

VZMOD: A Vadose Zone Model for Simulation of Nitrogen Transformation and Transport

User's Manual

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1 INTRODUCTION

This manual describes the functionality and usage of VZMOD, a Vadose Zone MODEL and python-based software that simulates transformation and one-dimensional (1-D) transport of ammonium and nitrate in vadose zone beneath the drain field of onsite wastewater treatment systems (OWTS), namely septic systems. VZMOD simulates adsorption and nitrification processes of ammonium and denitrification process of nitrate occurring in vadose zone. For each septic system, VZMOD produces vertical profiles of ammonium and nitrate concentrations in vadose zone as well as estimation of nitrate load to groundwater. The conceptual model behind VZMOD is based on simplification of nitrogen fate and transport, which reduces data requirement of the nitrogen modeling and can be easily integrated into a geographic information system (GIS) for ease of data management and pre- and post-processing.

The model is implemented using Python 2.6.5 that is available on any computers with ArcGIS 10 installed. A graphical user interface (GUI) is developed to facilitate the user interaction, in which a point and click approach is used and default values of parameters are provided based on literature.

VZMOD can be operated as a standalone tool to simulate nitrogen transformation and 1-D transport from a single septic system in various soil types. In this mode, VZMOD is independent to any software but Windows platform and installation of Python 2.6.5 on the user's computer.

When being used together with ArcGIS, VZMOD can be used to simulating nitrogen transformation and 1-D transport from multiple septic systems in vadose zone with heterogeneous hydraulic conditions. In this mode, using functions of ArcGIS, VZMOD reads input raster layers of hydraulic conductivity and soil porosity to assign heterogeneous parameters for individual septic system. This feature entails installation of ArcGIS Desktop 10.0 and license of its spatial analysis extension.

When VZMOD is used together with ArcGIS, VZMOD can be used as a pre-processing software for ArcNLET, an ArcGIS-based Nitrate Load Estimation Toolkit (Rios et al., 2011), developed to estimate nitrate load from OWTS to surface water bodies by simulating the fate and transport of nitrate in surficial groundwater aquifers. ArcNLET is a free software and the installation file associated with the documents files can be downloaded from <http://people.sc.fsu.edu/~mye/ArcNLET>. The ArcNLET modeling requires input of nitrate concentration at the water table beneath the drainfields, and this can be provided by VZMOD directly. In addition, VZMOD and ArcNLET share some common ArcGIS layers. The layers include hydraulic conductivity and soil porosity layers that describe the heterogeneity of hydraulic conditions, as well as ArcNLET input layers of DEM and output layer of smoothed DEM.

The focus of this manual is to describe the underlying model of nitrogen transformation and transport as well as the practical usage of the software. Readers of this manual should be familiar with the basics of working with ArcGIS and basic scientific and hydrological terminology.

1.1 Units

The measurement units used in this manual are fixed. The users need to use the units give in Section 3.3 for the model input data and files.

1.2 Organization of the Manual

The structure of the manual is as follows: the manual begins with an abbreviated description of the model of unsaturated flow and the model of nitrogen transformation and transport used in this software (Chapter 2), followed by the installation of the software, description of the VZMOD GUI, explanation of VZMOD input data and files, and organization of VZMOD output files (Chapter 3). Finally, in Chapter 4, an example problem is provided for executing the software and analyzing the modeling results.

1.3 Acronyms and Abbreviations

In this manual, acronyms or terms that are abbreviated are spelled out in full the first time they appear. The following is a list of acronyms and abbreviations used in this manual:

Table 1-1. Abbreviations.

DEM	Digital Elevation Model
DTW	Depth To Water table
GIS	Geographic Information System.
FDEP	Florida Department of Environmental Protection
GUI	Graphical User Interface
NED	National Elevation Dataset
OWTS	Onsite Wastewater Treatment System. A septic tank is an example of an OWTS
SA	Spatial Analyst (extension for ArcGIS)
STU	Soil Treatment Unit
SSURGO	Soil Survey Geographic Database

2 CONCEPTUAL – MATHEMATICAL MODELS

As shown in Figure 2-1, a conventional OWTS has four main components: a pipe from the home (waste water source), a septic tank (pretreatment unit), a drainfield/leachfield, and the soil. Waste water is collected from the source and piped to the septic tank. Pretreatment processes in the septic tank include sedimentation of solids, floatation of oils and greases as well as partial decomposition of the solid materials. The partially treated wastewater is pushed along into the drainfield, where it percolates through the vadose zone down to the ground water (McCray et al., 2010). The soil provides final treatment by removing harmful bacteria, viruses, and nutrients. Suitable soil and vadose zone thickness is necessary for successful wastewater treatment. Understanding the soil treatment processes is critical to design of OWTS and environmental protection of nitrogen contamination to groundwater and surface water bodies.

