Florida Onsite Sewage Nitrogen Reduction Strategies Study

Task D.12

Aquifer-Complex Soil Model Performance Evaluation

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TASK D.12
WHITE PAPER

Aquifer-Complex Soil Model Performance Evaluation

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Section 1.0
Introduction

1.0 Introduction

As part of Task D for the Florida Onsite Sewage Nitrogen Reduction Strategies Study a combined vadose zone and saturated zone model is being developed. This white paper, prepared by the Colorado School of Mines (CSM), documents the Task D.12 performance evaluation conducted on the combined complex soil model (STUMOD-FL) and the aquifer model (horizontal plane source, HPS).

The overreaching goal of Task D is to develop quantitative tools for groundwater contaminant transport that can be employed by users with all levels of expertise to evaluate onsite wastewater treatment systems (OWTS). The combined aquifer-complex soil model, STUMOD-FL-HPS, is intended to fill the gap that currently exists between end users and complex numerical models by overcoming the limitations in the application of complex models while maintaining an adequate ability to predict contaminant fate and transport. The aquifer model uses an analytical contaminant transport equation that is ideally suited for an OWTS that simplifies user input. The aquifer model is coupled with the Soil Treatment Unit Model (STUMOD-FL) providing the user with the ability to seamlessly evaluate contaminant transport through the vadose zone and aquifer underlying an OWTS. The model has been implemented as an Excel Visual Basic Application (Excel VBA) to make the final product readily available to and easily implemented by a wide range of users.

Section 2.0
Approach

Task D.12 includes performance evaluation of the aquifer-complex soil model implementation, corroboration/calibration, parameter sensitivity analysis and uncertainty analysis of the aquifer model described in Task D.11. Data sets from Florida were used. Metrics include average concentration observations and model output. Model-evaluation statistics were used to determine whether the model could appropriately simulate the observed data. Multiple methods for evaluating the model performance were used for model evaluation. Results from the evaluation show that STUMOD-FL-HPS is an effective tool for evaluating contaminant transport in the surficial aquifer beneath an OWTS.

The aquifer model is coupled with STUMOD-FL to obtain boundary concentrations for nitrogen species infiltrating through the soil treatment unit to the water table. Concentration reaching the water table is the only parameter calculated by STUMOD-FL that is used in the aquifer model. However, the aquifer model may also be run independently of STUMOD-FL with user provided values for contaminant concentrations at the water table. Thus it was determined that more valuable information would be obtained by doing model performance evaluation (calibration, parameter sensitivity and uncertainty analysis) independently on the aquifer model.

Calibration, parameter sensitivity and uncertainty analysis was done on STUMOD-FL based on unsaturated zone parameters as described in Task D.9. Saturated zone parameters have no relevance to STUMOD outputs, which is analogous to watershed modeling where a downstream gage or downstream catchment properties do not have effect on calibration to an upstream gage station. Only those parameters specific to zones contributing to the observation point (in this case, the water table) are relevant.

For an observation point in the saturated zone downstream of the soil treatment unit (STU), model predictions could be affected by the performance of the unsaturated zone model when the concentration input for the aquifer model is obtained from the unsaturated zone model. However, even for an observation point in the aquifer downstream of the STU, it is important to limit the number of parameters to be evaluated or estimated through calibration. Although optimization of many input parameter values at a time can lead to a better match between simulated and observed values, (1) the improved fit may simply capture errors in the observations rather than behavior of the system; and (2) it is often impossible to converge on a unique solution when estimating many parameters (Hill and Tiedeman, 2007). Thus, it is advised to limit the number of parameters to be estimated.

Fixing the values of some parameters to either some reasonable value based on field measurement or using a different approach that results in a better estimate of parameter values, can limit the number of parameters estimated. If there is a better approach to fix parameters values to some value for some compartment of an integrated model, it is advisable to do so to reduce uncertainty. It is customary to assign priority values to parameters using some generalized approach to reduce the number of parameters to calibrate. This means that a more accurate performance evaluation can be achieved by fixing the vadose zone parameters affecting concentration input to the saturated zone by calibrating the vadose zone model independently, based on observations at the water table, rather than simultaneously calibrating saturated and unsaturated zone parameters using observations in the subsurface downstream of the STU. A similar approach is used in watershed modeling where calibration starts with sub basins upstream using an observation at an upstream gage station, fixing parameter values for sub basins upstream and then moving to downstream locations. Calibration using an observation in the aquifer may result in an average performance for both compartments while calibration by compartment (vadose and/or saturated) would result in better performance for each zone. Calibration, parameter sensitivity and uncertainty on a zone by zone basis provides more details about parameter values, sensitivity of parameters and uncertainty pertinent to each zone rather than a black box approach based on observation points in the subsurface downsteam of STU.

Finally, again, concentration reaching the water table is the only input related to the vadose zone that is used in the aquifer model. This input was altered during the uncertainty analysis of the aquifer model as described in Section 3.3. Because the effluent concentration was not identified as a sensitive parameter in the parameter sensitivity analysis, this input is not likely to have a large effect in the model calibration or uncertainty analysis of the aquifer model.

Section 3.0
Model Parameter Sensitivity and Uncertainty Analysis

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.

3.1 Parameter Sensitivity Analysis

Parameter sensitivity analysis is a useful tool for model users; because it provides an idea of which parameters 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 are local and global methods (Geza et al., 2010; Saltelli et al., 2000). Global techniques evaluate the impact on model output from changes in multiple parameter values while local techniques evaluate only 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 continuous distributions rather than discrete distributions. Saturated hydraulic conductivity is an example of a parameter value that exists as a continuous distribution. Thus, 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 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.

3.2 Parameter Sensitivity 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 hydraulic loading rate (HLR) of 5.95 m/yr (1.6 cm/d) at the water table. This would be equivalent to an OWTS receiving approximately 5300 gal/d at a HLR of 0.39 gal/ft^2/d and a total nitrogen concentration equal to or greater than 30 mg-N/L in the septic tank effluent. Within a typical OWTS, 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 described in Task D.11 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 3-1 through 3-3. 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 3-3 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 to retardation was included to account for this effect, not for the case where retardation is greater than one and slows contaminant movements (e.g., ammonium). Sensitivity results show that retardation 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. As porosity decreases seepage velocity increases decreasing the transport time. 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.

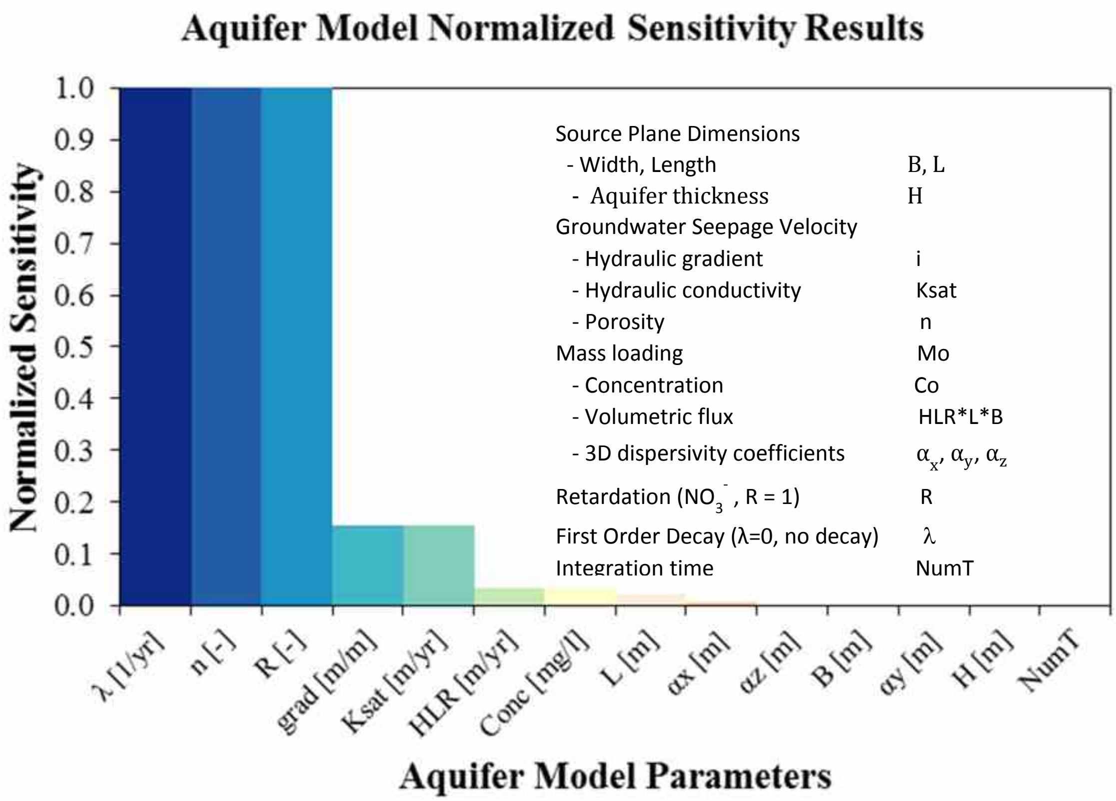

Figure 3.1: Normalized Sensitivity Analysis Results

Results show denitrification, porosity and retardation have the largest impact on model output and should be independently evaluated or calibrated to minimize uncertainty.

