Development of an Analytical Groundwater Contaminant Transport Model

by

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Abstract

Onsite wastewater systems (OWS) are utilized by approximately 20% of US households. Domestic wastewater contains a variety of contaminants that may result in degradation of water resources if the OWS is improperly designed, installed or operated. There is a large diversity in the contaminants composing the wastewater stream from household though nutrients (nitrogen, phosphorus, potassium) are the most ubiquitous. Within the underlying aquifers, nitrogen is of primary concern because of its mobility as well as its effects on human and ecosystem health.

Regulators, engineers and scientist working in the OWS industry require simple-to-use tools to evaluate the performance of an OWS. Currently the tools that are available to these professionals consist of complex mathematical models that are neither widely available nor easy to use. An analytical groundwater contaminant transport model (the aquifer model) was developed to provide professionals with robust simple-to-use tools to evaluate the performance of an OWS. The aquifer model uses an analytical contaminant transport equation that is ideally suited for an OWS that will simplify user input. The aquifer model Graphical User Interface (GUI) will facilitate user interaction making the model easy-to-use. In addition, the aquifer model is coupled with the Soil Treatment Unit Model (STUMOD) which will provide the user with the ability to seamlessly evaluate contaminant transport through the vadose zone and aquifer underlying an OWS.

The performance of the aquifer model has been evaluated through calibration to field data collected down gradient of an OWS installed at a Florida field site. Calibration results from the aquifer model have also been compared to calibration results from two complex numerical models (MODFLOW/MT3D). Calibration of the aquifer model to field data showed excellent results with a correlation coefficient of 0.66. The numerical models in contrast returned
correlation coefficients below 0.1 when compared to field data. Calibrated parameter values for the aquifer model and the numerical models are within the expected range though the calibrated numerical models did not successfully replicate observed nitrate concentrations. Results from the evaluation of the aquifer model show that it is an effective tool for evaluating contaminant transport in surficial aquifer beneath an OWS when compared to complex numerical models.
Table of Contents

Abstract .......................................................................................................................................................... iii
List of Figures ............................................................................................................................................... vii
List of Tables ................................................................................................................................................ x
Acknowledgments ........................................................................................................................................ xi
CHAPTER 1 ................................................................................................................................................... 1
  1.1 Scope .................................................................................................................................................... 3
    1.1.1 Purpose .......................................................................................................................................... 3
    1.1.2 Research Objective ......................................................................................................................... 5
  1.2 Background .......................................................................................................................................... 6
    1.2.1 Nitrogen cycle ................................................................................................................................. 6
    1.2.2 The Soil Treatment Unit Model (STUMOD) .................................................................................. 9
    1.2.3 Modeling Semantics and Terminology ............................................................................................. 9
    1.2.4 Governing Equations and Solution Techniques ............................................................................. 11
  1.3 Overview of the Aquifer Model .......................................................................................................... 12
    1.3.1 Inputs and Outputs ....................................................................................................................... 13
    1.3.2 Implementation .............................................................................................................................. 17
CHAPTER 2 ................................................................................................................................................... 19
  2.1 Derivation of the Analytical Solution ................................................................................................. 20
    2.1.1 Solutions Expressed as the Product of Simpler Solutions ............................................................ 20
    2.1.2 Deriving the Horizontal Plane Source Solution ........................................................................... 22
  2.2 Implementation in Excel VBA ............................................................................................................ 27
    2.2.1 Concentration ............................................................................................................................... 27
    2.2.2 Mass Flux ...................................................................................................................................... 29
  2.3 Automated Parameter Estimation ....................................................................................................... 33
    2.3.1 Dispersivity .................................................................................................................................. 33
    2.3.2 Hydraulic Gradient ......................................................................................................................... 35
  2.4 Model Performance Evaluation ......................................................................................................... 38
    2.4.1 Parameter Sensitivity Analysis ...................................................................................................... 39
    2.4.2 Sensitivity Analysis Results ......................................................................................................... 40
    2.4.3 Uncertainty Analysis ..................................................................................................................... 44
## List of Figures

Figure 1, the geometry of the Horizontal Plane Source Solution ........................................ 4
Figure 2, the geometry of the Vertical Plane Source Solution .............................................. 5
Figure 3, a typical OWS ....................................................................................................... 7
Figure 4, conceptual framework of the aquifer model and interface with STUMOD .......... 14
Figure 5, the STUMOD GUI ............................................................................................... 16
Figure 6, a graphic representation of a convolution integral .................................................... 26
Figure 7, plume discretization ............................................................................................... 30
Figure 8, plume cross sections constructed by the aquifer model ........................................... 31
Figure 9, VBA structure for the aquifer model ....................................................................... 32
Figure 10, normalized sensitivity analysis results ................................................................. 42
Figure 11, sensitivity analysis results for the five most sensitive parameters ......................... 42
Figure 12, sensitivity analysis results for the remaining parameters ...................................... 43
Figure 13, uncertainty analysis results for all reported denitrification rates ......................... 49
Figure 14, uncertainty analysis results for the 50th percentile and below denitrification rates .... 49
Figure 15, validation results for the HPS solution using a homogeneous velocity field ........ 52
Figure 16, validation results for the HPS solution using a heterogeneous velocity field .......... 53
Figure 17, RMSE comparison between a homogeneous and heterogeneous velocity field and the HPS solution ......................................................................................................................... 55
Figure 18, the Gulf Coast Research and Education Center (GCREC) field site .................... 60
Figure 19, conceptual model of the Floridian Aquifer system ............................................... 61
Figure 20, water table fluctuations at the GCREC field site .................................................... 62
Figure 21, the diagram used to calculate distances from the source to sample location ........ 72
Figure 22, calibration results from the aquifer model ................................................................. 76
Figure 23, hydraulic head versus smoothed land surface ......................................................... 80
Figure 24, MODFLOW calibration results for the transient numerical model ....................... 83
Figure 25, MT3D calibration results for the transient numerical model ................................ 84
Figure 26, MODFLOW calibration results for the steady state numerical model .................... 87
Figure 27, MT3D calibration results for the steady state numerical model ............................. 87
Figure 28, USGS groundwater monitoring wells near the GCREC field site ............................. 108
Figure 29, USGS monitoring well (1) .......................................................................................... 108
Figure 30, USGS monitoring well (2) .......................................................................................... 109
Figure 31, USGS monitoring well (3) .......................................................................................... 109
Figure 32, USGS monitoring well (4) .......................................................................................... 110
Figure 33, USGS monitoring well (5) .......................................................................................... 110
Figure 34, USGS monitoring well (6) .......................................................................................... 111
Figure 35, USGS monitoring well (7) .......................................................................................... 111
Figure 36, USGS monitoring well (8) .......................................................................................... 112
Figure 37, USGS monitoring well (9) .......................................................................................... 112
Figure 38, USGS monitoring well (10) ....................................................................................... 113
Figure 39, USGS monitoring well (11) ....................................................................................... 113
Figure 40, slug test locations for the GCREC field site ............................................................ 118
Figure 41, the interpolated hydraulic conductivity field (Hvorslev) ........................................ 119
Figure 42, the interpolated hydraulic conductivity field (Bouwer & Rice) .............................. 119
Figure 43, hydraulic conductivity field used in the numerical models ..................................... 120
Figure 44, GCREC well completion report (1) ......................................................................... 121
Figure 45, GCREC well completion report (2).................................................................................. 121

Figure 46, GCREC well completion report (3).................................................................................. 122

Figure 47, alternate calibration results for the aquifer model (33 observations)......................... 123

Figure 48, alternate calibration results for the aquifer model (33 observations & concentration)
.......................................................................................................................................................... 124

Figure 49, alternate calibration results for the aquifer model (23 observations & concentration).
.......................................................................................................................................................... 125
List of Tables

Table 1, uncertainty analysis parameter distributions .......................................................... 47
Table 2, descriptive statistics for all groundwater samples .................................................. 64
Table 3, descriptive statistics for groundwater samples down gradient of the OWS ........... 67
Table 4, descriptive statistics for STUMOD predictions ....................................................... 69
Table 5, descriptive statistics for hydraulic head ................................................................. 69
Table 6, descriptive statistics for hydraulic gradient & bearing .......................................... 69
Table 7, fixed parameters for calibration of the aquifer model ........................................... 74
Table 8, calibrated parameter values for the aquifer model ................................................ 75
Table 9, calibration results for the aquifer model ............................................................... 77
Table 10, calibration results for the transient state numerical model ................................. 85
Table 11, calibration results for the steady state numerical model ...................................... 86
Table 12, descriptive statistics of the heterogeneous hydraulic conductivity field ............ 107
Table 13, descriptive statistics of the heterogeneous velocity field .................................... 107
Table 14, hydraulic conductivity (Hvorslev and Bouwer & Rice) ...................................... 117
Table 15, calibration results for the aquifer model using all field data ............................... 123
Table 16, calibration results for the aquifer model (including concentration) ....................... 123
Table 17, calibration results for the aquifer model using 23 OWS groundwater samples
   (including concentration) ................................................................................................ 124
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CHAPTER 1
INTRODUCTION

Soil based onsite wastewater systems (OWS) are used by approximately 20% (26.1 million) of U.S. households [EPA, 2009]. The fraction of households that use OWS has remained relatively constant over the past three decades indicating that the OWS will remain an important part of the wastewater infrastructure for the foreseeable future. OWS are predominantly used in rural and suburban developments, with 50% and 47% of existing OWS installed at rural and suburban locations, respectively [EPA, 2009]. Many of these suburban and rural housing developments also use private water supply wells to provide drinking water. Because these communities depend heavily on local resources to provide both drinking water and wastewater disposal, a real danger exists that drinking water resources may become compromised.

Numerous studies have also linked OWS to degradation of surface water quality [Drake and Bauder, 2005; Fetter, 1999; Morgan et al., 2007]. Nutrients, present in household wastewater, enter groundwater and are transported in the direction of the regional hydraulic gradient. These nutrients are then discharged to surface water bodies such as streams and lakes through base flow. Nutrient limited surface water bodies may become degraded over time through eutrophication and hypoxia. Also, though limited studies have considered the movement of pharmaceuticals and other contaminants from OWS, a possibility exists that these contaminants may be transported to groundwater, drinking water sources, and surface water bodies.

The waste stream to OWS is variable and composed of numerous contaminants that may persist in the subsurface. Lowe et. al [2009] and Crites and Tchobanoglous [1998] provide extensive data on the composition of the modern waste stream from households. Nitrogen, a
nutrient prevalent in household wastewater, is of primary concern because of the mobility of nitrate in the subsurface and the potential impact to human health and aquatic ecosystems. Nitrate is widely known to cause methemoglobinemia, “blue baby syndrome,” in young infants where the oxygen carrying capacity of blood is reduced and the infant effectively suffocates [Johnson et al., 1987]. N-nitrosodimethlamine, a nitrate derived compound, has been shown to cause cancer in rats and has been identified in nitrate preserved foods suggesting that nitrate consumption can have negative health effects in adults as well [Ender et al., 1964; Magee and Barnes, 1956].

Because of the negative health effects and impacts to surface water bodies the U.S. Environmental Protection Agency (EPA) has established limits to protect both human health and aquatic environments. The EPA has established the maximum contaminant level (MCL) for nitrate in drinking water at 10 mg-N/L. Various limits exist for nitrogen loading to surface water bodies depending on their use and vulnerability. The total maximum daily loads (TMDL) protect surface water quality by limiting nitrate mass loading to levels that will not cause degradation.

In order to meet these criteria and ensure that groundwater and surface water resources are protected for future generations quantitative tools are needed to assess the design and performance of OWS. Mathematical models that consider the reactive transport of wastewater constituents in the subsurface are useful tools because they allow the user to evaluate the potential impact on groundwater and surface water quality relatively quickly and at minimal cost. Numerous models exist that have been used to evaluate contaminant transport from OWS ranging widely in complexity. Increasing mathematical complexity typically correlates with more flexibility allowing for better mathematical representation of the physical processes that are occurring. Increasing complexity, however, limits the user group, increases the input data
requirements and increases the cost of using the model. To date a limited number of models specifically consider OWS and fewer still are designed with a wide user group in mind.

1.1 Scope
This work documents the development of a screening-level model, referred to as the aquifer model here after, that is intended to answer questions concerning contaminant transport from an OWS. The question may come to mind of why yet another model is needed when a plethora of models exist that purport to address this question or similar questions [Conan et al., 2003; Jeong et al., 2011; Kinzelbach et al., 1991; Lee et al., 2006; Rios et al., 2013]. Many of the models that exist are not useful as screening-level models because they require too much input or technical expertise to be of practical use to most OWS professionals. These models require a high level of technical proficiency to correctly use due to the numerical techniques that are used to solve the governing equations and because of the input data requirements. Other models that have been developed as screening-level models either do not explicitly consider OWS or use analytical solutions that may introduce mathematical error in the results [Aziz et al., 2000a; Newell et al., 1996; Srinivasan et al., 2007].

1.1.1 Purpose
To address the lack of an adequate screening-level model to assess the impacts of an OWS on groundwater quality, the aquifer model was developed utilizing a mathematically correct analytical solution to the advection dispersion equation (ADE). The analytical solution will be referred to as the Horizontal Plane Source (HPS) solution in this work [Galya, 1987]. The geometry of the contaminant source that the HPS solution considers is consistent with that of an OWS, figure 1, because the contaminant source plane is oriented horizontally rather than vertically. Another widely used analytical solution originally derived by Domenico and Robbins [1985] considers a vertical contaminant source plane, figure 2, which requires a few assumptions
and estimations in order to be used to model an OWS. While the HPS solution does not exist in closed form, it avoids the assumptions used by the Domenico and Robbins [1985] solution which can introduce error under certain conditions [Srinivasan et al., 2007]. Others have already developed models based on the HPS solution; however their implementation does not specifically consider an OWS [Galya, 1987; Guyonnet, 2001]. Moreover these computer programs do not use a graphical user interface (GUI) to facilitate user input and do not provide graphical representation of the contaminant plume.

**Figure 1.** the orientation of the HPS analytical solution which considers a horizontally oriented contaminant source plane.

The aquifer model was developed in Excel as a Visual Basic Application. Excel was chosen as the platform to develop the aquifer model because it is widely available on most personal computers and because of the developer tools available within Excel that facilitate GUI construction. Development of the aquifer model within Excel has also allowed for seamless integration with the Soil Treatment Unit Model (STUMOD)[Geza et al., 2014]. STUMOD is a vadose zone model that describes the reactive transport of effluent constituents from the infiltrative surface of an OWS to the water table, figure 3. STUMOD is described in more detail in section 1.2.2.
Figure 2, the orientation of the analytical solutions derived using a vertical contaminant source plane.

1.1.2 Research Objective

The HPS solution used in the aquifer model is necessarily a simplification of the more general ADE. These simplifications are necessary in order to make the model available to a wide audience and reduce complexity. The research questions that are posed in this work are: 1) what are the limitations of the aquifer model given the simplifications of the analytical solution to the ADE? 2) Can this model reproduce field observations of nitrate in groundwater samples collected down gradient of an OWS at a study site in Florida?

These questions are answered by comparing an aquifer model simulation to results from a complex numerical model (MODFLOW/MT3D) constructed to simulate the transport of a synthetic contaminant in an aquifer with a one directional, uniform seepage velocity field. Results from the aquifer model are also compared to an additional numerical simulation that introduces a complex advection field to evaluate limitations of the HPS solution when used to model contaminant transport for real aquifers. These results validate the mathematical derivation of the HPS solution and provide insight into the effect that assumptions inherent to the HPS solution may have on model predictions.
Calibration of the analytical model to field observations provides an understanding of the ability of the aquifer model to replicate field observations. The calibrated parameter values from the analytical model are compared to parameters values from a numerical model constructed and calibrated for the same site. Model outputs for both the analytical and numerical models are also compared providing an understanding of the expected performance of the aquifer model and potential limitations. These results also illuminate the advantages of using steady state analytical tools over transient numerical models for evaluating OWS.

1.2 Background

A brief overview of the nitrogen cycle is given in the following section, with a particular focus on nitrogen in OWS. A short discussion on terminology related to mathematical modeling is also presented along with a framework that may be useful to the reader in evaluating model results. Finally, a brief description of the governing equations that describe contaminant transport in an aquifer are presented along with a brief comparison of two methods for solving these equations.

1.2.1 Nitrogen cycle

Nitrogen is an essential nutrient for plant growth and an important constituent of amino acids that make up proteins which make life possible for all living organisms. The atmosphere is a large reservoir of inert nitrogen (nearly 78% N₂) that until 1913, when ammonia was first produced on an industrial scale using the Haber-Bosch process, was largely unavailable for human use [Smil, 2001]. Anthropogenic activity has altered the natural nitrogen cycle greatly increasing the quantity of reactive nitrogen species, such as nitrate (NO₃⁻) and ammonium (NH₄⁺).
Nitrogen may enter groundwater from a variety of sources such as synthetic fertilizers, atmospheric deposition or animal wastes. All of these sources have been implicated in the degradation of water quality; however, the focus of this work is nitrogen from OWS because of the proximity to groundwater. The predominant nitrogen species in raw household wastewater are organic nitrogen and to a lesser degree ammonium. Organic nitrogen is transformed to ammonium within the septic tank and effluent applied to the Soil Treatment Unit (STU) is predominantly in the form of ammonium [Crites and Technobanogluos, 1998; Lowe, 2009].

\[
2\text{NH}_4^+ + 3\text{O}_2 \rightarrow 2\text{NO}_2^- + 2\text{H}_2\text{O} + 4\text{H}^+ \quad \text{(Nitrosomonas)} \tag{1.10}
\]

\[
2\text{NO}_2^- + \text{O}_2 \rightarrow 2\text{NO}_3^- \quad \text{(Nitrobacter)} \tag{1.11}
\]

Within the STU ammonium is transformed to nitrate in a two-step process, referred to as nitrification, mediated by the bacteria *Nitrosomonas* and *Nitrobacter*, equations 1.10 and 1.11.
Attenuation of ammonium can also occur via sorption to the negatively charged soil matrix. While ammonium sorption may be important for the removal of nitrogen from effluent in the STU it cannot be assumed to be the dominant process. In some soils it has been shown that ammonium is among the least competitive cation as other cations will sorb preferentially before ammonium [Sparks, 1995; Tan, 1998]. Because of this and because of the relatively high nitrification rate in most soils the sorption of ammonium is considered negligible by some [Heatwole and McCray, 2005]. Due to the high rate of nitrification in most soils the dominant form of nitrogen arriving at the water table is nitrate.

\[
\text{NO}_3^- \rightarrow \text{NO}_2^- \rightarrow \text{NO}^- + \text{N}_2\text{O} \rightarrow \text{N}_2 \quad \text{(denitrification)} \quad (1.12)
\]

\[
\text{NH}_4^+ + \text{NO}_2^- \rightarrow \text{N}_2 + 2\text{H}_2\text{O} \quad \text{(anammox)} \quad (1.13)
\]

Because of the nitrification and denitrification processes that occur within the STU, the STU is a critical component of an OWS and may mitigate the transport of nitrogen to groundwater. Denitrification is the anoxic reduction of nitrate to nitrogen gas mediated by various heterotrophic and autotrophic bacteria, equation 1.12 [Rivett et al., 2008]. Denitrification is considered the primary mechanism for nitrogen removal in the STU. While anoxic conditions typically do not persist in the STU, anoxic conditions do develop at micro sites where denitrification can occur. Within groundwater, denitrification is thought to be the dominant process for the attenuation of nitrogen if dissolved organic carbon is present. Ammonium that reaches groundwater, in comparison, has a propensity to accumulate [Postma et al., 1991]. The anammox process, equation 1.13, is the microbial oxidation of ammonium which produces nitrogen gas potentially removing ammonium from groundwater. Though it has been observed in anoxic wastewater, the importance of this process in mitigating nitrogen contamination of groundwater is considered relatively small [Mulder et al., 1995].
1.2.2 The Soil Treatment Unit Model (STUMOD)

Figure 3 and section 1.2.1 explain how a typical OWS functions and the various chemical reactions that occur in the treatment train. The vadose zone, lying beneath the infiltrative surface and above the phreatic surface, is a critical region for a properly functioning OWS. Contaminants in septic tank effluent are attenuated in this region in large part by microbes. STUMOD was developed as tool to predict the fate and transport of contaminants such as nitrogen within this region. With respect to nitrogen, STUMOD calculates the attenuation of ammonium via sorption and nitrification. It also calculates the amount of nitrogen removed via denitrification and plant uptake. STUMOD is capable of predicting total nitrogen, ammonium and nitrate concentrations at any point in the vadose zone. An important STUMOD output is the concentration of total nitrogen arriving at the water table. This gives the user the ability to estimate mass flux of nitrogen to the underlying aquifer. While STUMOD requires numerous parameters, a default set of parameter values have been established based on the soil textural classes from an extensive literature review. In the context of this work STUMOD is used to estimate the mass flux of nitrate to the surficial aquifer at the field site where data were gathered for corroboration of the aquifer model. The aquifer model has been designed to couple with STUMOD and provide the user with an estimate of nitrate concentration or mass flux down gradient of the STU.