VZMOD is focused on modeling the treatment processes and transport of nitrogen in the vadose zone. Since this toolkit aims at simulating long-term, vertical migration of OWTS effluent from drainfield in the Soil Treatment Unit (STU) to groundwater, the vadose zone flow and nitrogen transport is assumed to be 1-D in the vertical direction and in steady state. The simplified conceptual-mathematical models of vadose zone flow and transformation and transport of ammonium and nitrate are described in Sections 2.1 – 2.3, followed by the algorithm of numerical solution in Section 2.4. Numerical implementation and flow chart of VZMOD are given in Section 2.5.

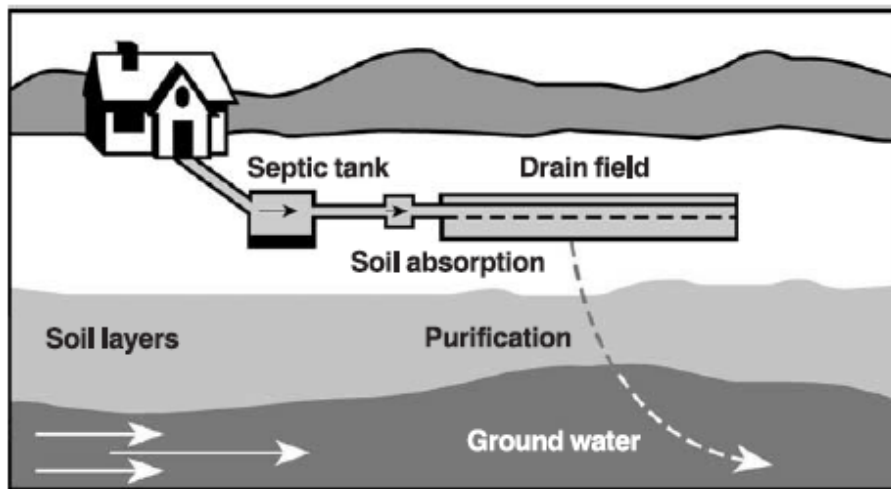


Figure 2-1. Diagram of conventional Onsite Wastewater Treatment System (from National Small Flows Clearinghouse, 2000).

2.1 Unsaturated Flow Model

The steady-state, 1-D vertical water movement in unsaturated porous medium can be described by the Darcy's Law,

$$K \left(\frac{\partial h}{\partial z} + 1 \right) = -q \quad (1)$$

where h is water pressure head [L], z is spatial coordinate [L] (positive upward), q is hydraulic loading rate of the septic system [LT^{-1}], and K is unsaturated hydraulic conductivity function [LT^{-1}]. The van Genuchten-Mualem model (*van Genuchten*, 1980; *Mualem*, 1976) is used to describe the relations between pressure head, moisture content, and degree of saturation:

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \quad (2)$$

$$K(h) = K_s S^l [1 - (1 - S^{1/m})^m]^2 \quad (3)$$

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (4)$$

where K_s is saturated hydraulic conductivity [LT^{-1}], S is degree of saturation [-], θ is volumetric water content [L^3L^{-3}], θ_r and θ_s are residual and saturated water content, respectively, α is inverse of the air-entry value (or bubbling pressure), n is a pore-size distribution index, m equals to $1-1/n$, and l is a pore-connectivity parameter, which usually takes 0.5. In soil sciences, α , n , θ_r , and θ_s are always referred to as soil retention parameters. Soil hydraulic parameters include the soil retention parameters and saturated hydraulic conductivity (K_s).

The upper boundary of the vadose zone is the bottom of drainfield, which is referred to as infiltrative surface hereinafter. It is treated as the constant flux boundary and the flux equals to the hydraulic loading rate (*HLR*) of the septic system. The lower boundary of the vadose zone is the water table, which is treated as the constant pressure head boundary with pressure head equals zero.

In VZMOD, the user inputs *HLR* and soil hydraulic parameters (K_s , α , n , θ_r , and θ_s) in the block of “Hydraulic Params” of the VZMOD graphic user interface (GUI) shown in the next chapter. By solving the nonlinear equations (1 – 4), VZMOD gives the vertical profile of moisture content and degree of saturation; the latter is used for simulating below transformation and transport of ammonium and nitrate.

2.2 Transformation Model of Ammonium and Nitrate

After being discharged to the soil, nitrogen in effluent is primarily inorganic (ammonium and nitrate); organic nitrogen is usually retained in the clogging zone at the infiltration surface of STU (*Heatwole and McCray*, 2007). In the vadose zone transport process, ammonium is subject to nitrification and nitrate to denitrification. During nitrification, ammonium-nitrogen is transformed to nitrite- and nitrate-nitrogen through biological aerobic oxidation by specific autotrophic microbes, *Nitrosomonas* and *Nitrobacter*. Using oxygen as a terminal electron acceptor, *Nitrosomonas* oxidizes ammonium-nitrogen to nitrite-nitrogen, and *Nitrobacter* converts nitrite-nitrogen to nitrate-nitrogen. The nitrification process usually occurs relatively fast in STU, and

complete nitrification usually occurs in the first 30 cm of STU (Fischer, 1999; Beach, 2001). Thus, nitrate is generally the pollutant of concern for OWTS systems.