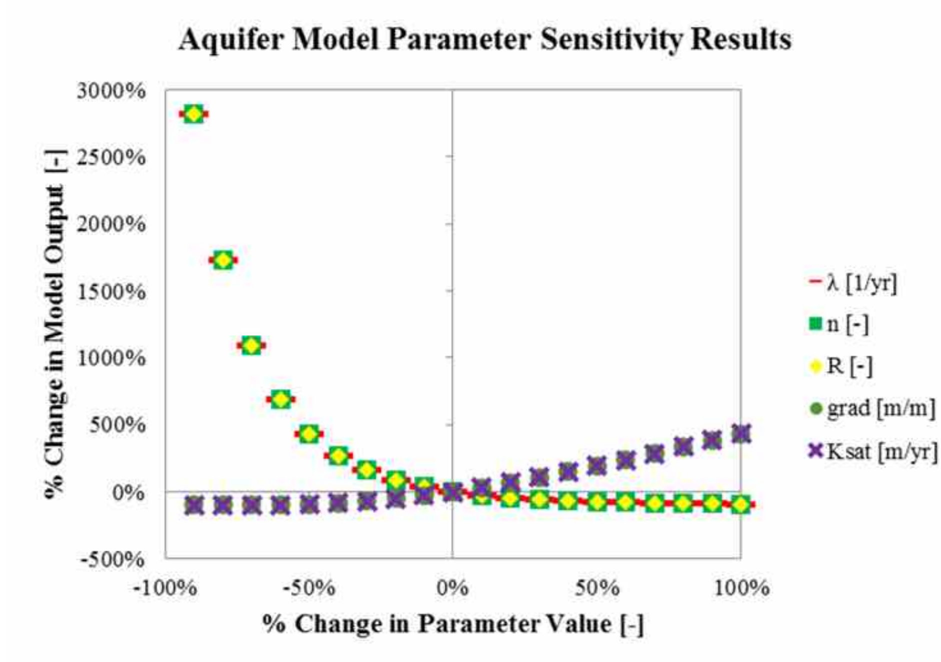

Figure 3.2: Sensitivity Analysis Results

Five parameters identified as most sensitive are shown (see Figure 3.1). Small porosity, retardation, and decay values have the largest impact on model output.

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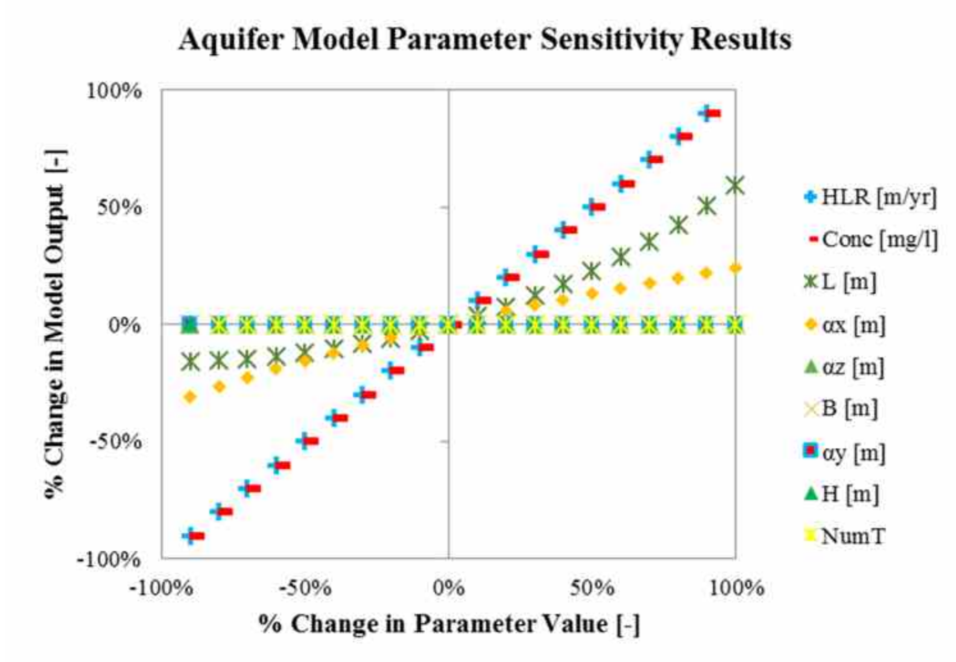

Figure 3.3: Additional Sensitivity Analysis Results

Model parameters not shown in Figure 3.2 with 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.

3.3 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 discussed, 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-FL to provide insight into probable model outcomes (Table 3.1). 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 included 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 3.1).

Table 3.1
Distributions Used for Each Parameter Included in the Uncertainty Analysis

Parameter	Distribution	Mean/Max	Std/Min
R [-]	random uniform	1	0.95
n [-] SMP	random log normal	0.3874	0.055
n [-] SLP	random log normal	0.3749	0.055
n [-] SCL	random log normal	0.38	0.061
grad [m/m]	random uniform	0.05	0.001
conc [mg-N/L]	random normal	30	3
λ [1/yr]	random uniform*	1	0
α_L [m]	random uniform	5	0.5
α_{TH} [m]	random uniform	1	0.005
α_{TV} [m]	random uniform	1	0.005
K_{sat} [cm/d] SMP	random log normal	2.83	0.59
K_{sat} [cm/d] SLP	random log normal	2.55	0.59
K_{sat} [cm/d] SCL	random log normal	1.39	0.85

Equation used for denitrification (McCray et al., (2005)):

$$y = 365.25 \cdot e^{(x-0.9288)/_{0.1348}} \tag{3-1}$$

Where, x is denitrification rate, and y is the probability that a denitrification rate is below x in the cumulative frequency distribution (CFD).

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 $\pm$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 3.1 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/d) meaning this function is incapable of considering the case of denitrification less than the minimum reported rate of 0.004 (1/d). To address this, the distribution function was modified considering only denitrification rates less than or equal to the 50th percentile value of 0.025 (1/d) 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 et al., 2010).

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 3.1

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).

3.4 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 (Figure 3.4 and 3.5). 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., (2005) 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 differences between the two uncertainty analysis results shown in Figure 3.4 and 3.5 demonstrate the importance of the denitrification parameter. 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. When the entire range in McCray et al., (2005) is used, there was higher probability for removal at 200 feet downgradient for all soil types, unlike the second case where the lower denitrification rate (rates below the median) are used. In the latter case, there is a considerably lower probability of removal at 200 feet. These results reveal that model output uncertainty changes in response to 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 (Figure 3.4 and 3.5). 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.

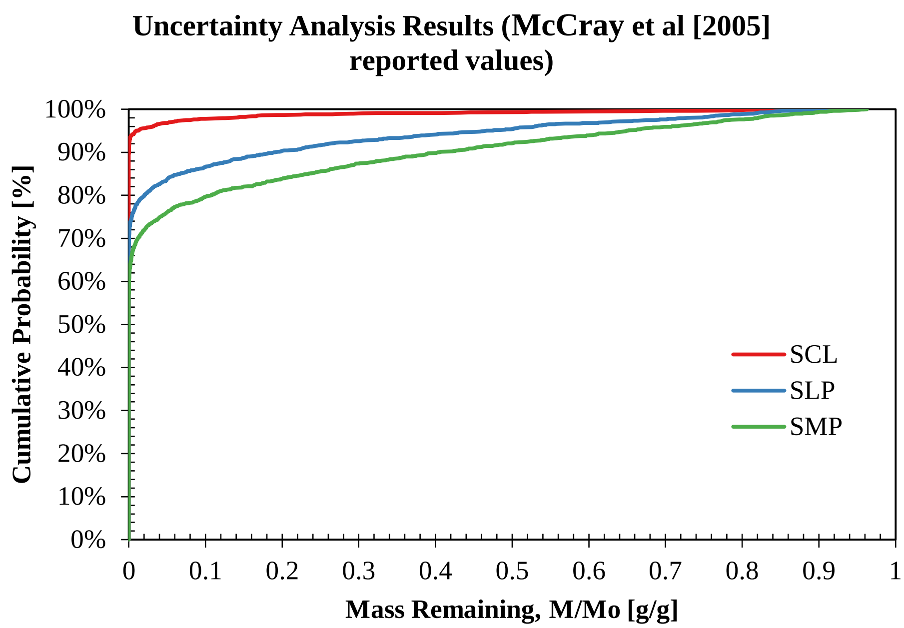

Figure 3.4: Uncertainty Analysis Results for Sandy Clay Loam (SCL), Less Permeable Sand (SLP) and More Permeable Sand (SMP) Utilizing Denitrification Values Reported by McCray et al., (2005)

Results do not consider the case of denitrification less than the minimum denitrification rate, 0.004 (1/d), reported by McCray et al., (2005).