1.2.3 Modeling Semantics and Terminology

In discussing the development of a mathematical model of a natural process it is helpful to discuss some of the semantics of modeling as well. It should first be recognized that models are necessarily approximations of reality [Beven and Young, 2013]. Even the well-established mathematical equations and “laws” that are widely employed, have been derived under a set of assumptions and or simplifications [Beven, 2013; Beven and Germann, 2013]. Thus it is critical that the developer and users of the model clearly understand and state the assumptions and
simplifications that have been made through the process of model development. Models based on the Dominico and Robbins [1985] analytical solution to the ADE are an example where the assumptions and simplifications have not been well understood by users leading to a misunderstanding of the model limitations [Srinivasan et al., 2007].

Though mathematical models are approximations of reality they can be used to answer questions about real systems. A model that has successfully reproduced independent observations is often said to be “validated,” though Beven and Young [2013] point out that these “validations” are often conducted for specific conditions. Because of the limited scope of most validation procedures a more descriptive term would be “conditionally validated.” A conditionally validated model can provide useful information about the future behavior of the system or answer questions about the current behavior of a system that cannot be easily observed. While a conditionally validated model may answer questions there is always some level of uncertainty surrounding model predictions given the scope under which it has been evaluated. Thus the only definitive conclusion that can be obtained from a mathematical model is when the model fails to accurately describe the observed phenomenon, i.e. falsification of the model [Beven and Young, 2013].

Because of uncertainty in model parameters or the simplifications and assumptions involved in the derivation of a particular model, blanket confidence should not be placed in model predictions. If, however, the model can meet a given set of criteria, the model may be useful as a screening-level model. Such a model is useful in answering general questions of whether a condition is likely to occur or not. The criterion that is often set for such a model is that the predictions be conservative and within an order of magnitude of observed values. For example Bioscreen and Biochlor are widely known groundwater screening-level models.
developed by the EPA that can answer questions of whether further work is warranted at sites contaminated with hydrocarbons and chlorinated solvents, respectively [Aziz et al., 2000a; Newell et al., 1996]. This framework has been adopted through the design and evaluation process of the aquifer model. Limitations of the aquifer model have been highlighted during calibration to observed data; however these limitations do not preclude its usefulness.

### 1.2.4 Governing Equations and Solution Techniques

The groundwater flow equation, equation 1.14, describes three dimensional flow of fluid in porous media [Fetter, 2001]. The basic principal underlying the groundwater flow equation is conservation of mass. The groundwater flow equation is given by the following where \( K_{x,y,z} \) is the anisotropic hydraulic conductivity of the porous media, \( S_s \) is specific storage, and \( \phi(x, y, z, t) \) is the hydraulic head.

\[
\frac{\partial}{\partial x} \left[ K_{xx} \frac{\partial \phi}{\partial x} \right] + \frac{\partial}{\partial y} \left[ K_{yy} \frac{\partial \phi}{\partial y} \right] + \frac{\partial}{\partial z} \left[ K_{zz} \frac{\partial \phi}{\partial z} \right] = S_s \frac{\partial \phi}{\partial t} \tag{1.14}
\]

The mass of fluid entering a representative elementary volume (REV) is balanced by a mass flux equal in magnitude out of the REV. The groundwater flow equation does not described the movement of a dissolved solute but when solved does provide the velocity field that serves as an input for the ADE. Equation 1.15 gives the ADE that describes the movement of solutes via advection and dispersion in three dimensions through an REV [Fetter, 1999]. The parameters \( D_{x,y,z} \) describe dispersion in the \( X, Y, \) and \( Z \) dimensions, \( v_{x,y,z} \) describes the three dimensional components of groundwater velocity, and \( C(x, y, z, t) \) the concentration of the solute.

\[
\left[ \frac{\partial}{\partial x} \left( D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_z \frac{\partial C}{\partial z} \right) \right] - \left[ \frac{\partial}{\partial x} (v_x C) + \frac{\partial}{\partial y} (v_y C) + \frac{\partial}{\partial y} (v_y C) \right] = \frac{\partial C}{\partial t} \tag{1.15}
\]

The ADE is also a conservation of mass equation which accounts for removal of mass from the system via processes such as microbially mediated degradation, chemical reactions and
sorption etc. An input required for the solution of the ADE is groundwater velocity which can be provided by solving the groundwater flow equation prior to the ADE.

Both the groundwater flow equation and the ADE are partial differential equations (PDE) that are difficult to solve without prior information of the system. Thus, in order to solve a PDE, the boundary conditions at the extent of domain must be known as well as the initial conditions. While numerous methods exist to solve a PDE, the solutions can be grouped as either analytical or numerical solutions. Numerical solutions approximate the PDE using a series of piece wise linear functions which are solved simultaneously. Due to the large number of equations that must be solved, and the iterative method that is required, numerical solutions can require a significant amount of time to solve.

Analytical solutions are derived for a specific set of boundary and initial conditions. Assumptions and simplifications are generally made in order to derive the solutions. Analytical solutions to the ADE are generally derived considering one dimensional advection and up to three dimensional dispersion. An analytical solution may exist in a closed form, meaning it can be expressed with a finite number of terms, or in an alternative form. An example of an alternative form is an infinite sum that cannot be express with a finite number of terms or constants.

1.3 Overview of the Aquifer Model

A brief overview of the functions available to users of the aquifer model is presented in this section. The outputs from the model as well as the inputs that are required to run the model are outlined in this section. Methods for estimating parameter values are also briefly discussed. Finally, this section presents a description of how this model can be used to evaluate contaminant transport from an OWS, and the conclusions that are possible to draw from the model results.
1.3.1 Inputs and Outputs

A number of options exist for the user to select the input and output methods that are suitable for their needs. Because the aquifer model is coupled with STUMOD through a GUI, running STUMOD prior to the aquifer model will automatically populate the appropriate fields in the aquifer model with nitrogen concentration of STU percolate arriving at the water table, hydraulic conductivity and porosity. The aquifer model may also be run independently of STUMOD though the user will need provide values for contaminant concentration, porosity and hydraulic conductivity. Because of this, the user is encouraged to independently evaluate site specific parameter values or run STUMOD to obtain those parameter values.

The aquifer model is designed to function with STUMOD. It uses STUMOD parameters and provides the user numerous options to estimate other needed parameters. In addition, the user is provided with several options to select different model outputs. The conceptual framework of the aquifer model is presented in figure 4.

Concentration can be calculated at any point within the aquifer specified by three dimensional Cartesian coordinates, figure 4. The origin of the coordinate system is the center of the STU footprint at the water table, i.e. where x = y = z = 0. Model outputs will give concentration of nitrate as nitrogen in units of mg-N/L. The user may also choose to construct a cross sectional image of the nitrate plume. The model is capable of constructing a cross section of the plume in y-z plane, which is perpendicular to the direction of flow, or x-y plane giving an aerial view of the plume. The user must specify a point in the x direction where the y-z plume is to be constructed, or for an x-y plume, points x and z to display the aerial view of the plume at a user chosen depth below the water table.
Mass flux is calculated by specifying a point, $x$, down gradient of the source, the extent of the plume in the $y$ and $z$ direction is estimated by the model, figure 4. Mass flux estimates are useful for users or regulatory agencies who wish to estimate the maximum contaminant load to a surface water body. The inherent assumptions made when calculating mass flux are: all nitrate contaminated groundwater reaches the surface water body as base flow, and the denitrification rate does not increase within the sediments or hyporheic zone of the lake or stream, respectively. These assumptions are conservative as the mass flux to the water body will likely be somewhat
less due to increased denitrification that may occur in the hyporheic zone or because all streamlines from the contaminant source do not intersect the water body.

This modelling approach is expected to be more practical and preferred to other analytical contaminant transport models because the user can interact with the model through a user friendly GUI, figure 5, and is not required to provide a significant amount of input data. The data that is required can be input through the GUI which simplifies data input and output for the user. Most users are familiar with GUI’s as most operating systems use a GUI interface. Models that use command line or text file inputs are less familiar and may present a barrier to some potential users.

The parameter input boxes are grouped by type, figure 5. The “Input Dimensions” are parameters specific to the OWS that will be evaluated. The width and length refer to the footprint of the STU which can easily be measured in the field as the width and length of the area where the distribution tubes have been installed or from design drawings. The hydraulic loading rate (HLR) is the flow rate applied to the STU per day divided by the STU footprint area. If STUMOD is run prior to running the contaminant transport model, the HLR input field is automatically populated and then multiplied by the footprint to get a volumetric loading rate. The latitude and longitude refer to the center of the STU and are only used if the user chooses to calculate the distance to the point where concentration or mass flux will be evaluated. In this case, the user needs to provide the latitude and longitude of the point where the concentration or mass flux is to be evaluated. Alternatively, the user can input the x, y and z distance of the point from the source.

The “Groundwater Velocity” or seepage velocity is calculated using Darcy’s law given by equation 2.57, in chapter 2. The user must specify the magnitude of the local hydraulic
gradient or it may be calculated. The user has the option to calculate the hydraulic gradient if they provide the latitude, longitude and observed hydraulic head at three locations (elevation of groundwater above any reference datum). If this data is available the model has the ability to accurately calculate both the magnitude and direction of the hydraulic gradient. The specifics of how this algorithm functions will be given in chapter 2.

Figure 5, users will interact with the aquifer model through the STUMOD GUI pictured above.
“Aquifer Properties” refer to the physical characteristics of the surficial aquifer where the OWS is constructed. The porosity and saturated hydraulic conductivity input fields are automatically populated with values from the STUMOD interface if a STUMOD simulation has been conducted prior to running the aquifer model. The values from STUMOD are based on the 12 soil textural classes defined by the United States Department of Agriculture (USDA) and represent class averages [Schaap et al., 2001]. The aquifer thickness is the thickness of the saturated zone or the distance from the water table to the first confining unit. The three dimensional dispersivity values must be input by the user or the user may select to calculate those values based on the longitudinal distance to the observation point. The method for calculating the dispersivity values will be described in the subsequent chapter.

“Contaminant Properties” refer to the chemical characteristics of the contaminant that affect its movement and transformation within the aquifer. Nitrate is generally not retarded in the subsurface but the option to change the retardation factor is given to allow a user the flexibility of modeling the transport of other contaminants that are retarded in the subsurface. The denitrification process has been represented using zero order, first order, and Monod kinetics by numerous other studies. However, under low concentrations the denitrification process can be accurately represented using first order reaction kinetics. Also, the use of first order kinetics to represent denitrification minimizes model parameters. Concentration refers to the concentration of nitrate (mg-N/L) in the percolate at the water table. STUMOD has been designed to calculate this value and is the recommended method for obtaining this value.

1.3.2 Implementation

The aquifer model has been designed to provide the user with a quantitative estimate of the impact that an OWS has on groundwater. An engineer, scientist or field technician may wish
to use this model for a variety of reasons. For example, a field technician who is assessing surface water quality could use this model along with engineering designs of the OWS installed at the site to evaluate the mass flux of nitrate from the OWS to the surface water body in order to meet the MCL regulations. The mass flux estimates can also be used to evaluate cost effective modifications to the OWS to reduce the mass flux of contaminants.

The aquifer model’s ability to calculate the magnitude and direction of the hydraulic gradient could be potentially useful for estimating whether or not a contaminant plume will reach a receptor. For example, this subroutine could be used to determine if a nitrate plume from an OWS could potentially reach drinking water wells installed down gradient. During construction or design of an OWS the model could be used to determine the optimal location for an OWS based on the direction of the hydraulic gradient.

An engineer or scientist designing an OWS may use this model to evaluate the impact of a particular design on groundwater quality such as a higher HLR or higher nitrogen loads. If the design does not meet the requirements for groundwater quality the relative impact of different design options can be quickly evaluated and the most economical can be selected.

These capabilities notwithstanding, as the cost of an incorrect prediction increases so should the investment in an independent method to evaluate model parameters thereby minimizing uncertainty. Also, the aquifer model is not intended to replace robust numerical models but rather it provides a first step to determine if additional work and expenditures are warranted.
CHAPTER 2

DERIVATION AND IMPLEMENTATION OF THE
ANALYTICAL ADVECTION DISPERSION EQUATION

Chapter 2 presents the derivation of the analytical solution to the ADE. This derivation provides the reader a general understanding of the methods that are used to derive analytical solutions as well as the assumptions and simplifications that have been made. This will also provide the reader the opportunity to scrutinize the validity of the solution. A basic description of the algorithms coded in Excel VBA is also provided. The methods that are used to calculate the hydraulic gradient and dispersivity are provided as well as the justifications.

An important part of model development is to understand the relative importance of model parameters and the impact they have on model predictions and uncertainty. The results from a local sensitivity analysis are presented to give the user an understanding of the most influential parameters on model outcome. These results will aid the user in the selection of parameters to independently establish to improve confidence in model predictions.

Given all the possible combinations of parameter values there is a large range of possible model outcomes. An uncertainty analysis quantifies the model behavior for the large number of possible parameter combinations. Results from an uncertainty analysis that was conducted using a Monte Carlo method, where parameter values were varied within valid ranges, are presented. The parameter distributions were established from literature to ensure the uncertainty analysis was physically based. These results allow the user to quickly assess the range of possible model outcomes and the probability of achieving a particular outcome.
2.1 Derivation of the Analytical Solution

Galya [1987] presents the derivation of an analytical solution to the ADE for a horizontal contaminant source plane based on the work of Carslaw and Jaeger [1959] and Crank [1975]. Carslaw and Jaeger [1959] derived numerous analytical solutions for heat transport problems which are similar in form to the advective and dispersive processes that control the movement of solutes in porous media. Galya [1987] derived the analytical solution for a horizontal contaminant source plane by employing simplifications originally derived by Carslaw and Jaeger [1959] and presented in sections 2.1.1 and 2.1.2. While this work was originally presented by Carslaw and Jaeger [1959] and Crank [1975] many of the intermediate steps were not provided in the original publications and have been added to provide a better understanding.

2.1.1 Solutions Expressed as the Product of Simpler Solutions

Consider the three dimensional partial differential equation describing diffusion in an isotropic media (the diffusion equation is analogous to the advection dispersion equation with no advection).

\[
\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} = \frac{1}{\rho} \frac{\partial c}{\partial t}
\]  

(2.10)

Carslaw and Jaeger [1959] show that the solution to complex equations, such as 2.10, may be expressed as the product of solutions to simplified one dimensional equations.

\[
a_1 < x < b_1, a_2 < y < b_2, a_3 < z < b_3
\]

(2.11)

Consider a solution to equation 2.10 that describes concentration within the region given by 2.11 as a function of location (x, y, z) and time (t). The solution must also satisfy specified initial and boundary conditions. The equation derived as the solution to 2.10 may be checked by substitution into 2.10 and performing the indicated partial derivatives.

Suppose \(c_1(x, t)\) satisfies the one dimensional diffusion equation:
The boundary conditions for \( c_1(x, t) \) are given by:

\[
\begin{align*}
\alpha_1 \frac{\partial c_1}{\partial x} - \beta_1 c_1 &= 0 \quad x = a_1, \quad t > 0 \\
\alpha_1' \frac{\partial c_1}{\partial x} + \beta_1' c_1 &= 0 \quad x = b_1, \quad t > 0
\end{align*}
\] (2.13, 2.14)

The coefficients \( \alpha_1 \) and \( \beta_1 \) are constants that specify flux and boundary concentration, either of which can equal zero. For \( \alpha_1 = 0 \), the flux at \( x = a \) is zero and for \( \beta_1 = 0 \), the surface concentration at \( x = a \) is zero.

The initial conditions that are honored by \( c_1(x, t) \) are given as:

\[
c_1(x, 0) = C_1(x) \quad a_1 < x < b_1 \quad t = 0
\] (2.15)

According to Carslaw and Jaeger [1959] the solution to 2.10 can be expressed as the product of one dimensional solutions:

\[
c(x, y, z, t) = c_1(x, t)c_2(y, t)c_3(z, t)
\] (2.16)

From this and equations 2.13, 2.14 and 2.15 the initial and boundary conditions for 2.10 are taken as:

\[
c(x, y, z, t) = C_1(x)C_2(y)C_3(z) \quad t = 0
\] (2.17)

\[
\alpha_{1,2,3} \frac{\partial c_{1,2,3}}{\partial x} - \beta_{1,2,3} c_{1,2,3} = 0 \quad x = a_{1,2,3} \quad t > 0
\] (2.18)

\[
\alpha_{1,2,3}' \frac{\partial c_{1,2,3}}{\partial x} + \beta_{1,2,3}' c_{1,2,3} = 0 \quad x = b_{1,2,3} \quad t > 0
\] (2.19)

Plugging 2.16 into 2.10 gives:

\[
c_2(y, t) c_3(z, t) \frac{\partial^2 c_1(x, t)}{\partial x^2} + c_1(x, t) c_3(z, t) \frac{\partial^2 c_2(y, t)}{\partial y^2} + c_1(x, t) c_2(y, t) \frac{\partial^2 c_3(z, t)}{\partial z^2} =
\]

\[
\frac{1}{D} \left[ c_2(y, t) c_3(z, t) \frac{\partial c_1(x, t)}{\partial t} + c_1(x, t) c_3(z, t) \frac{\partial c_2(y, t)}{\partial t} + c_1(x, t) c_2(y, t) \frac{\partial c_3(z, t)}{\partial t} \right]
\] (2.20)

Equation 2.20 can be rewritten according to the product rule as:
\[
\frac{\partial^2 c_1(x,t)c_2(y,t)c_3(z,t)}{\partial x^2} + \frac{\partial^2 c_1(x,t)c_2(y,t)c_3(z,t)}{\partial y^2} + \frac{\partial^2 c_1(x,t)c_2(y,t)c_3(z,t)}{\partial z^2} = \frac{1}{D} \left[ \frac{\partial c_1(x,t)c_2(y,t)c_3(z,t)}{\partial t} \right]
\] (2.21)

Where the product of \( c_1(x,t) \), \( c_2(y,t) \), and \( c_3(z,t) \) can be expressed as \( c(x, y, z, t) \) it follows that:

\[
\frac{\partial^2 c(x,y,z,t)}{\partial x^2} + \frac{\partial^2 c(x,y,z,t)}{\partial y^2} + \frac{\partial^2 c(x,y,z,t)}{\partial z^2} = \frac{1}{D} \left[ \frac{\partial c(x,y,z,t)}{\partial t} \right]
\] (2.22)

Equation 2.22 is equivalent to equation 2.10 which shows that the solution to 2.10 can be expressed as the product of one dimensional solutions, equation 2.16. Carslaw and Jaeger [1959] point out that the initial condition of 2.10 must be expressible as the product of the initial conditions for the one dimensional problems. If this condition is met then the solution to a three dimensional PDE can be expressed as the product of the individual one dimensional solutions.

