map module to develop a conceptual model of the site being modeled. The location of sources/sinks, layer parameters such as hydraulic conductivity, model boundaries, and all other data necessary for the simulation can be defined at the conceptual model level. Once this model is complete, the grid is generated and the conceptual model is converted to the grid model and all of the cell by cell assignments are performed automatically.

The modeler chose the conceptual model approach, as it is relatively new to the GMS platform and makes the calibration process faster. The conceptual model approach is a user-friendly precursor to the grid approach since input from the conceptual model approach is converted to a grid.

4.3.2 Modeling Protocol and Water Budget

4.3.2.1 Modeling Protocol

Table 4-2 presents the modeling protocol, or the process that the researcher used (adapted from Anderson and Woessner).

4.3.2.2 Background Image For Conceptual Model Approach

The tutorial for the conceptual model approach published by Brigham Young University was used as a guide for the researchers grid construction. The GMS manuals, tutorial, and related manuals may be referenced on the World Wide Web at:

http://chl.wes.army.mil/software/gms/docs.htp

The GMS tutorial for this conceptual model approach details the steps involved in creating the grid. GMS allows the researcher to use an image of the site as a background to place feature objects in the appropriate places. These feature objects are patterned after Geographic Information Systems (GIS) objects and include points, nodes, arcs, and polygons (BYU GMS v3.0 Reference Manual). Feature objects are grouped into coverages, defining particular sets of information. GMS uses these to create a three dimensional-grid and assign boundary conditions and model parameters to the appropriate cells.

The image started as an AutoCAD drawing of the Oneida Tie Yard Site provided by ARCADIS G&M. The researcher exported the AutoCAD drawing as a bitmap file, and then converted the bitmap file to a Tags Image File Format (TIFF) image using standard image file viewer software. The researcher imported the TIFF image into GMS and “registered” it by identifying three points on the image corresponding to locations with known real world x-,y- coordinates (BYU GMS v3.0 Reference Manual).
### Table 4-2: Modeling Protocol For This Research

<table>
<thead>
<tr>
<th>1) Purpose:</th>
<th>Model is to be used to predict future impact of phytoremediation systems (poplar trees) on groundwater flow.</th>
</tr>
</thead>
</table>
| 2) Conceptual Model: | Assume: heterogeneous, isotropic aquifer, variable recharge over entire area (no runoff, infiltration, depression calculations).  
No point/grid refinement due to small size of site.  
No alignment of grid necessary.  
Inputs/outputs of groundwater, sources, and sinks  
Water Budget |
| 3) Code Selection: | MODFLOW |
| 4) Model Design: | GMS Conceptual Model approach using Map Module to create grid, boundaries.  
Boundaries are stream lines (no-flow) and Pine Creek (drain).  
Preliminary selection of values |
| 5) Calibration: | Trial and error adjustments to variables so model produces known data. When converging, will use the PEST or UCODE inverse calculation software (included in GMS) to complete the calibration procedure. |
| 6) Sensitivity Analysis | Calibration is ultimately a first step to any sensitivity analysis. Change the input variables and observe changes in primary calibration statistics (that is, how does the residual mean and the residual standard deviation change when parameters are changed?). |
| 7) Non-Unique Solution Check and Verification | Adjust variables, but keep ratio of variables the same, to check for a unique solution. Then use calibrated model to reproduce another set of field data. |
| 8) Prediction | Presentation of design and results. |
The coordinates used to register the image are the coordinates of three multilevel samplers that were surveyed at the site. The three multilevel samplers used with their real world x-,y- coordinates appear in Figure 4-5. Point #1 is placed on Multilevel Sampler 5, Point #2 is placed on Multilevel Sampler 1, and Point #3 is placed on Multilevel Sampler 10.

![Figure 4-5: Registering Image in GMS](image)

After registering the image, the Map Module is used to place the feature objects on the image. Again, the GMS tutorial details the steps involved in creating the grid for this conceptual model approach. Feature objects that are placed on the image include arcs, polygons, and points, all given properties that will convert and translate to the grid. During calibration, new values can be assigned to the feature objects and then translated to the MODFLOW three-dimensional grid with greater ease than cell by cell editing.

Boundary features will consist of: (1) Pine Creek, represented as a drain, on the north and east sides of the model domain; (2) streamline on the west side of the model domain, perpendicular to Pine Creek; and (3) streamline on the south side of the model domain, also perpendicular to Pine Creek. Conductance will be varied within the Pine Creek Drain Package during calibration.
4.0 Modeling the Site

The groundwater interception trench will be modeled using the Drain Package, with conductance varied within the package for calibration. The areal polygons of the poplar trees will be associated with the ET Package. ET rates will be varied within the ET Package during calibration.

The inherent Basic and BCF Packages, as well as the aforementioned PCG2 Solver Package will be used. Areal polygons will be created in the Map Module within GMS to enter the recharge values and hydraulic conductivity values for different areas of the model. These will be converted to the MODFLOW grid, the recharge values going into the Recharge Package, and the hydraulic conductivity values going into the BCF Package. The recharge and hydraulic conductivity will be varied within the BCF package during calibration. Top and bottom elevation data of each layer will be entered by scatter-point files and mapped to the BCF Package.

4.3.2.3 Water Budget

It has been said, “the water budget method…is a very simple procedure, but it seldom produces reliable results (Viessman and Lewis, 1996).” Viessman and Lewis (1996) further explained that the water budget method’s “…adequacy is dependent upon the accuracy with which several terms in the budget equation can be evaluated.”

Before actually entering parameter values into the model, a water budget is analyzed. A water budget is “an evaluation of all sources of supply (inflow) and discharges with respect to an aquifer or drainage basin, using the hydrologic equation (Widdowson, 1995),” and is basically a single-cell model analysis. The hydrologic equation is a “quantitative means to evaluate the hydrologic cycle using the concept of continuity (Widdowson, 1995):”

\[
\text{Inflow} = \text{Outflow} + \Delta \text{Storage}, \text{ or } \\
Q_{in} = Q_{out} + \Delta S, \text{ or } \\
Q_{in} - Q_{out} = \Delta S 
\] (4-11)

Adapting this hydrologic equation to a water budget equation for the Oneida Tie Yard Site [by modifying Viessman and Lewis (1996) hydrologic equation]:

\[
(P + G_{in}) - (R + G_{out} + Q_{T} + \text{ET}) = \Delta S 
\] (4-12)

where: \( P \) = precipitation [L^3/T];
\( R \) = surface runoff [L^3/T];
\( G_{in} \) = groundwater inflow [L^3/T];
\( G_{out} \) = groundwater outflow [L^3/T];
\( Q_{T} \) = groundwater interception trench outflow [L^3/T];
\( \text{ET} \) = evapotranspiration [L^3/T]; and
\( \Delta S \) = change in water storage [L^3/T].
Loftis (1999) and Panhorst (2000) investigated the above components of the water budget. Each of their components varied, as did their Oneida Tie Yard Site size and orientation. This thesis will incorporate some of their findings. The November 1997 and May 1998 data will be used for water budget calculations. The November 1997 data will provide information before the trench was in operation and before the trees were significantly active. The May 1998 data will provide information during a time when the trench was operating, the poplar trees were active and using water, and there was plentiful rainfall in Oneida.

Area and length calculations are required to create a water budget. The GMS Map Module was used to construct the conceptual model, as partially described above. This allows GMS to calculate the lengths of Pine Creek and the streamline boundaries applicable to the study site, as well as calculate the areas of the study site and the poplar trees within the study site. Figure 4-6 shows the applicable values.

RAINFALL

Extensive rainfall data is available for the Oneida Tie Yard Site, the city of Oneida, and the region surrounding it. Appendices A and D present rainfall data used for calibrating the anticipated model. Figure 4-8 is taken directly from Panhorst (2000), showing monthly rainfall data (from April 1997 through February 2000) obtained from the Oneida Municipal Wastewater Treatment Plant, the on-site weather station installed by Virginia Tech, and the National Weather Service (for Knoxville, Tennessee).

The Oneida Treatment Plant data will be used to calculate total rainfall. From Figure 4-7, the November 1997 rainfall total was approximately 2 inches. Applied over the 9.26-acre site, 2 inches converts to approximately 67,000 cubic feet of precipitation in the month of November 1997. The gauging data was collected on November 12, 1997. Daily rainfall records provided by the Oneida Municipal Wastewater Treatment Plant detail that the majority of the November rainfall occurred before this date. The May 1998 rainfall total was approximately 7.7 inches, converting to approximately 260,000 cubic feet of precipitation.

RUNOFF

Calculating the surface runoff without extensive data requires many assumptions. Various correlations have been developed between precipitation and runoff; however, because various factors affect runoff (for example, the precipitation intensity and duration, initial soil-moisture conditions, and the time of year), calculating runoff as a function of rainfall “…does not produce satisfactory correlation (Chow, 1964).”
Figure 4-6: Conceptual Model From Map Module Showing Dimensional Data

Figure 4-7: Monthly Rainfall Data for Oneida, Tennessee (Panhorst 2000)
The Soil Conservation Service (SCS) developed runoff curve numbers for creating hydrographs to quantify runoff (Viessman and Lewis, 1996). The Rationale Method is also commonly used to calculate the amount of runoff from a small watershed based on soil types, surface conditions, and rainfall intensity, as well as empirical variables. Interception and depression storage have to be considered when calculating runoff.

There is a significant lack of data necessary to estimate the runoff during any given month at the Oneida Tie Yard Site. Therefore, the runoff analysis made by Panhorst (2000) will be accepted, and it will be assumed that 10 percent of monthly rainfall will result in runoff outflow. For example, in November 1997, the monthly runoff would be 10 percent of 67,000 cubic feet per month (6,700 cubic feet per month). The May 1998 runoff value will be 10 percent of 260,000, or 26,000 cubic feet per month.

**GROUNDWATER FLOW**

The estimated piezometric surface at the study site for November 1997 is presented in Figure 4-8, based on gauging data collected in November 1997.

Recall that water level contours using April 1997 gauging data were presented earlier in Figure 3-7, a figure produced by ARCADIS G&M. Although the trench was not in operation and the poplar trees were not planted yet in both April 1997 and November 1997, the figures are clearly different. This is due to the amount of gauging data available for each month. Figure 3-7 only uses gauging data from monitoring wells MW-1 through MW-5, while Figure 4-8, uses data from monitoring wells MW-1 through MW-7 as well as piezometers P-1 through P-19.