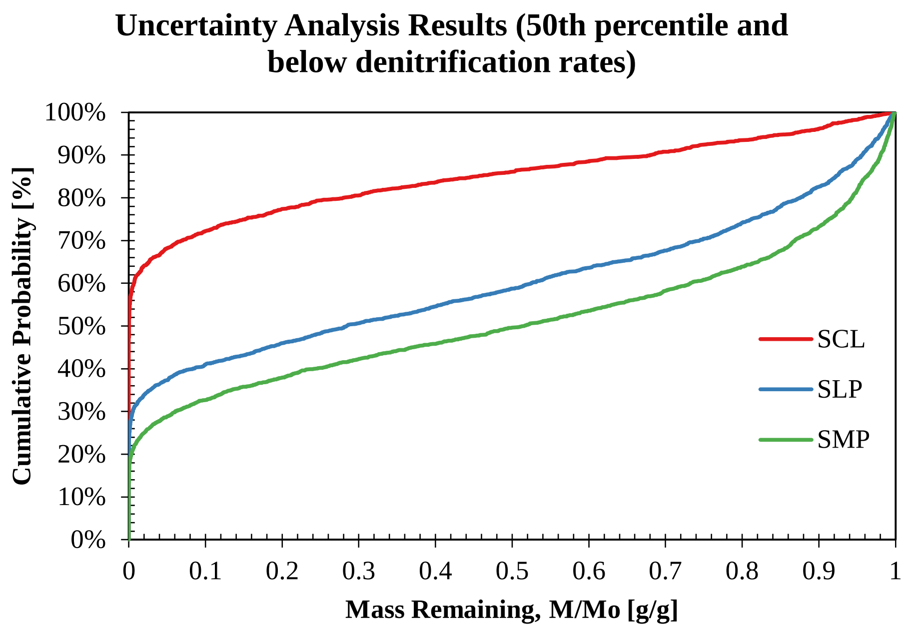

Figure 3.5: Uncertainty Analysis Results for Sandy Clay Loam (SCL), Less Permeable Sand (SLP) and More Permeable Sand (SMP) Utilizing Denitrification up to 0.025 (1/d)

Maximum denitrification rate is the 50th percentile value, 0.025 (1/d) reported by McCray et al., (2005).

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Section 4.0
Model Performance Evaluation-Corroboration/Calibration of Aquifer Model

The mathematical derivation, solution scheme and programing in Excel were checked to determine that it correctly describes the one dimensional advection and three dimensional dispersion of a contaminant. In order to establish the predictive capabilities of the aquifer model for OWTS and aquifers, the performance was evaluated using data collected from the surficial aquifer at the University of Florida Gulf Coast Research and Education Center (GCREC) mound. In an effort to evaluate accuracy of implementation of the model in Excel-VBA, the model outputs were compared to a numerical model as well. The calibration of the aquifer model and comparison to a numerical model was done to provide supporting evidence as to the utility of this tool for evaluating contaminant transport from OWTS to aquifers.

The veracity of the HPS solution was checked by a comparison between results obtained from the HPS solution to those from a numerical model for a non-decaying synthetic contaminant. The purpose of this comparison was to determine the accuracy of the mathematics, solution scheme, and programing in Excel used to derive and solve the HPS solution. The numerical models used were MODFLOW and MT3DMS (Harbaugh, 2005; Zheng and Wang, 1999). The results from this comparison indicated that the HPS solution implemented in Excel-VBA accurately calculates the contaminant concentration as estimated by a numerical model. These comparisons are not intended to replace the corroboration/calibration of the aquifer model, which compares the HPS solution, to observed field data; it was intended to verify the implementation of the HPS solution.

The following discussion focuses on corroboration/calibration of the aquifer model using observed field data. 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 provided a good estimation of the performance of the aquifer model.

4.1 Field Site and Data

Groundwater data were collected at the University of Florida GCREC mound as part of Task C. 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 account for 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. Also presented are the hydraulic head observations and the method that was used to estimate groundwater seepage velocity for the aquifer model.

4.1.1 Field Site Description

The GCREC site description has been provided in previous deliverables. However, a summary is recapped here in context of how Task C field data were utilized for model performance evaluation. The GCREC, located in southern Hillsborough county Florida approximately 30 miles from the city of Tampa, 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 mound OWTS designed for flows in excess of 2500 gallons per day serves the facility and receives primarily domestic wastewater from the offices. The OWTS was constructed approximately 6 years prior to the sampling campaign, which is sufficient time to approach steady state conditions in the STU (Parzen, 2007).

The GCREC mound OWTS design HLR was 0.65 gal/ft^2/d (2.65 cm/d), however based on a slightly larger infiltrative surface of 4,800 ft^2, the effective design HLR was 0.59 gal/ft^2/d. Review of flows to the mound (to each half and the combined total flow), suggest that the actual median HLR was 0.46 - 0.49 gal/ft^2/d (average HLR was 0.54 - 0.57 gal/ft^2/d). The infiltration area where effluent is dispersed is approximately 82 by 115 feet in dimension. Effluent is applied via low pressure dosing in an alternating pattern to half of the infiltrative area at each dose. The infiltrative area is elevated approximately 4-5 feet above the surrounding land surface. This ensures that an unsaturated region exists beneath the infiltrative area even during high water table conditions.

Twenty-two piezometers were installed in the surficial aquifer in the area surrounding the OWTS 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 points consisting of a stainless steel drive point and screened body connected to ¼-in. tubing were driven into the surficial aquifer at multiple depths on a grid pattern downgradient of the mound (Figure 4-1). These drive point samplers 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 locations installed in the surficial aquifer.

Groundwater samples were collected on four occasions: December 2010, April 2011, June 2011 and September 2011. Groundwater quality was not monitored throughout the entire study period 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, 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 (see Section 4.1.3) indicating that the majority of nitrogen exists as nitrate within the surficial aquifer.

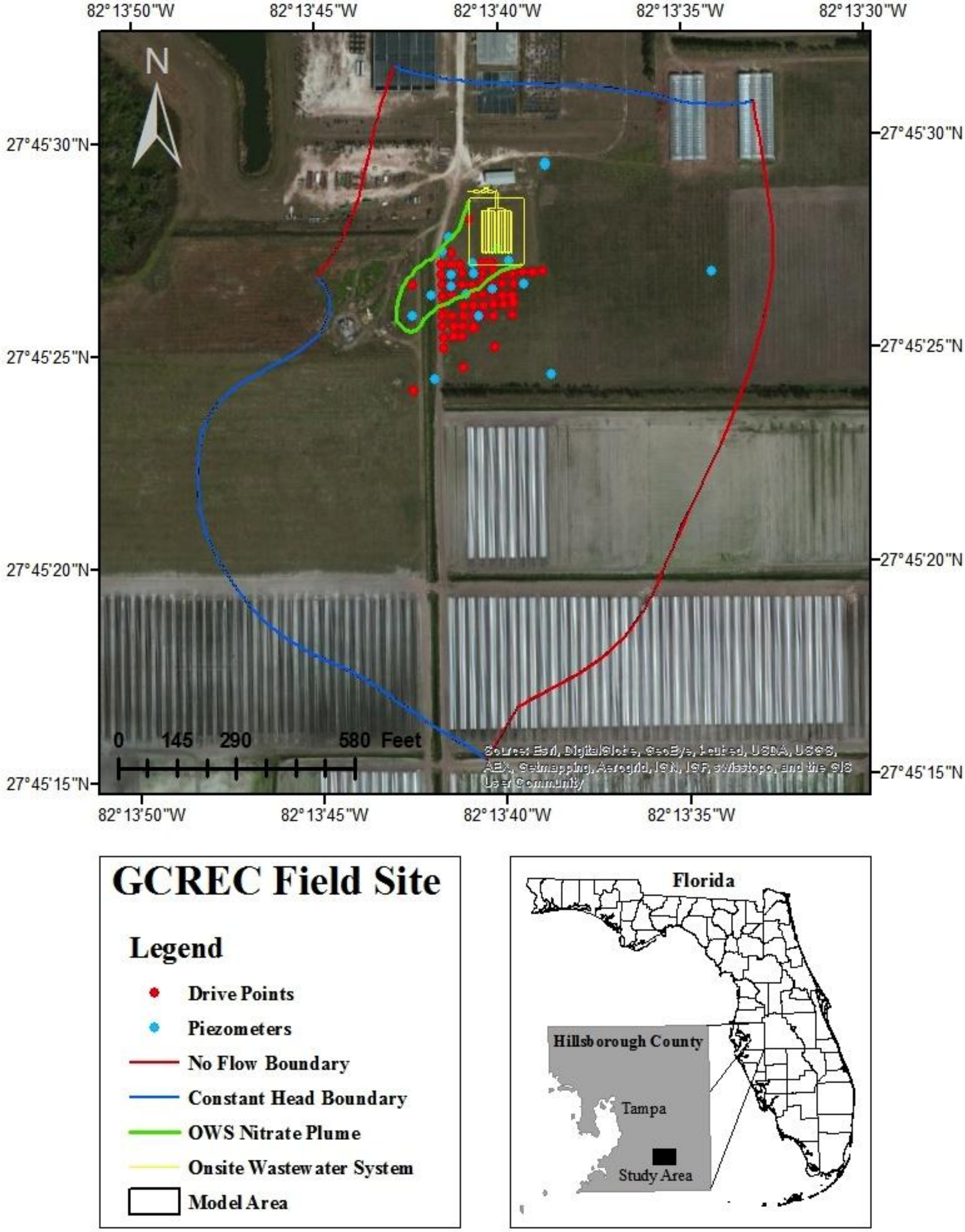

Figure 4-1: GCREC Field Site Layout

Surrounding area is agricultural where synthetic fertilizers are used. The delineated nitrate plume from the OWTS aligns well with the direction of the average hydraulic gradient which is directed towards a local stream.

