Florida Onsite Sewage Nitrogen Reduction Strategies Study

Task D.9

Complex Soil Model Performance Evaluation

White Paper

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TASK D.9
WHITE PAPER

Complex Soil Model Performance Evaluation

Prepared for:

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Section 1.0
Background

1.0 Background

As part of Task D for the Florida Onsite Sewage Nitrogen Reduction Strategies (FOS-NRS) Study, performance evaluation of the complex soil model developed in Task D.8 (STUMOD-FL) is required. This complex soil model performance evaluation was identified as a separate task, Task D.9 and involved model performance evaluation through corroboration/calibration to better understand the quality and quantity of data required by comparing simulated model outputs to the corresponding measured values (calibration targets). Calibration targets used were nitrogen species concentrations. Model evaluation included detailed performance evaluation using model-evaluation statistics to determine whether the model can appropriately simulate the observed data. In addition, a parameter sensitivity analysis has been performed to identify the most relevant model parameters. Finally, an uncertainty analysis was performed where probability-based ranges for model input parameters were used to generate probable model outcomes. This white paper was prepared by the Colorado School of Mines (CSM) to document completion of Task D.9. Descriptions included herein are intended to highlight Task D progress with final reporting to be conducted as part of Tasks D.16 and D.17.

Section 2.0
Model Performance Evaluation

The general user will likely evaluate model performance by comparing STUMOD-FL outputs to available field data. It is vital that the general user understands the requirements for the quality and quantity of field data needed in order to make a valid comparison. Also, for the more advanced user a more rigorous approach, using quantitative model evaluation measures is needed to establish the capability and limitations of STUMOD-FL. As part of Task D.9, observed field data representing field conditions were compared to STUMOD-FL outputs. Reported operational conditions (hydraulic loading rate, effluent quality, soil texture, and depth) were entered into the model and the percent removal estimated by the model was compared to the observed values. Because STUMOD-FL is a vadose zone model, field data required must include vadose zone analyses. The data set used for implementation checks and corroboration were from the Gulf Coast Research and Education Center (GCREC) Soil and Groundwater (S&GW) test facility (data reported in the Task C.17 Data Summary Reports) and the University of Southern Florida (USF) Lysimeter Station.

There are 6 test areas (mini-mounds) at the GCREC S&GW test facility receiving either septic tank effluent (STE) or nitrified effluent delivered to the soil via a pressure dosed mound or a shallow drip dispersal system. Initially corroboration was limited to Test Area 1, but evaluating each individual sampling event. Additional corroboration included Test Areas 2, 3, and 4 as well as comparison to USF Lysimeter Station observations. Test Areas 5 and 6 are not relevant to the work described here, they were constructed as vertically stacked, in-situ stage 1/stage 2 biofilters for treatment performance evaluation as part of Task A.

Because flow is constant (steady state conditions), mass loading is proportional to the concentration. STUMOD-FL estimates mass loading based on center line concentration (mass per unit area per day). As presented in Task D7, velocities estimated based on tracer test were 0.17, 0.30 and 0.33 ft/d for 1, 2 and 3.5 ft, respectively. The average velocity in STUMOD-FL (HLR/porosity) for a hydraulic loading rate of 3.26 cm/day and a porosity of 0.38 is 0.28 ft/day. Corroboration results on concentration apply to the mass flux as well since the flux from STUMOD-FL agrees well with the range obtained from tracer test data in the field.

A soft calibration was conducted during corroboration to better fit the STUMOD-FL soil moisture profile to field measurements at the GCREC. STUMOD-FL moisture profile was also compared to HYDRUS-2D moisture profile for the three soil types and it was demonstrated that the moisture profile from STUMOD-FL captured the moisture profile from Hydrus 2D. In most cases, the default parameter values were used during corroboration to field data. In some cases, parameter values were adjusted to improve model fit. By calibrating the model users can obtain a relatively better fit than what was obtained during corroboration. However, because even after calibration there is uncertainty in the outputs simply due to variability in observational data, no simulation model is an entirely true reflection of the physical process being modeled. Therefore, applying the new ‘calibrated’ parameter values to other sites may not necessarily improve predictions. This was especially evident in the additional corroboration added for the GCREC test areas 2, 3, and 4 (see Section 2.1.2) and as was observed during corroboration at the USF site based on soft calibration parameter values from the GCREC corroboration (see Task D.7 report).

2.1 Initial GCREC Corroboration

Data from Test Area 1 (TA1) represents a mound system receiving pressure dosed STE at 0.8 gpd/ft^2 (3.26 cm/d). A hydraulic loading rate of 3.26 cm/d was used in STUMOD-FL as the representative hydraulic loading rate. Soil in this area has been identified as Seffner fine sand. Because there were no data records for the Seffner series in the Florida Soil Characterization Data Retrieval System (University of Florida, 2007), soil properties and relevant model input parameters (θ_r, θ_s, α, and n) were set as equal to the less permeable sand (see Tasks D.7 and D.8). Variations in ET were assumed to be small, at least within a month timeframe specific to each sample event, so ET was not considered. STE input concentrations were equal to the STE field measured value at the time of sampling (i.e., six runs with different effluent input concentrations ranging from 60.5 to 89 mg-N/L). Rainfall is a variable input and cannot be input into STUMOD-FL. A single homogenous soil layer was assumed. Operational conditions for each STUMOD-FL run are found in Table 2.1.

Table 2.1
STUMOD-FL Simulation Parameters Selected to Replicate TA1 Field Conditions during Sample Events (input ammonium and nitrate concentrations obtained from sample analyses)

	K_s (cm/d)	Water Table Depth (ft below IS)	HLR (cm/d)	Tmax (C^o)	Tmin (C^o)	C_o NH_4^+ *(mg-N/L)*	C_o NO_3^- *(mg-N/L)*
6/18/12	352.6	5.58	3.26	32.1	20.8	64.0	0.04
8/20/12	352.6	5.54	3.26	33.1	22.4	60.5	0.04
10/15/12	352.6	3.40	3.26	28.0	17.1	65.0	0.04
1/7/13	352.6	5.95	3.26	23.1	9.1	56.0	0.15
3/11/13	352.6	6.59	3.26	26.1	11.2	89.0	0.98
6/13/13	352.6	2.48	3.26	32.1	20.8	69.5	0.08

Relevant for model calibration, the vadose zone was monitored with suction lysimeters at 1, 2 and 3.5 ft (30, 60, and 107 cm) below the infiltrative surface for temperature, TKN, NOx, and ammonium-nitrogen for six sampling events. The options in STUMOD-FL for boundary conditions allows users to enter either a known water table depth or use the model calculated water table as determined by a water table fluctuation model. The option for a known water table depth was used as the constant head boundary condition at the bottom of the vadose zone in STUMOD-FL based on groundwater elevation measurements within the test areas.

Results for STUMOD-FL calibration and corroboration are shown in Table 2.2. Graphical outputs from these STUMOD-FL runs compared to the observed data are provided in Appendix A. Modifications made to STUMOD-FL parameters to improve model performance are presented in Task D.10 (Validate/Refine Complex Soil Model).

These results show that STUMOD-FL predictions captured ammonium concentrations as observed in the field with both field data and model predictions showing quick conversion of nitrogen within one foot of the infiltrative surface. Results indicate that the conceptual model for nitrification as well as the input parameters sufficiently represent the processes occurring within the soil treatment unit (STU). However, STUMOD-FL nitrate predictions were observed to be more conservative (i.e., less removal) compared to field data as shown by most cases where STUMOD-FL predicted nitrate concentrations relatively higher than field observations, particularly at shallow depth.

Table 2.2
Field Observations Compared to STUMOD-FL Simulations

Lysimeter	Field Data (mg-N/L)			STUMOD-FL Simulations (mg-N/L)		
Depth (ft below IS)	TN	NO_x	NH_4^+	TN	NO_x	NH_4^+
	Sample Event 1 (6/18/12)					
1 ft	49.0	46.0	0.01	58.8	58.8	0
2 ft	59.6	53.0	0.05	53.4	53.4	0
3.5 ft	46.0	36.0	0.01	45.3	45.3	0
	Sample Event 2 (8/20/12)					
1 ft	14.7	13.0	0.01	55.4	55.4	0
2 ft	41.4	39.0	0.01	50.0	50.0	0
3.5 ft	51.8	50.0	0.01	42.1	43.5	0
	Sample Event 3 (10/15/12)					
1 ft	49.4	48.0	0.01	59.8	59.8	0
2 ft	45.7	45.0	0.01	54.2	54.2	0
3.5 ft	53.7	53.0	0.01	44.0	44.0	0
	Sample Event 4 (1/7/13)					
1 ft	52.0	50.0	0.01	50.9	50.9	0
2 ft	51.2	47.0	0.01	45.6	45.6	0
3.5 ft	55.1	52.0	0.01	37.9	37.9	0
	Sample Event 5 (3/11/13)					
1 ft	59.5	55.0	0.01	84.4	84.4	0
2 ft	64.2	60.0	0.01	79.1	79.1	0
3.5 ft	70.5	68.0	0.01	71.0	71.0	0
	Sample Event 6 (6/13/13)					
1 ft	33.6	32.0	0.02	64.1	64.1	0
2 ft	26.7	25.0	0.01	57.2	57.2	0
3.5 ft	49.6	46.0	0.01	-	-	-

2.2 Root Mean Square Error

The following evaluation is applicable to the initial corroboration described in Section 2.1. The additional corroboration described in Sections 2.3 and 2.4 illustrate the difficulties in corroborating to field data. Model statistics are not provided for these additional corroboration runs.

Since STUMOD-FL will be utilized both by general and technical users, it is important to understand the effect of the quality and quantity of field data in calibration and/or corroboration procedures. In light of the general comparison between STUMOD-FL simulation results and field data, users should understand that a robust field data set is required to adequately calibrate STUMOD-FL results. Field data collection must be designed with calibration in mind such that both spatial and temporal data ensures that the behavior of the system is adequately captured and model limitations are considered. It is likely that as more exhaustive data sets that consider model limitations (e.g., data that captures steady state behavior) become available, STUMOD-FL can be further refined to better predict removal under various field conditions.

STUMOD-FL has built-in default parameter values; however, STUMOD-FL can also be calibrated to site specific observations if the required data is available. The use of default or calibrated parameter values specific to a site depends on specific goals of site assessment. For example, utilization of STUMOD-FL with built-in default parameter values provides simulation results adequate for a screening procedure rather than an exhaustive performance analysis. The results of the performance screening (e.g., nitrate concentration at a specific depth greater than a desired target concentration) may indicate a potential environmental concern at the site and need for further data analysis or collection (e.g., obtaining more certain denitrification rates and/or data on soil properties) to refine the output. Alternatively, the screening results may suggest the need to improve predictions at the site requiring implementation of a more complex numerical model.

A more rigorous evaluation of STUMOD-FL performance is helpful to understand its capabilities and limitations. Root Mean Square Error (RMSE) and the coefficient of determination (R^2) can be used to evaluate model performance. Multiple calibration statistics are necessary to evaluate model performance because each statistic has inherent limitations. R^2 is a measure of co-linearity between observed and model predicted values. R^2 is not strongly affected by the number of observations, because of this R^2 can be used to compare model runs for different numbers of observations. R^2 is also helpful because it ranges between 0 and 1 regardless of the magnitude of the observation and model values. An inherent weakness of R^2 is its inability to reproduce observation data with a large variance when it is used as an objective function.

R^2 is also limited because it is relatively insensitive to additive and proportional differences between model predictions and observed data (Legates and McCabe, 1999). Equation 2-1 gives R^2 where it can be seen that a large variance in the observation data or proportional and additive differences between observation data and model predictions can yield R^2 values closer to 1.

$$R^2 = \left(\frac{\sum(x-\bar{x})(y-\bar{y})}{\sqrt{\sum(x-\bar{x})^2(y-\bar{y})^2}}\right)^2 \qquad 2\text{-}1$$

RMSE is a useful calibration statistic though standard values for excellent model performance have not been established because RMSE is strongly affected by the magnitude of the model and observation data. Large values, such as large hydraulic heads, lead to large RMSE values while small values such as contaminant concentrations yield small RMSE values. In such a situation a model that has large RMSE values may provide a relatively good fit of the data while another model with small RMSE values may be completely inaccurate. Equation 2-2 gives RMSE, which was calculated using the observation data from the six sample events for each depth.

$$RMSE = \sqrt{\frac{\sum_{i}^{n} (p_i - o_i)^2}{n}} \qquad 2\text{-}2$$

Equation 2-2 shows that RMSE can also be strongly affected by outliers, because of the squared term in the numerator, similar to R^2. For a steady state model R^2 could be influenced by sampling events with variable inputs (e.g., rainfall or higher effluent concentrations). The squared term prevents positive and negative values from canceling each other but may bias a model that is calibrated using RMSE as the objective function to extreme behavior. This fact also allows RMSE objective functions to better capture the behavior of data sets with large variances when compared to R^2.

Table 2.3 lists STUMOD-FL corroboration results as measured by R^2 and RMSE. The calibration statistics were calculated using all the data for each depth. STUMOD-FL performance was evaluated at the three depths where samples were taken in the vadose zone using both R^2 and RMSE.

Table 2.3
STUMOD-FL evaluation statistics quantifying model performance

Depth	**TN**	**NO_x**	**NH_4^+**
		R^2	
1 ft	0.18	0.15	-
2 ft	0.17	0.20	-
3.5 ft	0.71	0.50	-
		RMSE (mg-N/L)	
1 ft	23.85	25.82	0.01
2 ft	15.10	16.38	0.02
3.5 ft	9.87	9.16	0.01

Most papers discussing calibration of models (e.g., Anand et al., 2007; White and Chaubey, 2005) use the coefficient of determination, R^2, to measure the quality of calibration, which describes the degree of co-linearity between simulated and measured values and ranges from 0 to 1. The model fit obtained in this work is relatively good at the 3.5 ft depth (R^2 = 0.71), given that typically R^2 values greater than 0.5 are acceptable. This indicates that although STUMOD-FL generally over predicts nitrate in the upper vadose zone it achieves better accuracy with depth (Santhi et al., 2001). The discrepancies between observed and model predicted concentrations and consequently lower R^2 values occurred particularly at 1 and 2 ft. This is attributed to variable and low observed nitrate concentrations that could not be well explained (e.g., various factors in the field, input variability that cannot be captured by the model, such as precipitation, etc.)

Agreement between R^2 and RMSE indicates that the model is adequately predicating nitrogen in the vadose zone as designed. Because both RMSE and R^2 values show similar behavior, the calculated performance of the model does not appear to be influenced by large variance or data outliers particularly at the deeper observation point. Processes that cause the large discrepancies between model predictions and observations at shallower depths appear to be eliminated deeper in the vadose zone which is indicated by improved evaluation statistics at the 3.5 ft depth. Figures 2.1 through 2.3 show how the variance and the outliers at the 1ft and 2ft depths affect the calculation of the evaluation statistics and that STUMOD-FL is indeed capable of predicting observed nitrogen concentrations as the influences of unexplained process are removed.