2.1.2 Deriving the Horizontal Plane Source Solution

Considering the one dimensional advection and three dimensional dispersion equation given in 2.23, the solution can be derived as the product of two diffusion equations and one advection/diffusion equation [Galya, 1987]. Equation 2.23 also considers retardation, \( R[-] \) and first order decay, \( \lambda [1/\text{yr}] \) and accounts for a contaminant source, \( M_s [\text{kg/yr}] \).

\[
\frac{\partial c}{\partial t} + \frac{v}{R} \frac{\partial c}{\partial x} = \frac{D_x}{R} \frac{\partial^2 c}{\partial x^2} + \frac{D_y}{R} \frac{\partial^2 c}{\partial y^2} + \frac{D_z}{R} \frac{\partial^2 c}{\partial z^2} - \lambda c - \frac{M_s}{\theta}
\] (2.23)

Considering transport in the ‘Z’ dimension there are two possible boundary conditions that must be considered at the lower extent; An infinitely thick aquifer where the concentration approaches zero at infinity, equation 2.25, and an aquifer of finite thickness (\( H \)) where the lower boundary condition is a no flux boundary, equation 2.26. The upper boundary condition in both cases is a no flux boundary given by equation 2.24.
\[ D_z \frac{\partial c}{\partial z} = 0 \quad z = 0 \quad (2.24) \]
\[ c = 0 \quad z = \infty \quad (2.25) \]
\[ D_z \frac{\partial c}{\partial z} = 0 \quad z = H \quad (2.26) \]

Consider the one dimensional diffusion equation, equation 2.27:

\[ \frac{\partial^2 c}{\partial z^2} - \frac{1}{D} \frac{\partial c}{\partial t} = 0 \quad (2.27) \]

A particular solution for equation 2.27 is given by Carslaw and Jaeger [1959] in equation 2.28:

\[ u = t^{-\frac{1}{2}} e^{-z^2/4Dt} \quad (2.28) \]

Equation 2.28 can be integrated with respect to \( z \) giving equation 2.29 which is the concentration of solute diffusing from a point into an infinite plane where \( z \) is the point where the concentration is evaluated and \( z' \) is the location of the source.

\[ c(z, t) = \frac{1}{2\sqrt{\pi Dt}} e^{-(z-z')^2/4Dt} \quad (2.29) \]

Considering the case of an aquifer of infinite thickness with boundary the conditions presented in equations 2.24 and 2.25 the solution is expressed by equation 2.30 which uses the method of images outlined in Carslaw and Jaeger [1959] to account for the no flux boundary at the water table (\( z=0 \)) [Galya, 1987].

\[ c(z, t) = \frac{1}{2\sqrt{\pi Dz}} e^{-(z-z')^2/4Dz} + \frac{1}{2\sqrt{\pi Dz}} e^{-(z+z')^2/4Dz} \quad (2.30) \]

\[ c(z, t) = \frac{1}{2\sqrt{\pi Dz}} \left[ e^{-(z-z')^2/4Dz} + e^{-(z+z')^2/4Dz} \right] \quad (2.31) \]

Accounting for retardation;

\[ c(z, t) = \frac{1}{2\sqrt{\pi Dz/R}} \left[ e^{-(z-z')^2/(4Dzt/R)} + e^{-(z+z')^2/(4Dzt/R)} \right] \quad (2.32) \]
For the case of an aquifer of finite thickness with boundary conditions given in equations 2.24 and 2.26 and utilizing the method of images at $z = 0$ and $z = \infty$ the solution is given by equation 2.33.

$$c(z, t) = \sum_{n=-\infty}^{\infty} \frac{1}{2\sqrt{(\pi D_z t / R)}} \left[ e^{-(2nH-z'+z)^2/(4D_z t / R)} + e^{-(2nH+z'+z)^2/(4D_z t / R)} \right]$$  \hspace{1cm} (2.33)

An alternate solution that is more conducive to implementation in Excel VBA is derived by Carslaw and Jaeger [1959] using the method of Green’s functions and presented below:

$$c(z, t) = \frac{1}{H} \left[ 1 + 2 \sum_{n=1}^{\infty} e^{-\left(\frac{n^2 \pi^2 D_z t}{H^2 R}\right)} \cos \left(\frac{n \pi z}{H}\right) \cos \left(\frac{n \pi z'}{H}\right) \right]$$  \hspace{1cm} (2.34)

Where $R = \textit{retardation coefficient}$

$$D_z = \alpha_z \cdot v$$

$H = \textit{aquifer thickness}$

The solution for 2.27 in the ‘Y’ dimension is similar in form to equation 2.32; however, the solution considers a line source between $-B/2 \text{ to } +B/2$ where $B$ is the length of the line or OWS in the case of the aquifer model. Also the boundary conditions are slightly different because the aquifer under consideration is assumed to be of infinite areal extent. The boundary conditions defined by Galya [1987] for this solution are as follows:

$$c = 0 \quad \text{at} \quad y \pm \infty$$  \hspace{1cm} (2.35)

Again beginning with equation 2.28 but in the ‘Y’ dimension and considering the boundary conditions expressed by equation 2.35, the solution outlined by Crank [1975] is given as:

$$c(y, t) = \frac{1}{2\sqrt{(\pi D_y t)}} e^{-(y-y')^2/(4D_y t)}$$  \hspace{1cm} (2.36)

The solution presented by equation 2.37 is obtained by integrating 2.36 between $-B/2 \text{ and } +B/2$ [Galya, 1987] giving:
\[ c(y, t) = \frac{1}{2B} \left[ \text{erf}\left(\frac{B}{2} - y - y'\right) + \text{erf}\left(\frac{B}{2} - y + y'\right) \right] \] (2.37)

Considering retardation:
\[ c(y, t) = \frac{1}{2B} \left[ \text{erf}\left(\frac{B}{2} - y - y'\right) + \text{erf}\left(\frac{B}{2} - y + y'\right) \right] \] (2.38)

Where \( B = OWS \text{ width} \)
\( D_y = \alpha_y \cdot v \)

The solution for a line source in the ‘X’ dimension was developed by Galya [1987] by first noting that the form of the solution is similar to that of 2.38.
\[ c(x, t) = \frac{1}{2L} \left[ \text{erf}\left(\frac{L}{2} - x - x'\right) + \text{erf}\left(\frac{L}{2} - x + x'\right) \right] \] (2.39)

Note that the ‘X’ dimension is also the direction in which advection occurs, thus 2.39 must account for translation in that direction. According to Galya [1987] to obtain a solution for a fixed coordinate system a coordinate transformation must be performed. The coordinate transform that is proposed is given in equation 2.40, where \( x \) is the distance in the \( x \) direction to the calculation point for a fixed coordinate system.
\[ x'' = x - \frac{vt}{R} \] (2.40)

Substituting equation 2.40 into equation 2.39 gives the solution to equation 2.27 for a line source in the ‘X’ dimension, equation 2.41.
\[ c(x, t) = \frac{1}{2L} \left[ \text{erf}\left(\frac{L}{2} - x - x' + \frac{vt}{R}\right) + \text{erf}\left(\frac{L}{2} - x + x' + \frac{vt}{R}\right) \right] \] (2.41)

Where \( L = OWS \text{ length} \)
\( D_x = \alpha_x \cdot v \)
The solution to equation 2.23 is then given as the product of equations 2.32 or 2.34 where appropriate and equations 2.38 and 2.41 which follows the proof outlined by Carslaw and Jaeger [1959] in equations 2.10-2.22.

\[ c(x, y, z, t) = c(x, t)c(y, t)c(z, t) \] (2.42)

The solution presented by Galya [1987] is for a continuous or time varying contaminant source. The solution considers a mass loading function and contaminant decay function and is given as a convolution integral, equation 2.43.

\[ C(x, y, z, t) = \frac{1}{\theta R} \int_{0}^{t} M_s(\tau)c(x, t - \tau)c(y, t - \tau)c(z, t - \tau)T(t - \tau)d\tau \] (2.43)

The first order decay function and contaminant source functions are given as follows:

\[ T(t) = e^{-\lambda t} \] (2.44)

\[ M_s(\tau) = \text{Constant} \] (2.45)

Where \( \lambda = 1st \ order \ decay \ coefficient \)

The convolution integral considers the impulse response of a system where the impulse is the solution to equation 2.23 in the ‘X’, ‘Y’ and ‘Z’ dimensions, equations 2.32, 2.34, 2.38, 2.41 and the mass loading and decay functions, equations 2.44 and 2.45. The concentration of a contaminant in an aquifer is then the impulse response from elementary solutions superimposed upon one another from time zero to time \( t \) which is best illustrated by figure 6.

**Figure 6.** The convolution integral can best be visualized as the response of a system to multiple impulses. Here the black line is the system response to two different impulses, the pink and cyan lines.
2.2 Implementation in Excel VBA

Equation 2.43 can be solved via numerical integration relatively easily though the infinite sum requires special treatment. Galya [1987] was the first to present a FORTRAN code to numerically integrate 2.43 using a simple trapezoidal rule. The model developed by Galya [1987] is capable of considering multiple sources and computing the concentration at up to forty locations. User input is taken via text files or command line prompts on a DOS based computer. Currently the program is out of date and must be run through a DOS emulator as it was compiled for a 16 bit system.

2.2.1 Concentration

The current implementation in Excel makes simplifications to 2.43 to simplify the user interface and make the program as user friendly as possible. The primary simplification to 2.43 is the integration time, which is assigned a large value to simulate steady state conditions. Steady state conditions are sufficient for screening level purposes because they capture the average behavior of the system under evaluation. The user cannot specify a variable contaminant source concentration in the aquifer model which also minimizes the input requirements without greatly limiting the model. The current implementation does not account for multiple OWS but future development will focus on this capability. The temporal discretization of 2.43 is hardcoded and cannot be changed by the user but the value that was selected provides accurate results for evaluating OWS. Again the motivation for this was to simplify user inputs.

Galya [1987] presents algorithms adapted from the work of Codell and Schriber [1977] that improve the computational efficiency by minimizing the number of calculations necessary for evaluating equation 2.43. New integration limits may be calculated via equations 2.46 and 2.47 as only a portion of the curve significantly contributes to the calculated concentration.
\[ t_1 = t - \frac{C_{tA}}{C_{tB}} - \left[ \left( \frac{C_{tA}}{C_{tB}} \right)^2 - \left( \frac{4x^2}{C_{tB}} \right) \right]^{1/2} \]  

(2.46)

\[ t_2 = t + \frac{C_{tA}}{C_{tB}} - \left[ \left( \frac{C_{tA}}{C_{tB}} \right)^2 - \left( \frac{4x^2}{C_{tB}} \right) \right]^{1/2} \]  

(2.47)

Where \( t_1 \) and \( t_2 \) are the new lower and upper integration limits, respectively. Within the aquifer model the number of sums used to compute the convolution integral is fixed at 250 to provide the optimal combination of efficiency and accuracy. For each model run the \( \Delta t \) value changes because \( t_1 \) and \( t_2 \) change while the number of sums used to compute the convolution integral remains constant. The values \( C_{tA} \) and \( C_{tB} \) are defined below:

\[ C_{tA} = \frac{2xV}{R} + \frac{100D_z}{R} \]  

(2.48)

\[ C_{tB} = \left( \frac{V}{R} \right)^2 + \frac{4D_z\lambda}{R} \]  

(2.49)

Equation 2.34 is an infinite sum, however the number of terms needed can be limited by the following [Galaya, 1987]:

\[ N_{INF} = \left( \frac{H}{\pi} \right) \left[ \frac{25R}{D_z} (t - \tau) \right]^{1/2} + 1 \]  

(2.50)

With equations 2.46-2.50, equation 2.43 is implemented within Excel following the design in figure 9. There are two options to specify aquifer thickness which provides the user the ability to evaluate the effect of a no flow boundary along the bottom of the aquifer, such as a confining unit, on contaminant transport. By entering a value of ‘0’ for ‘H’ equation 2.32 is used rather than equation 2.34. For all other values of H equation 2.34 is used. In theory, for any combination of relatively large ‘H’ and small ‘D_z’ the solution of equation 2.34 approaches that of equation 2.32. Further improvements could be made to determine the ratio of H:D_z where equation 2.34 approaches equation 2.32 enabling the model to automatically select the solution method, possibly resulting in an improvement in the computation time.
2.2.2 Mass Flux

The aquifer model can also be used to estimate mass flux. Mass flux is an important model output that can be used in a variety of ways. For example a user may wish to estimate nitrate loads from an OWS to a stream or lake and the likelihood of exceeding the nitrate TMDL for that water body. In addition to a mass flux estimate, a plume cross section can also be generated in the y-z or x-y plane with this algorithm.

\[ M \left[ \frac{kg - N}{yr} \right] = \sum_{i=1}^{n} v \cdot c_i(t, x, y, z) \cdot dy \cdot dz \quad (2.51) \]

The mass flux algorithm is constructed using equation 2.51, which calculates mass flux for a cross section perpendicular to the hydraulic gradient, figure 7. The extent of the plume in the ± y and z direction is determined by calculating the location where the plume concentration is approximately 0.0004 mg/l. These locations mark the maximum extent of the plume. This concentration value was chosen to delineate the extent of the plume after testing several different values including zero concentration. Smaller concentration values require significantly more calculations and can cause the model to fail. While smaller values are preferable for accuracy, larger concentration values increase the speed of the model but reduce the accuracy of the mass flux calculation. Upon determining the extent of the plume it is then discretized into N rows and M columns where the total number of cells across the entire cross section is 1600. For most situations increasing the discretization of the plume will minimally improve the precision of the mass flux calculation at a great cost to the computation time.

The number of rows and columns is determined by the ratio of the plume depth to height. This is necessary to avoid errors that could arise when there is a large difference between the transverse dispersivity values. By determining the number of rows and columns based on plume width and depth the mass flux algorithm will increase the discretization along the dimension.
where the concentration gradient is the highest. The concentration in equation 2.51 is calculated at the center of each cell and mass flux is calculated as the product of the volumetric flux and the cell concentration. Leveraging the symmetry of the plume the computation time is reduced in half by calculating the mass flux for half of the plume and then doubling the calculated mass flux.

**Figure 7.** illustrates how the plume is discretized into M columns and N rows. Mass flux is then calculated for each element.

The plume cross sections, in the y-z and x-y planes, are generated using equation 2.51 in a manner similar to the method described to calculate mass flux. The x-y plume cross is essentially an aerial view of the plume. The user must specify the ‘x’ location where the plume cross section is to end and the ‘z’ plane where the plume is to be located. The number of rows and columns that are used to generate the plume cross sections are fixed. For both the y-z and x-y cross sections there are exactly 40 rows and 40 columns. This was necessary because of the limited graphics capabilities in Excel. The one disadvantage of fixing the number of rows and columns is that the image that is generated is at times distorted. For example, a y-z cross section with a depth of 10 feet and a width of 50 feet will look square because it contains the same number of rows in the ‘Z’ dimension as it has columns in the ‘Y’ direction, figure 8. However the width and depth or length of the plume is always reported so the user will have an understanding of the actual dimensions of the plume.
**Figure 8**, plume cross sections constructed by the aquifer model utilizing the technique described above. The images are not proportional but plume dimensions are listed on the graphics to allow the user to understand the geometry of the plume.
Figure 9, the design of the VBA code used by the aquifer model to solve the HPS solution. Future development may focus on methods to allow the aquifer model to select the appropriate equation for the aquifer under consideration, equations 2.34 and 2.32.
2.3 Automated Parameter Estimation

There are several methods for the user to obtain the parameter values for the aquifer model. Several of the parameter values are automatically obtained from STUMOD if a vadose zone simulation is conducted prior to running the aquifer model. The user is given the option to change these values if needed. Other parameter values such as STU dimensions can be easily obtained in the field or from design drawings. Dispersivity values and the hydraulic gradient are somewhat more difficult to measure accurately in the field and literature values are often site specific. Because of this, methods have been developed and incorporated in the aquifer model to allow the user to estimate these values from data that can be gathered in the field.

2.3.1 Dispersivity

Dispersion is the term that describes the irreversible spreading of a solute within an aquifer beyond the volume expected by advection alone [Bear, 1979]. This spreading is due to diffusion driven by concentration gradients, known as molecular diffusion, and by diverging flow paths of the solute particles, known as mechanical dispersion. The sum effect of these spreading forces is termed hydrodynamic dispersion, equation 2.52. In practice the effect of mechanical dispersion is much greater than the effect of molecular diffusion and hydrodynamic dispersion will be largely described by mechanical dispersion, equation 2.53.

\[ D_h = \alpha_m v + D^* \]  \hspace{1cm} (2.52)
\[ D_h = \alpha_m v \]  \hspace{1cm} (2.53)

Molecular diffusion was first described by Adolf Fick in 1855 [Fick, 1855]. Fick’s first law states that diffusive flux is proportional to the concentration gradient. Mechanical dispersion is commonly assumed to also be a Fickian type process and the amount of dispersion to be proportional to the seepage velocity [Bear, 1979; Fetter, 1999]. While mechanical dispersion
could in theory be described by a mathematical model for each flow path within a porous media such an approach is impractical. Describing mechanical dispersion as a Fickian process, however, is far more practical. The proportionality constant in equation 2.52 and 2.53 is 

dispersivity, which is a parameter that in theory describes the tortuosity of the flow paths within the porous media. The magnitude of dispersivity however, has been found to be largely dependent on the transport scale. Numerous studies have attempted to quantify the relationship between flow length and dispersivity. Lallemand-Barres and Peaudecerf [1978] were the first to publish a log-log plot of dispersivity and flow length which suggests that dispersivity can be approximated as \(1/10\)th the flow length. More recent work by Gelhar [1986] and Gelhar et al [1992] show that this common assumption is perhaps flawed and could lead to excessively high dispersivity values and consequently low concentrations. The work of Gelhar et al [1992] suggests that dispersivity may reach some asymptotic value at large flow lengths and several methods have been developed to estimate dispersivity given these observations [Neuman, 1990; Xu and Eckstein, 1995].

\[
\alpha_x = 0.83 (\log_{10}(x))^{2.414} \tag{2.54}
\]

\[
\alpha_y = \frac{1}{10} \alpha_t = 0.083 (\log_{10}(x))^{2.414} \tag{2.55}
\]

\[
\alpha_z = \frac{1}{100} \alpha_t = 0.0083 (\log_{10}(x))^{2.414} \tag{2.56}
\]

The aquifer model provides a method whereby the user can choose to allow the model to estimate dispersivity values based on flow length. The method that was selected was chosen based on a literature review of studies that reported dispersivity values for surficial sand aquifers [Bitsch and Jensen, 1990; Mallants et al., 2000; Sudicky et al., 1983]. The selection criteria also incorporated the observations of studies that considered dispersivity values measured in other types of aquifers [Gelhar, 1986; Gelhar et al., 1992]. The criteria that were established were that
the method follow the observations of dispersivity reaching asymptotic values over large flow lengths and that it must also reproduce the observed dispersivity values reasonably well. The relationship developed by Xu and Exstein [1995], equation 2.54, meets these criteria and was chosen as the method to estimate dispersivity in the model. This method has precedence as well, as it is a method used by the EPA for estimating dispersivity values and has been incorporated as standard practice in contaminant transport modeling by some state environmental protection agencies [EPA, 2013; Howarth et al., 2002]. Equations 2.55 and 2.56 determine the transverse lateral and transverse vertical dispersivity. These relationships are based on the observations of many that contaminant plumes are generally flat and narrow in comparison to the longitudinal length. These relationships are not based on any physical data but are generally conservative estimates of dispersivity. If more accuracy is required in model predictions, the user should independently evaluate dispersivity at the location under consideration.

2.3.2 Hydraulic Gradient

The hydraulic gradient and groundwater seepage velocity are critical parameters that are often difficult to measure. The seepage velocity can be calculated using a simple relationship between Darcy velocity, porosity and by making use of the Dupuit approximation that flow is essentially horizontal, equation 2.57 [Bear, 1979; Dupuit, 1863]. The challenge is determining the hydraulic gradient. One common method is the graphical ‘Three-point Problem’ where the strike and dip of a plane can be determined using three points [Fetter, 2001]. This method requires a pencil and paper approach which is relatively simple but time consuming. In order to provide the user a way to quickly and accurately determine both the magnitude and direction of the hydraulic gradient an algorithm was developed based on the work of Fienen [2005] that solves the ‘Three-point Problem’ using vector analysis. The input data required from the user are
three hydraulic head measurements using any reference datum and the associated latitude and longitude coordinates of those measurements.

\[ v_x = \frac{q}{n} = -\frac{k_{sat}}{n} \frac{dh}{dl} \] (2.57)

Using three spatially located head measurements, two vectors can be constructed that lay in the plane defined by the three head measurements. Let \( \mathbf{p}_1 = (x_1, y_1, z_1) \), \( \mathbf{p}_2 = (x_2, y_2, z_2) \) and \( \mathbf{p}_3 = (x_3, y_3, z_3) \) be the head measurements where the ‘x’, and ‘y’ points represent latitude and longitude coordinates projected on a flat surface and ‘z’ the observed hydraulic head. Then two vectors that are positioned end to end can be constructed by subtracting \( \mathbf{p}_1 \) from \( \mathbf{p}_2 \) and \( \mathbf{p}_1 \) from \( \mathbf{p}_3 \).

\[ \mathbf{v}_1 = \begin{bmatrix} v_{1i} \\ v_{1j} \\ v_{1k} \end{bmatrix} = \mathbf{p}_2 - \mathbf{p}_1 = \begin{bmatrix} (x_2 - x_1) \\ (y_2 - z_1) \\ (z_2 - z_1) \end{bmatrix} \] (2.58)

\[ \mathbf{v}_2 = \begin{bmatrix} v_{2i} \\ v_{2j} \\ v_{2k} \end{bmatrix} = \mathbf{p}_3 - \mathbf{p}_1 = \begin{bmatrix} (x_3 - x_1) \\ (y_3 - z_1) \\ (z_3 - z_1) \end{bmatrix} \] (2.59)

Selecting \( \mathbf{v}_1 \) such that it always lies to the right of \( \mathbf{v}_2 \) and calculating the cross product of \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) will give a vector normal to the plane containing \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) pointing in the positive ‘z’ direction, equation 2.60.

\[ \mathbf{v}_1 \times \mathbf{v}_2 = \det \begin{bmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ v_{1i} & v_{1j} & v_{1k} \\ v_{2i} & v_{2j} & v_{2k} \end{bmatrix} = \begin{bmatrix} (v_{1j}v_{2k} - v_{2j}v_{1k}) \mathbf{i} \\ (v_{2i}v_{1k} - v_{1i}v_{2k}) \mathbf{j} \\ (v_{1i}v_{2j} - v_{2i}v_{1j}) \mathbf{k} \end{bmatrix} \] (2.60)

Where the unit vector of \( \mathbf{v}_1 \times \mathbf{v}_2 \) can be calculated by equation 2.55, where \( \| \cdot \| \) indicates magnitude:

\[ \mathbf{n} = \frac{1}{\| \mathbf{v}_1 \times \mathbf{v}_2 \|} (\mathbf{v}_1 \times \mathbf{v}_2) \] (2.61)
Defining the projection of $\vec{n}$ onto the horizontal x-y plane as $\vec{n}_{proj}$, will give a vector that can be used to find the direction of the hydraulic gradient. This vector can be thought of as the shadow of the unit normal vector, $\vec{n}$ on a horizontal plane if illuminated from directly above.

$$\vec{n}_{proj} = \vec{n} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} \vec{n}_x \\ \vec{n}_y \\ 0 \end{bmatrix} \quad (2.62)$$

The angle between the unit vector pointing in the direction of North $\vec{a}_x^T$ (where North is $0^0$) and $\vec{n}_{proj}$ can be calculated using equation 2.63, giving the direction of the hydraulic gradient in degrees relative of North, where $^T$ indicates the transpose, as:

$$\theta = \cos^{-1}\left( \frac{\vec{a}_x^T \cdot \vec{n}_{proj}}{\|\vec{a}_x\| \|\vec{n}_{proj}\|} \right) = \cos^{-1}\left( \frac{\vec{a}_x^T \vec{n}_{proj}}{\sqrt{\vec{a}_x^T \vec{a}_x \vec{n}_{proj}^T \vec{n}_{proj}}} \right) \quad (2.63)$$

Equation 2.63 will give the inner angle between $\vec{a}_x$ and $\vec{n}_{proj}$ which is always less than $180^0$ but the true angle can easily be determined by observing the sign of the ‘x’ and ‘y’ components of $\vec{n}_{proj}$. A positive value for both ‘x’ and ‘y’ or a positive and negative value for ‘x’ and ‘y’, respectively, indicates an angle between $\vec{a}_x$ and $\vec{n}_{proj}$ less than $180^0$ lying in quadrant one or four. If the values of ‘x’ and ‘y’ are both negative or negative and positive, respectively, then the angle is greater than $180^0$ when measured clockwise from north and the angle lies in quadrant two or three.