4.1.2 Hydrogeologic Description

The aquifer system underlying most of Florida 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 Floridan aquifer, a middle confining unit, and the Lower Floridan aquifer (McGurk, 1998; Sepúlveda et al., 2012; Yager and Metz, 2004). Drinking water wells are typically located within the Upper Floridan aquifer though in some areas the upper confining unit can also be an important source of fresh water (Figure 4-2). The surficial aquifer is generally not used as a drinking water source directly in most of Florida, but serves as an important source of recharge for the Upper Floridan 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 and Metz, 2004).

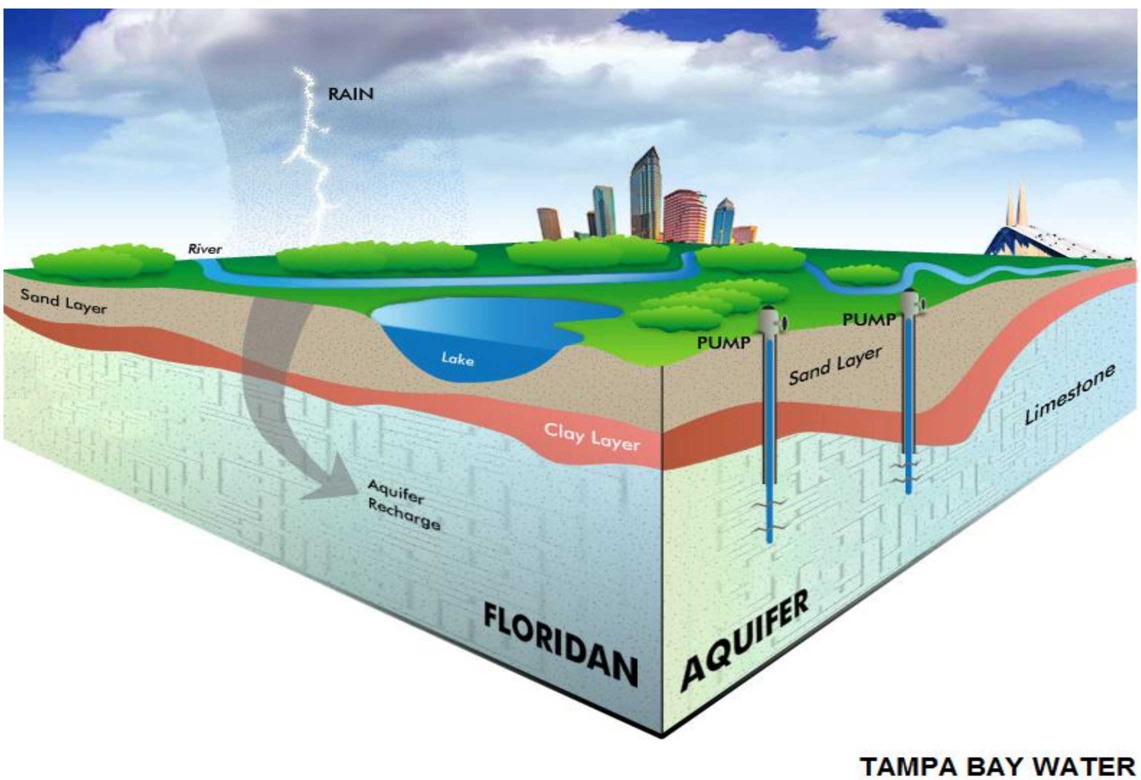

Figure 4-2: Conceptual Model of the Surficial Aquifer System

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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. The depth to the upper confining unit (Hawthorn Layer) at the GCREC field site is approximately 25-30 feet. The surficial aquifer is characterized by a free water table and receives direct recharge from precipitation and OWTS 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 4-3. 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.

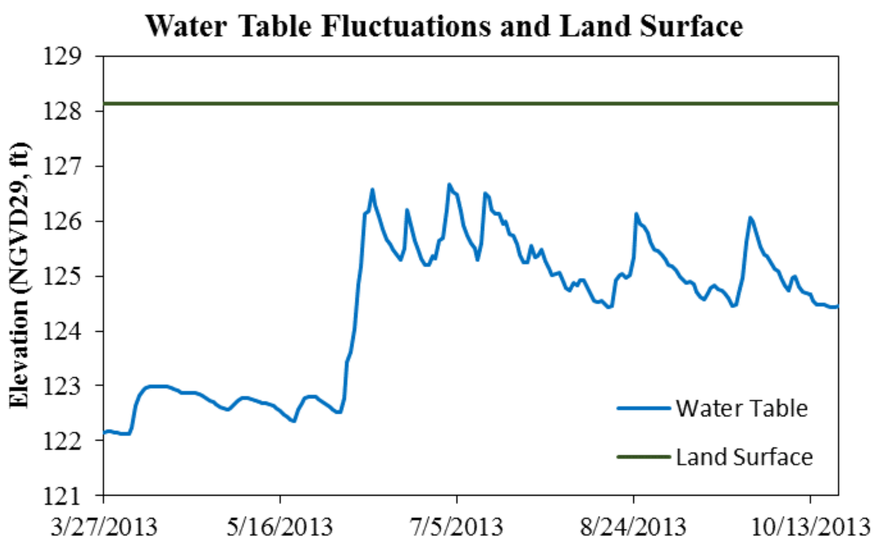

Figure 4-3: Water Table Fluctuations

Water table measured by a pressure transducer and indicates 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 1986; Yager and Metz, 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 and Metz, 2004). Vertical hydraulic conductivities for this layer are reported to range between 7.6 x 10^{-5} - 0.34 ft/d (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.

The Upper Floridan aquifer includes portions of the Hawthorn group, including the Suwanee limestone, the Ocala limestone and the top of the Avon Park formation, where present (Merritt 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 surface. The Upper Floridan aquifer is the primary production zone for groundwater and wells are typically screened within the Suwanee and Ocala limestone or Avon Park formation (Merritt 2004). The secondary porosity within these zones is the principal source of extracted groundwater.

4.1.3 Data Analysis

Groundwater samples were collected within the surficial aquifer immediately down gradient of the infiltrative surface of the OWTS. Groundwater quality within the confining unit and the Upper Floridan 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 OWTS any effects on groundwater quality are likely mitigated to a certain degree which makes identification of the contaminant plume more difficult.

Table 4.1 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 maximum contaminant levels (MCL) of 10 mg-N/L, approximately a third of the groundwater samples exceeded the MCL. Groundwater samples also reveal that the mound appears to be functioning correctly by attenuating the movement of ammonium to groundwater via transformation of ammonium 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-FL.

Table 4.1
Descriptive Statistics of Groundwater and Effluent Samples Collected at the GCREC Mound Field Site

	GW Samples		Effluent Samples	
	NO_3^- [mg-N/L]	NH_4^+ [mg-N/L]	NO_3^- [mg-N/L]	NH_4^+ [mg-N/L]
Mean	9.5	0.12	0.11	34.5
Median	8.4	0.013	0.065	30.5
Mode	12.0	0.005	0.24	28
Standard Deviation	7.9	0.34	0.11	13.8
Max	46.0	3.0	0.24	61
Min	0.015	0.005	0.01	22
Count	306	306	6	6

While sorption of ammonium in the surficial aquifer could account for the low ammonium concentrations observed, this is not likely as the soils 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 OWTS 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 OWTS effluent, indicates 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 OWTS. 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 account for the effect of the agricultural nitrate plume and improve identification of those samples representative of the OWTS effluent plume. This method was developed from observations that indicated that samples taken near the OWTS infiltrative area had a relatively high specific conductance. The higher specific conductance is attributed to OWTS effluent, because natural recharge from precipitation is not as likely to contain high levels of dissolved anionic species. OWTS 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 OWTS effluent plume or not.

Using the methodology described above, the area in Figure 4-4 was determined to be part of the OWTS effluent plume. A limitation of the method is that it does not account for dilution that would reduce the specific conductance of the groundwater and may cause omission of some OWTS plume data in the evaluation. Vertical hydraulic gradients and water table fluctuations that cause mixing of the OWTS and agricultural plumes also make it difficult to locate the vertical extent of the OWTS effluent plume. It is highly likely that this location is variable throughout the aquifer due to water table fluctuations.

Therefore, the data within the area marked in Figure 4-4 were used for model calibration and evaluation of the aquifer model. 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 OWTS 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 OWTS effluent. Additional descriptive statistics for the OWTS plume samples are presented in Table 4.2.