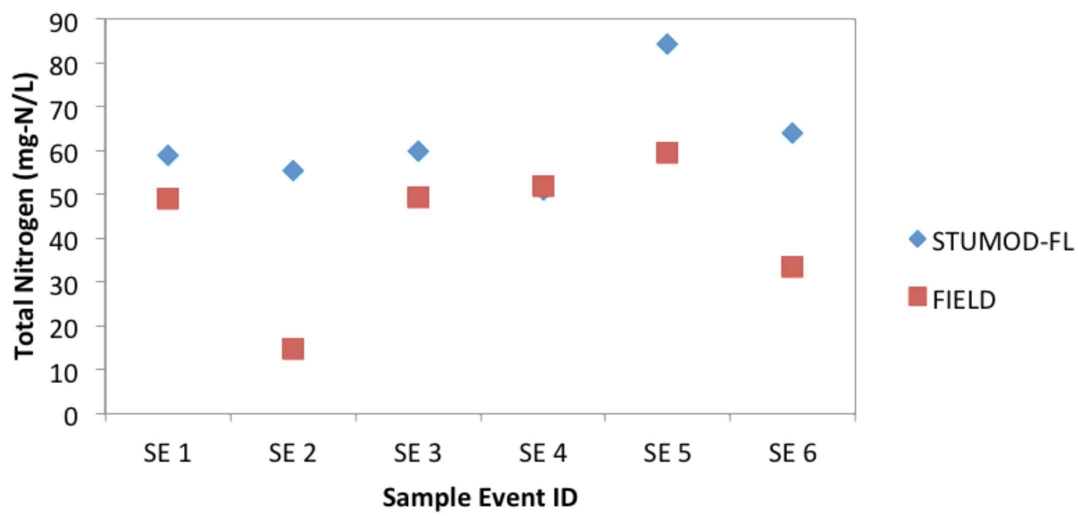

Figure 2.1: Comparison of Total Nitrogen Concentration Predicted by STUMOD-FL to Field Observations at 1 ft. Large differences between the observed data and STUMOD-FL predictions during SE 2, SE 5, and SE 6 negatively impact the performance evaluation (Table 2.3; SE 2 and SE 6 had substantial rainfall preceding the sampling events)

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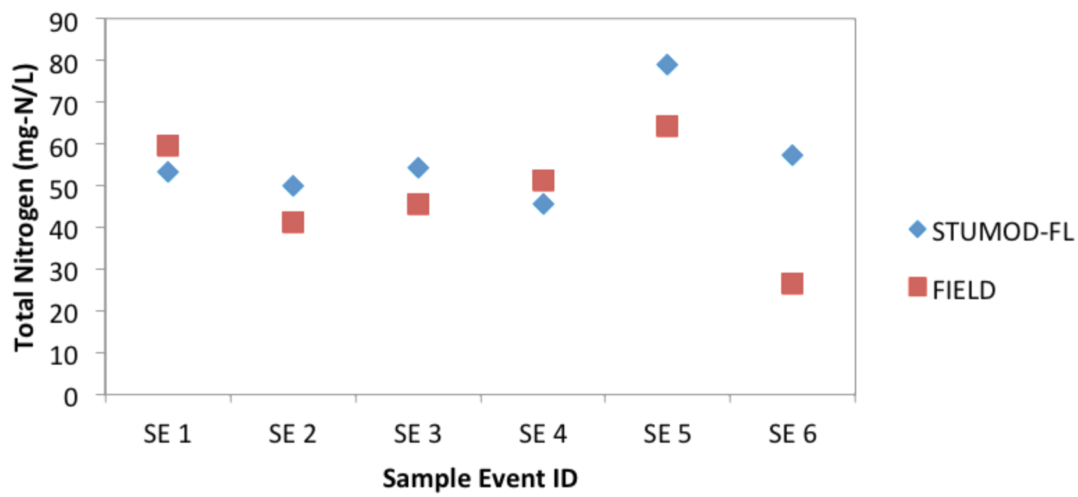

Figure 2.2: Comparison of Total Nitrogen Concentration Predicted by STUMOD-FL to Field Observations at 2 ft. Observed nitrogen concentrations follows a more predictable pattern though a large difference between STUMOD-FL and field observations for SE 6 significantly impact performance evaluation at the 2 ft level

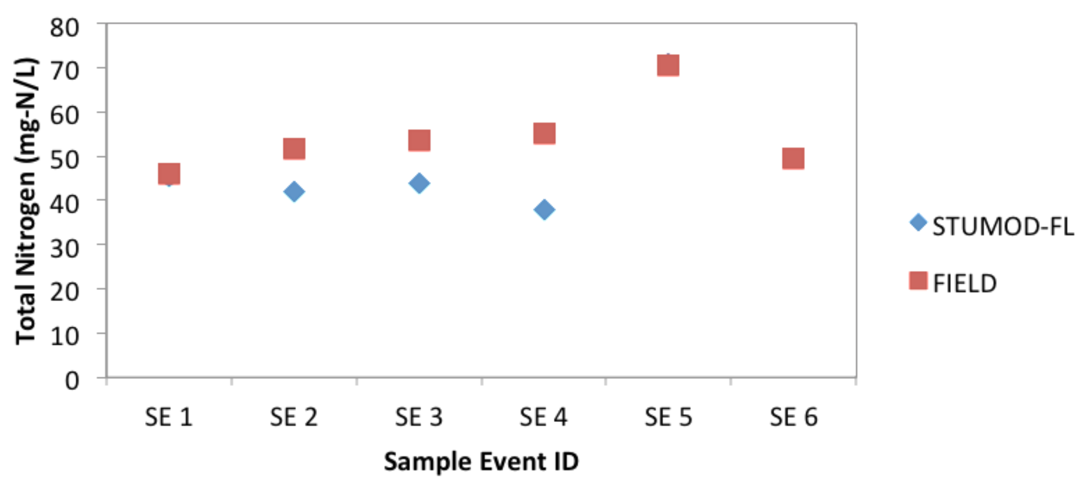

Figure 2.3: Comparison of Total Nitrogen Concentration Predicted by STUMOD-FL to Field Observations at 3.5 ft. Model predictions seem to improve at the 3.5 ft depth (compared to Figures 2.1 and 2.2) though data collected for SE 6 is likely not accurate because the suction lysimeter was below the water table

Total nitrogen behaves in much the same way as nitrate because a large fraction of total nitrogen is nitrate as ammonium is quickly converted to nitrate as observed in the field and predicted by the model. Figures 2.4 and 2.5 also highlight that STUMOD-FL produced conservative estimates (relatively less removal) particularly at shallow depth (1 ft and 2 ft). This could be a desired outcome in most cases given the uncertainties in the field observations in addition to uncertainties that may arise due to parameter inputs and inherent model behavior. Thus, it is useful to note that the outputs are good first estimates of removal rates under different conditions. However, further adjustments can be made to STUMOD-FL input parameters (e.g., denitrification rate) to match measured data or to reflect site specific observations and apply the model for a scenario different from the corroboration condition (e.g., different loading rate).

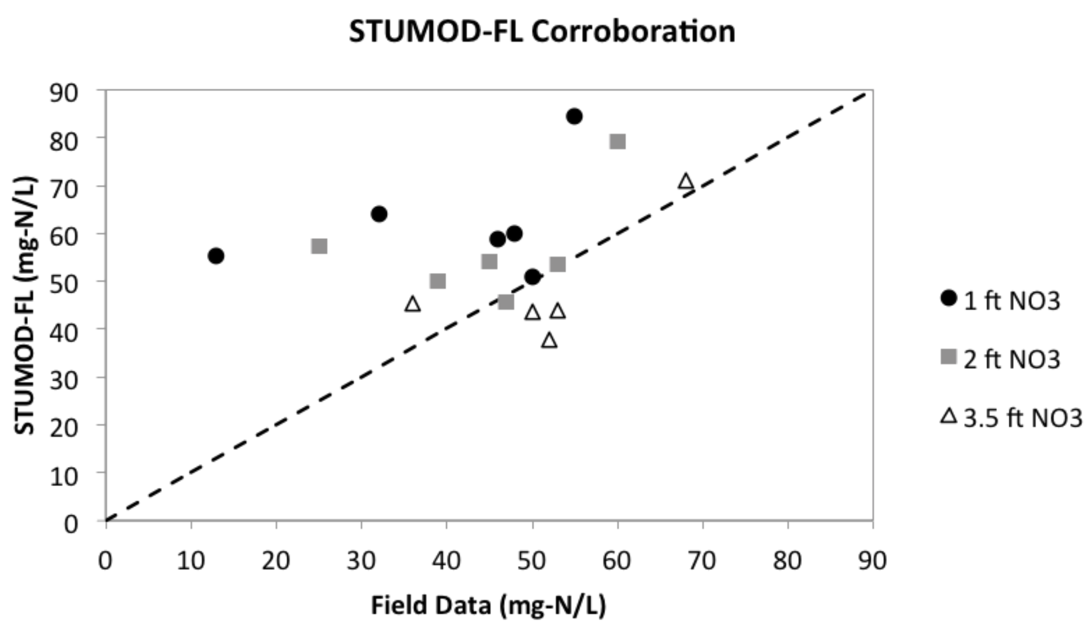

Figure 2.4: STUMOD-FL Nitrate Corroboration Results from the GCREC S&GW Test Area 1. The conservative nature of the model as well as its ability to better predict nitrate concentrations at lower depths is shown

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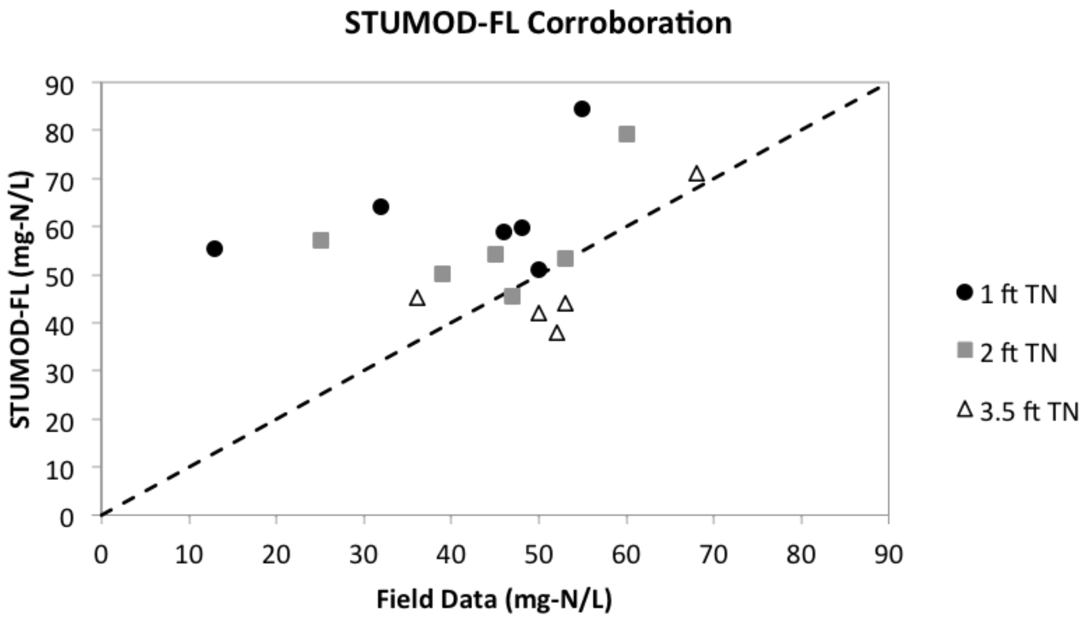

Figure 2.5: STUMOD-FL Total Nitrogen Corroboration Results from the GCREC S&GW Test Area 1. Results similar to Figure 2.4 because of the high fraction of nitrate making up total nitrogen

2.3 USF Lysimeter Station Corroboration

Additional corroboration of STUMOD-FL to field data was done for the USF Lysimeter Station. Three sets of parameter values were used during comparison shown in Table 2.4. As was done for Task D.7, parameter values were based on the generalized more permeable sand (see Tasks D.7 and D.8), Candler fine sand (University of Florida, 2007), and site properties measured at the site (Ayres Associates 1993). The relevant parameters (θ_r, θ_s, α, and n) were estimated specific to the Candler fine sand discussed in previous reports. The applied effluent quality was represented as 40.5 mg-N/L as ammonium + 0.04 mg-N/L as nitrate delivered to the soil at two HLRs, 3.06 and 6.12 cm/d (0.75 and 1.5 gpd/ft^2).

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Table 2.4
HYDRUS-2D Simulation Parameters Selected to Replicate USF Field Conditions

Run ID[1]	K_s (cm/d)	Water Table Depth (ft)	HLR (cm/d)	θ_r	θ_s	α	n	C_o NH_4 (mg/L)	C_o NO_3 (mg/L)
1	670.8	2, 4	3.06	0.013	0.3874	0.024	2.52	40.5	0.04
2	670.8	2, 4	6.12	0.013	0.3874	0.024	2.52	40.5	0.04
3	890.4	2, 4	3.06	0.0079	0.3856	0.023	3.57	40.5	0.04
4	890.4	2, 4	6.12	0.0079	0.3856	0.023	3.57	40.5	0.04
5	633.4	2, 4	3.06	0.0368	0.3978	0.017	6.24	40.5	0.04
6	633.4	2, 4	6.12	0.0368	0.3978	0.017	6.24	40.5	0.04

[1]Parameters for runs 1 and 2 are based on generalized more permeable sand (data set I). Parameters for runs 3 and 4 are based on generalized Candler fine sand data set II (University of Florida, 2007). Parameters for runs 5 and 6 are based on site specific data set III (Ayres Associates, 1993).

For corroboration, the model output was compared to observed nitrate nitrogen concentrations. Field observations were determined as the average of measured concentrations for sampling events with at least 4 days without rainfall prior to the sampling events, for two loading rates and two water table depths (2 and 4 ft). These nitrate nitrogen targets were: 27.5 mg-N/L at 2 ft for a HLR of 3.06 cm/d; 29.0 mg-N/L at 4 ft for a HLR of 3.06 cm/d; 18.0 mg-N/L at 2 ft for a HLR of 6.12 cm/d; and 26.0 mg-N/L at 4 ft for a HLR of 6.12 cm/d. For each hydraulic loading rate the water table depth in STUMOD-FL was set to 2 and 4 ft. Default nitrification and denitrification rates were used (56 mg N L^{-1} d^{-1} and 2.58 mg N L^{-1} d^{-1} respectively for nitrification and denitrification).

The model predictions matched field observations relatively well as shown in Figures 2.6, 2.7, and 2.8 with R^2 values > 0.7 for all the three datasets. The average relative error was 11.9%, 15% and 9.9% for the generalized medium sand (K_s 670.8 cm/d), Candler fine sand (K_s of 890.4 cm/d), and site-specific (K_s of 633.4 cm/d) respectively. STUMOD-FL predicted better with default parameters than HYDRUS-2D runs described in the previous D.7 report. STUMOD-FL also captured the nitrification process with total nitrification occurring within a foot distance from the infiltrative surface.

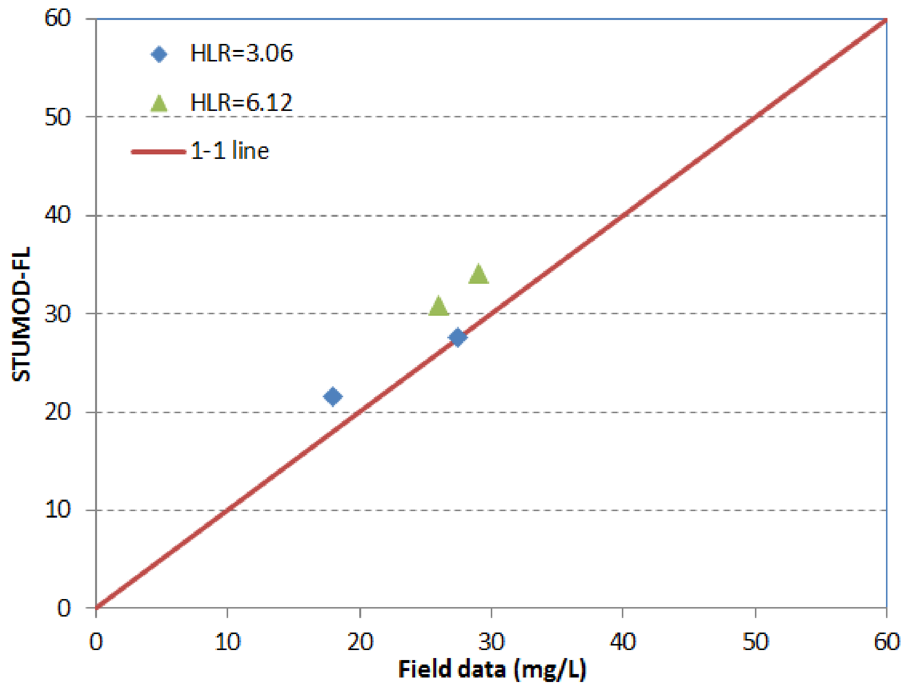

Figure 2.6: STUMOD-FL Nitrate-Nitrogen Corroboration Results from the USF Lysimeter Station using Parameters based on the Generalized More Permeable Sand
(in mg/L as N)

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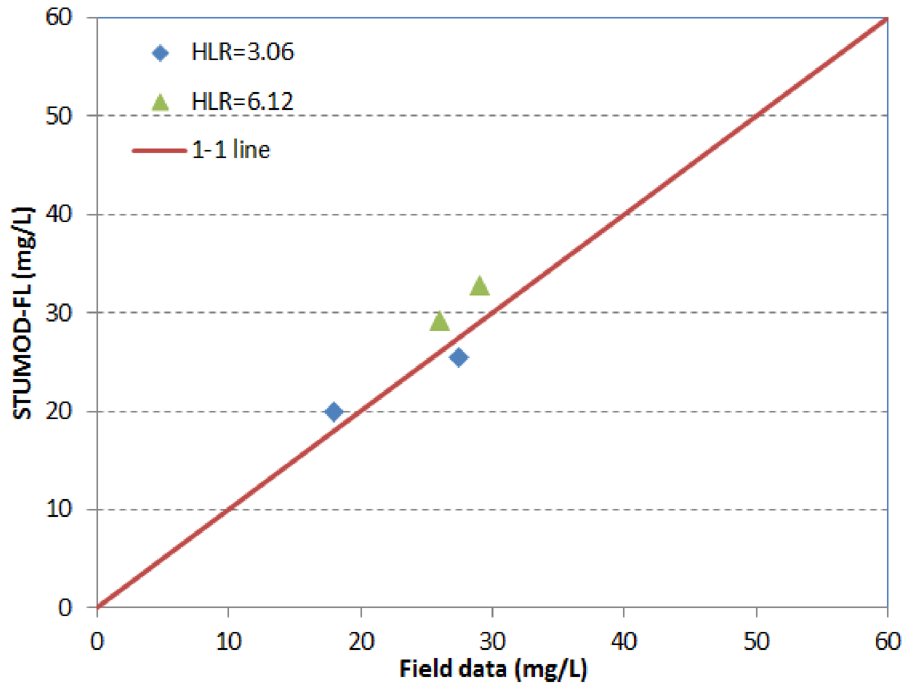

Figure 2.7: STUMOD-FL Nitrate-Nitrogen Corroboration Results from the USF Lysimeter Station using Parameters based on Candler Fine Sand (in mg/L as N)

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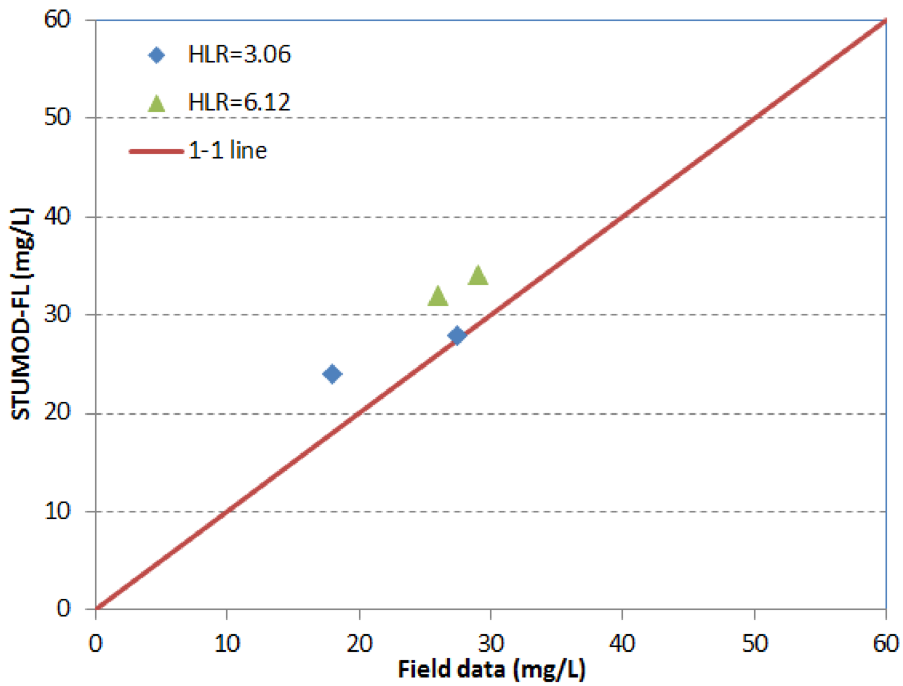

Figure 2.8: STUMOD-FL Nitrate-Nitrogen Corroboration Results from the USF Lysimeter Station using Parameters based on Site Specific Data (in mg/L as N)

It was observed that percent removal decreased with increasing hydraulic loading rate (better removal for 3.06 cm/d loading than 6.12 cm/d loading in all cases) for both STUMOD-FL runs and field observations which could be attributed to the increased velocity/reduced travel time at higher loading rates. It was also observed that the reduction in removal efficiency with increasing hydraulic loading rates was not as large in STUMOD-FL as compared to the reduction in field observations (note consistently higher concentrations in Figures 2.6, 2.7, and 2.8 for the higher loading rate). This suggested that under field conditions, there are additional factors that compensated for the effect of reduced travel time due to increased hydraulic loading rate which were not captured in the model. For instance, an increased carbon loading and subsequent accumulation of more carbon in the unsaturated zone as a result of increasing hydraulic loading may compensate for reduced travel time although this dataset alone may not be sufficient to generalize. Future investigation of field measurement under a range of loading rates is needed to prove the consistency of this observation or lead to further modification in the model. A similar trend was observed during HUDRUS-2D runs (Task D.7). However, the predicted values for STUMOD-FL runs are relatively closer to the observed values as demonstrated by a lower relative error, as compared to 20% in HYRDUS-2D runs.