The direction of the hydraulic gradient being established, it is relatively easy to then calculate the magnitude of the hydraulic gradient. The magnitude is measured off a horizontal reference plane giving the magnitude of the gradient in slope form or length per length which is a form familiar to many and can be used directly in computing the seepage velocity. Observing the unit normal vector calculated by equations 2.60 and 2.61 it is easy to see that the dip angle of the plane defined by the three head observations is equal to the angle between the unit normal
vector and a vector normal to the horizontal plane. The magnitude is then calculated by the following:

\[
g_{\text{ad}} = \frac{\vec{n}_k}{\|\vec{n}_{\text{proj}}\|}
\]  (2.64)

Equations 2.57 through 2.64 are implemented in Excel VBA as part of the aquifer model and provide the user a quick and accurate method to determine the direction and magnitude of the hydraulic gradient. This algorithm alone may provide the user with useful information about the potential for contamination of a receptor. By observing the magnitude and direction of the hydraulic gradient over time it may be possible to rule out the possibility of contaminant transport from an OWS to a potential receptor. For example, if the direction of the hydraulic gradient is consistently directed away from a potential receptor then contamination is likely not to occur. In the case of a well it may be possible to determine if the cone of depression is likely to alter the local direction of the hydraulic gradient and take preventative measures. The obvious limitation is that three locations must be available to measure the elevation of the water table.

### 2.4 Model Performance Evaluation

The purpose of model performance evaluation is to quantify prediction uncertainty. Parameter sensitivity analysis evaluates the impact a parameter value has on model predictions. Sensitivity analysis results provide the user with information that can be used to reduce uncertainty in model predictions in a cost effective manner. Model uncertainty analysis calculates the range of possible model outcomes given the range in model input parameters. Uncertainty analysis results give the user a method for easily estimating the likelihood of achieving a particular model outcome.

Model performance evaluation was conducted on the aquifer model using a local parameter sensitivity technique and a Monte Carlo type uncertainty analysis. The results from
this performance evaluation are presented below giving the user an understanding of which model parameters have the greatest impact on model output. Also presented is a cumulative frequency diagram of model outputs for a large range of input parameters. These results can be used to estimate the likelihood of achieving a reduction in nitrate mass flux over a distance of 200 feet.

2.4.1 Parameter Sensitivity Analysis

Parameter Sensitivity Analysis is a useful tool for model users because it will give users an idea of which parameters will have the most impact on model predictions. In a situation where the user wishes to minimize uncertainty in model predictions but has limited resources to do so, parameter sensitivity analysis will indicate whether measurement of a specific parameter will likely yield a large reduction in uncertainty, or if it would likely cause no improvement in model performance. There are several standard methods to conduct sensitivity analysis which are classified by the way the parameters are handled. The two general categories that sensitivity analysis techniques fall into are local and global methods [Geza et al., 2010; Saltelli et al., 2000]. Global techniques function by evaluating the impact on model output from changes in multiple parameter values while local techniques will only evaluate the change in model output from a change in a single parameter value.

For most models there are an infinite number of possible parameter values because parameter values are typically taken from a continuous distribution rather than discrete distributions. Saturated hydraulic conductivity is an example of a parameter value that exists as a continuous distribution because, for example, it may have a value of 12.0 [ft/d] or 10.25 [ft/d]. Because of this there are an infinite number of possible parameter combinations as well. Parameters may have a correlative effect on model output, meaning that a slight change in two or
more parameter values may produce a much larger change in model output than a single large change in only one parameter value. Global sensitivity analysis techniques are capable of sampling the entire parameter space and capturing these correlative effects between parameters. Parameters that are correlated cannot be independently estimated. These methods are especially useful for large complex models that have many parameters.

Local sensitivity techniques do not capture the correlative effect of parameters but these techniques are still useful for evaluating models. Local techniques are particularly suited for evaluating models with relatively fewer parameters because the parameter space may be less complex. Also, local techniques are likely to capture the behavior of the model that a user might experience when they refine parameter values. For example a user who wishes to improve confidence in model predictions will likely choose to independently evaluate one parameter at a time to minimize cost. Local sensitivity analysis results can provide guidance that the user can follow for refining the model as well as the expected results for each refinement. Because of this, a local sensitivity analysis technique was used to evaluate parameter sensitivity for the aquifer model.

2.4.2 Sensitivity Analysis Results

The initial parameter values were established for a 35 meter by 35 meter source plane receiving a nitrate load of 219 kg/yr or 30 mg-N/L at a HLR of 5.95 m/yr (1.6 cm/day) at the water table. This would be equivalent to an OWS receiving approximately 5300 gal/day and a total nitrogen concentration equal to or greater than 30 mg-N/L in the septic tank effluent. Within a typical OWS, nitrate is removed via denitrification within the STU before percolate reaches the water table. For this reason the nitrogen concentration in effluent applied to the infiltrative surface would likely be greater than 30 mg-N/L. The dispersivity values were calculated using
equations 2.54 through 2.56 at a distance of 200 feet. The mass flux at a plane 200 feet down
gradient was calculated for each change in parameter value. Parameter sensitivity was calculated
by incrementally changing one parameter at a time through values of -90% to +100% of the
initial value while holding all other parameter values at their initial values.

Results from this sensitivity analysis are presented in figures 10, 11 and 12. Parameter
sensitivity analysis results indicate that model output is sensitive to retardation, porosity, and the
first order denitrification coefficient. These results fit with the widely held conceptual model that
denitrification is the most critical process in controlling nitrate transport in groundwater. The
initial first order denitrification value that was used was the median value reported by McCray et
al. [2005]. Figure 11 indicates that model output was sensitive to retardation coefficients less
than one. While retardation coefficients greater than unity are common, retardation values less
than unity are possible and have important implications for nitrate transport in groundwater.
Anion exclusion, caused by the repulsion between soils with a negative surface charge and
anionic solutes, may restrict solutes to faster moving pore water [James and Rubin, 1986;
McMahon and Thomas, 1974]. Sensitivity results show that this will have a large effect on the
calculated concentration because the faster travel time will minimize the amount of nitrate lost to
denitrification. Porosity is an important factor controlling seepage velocity and thus transport
time (equation 2.57). As porosity decreases seepage velocity increases decreasing the transport
time, as can be seen in equation 2.57. A decrease in porosity also results in a smaller pore
volume available to dissolve the contaminant mass which results in higher concentrations. The
sensitivity of model output to porosity is likely due to both the increased pore water velocity and
decrease in volume.
Figure 10, the normalized sensitivity analysis results. These results show that denitrification, porosity and retardation have the largest impact on model output. These parameters should be independently evaluated or calibrated to minimize uncertainty.

Figure 11, the sensitivity analysis results for five parameters identified in figure 10 as most sensitive. These results show that small porosity, retardation, and decay values have the largest impact on model output.
Figure 12. The results for the remaining parameters not shown in Figure 11. These parameters have little impact on model output relative to the first order decay, retardation and porosity parameters. However, changes in these parameters do have an impact on model output, primarily HLR and concentration.

While sensitivity analysis results indicate denitrification, porosity and retardation are critical parameters for the aquifer model, the probable range of these parameter values and uncertainty in actual measurements is also important to consider. Denitrification rates ranging over several orders of magnitude are reported in literature [McCray et al., 2005]. This large range is due to the temporal and spatial variation in microbial processes occurring within an aquifer. Because of this, independently measured denitrification rates may not significantly reduce uncertainty in model outputs. Retardation and porosity in contrast do not vary over several orders of magnitude. Under most conditions nitrate is not retarded eliminating uncertainty related to this parameter. Measurements of porosity commonly are within 20% of the actual value thus greatly reducing model uncertainty. Moreover, porosity values are always within a range of 0 -1 and generally do not exceed a value of 0.5 for most aquifers.
Results indicate that hydraulic conductivity and hydraulic gradient are not sensitive parameters, but due to the large range of possible values these should also be considered critical parameters for the aquifer model. Both hydraulic conductivity and hydraulic gradient control the transport time of solutes when retardation does not occur. Under denitrifying conditions longer transport times may result in a larger mass removal from the aquifer. As a result, in the application of the aquifer model the denitrification rate should be regarded as the most critical parameter followed by hydraulic conductivity, hydraulic gradient and finally retardation and porosity.

**2.4.3 Uncertainty Analysis**

Model uncertainty analysis seeks to quantify model behavior so that the user can have an understanding of the probable model outcomes. As previously mentioned there are an infinite number of probable parameter values and combinations. Uncertainty analysis is a method that can be used to quantify probable model outcome for this large parameter space. This is done by selecting random combinations of parameter values and observing model outcome, known as the Monte Carlo Simulation method [Mishra, 2009]. Parameter values are selected from probability distributions that honor the natural or observed distributions of these parameter values, i.e. normal, log normal, linear etc. Selection of the probability distribution functions for the parameter values is critical for correctly mapping input uncertainty to model output uncertainty. Another critical aspect of the uncertainty analysis is running the model a sufficient number of times such that the output, when plotted as a cumulative frequency diagram, does not change with additional model runs [Mishra, 2009].

Model uncertainty analysis was conducted for three soil textures (two sands and a sandy clay loam) supported by STUMOD to provide insight into probable model outcomes. The
parameter sensitivity analysis indicates that model output is sensitive to the denitrification, retardation and porosity parameters. Establishing correct probability distribution functions for these parameters is critical, however little data exists for nitrate retardation as this phenomenon is not regularly observed. As previously mentioned anion exclusion has been observed in lab experiments but has not been reported in aquifers for nitrate transport. Because sandy soils are not characterized by a strong surface charge it is safe to assume that anion exclusion is not an important process. As a result, though retardation is a sensitive parameter it was not include in the uncertainty analysis for the two sands and only included to a limited extent for the sandy clay loam using a random uniform distribution, table 1.

The input concentration of nitrate as nitrogen at the water table was the same as was used for the parameter sensitivity analysis (30 mg-N/L). This value was allowed to vary uniformly within ±3 mg-N/L to include the effect of uncertainty in nitrogen effluent concentration at the water table. Because the effluent concentration was not identified as a sensitive parameter in the parameter sensitivity analysis this input in the model uncertainty analysis is not likely to have a large effect.

The probability distribution for the first order denitrification parameter was obtained from McCray et al. [2005] who developed a cumulative probability distribution function to describe denitrification rates reported in literature. This study is the most comprehensive review of reported first order denitrification values. The probability distribution function for this parameter is reported in table 1 where the independent variable is a cumulative probability between zero and one selected by a random number generator. The output of this function strongly favors smaller, rather than larger, first order denitrification values, however it does not yield values less than 0.004 (1/day) meaning this function is incapable of considering the case of
no denitrification. To address this, the distribution function was modified such that it would generate values less than or equal to the 50\textsuperscript{th} percentile value reported by McCray et al. [2005].

Porosity and hydraulic conductivity are important parameters for the aquifer model. There are numerous probability distribution functions that can be used to describe these parameters if viewed from a geostatistical standpoint. For example the hydraulic conductivity field of an aquifer may be adequately described by a particular geostatistical function because of its geomorphology (alluvial, colluvial etc.) [Goovaerts, 1997]. However, the purpose of this model uncertainty analysis is not to evaluate the uncertainty due to a lack of understanding of the geomorphology of an aquifer, which would be somewhat specific in scope. Rather, the purpose is to evaluate uncertainty in model output for all aquifers composed of soils that fall into the previously defined textural classes, a somewhat more general approach. The shape of the distributions for porosity and hydraulic conductivity were obtained from Rosetta. Rosetta is a program that uses pedo transfer functions to generate soil hydraulic properties from basic soil data such as texture [Schaap et al., 2001]. The mean and standard deviation for each soil texture that was used in the uncertainty analysis was derived via an independent statistical analysis of reported soil data [McCray, 2011].

The hydraulic gradient is an important parameter that can control the transport time of solutes. Hydraulic gradients are likely to vary significantly for any number of reasons including geologic structure, preferential recharge, and anthropogenic activities such as groundwater extraction. The probability distribution function for hydraulic gradient was selected to be a random uniform distribution ranging between 0.1 – 5\%. This range was selected because under low hydraulic gradients complex advection fields are not as likely to develop. Because the HPS
solution only considers one dimensional advection it would not be appropriate to apply this model to aquifers where complex advection fields are likely to exist.

Gelhar et al. [1992] presents dispersivity values from an extensive literature review. These results appear to indicate that a relationship may exist between transport distance and dispersivity. The reported data indicate multiple dispersivity values have been observed for equal transport distances. While Xu and Eckstein [1995] provide a method to estimate dispersivity this method does not provide insight into the probable range of dispersivity values for a particular transport distance. Due to a lack of an adequate probability distribution function for dispersivity, these values were drawn from a random uniform distribution. The upper and lower limits of this uniform distribution are presented in table 1 and represent a wide range of dispersivity values that fall within the observations of Gelhar et al. [1992] and are reasonably predicted by the method of Xu and Eckstein [1995].

Table 1, the distributions used for each parameter included in the uncertainty analysis. The equations used for denitrification are presented below.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Distribution</th>
<th>Mean/Max</th>
<th>Std/Min</th>
</tr>
</thead>
<tbody>
<tr>
<td>R [-]</td>
<td>Random Uniform</td>
<td>1</td>
<td>0.95</td>
</tr>
<tr>
<td>n [-]</td>
<td>Random Log Normal</td>
<td>0.4</td>
<td>0.06</td>
</tr>
<tr>
<td>grad [m/m]</td>
<td>Random Uniform</td>
<td>0.05</td>
<td>0.001</td>
</tr>
<tr>
<td>Conc. [mg-N/L]</td>
<td>Random Normal</td>
<td>30</td>
<td>3</td>
</tr>
<tr>
<td>λ [1/yr]</td>
<td>Random Uniform*</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>αT [m]</td>
<td>Random Uniform</td>
<td>5</td>
<td>0.5</td>
</tr>
<tr>
<td>αTH [m]</td>
<td>Random Uniform</td>
<td>1</td>
<td>0.005</td>
</tr>
<tr>
<td>αTV [m]</td>
<td>Random Uniform</td>
<td>1</td>
<td>0.005</td>
</tr>
<tr>
<td>Ksat [m/yr]</td>
<td>Random Log Normal</td>
<td>1.4</td>
<td>0.9</td>
</tr>
</tbody>
</table>

\[
y = 365.25 \cdot e^{(x-\frac{1.423}{0.1348})} \quad \text{or} \quad y = 365.25 \cdot e^{(x-\frac{0.923}{0.1348})}
\]

2.4.4 Uncertainty Analysis Results

Results from the uncertainty analysis for the three soil textures indicate that the aquifer model predicts substantial removal of nitrate for a 200 foot setback distance, figures 13 and 14. These results suggest that the denitrification parameter is controlling model output uncertainty. More specifically, denitrification values greater than the 50th percentile reported by McCray et al.
have a large impact on model output uncertainty. This conclusion is supported by the alternate uncertainty analysis that was conducted using values equal to or less than the 50th percentile denitrification value. The model outputs for these two uncertainty analyses are significantly different though the only difference was the range of denitrification values that were used.

Model output is also dependent on transport parameters such as hydraulic conductivity, hydraulic gradient and porosity. The two uncertainty analyses that were conducted reveal that when denitrification rates following the distribution reported by McCray et al. [2005] are used the differences in model outputs are not as large. However as smaller denitrification values are used, model output uncertainty will be increasingly controlled by the other parameters. These results reveal that model output uncertainty changes in response denitrification and under conditions of low denitrification output uncertainty is largely controlled by the physical transport parameters, hydraulic conductivity, hydraulic gradient and porosity.

From a user perspective these results reveal the likelihood of achieving a particular model outcome given uncertainty in model input parameters. Specifically, for two sands and a sandy clay loam the aquifer model predicts a high probability of achieving excellent nitrate removal. However, for an alternate case with lower denitrification values the amount of nitrate remaining in the aquifer can be significant, figures 13 and 14. Model uncertainty analysis results can be used directly to estimate nitrate removal if the user has a qualitative understanding of the extent to which denitrification is occurring, i.e. high or low. If not, however, the user should evaluate the potential for denitrification independently to better understand nitrate transport for their specific location.
Figure 13, uncertainty analysis results for a Sandy Clay Loam (SCL), Less Permeable Sand (SLP) and More Permeable Sand (SMP) utilizing denitrification values reported by McCray et al. [2005]. These results do not consider the case of no denitrification or little denitrification. The minimum denitrification value used is 0.004 (1/day).

Figure 14, uncertainty analysis results for a Sandy Clay Loam (SCL), Less Permeable Sand (SLP) and More Permeable Sand (SMP) utilizing denitrification up to 0.025 (1/day) which is the 50th percentile value reported by McCray et al. [2005].
2.5 Validation of the HPS Solution with a Numerical Model

This section presents a comparison between results obtained from the HPS solution to those from a numerical model for a non-decaying synthetic contaminant. This comparison serves as validation of the mathematics, solution scheme, and programing in Excel used to derive and solve the HPS solution. The numerical models that were used were MODFLOW and MT3DMS [Harbaugh, 2005; Zheng and Wang, 1999]. Two simulations using the numerical models were carried out for comparison to the HPS solution. The first simulation considers a homogeneous one dimensional velocity field, while the other considers a heterogeneous one dimensional velocity field; the HPS solution was derived to consider the latter. The first comparison establishes the mathematical soundness of the HPS solution while the second comparison examines potential limitations of the HPS solution for a specific case. The term validation has been carefully selected for the title of this section to set the results apart from those that will be presented in the subsequent chapter. The use of validation implies the act of establishing the veracity of the HPS solution, which is a stronger term then corroboration, meaning to provide supporting evidence [Merriam-Webster Inc., 2005]. These comparisons are not intended as a corroboration of the aquifer model, which uses the HPS solution, to observed field data. Corroboration of the aquifer model is presented in chapter three and while that analysis provides supporting evidence it does not establish the veracity of the aquifer model for evaluating contaminant transport from OWS in real aquifers.

2.5.1 The One Dimensional Homogenous Velocity Case

A numerical model (MODFLOW/MT3DMS) was created using 161 columns, 624 rows and 21 layers. The finite difference grid was refined along the portion of the model where concentration was monitored. The grid spacing for this area was 1.25 meters by 0.625 meters by
0.625 meters in the ‘X’, ‘Y’ and ‘Z’ directions, respectively. The total dimensions of the finite difference grid were 50 meters deep by 2172 meters wide by 780 meters long. These dimensions are intended to represent and aquifer of infinite areal extent and of finite thickness. Dispersivity values were assigned to ensure a grid peclet number less than one, 5 meters in the longitudinal direction and 2.5 meters in the transverse horizontal and vertical directions. The grid Peclet number is a measure of the degree to which the transport problem is dominated by advection. It is critical for understanding potential error introduced by the numerical solution schemes [Zheng and Bennett, 2002]. The hydraulic conductivity was 120 m/yr and a porosity/specific yield of 0.3 was assigned to the entire domain. “Constant Flux” boundary conditions were used for the upper and lower boundaries of the model and “No Flow” boundaries were assigned along the lateral extent of the model. The constant flux across each cell at the upper and lower extent of the finite difference grid was calculated using equation 2.57 such that the seepage velocity was constant, at 10 m/yr. This was later verified by examining the cell-by-cell flow file produced by MODFLOW.