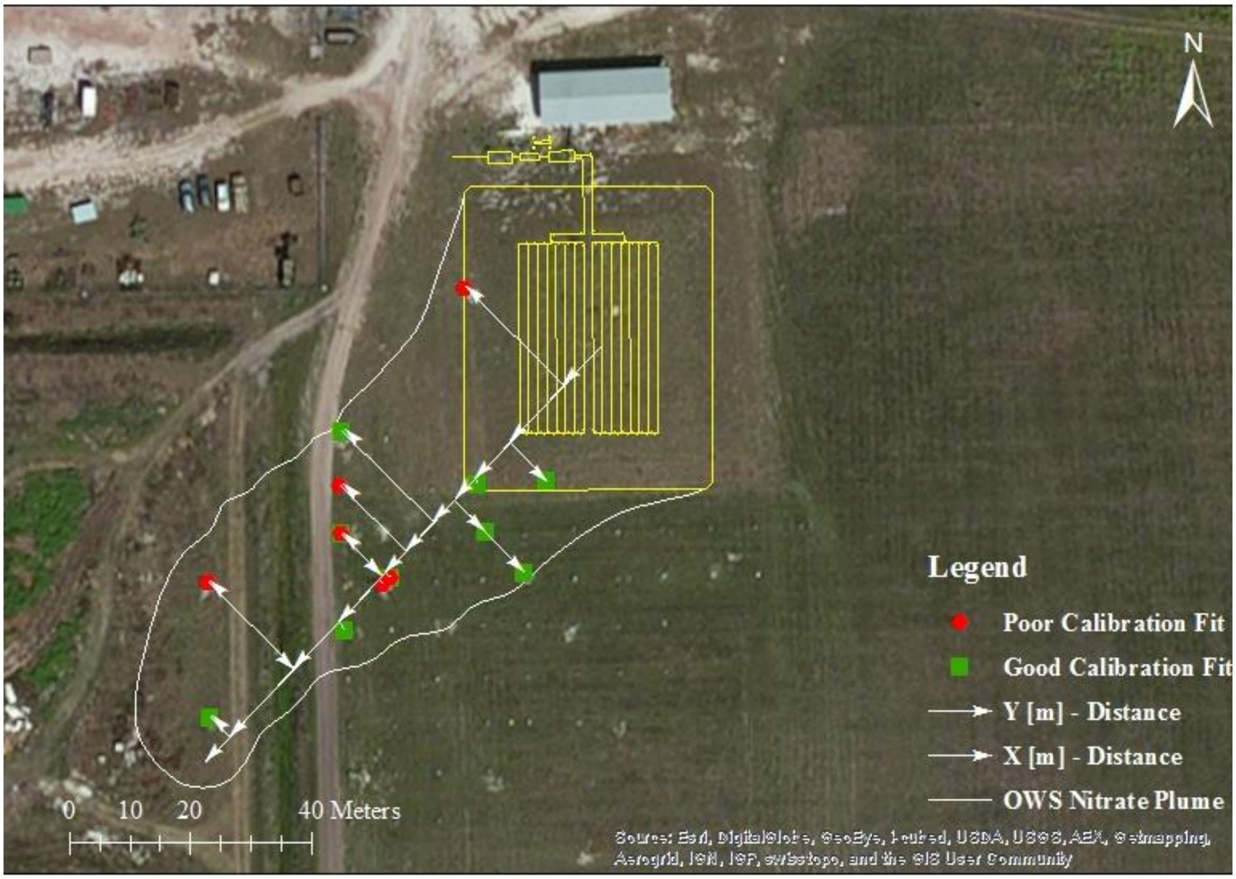

Figure 4-4: Method Used to Estimate X, Y and Z Values Required by the Aquifer Model to Calculate Concentration.

Table 4.2
Descriptive Statistics for Groundwater Samples in the Area Directly Affected by Percolate from the Mound

	GW Samples	
	NO_3^- [mg-N/L]	NH_4^+ [mg-N/L]
Mean	14.7	0.11
Median	12	0.028
Mode	12	0.005
Standard Deviation	8.6	0.21
Max	46	1.5
Min	0.17	0.005
Count	101	101

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 OWTS, 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 calibration. In order to minimize the effects, observations used for calibration of the aquifer model were averaged for each sampling location. The objective was to approximate the long term nitrate concentration at those points within the aquifer. Several locations were sampled only one or two times due to budget limitations. These data were not used for calibration of the aquifer 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 4.8) for calibration of the aquifer model.

The aquifer model constructed for calibration requires 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. Nitrate mass flux to groundwater was estimated using STUMOD-FL nitrate concentration predictions. Ammonium input concentrations to STUMOD-FL were assumed to be equivalent to what was observed in the septic tank effluent samples presented in Table 4.1. Parameter values and other site specific conditions were input into STUMOD-FL for each simulation. Because the NRCS soil survey for the area indicates a transition between Zolfo and Seffner sands within the field site, STUMOD-FL simulations were conducted using two groups of parameters representative of the more permeable sand and less permeable sand for a total of 12 STUMOD-FL simulations. STUMOD-FL results for nitrate concentration at the water table are presented in Table 4.3 and are an average of the outputs using the two different sands (the input concentration was later modified to 25 mg-N/L, see Table 4.6). These results were initially used as direct inputs for nitrate loading for the aquifer model during calibration.

Table 4.3
Descriptive Statistics for the Twelve STUMOD-FL Predictions of Nitrate Concentration in Mound Percolate at the Water Table

	NO_3^- [mg-N/L/d]
Mean	3.9
Median	1.6
Mode	1.9
Standard Deviation	6.3
Max	21.7
Min	0.2
Count	12

In addition to the groundwater samples that were gathered, hydraulic head observations were also collected. Hydraulic head was measured at piezometers shown in Figure 4-1 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 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 4.4).

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Table 4.4
Descriptive Statistics for Average Hydraulic Head

	Mean	Median	Mode	Std	Range	Min	Max	Count
PZ02	119.55	119.57	118.87	1.20	7.26	118.11	125.37	36
PZ03	120.24	120.16	120.50	1.24	8.11	119.04	127.15	42
PZ04	122.85	122.73	#N/A	1.55	9.74	119.19	128.93	47
PZ05	122.42	122.23	120.68	1.59	8.87	120.68	129.55	32
PZ07	121.42	121.31	120.67	1.34	7.95	119.72	127.67	40
PZ08	120.79	120.63	119.93	1.30	7.76	119.33	127.09	38
PZ09	120.21	120.08	120.57	1.03	5.73	119.06	124.79	35
PZ10	121.80	121.61	#N/A	1.80	10.71	119.90	130.61	33
PZ11	120.72	120.78	121.29	1.01	6.00	118.21	124.21	36
PZ13	121.06	121.01	121.65	0.80	3.37	119.68	123.05	40
PZ14	119.75	119.66	119.44	1.09	6.02	118.71	124.73	31
PZ15	120.91	120.89	120.16	1.26	6.91	119.36	126.27	31
PZ16	120.41	120.45	120.91	0.88	4.44	119.07	123.51	30
PZ17	119.44	119.21	118.56	1.67	9.02	118.26	127.28	26
PZ18	119.32	119.35	119.35	0.70	3.86	117.98	121.84	28
PZ19	120.40	120.22	120.66	1.51	8.64	119.02	127.66	31
PZ20	120.42	120.25	120.57	1.51	8.69	119.03	127.72	31
PZ21	120.47	120.37	#N/A	1.50	8.58	119.01	127.59	30
PZ22	120.43	120.26	119.37	1.51	8.46	119.00	127.46	29
PZ23	120.90	120.77	119.64	1.49	8.25	119.31	127.56	31
PZ24	123.01	122.71	#N/A	2.05	11.03	120.52	131.55	33

This algorithm incorporated into STUMOD-FL-HPS was then used to calculate the average hydraulic gradient magnitude and direction for all combinations (Table 4.5). The groundwater seepage velocity was calculated using Darcy's equation using 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. This is very similar to the estimated velocity from the first tracer test if a similar Ksat is used (see Task C.15, Tracer Test No. 1 Report). The calculated direction of the hydraulic gradient also aligns well with the area that is thought to be directly affected by the GCREC mound effluent.

Table 4.5
Descriptive Statistics for the Calculated Hydraulic Gradient and Bearing

Gradient (ft/ft)		Bearing (degrees)	
Mean	0.028	Mean	221
Median	0.025	Median	228
Mode	0.029	Mode	240
Standard Deviation	0.014	Standard Deviation	47
Max	0.080	Max	360
Min	0.00048	Min	0.6
Count	8015	Count	8015

4.2 Aquifer Model Performance and Evaluation

4.2.1 Model Parameter Values and Observations

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 mound at the GCREC 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 4-4). 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.

The aquifer model requires a number of parameters that were not included in the calibration procedure because independent methods were used to establish these values (Table 4.6). The methods used to independently obtain parameters are discussed below.

Table 4.6
Fixed Parameter Values used for Calibration of the Aquifer Model

Fixed Parameters		
Parameter	Symbol [units]	Parameter Value used in Model
Retardation factor	R [-]	1
Porosity	n [-]	0.39
Aquifer thickness	H [m]	39.62
Trench width	B [m]	26
Trench Length	L [m]	35
Hydraulic gradient	grad [m/m]	0.025
Hydraulic loading rate	HLR [m/yr]	5.95[1]
Concentration	conc [mg-N/L]	25
Integration time	time [yr]	1000
Saturated hydraulic conductivity	K_{sat} [m/yr]	761

[1]HLR equivalent to 0.41 gal/ft^2/d (1.6 cm/d) or approximately the actual median mound HLR.