Denitrification is a microbially facilitated process of nitrate reduction, a mechanism of nitrogen removal in STU. Denitrification is the reduction of nitrate through the intermediates nitrite, perhaps nitric oxide, and nitrous oxide to form dinitrogen gas returning to the atmosphere. This respiratory process reduces oxidized forms of nitrogen in response to the oxidation of an electron donor such as organic matter. In the order of most to least thermodynamically favorable, the preferred nitrogen electron acceptors are nitrate, nitrite, nitric oxide, and nitrous oxide. Complete denitrification in most STU does not occur (Heatwole and McCray, 2007). Because denitrification rates are usually significantly smaller than nitrification rates in natural soils, denitrification is the limiting reaction for nitrogen removal in STU.

The nitrification and denitrification processes can be modeled as either zero-order reactions (Yamaguchi et al., 1996; Anderson, 1998; Korom et al., 2005; Heatwole and McCray, 2007) or first-order (Kirda et al., 1974; Misra et al., 1974a,b,c; Yamaguchi et al., 1996). McCray et al., (2005) and Tucholke (2007) suggested modeling denitrification as the zero-order process at higher nitrate concentrations and first-order at lower concentrations. In VZMOD, the first-order nitrogen transformation is used, but the code can be extended to include the zero-order transformation. Considering effects of temperature and soil saturation on the rates, the first-order reactions of nitrification and denitrification are

$$\frac{\partial[NH_4^+]}{\partial t} = -k_{nit} f_{t,nit} f_{sw,nit} [NH_4^+] \quad (5)$$

$$\frac{\partial[NO_3^-]}{\partial t} = k_{nit} f_{t,nit} f_{sw,nit} [NH_4^+] - k_{dnt} f_{t,dnt} f_{sw,dnt} [NO_3^-] \quad (6)$$

where k_{nit} and k_{dnt} are the maximum first-order reaction rates of nitrification and denitrification, respectively. The two parameters are specified in the blocks of “Nitrification Params” and “Denitrification Params” of the VZMOD GUI shown in the next chapter. The actual reaction rates are adjusted by temperature function, f_t , and saturation function, f_{sw} , to account for the effect of temperature and soil saturation on the reaction rates. These functions, defined below, are first used in software DRAINMOD-N2 (Skaggs, 1978; Youssef et al., 2005) and also in STUMOD (McCray et al., 2010).

The nitrification and denitrification rates are functions of temperature. As shown in Figure 2-2, the function is a Gaussian-type bell curve. For both nitrification and denitrification, the temperature function, f_t (between 0 and 1),

$$f_t = \exp \left[-0.5\beta T_{opt} + \beta T \left(1 - \frac{0.5T}{T_{opt}} \right) \right] \quad (7)$$

has the same form (McCray et al., 2010), where T is temperature, T_{opt} is the optimum temperature for nitrification or denitrification, and β is a fitting parameter. According to this function, the peak of the f_t curve (Figure 2-2) occurs at the optimum temperature (T_{opt}) and the width is determined by β .

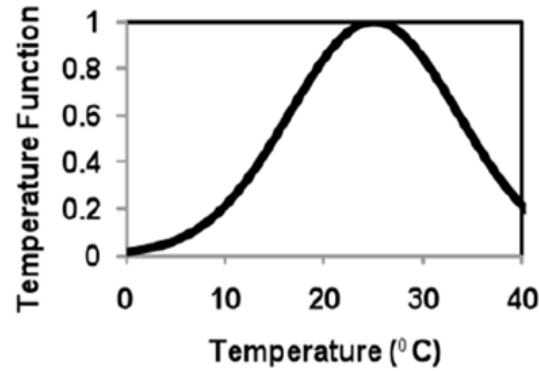


Figure 2-2. Illustration of temperature function of nitrification and denitrification (from McCray et al., 2010).

In VZMOD, the temperature function is calculated using equation (7) for nitrification and denitrification processes separately. The calculation uses parameters $T_{opt-nit}$ and β_{nit} for nitrification and $T_{opt-dnt}$ and β_{dnt} for denitrification. Parameter T is specified in the block of “Temperature Param” of the VZMOD GUI shown in the next chapter; $T_{opt-nit}$ and β_{nit} are specified in the block of “Nitrification Params” and $T_{opt-dnt}$ and β_{dnt} in “Denitrification Params”.

The actual rates of nitrification and denitrification are also functions of soil saturation, since the saturation affects diffusion of oxygen into soil pores. The solid line in Figure 2-3 shows the diagram of the saturation function for nitrification. As nitrification is an aerobic process, it is not likely that nitrification will occur in nearly saturated soils due to limited oxygen supply (McCray et al., 2010). On the other hand, when the degree of saturation is low, because connection of wetted soil pores is poor, diffusion of ammonium and aqueous CO_2 between soil pores is limited. In other words, nitrification is limited or prohibited by low saturation limits (McCray et al., 2010). Optimal nitrification occurs between the low and high degrees of saturation. The saturation function, $f_{sw,nit}$ (between 0 and 1), is defined as (McCray et al., 2010)