A contaminant source was created to replicate a horizontal plane 2.5 by 3 meters with a HLR of 1 m/yr. The concentration of the synthetic contaminant in the recharge water was 32 mg/l, no decay was considered. The total mass flux of contaminant to the aquifer was 240 g/yr. Forty monitoring wells were placed along the centerline of the expected plume at the surface of the finite difference grid and at 1, 3, 5, and 9 meters below the surface. The wells were located from 20 to 755 meters from the contaminant source plane. The simulation was run to steady state conditions.

While the numerical model requires a finite difference grid and complex algorithms to accurately solve the governing equations the HPS solution does not. The same conceptual model
used to build the numerical model was also used to construct an HPS simulation. The contaminant transport problems considered by the HPS solution and the numerical model were identical in every way except the manner in which they were solved. The HPS solution was used to calculate contaminant concentrations at the same locations within the hypothetical aquifer. Because the HPS solution does not consider volumetric flux a mass flux of 240 g/yr was applied at the contaminant source plane. The dimensions of the source plane, porosity, seepage velocity and dispersivity values were identical to those that were used in the MODFLOW/MT3DMS model. The results from this comparison are presented in figures 15 and 16 which indicate that the HPS solution accurately calculates the contaminant concentration at all locations. This comparison is a validation of the mathematical derivation of the HPS solution. These results also validate the numerical integration technique that is used to solve equation 2.43 and the Excel program that was developed. While the trapezoidal integration technique can introduce error for functions that change rapidly the HPS solution is relatively constant under steady state conditions and thus the integration technique is appropriate.

**Homogeneous K-field**

![Graph](image)

**Figure 15.** validation results for the HPS solution indicate that it will accurately calculate concentration for a homogeneous velocity, one dimensional advection and three dimensional dispersion transport problem.
2.5.2 The One Dimensional Heterogeneous Velocity Case

A one dimensional homogeneous velocity is not likely to occur within an actual aquifer due to heterogeneities in hydraulic conductivity, variable recharge, and anthropogenic activity such as extraction wells. The question that is likely to arise is whether the HPS solution can be successfully applied in situations where these ideal conditions do not exist. It would be difficult to quantify all the possible error that may be incurred by applying the HPS solution to situations where a one dimensional advection field does not exist. However, one specific case is presented here where the HPS solution was compared to results from a numerical model with a heterogeneous velocity field in one dimension.

Figure 16, results from a comparison of the HPS solution to a numerical model with a one dimensional heterogeneous velocity field.

The numerical model presented in the previous section was used as a base to build a new numerical model with a heterogeneous velocity field. The same parameter values were used to construct this model with one difference. The hydraulic conductivity field was constructed using a random number generator. The hydraulic conductivity field of the new model possessed the same mean hydraulic conductivity as did the previous model. The hydraulic conductivity values
that were generated were drawn from a log normal distribution and ranged over three orders of magnitude. The resultant seepage velocities within the finite difference cells varied from 0 – 4387 m/yr but maintained a mean velocity of 10 m/yr which was verified in the cell-by-cell flow file produced by MODFLOW. Because of this a direct comparison to the HPS solution was possible. Descriptive statistics for the hydraulic conductivity field as well as the calculated seepage velocity for this setup are found in appendix A.

Concentrations calculated by the HPS solution presented in the previous section were also used for comparison to the results from the numerical model with a heterogeneous hydraulic conductivity field. Because the mean velocity remained the same for the heterogeneous hydraulic conductivity numerical model it may be expected that no possible differences could exist in the results. However, the working hypothesis was that two possible phenomenon could occur which would result in differences between the HPS solution and the heterogeneous hydraulic conductivity numerical model. The first condition is that increased longitudinal and transverse dispersion due to local differences in velocity could occur. The result from this would be decreased concentrations at the observation points in the heterogeneous model. Results in figure 16 would not fall along the one-to-one line and the RMS error displayed in figure 17 would be larger than the homogeneous case. The second phenomenon that could have occurred would have been transverse advection instead of purely longitudinal advection. This could occur if adjacent cells had higher hydraulic conductivities then the cells immediately down gradient. This arrangement of hydraulic conductivity might promote advective movement around cells of lower hydraulic conductivity.

Results from the numerical model indicate that heterogeneities in velocity do not have a significant impact and that the HPS solution is still valid under these conditions, figures 16 and
17. The results are important because they show that velocity heterogeneities do not have a substantial impact so long as they do not cause preferential flow or transverse advection to occur. In regards to the working hypothesis, local variations in velocity do not appear to increase dispersion in any dimension under steady state conditions. The variations in velocity may be significant if the timing of contaminant break-through is critical, however this condition is not of interest for evaluating an OWS. Contaminant break-through is generally not critical for an OWS because the long term transport behavior of the system is more important than the behavior at start-up when considering potential contamination of receptors. With respect to transverse advection the cell-by-cell flow file created by MODFLOW revealed that it did not occur for this case. One possible explanation is that the random nature of the hydraulic conductivity field does not create a situation where multiple cells with similar hydraulic conductivities are adjacent and thus advection remains one-dimensional.

![Root Mean Squared Error (HPS - MODFLOW/MT3D)](image)

**Figure 17.** Comparison of the root mean squared error between the HPS predicted concentrations and the numerical models with a homogeneous and heterogeneous hydraulic conductivity fields. It is unknown why a larger discrepancy exists between predictions from the numerical model with a homogeneous hydraulic conductivity field and the HPS solution at the aquifer surface.
CHAPTER 3
CALIBRATION AND CORROBORATION OF THE
ANALYTICAL MODEL

Validation of the HPS solution is presented in chapter 2 and shows that the mathematical derivation, solution scheme and programming in Excel are correct and accurately describe one dimensional advection and three dimensional dispersion of a contaminant. In order to establish the predictive capabilities of the aquifer model for real OWS and aquifers the performance was evaluated using data collected from a surficial aquifer in central Florida and comparison to two numerical models. The calibration of the aquifer model and comparison to numerical models is presented to provide supporting evidence as to the utility of this tool for evaluating contaminant transport from an OWS in aquifers. Groundwater data from a surficial aquifer receiving OWS effluent is used for the corroborations of the aquifer model by calibrating the aquifer model and two numerical models to these data and drawing a comparison between the results for the calibrated models (both calibrated parameters and goodness of fit). The numerical models were used to establish a performance baseline for the aquifer model. In this manner corroborations of the aquifer model is conducted by comparison to robust numerical models and field observations.

Section 1.2.2 in chapter 1 is a useful framework for evaluating the results presented within this chapter. Regardless of the complexity of a mathematical model it should be recognized that all models are to some degree, simplifications of reality. Because of this a quantitative measure of model performance is desirable; such analysis, however, can be misleading. Model performance with respect to observed data is specific to the conditions under which the observed data were collected and should not be taken as the expected performance for all conditions [Beven and Young, 2013]. The observations from calibration of the aquifer model as well as the
comparison to state of the art numerical models provides a good estimation of the performance of the aquifer model as these highlight the differences between the numerical models and the aquifer model. Because the numerical models that have been used are well researched and documented differences between the numerical models and aquifer model can be explained. However, since the calibrated aquifer model is not compared in a forward simulation to observed data no quantitative measure of future model performance is provided (such a measure would be site specific anyway). Rather, the user must understand the limitations of the aquifer model and use the results presented in section 2.4 to minimize uncertainty or use a more complex model and obtain higher quality input data if the cost of an incorrect prediction is high.

3.1 Field Site and Data

Groundwater data were collected at the University of Florida Gulf Coast Research and Education Center (GCREC). Data consisted of hydraulic head measurements as well as groundwater samples for a period spanning approximately four years. Groundwater samples were analyzed for nitrate and ammonium among other constituents. Because of high background nitrate concentrations a process was developed to mitigate the influence of data that were thought to be part of the background nitrate plume to facilitate model calibration. The following sections present the methodology that was used to process the nitrate concentration data for calibration of the numerical and analytical models. Also presented are the hydraulic head observations and the method that was used to estimate groundwater seepage velocity for the aquifer model.

A brief description of the hydrogeologic units within the field site is also presented in the following sections. The Floridian aquifer system is composed of several distinct hydrogeologic units that are interconnected. An understanding of these connections and flow within these units has been fundamental in the construction and evaluation of the numerical models. Significant
effort was devoted to developing a conceptual model of the site that could be defended by the hydrogeologic record. Figure 19 displays the conceptual model that was used for the construction and calibration of the contaminant transport models. Results from the calibration of the numerical models to the observed hydraulic head indicate that the conceptual model is correct and that the hydrogeologic units within the study site are hydraulically connected rather than independent units.

3.1.1 Field Site

The GCREC is located in southern Hillsborough county Florida approximately 30 miles from the city of Tampa. The facility primarily serves as an agricultural research center for the University of Florida and has numerous agricultural demonstration plots located around the facility. The facility serves as office and research laboratory space where approximately 71 people work. A large soil based OWS designed for flows in excess of 2500 gallons per day serves the facility and receives primarily domestic waste water from the offices. The OWS was constructed approximately 6 years prior to the sampling campaign, which is sufficient time to approach steady state conditions in the STU [Parzen and Siegrist, 2007].

The design HLR of the OWS is 3.26 cm/day or 0.4 gal/ft$^2$/day. The infiltration area where effluent is dispersed is approximately 82 by 115 feet in dimension. Effluent is applied in an alternating pattern to half of the infiltrative area to prevent saturated conditions from forming within the vadose zone. Because effluent is only applied to half of the total infiltrative area per dose the maximum volume applied to the infiltrative area never exceeds 5000 gallons. The infiltrative area is elevated approximately 4-5 feet above the surrounding land surface. This ensures that an unsaturated region will exist beneath the infiltrative area even during high water table conditions.
Twenty-two piezometers were installed in the surficial aquifer in the area surrounding the OWS for the purposes of this study. The piezometers have been used to collect hydraulic head measurements beginning about March 2009 through July of 2013, or approximately 4 years. In addition, groundwater sampling wells consisting of a stainless steel point and screened body connected to ¼ tubing were driven into the surficial aquifer at multiple depths on a grid pattern down gradient of the OWS, figure 18. The wells function in a manner similar to multilevel piezometers and allow groundwater samples to be drawn from multiple depths; sampling locations however cannot be used to measure hydraulic head. There are 118 groundwater sampling wells installed in the surficial aquifer.

Groundwater samples were collected from sampling wells and piezometers on four occasions: December 2010, April 2011, June 2011 and September 2011. Groundwater quality was not monitored throughout the entire study period as hydraulic head was, due to budget limitations. Groundwater samples were analyzed for various constituents including nitrate, nitrite and ammonium. Concentrations of nitrate and nitrite were reported as a sum of the NOx species. For the purposes of model calibration and corroboration the reported NOx as nitrogen concentrations were assumed to be representative of nitrate because nitrite is relatively unstable in the natural environment and is readily converted to other forms of nitrogen [Tan, 1998]. This assumption was verified by a group of samples where both nitrate and nitrite concentrations were reported all of which contained very small amounts of nitrite, less than 0.3 mg-N/L. Nitrification as well as ammonium transport were not considered during the corroboration of the aquifer model. The reported ammonium concentrations in groundwater samples did not exceed 3 mg-N/L and the mean concentration was 0.12 mg-N/L, table 2, indicating that the majority of nitrogen exists as nitrate within the surficial aquifer.
Figure 18, the layout of the GCREC field site near Tampa, Florida. The surrounding area is agricultural where synthetic fertilizers are used. The delineated nitrate plume from the OWS aligns well with the direction of the average hydraulic gradient which is directed towards a local stream.
3.1.2 Hydrogeologic Description

The Floridian aquifer system consists of several hydrogeologic units separated by confining or semi confining units. The aquifer system generally consists of a surficial aquifer, upper confining unit sometimes referred to as the intermediate aquifer, the Upper Floridian aquifer, a middle confining unit, and the Lower Floridian aquifer [McGurk, 1998; Sepúlveda et al., 2012; Yager et al., 2004]. Drinking water wells are typically located within the Upper Floridian aquifer though in some areas the upper confining unit can also be an important source of fresh water, figure 19. The surficial aquifer is generally not used as a drinking water source directly but serves as an important source of recharge for the Upper Floridian aquifer. Recharge occurs through the upper confining unit and through localized breaches that form from subsidence features such as sinkholes that have filled with sand from the surficial aquifer [Yager et al., 2004].

Figure 19, the conceptual model used to construct the numerical models and setup the calibration of the aquifer model.
The surficial aquifer is primarily composed of fine to medium fine sands [Doolittle et al., 1989]. The hydraulic conductivity of these sands within the study area ranges from less than a foot per day to tens of feet per day according to slug tests conducted at the piezometers (see Appendix C). The depth to the upper confining unit (Hawthorn Layer) at the GCREC field site is approximately 25-30 feet. The aquifer is characterized by a free water table and receives direct recharge from precipitation and OWS effluent. Water table fluctuations in response to precipitation recharge are several feet and it is not uncommon for the water table to be within one or two feet of the land surface during the summer months which is shown in figure 20. A spodic layer is present within the soil profile and is distinguished by a dark color. The spodic layer is formed by the precipitation of minerals that have been dissolved and transported through the soil profile by organic acids [Huang et al., 2012]. Precipitation of these minerals is speculated to take place due to changing redox conditions near the water table or microbial degradation of the organic acids. Chemical and physical attributes of this layer do not appear to control the migration of nitrate within the surficial aquifer.

![Water Table Fluctuations and Land Surface](image)

**Figure 20.** Water table fluctuations measured by a pressure transducer through the summer months indicate that the water table comes within a few feet of the land surface during the summer.
The upper confining unit is composed of undifferentiated deposits collectively known as the Hawthorn Group [Florida. Bureau of Geology. et al., 1986; Yager et al., 2004]. This geologic unit is an important economic resource as the phosphate deposits that are mined in Florida are located within this group. The Hawthorn group is principally composed of clay with varying amounts of sand, phosphate, and limestone. Dissolution of the limestone within the clay can cause subsidence features to form that can fill with surficial sand deposits forming direct connections between the surficial aquifer and lower aquifer units [Stewart and Parker, 1991; Yager et al., 2004]. Vertical hydraulic conductivities for this layer are reported to range between $7.6 \times 10^{-5} – 0.34$ ft/day [McGurk, 1998; Phelps, 1984]. Sand lenses within the Hawthorn group can form important artesian aquifers that are used for drinking water or form important springs. Well logs from the installation of three wells at the GCREC facility reveal that these features do exist within the vicinity of the field site. Data obtained from the well logs also reveal that the upper portion of the Hawthorn group at the GCREC facility is primarily clay, interbedded with limestone, shale and sand. Void spaces were also recorded during the installation of one well suggesting that direction connections between the surficial aquifer and lower hydrogeologic units exist here as well (see Appendix D).

The Upper Floridan aquifer includes portions of the Hawthorn group, where present the Suwanee limestone, the Ocala limestone and the top of the Avon Park formation [Merritt et al., 2004]. The Suwanee limestone is present throughout Hillsborough County and dips towards the south southwest and is approximately 300 feet below mean sea level along the southern border of the county [Campbell, 1984]. The location of the Suwanee limestone can be used to estimate the thickness of the overlying Hawthorn group. Well logs appear to indicate a contact between the lower member of the Hawthorn group and the Suwanee limestone 100-200 feet below land
The Upper Floridian aquifer is the primary production zone for groundwater and wells are typically screened within the Suwanee and Ocala limestone or Avon Park formation [Merritt et al., 2004]. The secondary porosity within these zones is the principle source of extracted groundwater.

3.1.3 Data Analysis

Groundwater samples were collected within the surficial aquifer immediately down gradient of the infiltrative surface of the OWS. Groundwater quality within the confining unit and the Upper Floridian aquifer was not tested because these aquifer units are located further from the source and the flow paths within these units are not as well understood. Initially it was thought that nitrate transport to these units would not be significant, though results from the numerical model suggest it could be. Also, as groundwater travels away from the OWS any effects on groundwater quality are likely mitigated to a certain degree which makes identification of the contaminant plume more difficult.

Table 2 presents descriptive statistics of groundwater samples and effluent samples collected during four sampling events from within the surficial aquifer. A total of 306 groundwater and 6 effluent samples were collected and analyzed during the four sampling events. While the mean and median nitrate concentrations in groundwater were below the EPA MCL (10 mg-N/L), approximately a third of the groundwater samples exceeded the MCL.
Groundwater samples also reveal that the STU appears to be functioning correctly by attenuating the movement of ammonium to groundwater via transformation of ammonium (the primary form of nitrogen leaving a septic tank) to nitrates in the unsaturated zone. Effluent samples collected at the septic tank are in line with the observations of Lowe et al. [2009] that show that the primary form of nitrogen in the septic tank is ammonium. Effluent samples show a relatively large range of ammonium concentrations which poses a challenge when estimating the mass flux of nitrate to the water table using STUMOD.

While sorption of ammonium in the surficial aquifer could account for the low ammonium concentrations observed this is not likely as the soils that compose the surficial aquifer are primarily quartz sands that have little cation exchange capacity [Tan, 1998]. In addition, ammonium sorption is generally thought to be reversible and would not likely serve as an effective sink for nitrogen from a nearly constant input over many years.

Two piezometers were located up gradient of the OWS infiltrative area at a sufficient distance to ensure effluent percolate would not reach the screens. One piezometer is screened 12 feet below land surface while the other, located at the same position, is screened 24 feet below land surface. Groundwater samples collected at these piezometers were consistently high in nitrate and values for the deeper piezometer were consistently over 10 mg-N/L. This evidence as well as the steady state direction of the hydraulic gradient and other piezometers that are located in areas that were not expected to receive OWS effluent indicate the existence of a background nitrate plume. The high ambient nitrate concentrations are most likely due to the use of synthetic nitrate fertilizers in the surrounding agricultural plots up gradient of the OWS. The agricultural nitrate plume is located deeper in the surficial aquifer due to recharge through the Hawthorn layer that causes it to descend as it travels and recharge from precipitation.
A method was developed to mitigate the effect of the agricultural nitrate plume and improve identification of those samples representative of the OWS effluent plume. This method was developed from observations that indicated that samples taken near the OWS infiltrative area had a relatively high specific conductance. The higher specific conductance is attributed to OWS effluent because natural recharge from precipitation is not as likely to contain high levels of dissolved anionic species. OWS effluent in contrast contains higher concentrations of anions from human and other wastes. Samples drawn from areas unaffected by effluent percolate were characterized by much lower specific conductance values. The agricultural nitrate plume also appeared to be located in the lower portion of the surficial aquifer above the confining layer. These observations were used to determine if a piezometer or drive point was likely to be within the OWS effluent plume or not.

Using the methodology described above the area in figure 21 was determined to be part of the OWS effluent plume. A limitation of the method is that it does not account for dilution which would reduce the specific conductance of the groundwater and may cause some OWS plume data not to be included in the evaluation. Vertical hydraulic gradients and water table fluctuations that cause mixing of the OWS and agricultural plumes also make it difficult to locate the vertical extent of the OWS effluent plume. It is highly likely that this location is variable throughout the aquifer due to water table fluctuations. The data within the area marked in figure 21 were used for model calibration and evaluation of the aquifer model and numerical models. Other data from piezometers and drive points outside of the delineated plume were not used. Approximately a third of the groundwater samples that were collected were identified as pertaining to the OWS effluent plume using this method. The mean nitrate concentration for these samples is slightly higher than for the complete data set while the standard deviation also
increases. This indicates that there is a large variation in the observed nitrate concentration even within the area that is speculated to be directly affected by OWS effluent. Additional descriptive statistics for the OWS plume samples are presented in table 3.

The aquifer model has been designed as a steady-state model and considers a constant mass flux contaminant source and a constant denitrification rate. While steady state conditions may persist within the aquifer down gradient of the OWS the groundwater samples can be affected by the temporal fluctuations in contaminant loading and denitrification. In order to accurately evaluate the aquifer model, these effects should be minimized in the observations as this provides a better indication of the long term behavior of the system and facilitates model corroboration. In order to minimize the effects, observations used for calibration of the aquifer model and the steady state numerical model were averaged for each sampling location. The objective was to approximate the long term nitrate concentration at those points within the aquifer. Several of the locations were sampled one or two times due to budget limitations. These data were not used for corroboration of the aquifer model or steady state numerical model because of a concern that these data could still be heavily influenced by temporal variations in contaminant loading or denitrification. Averaging and exclusion of sample locations with fewer than three reported concentrations left 33 observations (reported in Table 7) for corroboration of the aquifer model and the steady state numerical model.