The dimensions of the infiltrative area and the HLR, 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, also used to calculate mass loading to the aquifer, was estimated as the average of STUMOD-FL simulations presented in Table 4.3. However, due to poor calibration results the input concentration was later modified to 25 mg-N/L (Table 4.6) based on sampling results from PZ-25 and the maximum STUMOD-FL prediction.

The aquifer thickness is a parameter used directly by the HPS solution. Initially, a no flow boundary was assumed below the surficial aquifer at the top of the Hawthorn layer. However, due to poor calibration results, a low conductivity layer representing the Hawthorn was added below the surficial aquifer with the no flow boundary located at what is believed to be the contact between the Hawthorn layer and the Suwanee limestone. As shown in Figures 3.1 and 3.3, the model was more sensitive to dispersivity (α_x, α_y, α_z) compared to aquifer thickness (H). For conditions of “relatively large” aquifer thickness and “small vertical” dispersivity the effect of the aquifer thickness is limited and dispersivity becomes dominant (see Task D.11, equations 3-5 and 3-6).

Groundwater seepage velocity is a parameter in the HPS solution but the aquifer model calculates seepage velocity using the three-point problem algorithm described earlier. 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 4.1.3. The saturated hydraulic conductivity was the average reported value from slug tests conducted at piezometers down gradient of the mound infiltrative area.

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 (see Section 3.2), but 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. The soils at the GCREC site are 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-FL (see Task D.7) indicate that soils that fall into the sand textural class generally have porosities greater than 0.35 (McCray et al., 2010; Schaap et al., 2001). Thus, porosity was assigned an average value for sand and not included in the calibration.

The aquifer model parameters included in the calibration were the first-order denitrification parameter and the three dimensional dispersivity parameters (Table 4.7). McCray et al., (2005) present 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 compared to denitrification, the gradient and HLR. However, reported values for equivalent transport distances and porous media vary substantially (Gelhar et al., 1992). The method developed by Xu and Eckstein (1995) used by the aquifer model has not been corroborated for the GCREC site because no independent data exists to corroborate the estimated dispersivity values.

Table 4.7
Parameter Values Produced via Calibration of the Aquifer Model to Field Observations of Nitrate in Groundwater

Calibrated Parameter Values	
λ [1/yr]	2.8E-08
α_x [m]	13.3
α_y [m]	2.4
α_z [m]	0.4

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 and calculated using equations described in Task D.11. The input nitrate concentration was 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 and the observed results (19 and 20 mg-N/L) in PZ-25. The results from this calibration are presented in Figure 4-5, which contains 23 of the 33 observations, and in Table 4.7.

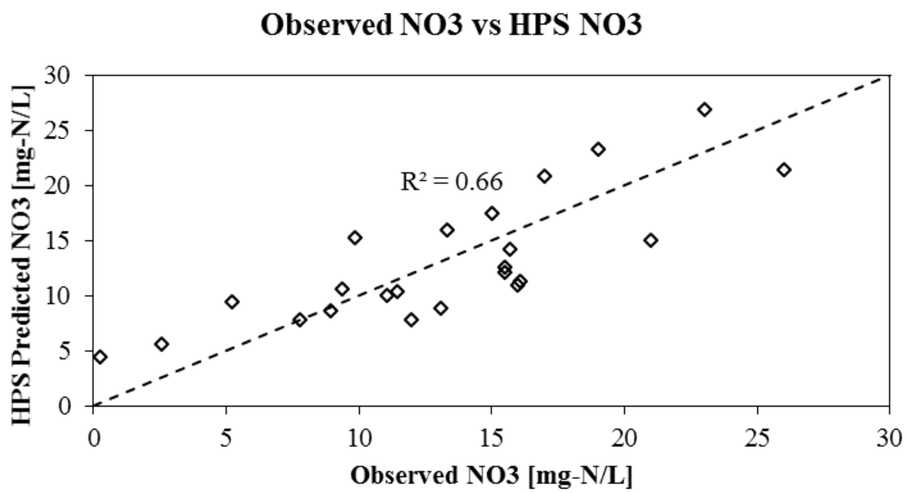

Figure 4-5: Aquifer Model Calibration Results for the 23 Observations
Subset of complete observations determined to pertain to the mound nitrate plume.

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. Of the 33 observations and model predictions (Table 4.8), 10 were “poor model fits” and 23 were “good model fits". These 10 “poor model fit” observations could only be marginally replicated by the aquifer model by using high nitrate concentrations to the top of the water table (above 60 mg-N/L) indicating that these points are heavily influenced by the agricultural nitrate plume. In addition, six of the 10 poor model fit observations were located at least 15 m off the plume center line. The distance off of the plume center line may also affect calibration results because the HPS solution does not consider transverse 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. Of the poor model fits, the observed concentrations were under predicted by the calibrated aquifer model in nine cases with only one over predicted (Table 4.8). 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 (Table 4.7).

Table 4.8
Complete Calibration Results for the 33 Observations within the Mound Nitrate Plume Area
Residuals (Res) are computed as *model – obs.*

Observation ID	x_i [m]	y_i [m]	z_i [m]	Obs [mg-N/L]	Model [mg-N/L]	Res [mg-N/L]
Poor Model Fit						
DP-AA9-14	9.1	22.6	2.1	24.0	5.3	-18.6
PZ03	52.7	1.1	0.6	1.0	18.3	17.3
DP-F15-14	72.7	19.9	3.1	21.7	7.2	-14.4
DP-F15-20	72.7	19.9	4.9	18.6	6.4	-12.3
DP-E12-15	51.7	9.5	3.2	23.7	13.4	-10.2
DP-F11-15	51.2	1.3	3.3	25.3	15.8	-9.6
DP-G12-15	62.3	1.8	3.4	21.3	13.6	-7.6
DP-AA9-22	9.1	22.6	4.6	11.0	3.8	-7.2
DP-F15-26	72.7	19.9	6.7	12.3	5.4	-7.0
DP-AA9-27	9.1	22.6	6.1	8.8	2.9	-5.9
Good Model Fit						
DP-E12-10	51.7	9.5	1.7	21.0	15.1	-5.9
DP-G12-09	62.3	1.8	1.6	9.8	15.2	5.4
DP-F11-24	51.2	1.3	6.1	16.0	10.9	-5.1
DP-G12-21	62.3	1.8	5.2	16.1	11.3	-4.7
DP-D7.5-14	21.7	8.8	1.9	26.0	21.5	-4.5
DP-D09-15	30.1	1.1	2.3	19.0	23.3	4.3
DP-G12-27	62.3	1.8	7.1	13.1	8.9	-4.2
DP-F11-27	51.2	1.3	7.0	5.2	9.4	4.2
PZ16-C12-28	39.8	20.9	7.1	0.3	4.4	4.2
PZ17-I15-26	88.0	4.4	6.9	12.0	7.8	-4.1
DP-D09-08	30.1	1.1	0.2	23.0	26.9	3.9
PZ11-E09-10	34.7	7.1	1.8	17.0	20.8	3.8
DP-D12-11	46.3	15.0	2.0	15.5	12.1	-3.4
DP-F08-28	34.9	16.4	7.2	2.6	5.6	3.0
DP-F11-21	51.2	1.3	5.1	15.5	12.5	-3.0
DP-D7.5-20	21.7	8.8	3.7	13.3	16.0	2.7
DP-F11-11	51.2	1.3	2.1	15.0	17.5	2.5
DP-F11-18	51.2	1.3	4.2	15.7	14.2	-1.5
DP-D7.5-26	21.7	8.8	5.6	9.4	10.7	1.3
DP-G12-24	62.3	1.8	6.2	11.1	10.0	-1.1
DP-E12-22	51.7	9.5	5.4	11.4	10.4	-1.0
DP-F08-20	34.9	16.4	4.7	8.9	8.6	-0.3
DP-E12-28	51.7	9.5	7.2	7.8	7.9	0.1

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4.2.2 Model Evaluation Statistics

Model performance was evaluated using multiple model performance measures including the common correlation measures; coefficient of determination (R^2), Root Mean Square Error (RMSE), the RMSE-observations standard deviation (SD) ratio (RSR) and The Nash-Sutcliffe Efficiency (NSE).

The correlation coefficient, R, or the coefficient of determination (R^2) is a common performance measure. R^2 ranges from 0 to 1, with higher values indicating less error variance, and typically values greater than 0.5 are considered acceptable (Santhi, et al., 2001, Van Liew et al., 2003). The R^2 value obtained for the aquifer model was 0.66 which is within an acceptable range. R^2 is oversensitive to high extreme values (outliers) and insensitive to additive and proportional differences between model predictions and measured data (Legates and McCabe, 1999). That means it is possible to obtain a good R^2 value as long simulation results capture the trend in observed values even when the absolute differences are large. Thus, we looked at other measures of performance. The second measure performance we used was the RMSE.
RMSE is given by:

$$RMSE = \sqrt{\frac{\sum_{i}^{n}(p_i - o_i)^2}{n}} \tag{4-1}$$

where p_i is simulated value, o_i is measured value and n is the number of observations. The stated rationale for squaring each error is to remove the sign and get the magnitude of the errors. RMSE value closer to zero indicates a better fit to observed values. If the RMSE value is close to zero, model results are acceptable. The RMSE value obtained for the aquifer model was 3.6. Although it is commonly accepted that the lower the RMSE, the better the model performance, it important to assess how to qualify the value when RMSE is greater than zero.