The estimated piezometric surface at the study site for May 1998 is presented in Figure 4-9, based on the water level elevations calculated from gauging data collected in June 3, 1998. The June 3, 1998, estimated water level contours are presented since they represent the effect of the May 1998 rainfall total. The May 5, 1998, gauging data would be representative of the April 1998 stresses. Figure 4-9 differs slightly from Figure 4-8 (and Figure 3-7) because the groundwater interception trench was in operation and the poplar trees were planted and active.

The groundwater inflow to and outflow from the study site is estimated using Darcy’s Law, Figure 4-6, and Figure 4-8. An alternative form of Darcy’s Law presents the flow rate through an aquifer as a function of hydraulic conductivity, hydraulic gradient, and the cross-sectional area to flow (Freeze and Cherry, 1979):

\[
Q = -KiA
\]

where:  
\( Q \) = Groundwater flow [L^3/T];  
\( K \) = hydraulic conductivity [L/T];  
\( i \) = hydraulic gradient [Δh/L or L/L];  
\( A \) = cross-sectional area to flow direction [L^2];
Figure 4-8: Estimated Water Level Contours for November 12, 1997
Figure 4-9: Estimated Water Level Contours for June 3, 1998 (for May 1998 contours)
As mentioned in Section 3.1.2, based on the soil composition of the site (that is, unconsolidated intervals of clay, silt, and sand) the approximate site-wide hydraulic conductivity was estimated to be $3.28 \times 10^{-2}$ feet per day according to ARCADIS G&M. Virginia Tech slug tests at the site determined a hydraulic conductivity of approximately 0.2 feet per day. The upper portion of the site has the low permeability coal layer, which may have also been a factor in ARCADIS G&M’s estimation of the hydraulic conductivity.

Panhorst (2000) assumed a hydraulic conductivity of 10 feet per day for his water budget calculations. Loftis (1999) used 4 feet per day for his Darcy Velocity calculations, acquiring the value from his calibrated model.

The water budget calculations are more simplistic than the numerical model. The modeler will adjust many variables, including the hydraulic conductivity, during calibration of the model. The modeler has an intimate knowledge of the study site subsurface geology; especially after hand-augering many of the piezometer and/or multi-level sample boreholes to bedrock, and even trying one of the slug tests. The site-specific slug test data would tend to be what is used in the professional consulting realm, but the assumptions of the previous modelers are also credible. The average of all of the previously used values (that is, 0.0328, 0.2, 10, and 4) would be approximately 3.5, somewhat high compared to the slug test results. For the water budget calculations in this thesis, the hydraulic conductivity was assumed 4.5 feet per day, since most of the flow out of the site will be through sandy media with higher hydraulic conductivities.

Panhorst (2000) calculated hydraulic gradients based on water level data from various wells and piezometers over eight months. Panhorst determined an average hydraulic gradient of 0.025 to use in his water budget calculations. Loftis (1999) also calculated the hydraulic gradient, but only used the December 1997 gauging data (for piezometers P-9, P-10, and P-11). Loftis determined the hydraulic gradient for December 1997 to be approximately 0.007 for the site. For these water budget calculations, the hydraulic gradients are calculated for both the November 1997 and May 1998 data in the same manner (that is, using Widdowson, 1997, CE 5374 gradient magnitude method). Hydraulic gradient calculations appear in Appendix B. The average November 1997 site-wide hydraulic gradient was determined to be 0.028, while the May 1998 (using June 5, 1998, gauging data) average site-wide hydraulic gradient was determined to be 0.043.

Calculating the cross-sectional area perpendicular to flow for the groundwater inflow and outflow requires more assumptions. The outflow portion seems to be the most obvious, since the groundwater outflow from the site mostly goes to Pine Creek. Therefore, only the saturated thickness of the aquifer has to be assumed for the groundwater outflow cross-sectional area. Loftis (1999) did actually perform manual water budget calculations. Panhorst (2000) assumed the aquifer’s saturated thickness across the site of four feet. For this thesis, the average saturated thickness was calculated for each month. Subtracting the bedrock elevation from the water level elevation at each respective well or piezometer allowed for this calculation (refer to
Appendix B). The November 12, 1997, average saturated thickness was 4.66 feet, while the June 3, 2002 (for May 1998), average saturated thickness was 6.29 feet. Therefore, the groundwater outflow for November 12, 1997, would be:

\[ Q_{\text{out}} = K_iA \]
\[ = \frac{4.5 \text{ feet}}{\text{day}} \times 0.028 \times (4.66 \text{ feet} \times 1,143.48 \text{ feet}) \]
\[ = 670 \text{ feet}^3/\text{day} \times \frac{30 \text{ days}}{\text{month}} \]
\[ = 20,100 \text{ feet}^3/\text{month} \]

Performing the same calculation for May 1998 yields approximately 41,800 cubic feet per month for groundwater outflow.

The conceptual model for this thesis does not allow for groundwater inflow since the two streamline boundaries are no-flow, and the Pine Creek drain cannot add water to the system. Loftis (1999) used the same boundary conditions, and concluded that flux (wells) should be added to southwest streamline to calibrate the model better for future studies. The lack of geologic features or an obvious groundwater divide practically necessitated the use of streamlines as boundaries; however, the water budget calculations assume groundwater inflow into the system, and assume a cross-sectional area for the groundwater inflow.

For purposes of the water budget, the equivalent of 400 feet [out of the total 1,421 feet of stream line boundaries, as shown in Figure 4-6] will accept groundwater inflow; however, the MODFLOW model will not include flux across the streamlines, despite Loftis’s recommendation. With the 400 feet of boundary accepting groundwater inflow for the water budget calculation, the groundwater inflow total is calculated for November 1997:

\[ Q_{\text{in}} = K_iA \]
\[ = \frac{4.5 \text{ feet}}{\text{day}} \times 0.028 \times (4.66 \text{ feet} \times 400 \text{ feet}) \]
\[ = 235 \text{ feet}^3/\text{day} \times \frac{30 \text{ days}}{\text{month}} \]
\[ = 7,000 \text{ feet}^3/\text{month} \]

Similarly, using 0.043 for the hydraulic gradient and 6.29 feet for the average saturated thickness, the May 1998 groundwater inflow would be approximately 14,600 cubic feet per month.

**GROUNDWATER INTERCEPTION TRENCH**

The groundwater interception trench at the Oneida Tie Yard Site began operation in 1991, but was in ill repair for some time until it was fixed and turned back on in February 1998 (refer to Section 3.1.3). Monthly flow data are available from ARCADIS G&M (refer to Table A-2 in Appendix A). The trench
was not operating during November 1997, making \( Q_T = 0 \). Table A-2 shows that the \( Q_T = 60,001 \) gallons (8,021 cubic feet) during May 1998.

**Change in Water Storage**

The change in water storage in an unconfined aquifer can be defined as (Spitz and Moreno, 1996):

\[
\Delta S = A \times S_y \times (h(t+\Delta t)-h(t))
\]

where:
- \( \Delta S = \) change in water storage over time period \( \Delta t \) [L^3/T];
- \( A = \) area of site [L^2];
- \( S_y = \) specific yield of unconfined aquifer;
- \( (h(t+\Delta t)-h(t)) = \) head difference over time period \( \Delta t \) [L];

The area of the site is 403,180 square feet (Figure 4-6). The specific yield is the storage term for unconfined aquifers. Specific yield values typically range from 0.1 to 0.3, depending on the soil type (Viessman and Lewis, 1996). Sandy clays, the prevalent soil type at the Oneida Tie Yard Site, typically have a specific yield of 0.1 to 0.2. For the water budget, a specific yield of 0.1 will be assumed.

The head difference over the time period of one month is determined for November 1997 and May 1998 by averaging the head changes from the monitoring wells and piezometers (Appendix B). The average change in head over the site for November 1997 was 1.37 ft. The average change in head over the site for May 1998 was –0.81 feet. Therefore, the change in water storage for the month of November 1997 was:

\[
\Delta S = 403,180 \text{ feet}^2 \times 0.1 \times 1.37 \text{ feet} \\
= 55,000 \text{ feet}^3
\]

Similarly, for the month of May 1998, \( \Delta S \approx -33,000 \) cubic feet.

**Evapotranspiration**

ET can be estimated using various equations and relationships, as described in Section 2.3. For the water budget, the ET will actually be the unknown, rather than \( \Delta S \). Rearranging Equation 4-17 to solve for the November 1997 ET:

\[
P + G_i = R + G_o + Q_T + ET + \Delta S, \text{ or} \\
ET = P + G_i - R - G_o - Q_T - \Delta S \\
= 67,000 \text{ ft}^3 + 70,100 \text{ ft}^3 - 6,700 \text{ ft}^3 - 7,000 \text{ ft}^3 - \Delta S \\
= 113,000 \text{ ft}^3 \text{ for the November 1997 time period}
\]

For the May 1998 period, the calculated ET is 254,000 cubic feet.
WATER BUDGET RESULTS

After the various assumptions and calculations described above, the individual parameters for Equation 4-18 were determined as shown in Table 4-3.

<table>
<thead>
<tr>
<th>Water Budget Component</th>
<th>November 1997</th>
<th>May 1998</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rainfall</td>
<td>P 67,000 cubic feet per month</td>
<td>260,000 cubic feet per month</td>
</tr>
<tr>
<td>Runoff</td>
<td>R 6,700 cubic feet per month</td>
<td>26,000 cubic feet per month</td>
</tr>
<tr>
<td>Groundwater</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydraulic Conductivity</td>
<td>K 4.5 feet per day</td>
<td>4.5 feet per day</td>
</tr>
<tr>
<td>Hydraulic Gradient</td>
<td>i 0.028</td>
<td>0.043</td>
</tr>
<tr>
<td>Saturated Thickness</td>
<td>Q_{in} 4.66 feet</td>
<td>6.29 feet</td>
</tr>
<tr>
<td>Inflow</td>
<td>Q_{in} 20,100 cubic feet per month</td>
<td>41,800 cubic feet per month</td>
</tr>
<tr>
<td>Outflow</td>
<td>Q_{out} 7,000 cubic feet per month</td>
<td>14,600 cubic feet per month</td>
</tr>
<tr>
<td>Groundwater Interception</td>
<td>Q_{T} 0</td>
<td>8,021 cubic feet per month</td>
</tr>
<tr>
<td>Trench</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Change in Water Storage</td>
<td>∆S 55,000 cubic feet per month</td>
<td>33,000 cubic feet per month</td>
</tr>
<tr>
<td>Evapotranspiration</td>
<td>ET 102,000 cubic feet per month</td>
<td>113,800 cubic feet per month</td>
</tr>
</tbody>
</table>

Solving for ET with Equation 4-18 gave approximately 102,200 cubic feet for the November 1997 period and approximately 113,800 cubic feet for the May 1998 period. This possibly shows that in the active season (and when more precipitation was occurring) the poplar trees doubled the ET at the site (when they had been growing for a year). Not only does precipitation typically increase in the spring time, but ET rates have the opportunity to increase due to the additional subsequent recharge.