$$f_{sw,nit} = \begin{cases} f_s + (1 - f_s) \left(\frac{1 - S}{1 - S_h} \right)^{e_2} & S_h < S \leq 1 \\ 1 & S_l \leq S \leq S_h \\ f_{wp} + (1 - f_{wp}) \left(\frac{S - S_{wp}}{S_l - S_{wp}} \right)^{e_3} & S_{wp} \leq S \leq S_l \end{cases} \quad (8)$$

where f_s is the value of $f_{sw,nit}$ at full saturation, f_{wp} and S_{wp} are the value of $f_{sw,nit}$ and degree of saturation at wilting point, S_l and S_h are the lower and upper saturation boundaries, respectively, for optimal nitrification, and e_2 and e_3 are fitting exponent parameters. In VZMOD, the degree of saturation, S , is computed in the flow model, and f_s , f_{wp} , S_{wp} , S_l , S_h , e_2 , and e_3 are input parameters specified in the block “Nitrification Params” in the VZMOD GUI shown in the next chapter.

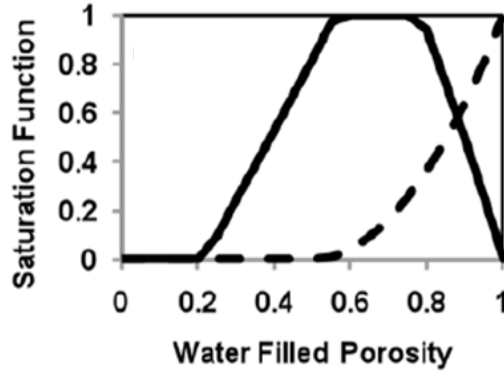


Figure 2-3. Illustration of saturation functions for nitrification (solid) and denitrification (dashed). The figure is from McCray et al. (2010).

Unlike nitrification, denitrification takes place under anaerobic conditions. As shown in the dashed line in Figure 2-3, after a threshold saturation value, the saturation function of denitrification increases with the degree of saturation, because higher degree of saturation leads to more anaerobic conditions and enhances denitrification. The saturation function of denitrification, $f_{sw,dnt}$ (between 0 and 1), is defined as (McCray et al., 2010)

$$f_{sw,dnt} = \begin{cases} 0 & S < S_{dnt} \\ \left(\frac{S - S_{dnt}}{1 - S_{dnt}}\right)^{e_1} & S \geq S_{dnt} \end{cases} \quad (9)$$

where S_{dnt} is a threshold value of degree of saturation for denitrification, and e_1 is a fitting exponent parameter. The two parameters are inputs through the block of “Denitrification Params” in VZMOD GUI shown in the next chapter.

While pH and organic carbon are commonly considered to impact nitrification and denitrification rates, they are not considered in this study for the reasons below:

- (1) Nitrification process produces acid and low pH can cause a reduction of the growth rate of nitrifying bacteria. The optimum pH for Nitrosomonas and Nitrobacter of nitrification is between 7.5 and 8.5; nitrification stops at a pH below 6.0. According to McCray et al. (2010), since the pH (7.1 to 7.7) of septic tank effluent is normally at the optimum level, it is reasonable to ignore the effect of pH on nitrification.
- (2) Denitrification is an alkalinity producing process, and it can partially mitigate the effect of lowering pH caused by nitrification. Optimum pH values for denitrification are between 7.0 and 8.5. Because the microbes responsible for denitrification are very tolerant and adaptable to environmental changes, the pH of the effluent is not of primary importance to the denitrification (McCray et al., 2010). Therefore, pH is assumed not to be a restraint factor of denitrification in this study.
- (3) Organic carbon is another factor that affects denitrification. Since organic carbon can be found both in the septic tank effluent and natural soil, it is assumed in this study that organic carbon is not a restraint factor.

2.3 Transport Model of Ammonium and Nitrate

Assuming that sorption of ammonium to soils follows the linear isotherm, the coupled steady-state advection – dispersion equations for 1-D, vertical transport of ammonium and nitrate are

$$D \frac{\partial^2 C_{NH4}}{\partial z^2} - \frac{q}{\theta} \frac{\partial C_{NH4}}{\partial z} - k_{nit} f_{t,nit} f_{sw,nit} \left(1 + \frac{\rho k_d}{\theta} \right) C_{NH4} = 0 \quad (10)$$

$$D \frac{\partial^2 C_{NO3}}{\partial z^2} - \frac{q}{\theta} \frac{\partial C_{NO3}}{\partial z} + k_{nit} f_{t,nit} f_{sw,nit} \left(1 + \frac{\rho k_d}{\theta} \right) C_{NH4} - k_{dnt} f_{t,dnt} f_{sw,dnt} C_{NO3} = 0 \quad (11)$$

where C_{NH4} and C_{NO3} are concentrations of ammonium and nitrate, respectively, D is dispersion coefficient [L^2T^{-1}], ρ is soil bulk density [ML^{-3}], k_d is distribution coefficient of linear adsorption [$M^{-1}L^3$]. The last term at the left hand side of equation (10) indicates that nitrification occurs for the adsorbed ammonium; similarly, the last term at the left hand side of equation (11) is to account for the denitrification process. The value of D is specified in the block of “Transport Param” and the values of ρ , and k_d are in “Adsorption Params” in the VZMOD GUI shown in the next chapter.