**Table 3.** the descriptive statistics for the groundwater samples obtained in the area directly affected by percolate from the STU.

<table>
<thead>
<tr>
<th>GW Samples</th>
<th>NO\textsubscript{3} [mg-N/L]</th>
<th>NH\textsubscript{4}⁺ [mg-N/L]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>14.7</td>
<td>0.11</td>
</tr>
<tr>
<td>Median</td>
<td>12</td>
<td>0.028</td>
</tr>
<tr>
<td>Mode</td>
<td>12</td>
<td>0.005</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>8.6</td>
<td>0.21</td>
</tr>
<tr>
<td>Max</td>
<td>46</td>
<td>1.5</td>
</tr>
<tr>
<td>Min</td>
<td>0.17</td>
<td>0.005</td>
</tr>
<tr>
<td>Count</td>
<td>101</td>
<td>101</td>
</tr>
</tbody>
</table>
The aquifer model and numerical models that were constructed for calibration and corroboration require nitrate loading data at the water table, below the infiltrative area. Nitrogen transformation and attenuation occurs within the STU and heavily controls the mass flux of nitrogen to groundwater. Because no samples were collected within this area, nitrate mass flux to groundwater was estimated using STUMOD nitrate concentration predictions. STUMOD is designed to model nitrogen transformations within the STU and is capable of accurately predicting concentrations throughout the vadose zone and at the water table [Geza et al., 2009]. Ammonium input concentrations to STUMOD were assumed to be equivalent to what was observed in the septic-tank effluent samples presented in table 2. Parameter values and other site specific conditions were input into STUMOD for each simulation. Because the NRCS soil survey for the area indicates a transition between a fine and course sand within the field site, STUMOD simulations were conducted using two groups of parameters representative of the two sand types for a total of 12 STUMOD simulations. The STUMOD results for nitrate concentration at the water table are presented in table 4 and are an average of the outputs using the two different sands. These results were initially used as direct inputs for nitrate loading for the aquifer model and numerical models during calibration.

In addition to the groundwater samples that were gathered, hydraulic head observations were also collected. Hydraulic head was measured at piezometers shown in figure 18 utilizing the NGVD 29 datum. Over the course of the four year field campaign several hundred observations were manually recorded using a drop tape. These observations were used for calibration of the two numerical models and to calculate the seepage velocity for the aquifer model. The steady-state hydraulic gradient was calculated by averaging the observed hydraulic head at each piezometer, table 5.
Table 4, the descriptive statistics for the twelve STUMOD predictions of nitrate concentration in STU percolate. The soils (more permeable and less permeable sand) are characteristic of the field site. The EPA MCL for nitrate nitrogen is 10 mg-N/L.

<table>
<thead>
<tr>
<th>NO$_3^-$ [mg-N/L/day]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
</tr>
<tr>
<td>Median</td>
</tr>
<tr>
<td>Mode</td>
</tr>
<tr>
<td>Standard Deviation</td>
</tr>
<tr>
<td>Max</td>
</tr>
<tr>
<td>Min</td>
</tr>
<tr>
<td>Count</td>
</tr>
</tbody>
</table>

Table 5, presents descriptive statistics for average hydraulic head. These data were used to calculate the average hydraulic gradient, bearing and to construct boundary conditions.

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>Median</th>
<th>Mode</th>
<th>Std</th>
<th>Range</th>
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</thead>
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<td>PZ02</td>
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<td>119.57</td>
<td>119.87</td>
<td>1.20</td>
<td>7.26</td>
<td>118.11</td>
<td>125.37</td>
<td>36</td>
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<td>PZ03</td>
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<td>120.50</td>
<td>1.24</td>
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<td>2.05</td>
<td>11.03</td>
<td>120.52</td>
<td>131.55</td>
<td>33</td>
</tr>
</tbody>
</table>

Table 6, descriptive statistics for the calculated hydraulic gradient and bearing.

<table>
<thead>
<tr>
<th>Gradient (ft/ft)</th>
<th>Bearing (degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.028</td>
</tr>
<tr>
<td>Median</td>
<td>0.025</td>
</tr>
<tr>
<td>Mode</td>
<td>0.029</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>0.014</td>
</tr>
<tr>
<td>Max</td>
<td>0.080</td>
</tr>
<tr>
<td>Min</td>
<td>0.00048</td>
</tr>
<tr>
<td>Count</td>
<td>8015</td>
</tr>
</tbody>
</table>
After averaging, all possible combinations of three piezometers were created. The combinations represent all of the possible groups of piezometers, choosing three at a time, where order does not matter. The algorithm described in section 2.3.2 was then used to calculate the average hydraulic gradient magnitude and direction for all combinations, table 6. The groundwater seepage velocity was calculated using equation 2.57, the calculated hydraulic gradient, the reported hydraulic conductivity (from slug tests) and porosity for the field site. The estimated average groundwater seepage velocity within the study site is 49 m/yr and the steady state direction of the local hydraulic gradient is south southwest, in the direction of Carlton Branch Creek a local stream that empties to Tampa Bay. The calculated direction of the hydraulic gradient also aligns well with the area that is thought to be directly affected by OWS effluent.

### 3.2 Model Corroboration

The observed data presented in section 3.1 was used to calibrate the aquifer model and two numerical models. The purpose of the calibration was to evaluate the behavior of the aquifer model and gain an understanding of the limitations of the HPS solution that is used by the aquifer model. A common approach for model evaluation is a comparison between observed data and a forward simulation of a calibrated model. However, a large portion of the collected data appeared to be heavily influenced by the agricultural nitrate plume that is present. Also, uncertainty surrounding the temporal variability in contaminant loading and denitrification affected the observed data. Because of these limitations there was significant uncertainty in the calibration results of the aquifer model. In light of this uncertainty it was determined that a better approach for model evaluation would be a comparison between the calibration results from the aquifer model and two numerical models. Because the numerical models
(MODFLOW/MT3DMS) are state of the art, they are used as a benchmark for evaluating the aquifer model. The corroboration of the aquifer model is presented as its performance during calibration relative to the numerical models which also highlights any limitations of the HPS solution for evaluating contaminant transport.

A transient numerical model of the GCREC field site was initially constructed for comparison to the aquifer model. The transient numerical model is capable of considering three dimensional advection and dispersion as well as transient processes such as precipitation, evapotranspiration and contaminant loading. During the construction and calibration, limitations of the transient numerical model became apparent. A steady state numerical model was constructed in order to evaluate those limitations and gain an understanding of the best methodology for constructing mathematical models of an OWS where input data is limited. Results from the steady state numerical model are also an important part of the corroboration of the aquifer model. Details of the construction and calibration of the numerical models are presented in the following sections.

3.2.1 Calibration of the Aquifer Model

The aquifer model calculates nitrate concentration as a function of time and position using three dimensional Cartesian coordinates. The time component is assigned a large value to approximate steady state conditions. The estimated groundwater seepage velocity at the GCREC site is 49 m/yr and given that the OWS at the site had been in operation for 6 years prior to the commencement of this study a steady state assumption is appropriate. The three dimensional position where each groundwater sample was obtained was estimated as the distance between the center of the infiltrative area and the position of the drive point or piezometer. The distance in the ‘X’ direction was estimated as the distance along a centerline drawn from the center of the
infiltrative surface to a point adjacent to the sample location. The distance ‘Y’ was estimated as the distance from the sample location to a point on the centerline creating perpendicular lines, figure 21. The ‘Z’ distance or depth below the water table was calculated as the distance between the observed hydraulic head and the piezometer screen. This distance was estimated for groundwater sampling wells as the difference between an interpolated water table created using the average observed hydraulic head and the drive point location. This method was used to calculate the position of the 33 nitrate observations that were used for calibration of the aquifer model.

**Figure 21.** the method used to estimate the X, Y and Z values that are required by the aquifer model to calculate concentration.
The aquifer model requires a number of parameters which were not included in the calibration procedure because independent methods were used to establish these values, which are presented in table 7. The methods used to independently obtain parameters are discussed below. The dimensions of the infiltrative area and the HLR, which are used to calculate mass flux of nitrate at the water table, were obtained from the engineering designs and the operating permit. Initially the nitrate concentration in the STU percolate, which is also used to calculate mass loading to the aquifer, was estimated as the average of STUMOD simulations described in section 3.1.3 and presented in table 4. However, due to poor calibration results the input concentration was later modified. The aquifer thickness, which is a parameter used directly by the HPS solution, was estimated as the depth from the average water table elevation to what is believed to be the contact between the Hawthorn layer and the Suwanee limestone (see Appendix D). Groundwater seepage velocity is a parameter in the HPS solution but the aquifer model calculates seepage velocity using equation 2.57. Because of this, the aquifer model requires inputs of hydraulic gradient, porosity and saturated hydraulic conductivity. The hydraulic gradient was calculated as mentioned in section 3.1.3. The saturated hydraulic conductivity was the average reported value from slug tests conducted at piezometers down gradient of the OWS infiltrative area. Slug test data are presented in Appendix C. The retardation coefficient was assigned a value of one indicating no retardation, which is generally appropriate for nitrate in an aquifer composed of quartz sands with small cation exchange capacity. Quartz sands have no surface charge making anion exclusion unlikely. Porosity was identified as a sensitive parameter in the sensitivity analysis presented in section 2.4 but this parameter was not included in the calibration. Porosity was not included in the calibration because sensitivity analysis results indicated that model outputs were primarily sensitive to small porosity values less than 0.3.
However, the soils at the GCREC site were identified as sands by NRCS soil survey data, which generally have larger porosities. Data from the Rosetta program as well as independent work done to identify default parameter values for STUMOD indicate that soils that fall into the sand textural class generally have porosities greater than 0.35 [McCray, 2011; Schaap et al., 2001]. Because of this porosity was assigned an average value for sand and not included in the calibration.

**Table 7**, the fixed parameter values used for calibration of the aquifer model. These values were obtained via independent methods.

<table>
<thead>
<tr>
<th>Fixed Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>R [-]</td>
<td>1</td>
</tr>
<tr>
<td>n [-]</td>
<td>0.39</td>
</tr>
<tr>
<td>H [m]</td>
<td>39.62</td>
</tr>
<tr>
<td>B [m]</td>
<td>26</td>
</tr>
<tr>
<td>L [m]</td>
<td>35</td>
</tr>
<tr>
<td>grad [m/m]</td>
<td>0.025</td>
</tr>
<tr>
<td>HLR [m/yr]</td>
<td>5.95</td>
</tr>
<tr>
<td>Conc. [mg-N/L]</td>
<td>25</td>
</tr>
<tr>
<td>Time [yr]</td>
<td>1000</td>
</tr>
<tr>
<td>Ksat [m/yr]</td>
<td>761</td>
</tr>
</tbody>
</table>

The aquifer model parameters that were included in the calibration were the first-order denitrification parameter and the three dimensional dispersivity parameters, table 8. McCray et al. [2005] presents a compilation of first-order denitrification values that have been published in literature. These values were presented on a cumulative frequency diagram with an equation to estimate denitrification values based on percentile rank. These data have a range of approximately three orders of magnitude and cannot be used to determine the correct denitrification value for a specific field site. Rather these data were intended to be used for risk assessment when site data is not available. Calibration of the denitrification parameter was also justified by results from the sensitivity analysis which found that model output was highly sensitive to this parameter. The dispersivity parameters were not identified as sensitive parameters, but reported values for equivalent transport distances and porous media vary...
substantially [Gelhar et al., 1992]. The method developed by Xu and Eckstein [1995], which is used by the aquifer model, has not been corroborated for the field site. Because no independent data exists to corroborate the estimated dispersivity values for the field site these parameters were also included in the calibration procedure.

Table 8, the parameter values produced via calibration of the aquifer model to field observations of nitrate in groundwater samples.

<table>
<thead>
<tr>
<th>Calibrated Parameter Values</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$ [1/yr]</td>
<td>2.8E-08</td>
</tr>
<tr>
<td>$\alpha_x$ [m]</td>
<td>13.3</td>
</tr>
<tr>
<td>$\alpha_y$ [m]</td>
<td>2.4</td>
</tr>
<tr>
<td>$\alpha_z$ [m]</td>
<td>0.4</td>
</tr>
</tbody>
</table>

A Levenberg-Marquardt optimization algorithm developed by the University of Chicago was adapted for calibration of the aquifer model within Excel VBA. The median denitrification value reported by McCray et al. [2005] was used as the initial denitrification value. Initial dispersivity values were estimated using the equation developed by Xu and Eckstein [1995] and the method described in section 2.3.1. The input nitrate concentration as assumed to be the average value reported from the twelve STUMOD simulations. Calibration attempts using these initial values were unsuccessful as the model predicted concentrations were well below the observed values. Initially it was thought that these results were due to model convergence on local minima possibly due to an initial value for the denitrification rate constant that was too large. To determine if the initial parameter values were responsible for the unsuccessful calibration attempt, random values were chosen for the denitrification and dispersivity values. These values were chosen within the probable ranges for denitrification and dispersivity. It was concluded that the initial values had little impact on the final calibration results.

Adequate calibration results could only be obtained by increasing the input nitrate concentration at the water table. Reasonable results were achieved with an input nitrate concentration of 25 mg-N/L, slightly higher than the maximum value of 21.7 mg-N/L predicted
by STUMOD. The results from this calibration are presented in figure 22, which contains 23 of the 33 observations, and in table 8. Ten of the 33 observations could not be adequately fit with any combination of parameter values and an input nitrate concentration of 25 mg-N/L. All 33 observations and model predictions are given in table 9, where 10 “poor model fits” and 23 “good model fits” are annotated. The 10 “poor model fit” observations could only be marginally replicated by the aquifer model by using high input nitrate concentrations, above 60 mg-N/L. This appears to indicate that these points are heavily influenced by the agricultural nitrate plume. Six of the 10 observations were located at least 15 meters off the plume center line, which may also affect calibration results because the HPS solution does not consider transversal advection which could be responsible for the high concentrations observed off the centerline. The remaining four observations were less than 10 meters off the plume centerline. Nine of these 10 observed concentrations were under predicted by the calibrated aquifer model and only one was over predicted, these results are also presented in table 9. The optimized denitrification value was notably low while the longitudinal dispersivity value was approximately three times that of what was estimated using the Xu and Eckstein [1995] method. These values are presented in table 8.

![Observed NO3 vs HPS NO3](image)

**Figure 22**, calibration results from the aquifer model for the 23 observations determined to pertain to the OWS nitrate plume.
Table 9, complete calibration results for the 33 observations within the OWS nitrate plume area. Residuals (Res) are computed as $model - obs$.

<table>
<thead>
<tr>
<th>Name</th>
<th>$x_i$ [m]</th>
<th>$y_i$ [m]</th>
<th>$z_i$ [m]</th>
<th>Obs [mg-N/L]</th>
<th>Model [mg-N/L]</th>
<th>Res [mg-N/L]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poor Model Fit</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DP-AA9-14</td>
<td>9.1</td>
<td>22.6</td>
<td>2.1</td>
<td>24.0</td>
<td>5.3</td>
<td>-18.6</td>
</tr>
<tr>
<td>PZ03</td>
<td>52.7</td>
<td>1.1</td>
<td>0.6</td>
<td>1.0</td>
<td>18.3</td>
<td>17.3</td>
</tr>
<tr>
<td>DP-F15-14</td>
<td>72.7</td>
<td>19.9</td>
<td>3.1</td>
<td>21.7</td>
<td>7.2</td>
<td>-14.4</td>
</tr>
<tr>
<td>DP-F15-20</td>
<td>72.7</td>
<td>19.9</td>
<td>4.9</td>
<td>18.6</td>
<td>6.4</td>
<td>-12.3</td>
</tr>
<tr>
<td>DP-E12-15</td>
<td>51.7</td>
<td>9.5</td>
<td>3.2</td>
<td>23.7</td>
<td>13.4</td>
<td>-10.2</td>
</tr>
<tr>
<td>DP-F11-15</td>
<td>51.2</td>
<td>1.3</td>
<td>3.3</td>
<td>25.3</td>
<td>15.8</td>
<td>-9.6</td>
</tr>
<tr>
<td>DP-G12-15</td>
<td>62.3</td>
<td>1.8</td>
<td>3.4</td>
<td>21.3</td>
<td>13.6</td>
<td>-7.6</td>
</tr>
<tr>
<td>DP-AA9-22</td>
<td>9.1</td>
<td>22.6</td>
<td>4.6</td>
<td>11.0</td>
<td>3.8</td>
<td>-7.2</td>
</tr>
<tr>
<td>DP-F15-26</td>
<td>72.7</td>
<td>19.9</td>
<td>6.7</td>
<td>12.3</td>
<td>5.4</td>
<td>-7.0</td>
</tr>
<tr>
<td>DP-AA9-27</td>
<td>9.1</td>
<td>22.6</td>
<td>6.1</td>
<td>8.8</td>
<td>2.9</td>
<td>-5.9</td>
</tr>
<tr>
<td>Good Model Fit</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DP-E12-10</td>
<td>51.7</td>
<td>9.5</td>
<td>1.7</td>
<td>21.0</td>
<td>15.1</td>
<td>-5.9</td>
</tr>
<tr>
<td>DP-G12-09</td>
<td>62.3</td>
<td>1.8</td>
<td>1.6</td>
<td>9.8</td>
<td>15.2</td>
<td>5.4</td>
</tr>
<tr>
<td>DP-F11-24</td>
<td>51.2</td>
<td>1.3</td>
<td>6.1</td>
<td>16.0</td>
<td>10.9</td>
<td>-5.1</td>
</tr>
<tr>
<td>DP-G12-21</td>
<td>62.3</td>
<td>1.8</td>
<td>5.2</td>
<td>16.1</td>
<td>11.3</td>
<td>-4.7</td>
</tr>
<tr>
<td>DP-D7.5-14</td>
<td>21.7</td>
<td>8.8</td>
<td>1.9</td>
<td>26.0</td>
<td>21.5</td>
<td>-4.5</td>
</tr>
<tr>
<td>DP-D09-15</td>
<td>30.1</td>
<td>1.1</td>
<td>2.3</td>
<td>19.0</td>
<td>23.3</td>
<td>4.3</td>
</tr>
<tr>
<td>DP-G12-27</td>
<td>62.3</td>
<td>1.8</td>
<td>7.1</td>
<td>13.1</td>
<td>8.9</td>
<td>-4.2</td>
</tr>
<tr>
<td>DP-F11-27</td>
<td>51.2</td>
<td>1.3</td>
<td>7.0</td>
<td>5.2</td>
<td>9.4</td>
<td>4.2</td>
</tr>
<tr>
<td>PZ16-C12-28</td>
<td>39.8</td>
<td>20.9</td>
<td>7.1</td>
<td>0.3</td>
<td>4.4</td>
<td>4.2</td>
</tr>
<tr>
<td>PZ17-I15-26</td>
<td>88.0</td>
<td>4.4</td>
<td>6.9</td>
<td>12.0</td>
<td>7.8</td>
<td>-4.1</td>
</tr>
<tr>
<td>DP-D09-08</td>
<td>30.1</td>
<td>1.1</td>
<td>0.2</td>
<td>23.0</td>
<td>26.9</td>
<td>3.9</td>
</tr>
<tr>
<td>PZ11-E09-10</td>
<td>34.7</td>
<td>7.1</td>
<td>1.8</td>
<td>17.0</td>
<td>20.8</td>
<td>3.8</td>
</tr>
<tr>
<td>DP-D12-11</td>
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</tr>
<tr>
<td>DP-F08-28</td>
<td>34.9</td>
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<td>2.6</td>
<td>5.6</td>
<td>3.0</td>
</tr>
<tr>
<td>DP-F11-21</td>
<td>51.2</td>
<td>1.3</td>
<td>5.1</td>
<td>15.5</td>
<td>12.5</td>
<td>-3.0</td>
</tr>
<tr>
<td>DP-D7.5-20</td>
<td>21.7</td>
<td>8.8</td>
<td>3.7</td>
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</tr>
<tr>
<td>DP-F11-11</td>
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<td>2.1</td>
<td>15.0</td>
<td>17.5</td>
<td>2.5</td>
</tr>
<tr>
<td>DP-F11-18</td>
<td>51.2</td>
<td>1.3</td>
<td>4.2</td>
<td>15.7</td>
<td>14.2</td>
<td>-1.5</td>
</tr>
<tr>
<td>DP-D7.5-26</td>
<td>21.7</td>
<td>8.8</td>
<td>5.6</td>
<td>9.4</td>
<td>10.7</td>
<td>1.3</td>
</tr>
<tr>
<td>DP-G12-24</td>
<td>62.3</td>
<td>1.8</td>
<td>6.2</td>
<td>11.1</td>
<td>10.0</td>
<td>-1.1</td>
</tr>
<tr>
<td>DP-E12-22</td>
<td>51.7</td>
<td>9.5</td>
<td>5.4</td>
<td>11.4</td>
<td>10.4</td>
<td>-1.0</td>
</tr>
<tr>
<td>DP-F08-20</td>
<td>34.9</td>
<td>16.4</td>
<td>4.7</td>
<td>8.9</td>
<td>8.6</td>
<td>-0.3</td>
</tr>
<tr>
<td>DP-E12-28</td>
<td>51.7</td>
<td>9.5</td>
<td>7.2</td>
<td>7.8</td>
<td>7.9</td>
<td>0.1</td>
</tr>
</tbody>
</table>
3.2.2 Construction of Two Numerical Models

Two numerical models were constructed for the GCREC field site which considered transient and steady state conditions. These models used the MODFLOW and MT3DMS algorithms within Groundwater Vistas [Rumbaugh and Rumbaugh, 2011]. The construction of these models was similar in that they contained the same number of cells and boundary conditions. The transient conditions that were considered were precipitation and evapotranspiration. Temporally varying OWS effluent flows, and thus nitrogen flux to the aquifer, were not considered in the model because the discharge from the OWS septic tank was not metered. Also the nitrogen concentrations in the septic tank effluent were only sampled on four occasions with two replicates. Nitrate concentrations in STU percolate arriving at the water table beneath the infiltrative area were never sampled. Recharge and nitrogen mass flux from the OWS was estimated using the design HLR of 3.26 cm/day or 0.4 gal/ft²/day and the same input concentration used for the aquifer model calibration (25 mg-N/L). These values were also used for the steady state numerical model.