4.3.2.4 Steady-State Model – Pre-Remediation

CONCEPTUAL MODEL

The first MODFLOW design begins with creating a steady-state groundwater model that will simulate the site before the trees were active and when the trench was not in operation. This will allow for a more direct approach to calibration of the site-specific model parameters of hydraulic conductivity and recharge. Figure 4-10 depicts the conceptual model before it is converted to the MODFLOW three-dimensional, single-layer grid. An areal drain, northwest of poplar tree rows 6-8, was added to the conceptual model in an attempt to simulate the wooded area shown in Figure 3-9, where groundwater discharge was observed when the water table was near the land surface. The drains are transferred to MODFLOW through the Local Sources/Sinks Coverage.
Figure 4-10: Conceptual Image From Map Module
[for November 1997 (No Trees and No Trench)]

Figure 4-11 shows different polygons representing zones of different hydraulic conductivity and recharge. For calibration purposes, each zone is numbered so that it can be referenced. The boundaries were based on one or more of the following: bedrock and surface elevations, known soil types based on soil borings (presented in Section 3), the location of the poplar trees, the location of the trench, and the location of the coal layer.
The polygons in Figure 4-11 are used in the Hydraulic Conductivity [layer attributes] Coverage and the Recharge [areal attributes] Coverage. An “observation” coverage is created in the Map Module to enter the piezometer and monitoring well water level elevations for November 12, 1997, into the model. This will allow GMS to compare each MODFLOW solution set to the observed values in the Observation Coverage, and report a mean error (ME), mean absolute error (MAE), and root mean squared error (RMSE). The mean, mean absolute, and root mean squared errors are common statistical comparisons used in groundwater modeling to quantify the goodness of fit of the computed heads to the observed heads:

\[
\text{Mean Error} = \frac{1}{n} \sum_{i=1}^{n} (h_{\text{observed}} - h_{\text{computed}}) \tag{4-19}
\]

\[
\text{Mean Absolute Error} = \frac{1}{n} \sum_{i=1}^{n} \left| (h_{\text{observed}} - h_{\text{computed}}) \right| \tag{4-20}
\]

\[
\text{Root Mean Squared Error} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (h_{\text{observed}} - h_{\text{computed}})^2} \tag{4-21}
\]
MODFLOW GRID

The conceptual model is then converted to the MODFLOW grid. The one-layer MODFLOW grid, shown in Figure 4-12, consists of a 100 x 100 node grid, overlaid on the conceptual model image. Only cells within the model boundary are activated in MODFLOW (that is, 9,536 cells).

Figure 4-12: MODFLOW Grid

After converting the conceptual model to a three-dimensional grid, and subsequently transferring the information to the MODFLOW input files, bedrock and land surface elevations must be interpolated.
Using survey and field data, scatter point files are created for the bedrock and land surface elevations. The scatter point files are imported and interpolated to the MODFLOW layer using the X,Y-Scatter Point Module in GMS (using the inverse difference weighted interpolation method). Both Loftis (1999) and Panhorst (2000) noted the absence of data on the northwestern portion of the site, and both assumed a uniform bedrock elevation for this part of the site for their models. For the model design in this thesis, the modeler created “imaginary” points where elevation data was created based on assumptions and field observations. This allowed for more natural bedrock and surface contours. Figures 4-13 and 4-14 show the interpolated bedrock and land surface elevation contours, respectively.

Figure 4-13: Bedrock Elevation Contours
4.0 MODELING THE SITE

CALIBRATION

Calibration begins with running MODFLOW for the first time with the initial input values. The statistical comparisons are examined, and then various parameters are adjusted to try to make the computed heads match the observed heads. This is done with the following general relationships in mind: increasing the recharge will increase the computed heads, increasing the hydraulic conductivity will lower the computed heads, and increasing the drain conductance will lower nearby computed heads.

Table 4-4 presents the calibration steps and shows the progression to the solution parameters that resulted in satisfactory statistical errors. Table 4-5 shows the results of the error analysis for each model run. Note that for the calibrations in this thesis, the “R” represents recharge to the aquifer, not total rainfall.
Table 4-4: Calibration data for November 12, 1997, Solution
(Steady-State, No Trees, No Trench)

<table>
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<th>4</th>
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R = Recharge (ft/d);
K = Hydraulic Conductivity (ft/d);
(refer to Figure 4-11 for Area locations)
Table 4-5: Error Analysis for Calibration Model Runs
November 12, 1997, Solution
(Steady-State, No Trees, No Trench)

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<tr>
<th>Parameter</th>
<th>Area</th>
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<th>Areal Drain</th>
<th>Mean Error</th>
<th>Mean Absolute Error</th>
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</tr>
</tbody>
</table>

C = Conductance (ft^2/d/ft^2 or ft/d/ft)
(refer to Figure 4-11 for Area locations)

Figure 4-15 shows the calibrated water level contours (that is, the water level contours for Model Run 10). Included in the figure are the observation calibration results, showing the amount of error between the observed and computed heads. Also included are error plots and error analysis results provided by GMS. All MODFLOW input and output data are presented in Appendix C.

The “Error versus Simulation” error analysis plot shows how the ME, MAE, and RMSE [me, mae, and rme, respectively, in the modflow plot legend in Figure 4-15] typically move towards zero with each consecutive model run. This is a result of adjusting the recharge and hydraulic conductivity for different areas, as well as changing the conductance for the drains. For example, to increase the computed head to match an observed head at an observation well, one increases the recharge and/or decreases the hydraulic conductivity in the area that the observation well is located. Then the error analysis reveals whether the residual increases or decreases.

The water budget summary [for the calibrated Model Run 10] provided in the MODFLOW output file (presented in Table 4-6) shows that approximately 640 cubic feet per day of water entered the site through recharge while the same amount left the site via the drains. The computed output flow rate through the drain (Pine Creek) is similar to the 670 cubic feet per day (20,100 cubic feet per month groundwater leaving the site) calculated earlier in Section 4.3.2.3.
Table 4-6: November 12, 1997, Water Budget Summary from MODFLOW Model Run 10 Output File

<table>
<thead>
<tr>
<th>November 12, 1997</th>
<th>In (cubic feet per day):</th>
<th>Out (cubic feet per day):</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant Head</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Drains</td>
<td>0</td>
<td>638.8331</td>
</tr>
<tr>
<td>Recharge</td>
<td>638.9019</td>
<td>0</td>
</tr>
<tr>
<td>Total</td>
<td>638.9019</td>
<td>638.8331</td>
</tr>
<tr>
<td>In – Out</td>
<td></td>
<td>0.068848</td>
</tr>
<tr>
<td>Percent Discrepancy</td>
<td></td>
<td>0.01</td>
</tr>
</tbody>
</table>

Figure 4-15: Calibrated Steady-State Model for November 12, 1997 (Steady-State, No trees, No trench)
UNIQUENESS OF SOLUTION

After the model is calibrated, a non-unique solution analysis is performed. The hydraulic conductivity and recharge input parameters are varied, but the ratio between the two is kept the same. For example, Area 1 (refer to Figure 4-12) had a calibrated hydraulic conductivity (K) of 4 feet per day and a recharge (R) of 0.001 feet per day, giving a ratio of \( \frac{K}{R} = \frac{4}{0.0001} = 40,000 \). For the non-unique solution check, this ratio will remain constant while the hydraulic conductivity and recharge values are varied for Area 1. After Area 1 is examined, Area 7 will also be examined. Table 4-7 summarizes the non-unique solution analysis.

Table 4-7 shows that varying the K and R (but keeping the K/R ratio the same) in Area 1 did not have a significant effect on the rest of the model. This is likely because Area 1 is at the upgradient end of the model in an area that only affects one or two piezometers directly. Changing the K and R values for Area 7, however, demonstrated a significant effect on the rest of the model, causing the RMSE statistical comparison value to vary from 0.92 to 7.39. This suggests that the calibrated model is a unique solution, and cannot be replicated using different hydraulic conductivities or recharges.

<table>
<thead>
<tr>
<th>Analysis 1</th>
<th>Area 1</th>
<th>Mean Error</th>
<th>Mean Absolute Error</th>
<th>Root Mean Squared Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>R (ft/d)</td>
<td>K (ft/d)</td>
<td></td>
</tr>
<tr>
<td><strong>INITIAL MODEL</strong></td>
<td>0.0001</td>
<td>4</td>
<td>0.002</td>
<td>0.8</td>
</tr>
<tr>
<td>Check 1</td>
<td>2.50E-07</td>
<td>0.01</td>
<td>0.1</td>
<td>0.43</td>
</tr>
<tr>
<td>Check 2</td>
<td>2.50E-06</td>
<td>0.1</td>
<td>0.09</td>
<td>0.44</td>
</tr>
<tr>
<td>Check 3</td>
<td>2.50E-05</td>
<td>1</td>
<td>0.07</td>
<td>0.48</td>
</tr>
<tr>
<td>Check 4</td>
<td>2.50E-04</td>
<td>10</td>
<td>0.09</td>
<td>0.56</td>
</tr>
<tr>
<td>Check 5</td>
<td>2.50E-03</td>
<td>100</td>
<td>0.59</td>
<td>0.8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Analysis 2</th>
<th>Area 7</th>
<th>Mean Error</th>
<th>Mean Absolute Error</th>
<th>Root Mean Squared Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>R (ft/d)</td>
<td>K (ft/d)</td>
<td></td>
</tr>
<tr>
<td><strong>INITIAL MODEL</strong></td>
<td>0.004</td>
<td>6</td>
<td>0.30</td>
<td>0.60</td>
</tr>
<tr>
<td>Check 1</td>
<td>6.67E-06</td>
<td>0.01</td>
<td>7.09</td>
<td>7.09</td>
</tr>
<tr>
<td>Check 2</td>
<td>6.67E-05</td>
<td>0.1</td>
<td>5.7</td>
<td>5.7</td>
</tr>
<tr>
<td>Check 3</td>
<td>6.67E-04</td>
<td>1</td>
<td>1.81</td>
<td>1.83</td>
</tr>
<tr>
<td>Check 4</td>
<td>6.67E-03</td>
<td>10</td>
<td>0.54</td>
<td>0.77</td>
</tr>
<tr>
<td>Check 5</td>
<td>6.67E-02</td>
<td>100</td>
<td>3.15</td>
<td>3.15</td>
</tr>
</tbody>
</table>

R = Recharge  
K = Hydraulic Conductivity
SENSITIVITY ANALYSIS

A sensitivity analysis is performed to see how varying the values of the hydraulic conductivity and recharge would affect the model. This analysis is similar to the non-unique solution check, except that the goal is not to show a unique solution set, but to show how varying the input parameters can affect the MODFLOW output, and to what degree. A sensitivity index can be computed (Spitz and Moreno, 1996):

\[
S = \frac{|dP|}{P} \tag{4-22}
\]

where:
- \( S \) = normalized sensitivity index which is a measure of the average change in the predicted variable per fractional change in the input parameter;
- \(|dP|\) = difference in predicted variable, at one or more key locations, between the base case and the sensitivity case;
- \( dP \) = change in input parameter value; and
- \( P \) = initial input parameter value.