The upper boundary of the vadose zone (i.e., infiltrative surface) is treated as the constant mass flux boundary, and the flux equals the mass loading rate of nitrate and ammonium calculated by multiplying nitrate and ammonium concentrations in septic tank effluent by hydraulic loading rate. The concentrations are specified in the block of “Effluent Params” of the VZMOD GUI shown in the next chapter, and mass flux is calculated in the VZMOD code. The lower boundary of the vadose zone is the water table, and the boundary condition is zero concentration gradient for transport model.

2.4 Algorithms of Numerical Solutions

The vadose zone flow and solute transport equations are solved numerically in VZMOD. The modeling domain from infiltrative surface to water table is discretized into $N = 100$ (the number is hardcoded in VZMOD) adjoining elements with $N + 1$ nodes; node 1 is at the top boundary and node $N + 1$ at the bottom boundary. Following HYDRUS-1D (Simunek et al., 2009), the mass-lumped linear finite elements scheme is used for discretization of the Darcy equation (equation 1). This results in the following discrete equation,

$$\frac{K(h_i) + K(h_{i+1})}{2} \times \left[\frac{h_i - h_{i+1}}{\Delta z} + 1 \right] = -q \quad (12)$$

for element i , where subscripts i and $i + 1$ are indices of finite element nodal points. Given that the bottom boundary is the water table, $h_{N+1} = 0$. With this condition, h_N can be solved by virtue of equation 12. In the same manner, pressure head at nodes $N - 1$ to 1 are solved. For solving the transport equations 10 and 11, the Galerkin finite element method of HYDRUS-1D (Simunek et al., 2009) is used and the details of the algorithm are referred to the manual of HYDRUS-1D. The numerical solutions may subject to numerical oscillation and dispersion. This can be resolved by using advanced numerical techniques (e.g., higher-order TVD method), which however have not been implemented in the current version.

2.5 Design of VZMOD and Python Implementation

Figure 2-4 is the flow chart of VZMOD. The first step is to read the parameters of flow and nitrogen transformation and transport for a given soil type. If VZMOD is used for a single septic system, these parameters will be used to solve the flow and transport equations sequentially, and the concentration profiles are saved for post-processing.

If VZMOD is used for multiple septic systems at a neighborhood scale, ArcGIS layers are needed to take into account of spatial variability of septic tanks, hydraulic conductivity, porosity, and depth to water table (DTW). As shown in Figure 2-4, three ArcGIS layers of OWTS locations, DEM raster, and Smoothed DEM Raster are used to calculate DTW. The calculation procedure is given in the next chapter. The next step is to determine whether homogeneous or heterogeneous hydraulic conductivity (K_s) and porosity (θ_s) are used. The homogenous parameter values are those read from VZMOD GUI when VZMOD is used for a single OWTS. The heterogeneous data are extracted from the Hydraulic Conductivity Raster and Soil Porosity Raster to the locations of OWTS. After this, VZMOD solves the flow and transport models for each individual OWTS until all the OTWS are calculated.