Singh et al. (2004) have published a guideline to qualify what is considered a low RMSE based on the observations standard deviation. Based on the recommendation by Singh et al. (2004), a model evaluation statistic, named the RMSE-observations standard deviation (SD) ratio (RSR), was developed. It is recommended that this measure of model performance be used instead of RMSE to account for the bias due to variability in the data set. RSR standardizes RMSE using the observations SD. Thus, we considered a third statistic in our aquifer model evaluation; the RSR. RSR is calculated as the ratio of the RMSE and SD of measured data:

$$RSR = \frac{RMSE}{STDEV_{obs}} = \frac{\sqrt{\sum_{i}^{n}(o_i - p_i)^2}}{\sqrt{\sum_{i}^{n}(o_i - o_{mean})^2}} \tag{4-2}$$

RSR incorporates the benefits of error index statistics and includes a scaling or normalization factor, so that the resulting statistic and reported values can apply to various constituents. RSR varies from the optimal value of 0, which indicates zero RMSE or residual variation and therefore perfect model simulation, to a large positive value. The lower the RSR, the lower the RMSE, and the better the model simulation performance. RSR of 0 to 0.5 is considered to be very good, 0.50 to 0.60 is good, and 0.60 to 0.70 is satisfactory and greater than 0.70 is unsatisfactory. The RSR value for the aquifer model was 0.6 indicating a good representation of observations by the aquifer model.

The last measure of model performance we used was the Nash-Sutcliffe Efficiency (NSE). The NSE (Nash and Sutcliffe, 1970) determines the model efficiency as a fraction of the measured value variance that is reproduced by the model. NSE is given is calculated as:

$$NSE = 1 - \frac{\sum(o_i - p_i)^2}{\sum(o_i - \overline{o_i})^2} \tag{4-3}$$

where: o_i = measured value, p_i = simulated value and $\overline{o_i}$ is mean of measured values. The closer the NSE value to 1.0 the better is the model estimation. NSE $\geq$ 0.75 is considered to be an excellent estimate while a NSE value between 0.75 and 0.36 is regarded to be satisfactory (Motovilov et al., 1999). The NSE value for the aquifer model was 0.6 indicating the NSE value was in the satisfactory range but closer to the "excellent" value of 0.75.

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 (note, total nitrogen concentration in PZ-25, located within the mound, was observed to be <25 mg-N/L in SE2 and SE4). Because more mass was needed to fit these observations than existed in the observations, 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 4.7 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. Thus, further investigation was made to evaluate the effect of including these 10 observations on the calibrated parameter values. This situation was examined by using all the available observations for a calibration run and comparing the calibrated parameters to those in Table 4.7. The parameter values for this calibration run were similar though not identical.

Three additional calibration approaches were investigated. The first 2 approaches included all the 33 nitrate observations; the first one with input nitrate concentration fixed at 25 mg-N/L as described in Section 4.2.2 and the second one with input concentration allowed to vary during calibration process. The third approach included the 23 observations and the input concentration was allowed to vary.

Notably, the first order denitrification coefficient for all calibration attempts (either 23 or 33 observations) was small while the horizontal and transverse dispersivity value for the calibrations with the 33 observations were generally higher. However, an independent evaluation of the denitrification potential of soils collected at the GCREC field site concluded that it was exceedingly low (~0.002 mg-N/d per L of pore volume) affirming the conclusion from model corroboration (Farrell, 2013; Farrell et al., 2014). Table 4.9 shows calibrated parameter values for the first approach utilizing 33 observations but with fixed input concentration. Figure 4-6 shows the model fit for this case. Table 4.10 shows calibrated parameter values for the second approach utilizing 33 observations but with variable input concentration. Figure 4-7 shows the model fit for this case. The calibrated input concentration was higher than the range of OWTS effluent concentrations. Table 4.11 shows calibrated parameter values for the third approach utilizing 23 observations but with fixed input concentration.

Table 4.9
Aquifer Model Calibration Results Using the 33 Nitrate Observations
The longitudinal dispersivity decreases while the transverse dispersivity increases.

Calibrated Parameter Values	
λ [1/yr]	1.8E-10
α_x [m]	11.3
α_y [m]	3.2
α_z [m]	0.4

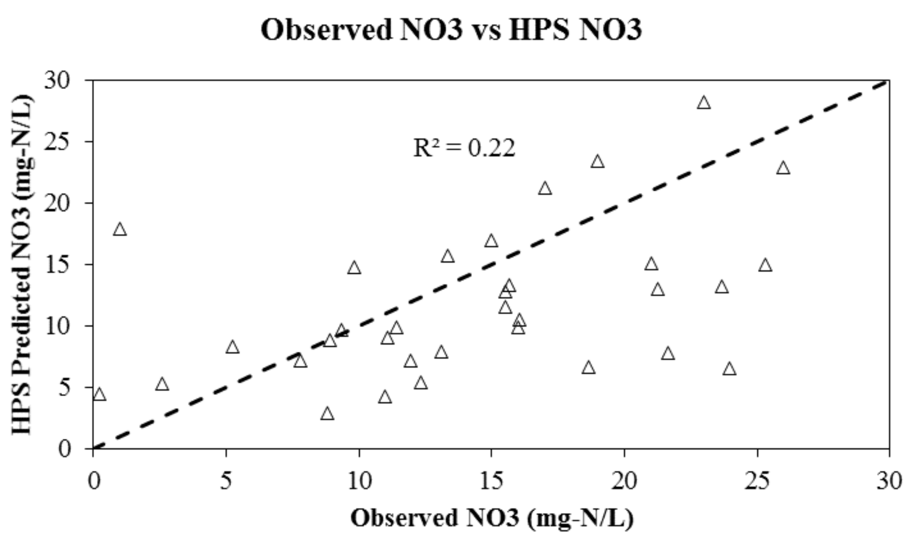

Figure 4-6: Calibration Results from Calibration to the 33 Nitrate Observations
Results are affected by those observations believed to be heavily influenced by the agricultural nitrate plume.

Table 4.10
Calibration Results Obtained from the Calibration of Parameters Identified in Section 4.2
Input concentration using 33 nitrate observations. The longitudinal dispersivity and input concentration have notably increased.

Calibrated Parameter Values	
λ [1/yr]	6.9E-05
α_x [m]	245.0
α_y [m]	18.7
α_z [m]	0.1
conc [mg-N/L]	251.577

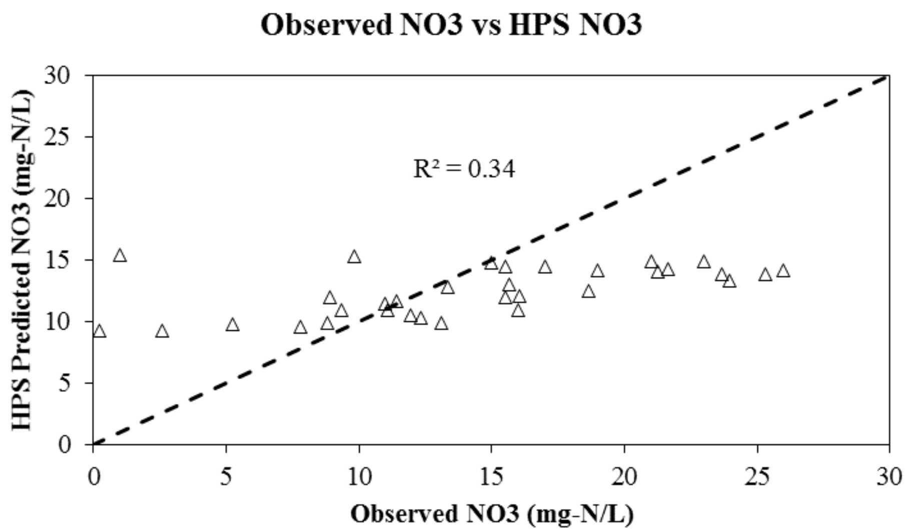

Figure 4-7: Calibration Results for the Calibrated Parameters Presented in Table 4.10
Results obtained by including input concentration as a calibration parameter. The results are improved over Figure 4-6 but the input concentration and dispersivity values do not appear realistic.

Table 4.11
Calibration Results from Calibration that Included the Input Concentration and the 23 observations that are part of the Mound Nitrate Plume

Points thought to be heavily influenced by the agricultural plume were eliminated and resulted in calibrated parameter values very similar to those presented in Section 4.2.1 (Table 4.7).

Calibrated Parameter Values	
λ [1/yr]	6.5E-07
α_x [m]	17.8
α_y [m]	2.2
α_z [m]	0.5
Conc. [mg-N/L]	27.2

In summary, the results from the calibration of the aquifer model to the 33 observations resulted in increased calibrated dispersivity value. This 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 4.7. 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 (second case) 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/d)). In comparison, dispersivity values decreased and in general the calibration results improved relative to the case with a lower input nitrate concentration (first case). Because the measured nitrogen concentration in the septic tank did not exceeded 61 mg-N/L coupled with a likely net nitrogen removal within the vadose zone, input concentrations to the aquifer are likely not this high. As a result the parameter values for second 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 4.7.