2.4 Additional GCREC Corroboration

Based on the results from the initial corroboration (Section 2.1) and in tandem with the corroboration approach used for the Task D.7 HYDRUS 2-D simulations, additional modifications were made to STUMOD-FL and additional corroboration was conducted.

In the initial corroboration, the effluent input was varied for each run based on the measured effluent concentration for each sampling event and was assumed to be equal to TKN. For a steady state model, it was found necessary to test the model based on average effluent concentration, although this may have limitations when the average concentration is much different than the days on and before the sampling events (SE). Due to the organic fraction of nitrogen within TKN measurements, the input concentrations were high. Thus for this subsequent corroboration, the average effluent input concentration for TA1 and TA3 was 57.5 mg-N/L of ammonium and 0.37 mg-N/L nitrate. The effluent applied to TA2 and TA4 was from an ATU; however, for some of the sampling events it was observed that substantial ammonium was present due to less than anticipated nitrification. Thus, STUMOD-FL was run assuming both totally and partially nitrified effluent for TA2 and TA4.

Plant uptake was also considered; however, plant uptake did not have a significant effect due to the STU configuration. Specifically, in TA1 and TA2 the infiltrative surface is 1.5 ft below land surface: 1 ft of gravel and 0.5 ft of mound sand on top of the infiltrative surface. For TA3 and TA4, the infiltrative surface was 0.5 ft (~15 cm) from the land surface. The grass on TA1 is St. Augustine turf grass with a maximum root depth of 40 cm (16 inches) (Miller, 2014). For a root depth of 40 cm, there is no rooting depth below the infiltrative surface for TA1 and TA2 and only 25 cm of the rooting depth is below the infiltrative surface for TA3 and TA4. In STUMOD-FL, plant uptake from applied STU is neglected when plant roots are above the infiltrative surface. Operational conditions for STUMOD-FL corroborations specific to the GCREC S&GW test areas are found in Table 2.5. Operational conditions for STUMOD-FL corroborations specific to the S&GW sampling events are found in Table 2.6.

Table 2.5
STUMOD-FL Simulation Parameters Selected to Replicate Field Conditions at Different GCREC Test Areas (average input ammonium and nitrate concentrations obtained from sample analyses)

	K_s (cm/d)	HLR (cm/d)	C_o NH_4^+ (mg-N/L)	C_o NO_3^- (mg-N/L)	Depth to IS (cm)	Rooting Depth (cm)	Plant Uptake (kg/ha/yr)
TA1	352.6	3.26	57.5	0.4	45	40	296
TA2	352.6	3.26	0.0	33.4	45	40	296
TA2	352.6	3.26	20.78	12.61	45	40	296
TA3	352.6	3.26	57.5	0.4	15	40	296
TA4	352.6	3.26	0.0	33.4	15	40	296
TA4	352.6	3.26	20.68	12.61	15	40	296

Table 2.6
STUMOD-FL Simulation Parameters Selected to Replicate Field Conditions during Sample Events

	Water Table Depth (ft below IS)	Tmax (C°)	Tmin (C°)	ET (cm/day)	C_o NH_4^+ (mg-N/L)[1]	C_o NO_3^- (mg-N/L)[1]
6/18/12	5.58	32.1	20.8	0.46	53.0	0.3
8/20/12	5.54	33.1	22.4	0.39	11.0	12.0
10/15/12	3.40	28.0	17.1	0.28	6.3	3.7
1/7/13	5.95	23.1	9.1	0.19	22.0	5.7
3/11/13	6.59	26.1	11.2	0.29	31.0	19.0
6/13/13	2.48	32.1	20.8	0.46	1.4	34.0

[1]Variable input ammonium and nitrate concentrations obtained from sample analyses applied to TA2 and TA4. See Table 2.1 for variable input ammonium and nitrate concentrations applied to TA1 and TA3.

Results for TA1 are shown in Figure 2.9. Points closer to the 1-1 line illustrate STUMOD-FL predictions that are closer to the field observations. Most of the points furthest from the 1-1 line occurred for the sampling events where there was considerable rainfall on the days preceding the sampling events (SE2, SE4, and SE6). Because STUMOD-FL is a steady state model it does not capture this variability in the inputs (e.g., precipitation, variable effluent concentrations, diurnal changes).

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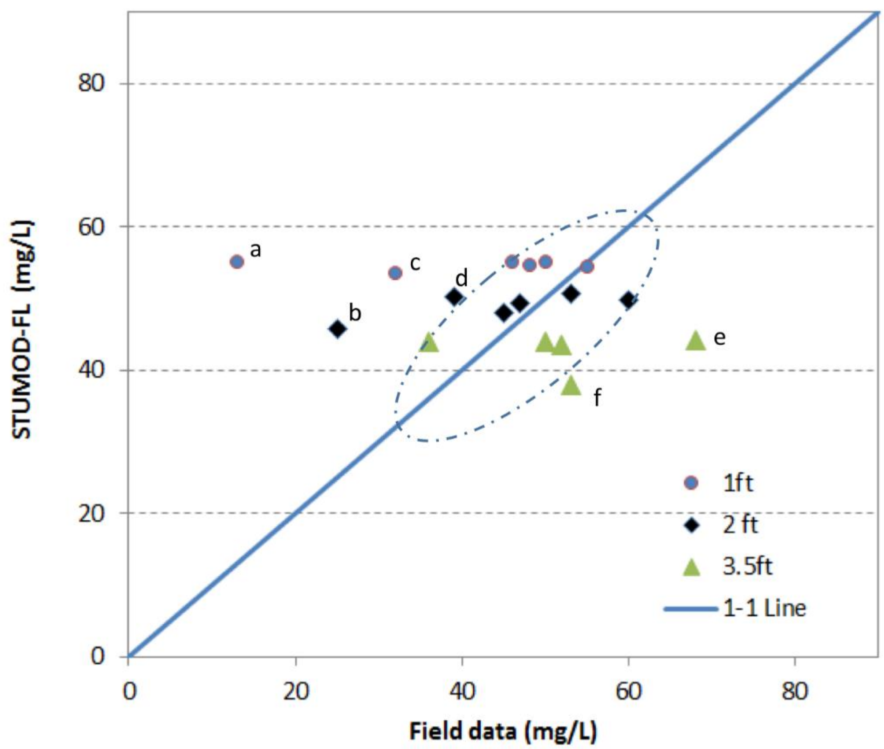

Figure 2.9: STUMOD-FL Total Nitrogen Corroboration Results from the GCREC S&GW Test Area 1 using an Averaged Effluent Concentration and ET
(in mg/L as N)

The points furthest from the 1-1 line (poorest fits) are labeled “a” to “f”. Point “a” represents an exceptionally low field observation of 13 mg-N/L at 1 ft depth on SE2 whereas most of the 1 ft observations were 25 mg-N/L and above. Points “b”, “c” and “d” are also relatively low concentrations measured in the field on SE2 and SE6. The precipitation data shows substantial rainfall on the days preceding SE6. SE2 and SE4 also had substantial rainfall recorded on the days preceding the sampling events although relatively low as compared to SE6.

Point “e” represents the 3.5 ft suction lysimeter depth during SE5. The model predicted 44 mg-N/L while the field observation was 68 mg-N/L which is greater than the averaged input value of 57.9 mg-N/L. The high field observation is attributed to the higher STE concentration of 81.9 mg-N/L measured during SE5. The actual input concentration above the averaged input concentration is assumed to be responsible for the discrepancy between the field observation and model prediction. Thus, the points marked “a” to “f” are samples not appropriate for corroborating a steady state model (sampling events with rainfall inputs and higher effluent input concentrations) but included to demonstrate the impact of variable inputs to model corroboration results. In most cases, points “a” to “f” had a sharp decrease in concentration at the shallower depth (attributed to the dilution effect from rainfall) followed by an increasing concentration with increasing depth. The model in contrast shows decreasing concentration with depth. The average relative error when these points are excluded was less than 15% with R^2 values of 0.6, 0.5 and 0.6 for 1, 2 and 3.5 ft respectively.

Generally the model predicted relatively higher concentration at 1 and 2 ft (most points for 1 ft and 2 ft lie above the 1-1 line) compared to 3.5 ft. This is attributed to the effect of rainfall that is not accounted for in a steady state model. Previous HYDRUS-2D simulations showed the match between field and model predicted values improved particularly for 1 ft and 2 ft when precipitation effects were included (see Task D.7 report). Comparison of Figure 2.5 to Figure 2.9 shows that using a variable input concentration specific to the sampling event only improved point “e” (SE5 at 3.5 ft). This is the specific case where the actual input concentration (81.9 mg-N/L) was higher than the averaged input concentration (57.9 mg-N/L).

The field observations between TA1 and TA3 had substantial differences as shown in Figure 2.10 further indicating that calibrating to a specific site and applying parameter values to other sites cannot produce a good model fit at the new site since observations also vary due to heterogeneity in the field. Observed concentrations for TA3 were lower than concentrations for TA1. The differences ranged from 1 mg-N/L to as high as 42 mg-N/L with more than 50% of the differences larger than 22 mg-N/L. Generally, the smaller differences occurred for sampling events preceded by substantial rainfall events (SE2, SE4 and SE6) and could be due to dilution during these sampling events masking the differences. The differences were not as consistent with depth, thus no conclusion could be made with depth since both small and large differences were observed at shallow and deeper depth.

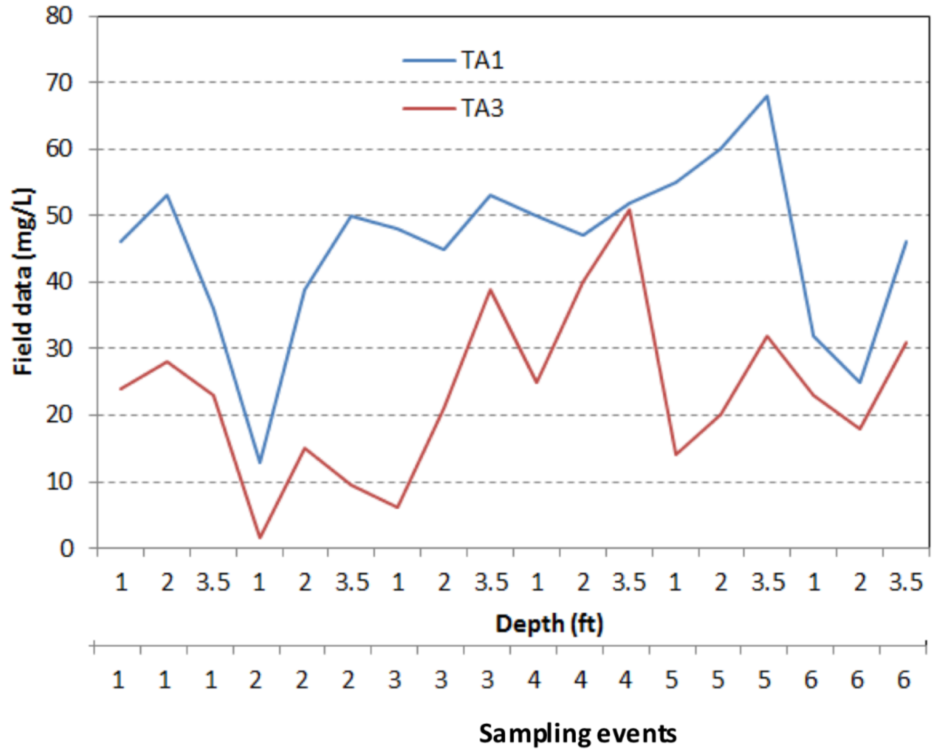

Figure 2.10: Comparison of TA1 and TA3 Field Measurements by both Depth and Sampling Event (in mg/L as N)

The two test areas received the same effluent input and precipitation was the same. While the soils are expected to be heterogeneous, homogeneity is assumed during modeling because the test areas are very close in proximity, and there is not sufficient data available to represent the variability on that scale. This means that the field data suggests differences either in the inputs or site characteristics but these differences are not included in the model.

Two differences between TA1 and TA3 are the depth to the infiltrative surface and effluent application method. TA3 was 0.5 ft (~15 cm) from the land surface with effluent applied to the infiltrative surface soil via drip irrigation, while TA1 was 1.5 ft from the land surface with effluent applied to a 12 in gravel filled trench. For a root depth of 40 cm, 25 cm of the rooting depth is below the infiltrative surface for TA3. This plant uptake in STUMOD-FL was considered and resulted in lower nitrogen concentrations in TA3, but was not large enough to match the observed differences in the field concentrations between the two sites.

Erickson et al. (2001) evaluated nitrogen leaching in newly established St. Augustine grass turf in Florida. For a fertilizer application rate of 300 kg N/ha/year, the leaching loss for the St. Augustine grass was only 4.1 kg N/ha/Year and runoff was negligible. Assuming that the remaining N is consumed, the plant uptake of 296 kg/ha/year was used in STUMOD-FL resulting in concentration reductions, but was not as high as the observed differences between TA1 and TA3. The University of Florida recommends applying a half pound (water-soluble nitrogen source) to one pound (slow-release nitrogen source) of nitrogen per 1000 square feet of turf grass (http://edis.ifas.ufl.edu/ep221) per month (up to 600 kg/ha/year) which is about twice the amount estimated based on Erickson et al. (2001). Thus, the effect of the plant uptake was further evaluated based on 1 lb per 1000 sq ft per month rate which reduced the concentrations further, but again did not match the observed differences between the two sites. It was assumed that there are differences in site characteristics between the two sites in addition to the observable differences in STU configuration.

To compensate for the difference, the denitrification rate was adjusted to 5.5 mg/L/day from a default rate of 2.58 mg/L/day to increase removal in TA3 to account for heterogeneity in the field. This adjustment further improved predictions in TA3; however, since the differences in the observed data were more influenced by the sampling events (weather variability) and soil heterogeneity than by the treatment depth as discussed earlier, change in the denitrification rate coefficient alone could not capture the differences. STUMOD-FL total nitrogen corroboration results for TA3 are shown in Figure 2.11. Even after adjustments to plant uptake and denitrification rate, the STUMOD-FL predicted higher concentrations particularly at shallow depth as compared to field data. Similar to TA1, most of the points away from the 1:1 line occurred at 1 ft with a few at 3.5 ft. Again, the field data show a sharp decrease in concentration at the shallower depth followed by an increasing concentration with increasing depth. The model in contrast shows decreasing concentration with depth that resulted in STUMOD-FL over predicting concentrations at shallow depth as observed in TA1.