The sensitivity index can be developed further in terms of the RMSE as the predicted variable (Spitz and Moreno, 1996; Widdowson, 1997):

\[
X_n = \left| \frac{\partial \text{RMSE}}{\partial a_n} \right| = \left| \frac{\text{RMSE}(a_n + \Delta a_n) - \text{RMSE}(a_n)}{\Delta a_n / a_n} \right| \quad \tag{4-23}
\]

where:
- \( X_n \) = normalized global sensitivity coefficient for the \( n^{th} \) parameter;
- \( \text{RMSE}(a_n) \) = RMSE for the calibrated model;
- \( \text{RMSE}(a_n + \Delta a_n) \) = RMSE for the perturbed-parameter simulation;
- \( \Delta a_n \) = amount of disturbance in the \( n^{th} \) parameter; and
- \( a_n \) = \( n^{th} \) parameter value in the calibrated model.

The higher the normalized coefficient, the more sensitive the model is to the change in the input parameter. Using Equation 4-27, the input parameters (hydraulic conductivity, drain conductance, and recharge) were adjusted to assess the effect on the RMSE. Just as for the non-unique solution check, only certain areas are investigated. For the sensitivity analysis (refer to Table 4-8), input parameters for Area 7 were varied as well the drain conductance.

For the first check, the hydraulic conductivity was changed in Area 7 from 6 feet per day in the initial model to 0.01 feet per day (that is, \( \Delta a_n = -5.99 \)). Accordingly, the Sensitivity coefficient was calculated as:

\[
X_n = \left| \frac{\text{RMSE}(a_n + \Delta a_n) - \text{RMSE}(a_n)}{\Delta a_n / a_n} \right| = 10.49 \quad \tag{4-24}
\]
Table 4-8: Sensitivity Analysis of Area 7

<table>
<thead>
<tr>
<th>Area 7</th>
<th>Recharge (ft/d)</th>
<th>Hydraulic Conductivity (ft/d)</th>
<th>Pine Creek Drain Conductance (ft²/d/ft)</th>
<th>Δa_n</th>
<th>Mean Error</th>
<th>Mean Absolute Error</th>
<th>Root Mean Squared Error</th>
<th>Sensitivity Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Model</td>
<td>0.004</td>
<td>6</td>
<td>4</td>
<td>0.30</td>
<td>0.60</td>
<td>0.69</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Perturbed Parameter = Hydraulic Conductivity</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Check 1</td>
<td>0.004</td>
<td>0.01</td>
<td>4</td>
<td>-5.99</td>
<td>10.15</td>
<td>10.15</td>
<td>11.17</td>
<td>10.49</td>
</tr>
<tr>
<td>Check 2</td>
<td>0.004</td>
<td>0.1</td>
<td>4</td>
<td>-5.9</td>
<td>7.33</td>
<td>7.33</td>
<td>7.62</td>
<td>7.04</td>
</tr>
<tr>
<td>Check 3</td>
<td>0.004</td>
<td>1</td>
<td>4</td>
<td>-5</td>
<td>2.34</td>
<td>2.34</td>
<td>2.54</td>
<td>2.22</td>
</tr>
<tr>
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<td>0.004</td>
<td>10</td>
<td>4</td>
<td>4</td>
<td>-0.03</td>
<td>0.49</td>
<td>0.59</td>
<td>0.15</td>
</tr>
<tr>
<td>Check 5</td>
<td>0.004</td>
<td>100</td>
<td>4</td>
<td>94</td>
<td>-0.97</td>
<td>0.99</td>
<td>1.12</td>
<td>0.03</td>
</tr>
<tr>
<td>Perturbed Parameter = Recharge</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Check 6</td>
<td>0.0004</td>
<td>6</td>
<td>4</td>
<td>-0.0036</td>
<td>-0.24</td>
<td>0.5</td>
<td>0.61</td>
<td>0.09</td>
</tr>
<tr>
<td>Check 7</td>
<td>0.04</td>
<td>6</td>
<td>4</td>
<td>0.036</td>
<td>4.36</td>
<td>4.36</td>
<td>4.5</td>
<td>0.42</td>
</tr>
<tr>
<td>Check 8</td>
<td>0.4</td>
<td>6</td>
<td>4</td>
<td>0.396</td>
<td>20.82</td>
<td>20.82</td>
<td>21.23</td>
<td>0.21</td>
</tr>
<tr>
<td>Perturbed Parameter = Pine Creek Drain Conductance</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Check 9</td>
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<td>6</td>
<td>0.1</td>
<td>-3.9</td>
<td>5.54</td>
<td>5.54</td>
<td>5.73</td>
<td>5.17</td>
</tr>
<tr>
<td>Check 10</td>
<td>0.004</td>
<td>6</td>
<td>1</td>
<td>-3</td>
<td>0.62</td>
<td>0.78</td>
<td>0.9</td>
<td>0.28</td>
</tr>
<tr>
<td>Check 11</td>
<td>0.004</td>
<td>6</td>
<td>10</td>
<td>6</td>
<td>0.19</td>
<td>0.54</td>
<td>0.65</td>
<td>0.029</td>
</tr>
<tr>
<td>Check 12</td>
<td>0.004</td>
<td>6</td>
<td>100</td>
<td>96</td>
<td>0.14</td>
<td>0.52</td>
<td>0.63</td>
<td>0.003</td>
</tr>
</tbody>
</table>

Note: All Δa_n’s are the difference between the perturbed parameter and the respective initial model value.

Table 4-8 suggests that the model was most sensitive to changes in hydraulic conductivity and comparably less sensitive to changes in recharge and conductance. Equation 4-10 describes groundwater flow under non-equilibrium conditions in a heterogeneous and anisotropic aquifer.

\[
\frac{\partial}{\partial x} \left( K_x h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y h \frac{\partial h}{\partial y} \right) = S_y \frac{\partial h}{\partial t} - R - Q
\]  

(4-10)

where:  
\( K_x, K_y \) = components of the hydraulic conductivity in two dimensions [L/T];  
\( S_y \) = specific yield;  
\( R \) = recharge rate [L/T]; and  
\( Q \) = source or sink term [L/T].

The hydraulic conductivity, \( K \), is part of the governing equation, while the recharge, \( R \), is just part of the boundary, or stress on the system. For a steady-state model run, the change in head with time differential becomes zero, making the equation for head at any point equal to the boundary, \( R \); however, \( K \) directly affects how much groundwater a cell can transmit. Varying \( R \) for a cell can only affect surrounding cells depending on \( K \). Thus, the statistical error of any model run would rely more on \( K \) than \( R \).
4.3.2.5 Steady-State Model With the Trench in Operation

CONCEPTUAL MODEL AND MODFLOW GRID

Adding in the operating groundwater interception trench added to the model’s complexity. The model is calibrated with the December 1998 gauging data, since the trees were mostly inactive while the trench was operating during this month. The conceptual model from Section 4.3.2.4 is modified by incorporating the groundwater interception trench as a drain (Figure 4-16).

![Figure 4-16: Conceptual Image From Map Module (for December 1998 [Steady-State, No Trees, and Operating Trench])](image)

The MODFLOW grid is the same as in Section 4.3.2.4, except that the trench drain cells are added in. The interception trench is initially given a drain conductance of 50 ft²/d/ft and an elevation of 1422 feet. The elevation is based on the bedrock elevations around the trench and the background information found in Section 3.

CALIBRATION

MODFLOW calculates a water budget giving the total drain outflow for all the drains in the model, but not individually. The individual groundwater interception trench output is determined by selecting the interception trench drain arc in the Local Sources/Sinks Coverage in the Map Module in GMS (that is, the flux out will appear in the information bar at the bottom of the screen when the arc is selected in the Local
Source/Sink Coverage). The total water out of the site through each individual drain can be determined this way. This allows observation well data and trench flux to be utilized for the calibration. ARCADIS G&M and VT Records show that the volume of fluids collected by the interception trench in December 1998 totaled approximately 241,300 gallons, or approximately 32,200 cubic feet. This corresponds to a flux of approximately 1,000 cubic feet per day (32,200 cubic feet / 31 days). A new Observation Coverage was created with the water level elevations for December 1998.

Table 4-9 presents the calibration steps and shows the progression to the solution parameters that resulted in satisfactory statistical errors. Note that the trench output flux is also monitored, but was not included in statistical calculations for solution error. Table 4-10 presents the results of the error analysis for each model run. Figure 4-17 shows the calibrated water level contours with the interception trench in operation. Again, the observation well errors are displayed, as well as the error plots and summary.