The conclusions 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
- 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.

4.2.3 Calibration of Two Numerical Models - Steady State vs Transient Modeling.

The HPS aquifer model is a steady state model. Two numerical models were constructed for the GCREC mound that considered transient and steady state conditions (Tonsberg, 2014). The two models were constructed to compare the limitation and strength of transient and steady modeling and to infer possible shortcomings in the steady state aquifer model due it steady state formulations. The two numerical models were constructed and calibrated with both hydraulics and contaminant transport.

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 OWTS effluent flows, and thus nitrogen flux to the aquifer, were not considered in the model because the discharge from the OWTS septic tank was not metered continuously in real time. 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 measured twice at 19 and 20 mg-N/L. Recharge and nitrogen mass flux from the OWTS was estimated using the a HLR of 1.6 cm/d or 0.4 gal/ft^2/d 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 and the HPS model (Section 4.2.1).

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 likely preclude improvements to the calibration results previously discussed.

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 4-8. A noteworthy observation of Figure 4-8 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.

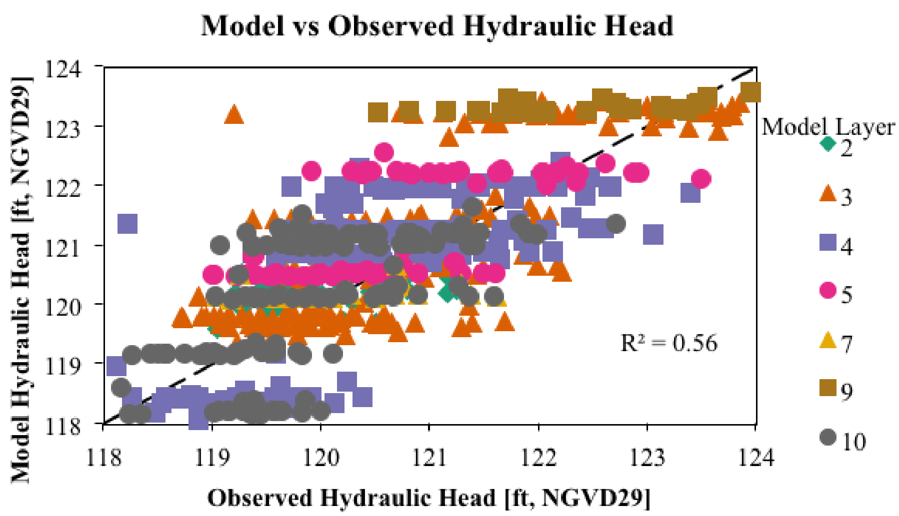

Figure 4-8: Calibration Results for the Groundwater Flow Portion of the Transient Numerical Model.

The vertical hydraulic conductivity of the Hawthorn layer (layer 11) was the only calibrated parameter.

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 a R^2 greater than 0.0001 (Figure 4-9). 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, but also is in agreement with the low denitrification potential of soils measured at the GCREC (Farrell, 2013; Farrell et al., 2014). 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.

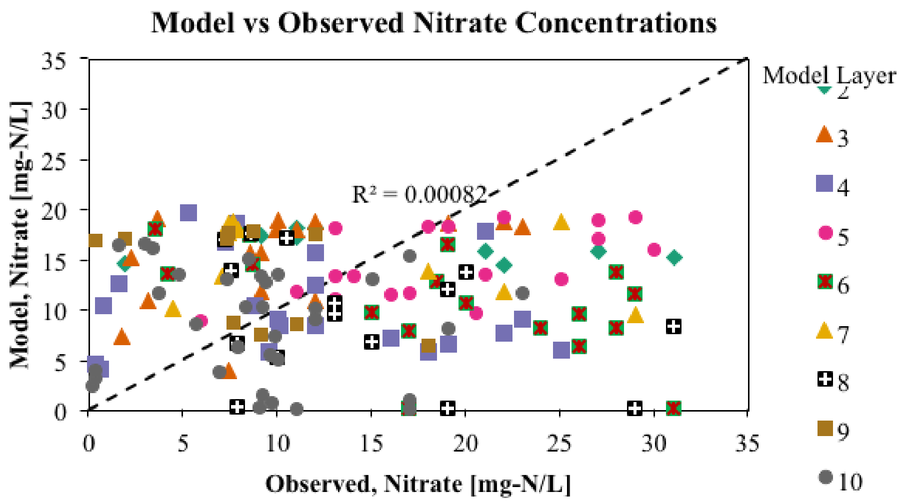

Figure 4-9: Calibration Results for the Groundwater Transport Portion of the Transient Numerical Model.

The first order denitrification and dispersivity parameters where calibrated parameters.

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 OWTS 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 (Figure 4-10). 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 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 OWTS could be answered via a steady state model.

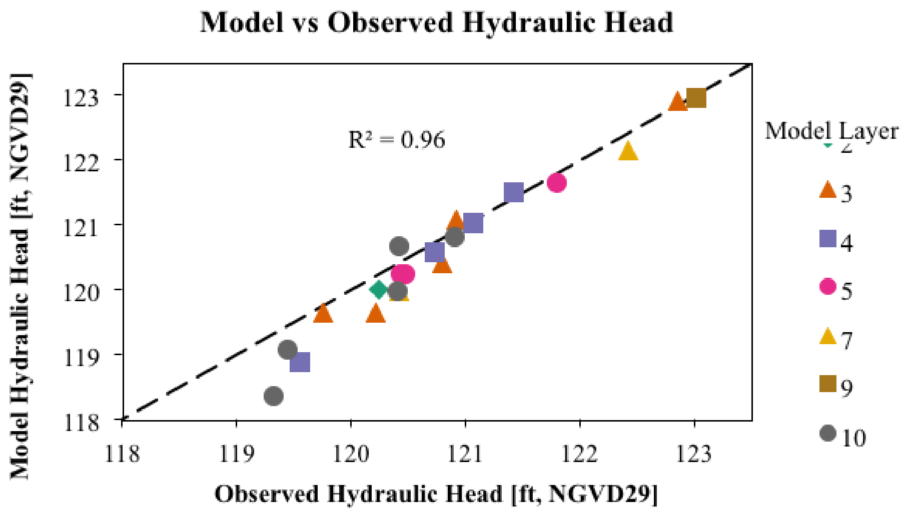

Figure 4-10: model predicted hydraulic head versus observed average hydraulic head

The model layer where hydraulic head was calculated is indicated by numbers 2 – 10.

Calibration of the contaminant transport portion of the steady state model did not produce an excellent fit of the observed data (R^2 = 0.00002). 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. 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 im-

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plication 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 OWTS 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., $y = z = 0$).

Section 5.0
Discussion and Conclusions

The aquifer model has been designed to provide the user with an estimate of nitrate concentration or mass flux down gradient of an OWTS. It has many additional features that allows 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 as a decision or design aid to test different hypothesis and if necessary make adjustments. Models in-turn should be refined based on feedback from field experiments.

The sensitivity analysis indicated that hydraulic conductivity and hydraulic gradient are not sensitive parameters, relative to other parameters evaluated; however 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.

The uncertainty analysis revealed that model output distribution changed significantly in response to a change in the range of denitrification values. Under conditions of low denitrification (with denitrification rates below a median value), only 20 to 60 percent of outputs demonstrated a 100% removal of nitrogen at a 200 ft setback distance. When the entire range of denitrification (0 to 100 percentile values) is used, 60 to 90 percent of the outputs demonstrated a 100% removal. This is an example of how the uncertainty analysis can be used to make an informed decision. For instance, for a median denitrification rate, there is a 60% probability that all the nitrate is removed at the setback distance for one soil type and only a 20% probability that this would occur for another soil type.

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 a 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 have important implications for parameter values estimated via model calibration to field observations. Model corroboration 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.

The aquifer model is a steady state model. To highlight the limitations of the aquifer model due to its steady state formulation, two numerical models (transient and steady state models) were also constructed and calibrated to observed field data. The comparison between the transient and steady numerical models and the limitation of each was used to infer the strength and weakness of the steady state aquifer model formulation.

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 OWTS 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 OWTS is more useful and minimizes error. This analysis demonstrated that although transient models attempt to mimic the field conditions better than steady state models, their usefulness is significantly limited by the availability of data. Thus, for long term nitrate plumes within the aquifer, the steady state aquifer model is a more useful tool.

While these limitations of the aquifer model should be considered, they do not preclude the usefulness of model estimates. During model corroboration it was concluded that denitrification was not as low as estimated by the aquifer model via calibration, though it was likely limited within the area monitored at the GCREC mound. An independent evaluation of the denitrification potential of soils collected at the GCREC site concluded that it was exceedingly low affirming the conclusion from model corroboration (Farrell 2013; Farrell et al., 2014). Estimates of transverse horizontal dispersivity were likely less than reported from calibration of the aquifer model. 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.

Section 6.0
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