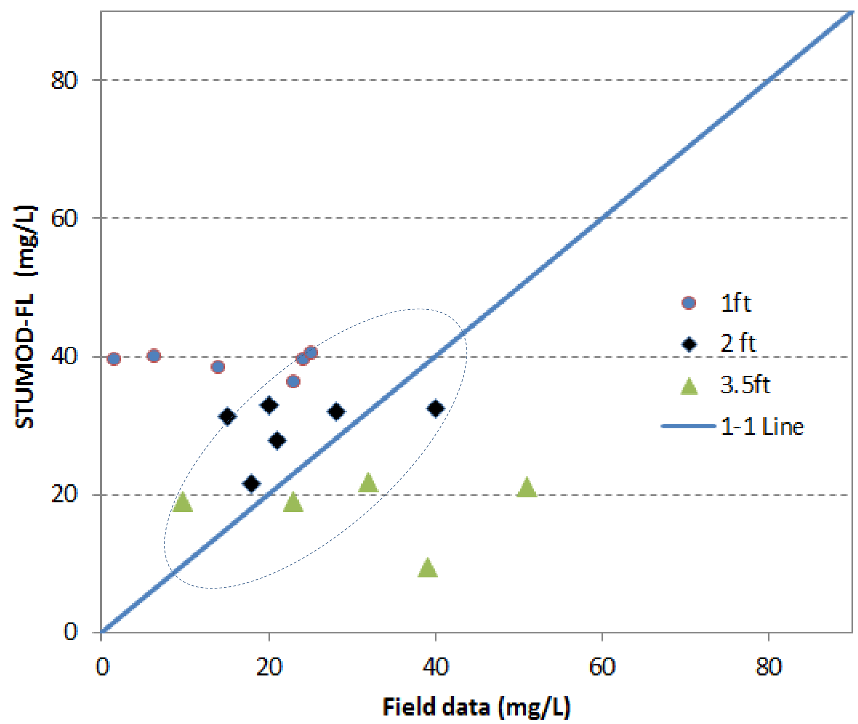

Figure 2.11: STUMOD-FL Total Nitrogen Corroboration Results from the GCREC S&GW Test Area 3 using an Averaged Effluent Concentration and ET
(in mg/L as N)

TA2 and TA4 received nitrified effluent. The average TIN concentration was 33.4 mg-N/L with substantial variability among the sampling events. Thus, using the average input resulted in over prediction in some cases and under prediction in other cases. To take this into account, STUMOD-FL was run using both variable (i.e., six runs with different effluent input concentrations, see Table 2.7) and averaged inputs (see Table 2.5). In addition, for some of the sampling events it was observed that substantial ammonium was present due to less than anticipated nitrification. Thus, STUMOD-FL was also run assuming both totally and partially nitrified effluent for both TA2 and TA4. There was no substantial difference in concentration of total nitrogen at 1, 2, or 3.5 ft between totally and partially nitrified effluent input because ammonium was nitrified within the first one foot of soil from the surface in both the model and in the field observations.

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Table 2.7
STUMOD-FL Simulation Parameters Selected to Replicate TA2 and TA4 Field Conditions during Sample Events (input ammonium and nitrate concentrations obtained from sample analyses)

	K_s (cm/d)	Water Table Depth (ft below IS)	HLR (cm/d)	Tmax (C°)	Tmin (C°)	C_o NH_4^+ (mg-N/L)	C_o NO_3^- (mg-N/L)
6/18/12	352.6	5.58	3.26	32.1	20.8	53.0	0.3
8/20/12	352.6	5.54	3.26	33.1	22.4	11.0	12.0
10/15/12	352.6	3.40	3.26	28.0	17.1	6.3	3.7
1/7/13	352.6	5.95	3.26	23.1	9.1	22.0	5.7
3/11/13	352.6	6.59	3.26	26.1	11.2	31.0	19.0
6/13/13	352.6	2.48	3.26	32.1	20.8	1.4	34.0

The configuration for TA2 was similar to TA1 with the infiltrative surface 1.5 ft below the land surface with a gravel trench application, so again plant uptake did not have an effect on concentration since the infiltrative surface was below the root depth. Figure 2.12 shows STUMOD-FL total nitrogen corroboration results from the GCREC S&GW for TA2 based on average effluent concentration input. It can be seen that most of STUMOD-FL predicted values fall between 20 to 30 mg-N/L for an average input concentration of 33.4 mg-N/L while the observed values varied between 15 to 53 mg-N/L. This illustrates the limitations of using the average input in capturing the variability observed in the field particularly when the input varies substantially as in this case. For most of the points furthest away from the 1-1 line, the effluent input concentrations during those sampling events were relatively higher than the average value used in the model, and in those cases the model under predicted concentration. If the variability in the effluent input was less, then use of an average value would have been sufficient. The model was re-evaluated using the variable input and the results are shown in Figure 2.13. With the average effluent input concentration, the model performance was poor at 1 ft as compared to 2 ft and 3.5 ft. With the variable input, the model was able to capture the trends better at 1 ft and equally good performance at 2 ft and 3.5 ft (Figures 2.12 and 2.13).

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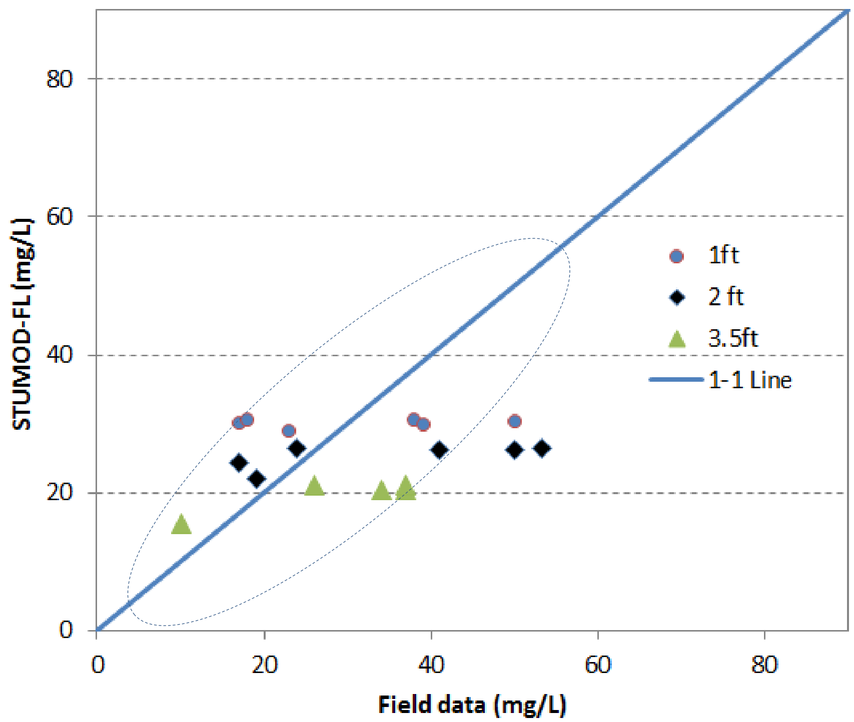

Figure 2.12: STUMOD-FL Total Nitrogen Corroboration Results from the GCREC S&GW Test Area 2 using an Averaged Effluent Concentration and ET (in mg/L as N)

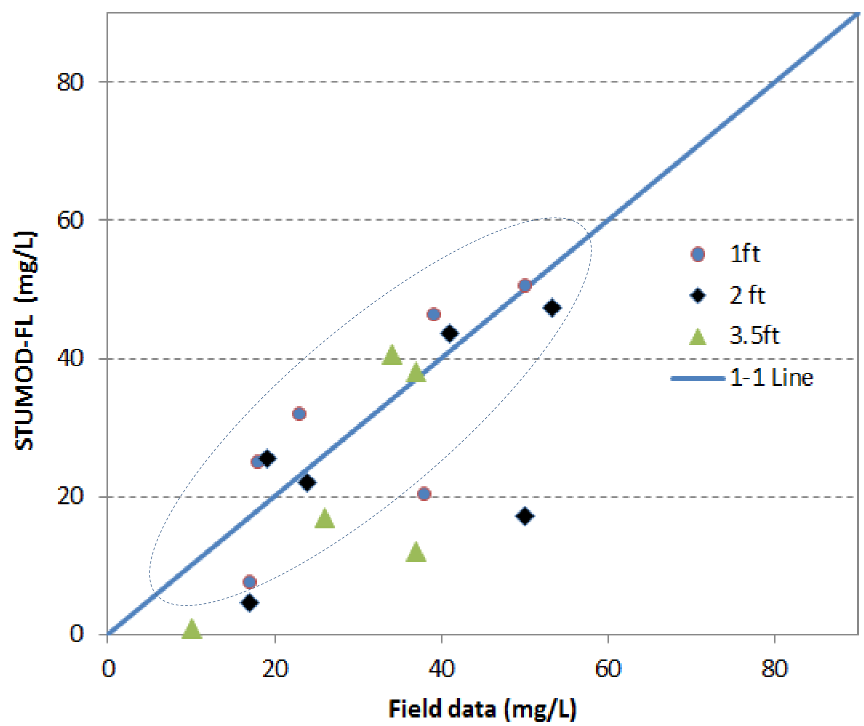

Figure 2.13: STUMOD-FL Total Nitrogen Corroboration Results from the GCREC S&GW Test Area 2 using Variable Effluent Concentrations and ET (in mg/L as N)

Like TA1/TA3, TA2 and TA4 received the same effluent input, precipitation, and the soils were assumed homogeneous, but the effluent application methods differed in that TA2 was applied in a gravel trench to the infiltrative surface while TA4 was applied by drip irrigation directly to the infiltrative surface soil. The suction lysimeter field observations in TA2 and TA4 differed (Figure 2.14), but not as substantial as TA1/TA3. The maximum difference between TA2 and TA4 was 13 mg-N/L. Again field data show relatively higher nitrogen concentrations in TA2 where the infiltrative surface is deeper compared to TA4 (1.5 ft for TA2 vs 0.5 ft for TA4) which is consistent with TA1/TA3. Due to the assumed root depth of 40 cm, 25 cm of the rooting depth is below the infiltrative surface for TA4 and resulted in a reduction in concentration in TA4 similar to the observed difference in the field data using the lower rate of 296 kg/ha/year.

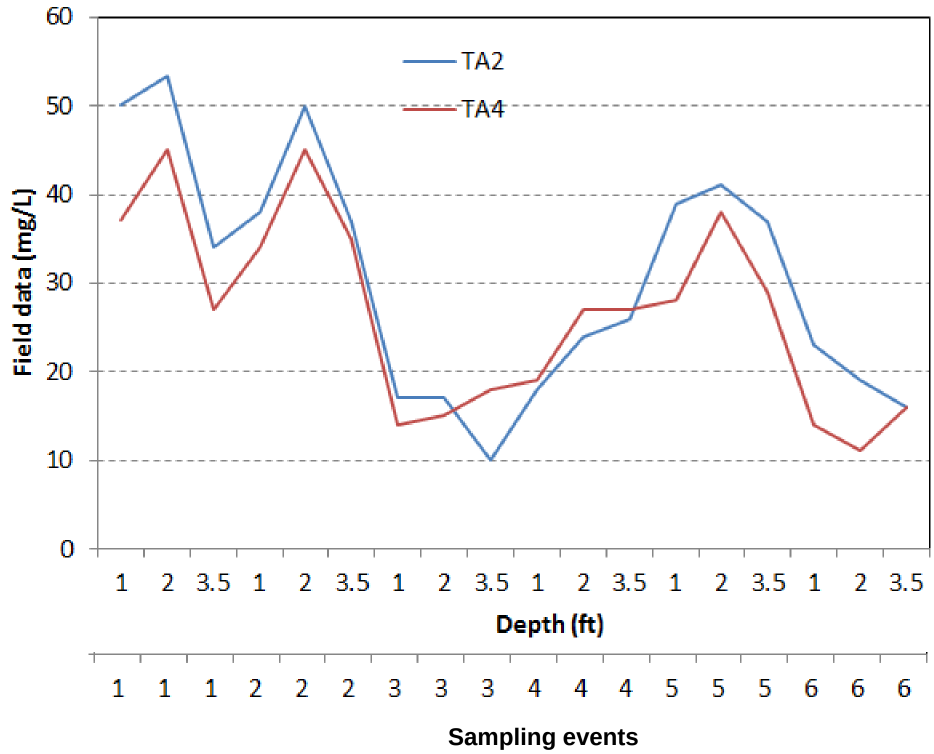

Figure 2.14: Comparison of TA2 and TA4 Field Measurements by both Depth and Sampling Event (in mg/L as N)

Again, due to nitrified effluent variability, STUMOD-FL was run assuming both totally and partially nitrified effluent for TA4; and again, there was no difference in concentration of total nitrogen at 1, 2, or 3.5 ft. Figure 2.15 shows STUMOD-FL total nitrogen corroboration results from the GCREC S&GW TA4 based on average effluent concentration input. It can be seen that most of STUMOD-FL predicted values fall between 10 to 25 mg/L for an average input concentration of 33.4 mg/L while the observed values varied between 10 to 45 mg/L. As with TA2, this illustrated the limitations of using the average input in capturing the variability observed in the field. The model was re-evaluated using the variable input and the results are shown in Figure 2.16. Using the variable input concentrations improved model corroboration results, although there are outliers as in the other test areas for reasons discussed earlier.

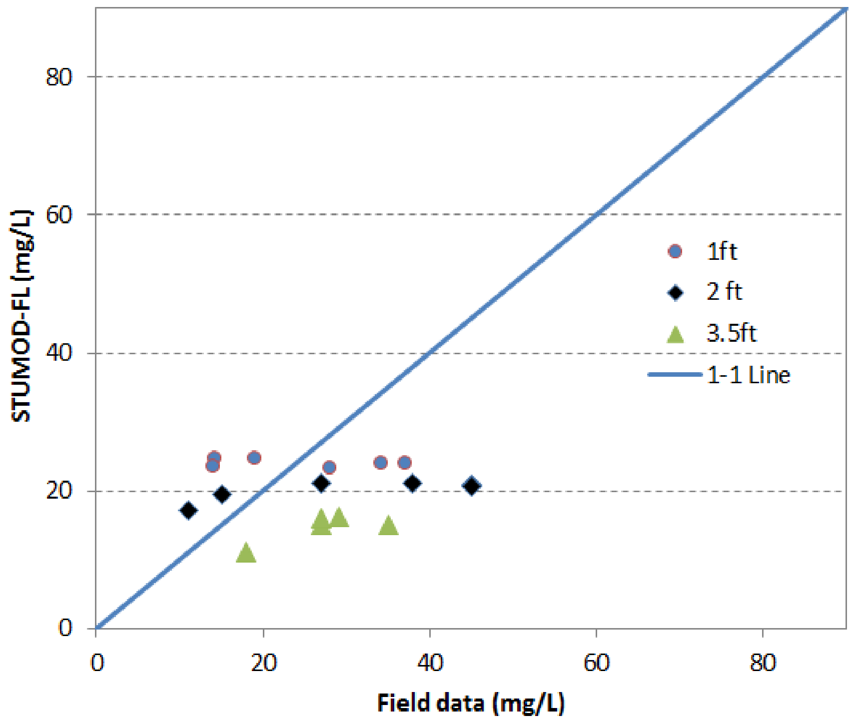

Figure 2.15: STUMOD-FL Total Nitrogen Corroboration Results from the GCREC S&GW Test Area 4 using an Averaged Effluent Concentration and ET (in mg/L as N)

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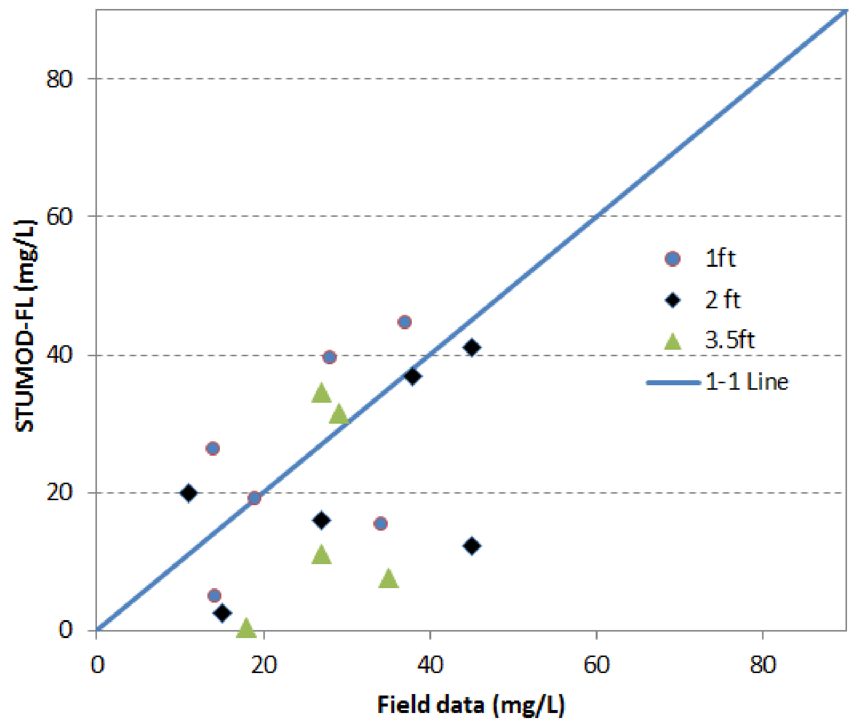

Figure 2.16: STUMOD-FL Total Nitrogen Corroboration Results from the GCREC S&GW Test Area 4 using Variable Effluent Concentrations and ET (in mg/L as N)

2.5 Moisture Content Corroboration

STUMOD-FL soil moisture profiles were also corroborated to measured field data at the GCREC S&GW test areas. Soil moisture was measured in the field using a Sentek Diviner to a maximum depth of 100 cm below the infiltrative surface. Measurements were taken at 13 locations throughout the test areas on 105 occasions. Figure 2.17 illustrates the variability of the measurements at one location (TA1, south). Figure 2.18 shows the field measured values during each sampling event with depth compared to the STUMOD-FL profiles using generalized more permeable sand parameters for the top 1 ft of mound sand and using less permeable sand parameters for the underlying soil. An increase with soil moisture can be observed in SE3 and SE6 field measurements suggesting the deeper measurements were taken in the capillary zone. STUMOD-FL over predicted the moisture content and did not capture the increased soil moisture content with depth specific to SE3 and SE6. Approximately 12-inches of rain was received in the 10 days prior to SE6. However, significant rainfall was not recorded prior to SE3 and suggests other field variability which cannot be explained.