Precipitation and evapotranspiration data were collected from a meteorological station located approximately 500 meters from the field site. Precipitation is measured with a tipping bucket range gauge at a precision of 0.01 inches. Evapotranspiration is not measured directly at the weather station, rather it is calculated using the Penman-Monteith method [Brutsaert, 2005]. The Penman-Monteith method is commonly used to estimate evapotranspiration but is known to be sensitive to vegetation specific parameters such as stomatal resistances causing over or under estimations [Beven, 1979]. Precipitation and evapotranspiration data were obtained from January 1\textsuperscript{st} 2008 through November 5\textsuperscript{th} 2013 for the transient numerical model. The average precipitation and evapotranspiration for this period was assigned to the steady state numerical model. Runoff
was not considered in either numerical model because the soils within the study site are sands and are characterized by a relatively high infiltration rate and are well vegetated which also mitigates runoff [Doolittle et al., 1989].

No physical features exist in relative proximity to the field site that could be used to define boundary conditions. The storm water detention basin pictured at the top left in figure 18 contains water for most of the year so it could be assumed that this is a manifestation of the water table which is typically close to the land surface. Water levels in the detention basin, however, were never monitored during the four year study period. Long term groundwater monitoring is conducted by the U.S. Geologic Survey (USGS) at numerous wells throughout Florida and these data have been used to construct steady state hydraulic head maps on a regional scale. These maps are often constructed using hydraulic head data obtained from the Floridian aquifer rather than the surficial aquifer which precludes their usefulness for this investigation.

Because of these limitations an alternate method was developed to define boundary conditions for the surficial aquifer at the field site. This method was developed after observing that a linear correlation existed between mean groundwater elevation and land surface. This follows the observations of many that the water table is often a subdued replica of the land surface [Rios, 2010]. Boundary conditions for both numerical models were defined using a smoothed three meter resolution digital elevation model (DEM) of the field site. Smoothing of the DEM was accomplished by a 7 x7 moving window average algorithm written in Excel VBA, a method developed by Rios et al. [2013] to estimate steady state hydraulic gradients for surficial aquifers in Florida. The average groundwater elevations observed at the piezometers within the study site were plotted against land surface elevations extracted from the smoothed DEM. A linear trend line was fit to these data using the least squared method which returned an $R^2$
correlation coefficient of 0.96 indicating that the water table can indeed be approximated as a smoothed replica of the land surface, figure 23. ArcGIS was used to construct elevation contours from the smoothed DEM every 0.1 feet. Constant head boundaries in figure 18 were defined using the equation given in figure 23 to calculate the water table elevation, where the independent variables were the smoothed DEM elevations. No-flow boundaries were assigned to the lateral boundaries shown in figure 18 and were constructed approximately perpendicular to the contours.

Elevation vs Observed Head

![Graph](attachment:image.png)

**Figure 23.** The average observed hydraulic head versus land surface elevation extracted from the smoothed DEM.

Isotropic hydraulic conductivity values for the surficial aquifer in both numerical models were gathered from NRCS soil survey geospatial data and data obtained from slug tests. While the vertical hydraulic conductivity of the Hawthorn layer was obtained through calibration. The hydraulic conductivity measurements obtained from the slug tests pertain to the immediate area where the piezometers were installed. A hydraulic conductivity field was constructed by interpolating these point data using a kriging algorithm in ArcGIS. The hydraulic conductivity data obtained from the NRCS soil survey is approximate and does not have the same spatial
resolution as the elevation data that were used. Because of this the hydraulic conductivity values from the NRCS soil survey geospatial data were only used in the areas beyond the hydraulic conductivity field constructed from slug tests. Slug test results as well as a map of the piezometers where slug tests were performed and images of the hydraulic conductivity field used in the numerical models are found in Appendix C.

The finite difference grid was constructed using 172 columns, 201 rows and 12 layers. The 11\textsuperscript{th} layer was assigned a thickness of 100 feet which is approximately the thickness of the Hawthorn layer at the GCREC field site. The 12\textsuperscript{th} layer was assigned a nominal thickness of one foot because it was used as a lower boundary condition representing the Upper Floridian aquifer. The remaining 10 layers were assigned a uniform thickness, approximately three feet, and represented the surficial aquifer. The grid size within the area where nitrate concentrations were monitored was 5.3 feet and a grid size of 10.6 feet was used where contaminant transport was not monitored. The transient numerical model contained 2136 stress periods for precipitation and evapotranspiration, which represented the period from January 1\textsuperscript{st} 2008 through November 5\textsuperscript{th} 2013, each stress period was divided into four time steps. The steady state model was constructed using one stress period divided into 400 time steps. The lower boundary condition for both models, layer 12, was assigned as a constant head boundary. The constant head value was assigned based on observations from USGS wells in southern Hillsborough County that were screened in the Upper Floridian aquifer. The average hydraulic head in these wells was approximately 10 feet though there was large variability in between wells and throughout time (Appendix A).
3.2.3 Calibration of the Transient Numerical Model

The parameters identified in section 3.2.1, first order denitrification and dispersivity, were included in the calibration of the transient numerical model. Additionally the vertical hydraulic conductivity of the Hawthorn layer was also included in the calibration procedure. The porosity and specific yield and specific storage parameters are inputs for the MT3DMS and MODFLOW numerical codes that were used, respectively. Specific yield describes the volume of pore space available for water within an unconfined aquifer. Specific yield and specific storage are important parameters for simulating the surficial aquifer and the semi-confining Hawthorn layer. Porosity refers to the effective pore volume that solutes can occupy. In many cases specific yield, storage and porosity are not equal. However, in both numerical models these parameters did not appear to be sensitive and were all assigned the porosity value used in the calibrated aquifer model, 0.39. The vertical hydraulic conductivity of the Hawthorn layer (11th layer) was included because the range of reported hydraulic conductivities by other studies was large [McGurk, 1998].

Calibration was carried out using the PEST optimization algorithm which is distributed with Groundwater Vistas [Doherty, 2004]. Hydraulic head observations and nitrate concentrations within the area that was determined to be part of the plume coming from the OWS were included. The data for the transient numerical model were not averaged as was done for the aquifer model and steady state numerical model. The purpose of using these calibration targets was to determine if a numerical model with transient inputs (precipitation and evapotranspiration) could capture the observed variability in hydraulic head and concentration. Obvious limitations of this transient numerical model were the lack of transient boundary conditions, concentration histories of the STU percolate and the daily volumetric flux from the
The results from calibration are presented in figure 24 for the hydraulic portion of the transient model and figure 25 for the contaminant transport of nitrate.

The vertical hydraulic conductivity of the Hawthorn layer (layer 11) was the only parameter calibrated using the hydraulic head observations. The hydraulic conductivity of the Hawthorn layer was assigned a uniform value, though it likely varies spatially. Because no geostatistical data exists to constrain the range and distribution of calibrated vertical hydraulic conductivities for the Hawthorn layer a single hydraulic conductivity zone was used to describe the Hawthorn layer. Without geostatistical data, using multiple zones of vertical hydraulic conductivity for the Hawthorn layer would provide too much flexibility to the model resulting in potentially misleading results. This, as well as the constant head boundary conditions that were used may cause the stratification visible in figure 24. The general trend of model values, however, do fall along the one to one line indicating that the transient model is capturing the general behavior of hydraulic head.

![Model vs Observed Hydraulic Head](chart.png)

**Figure 24.** calibration results for the groundwater flow portion of the transient numerical model. The vertical hydraulic conductivity of the Hawthorn layer (layer 11) was the only calibrated parameter.
Figure 25. calibration results for the contaminant transport portion of the transient numerical model. The first order denitrification and dispersivity parameters where calibrated parameters. The calibration of the contaminant transport parameters, denitrification and dispersivity, did not produce a good fit of the observed nitrate data, figure 25. Nitrate input to the aquifer was simulated using a constant value calculated from the design HLR and a concentration of 25 mg-N/L (the same as was used for the aquifer model). The volumetric flux to the aquifer from STU percolate was estimated as the design HLR because observed HLR data were not available. Eliminating observation data that appeared to pertain to the agricultural nitrate plume, as was done with the aquifer model calibration, was not possible. The misfit between model calculated values and observations was large and observation data could not be separated into distinct groups based on goodness of fit or location within the aquifer as was done with the aquifer model. This could be, because these data contain information regarding some potentially important temporally variable processes, such as denitrification, that were not measured and could not be included in the model as a temporally variable calibration parameter. The calibrated parameter values are presented in table 10. Calibrated hydraulic conductivity values for the Hawthorn layer fall within the reported range. Calibrated dispersivity values are smaller than
those produced by the calibration of the aquifer model. The calibrated denitrification rate in contrast is several orders of magnitude larger than the value returned by the aquifer model. The denitrification value falls within the 43rd percentile of values reported by McCray et al. [2005]. The results from calibration of the contaminant transport portion of the transient numerical model are presented in figure 25.

**Table 10.** calibration results from calibration of the transient state numerical model.

<table>
<thead>
<tr>
<th>Calibrated Parameter Values</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>λ [1/yr]</td>
<td>0.025</td>
</tr>
<tr>
<td>αx [m]</td>
<td>2.2</td>
</tr>
<tr>
<td>αy [m]</td>
<td>0.4</td>
</tr>
<tr>
<td>αz [m]</td>
<td>0.3</td>
</tr>
<tr>
<td>Kz [m/yr]</td>
<td>0.72</td>
</tr>
</tbody>
</table>

### 3.2.4 Calibration of the Steady State Numerical Model

The parameters that were included in the calibration of the transient model were also included in the calibration of the steady state model (Kz\textsubscript{sat}, dispersivity, decay). Construction of the steady state model was identical to that of the transient model. However, average precipitation and evapotranspiration from the five and a half year period from 2008 to 2013 were assigned to the model. The calibration targets for hydraulic head and nitrate concentration were the average observed value at each piezometer or groundwater sampling well. The nitrate concentration targets that were used for calibration were the same targets used for calibration of the aquifer model which were averages of a minimum of three observations. The hydraulic head calibration targets consisted of the average hydraulic head observed at each piezometer through the entire four year study period. Averages consisted of a minimum of 16 observations and up to a maximum of 47 observations.

The calibration results for hydraulic head and nitrate concentration are presented in figures 26 and 27 and table 11. Calibration results for hydraulic head are significantly improved over the transient numerical model while nitrate concentrations are not successfully replicated.
The hydraulic head observations were replicated well by the steady state model possibly because temporal variability in observations was eliminated. The calibrated value for vertical hydraulic conductivity of the Hawthorn layer is similar to that of the transient state model though not identical. Results from the calibration of the contaminant transport portion of the steady state model are not improved over calibration results of the transient model and the calibration should be considered unsuccessful due to the low correlation coefficient. Numerical dispersion or error in the solution of the ADE may cause mass balance errors that are not present in the aquifer model. The grid peclet number for both numerical models is greater than one if estimated with the smallest calibrated dispersivity value. The Total Variation Diminishing algorithm, which is reported not to be affected by numerical dispersion, was used to calculate contaminant transport [Zheng and Wang, 1999]. Regardless, it appears that both numerical models are unable to successfully replicate the nitrate observations.

**Table 11**, calibration results for parameters included in the calibration of the steady state numerical model.

<table>
<thead>
<tr>
<th>Calibrated Parameter Values</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(\lambda \text{ [1/yr]})</td>
<td>0.10</td>
</tr>
<tr>
<td>(\alpha_x \text{ [m]})</td>
<td>3.0</td>
</tr>
<tr>
<td>(\alpha_y \text{ [m]})</td>
<td>0.3</td>
</tr>
<tr>
<td>(\alpha_z \text{ [m]})</td>
<td>2.4</td>
</tr>
<tr>
<td>(K_z \text{ [m/yr]})</td>
<td>1.3</td>
</tr>
</tbody>
</table>
Figure 26, model predicted hydraulic head versus observed average hydraulic head. The model layer where hydraulic head was calculated is indicated by numbers 2 – 10.

Figure 27, the calibration result for the contaminant transport portion of the steady state numerical model is only slightly improved. In general the calibration should be considered unsuccessful as the $R^2$ value is low.
CHAPTER 4
DISCUSSION AND CONCLUSION

The aquifer model has been developed as an Excel VBA program utilizing an analytical solution to the ADE, the HPS solution. The HPS solution has been derived to consider a horizontal contaminant source plane similar to the geometry of an OWS. This program has been designed to couple with STUMOD providing the user a method to estimate nitrate mass flux and concentration in an unconfined aquifer receiving STU percolate. The aquifer model considers three dimensional dispersion and one dimensional advection of nitrate under steady state conditions. The derivation and validation of the HPS solution is presented in chapter 2. Validation results have established the mathematical accuracy of the analytical solution, the VBA algorithm and the method used to solve equation 2.43. Results from the calibration of the aquifer model to field data suggest the model performs as well or better than a steady-state numerical model and a transient numerical model that included the transient impacts of evapotranspiration and precipitation. The calibration also highlighted some limitations of the analytical solution. These limitations have been examined in the context of the research objectives, outlined in chapter 1, to provide the user an understanding of where the aquifer model can be applied. This discussion has also presented an opportunity for future development of the aquifer model to address the limitations of the HPS solution.

4.1 Discussion

The aquifer model has been calibrated to field data obtained from a surficial aquifer in Florida down gradient of an OWS. Additionally two numerical models that accounted for precipitation, evapotranspiration and allowed for complex solute transport via three dimensional dispersion and advection, which the HPS solution does not, were constructed and calibrated to
the observed data. The following discussion presents an analysis of the calibration of the aquifer model and the two numerical models.

### 4.1.1 Calibration of the Aquifer model

Calibration of the aquifer model to the observed field data for nitrogen concentration was successful, achieving an $R^2$ of 0.66. However, 10 of the 33 observations produced relatively large residuals and were removed from the final calibration results because these points appeared to be heavily influenced by the agricultural nitrate plume. These observations were located relatively further off the plume centerline than other observations. Residuals for these 10 points, calculated as the difference between model predictions and observations were all less than zero except for one point. These observations, however, could be adequately fit by the aquifer model by increasing the input nitrate concentration above 60 mg-N/L. Such high input concentrations are not physically possible, however, because all septic tank effluent samples contained total nitrogen concentrations equal to or less than 61 mg-N/L for the six samples collected. Because more mass was needed to fit these observations then existed in the OWS it was concluded that these observations were more closely related to the observations of the agricultural nitrate plume.

The calibrated parameter values presented in table 6 were obtained from the calibration to the 23 observations that produced low residuals during the initial calibration attempt. While the 10 observations that could not be fit are speculated to pertain to the agricultural nitrate plume, excluding the 10 observations during the final calibration may have selectively biased the calibrated parameters and produced artificially good calibration results. This situation was examined by using all the available observations for a calibration run and comparing the calibrated parameters to those in table 6. The parameter values for this calibration run were similar though not identical. Notably, the first order denitrification coefficient for both
calibration attempts was small while the horizontal transverse dispersivity value for the calibration with the 33 observations was larger. The results from the calibration of the aquifer model to the 33 observations are presented in Appendix E for comparison to table 8. The increased dispersivity value was likely due to fact that the HPS solution only considers one dimensional advection though two or three dimensional advection is likely occurring within the model area. An increase in transverse horizontal dispersivity would promote movement of the contaminant off the plume centerline. Because the 10 observations were located generally further off the plume centerline, model misfit may be due to the inability of the HPS solution to consider transverse advection.

The agricultural nitrate plume has likely influenced the calibrated parameter values reported in table 6. Due to superposition of the two plumes, nitrate concentrations within the area determined to be directly affected by STU percolate were likely higher than they otherwise would be. The effect of this on the final calibrated parameter values would likely be to decrease the denitrification value and increase the dispersivity values. During calibration, a decrease in the denitrification value would be the only way available to preserve the mass needed to produce the observed concentrations. Similarly, increases in dispersivity values would be the only available mechanism to fit the higher concentrations along the plume fringes. These conclusions were tested by including the input nitrate as a calibration parameter in one test calibration and allowing values above 60 mg-N/L. During this test calibration, the denitrification value increased, though it remained below the lowest value reported by McCray et al [2005] (0.004 (1/day)). In comparison, dispersivity values decreased and in general the calibration results improved relative to the case with a lower input nitrate concentration. These results are presented in Appendix E. Because the measured nitrogen concentration in the septic tank never exceeded
61 mg-N/L and because there is likely a net nitrogen removal within the vadose zone, input concentrations to the aquifer are likely not this high. As a result the parameter values for this test calibration are not based on conditions that are likely to exist. However, they were helpful in drawing qualitative conclusions concerning the values reported in table 6.

An additional limitation of the HPS solution, used by the aquifer model, was noted when plotting concentrations along the plume centerline. For a particular combination of HLR and input concentration the calculated concentration along the centerline was greater than the input concentration. It was determined that this occurs for high HLR because the HPS solution requires the contaminant source in terms of mass flux. Mass flux is calculated for the horizontal contaminant source plane as the input concentration times the design HLR times the dimension of the STU foot print. A contaminant arriving at the water table is applied as a mass rather than a solute effectively losing the volume in which the solute was dissolved. For a low HLR this issue may not be significant, however, this will cause all concentrations along the plume center line to be greater than they otherwise would be or in the case of calibration to observed data may cause the dispersivity values to be high.

The conclusions that have been drawn from these observations are: denitrification is occurring to a greater extent than the calibrated denitrification coefficient suggests but may be limited, the calibrated denitrification rate is likely depressed due to the agricultural nitrate plume, and finally the calibrated transverse values may be affected where complex advection fields exist in an aquifer because transport in those directions is only considered via dispersion within the HPS solution.
4.1.2 Calibration of two Numerical Models

Numerical models were constructed to evaluate any improvement in calibration provided by the increased flexibility. These models provided the ability to evaluate possible improvements in calibration by considering three dimensional advection as well as other spatially and temporally variable conditions. However, a primary limitation of the transient numerical model has been a lack of input data. Temporal variations in the contaminant source, spatial and temporal variations in denitrification, spatial variations in precipitation and evapotranspiration as well as the spatial and temporal fluctuation of hydraulic head along the model boundaries could not be accounted for in the construction of the model. These limitations have likely precluded any possible improvements to the calibration results presented in the previous chapter.

Calibration of the transient numerical model to observed hydraulic head produced adequate results with an $R^2$ of 0.56. However, the model was limited in that it could not capture the variability of observations as evidenced by the grouping around the 1:1 line in figure 24. A noteworthy observation of figure 24 is that results appear to be stratified or approximately separated by model layer. The transient numerical model appears to have behaved more like a steady state model, producing constant hydraulic head values within each model layer. While a significant effort was made to collect transient data for this model there were many limitations, for example; the limited spatial extent of the model may have allowed the boundary conditions to excessively control model behavior. Precipitation and evapotranspiration data were site specific but could not capture spatially variable recharge that is likely to occur due localized recharge from ponding and variable plant rooting depth. The spatial resolution of the hydraulic conductivity field used by the model likely did not capture local heterogeneities that may have also been responsible for the observed variability in hydraulic head. Improving the calibration
results of the transient numerical model would require better temporal and or spatial resolution in input data.

Contaminant transport within the transient state numerical model was solved using the MT3DMS algorithm [Zheng and Wang, 1999]. Nitrate concentrations observed in groundwater samples collected within the OWS plume were used as calibration targets. The three dimensional dispersivity parameters as well as the first order denitrification parameter were calibrated using the PEST algorithm [Doherty, 2004]. Calibration to nitrate concentration observations was unsuccessful and did not produce and R^2 greater than 0.0001. While the calibration results are not reliable, the first order denitrification value was low, similar to the value returned by the calibrated aquifer model. This supports the conclusion that the agricultural nitrate plume is the cause for the low calibrated denitrification parameter values. While it would be difficult to determine the amount of nitrate in each sample from the agricultural plume, adjusting the observed concentrations by that amount would allow for an improved estimation of denitrification at the site.