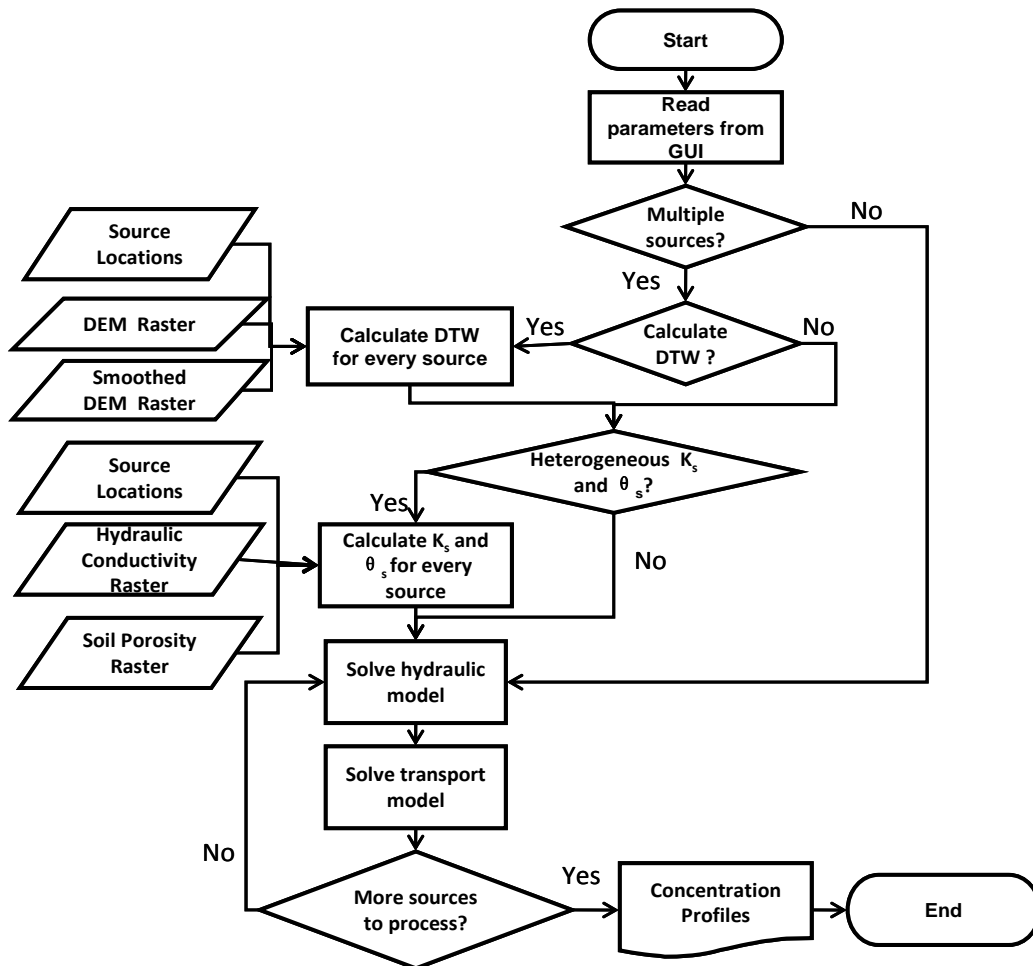


Figure 2-4. Flowchart of VZMOD.

The flowchart is implemented using the Python programming language, which is selected because it is free and compatible of crossing different computer platforms. More importantly, Python has been used as a scripting language by ESRI in ArcGIS 10 geoprocessing. Using the ArcPy site-package of ArcGIS 10, geoprocessing functionality is accessible through Python. This is critical to the functionality of VZMOD that uses GIS data to address spatial variability of VZMOD components, such as hydraulic parameters, septic tank locations, and water table.

3 USAGE

This chapter describes installation, graphic user interface, and execution of VZMOD. An example of “Run”ning the software is given in the next chapter.

3.1 System Requirement and Installation

In order to use the software, the following is required:

- (1) A Microsoft Windows computer (32 or 64 bit) that meets the minimum requirements for ArcGIS 10.0
- (2) ArcGIS 10.0 with Python 2.6.5 and Spatial Analyst extension

While “Run”ning VZMOD does not require installation of ArcNLET, ArcNLET may be needed to prepare input files of VZMOD. Therefore, it is recommended to install ArcNLET before using VZMOD.

Installation of VZMOD is not needed. After downloading the zip file, VZMOD.zip, from the software release website, extract the VZMOD.zip into a folder wherever you want to “Run” VZMOD. By double clicking the file VZMOD.pyw, the GUI of VZMOD will pop up. If the pop-up does not occur, one can open the GUI using pythonw.exe (version 2.6.5) included in ArcGIS 10.0. When multiple versions of Python are installed on a computer, it may cause error to open the VZMOD.pyw file by pythonw.exe of Python version 2.6.5. When this happens, one can open VZMOD.pyw in command window by typing “*path1/python path2\VZMOD.pyw*” after the prompt, where *path1* is the path where Python 2.6.5 is installed and *path2* is the path where VZMOD.pyw is. When ArcGIS 10.0 is installed, the default path of Python 2.6.5 is “*C:\Python26\ArcGIS10.0*”.

3.2 Graphic User Interface and Execution

Figure 3-1 is the GUI after launching the program by opening “VZMOD.pyw” using Python. We will give descriptions of the input parameters and data files in the sections below; in this section, we explain the three process control buttons: “Run”, “Check Results”, and “Quit”. After all input parameters and data files are specified through the GUI, by clicking the “Run” button, the program begins to execute. During the execution, if it is for a single septic system, calculated concentrations of ammonium and nitrate at discretized *z* coordinates are displayed in the window above the “Run” button at the right-most block of the GUI. Otherwise, this block displays only the index of septic system (FID) that is being processing.

After the execution is completed, by clicking the “Check Results” button, a new window will pop up that plots the calculated concentration profiles of ammonium and nitrate. Figure 3-2 is an example of the plot for a single septic system for clay soil texture with default parameters. If VZMOD is executed for multiple septic systems at a neighborhood scale (the feature will be discussed in the next section), concentration profiles of individual septic systems can be plotted by changing the FID of the septic systems at the top of pop-up window and then clicking the “OK” button shown in Figure 3-2. After simulation is completed, the GUI can be closed by clicking the “Quit” button.