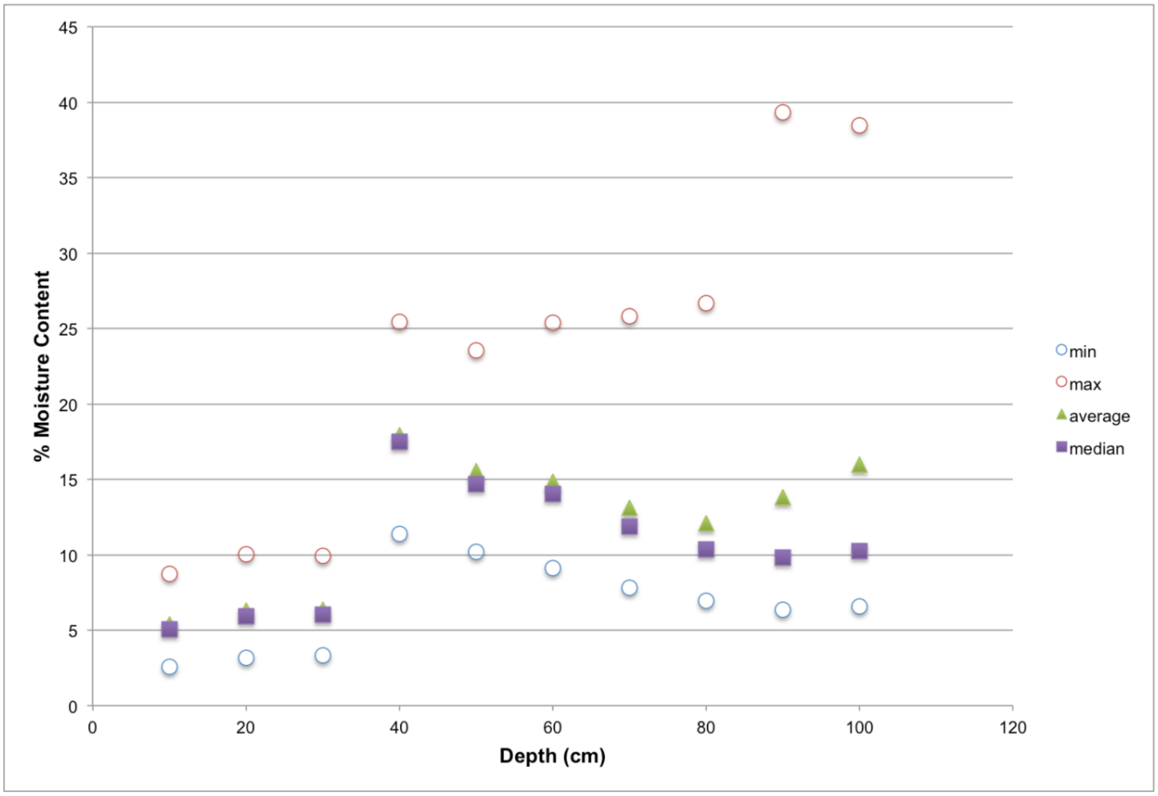

Figure 2.17: Measured Soil Moisture Content at the GCREC S&GW Test Area 1

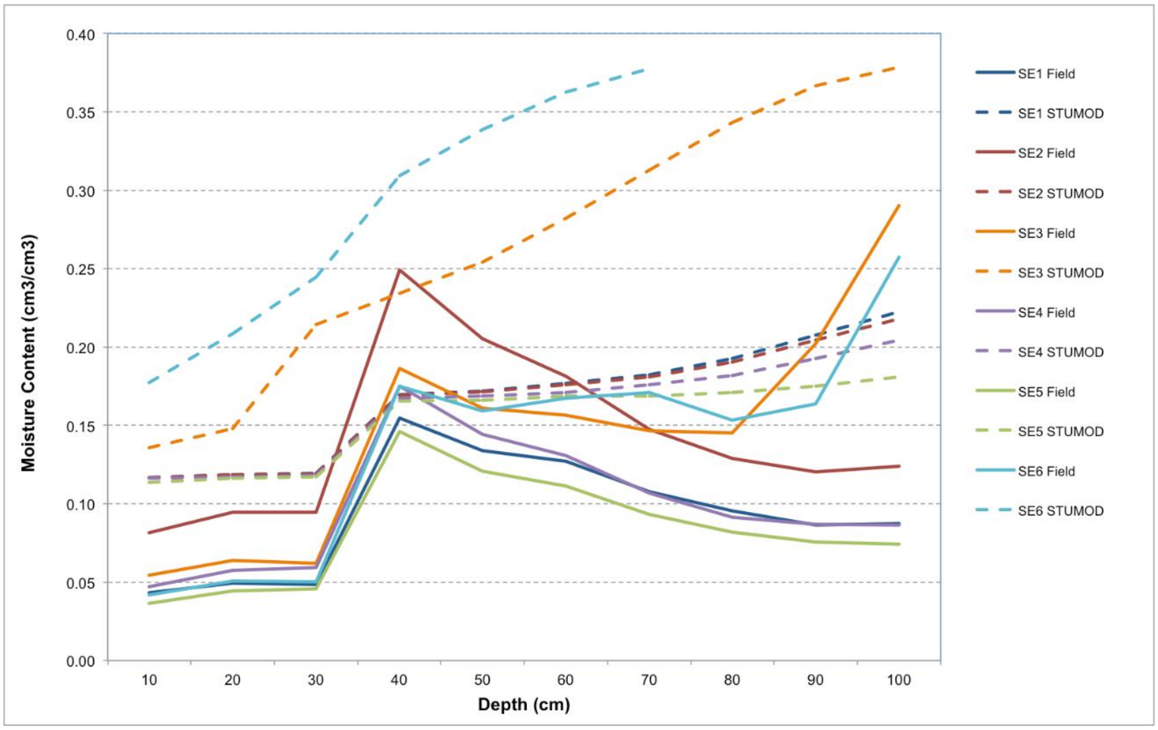

Figure 2.18: Moisture Content Comparison of Field Measurements to STUMOD-FL for TA1 (south) using Generalized Default Soil Parameters

Figure 2.19 shows an improved STUMOD-FL fit to the field moisture content profile when the model was soft calibrated by increasing the van Genuchten α parameter. In this case, more permeable sand parameters were again used for the top 1 ft of soil and less permeable sand parameters were again used for the underlying soil. The van Genuchten α parameter was modified for both layers; from 0.024 to 0.05 for the top more permeable sand layer and from 0.02 to 0.03 for the underlying less permeable sand layer. This soft calibration was not intended to alter the default parameters, since these measurements are site specific and calibrated values may not produce better fit in other sites. Corroboration of STUMOD-FL moisture profile to steady state HYDRUS-2D moisture profiles showed that STUMOD-FL resulted in a similar moisture profile as the numerical model and demonstrates the robustness of the analytical model for soil moisture profile calculation (Figure 2.20).

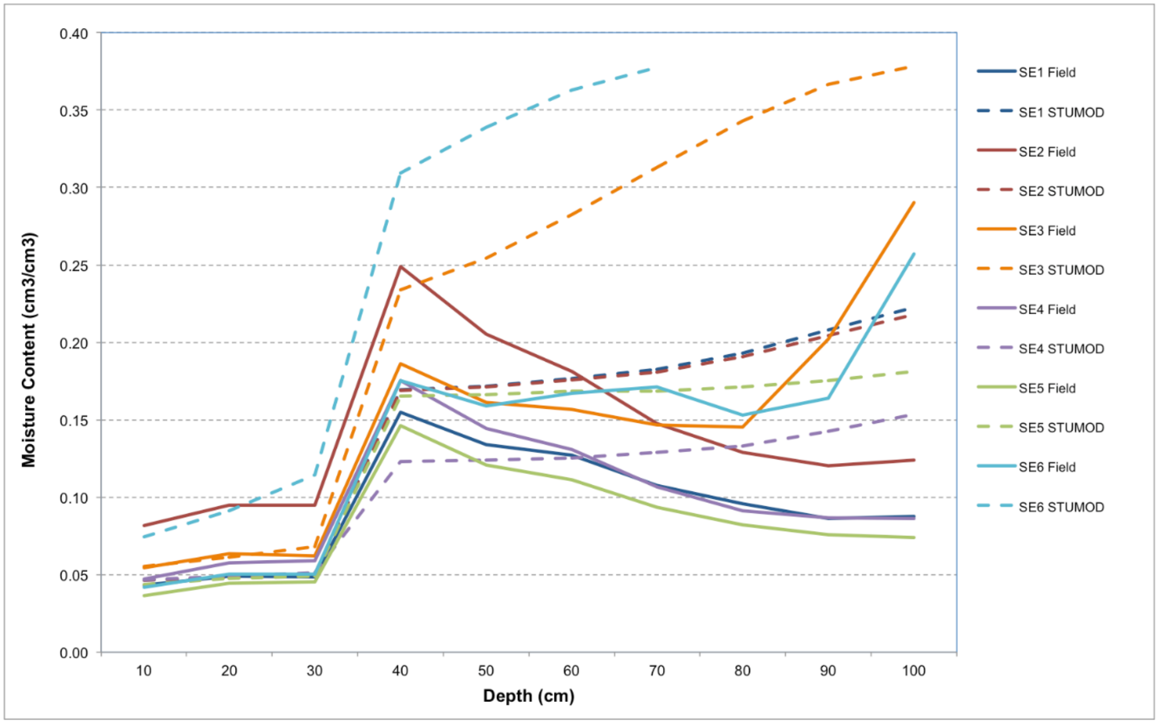

Figure 2.19: Moisture Content Comparison of Field Measurements to STUMOD-FL for TA1 (south) using Soft Calibrated Soil Parameters

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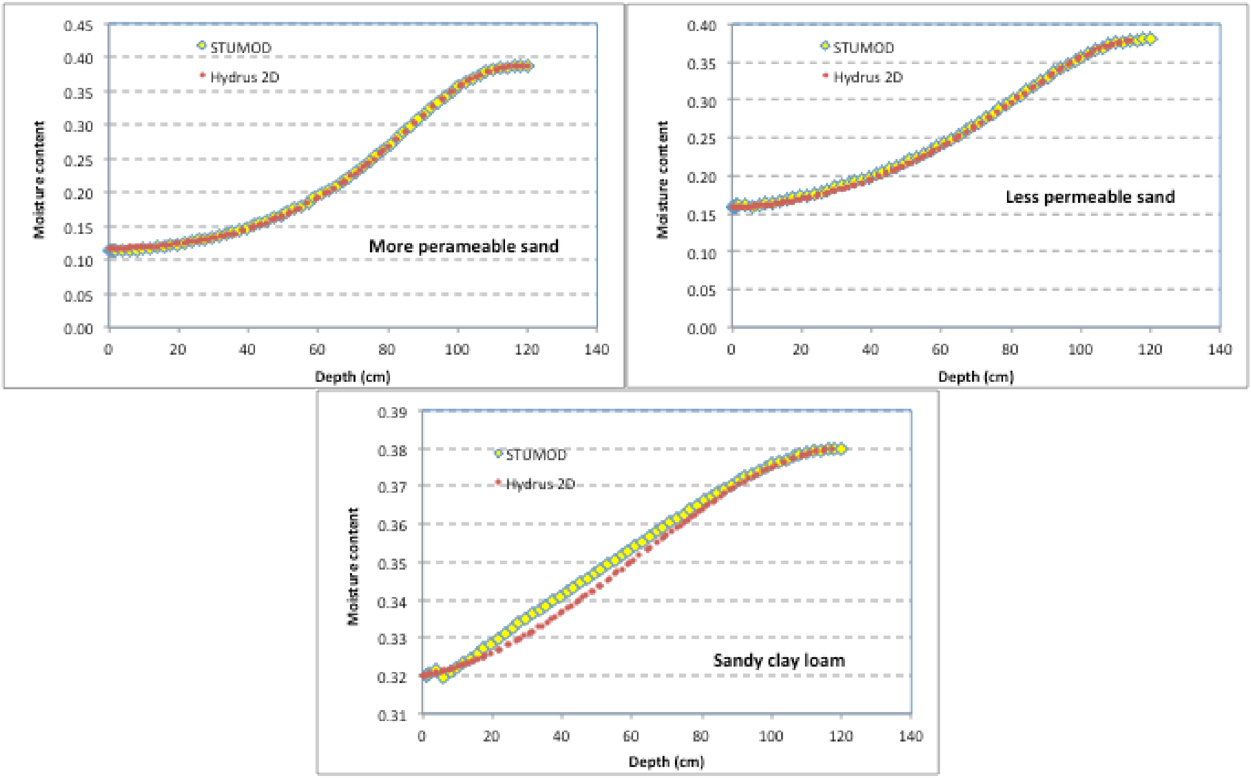

Figure 2.20: Moisture Content Comparison of STUMOD-FL Predictions to HY-DRUS-2D Predictions

2.6 Discussion

The corroboration at the GCREC S&GW TA1 indicated STUMOD-FL nitrate predictions to be more conservative (i.e., less removal) as compared to field data (i.e., STUMOD-FL predicted nitrate concentrations relatively higher than field observations) particularly at shallow depth. This could be attributed to environmental factors including dilution due to rainfall which would have a more pronounced effect at a shallow depth. This same trend was demonstrated using HYDRUS-2D for evaluation of the observed and model predicted concentrations for each sampling event (see Task D.7) when rainfall input was not used. Because flow is constant (steady state conditions) and given that STUMOD-FL predicted flux was within the range determined from the tracer test, mass loading is proportional to the concentration. Thus, corroboration results based on concentration are applicable to prediction of mass loading as STUMOD-FL estimates mass per unit area per day at the center line.

STUMOD-FL predictions show increasing nitrate concentrations at a shallow depth to a maximum value due to nitrification, and then decreasing nitrate concentrations with depth from this maximum value due to denitrification. Field observations do not show such a consistent trend with depth (Parzen 2007; Dimick et al., 2006; Tackett et al., 2004; Bohrer and Converse 2001; and Feigin 1984). Some studies have shown very low concentrations at shallow depth with an increase at some lower depth while other studies have shown consistent decreases in concentration with depth. Though Parzen (2007) observed a few locations where nitrate concentrations varied with depth, the majority of the locations showed a general consistent decrease in nitrate with depth. Bohrer and Converse (2001) also observed this consistent decrease with depth though relatively more observations indicated variable nitrate concentrations with depth. Feigin (1984) observed a consistent decrease in nitrate with depth in all but one of the sample locations. In each study, no definitive cause was determined that explained these variations in nitrate concentration with depth. While the exact causes of these observations have not been well explained, it could be due to preferential flow, experimental study artifacts, the effect of the biozone, and/or a more prevalent effect from dilution at shallow depth. In addition, simplifying assumptions incorporated into STUMOD-FL cannot capture this observed variability.

Parzen (2007) found that effluent in a sandy loam moved preferentially along drip emitter tubing as evidenced by the formation of a thick biomat directly under an emitter and suggested that the preferential flow paths affected observations in nitrate concentration with depth. At the GCREC, a vertical preferential flow path could cause effluent to migrate beyond the radial zone of influence captured during lysimeter sampling; however, this is unlikely due to the sandy soils at the GCREC. More likely is the fact that low suction pressures are required during vadose zone sampling, and this limits the radial area around the lysimeter that is collected in the sample, especially in sandy soils where retention of soil pore moisture is low. While preferential flow paths may form for a number of reasons, many other factors contribute to field measurements and the subsequent interpretation including lysimeter installation, operational conditions, hydrogeology conditions, sample collection conditions, duration of testing and sampling, and frequency of sampling. As is typical with field measurements, the observations are not consistent across field studies due to this wide range of factors that contribute to the measurement. Furthermore Parzen (2007), Bohrer and Converse (2001) and Feigin (1984) all investigated nitrogen occurrence in soils through soil sampling and analysis while other studies (Dimick 2006, Tackett 2004) and the sampling at the GCREC S&GW investigated nitrogen occurrence in soil pore water through vadose zone suction lysimeter sampling and analyses. Comparison of data from soil sampling and lysimeter sampling introduces the added complication of soil sample extraction effects, heterogeneity, and correlating reported concentrations between sample matrices. It is important to recognize that STUMOD-FL simulates the mobile water phase within the vadose zone.

Finally, development of STUMOD-FL required simplifying assumptions such as steady state behavior. Hence the variability observed in the field due to changes in applied nitrogen cannot be captured by a steady state assumption. Similarly, sorbed ammonium at deeper soil depths (Parzen 2007) and the resulting effects on nitrate occurrence also cannot be captured. However, the behavior of predicted nitrate concentration in STUMOD-FL is corroborated by numerous observations where concentrations generally decreased with depth although STUMOD-FL conservatively estimates the nitrate concentration (i.e., STUMOD-FL nitrate concentrations are higher than field observed concentrations). In cases where field measurements showed a more substantial decrease of nitrate and a subsequent increase deeper in the soil profile (compared to STUMOD-FL), the potential contributing factors were not well explained. Because the variability in the inputs including effluent concentration and rainfall input and other unknown factors, STUMOD-FL was not altered to fit the observed fluctuations. Doing so would bias the model to site specific processes or to artifacts of site instrumentation/monitoring. A field dataset representative of the model capabilities is required to adequately calibrate STUMOD-FL results.