It was not possible to identify samples that appeared to be sourced primarily from the agricultural plume and remove them for the calibration of the contaminant transport portion of the transient model as was done for the aquifer model. Temporal variations in nitrate mass flux and denitrification make it impossible to identify whether a sample primarily belongs to the agricultural plume or not. By averaging the collected samples, as was done for the aquifer model and the steady state numerical model, the effect of temporal variability is minimized and it becomes possible to determine if the sample pertains to the agricultural plume. These results support the use of steady state models for evaluating OWS as temporal variability makes meaningful interpretation of model results difficult or impossible.
Construction of a steady state numerical model addressed the limitations of the transient model by eliminating temporal variability and provided insight as to the importance of spatial versus temporal resolution of input data. Temporal variability was eliminated by averaging the observed hydraulic head, precipitation and evapotranspiration. Results from the calibration to observed hydraulic head for the steady state model indicate a significant improvement over the transient model. This suggests that the spatial resolution of input data, such as precipitation, evapotranspiration and hydraulic conductivity is not significantly limiting. The temporal resolution of input data is far more important for improvements in the transient model. The boundary conditions of the transient numerical model could be limiting the model’s ability to replicate the observed variability in hydraulic head. Defining variable boundary conditions would likely improve calibration results for the transient model but would be a significant undertaking. The question would also arise as to the benefit of constructing a transient model as most questions concerning an OWS could be answered via a steady state model.

Calibration of the contaminant transport portion of the steady state model did not produce an excellent fit of the observed data. It was anticipated that calibration results for the steady state model would be equal to or better than the aquifer model. However the numerical solution of the governing equations could result in error that prevented the model from replicating the observed nitrate concentrations. Any benefit that was provided by the ability of the model to consider three dimensional advection may be precluded by the numerical error. Additional work should be done to investigate the effect of solution error on model calibration results; however, this is not within the scope of this work. Though these results were not anticipated this illustrates the benefit of utilizing analytical solutions for some modeling applications.
Groundwater flow calculated by both numerical models also revealed that the assumption of one dimensional advection by the HPS solution is limiting. Both numerical models indicated that transverse advection occurs within the vicinity of the STU. The hydraulic head contours, and cell by cell flow data obtained from MODFLOW, show that the advective movement of water is directed radially away from the center of the STU within the immediate vicinity. This flow regime, however, does not persist down gradient of the STU, and flow can be approximated as one dimensional further down gradient. The implication for the aquifer model is that nitrate rich STU percolate may be transported laterally which will result in higher concentrations off the plume centerline but lower concentration along the centerline. For a smaller OWS or a reduced HLR the effect of lateral transport within or near the STU may be insignificant and the assumption of one dimensional flow appropriate. If conservative estimates are desired, nitrate concentrations should be calculated along the plume centerline, i.e. $y = z = 0$.

4.2 Conclusion

The aquifer model has been designed to provide the user with an estimate of nitrate concentration or mass flux down gradient of an OWS. It has many additional features that will allow the user to quickly and effectively evaluate contaminant transport. Its user friendly design will make it available to a large user group that has not had access to such a tool. While providing a tool of this type to a wider audience can be beneficial, the risk may be that users do not understand the limitations of a mathematical model. Mathematical models are necessarily simplifications of reality and taking model predictions as literal or expecting perfect performance from a model is not prudent. Rather, models should be used to test different hypothesis and if necessary make refinements. The research objectives of this work are to evaluate the limitations
of the aquifer model and determine if it is capable of replicating observed data to allow the user to align their expectations with the capability of the model.

4.2.1 Model Scope

Nitrate concentration can be calculated at any point within an aquifer receiving STU percolate. The HPS solution assumes a mass flux contaminant source and one dimensional advection. OWS that use high HLR may produce mounding of the water table beneath the infiltrative surface promoting transverse advection within the vicinity of the STU. In addition to this, because the HPS solution considers a mass flux contaminant source plane rather than a constant concentration contaminant source plane, dilution of nitrate by effluent is not accounted for. The transverse advection occurring due to water table mounding and the concentration effect caused by not accounting for dilution will result in over prediction of nitrate concentrations along the plume center line and under prediction along the plume edges.

Mass flux calculations estimate the mass of nitrate passing through a plane at point down gradient of the source specified by the user. If this method is used to estimate the potential mass flux of nitrate to a water body the estimate is inherently conservative as the model cannot account for streamlines that do not intersect the water body. In addition, the estimate may be conservative because the model will not account for increased denitrification that may occur within the hyporheic zone. In contrast, mass flux can be underestimated in some situations because denitrification is simulated via first order reaction kinetics. First order reaction kinetics are concentration dependent meaning higher concentrations along the plume centerline result in increased mass removal from the system. Finally, understanding the direction of the hydraulic gradient is critical for estimating potential mass flux. Incorrectly estimating the direction or
magnitude of the hydraulic gradient can significantly impact estimates of mass flux for a potential receptor.

The limitations of the aquifer model and HPS solution mentioned above also have important implications for parameter values estimated via model calibration to field observations. Model corroboration presented in chapter three shows that calibration of the denitrification parameter may result in an artificially low value due to agricultural nitrate concentrations or transverse advection due to water table mounding for points off the plume centerline. However, calibration utilizing observations approximately along the plume centerline may result in over estimation of the denitrification coefficient as the HPS solution tends to concentrate mass within this area. Other parameters estimated via calibration to field observations may also be over or under predicted for similar reasons.

While these limitations should be considered when utilizing the aquifer model, they do not preclude the usefulness of model estimates. During model corroboration it was concluded that denitrification was not as low as reported by the aquifer model thought it was likely limited within the area monitored at the GCREC field site. An independent evaluation of the denitrification potential of soils collected at the field site by Farrell [2013] concluded that it was exceedingly low affirming the conclusion from model corroboration. Estimates of transverse horizontal dispersivity were likely less than reported from calibration of the aquifer model. However, if the user desires to estimate dispersivity with more accuracy a tracer test can be conducted. This illustrates that the aquifer model is a versatile and powerful tool but that it does have limitations that should be recognized before using the model.

4.2.2 Transient versus Steady Modeling Approach

Two numerical models were constructed and calibrated to observed field data. A transient numerical model was constructed to examine limitations of the aquifer model. The transient
model considered daily changes in the hydraulic gradient due to precipitation and evapotranspiration. Because no data were available to account for daily fluctuations of nitrate mass flux to the aquifer, steady state contaminant loading was used. Also, boundary conditions were not capable of accounting for daily fluctuations in hydraulic head along model boundaries. These limitations in input data significantly limited the ability of the transient model to replicate observations. The groundwater flow portion of the model adequately replicated hydraulic head observations, though it was not capable of producing the observed variability within the observations. The contaminant transport portion of the model was unsuccessful in replicating the observed nitrate concentrations. The temporal variability in processes that control nitrate concentrations within the aquifer such as denitrification and mass flux as well as the limited input data for the model precluded any improvements.

Due to the poor results returned by the transient state model a steady state model was constructed for comparison to the aquifer model. The steady state numerical model eliminated temporal variability and examined the average behavior over time of the aquifer and contaminant transport within the aquifer. While this model was primarily constructed for comparison to the aquifer model to examine the significance of a three dimensional advection field, it revealed the limitations of transient state models. Transient state models require a significant amount of input data that may not be possible to obtain. Without this input data results from a transient model may be incorrect or difficult to interpret precluding the usefulness of such a model. Though it may seem desirable to evaluate an OWS utilizing transient state models, results from the construction and calibration of the two numerical models demonstrates that this is not an effective approach. Capturing the average or long term behavior of the OWS is far more useful and minimizes error.
4.2.3 A New Approach for Defining Boundary Conditions

Defining accurate boundary conditions is critical for constructing accurate models. Chapter three describes a method to construct accurate boundary conditions for numerical models of surficial aquifers in Florida. While the purpose of this work was not to develop a new method for defining boundary conditions, it may prove useful to others wishing to construct models that accurately capture the physics of a groundwater flow system. If constant head maps of the surficial aquifer do not exist a smoothed DEM can provide the necessary data to define constant head boundary conditions for locations with relatively smooth topography. Smoothing is accomplished by a moving window average algorithm that is relatively easy to construct. For this project the smoothing was done by an algorithm written in Excel VBA, though Python may be preferable as this will allow smoothing to be done within programs such as ArcGIS that are designed to handle DEM data directly.

4.2.4 Future Work

The capability of the aquifer model has been demonstrated by calibration to observation data. However, additional work can be done to address some of the limitations of the HPS solution. The HPS solution is desirable because it considers the geometry of an OWS but it is limited to considering a mass flux contaminant source. A viable solution to this problem is the analytical solution derived by Wexler [1992] that considers a vertical constant concentration contaminant source plane. This solution is similar to the solution derived by Domenico and Robbins [1985] however it does not make the same mathematical assumptions that are known to introduce error under certain conditions. In order to be included in the aquifer model, however, a method must be developed to accurately estimate the concentration value and the dimensions of the vertical source plane. Use of this solution will improve the aquifer model predictions along
the plume centerline and may allow the model to better predict concentrations along the plume fringes. The vertical contaminant source plane may also allow the aquifer model to account for transverse advection due to water table mounding for OWS that use high HLR. The HPS solution should still be used to estimate mass flux but calculations of concentration could be improved by this analytical solution.

The aquifer model currently does not provide the user with a calibration algorithm because calibration is a complex process. No doubt this model will be used by users that have sufficient expertise to accurately conduct a model calibration. The Levenberg–Marquardt algorithm used to calibrate the aquifer model can be added to the aquifer model to provide users with a robust calibration tool. Providing calibration capabilities with the aquifer model will require redesign of the Levenberg-Marquardt algorithm to ensure that it functions properly and provides users with accurate results. However, once added the calibration algorithm will provide unparalleled capabilities to an audience that has not had access to such tools.

4.2.5 Summary

- Concentration along the plume centerline is likely over estimated
- Concentration along the plume edges is likely underestimated
- Mass flux may be overestimated for receptors such as streams and lakes
- Mass flux for other receptors may be underestimated under certain conditions
- Calibrated parameter values can be under or overestimated depending on the location of the observation relative to the plume centerline
- The HPS solution is not adequate for OWS with high HLR
- Steady state models are preferable for evaluating OWS
- The aquifer model accurately replicated field observation for a large OWS
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104


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Appendix A

Table 12, descriptive statistics of the heterogeneous hydraulic field used in the numerical model to validate the HPS solution described in section 2.5.2.

<table>
<thead>
<tr>
<th>Hydraulic Conductivity [m/yr]</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>119.97</td>
</tr>
<tr>
<td>Median</td>
<td>84.84</td>
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<tr>
<td>Mode</td>
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</tr>
<tr>
<td>Standard Deviation</td>
<td>119.95</td>
</tr>
<tr>
<td>Range</td>
<td>7331.05</td>
</tr>
<tr>
<td>Minimum</td>
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<tr>
<td>Maximum</td>
<td>7332.49</td>
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<tr>
<td>Count</td>
<td>2109744</td>
</tr>
</tbody>
</table>

Table 13, descriptive statistics of the resultant velocity field produced by the random hydraulic conductivity field described in the table above and in section 2.5.2.

<table>
<thead>
<tr>
<th>Seepage Velocity [m/yr]</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
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</tr>
<tr>
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<td>Mode</td>
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<td>Standard Deviation</td>
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<tr>
<td>Range</td>
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</tr>
<tr>
<td>Minimum</td>
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<td>Maximum</td>
<td>4387.1</td>
</tr>
<tr>
<td>Count</td>
<td>2109744</td>
</tr>
</tbody>
</table>
Figure 28, the locations of the USGS monitoring wells where hydraulic head in the Floridian Aquifer has been monitored. These data informed the selection of the head value for the lower boundary condition in the two numerical models.

Figure 29, USGS Well (1)
Figure 30, USGS Well (2)

Figure 31, USGS Well (3)
Figure 32, USGS Well (4)

Figure 33, USGS Well (5)
Figure 34, USGS Well (6)

Figure 35, USGS Well (7)
Figure 36. USGS Well (8)

Figure 37. USGS Well (9)
Figure 38, USGS Well (10)

Figure 39, USGS Well (11)
Appendix C

Slug Test Analysis

Hydraulic conductivity for the saturated zone near the Soil Treatment Unit (STU) and directly
down gradient from it was inferred using the Bouwer and Rice method. The Hvorslev method was used to
corroborate results. The Bouwer and Rice and the Hvorslev method should be in relative agreement
provided assumptions inherent to both analysis are correct.

Hvorslev Slug-Test Analysis

The Hvorslev method is appropriate for wells that do not fully penetrate the aquifer, meaning the
screen length is less than the aquifer thickness. This method is appropriate for either addition or
withdrawal of water from the well. It is important prior to testing to know the well geometry and how it
was installed. If the ratio of the screen length to the screen radius is greater the 8 then the governing
equation given by equation 1 applies.

\[
K = \frac{r^2 \ln \left( \frac{L_e}{R} \right)}{2L_e t_{37}} \quad [\text{Hvorslev, 1951}]
\]

Where
- \( K \) (cm/d) = hydraulic conductivity
- \( r \) (cm) = radius of the well casing
- \( L_e \) (cm) = length of the well screen
- \( R \) (cm) = radius of the well screen
- \( t_{37} \) (s) = time for water level to fall to 37% of the initial change

The water level in the well is monitored before during and after the displacement of some volume
of water, either addition or withdrawal. The displacement at time \( t \) divided the by the initial \( \frac{H_t}{H_o} \),
maximum, displacement is plotted against time. The value \( t_{37} \) is selected by reading the x axis when the
ratio, \( \frac{H_t}{H_o} \), equals 0.37. Equation 1 can then be solved for hydraulic conductivity given in units that are
consistent with the plot of \( \frac{H_t}{H_o} \) vs \( t \). For the slug test data collected at the GCREC field site, it was
assumed that the radius of the well screen was the radius of the tubing used for the well and the length of
the well screen was the length of the slotted portion of the tubing. In situations where the well is installed
in a low permeable material and a higher permeable material such as gravel is used to fill between the
well screen and the bore wall, the screen length \( L_e \) becomes the length of the gravel pack and the radius
of the well screen \( R \) becomes the radius of the bore hole (Fetter 2001). The wells at the Florida field site
were installed using fine sand as backfill between the well casing and the bore wall. Because the backfill
materials is very similar to the native aquifer material it was assumed that the radius of the well screen
was the radius of the well casing and the length of the well screen was the length of the slotted portion of
the well casing. Results from both the Hvorslev and Bouwer and Rice analysis are given in the following table.

**Bouwer and Rice Slug-Test Analysis**

The Bouwer and Rice method provides an alternative analysis for slug tests which is useful for comparison with the Hvorslev method. It was anticipated that both methods would give values that are in relative agreement with each other. The Bouwer and Rice method uses a subset of the \(H_t/H_0\) vs Time data rather than a point value as the Hvorslev method does which can help eliminate effects of the borehole fill. Equation 2 gives the hydraulic conductivity for wells that penetrate an unconfined aquifer.

\[
K = \frac{r_c^2 \ln\left(\frac{R_e}{R}\right)}{2L_e} \cdot \frac{1}{t} \ln\left(\frac{H_0}{H_t}\right) \quad [\text{Bouwer and Rice, 1976}]
\]

Where
- \(K\) (cm/d) = hydraulic conductivity
- \(r_c\) (cm) = radius of the well casing
- \(R\) (cm) = Radius of the gravel envelop
- \(R_e\) (cm) = radial distance over which the head is dissipated
- \(L_e\) (cm) = length of the well screen
- \(H_0\) (cm) = initial displacement of the water table at time \(t = 0\)
- \(H_t\) (cm) = the displacement of the water table at time \(t = t\)
- \(t\) (s) = time since \(H = H_0\)

Where \(\ln\left(\frac{R_e}{R}\right)\) is given by equation 3 for wells that are not screened over the entire length of the aquifer and by equation 4 for wells that are screened over the entire length of the aquifer.

\[
\ln\left(\frac{R_e}{R}\right) = \left[\frac{1.1}{\ln\left(\frac{L_e}{R}\right)} + \frac{A + B \ln\left(\frac{H_t - L_e}{R}\right)}{\frac{L_e}{R}}\right]^{-1}
\]

\[
\ln\left(\frac{R_e}{R}\right) = \left[\frac{1.1}{\ln\left(\frac{L_e}{R}\right)} + \frac{C}{\frac{L_e}{R}}\right]^{-1}
\]

Where A, B, and C are dimensionless numbers that were empirically derived and are given by the following equations.

\[
A = 1.63844567 + 0.166908063 \times \log\left(\frac{L_e}{R}\right) + 0.000740459 \times e^{\left(6.17105281 \times \log\left(\frac{L_e}{R}\right) - 1.054747686 \times \log\left(\frac{L_e}{R}\right)^2\right)}
\]

\[
B = 0.174811819 + 0.060056188 \times \log\left(\frac{L_e}{R}\right) + 0.0007965502 \times e^{\left(2.053376868 \times \log\left(\frac{L_e}{R}\right) - 0.007990328 \times \log\left(\frac{L_e}{R}\right)^2\right)}
\]
Similar to the Hvorslev method, the Bower and Rice slug test analysis observes the time required for the water level in the well to return to its equilibrium level after the initial disturbance. The ratio of the displacement at time $t$ to the initial (maximum) displacement is plotted versus time on a semi log plot. The exponential rate constant given by the trend line fitted to the data gives the value of the last part of of equation one, i.e. $\left[\frac{1}{\tau} \cdot \ln(H_0/H_t)\right]$

\[
C = 0.074711376 + 1.083958569 \cdot \log\left(\frac{L_e}{R}\right) + 0.00557352 \cdot e^{2.929493814 \cdot \log\left(\frac{L_e}{R}\right) - 0.001028433 \cdot \left(\log\left(\frac{L_e}{R}\right)\right)^2}
\]
Table 14. hydraulic conductivity estimates for the GCREC field site produced the Hvorslev and Bouwer & Rice analysis methods

<table>
<thead>
<tr>
<th>Well ID</th>
<th>Date</th>
<th>Bouwer &amp; Rice (ft/d)</th>
<th>Hvorslev (ft/d)</th>
<th>Bouwer &amp; Rice (m/yr)</th>
<th>Hvorslev (m/yr)</th>
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<th>Well ID</th>
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Figure 40, the locations of the piezometers where slug tests were conducted relative to the OWS STU.
Figure 41, the interpolated hydraulic conductivity field constructed using results from the Hvorslev analysis method. Interpolation was carried out using a kriging algorithm in ArcGIS.

Figure 42, the interpolated hydraulic conductivity field constructed using results from the Bouwer & Rice analysis method. Interpolation was carried out using a kriging algorithm in ArcGIS.
**Figure 43**, the hydraulic conductivity field used in the two numerical models. The blue and green regions represent areas that were identified as a course sand and fine sand by the NRCS soil survey data. The multicolored region in the middle was created by interpolating hydraulic conductivity data obtained from slug tests with a kriging algorithm in ArcGIS.
Appendix D

Figure 44, well completion report for a water supply well completed on the GCREC property.

Figure 45, well completion report for a water supply completed on the GCREC property. This well log indicates a large void space between 260 – 263 feet below land surface.
**Figure 46.** Well completion report for a water supply well completed on the GCREC property.
Appendix E

Table 15, the calibration results from the calibration of the aquifer model utilizing the 33 nitrate observations. The longitudinal dispersivity decreases while the transverse dispersivity increases.

<table>
<thead>
<tr>
<th>Calibrated Parameter Values</th>
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<tr>
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<tr>
<td>$\alpha_z$ [m]</td>
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</table>

Observed NO3 vs HPS NO3

Figure 47, the calibration results from calibration to the 33 nitrate observations. These results are affected by those observations which are believed to be heavily influenced by the agricultural nitrate plume.

Table 16, calibration results obtained from the calibration of the parameters identified in section 3.2.1 and input concentration using the 33 nitrate observations. The longitudinal dispersivity and input concentration have notable increased.

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<td>Conc. [mg-N/L]</td>
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Figure 48, calibration results for the calibrated parameters presented in table 15. These results were obtained by including input concentration as a calibration parameter. The results are improved over figure 48 but the input concentration and dispersivity values do not appear realistic.

Table 17, calibration results from a calibration that included the input concentration and the 23 observations that are part of the OWS nitrate plume. Eliminating the points that were thought to be heavily influenced by the agricultural plume resulted in calibrated parameter values very similar to those presented in section 3.2.1.

<table>
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<td>Conc. [mg-N/L]</td>
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</table>
Figure 49. calibration results for the parameters in table 16. These results are identical to those presented in section 3.2.1 however these results were achieved by also calibrating the input nitrate concentration.