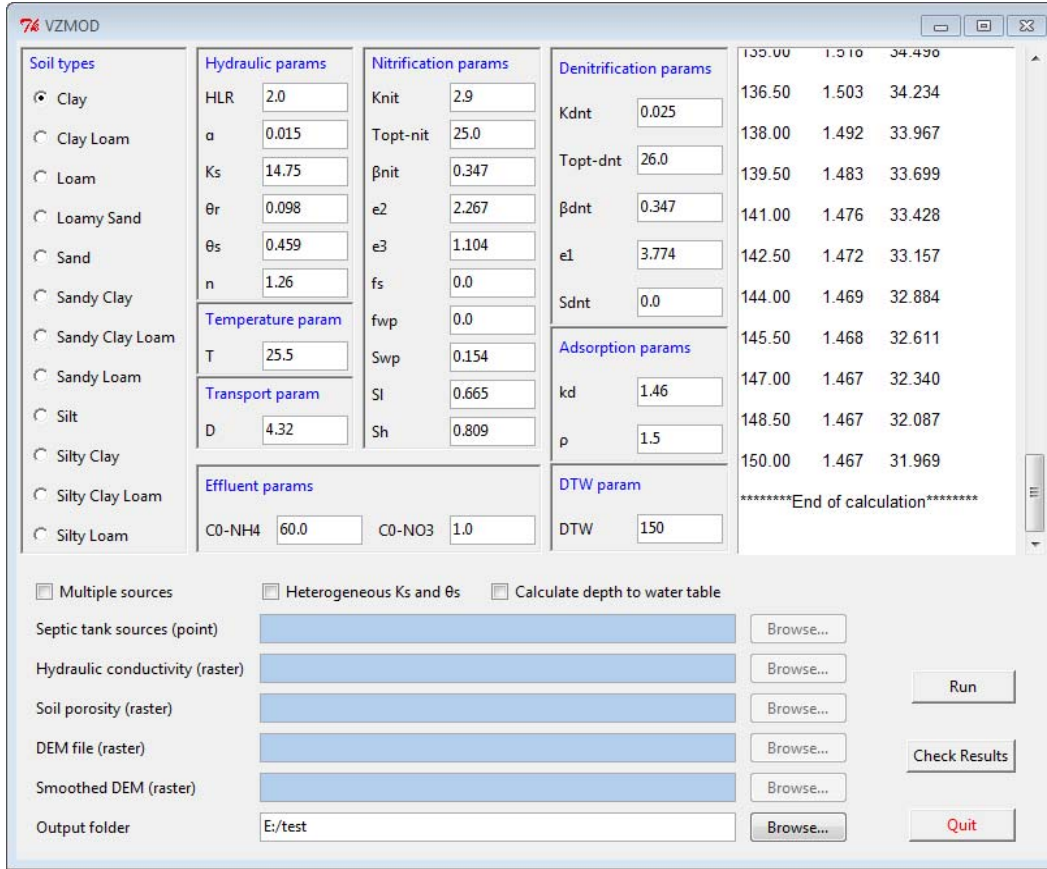


Figure 3-1. Graphic user interface (GUI) of VZMOD user interface. The input parameter values are default for clay soil adopted from McCray et al. (2010), and the output values at the right-most panel are concentrations of ammonium and nitrate for a single septic system.

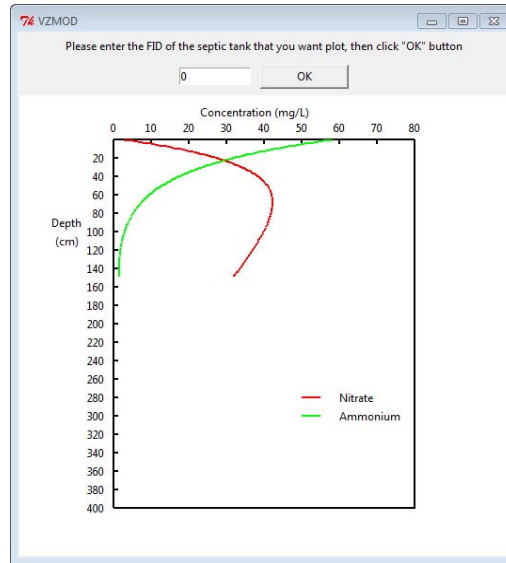


Figure 3-2. Plot of calculated concentration profiles of ammonium and nitrate for clay soil texture with default parameters.

3.3 Model Inputs and Outputs

This section explains the input data and files shown on the VZMOD GUI (Figure 3-1) and the outputs for plotting and post-processing.

3.3.1 Model Input Data

The VZMOD GUI has two segments for model inputs. The first one is for input data of model parameters; the second one is for input files that used to address the spatial variability of hydraulic conductivity, soil porosity and Depth To Water table (DTW).

Table 3-1 lists the input parameters of VZMOD, their units required for the simulation, and descriptions of the parameters. Based on an extensive literature review, McCray et al. (2005, 2010) provided in STUMOD default values of hydraulic parameters, temperature parameters, nitrification parameters, effluent parameters, denitrification parameters, and adsorption parameters. The default values are used in VZMOD except that the values of the first-order reaction rate of nitrification (K_{nit}) and denitrification (K_{dnt}) are from McCray et al. (2005). In addition, the value of dispersion coefficient (D), temperature (T) and depth to water table (DTW) are given arbitrarily, since they are site-specific. In other words, users should specify appropriate D , T and DTW values to the sites of their interest. The hydraulic parameters, the coefficient, e_l , of saturation function of denitrification, and the coefficient, k_d , of adsorption are specific to soil types, other parameters are the same for different soil types. Note that the default parameters are just provided as a reference and users of VZMOD are responsible of determining appropriate values for their nitrogen modeling.