STUMOD-FL is a very useful tool for evaluating impacts of numerous parameters on nitrogen contribution from STUs to groundwater although the model generally provides conservative estimations (higher nitrogen concentrations). As expected, field observations appear to be diluted by precipitation. Because the model can not handle variable inputs such as precipitation and changes in effluent quality, lower mass flux could be estimated by the user (e.g., effluent concentration x estimate of the volume of fluid applied [volume of effluent + volume of rainfall]) if the data is available. Refinements to the model parameters based on specific site data as available and/or calibration will improve the STUMOD-FL nitrogen estimates for that site.

Section 3.0
Sensitivity Analysis

A list of STUMOD-FL input parameters that were evaluated in the sensitivity analysis is given in Table 2.8. Sensitivity analysis indicates which input parameters are critical and which parameters have less influence on the final model output. Ultimately this information allows the user to understand and focus on the parameters that will have the most effect on STUMOD-FL predicted STU performance and to understand how potentially small changes in the parameter may produce a wide range of model outputs.

An automated sensitivity analysis tool was developed for the analysis of multiple STUMOD-FL input parameters. For sensitivity analysis using the automated process, one input parameter was selected and its value increased and decreased by a specific percentage (+10%, +25%, +50%, +75%, -10%, -25%, -50%, and -75%) from a default base value (within a range obtained from a literature search) while all other input parameters were held at their default value. STUMOD-FL was run to produce a corresponding output distribution for that particular input parameter. The process was repeated for the other input parameters producing output distributions for each input parameter. The van Genuchten α and n, K_s, θ_r, and θ_s are log normal distributions while K_{rmax}, V_{mas}, and K_d are natural log normal distributions. The percent change in model output from the default output value was calculated for each change in parameter value. Default parameter values were increased and decreased by a specific percentage around their default value (again, +10%, +25%, +50%, +75%, -10%, -25%, -50%, and -75%). The resulting data revealed the percent change in model output as a function of the percent change in the parameter value. For the purposes of comparison the percent change in model output for each percent change in parameter value was normalized by dividing by the largest calculated change in model output. The results for the sensitivity analysis are in Table 3.2 in order of the most sensitive parameters at the top to the least sensitive at the bottom.

Table 3.1
STUMOD-FL Input Parameters Evaluated in the Sensitivity Analysis

Parameter	Parameter Description
HLR	Hydraulic loading rate
α_G	Parameter α in Gardner's analytical equation for pressure distribution
α_{VG}	Parameter α in the soil water retention function
bnit	Empirical coefficient for temperature function for nitrification
$C_o\ NH_4$	Effluent ammonium concentration
e_{dnt}	Empirical exponent for denitrification
kd	Adsorption Isotherm
kr max	Maximum nitrification rate
K_s	Hydraulic conductivity
n	Parameter n in the soil water retention function
θ_r	Residual soil moisture
θ_r	Saturated soil moisture
s_{dn}	A threshold relative saturation
sh	Relative saturation for biological process (upper limit
sl	Relative saturation for biological process (lower limit)
T	Soil Temperature
V_{max}	Adjusted Denitrification Rate

Table 3.2
Order of Sensitive STUMOD-FL Parameters as Determined by Sensitivity Analysis

Normalized % Change in Model Output	Parameter	Parameter Description
100.00 %	*n*	Parameter n in the soil water retention function
78.09 %	s_{dn}	A threshold relative saturation
74.33 %	*T*	Soil temperature
74.25 %	V_{max}	Maximum denitrification rate
72.68 %	θ_s	Saturated soil moisture content
61.07 %	*HLR*	Hydraulic loading rate
60.34 %	$C_o\ NH_4$	Effluent ammonium concentration
59.77 %	α_{VG}	Parameter α in the soil water retention function
53.24 %	e_{dnt}	Empirical exponent for denitrification
41.36 %	α_G	Parameter α in Gardner's analytical equation for pressure distribution
29.27 %	*sh*	Relative saturation for biological process (upper limit)
21.58 %	K_s	Hydraulic conductivity
13.13 %	*kr max*	Maximum nitrification rate

Of the 17 parameters that were evaluated for sensitivity, 13 produced at least a 10% change from the default model output as listed in Table 3.2. Table 3.2 indicates that many of the sensitive parameters in STUMOD-FL are hydraulic parameters. The pore size distribution parameter (n), saturated soil moisture content (θ_s), air entry pressure (α_{VG}), pressure distribution (α_G), hydraulic loading rate (HLR), and hydraulic conductivity (K_s) all produced significant changes in model output during the sensitivity analysis. The sensitivity results show that other parameters such as effluent quality (C_o NH_4) and the maximum denitrification rate (V_{max}) were also important. It should be particularly noted that the model is sensitive to operation parameters (hydraulic loading rate and effluent quality) that can be controlled by designers and operators. Previously we noted that other researchers have observed differences with respect to consistent gradual decline of nitrate in the soil profile as we did during the corroboration and calibration procedure. Parzen (2007) indicated that preferential flow along drip tubing could cause unequal distribution of nitrate in the STU. Sensitivity results appear to corroborate this hypothesis and suggest that any factor that affects the hydraulic regime of the STU can have significant impacts on nitrogen concentrations throughout the soil profile. Vertical preferential flow paths that bypass monitoring instrumentation in the upper soil layers or variations in effluent concentrations could also explain field observations.

Figures 3.1 through 3.3 illustrate the relative sensitivity of the input parameters listed in Table 3.1 for three prevalent soil textures.

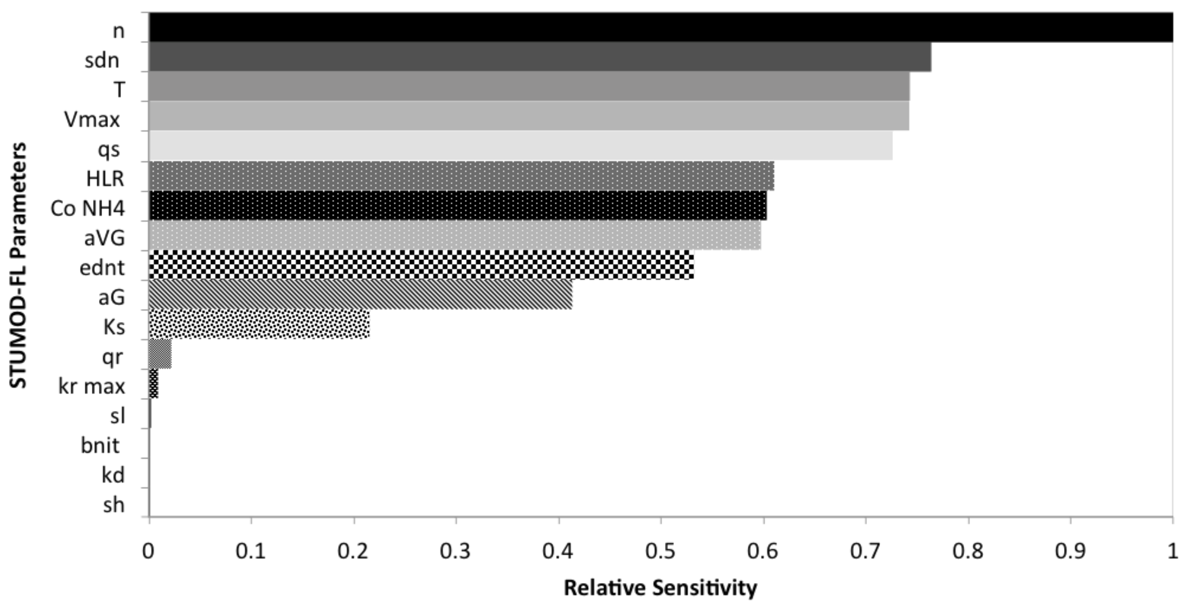

Figure 3.1: STUMOD-FL Relative Parameter Sensitivity in "More Permeable Sand"

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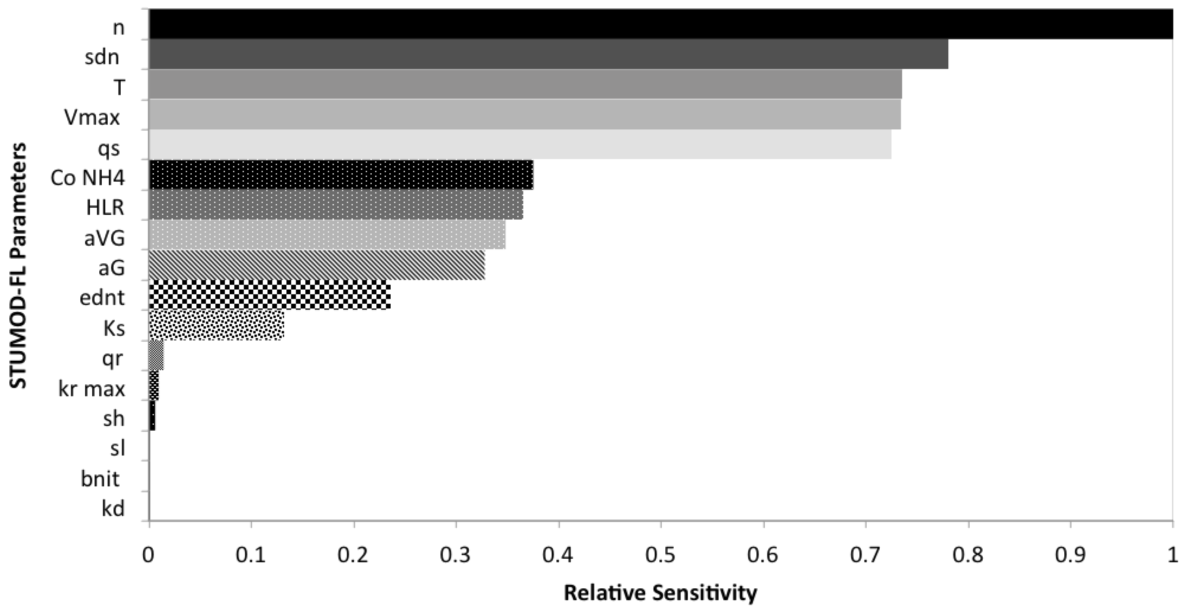

Figure 3.2: STUMOD-FL Relative Parameter Sensitivity in "Less Permeable Sand"

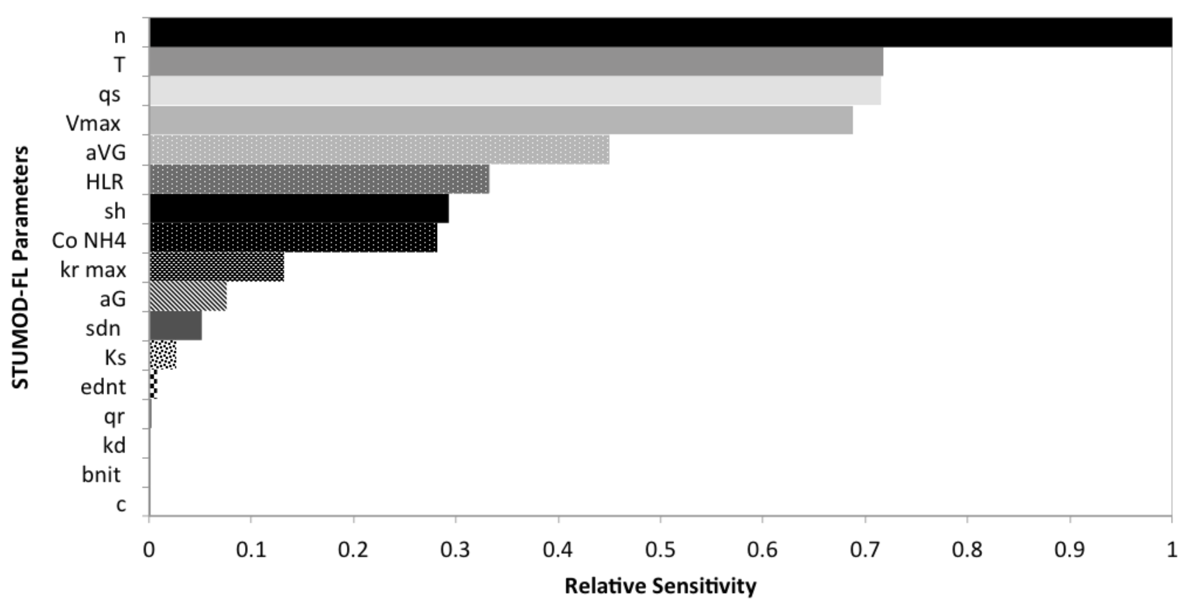

Figure 3.3: STUMOD-FL Relative Parameter Sensitivity in Sandy Clay Loam

To ensure the most accurate results, the STUMOD-FL user should establish the value of the parameters in Table 3.2 by independent methods. While the general user may not be capable of independently measuring many of the parameters in Table 3.2, results from the corroboration procedure (Section 2) indicate that STUMOD-FL results provide a conservative first approximation that may be sufficient for the general user. If STUMOD-FL users require more precision, steps should be taken to evaluate hydraulic parameters first, as it appears these parameters have the most impact on model output. Both general and technical users can easily access soil survey data, using online databases, which often report parameter values for several of the hydraulic parameters. Users who have the expertise and resources are encouraged to independently evaluate the soils at their site to establish parameter values.

Section 4.0
Uncertainty Analysis

Predictive uncertainties arise due to simplification of the system, errors in the conceptual model, and inadequate quantity and quality of data. Even models of relatively low predictive accuracy can be useful to decision makers if the predictive accuracy is quantified appropriately (Geza et al., 2010) because it provides information about the level of risk associated with accepting model predictions. For Task D.9, Monte Carlo simulation was used to quantify the uncertainty of model outcome in STUMOD-FL. Monte Carlo simulations rely on random selection of input values for a model from a known parameter range producing a method for statistically quantifying the uncertainty of a model outcome. The van Genuchten α and n, K_s, θ_r, and θ_s are log normal distributions while K_{rmax}, V_{mas}, and K_d are natural log normal distributions. A model is run numerous times with the input parameters selected randomly from ranges of expected values. The output of the model runs is then statistically analyzed and the probability of realizing any one particular outcome can be quantified, thus allowing the modeling results to be viewed in a risk-based framework (similar to a cumulative frequency diagram [CFD]) by displaying the cumulative uncertainty of a particular model output due to individual input data. Such an analysis is ideal for modeling processes such as nitrogen attenuation in a STU where large ranges of uncertainty exist or where certain data parameters are unknown or highly variable.

A VBA code was written to run STUMOD-FL through multiple iterations with the input parameter values randomly generated from ranges of values. The code allowed random generation of multiple input parameters across specified ranges or from a normal distribution of probable input parameters. The number of Monte Carlo simulations that are run is critical in establishing a valid cumulative probability plot. An insufficient number of runs will produce cumulative probability plots that are non-unique, meaning that if the same numbers of simulations are run again, the shape of the subsequent cumulative probability plot will be slightly different. The number of runs sufficient to produce a unique cumulative probability plot was identified by producing multiple plots from a varying number of simulations. Up to 4000 Monte Carlo simulations were run to determine if there was a change in the cumulative probability plot. From these simulations it was determined that beyond 2000 simulations the plot did not change.

By statistically analyzing thousands of model output results, the probability of realizing one particular outcome (concentration at a particular depth relative to effluent concentration - i.e., C/C_o), was quantified. The resulting model output can be viewed in a probabilistic framework allowing the user to determine which percentiles and outcomes are acceptable or unacceptable, or which outcomes represent “best,” and “worst” cases. Rather than a single output, this approach gives the probability of realizing any one specific outcome, based on the cumulative uncertainty of all model input parameters. The probability of realizing C/C_o values was calculated for different soil depths (1, 2, 4 and 6 ft) and two hydraulic loading rates (2 and 5 cm/d) for Florida soil temperature regimes. Two different boundary conditions were used to simulate the effect of a fixed water table (6 ft) and a deep water table (free drainage) on nitrogen removal. These hydraulic loading rates and boundary conditions were selected to bracket the range of probable conditions for Florida systems.

Monte Carlo simulations were then converted to cumulative probability plots of the model outputs (Figures 4.1 through 4.4). With a total of 24,000 Monte Carlo simulations represented in Figures 4.1 through 4.4, the behavior of the model is well defined for an array of field conditions. All simulations were run for the 3 soil textures prevalent in Florida (more permeable sand, less permeable sand, and sandy clay loam) with STE represented as 60 mg-N/L of ammonium.

Both measured data (e.g., Long 1995) and STUMOD-FL output (Figures 4.1 through 4.4) show a relatively higher removal in less permeable soils compared to more permeable sandy soils. Long (1995) reviewed studies of N transformation in STUs to develop a methodology for predicting N loading to the environment and indicated that STUs remove 23 to 100% of the N correlating greater removals with finer grained soils because anoxic conditions would be achieved more frequently. This observation is consistent with STUMOD-FL outputs. Studies conducted on N attenuation and transformation in soil shows that ammonium present in wastewater is rapidly oxidized to nitrate below the STE infiltrative surface (Cogger et al, 1988; Fischer, 1999; Kristiansen, 1981; Walker et al, 1973). STUMOD-FL predicted that ammonium conversion to nitrate occurred within the first foot below the infiltrative surface. However, in sandy clay loam STUMOD-FL results showed that ammonium persisted relatively deeper in the profile due to lower nitrification rates caused by higher predicted soil water content.