**Table 4-9: Calibration data for December 10, 1998, Solution (Steady-State, No Trees, and Operating Trench)**

<table>
<thead>
<tr>
<th>Area</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
<td>R</td>
<td>K</td>
<td>R</td>
<td>K</td>
<td>R</td>
</tr>
<tr>
<td>1</td>
<td>0.001</td>
<td>4</td>
<td>0.002</td>
<td>0.8</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
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<td>4</td>
<td>0.003</td>
<td>0.8</td>
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</tr>
<tr>
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<tr>
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<table>
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<th>9</th>
<th>10</th>
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<tbody>
<tr>
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<td>R</td>
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<td>R</td>
<td>K</td>
<td>R</td>
</tr>
<tr>
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</tr>
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<td>0.005</td>
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<td>0.01</td>
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<td>5</td>
<td>0.01</td>
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<td>10</td>
<td>0.02</td>
<td>5</td>
<td>0.01</td>
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<tr>
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<td>10</td>
<td>0.02</td>
<td>5</td>
<td>0.01</td>
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<td>9</td>
<td>0.002</td>
<td>10</td>
<td>0.02</td>
<td>5</td>
<td>0.01</td>
</tr>
</tbody>
</table>

R = Recharge (ft/d);
K = Hydraulic Conductivity (ft/d);
(refer to Figure 4-11 for Area locations)
Table 4-10: Error Analysis For Calibration Model Runs
December 10, 1998, Solution
(Steady-State, No Trees, and Operating Trench)

<table>
<thead>
<tr>
<th>Model Run Number</th>
<th>Parameter</th>
<th>Pine Creek Drain</th>
<th>Areal Drain</th>
<th>Intercept Trench</th>
<th>Trench Elevation (feet)</th>
<th>Trench Output (cubic feet per day)</th>
<th>Mean Error</th>
<th>Mean Absolute Error</th>
<th>Root Mean Squared Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
<td>4</td>
<td>1</td>
<td>50</td>
<td>1,422</td>
<td>519</td>
<td>-1.63</td>
<td>1.68</td>
<td>1.90</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>1</td>
<td>100</td>
<td>1,423</td>
<td>616</td>
<td>-0.55</td>
<td>0.91</td>
<td>1.15</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>1</td>
<td>100</td>
<td>1,423</td>
<td>573</td>
<td>-0.06</td>
<td>0.88</td>
<td>1.06</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>1</td>
<td>100</td>
<td>1,423</td>
<td>719</td>
<td>-0.20</td>
<td>0.84</td>
<td>1.00</td>
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</tr>
<tr>
<td>5</td>
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<td>1</td>
<td>100</td>
<td>1,423</td>
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<td>0.97</td>
<td>1.22</td>
<td>1.46</td>
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<td>4</td>
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<td>100</td>
<td>1,423</td>
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<td>1.27</td>
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<td>1,423</td>
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<td>0.02</td>
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<td>1,423</td>
<td>1,207</td>
<td>0.15</td>
<td>0.76</td>
<td>0.93</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>4</td>
<td>1</td>
<td>100</td>
<td>1,423</td>
<td>1,188</td>
<td>0.15</td>
<td>0.76</td>
<td>0.93</td>
<td></td>
</tr>
</tbody>
</table>

C = Conductance (ft²/d/ft² or ft²/d/ft)

(refer to Figure 4-11 for Area locations)

Figure 4-17: Calibrated Steady-State Model for December 10, 1998
(Steady-State, No Trees, Operating Trench)
The R and K parameters were varied to minimize the RMSE. The final model run (that is, Model Run 9) had an RMSE of 0.93. This steady-state calibration with the trench in operation proved slightly more complex. The majority of the model domain is not sensitive to drain conductance; however, the observation wells near a drain, such as P-9 and P-10 near the interception trench, did prove to be most sensitive to the drain conductance, as well as the recharge in Area 7. The groundwater contours in Figure 4-17 show how the active groundwater interception trench captures groundwater moving towards the creek under steady-state conditions.

The water budget summary (Table 4-11) from the MODFLOW output file from Model Run 9 shows that approximately 1,874 cubic feet per day of water left the site through the drains. Manually clicking on each drain while the Local Sources/Sinks Coverage is active allows the determination of the outflow through the interception trench drain, only (1,188 cubic feet). This trench output compared well with the 1,000 cubic feet per day estimation for the month of December 1998. The results also shows that approximately 1,874 cubic feet per day entered the site through recharge, while virtually the same amount left the site via the drains (that is, Pine Creek drain, the areal groundwater seep drain, and the groundwater interception trench drain).

<table>
<thead>
<tr>
<th>December 10, 1998</th>
<th>In (cubic feet per day):</th>
<th>Out (cubic feet per day):</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant Head</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Drains</td>
<td>0</td>
<td>1,873.5737</td>
</tr>
<tr>
<td>Recharge</td>
<td>1,874.3440</td>
<td>0</td>
</tr>
<tr>
<td>Total</td>
<td>1,874.3440</td>
<td>1,873.5737</td>
</tr>
<tr>
<td>In – Out</td>
<td>0.7703</td>
<td></td>
</tr>
<tr>
<td>Percent Discrepancy</td>
<td>0.04</td>
<td></td>
</tr>
</tbody>
</table>

4.3.2.6 Transient Model with Active Poplar Trees and Operating Trench

CONCEPTUAL MODEL AND MODFLOW GRID FOR TRANSIENT MODELS

The final step of the model design was simulating the transpiration of groundwater by the poplar trees. This is accomplished by using the ET Package in MODFLOW to simulate transient groundwater data collected in year 2000. This approach involves two steps: (1) modeling water level data during the winter and (2) modeling water level data during the summer with both the active poplar trees and the operating interception trench.

During the year 2000, continuous water levels were collected (via pressure transducers) from piezometers P-4, P-6, and P-7, as well as monitoring well MW-6. The transducer data from P-4, P-6, P-7, and MW-6 were utilized to calibrate the model (refer to Figure D-1 in Appendix D for transducer data from
Panhorst 2000). Subsequently, only four observation wells, at most, could be used for the calibration. This limits the validity of the model, especially in the northwestern portion of the site, as compared to the earlier steady-state model calibrations in this thesis. Figure D-1 also shows the daily rainfall totals at the site as determined from a nearby National Oceanic and Atmospheric Administration (NOAA) weather station (Panhorst 2000).

Figure 4-18a shows the conceptual model for both the precursory steady-state calibration (to get the starting heads for the transient calibration) and the transient calibration. The ET Coverage coincides with the poplar tree area – the ET Coverage will be explained further after the ET rates are calibrated later in this thesis. Figure 4-18a shows the following modifications to the area assignments in the model (Figure 4-18b shows new Areas more clearly): (1) Area 2 now includes observation well MW-6; and (2) The border between Areas 6 and 7 is changed in order to split Area 7 into new Areas 7 and 11. The modification to Area 2 allowed MW-6 to have a different recharge rate than P-4, P-6, and P-7 for the more intricate transient calibrations (since MW-6 is just outside the poplar tree vegetative cover, based on field observations). Splitting Area 7 into new Areas 7 and 11 allowed P-4, P-6, and MW-6 to be influenced by different recharge rates when the poplar trees are added into the model.

![Figure 4-18a: Conceptual Image From Map Module](image)

[Steady-State and/or Transient, Active and/or Not Active Trees, and Operating Trench]
INITIAL TRANSIENT CALIBRATION (NO EVAPOTRANSPIRATION)

The first data set used for the transient calibration is February 2000, when the trees were assumed to be dormant and rainfall data and transducer data are available. This initial step is needed to calibrate the model to groundwater recession in response to a recharge event and determine specific yield and variation in recharge rates by area. Figure 4-19 shows a close-up of Figure D-1 (from Panhorst 2000), showing more detail of the February 2000 precipitation events. The February 14, 2000, precipitation event was examined to investigate the groundwater recession in P-4, P-6, and MW-6 after the event (that is, with no active poplar trees contributing ET), as this is a precipitation event where there is an exceptional amount of rainfall followed by more than one day of no rainfall.
**Figure 4-19: February 2000 Transducer and Rainfall Data**

**Precursory Steady-State Calibration**

A precursory steady-state calibration is performed to determine starting heads for the transient calibration. The water levels from 10:00 p.m. on February 13, 2000 (just before the February 14, 2000, rainfall event), were entered into the observation coverage for calibrating the steady-state model. For both the steady-state and transient models, the known trench output of 193,910 gallons for the month of February 2000 was divided up evenly based on the time step and used to calibrate the model by comparing model output at the trench to these values.

Because the three observation wells and the groundwater interception trench yield the only data used to calibrate the model, the validity of the calibration is limited mainly to area in the phytoremediation system; however, this limitation does not conflict with the objectives of this thesis.

The calibrated precursory steady-state water level contours are presented in Figure 4-20. The calibrated trench output flux of 918 cubic feet per day compared well to the target steady-state flux of 894 cubic feet per day (193,910 gallons during February 2000 converts to approximately 894 cubic feet per day). The final calibration run yielded an RMSE of 0.46. The data associated with this calibration is presented in Appendix C.
TRANSIENT CALIBRATION
On February 14, 2000, approximately 0.75 inches of rain fell at the site. Recharge rates and specific yield were varied in each area until the transient computed water levels in P-4, P-6, and MW-6 most closely matched the observed values. The transient observed values were entered into the Observation Coverage. Data from observation wells P-4 and P-6 are only available in 2-hour increments, while MW-6 data are available in 15-minute increments. The rainfall event lasted approximately 16 hours, so a 16-hour stress period with eight time steps were followed by one no-recharge stress period. The time steps in the no-recharge stress period were 6 hours each in length, as this provided the best convergence.

Specific yields typically range from 0.1 to 0.4 (Anderson and Woessner, 1991). With such a small range of possible values, a preliminary specific yield of 0.25 was assigned to the entire grid [Panhorst (2000) determined a calibrated specific yield of 0.06]. The ET Package was inactive during this portion of the calibration. The solution set from the precursory steady-state calibration was used for the starting heads for this transient calibration of February 2000. Only recharge, specific yield, and the trench conductance were varied to calibrate this portion of the model. The hydraulic conductivities determined in the precursory steady-state calibration were not varied.
Figures 4-21 presents the water level contours at 12:00 p.m. on February 15, 2000, approximately 24 hours after the rainfall event ended. Associated data are included in Appendix C. The computed heads and the observed heads compare nicely for most of the time steps. The computed trench output of 3,174 cubic feet also compared well to the target trench output of 3,000 cubic feet for the transient period (converted from the observed monthly trench output).