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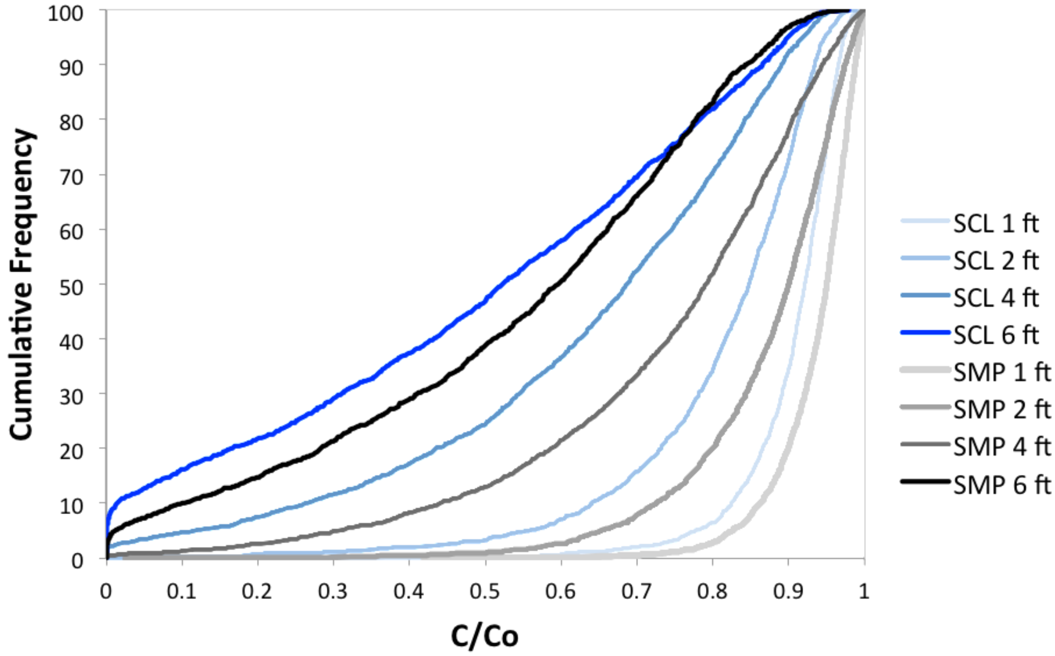

Figure 4.1: Uncertainty Analysis Results: 2 cm/d HLR with Fixed Water Table Boundary. Note: The 6 ft more permeable sand (SMP) curve crosses the sandy clay loam (SCL) curve at low removals due to the increased volumetric water content of the sand near the water table attributed to capillary rise

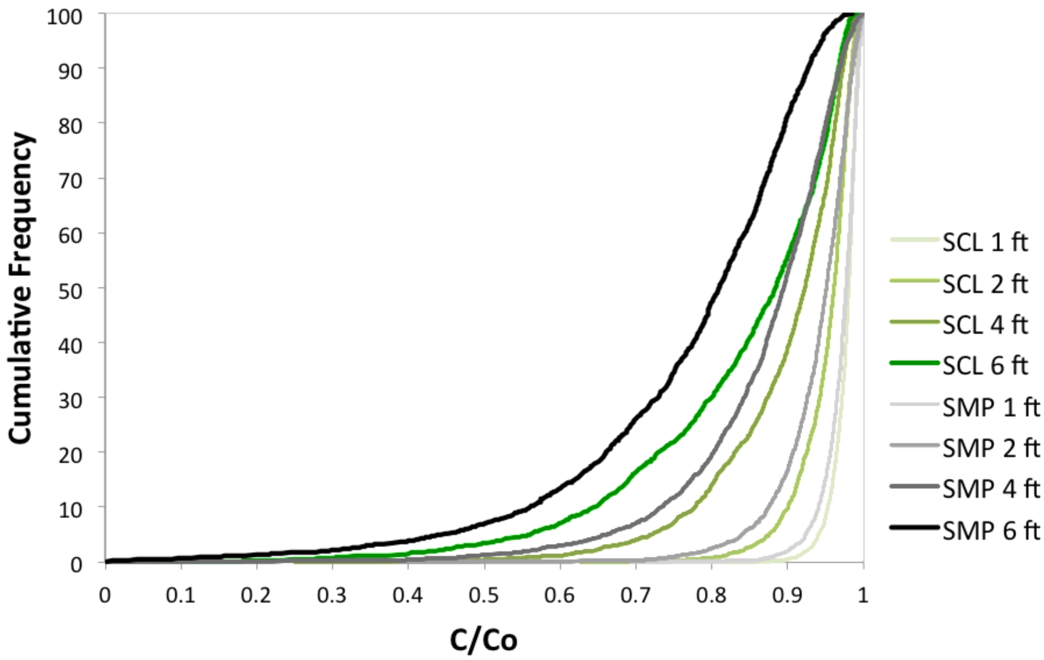

Figure 4.2: Uncertainty Analysis Results: 5 cm/d HLR with Fixed Water Table Boundary. Note: This shows that under high hydraulic loading rates sand soils remove more nitrogen relative to sandy clay loam because nitrification is not occurring as effectively in the sandy clay loam, thus limiting denitrification

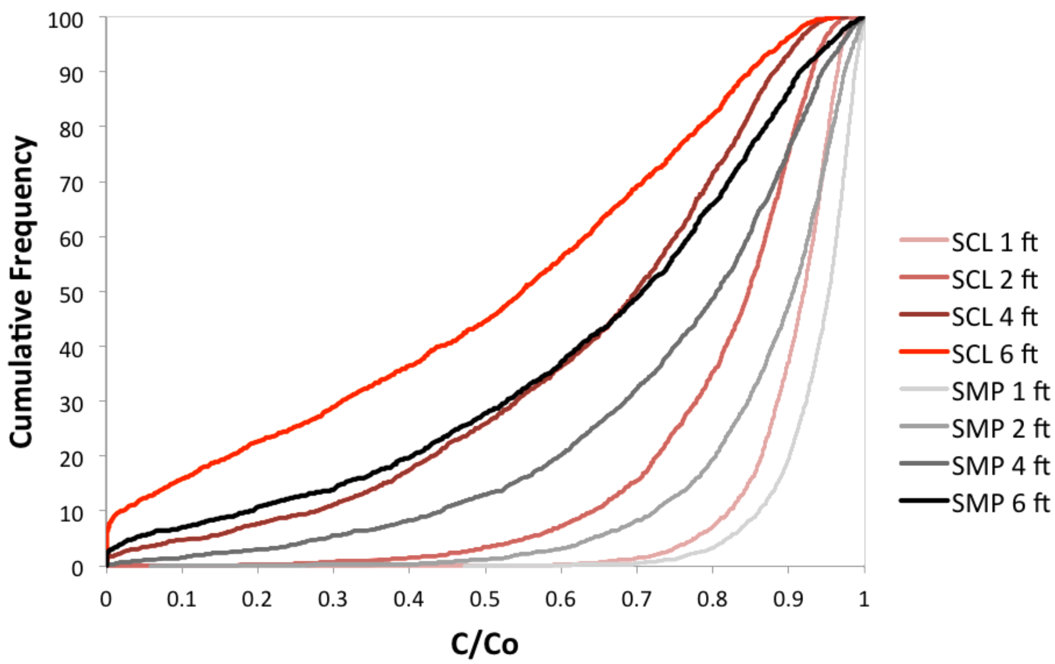

Figure 4.3: Uncertainty Analysis Results: 2 cm/d HLR with Deep Water Table Boundary (free drainage). Note: Because of the deep water table the capillary rise does not change the soil moisture profile at 6 ft and sandy clay loam removes more nitrogen relative to sand at all depths

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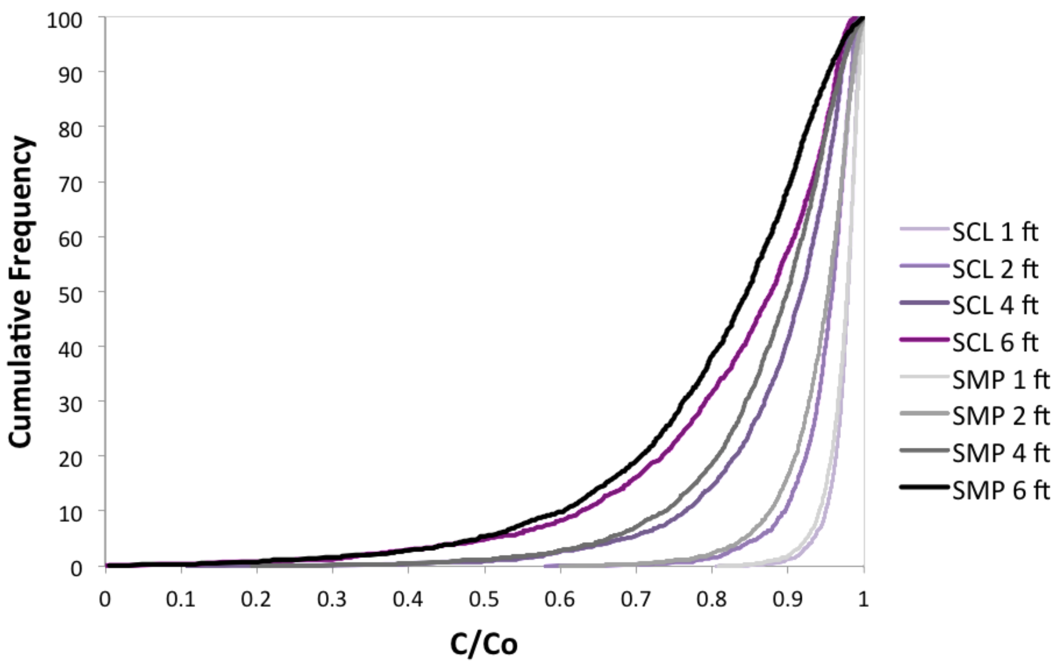

Figure 4.4: Uncertainty Analysis Results: 5 cm/d HLR with Deep Water Table Boundary (free drainage). Note: The behavior is similar to the behavior in Figure 4.2, sand removes more nitrogen relative to sandy clay loam because greater nitrification is occurring in the upper profile of sand, thus allowing greater denitrification lower in the profile.

In general, higher C/C_o values (i.e., higher fraction of N remaining) were typical at shallow depths for all three soil textures and less frequent for sandy clay loam compared to sandy soils particularly at the lower loading rate (2 cm/d) (Figure 4.1). Higher hydraulic loading rates result in less nitrogen removal for sandy clay loam compared to more permeable sand (Figure 4.2). This phenomenon, which may appear counter intuitive, is explained by the fact that the fine grained soils have high moisture holding capacity. Thus, as the loading rate increases the soil moisture content approaches saturation throughout the soil profile. Under saturated conditions nitrification does not occur and a larger fraction of the nitrogen remains as ammonium. While ammonium could potentially be removed from the soil profile via the annamox process, it is extremely rare and occurs at rates much less than the denitrification process. Alternatively, episodic periods of near saturation and less saturated conditions would facilitate nitrification. However, steady state models (e.g., STUMOD-FL, HYDRUS) do not capture these time variations in soil moisture content.

Figure 4.1 also shows interesting behavior beginning approximately at 25% removal (i.e., $C/C_o = 0.75$) at 6 ft below the infiltrative surface for the 2 cm/d loading rate. At this point on the cumulative probability plot, the more permeable sand shows more removal than the sandy clay loam which was not observed at 1, 2 or 4 ft. The shallow simulations were run with the water table at 6 ft below the infiltrative surface. The capillary effect extends only a few centimeters above the water table. The increase in moisture content right above the water table is assumed to be responsible for improved denitrification resulting in the increased removal observed. This behavior, where the more permeable sand showed more nitrogen removal than the sandy clay loam, was not observed at depths further away from the capillary fringe (e.g., 1, 2, or 4 ft) and led to evaluation of the effect of the capillary fringe in further detail across soil types and loading rates.

We were able to determine that this behavior, due to the capillary fringe, was more pronounced in the sandy soil because the moisture content was more limiting for denitrification compared to the sandy clay loam. Because of the high water holding capacity and high moisture content throughout the sandy clay loam profile, there was little change in moisture content at the capillary fringe resulting in a comparatively less significant change in denitrification rates and nitrification proceeded at a slightly slower rate when compared to the more permeable sand at locations well above the water table (i.e., 1, 2 and 4 ft). However, the denitrification rate is higher (as indicated by the higher removals illustrated on the Figure 4.1) at these same sandy clay loam locations due to the high water content. Within the capillary fringe, the more permeable sand shows better treatment relative to the sandy clay loam because more ammonium has been converted to nitrate that can subsequently be removed via denitrification. As Figure 4.1 shows, the more permeable sand only surpassed the treatment capacity of sandy clay loam under this specific condition - the capillary fringe. Thus, the relatively significant change in moisture content in the capillary zone in sandy soils along with an incoming high concentration to the capillary fringe (note a Monod function is used in STUMOD-FL) caused a significant increase in denitrification in the capillary zone.

Figure 4.2 does not show a similar capillary behavior for 5 cm/d loading rates under the same boundary conditions (a fixed water table – compare to Figure 4.1). Perhaps with the 5 cm/d loading rate even the more permeable sand had relatively high and uniform soil moisture content throughout the profile and there was no significant change in moisture content in the capillary zone unlike the 2 cm/d loading rate to cause a significant change in denitrification in the capillary zone. To test the hypothesis further, we ran additional simulations with a deep water table with no capillary effect. Thus, we were able to explain the phenomenon further as corroborated by Figures 4.3 and 4.4 which display the cumulative probability results for a deep water table boundary condition (free drainage). Under this boundary condition there was no apparent capillary effect. The results were consistent across all depths (1, 2, 4 and 6 ft) with the sandy clay loam showing a consistently higher removal.

The results from the Monte Carlo analysis, under the two water table boundary conditions are important in light of the field data that shows nitrate concentration variability with depth. The results also corroborate the sensitivity results in Table 3.2 that indicate the high sensitivity of the model to hydraulic parameters. While some field data shows the general trend of increasing nitrate concentrations followed by decreasing concentrations with depth, the same field studies also found similar generally decreasing nitrate concentrations with depth. While the exact causes of the variability in nitrate observations have not been proven conclusively, it could be due to preferential flow, experimental study artifacts, the effect of the biozone, and/or simplifying assumptions incorporated into STUMOD-FL all of which impact hydraulic parameters. Specifically the results in Figure 4.1 compared to Figures 4.2 through 4.4 show that changes in soil moisture movement and content can greatly affect the concentration of nitrogen observed. These findings also support the conclusion that modifying STUMOD-FL to better match the fluctuations in nitrate concentration with depth would bias the model to either site specific conditions or artifacts introduced by operation, instrumentation, or monitoring. The conceptual model programmed in STUMOD-FL, however, is corroborated by observed data from field studies that show a consistent decrease in nitrate with depth (Parzen 2007; Dimick et al., 2006; Tackett et al., 2004; Bohrer & Converse, 2001; Feigin et al, 1984).

While Monte Carlo results serve to corroborate previous findings, the curves generated by the uncertainty analysis can be utilized by users to understand the probability of achieving a particular treatment. Specifically the Monte Carlo analyses were used based on STUMOD-FL inputs to develop cumulative probability plots of the probability of the occurrence of a value (Figures 4.1 through 4.4). For example, in Figure 4.1, a horizontal line through a probability value of 50% suggests that the estimated nitrogen fraction remaining at 1 ft is ~90%, while at 6 ft, the nitrogen fraction remaining is ~50%. In other words, there is a 50% probability that 50% of the nitrogen is removed at 6 ft and a 50% probability that only 10% is removed at 1 ft. Alternatively, a vertical line through a specific fraction of nitrogen remaining enables the user to estimate the associated probability of the occurrence at depth of the selected value. A more practical approach is to determine the concentration of nitrogen in the expected effluent, and then determine how much removal is needed to reach a treatment goal. For example, if total nitrogen in STE is 60 mg-N/L and the goal is to reach 10 mg-N/L (approximately 80% removal), the cumulative probability plot can be used to determine at what depth such removal will likely occur for a given soil.

Section 5.0
Summary

Task D.9 involved model performance evaluation through corroboration/calibration, detailed performance evaluation using model-evaluation statistics, parameter sensitivity analysis, and an uncertainty analysis. Highlights from this Task include:

- Corroboration/calibration was conducted to better understand data required by comparing simulated model outputs to the corresponding measured values of nitrogen concentrations. Results from corroboration indicate that STUMOD-FL agrees with the conceptual model that was used to construct it and model outputs generally agree with field observations. Specifically, ammonium is removed quickly within the soil profile and subsequently nitrified with generally decreasing nitrate concentrations with depth.

- Additional corroboration/calibration was conducted using multiple data sets from the GCREC and data from the USF Lysimeter Station. Development of STUMOD-FL required simplifying assumptions such that variability observed in the field cannot be completely captured by a steady state assumption. When comparing STUMOD-FL to field data, more emphasis should be given to sampling events similar to steady state conditions (e.g., no rainfall) rather than sampling events with variable inputs not captured by the model (e.g., substantial rainfall that resulted in an outlier). STUMOD-FL was not altered to fit the observed fluctuations, as doing so would bias the model to site specific processes or to artifacts of site instrumentation/monitoring. A field dataset representative of the model capabilities is required to adequately calibrate STUMOD-FL results. Thus, further modification of STUMOD-FL requires additional field data, preferably from other locations throughout Florida, so as to not bias the model to site specific conditions.

- Detailed performance evaluation using model-evaluation statistics (R^2 and RMSE) determined whether the model could appropriately simulate the observed data. Agreement between R^2 and RMSE indicates that the model is adequately predicting nitrogen in the vadose zone as designed. Because both RMSE and R^2 values show similar behavior, the calculated performance of the model does not appear to be influenced by large variance or data outliers.

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- A parameter sensitivity analysis was performed to identify the most relevant model parameters. Thirteen parameters where shown to result in at least a 10% change from the default model output with many of the sensitive parameters in STUMOD-FL being hydraulic parameters. The pore size distribution parameter (n), saturated soil moisture content (θ_s), air entry pressure (α_{VG}), pressure distribution (α_G), hydraulic loading rate (HLR), and hydraulic conductivity (K_s) all produced significant changes in model output during the sensitivity analysis. Denitrification rate and initial effluent concentration were also determined to be influential parameters since the reactions are concentration dependent.

- An uncertainty analysis was performed where probability-based ranges for model input parameters were used to generate probable model outcomes. In general, higher nitrogen removal can be observed in lower hydraulic loading rates (2 cm/d removal > 5 cm/d removal), in finer grained soil textures (sandy clay loam removal > less permeable sand removal > more permeable sand removal), and with increasing depth (removal at 6 ft is > 4ft > 2 ft > 1ft). The effect of the capillary zone on nitrogen removal was observed due to a relatively significant change in moisture content in sandy soils with a lesser effect observed in sandy clay loam.

Section 6.0
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Appendix A
STUMOD-FL Graphical Outputs from Initial Corroboration

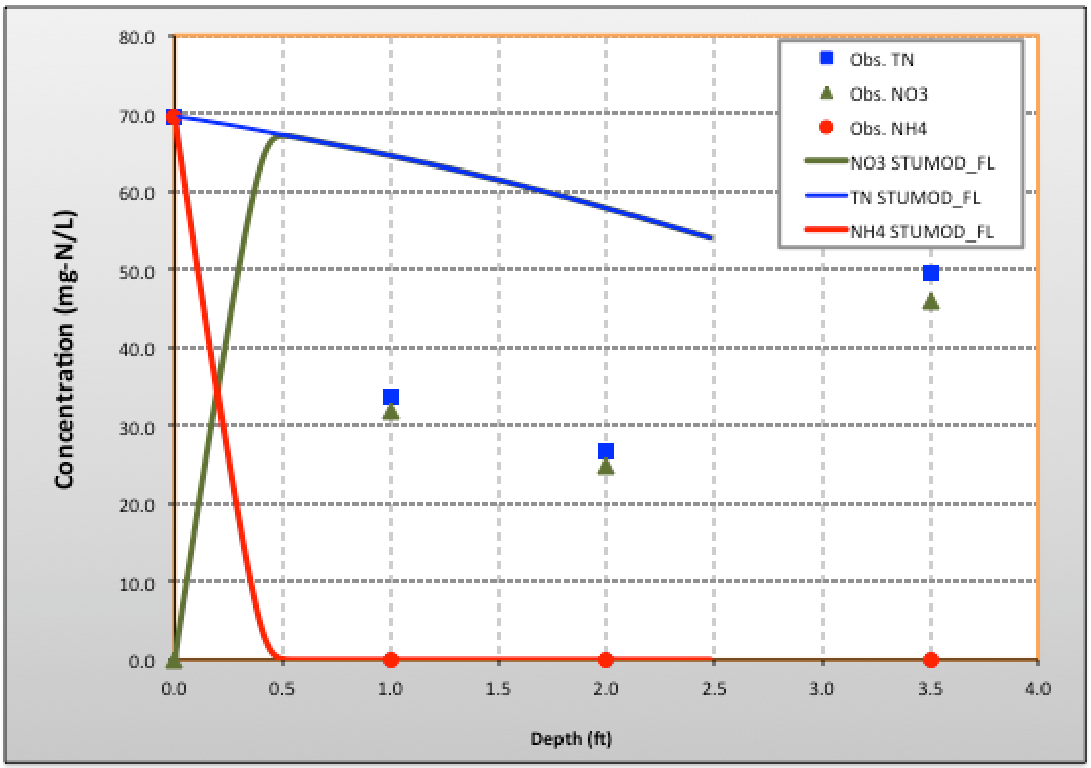

Figure A.1: STUMOD-FL Simulated Concentration with depth for Task C.16 Sample Event No. 1

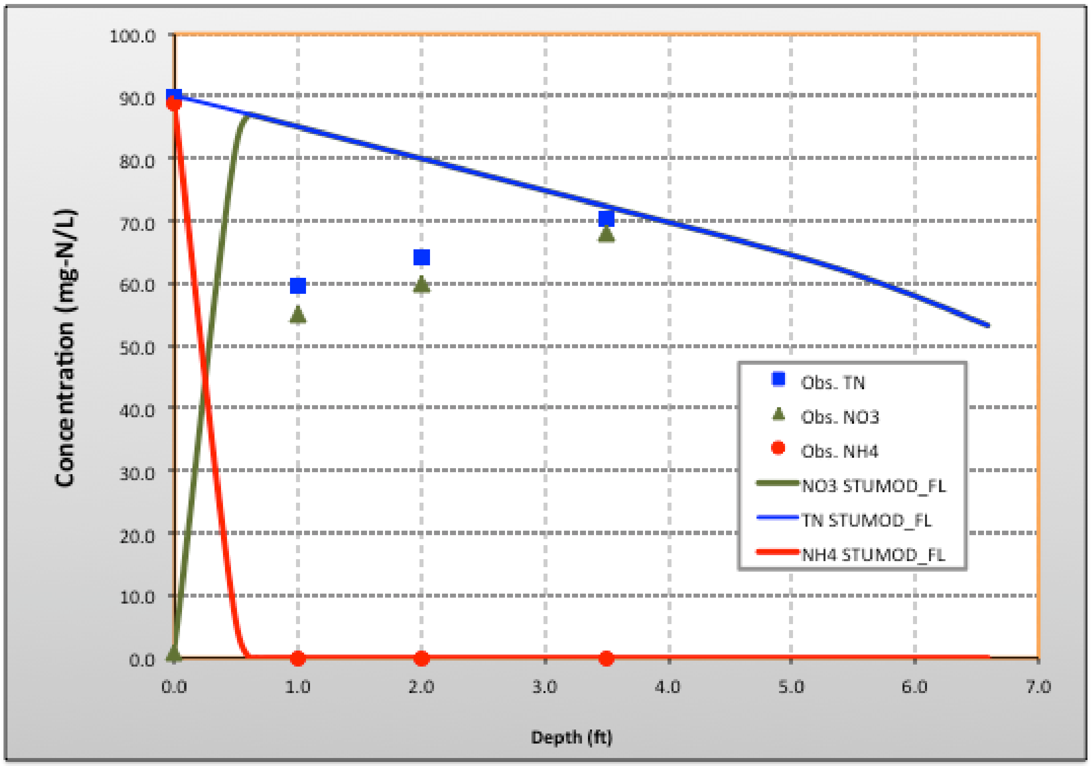

Figure A.2: STUMOD-FL Simulated Concentration with depth for Task C.16 Sample Event No. 2

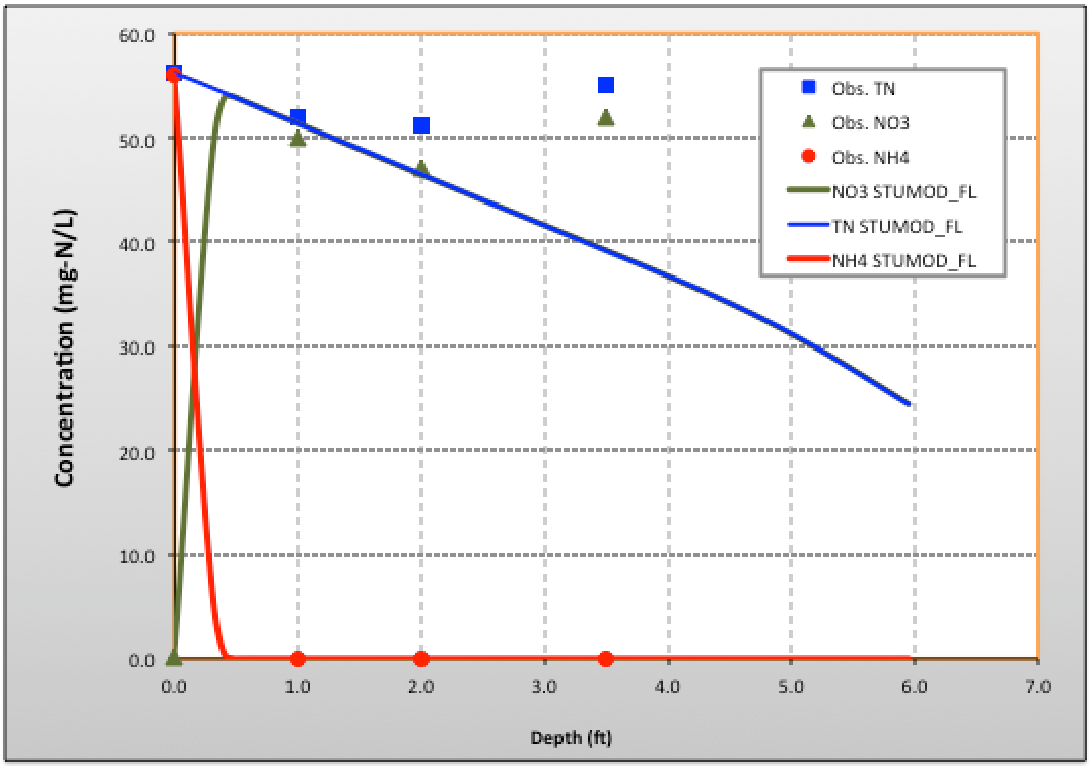

Figure A.3: STUMOD-FL Simulated Concentration with depth for Task C.16 Sample Event No. 3

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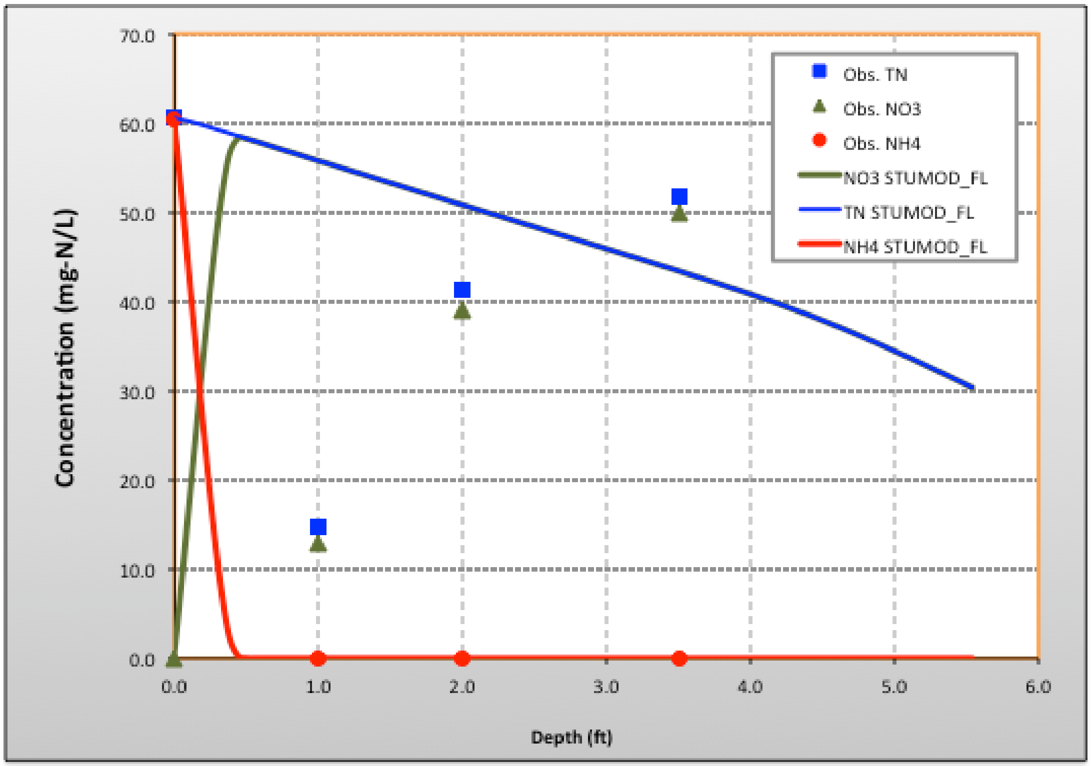

Figure A.4: STUMOD-FL Simulated Concentration with depth for Task C.16 Sample Event No. 4

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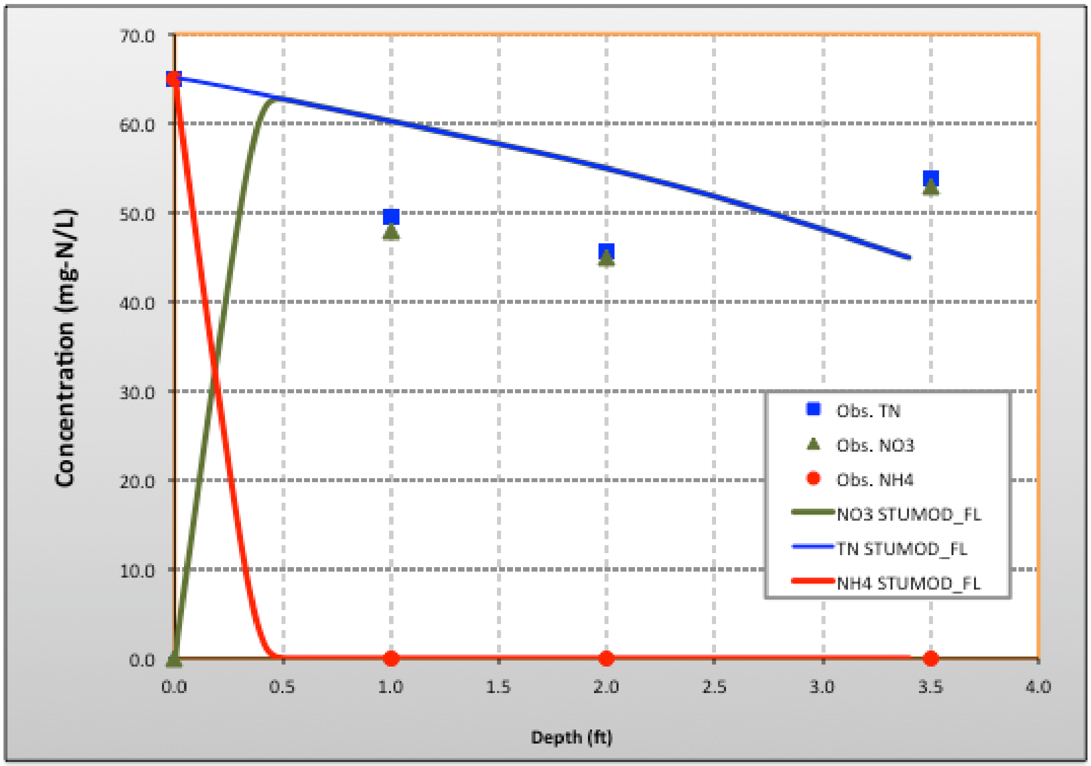

Figure A.5: STUMOD-FL Simulated Concentration with depth for Task C.16 Sample Event No. 5

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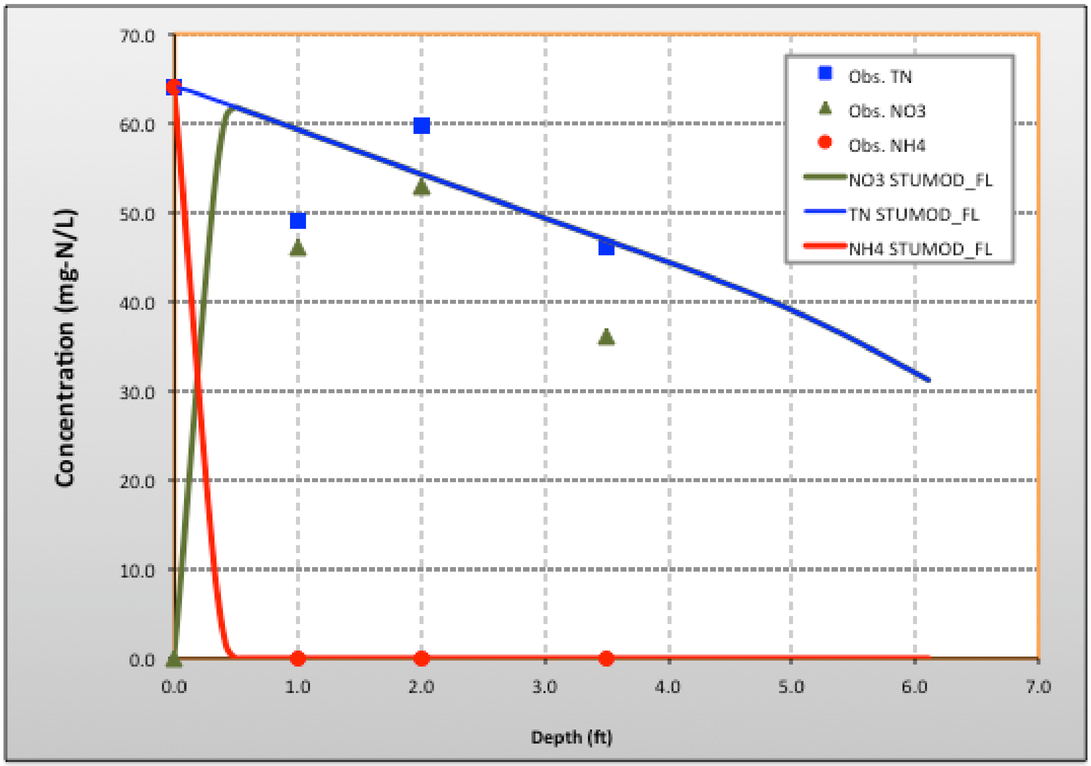

Figure A.6: STUMOD-FL Simulated Concentration with depth for Task C.16 Sample Event No. 6