The calibrated specific yield for the site ranged from 0.08 to 0.18, depending on the respective area. Lowering the specific yield to 0.08 in Area 5 allowed the groundwater rise (in response to the rainfall) and recession in P-4 and P-6 to most closely match the observed transducer data. The specific yield in Area 2 calibrated to 0.18 to match the MW-6 transducer data. Since specific yield (the effective porosity) is the water released per unit area of aquifer per unit decline in the water table, lowering the specific yield tends to shorten the wetting and drying times involved with the maximum storage and release of groundwater. In other words, when the specific yield was lowered, this typically allowed the water table to rise more quickly in response to rain, and subsequently, to recess faster when the recharge ended. Still, it proved difficult to make the water levels recess in P-4 and P-6 towards the end of the transient period, despite varying specific yield and recharge in Area 5 and surrounding areas. This is possibly due to a number of factors, including not accounting for possibly effectual ET in February 2000 in the model. Incorporating
the trees (that is, incorporating the ET Package) in the next transient calibration (refer to “Transient Calibration of ET” section, below) should allow for a better calibration of the groundwater recessions in P-4 and P-6.

The trench drain conductance was calibrated to 1.5 square feet per day per foot. This calibrated trench conductance proved to be lower than in the initial steady-state model runs. Since the trench has to be cleaned so frequently, this suggests that some of the finer silts and clays may be clogging the trench interface with the surrounding substrata. Also, the creosote NAPL likely tends to clog the interface, significantly lowering the conductance, and even the hydraulic conductivity in the surrounding substrata.

The recharge rates in each area were varied to simulate assumed rainfall intensities over time. These were estimated and were inherent to the transient calibration. This method was chosen since it would seemingly most closely match natural rainfall intensities during the respective rainfall event. This “random” approach influenced the rate of rise by having the higher rainfall intensity in the beginning, just as the transducer data shows the rise in the piezometers during this time. Figure 4-22 shows an example of how the transient recharge was input into one of the model areas.

![Figure 4-22: Transient Recharge Input](image)

Different recharge rate patterns were assigned to the areas at the site to provide the best calibration. All data associated with recharge are included in Appendix C.

**TRANSIENT CALIBRATION OF ET**

Figure 4-18a presented a view of the ET zones that were set up for the model based on an examination of the tree data in Appendix A, previous findings by Lawrence (2000), and field observations. Section 2.1.4
explained that Lawrence (2000) established that the root depths of the hybrid poplars at this site were approximately one-third of the total height of each of the respective trees. Therefore, the extinction depth of each zone was typically established by height (that is, one-third of the tree height) of the majority of the trees in each zone. Appendix A shows the tree heights for various months in 1998 and 1999 (from Lawrence 2000). The tree heights for summer 2000 were determined by adding 10 inches to the November 1999 heights. This would be the approximate expected overall growth of the trees during this time period according to Lawrence (2000). The calculated ET zone average root depths ranged from 2.7 – 8.0 feet. Within the coal layer (that is, Area 3), the ET extinction depth is approximately 2.5 feet. This corresponds to the average approximate depth to the coal layer at the site, keeping in mind that the poplar roots likely cannot penetrate the coal layer. The ET elevation is established by the most common land surface elevation in each ET zone. Note that transpiration is only simulated for the poplar trees and not the surrounding grassy areas. Also, note that any seasonal and/or diurnal ET cycles are ignored during this study (that is, the ET rates were all constant, rather than inputting transient ET rates). All input information for the ET Package may be found in Appendix C.

Figure 4-23: July 2000 Transducer and Rainfall Data

Figure 4-23 shows a close-up of Figure D-1 (from Panhorst 2000), showing more detail of the July 2000 precipitation events. The time of interest for the transient ET calibration was after the July 19, 2000, rainfall event, when there was eight days without precipitation at the site, so that the added effect of transpiration due to the poplar trees on the water levels can be determined. Note that the use of “ET” in
MODFLOW is a misnomer, since the model is actually calculating transpiration, only, or the groundwater removed from the model. It does not incorporate evaporation from the ground surface or from the foliage.

Once the initial ET rates and depths (that is, transpiration rates and depths) are chosen based on the above discussion, the transient calibration can begin. The recharge, transpiration rates, and transpiration extinction depths were varied during the calibration to best fit the observation data (that is, the groundwater rise and recession in P-4, P-6, P-7, and MW-6). The time period spans from 8:00 a.m. on July 19, 2000, through 8:00 p.m. on July 27, 2000.

**Precursory Steady-State Calibration**
A precursory steady-state calibration is performed to determine starting heads for the transient calibration. The water levels from 8:00 a.m. on July 19, 2000 (just before the July 19, 2000, rainfall event) were entered into the observation coverage for calibrating the steady-state model. For both the steady-state and transient models, the trench output of 48,610 gallons for the month of July 2000 was used for calibration (that is, 48,610 gallons per month was converted appropriately to the time step); however, this monthly total is likely erroneous since (1) it was taken early in the month on July 11, 2000, (2) the trench was just cleaned in June 2000, and (3) the trench flow meter recorded no flow from August 2000 through March 2001. Recall the previous explanation about clogging at the trench intake interface.

Figure 4-24 presents the calibrated precursory steady-state water level contours. The calibrated steady-state trench output was 289 cubic feet per day, just above the target steady-state trench output of 232 cubic feet per day. This is reasonable since the target flux is just an estimate of the flux that occurred on any given day based on the flow meter reading on July 11, 2000. The final calibration run yielded an MSE of 0.15. The data associated with this calibration is presented in Appendix C.

**Transient Calibration**
On July 19, 2000, approximately 0.42 inches of rain fell at the site over a 12-hour period from 8:00 a.m. to 8:00 p.m. Recharge was changed in each area until the transient computed water levels in P-4, P-6, P-7, and MW-6 most closely matched the observed values. The transient observed values were entered into the Observation Coverage. P-4, P-6, and P-7 data are only available in 2-hour increments, while MW-6 data are available in 15-minute increments. The rainfall event lasted approximately 12 hours, so a 12-hour stress period, with six time steps, was followed by eight 1-day no-recharge stress periods. The time steps in the no-recharge stress periods were changed to provide the best convergence. The specific yield for each area in the model was not varied from calibrated values determined during the February 2000 transient simulation (refer to Table 4-12 in this section for a summary of the calibrated specific yields).

The transpiration rates and extinction depths, recharge intensities, and the trench conductance were all varied to calibrate this portion of the model. The hydraulic conductivities determined in the precursory
steady-state calibration were preserved. The solution set from the precursory July 2000 steady-state calibration was used for the starting heads for this July 2000 transient calibration.

Figure 4-24: Calibrated Precursory Steady-State Model for July 2000
(Steady-State, Trees Active, Operating Trench)

Associated transient modeling input and output data are included in Appendix C. Table 4-12 presents the calibrated input parameters for the transient July 2000 model incorporating the poplar tree transpiration. Figure 4-25 presents one time step of the calibrated transient model incorporating transpiration. Water level contours at 10:00 a.m. on July 19, 2000, two hours after the rainfall event started, are presented in the figure. Figure 4-26 presents the water level contours at 8:00 p.m. on July 22, 2000, approximately 72 hours after the rainfall event ended. Additionally, Figure 4-25 displays ‘time step versus computed and observed heads’ graphs for MW-6 and P-4, while Figure 4-26 presents the graphs for P-6 and P-7. These graphs show the observed heads (with a plus or minus 0.5 foot confidence interval presented with highlighting) and the computed heads for each time step for the respective observation wells. Figure 4-27 presents a plot of the RMSEs for each time step in the calibrated July 2000 transient model.
Table 4-12: Calibration data for July 2000 Transient Solution
(Transien,t Active Poplar Trees, and Operating Trench)

<table>
<thead>
<tr>
<th>Area 1</th>
<th>Area 2</th>
<th>Area 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>R (ft/d)</td>
<td>0.01 – 0.9</td>
<td>R (ft/d)</td>
</tr>
<tr>
<td>K (ft/d)</td>
<td>6</td>
<td>K (ft/d)</td>
</tr>
<tr>
<td>Sy</td>
<td>0.08</td>
<td>Sy</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Area 4</th>
<th>Area 5</th>
<th>Area 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>R (ft/d)</td>
<td>0.01 – 0.9</td>
<td>R (ft/d)</td>
</tr>
<tr>
<td>K (ft/d)</td>
<td>3</td>
<td>K (ft/d)</td>
</tr>
<tr>
<td>Sy</td>
<td>0.15</td>
<td>Sy</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Area 7</th>
<th>Area 8</th>
<th>Area 9</th>
</tr>
</thead>
<tbody>
<tr>
<td>R (ft/d)</td>
<td>0.2 – 0.7</td>
<td>R (ft/d)</td>
</tr>
<tr>
<td>K (ft/d)</td>
<td>4</td>
<td>K (ft/d)</td>
</tr>
<tr>
<td>Sy</td>
<td>0.18</td>
<td>Sy</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Area 10</th>
<th>Area 11</th>
<th>Pine Creek</th>
<th>Areal Drain</th>
</tr>
</thead>
<tbody>
<tr>
<td>R (ft/d)</td>
<td>0.01 – 0.9</td>
<td>R (ft/d)</td>
<td>0.1 – 0.8</td>
</tr>
<tr>
<td>K (ft/d)</td>
<td>4</td>
<td>K (ft/d)</td>
<td>10</td>
</tr>
<tr>
<td>Sy</td>
<td>0.18</td>
<td>Sy</td>
<td>0.08</td>
</tr>
<tr>
<td>C (ft³/d/ft)</td>
<td>4</td>
<td>C (ft³/d/ft²)</td>
<td>1</td>
</tr>
</tbody>
</table>

**Interception Trench**

<table>
<thead>
<tr>
<th>Elevation</th>
<th>C (ft³/d/ft)</th>
<th>Target Total Flux over 8.5 day transient period</th>
<th>Computed Total Flux over 8.5 day transient period</th>
</tr>
</thead>
<tbody>
<tr>
<td>1424</td>
<td>1</td>
<td>2,000 cubic feet (15,000 gallons)</td>
<td>1,876 cubic feet (14,032 gallons)</td>
</tr>
</tbody>
</table>

**ET Package Input**

<table>
<thead>
<tr>
<th>Maximum ET Rate</th>
<th>ET Extinction Depth</th>
<th>ET Surface Elevation</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05 - 0.9 ft/d</td>
<td>2.5 - 8 ft</td>
<td>1430.5 - 1435.5 ft</td>
<td>0.16 - 0.33 (refer to Figure 4-27 and Appendix C)</td>
</tr>
</tbody>
</table>

ET = evapotranspiration (that is, transpiration for this model)
C = drain conductance  R = recharge  K = hydraulic conductivity
RMSE = root mean squared error  Sy = specific yield
(refer to Figure 4-11 for Area locations)
4.0 Modeling The Site

Figure 4-25: Calibrated Transient ET Model for July 19, 2000, at 10:00 a.m.

Figure 4-26: Calibrated Transient ET Model for July 22, 2000, at 8:00 p.m.


**Figure 4-27: RMSE for Calibrated Transient ET Model**
*(8:00 a.m. on July 19, 2000, through 8:00 p.m. on July 27, 2000)*

**DISCUSSION**

The water level contours in Figure 4-28 show the solution set for the final time step in the July 2000 transient model (that is, at 8:00 p.m. on July 27, 2000). ‘Time step versus computed and observed heads’ graphs are presented in the figure to show the observed heads (with a plus or minus 0.5 foot confidence interval presented with highlighting) and the computed heads for each time step for MW-6, P-4, P-6, and P-7. This provides a look at the piezometric surface eight days after a 0.41-inch rainfall event.

Comparing Figure 4-25 to Figures 4-26 and 4-28, it is clear that the trees did impact the groundwater flow at the site; however, it is not evident from this July 2000 transient model that the trees would completely contain a contaminant plume. Figure 4-28 also shows that the interception trench does not have the desired capture curve for the groundwater (to prevent contamination from migrating to Pine Creek).

The trench conductance did not significantly impact the transient model. The trench conductance was only varied slightly, mainly to match the target trench outflow for the time period. The various model runs produced varying trench outflows. The target outflow was determined from the July 11, 2000, oil/water separator flow meter reading; however, as previously mentioned, this data does not seem to be reliable. Regardless, a target outflow for the 204-hour simulation was approximated at 15,000 gallons (or approximately 2,000 cubic feet). The final calibrated model yielded a trench outflow that compared well to the target at just over 14,000 gallons (or 1,876 cubic feet over the time period).
Recall that the first stress period was divided into six 2-hour time steps. Each of following eight 1-day stress periods were divided into four 6-hour time steps to provide the best convergence. Figures 4-25, 4-26, and 4-28 result from the four 6-hour time step model run. The model did not prove to be sensitive to the choice of time step length and/or number. The recession curves stayed the same, but had either more or less data points depending on the time step chosen.

The model is inherently sensitive to the starting heads. The precursory steady-state solution set was precise by ‘steady-state’ statistical error standards (with an RMSE of 0.15); however, the transient model that followed tried to use head changes on the order of hundredths of a foot to calibrate. Therefore, if a starting head in an observation point were too high, by even 0.5 foot, the computed recession curve would never coincide with the observed curve (refer to the P-6 computed heads recession curve in Figure 4-26). Despite this extreme sensitivity, the model did show that it could simulate the recession, as can be seen in the ‘time step versus observed and computed heads’ graphs for P-4, P-6, P-7, and MW-6 (in Figures 4-25, 4-26, and 4-28).

Recharge certainly affected the groundwater rises, and depending on when the recharge ended (for this model, at the end of the first stress period), the groundwater recessions. One of the most valuable lessons of this research was that the known total rainfall does not directly translate to recharge. Instead, recharge is
dependant on many different site-specific [and often unknown] parameters. Further, it is used, perhaps even more than other input parameters, to allow the computed data to fit the observed data.

The ET rates (that is, the transpiration rates) would logically affect the water levels, but the ability of the trees to transpire groundwater depended mostly on the transpiration extinction depth (that is, the root depth). Using the initial transpiration extinction depths (calculated from an average of one-third the tree heights in each ET zone) did not impact the model at first, as the groundwater elevations were lower than expected in some of the ET zones. Therefore, the transpiration extinction depth values were generally increased. This seemed reasonable since the “one-third relationship” was determined by Lawrence (2000) with measurements from March and November 1999. Increasing the root depths closest to the observation wells allowed the groundwater recessions to be calibrated most effectively. Maximum transpiration depths in the calibrated model ranged from 2.5 feet, in the coal layer, to 8 feet, near the observation wells (refer to Table 4-12 and Appendix C).

Changing the transpiration rate within the ranges determined by Loftis (1999) and Panhorst (2000) (that is, 0.3 inches per day to 0.7 inches per day) did not impact the groundwater enough for the model to calibrate (that is, the groundwater did not recess enough in each observation well). Instead, transpiration rates ranging from 0.6 inches per day to 10 inches per day (that is, 0.05-0.9 foot per day) were utilized. The higher transpiration rates were assigned to the ET zones containing observation well P-4, while the lowest transpiration rate was required for the ET zone containing observation zone P-7. This was initially thought to be due to the closer proximity of P-7 to the groundwater interception trench (that is, perhaps the interception trench removed groundwater from the model cells close to P-7, so that a high transpiration rate in the respective ET zone was not required). By examining the water levels during the simulation, it was determined that the trees in the ET zone containing P-7 did not impact the groundwater, as the water levels were lower than the reasonably assumed extinction depth of over 5 feet. This is likely due, not only to the interception trench activity, but also to the transpiration occurring in surrounding ET zones, as well as the seemingly low storage capacity of the site (refer to Table 4-12 for calibrated specific yields).

The low end of the calibrated transpiration rates in the model domain occurred around P-7. The calibrated maximum transpiration rate for the ET zone containing P-7 (0.05 foot per day) actually corresponded to approximately 0.4 gallons per day per tree, or 1.4 liters per day per tree. This calculation resulted from converting the transpiration volumetric total out of the ET zone (approximately 24.7 cubic feet over the 8.5-day simulation, determined in GMS by selecting the ET zone with the ET Coverage active) by the approximate number of trees in the zone (approximately 60 trees, determined using the tree data in Appendix A):
4.0 Modeling the Site

\[
\text{Transpiration out of ET zone} = \frac{24.7 \text{ ft}^3 \times 7.48 \text{ gallons}}{8.5 \text{ days} \times 1 \text{ ft}^3} = 0.4 \text{ gallons per day per tree}\quad (4-25)
\]

Note that the referenced maximum transpiration rate for the ET zone is not used for the calculation of simulated individual tree transpiration rates. Recall that this maximum transpiration rate only occurs at the ET elevation, generally just below ground surface for this model. The groundwater at the site is typically below this elevation.

The high end of the calibrated transpiration rates in the model domain occurred around P-4. The maximum transpiration rate for the ET zone containing P-4 (0.9 foot per day), along with an ET extinction depth of 8 feet, caused an outflow (via transpiration) of approximately 119.9 cubic feet from the zone over the 8.5-day period (determined in GMS by selecting the ET zone with the ET Coverage active). This converts to approximately 5.3 gallons per day per tree, or 20 liters per day per tree, as shown below in Equation 4-26.

\[
\text{Transpiration out of ET zone} = \frac{119.9 \text{ ft}^3 \times 7.48 \text{ gallons}}{8.5 \text{ days} \times 1 \text{ ft}^3} = 5.3 \text{ gallons per day per tree}\quad (4-26)
\]

The transpiration rates calibrated in the model, and calculated in Equations 4-25 and 4-26, compare low to Ecolotree’s projection of 100 liters per day, although this projection assumes over five years of tree growth (refer to Section 2.1.5).

Loftis (1999) attempted to determine the steady-state minimum transpiration flux that would hydraulically control the creosote contaminant plume (that is, produce dry cells in MODFLOW). Loftis found the minimum transpiration rate that would accomplish this was 0.025 feet per day, or 0.3 inches per day. This corresponded to a transpiration flux of approximately 4.6 gallons per day per tree. Panhorst (2000) determined transpiration fluxes at the site by dividing the output of the trees (that is, the wells that simulated the trees) by the total number of trees. Using this method, Panhorst determined an average transpiration rate of 0.065 inches per day, or 1.34 gallons per tree per day, during a transient period in early September 1999. Panhorst noted that his calculated transpiration rate was significantly lower than normal values, and lower than expected values at the Oneida site.

Using the ET Package in a transient MODFLOW simulation seems to provide a more valid simulation of transpiration at the site, as compared to a using the Well Package to simulate transpiration. Using the Well Package (as Panhorst did) to simulate trees created a constant transpiration at the site, independent of depth to groundwater (that is, independent of a ET extinction depth). Therefore, the wells (that is, the trees) never stopped extracting groundwater. The ET Package in this model prevents transpiration from occurring when the groundwater water level elevation drops below the respective extinction depth.
A quick analysis of the total transpiration volumes and transpiration rates for the site during various time steps in the final transient model run can detail how MODFLOW’s ET package reacts to recessing water level elevations due to the end of a rainfall event. Recall that MODFLOW’s ET Package uses the transpiration elevation and the transpiration extinction depth to create a linear relationship for transpiration flux, depending on depth to groundwater. Figure 4-29 presents the overall transpiration volumetric totals for each time step, as well as the overall transpiration rate during each time step, from the calibrated transient model for July 2000. This figure was generated by reading the ET total volume (for the entire model domain) and the ET rate (for the entire model domain), during each time step, from the MODFLOW output file (included in Appendix C). The figure shows that after the rainfall event ends, the amount of groundwater transpired increases from approximately 500 gallons per time step to almost 1,400 gallons per time step. This is misleading since the time steps change from 2-hour time steps during the rainfall event to 6-hour time steps after the rainfall event. If the transpiration volumetric total per time step were normalized to a volume per unit time (that is, to a transpiration rate), it would be identical to the transpiration rate displayed in the figure.

Figure 4-29: Transpiration Volume Out of the Site and Site Transpiration Rate versus Time Step (Transient, July 19, 2000 to July 27, 2000)
Therefore, the transpiration rate is of most interest in Figure 4-29. The transpiration rate increases with each time step as the site is subjected to recharge throughout the rainfall event, causing the groundwater levels to rise closer towards the respective ET, or transpiration, elevations. The transpiration rate out of the site decreases with each time step after the end of the rainfall event. The declining transpiration rates with each time step are expected, as with the absence of recharge, the water levels at the site decrease, eventually to below the ET, or transpiration, extinction depths in some cases, thus decreasing the allowable ET rate in MODFLOW.
5.0 Summary and Conclusions

For steady-state calibrations, it is more straightforward to minimize the input parameters, determine a solution’s uniqueness and the model’s sensitivity to various parameters, and evaluate the validity of each model run. Sections 4.3.2.4 and 4.3.2.5 demonstrated these exercises. For transient calibrations, there are more variables and fewer checks available. Still, transient simulations offer the most realistic and authentic simulations. It is almost ironic that a steady-state solution is required to begin a transient modeling exercise.

For the final transient calibration in this research, transpiration was simulated at the Oneida site to demonstrate that a phytoremediation system was hydraulically controlling a contaminant plume. This model only looked at the groundwater hydraulics at the site, rather than the contaminant transport. Future research should continue with looking at the creosote contaminant fate and transport at the Oneida site.

The use of “ET” in MODFLOW is a misnomer, since the model is actually only calculating transpiration. It does not incorporate evaporation from the ground surface or from the foliage. The transpiration rates and extinction depths, recharge, specific yield, time steps, and the trench conductance were all varied to calibrate the transient model. The effects of changing recharge, specific yield, and time step length on the model were determined with the transient simulation of a February 2000 precipitation event. These lessons were carried forward to the transient simulation of a July 2000 precipitation event when the poplar trees were clearly transpiring groundwater. The hydraulic conductivities determined in precursory steady-state calibration for the July 2000 simulation were not changed during the transient simulation, so the transient simulation only required varying the transpiration rates and extinction depths in the ET Package. Trench conductance was only varied slightly to match the total groundwater removed from the site by the groundwater interception trench (per the flow meter reading in July 2000). The solution set from the precursory steady-state calibration’s final model run was used for the starting heads for the transient calibration.

The various model runs demonstrated the sensitivity of the model to several input parameters. Both steady-state and transient models were inherently sensitive to recharge input, as recharge is one of the main input parameter tools used to calibrate any model. Accordingly, the model showed sensitivity to the obvious hydraulic conductivity in the early steady-state model runs, and to specific yield and starting heads in the transient model runs. Still, once these parameters were determined for the site, the transient calibration involved varying the transpiration rates and extinction depths to most closely match the groundwater recessions in each observation well. The impact of the transpiration rates and extinction depths were most evident in the ET zones containing observation wells, such as the ET zone containing P-4. Observation well MW-6 was only calibrated using recharge and specific yield since its location lies outside of the
phytoremediation system (refer to the subsection titled, “Conceptual Model with Active Poplar Trees and Operating Trench,” within Section 4.3.2.6).

Transient recharge can affect groundwater rise and recession. One of the most valuable lessons learned during this research was that a known rainfall total, or intensity, could not be directly translated to recharge at a site. Instead, recharge was dependent on many different site-specific [often unknown] parameters, such as the heterogeneity of the site, the surface elevations (that is, the grade), and so on. Additionally, rather than a parameter that is a known observation, recharge is an input parameter that allows the modeler to fit the observed data.

This thesis determined the following:

- The ability of the trees to transpire groundwater depends on the transpiration extinction depth (that is, the root depth). Lawrence (2000) determined a “one-third relationship” using 1999 site data. This correlation between tree height and root depth did not work for the model calibrations of the site during the year 2000. Instead, the extinction depths had to be varied in areas depending on the presence of the coal layer and observation wells. Extinction depths at the site ranged from 2.5 feet to 8 feet (refer to subsection titled, “Transient Calibration of ET,” within Section 4.3.2.6).

- Loftis (1999) and Panhorst (2000) determined transpiration rates ranging from 0.3 inches per day to 0.7 inches per day. Loftis determined the steady-state site-wide minimum transpiration flux that would hydraulically control the creosote contaminant plume (that is, produce dry cells in MODFLOW) to be 0.3 inches per day, or approximately 4.6 gallons per day per tree. Panhorst determined the site-wide transpiration rates at the site by dividing the output of the trees (that is, the wells that simulated the trees) by the total number of trees. Using this method, Panhorst determined an average transpiration rate of 0.065 inches per day, or 1.34 gallons per tree per day, during a transient period in early September 1999. This thesis determined transpiration rate inputs (that is, maximum transpiration rates entered into the ET Package) ranging from 0.6 inches per day to 10 inches per day during calibration. These maximum transpiration rates do not correspond directly to calculated individual tree transpiration rates, since the groundwater rarely approaches the ET elevation. Dividing the ET volumetric total out of a particular ET zone (determined with the GMS Map Module, using the ET Coverage) by the approximate number of trees in the respective ET zone (determined with tree data in Appendix A) allowed for the computation of daily individual poplar tree transpiration rates. These calculated rates ranged from 0.4 gallons per day per tree to 5.3 gallons per day per tree (refer to “Discussion” in subsection titled, “Transient Calibration of ET,” within Section 4.3.2.6)
• Using the ET Package for a transient simulation in MODFLOW seemed to provide a more valid
determination of transpiration at the site, as compared to using a steady-state site-wide method
(Loftis 1999) or the Well Package (Panhorst 2000) to determine transpiration rates. Using a
steady-state method did not allow for the groundwater recessions to be examined. Using the Well
Package to simulate trees created a constant transpiration at the site, independent of depth to
groundwater (that is, independent of ET extinction depths). Therefore, the wells never stop
extracting groundwater. The ET Package in this model prevents transpiration from occurring
when the groundwater water level elevation drops below the respective extinction depth.

The transient modeling in this thesis should prove to be the first published transient study examining
MODFLOW’s capability to simulate direct transpiration with the ET Package. Pursuing the modeling in a
stepped approach (that is, starting with steady-state, practicing the transient, and so on) aided in the overall
understanding of how to maximize MODFLOW’s and the GMS platform’s capabilities.

The modeler does make the following recommendations for future developments of GMS/MODFLOW’s
ET Package:

• Allow the ET Package to import data. For example, rather than having to divide the ET into
zones, one may wish to import and interpolate scatter points that detail land surface elevations, ET
rates, and ET extinction depths. As it is now, these must be manually entered in cell by cell, or
with the Map Module, by creating polygon zones.

• Create some way, other than reprogramming MODFLOW, for the relationship between ET rates
and ET extinction depth to be defined. As it is now, the relationship is linear from the ground
surface (maximum ET rate) to the extinction depth (zero ET rate). Perhaps with future research, a
more intricate relationship will be developed.

• Devise some more analysis tools and/or improve the capabilities of the current post-simulation
statistical analysis tools.
6.0 References


Cooney, Catherine M. “Sunflowers remove radionuclides from water in ongoing phytoremediation field tests.” Environmental Science and Technology 30 (1996): 194A.


Wiley, John P., Jr. “Wastewater problem? Just plant a marsh: for some of the toughest environmental cleanups, plants can do it better and cheaper than we can.” Smithsonian July 1997: 24-25.


7.0 Epilogue

7.1 Regulators’ Perspectives On Phytoremediation

There seem to be three federal programs that have a remediation component: the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA); the Resources Conservation and Recovery Act (RCRA), and the Toxic Substances Control Act (ToSCA). In the USEPA Technology Innovation Office’s phytoremediation workshop in December 1996, a panel moderator from the USEPA, Jim Cummings, noted that “CERCLA, via the National Contingency Plan, has a remediation, versus regulatory, thrust… The statue itself provides relief from permit requirements [in section 121(e)].” He also said, “RCRA and ToSCA have regulatory requirements which impose duties and potential sanctions on researchers, technology developers and remediation practitioners.” Cummings said further:

…to date there have been few, if any situations where potential application of RCRA requirements to a phytoremediation project has arisen. Most projects to date appear to involve voluntary cleanup programs not involving wastes subject to RCRA. There are some unresolved policy issues regarding the extent to which phytoremediation may be subject to RCRA. The Technology Innovation Office has initiated discussion with the Office of General Counsel and the Office of Solid Waste.

These very circumstances may make it difficult for phytoremediation research and application to develop further. Cummings did mention, however, that discussions with federal and state regulators [as of December 1996] indicated a “general receptivity to phytoremediation.” He listed their concerns:

1. At present, how does the science compare with the practice of this technology? Are the two in some appropriate balance?
2. How can we evaluate potential efficacy? [clean-up timeframes and ability to reach desired cleanup levels]
3. How long will the technology take before contaminant levels begin to decrease? Is the proponent simply “stalling” in proposing/applying this technology, since “time is money” and phytoremediation is so cheap?
4. Is there potential for production of harmful daughter products and/or release of sequestered contaminants via transpiration?

He then relayed that the regulators seemed to be looking for rules of thumb to be able to determine whether there is an appropriate match between the site and the proposed approach.

7.2 Number One Issue to Allow Broad Application of Phytoremediation

USEPA’s Technology Innovation Office came up with a list of issues that, when resolved, would expedite phytoremediation’s acceptance. They presented these findings at often-mentioned USEPA
phytoremediation workshop at the end of 1996. Number one on the list: **Develop fate and transport models for certain contaminants within plants.** They further explained:

…existing groundwater models can be used to a limited extent in phytoremediation applications, but that **more integration of plant effects on groundwater need to be added to these models such as transpiration rates and their effects on groundwater.** Also, models need to be developed that integrate plant effects on contaminants and water availability in the unsaturated zone. As part of this integration of plants into existing groundwater and vadose zone models, further work needs to be done to model the fate of contaminants within the plant tissues: distributions of metabolites in different plant tissues (stem, root, leaf) are difficult to predict, as well as transpiration rates for water and contaminants such as volatile organics.

Hopefully, this thesis has started work in that direction.
Edward J. Corack, son of Edward W. and Mary T. Corack, was born on March 3, 1974, in Honolulu, Hawaii. After several homes and schools, Ed started second grade in Herndon, Virginia and spent the rest of his public education there. He attended the 1991 Virginia Governor’s School for the Gifted in Science. After graduating from Herndon High School in 1992, he went to Virginia Polytechnic Institute and State University in Blacksburg, Virginia, to pursue a Bachelor’s Degree in Civil Engineering (Environmental Option). He graduated Cum Laude, In Honors in May 1996. During summer 1996 he worked as a Science Assistant for the National Science Foundation in the Division of Bioengineering and Environmental Systems. Ed continued at Virginia Tech in fall 1996 for a Master’s Degree in Civil Engineering (Geoenvironmental Option). He left the program before completing his thesis to pursue a career at an environmental engineering consulting firm. He returned to complete his thesis and subsequently received his Master’s Degree in May 2003.