3.3.2 Model Input Files

The above model input data are sufficient when “Run”ning VZMOD for a single septic system. When using VZMOD for multiple septic systems at the neighborhood scale, more input files are needed to address spatial variability of hydraulic conductivity, soil porosity, and depth to water table. These files are ArcGIS files and can be used by both VZMOD and ArcNLET. Instructions for preparing the files are referred to the ArcNLET user manual (Rios et al., 2011). Table 3-2 lists the units of data in the input files.

What input files are needed depends on the functions of VZMOD selected by the user, and this has been automated in VZMOD. When VZMOD is used for modeling multiple septic systems, the user needs to check the box of “Multiple sources”. This activates the other two options of “Heterogeneous K_s and θ_s ” and “Calculate depth to water table” as well as the file input box of “Septic tank source (point)” to select a GIS point layer that specifies the locations of the contaminant sources (a.k.a the locations of drainfields). The user can use the two options of “Heterogeneous K_s and θ_s ” and “Calculate depth to water table” either separately or jointly.

Table 3-1. Input parameters of VZMOD, their required units, and descriptions.

Parameter	Unit	Description
Hydraulic parameters		
HLR	cmd ⁻¹	Hydraulic loading rate
α	-	Parameter of van Genuchten water retention function
Ks	cmd ⁻¹	Saturated hydraulic conductivity
θ_r	-	Residual moisture content
θ_s	-	Saturated moisture content
n	-	Parameter n of van Genuchten water retention function
Temperature parameters		
T	°C	Soil temperature
Transport parameters		
D	cm ² d ⁻¹	Dispersion coefficient
Nitrification parameters		
Knit	d ⁻¹	Maximum first-order nitrification rate
Topt-nit	°C	Optimum soil temperature for nitrification
e2	-	Empirical coefficient for saturation function of nitrification
e3	-	Empirical coefficient for saturation function of nitrification
β_{nit}	-	Empirical coefficient for temperature function of nitrification
fs	-	Saturation function of nitrification at full saturation
fwp	-	Saturation function of nitrification at wilting point
Swp	-	Degree of saturation at wilting point
Sl	-	Lower limit of relative saturation for nitrification
Sh	-	Upper limit of relative saturation for nitrification
Effluent parameters		
C0-NH4	mgL ⁻¹	Effluent concentration of ammonium-nitrogen
C0-NO3	mgL ⁻¹	Effluent concentration of nitrate-nitrogen
Denitrification parameters		
kdnt	d ⁻¹	Maximum first-order denitrification rate
Topt-dnt	°C	Optimum soil temperature for denitrification
e1	-	Empirical coefficient for saturation function of denitrification
β_{dnt}	-	Empirical coefficient for temperature function of denitrification
Sdn	-	Threshold degree of saturation for denitrification
Adsorption parameters		
kd	cm ³ g ⁻¹	Distribution coefficient describes adsorbed concentrations
ρ	gcm ⁻³	Soil bulk density
Depth to water table (DTW) parameters		
DTW	cm	Depth from infiltrative surface to water table

If “Heterogeneous K_s and θ_s ” is checked, the parameters K_s and θ_s in the block of “Hydraulic Params” above will be disabled and two boxes of “Hydraulic conductivity (raster)” and “Soil porosity (raster)” will be activated. The two boxes are used to input raster ArcGIS layers of heterogeneous saturated hydraulic conductivity and soil porosity

(approximately equals to saturated water content). The two files are also ArcNLET input files and can be generated base on soil survey data such as the SSURGO Database, instructions of which can be found in the application manual of ArcNLET (Wang et al., 2011).

Table 3-2. VZMOD input files and units of corresponding input data.

Input Files	Unit
Hydraulic conductivity	md ⁻¹
Soil porosity	-
DEM	m
Smoothed DEM	m

If “Calculate depth to water table” is checked, the user needs to input two raster GIS layers through the boxes of “DEM (raster)” and “Smoothed DEM (raster)”. This function calculates the depth from infiltrative surface to water table for every septic system. The DEM raster file is the same as that used as input of ArcNLET to generate an approximation to the water table by assuming that the water table is a subdued replica of topography. The smoothed DEM is the output raster file after smoothing the topography (DEM), and assumed to have the same shape of groundwater table. In other words, the smoothed DEM is assumed to be parallel to the water table. Based on this assumption and using the two files, the distance from the infiltrative surface to water table (DTW) for individual septic system can be calculated in the following procedure:

- (1) Calculate the elevation of water table by subtracting a constant (denoted as A) from the smoothed DEM, i.e., (Smoothed_DEM – A). This constant is the distance between the smoothed DEM and the water table. It can be estimated from field measurements of water level in monitoring wells. This requires first calibrating the smoothing factor of ArcNLET in the manner of Wang et al. (2011) described in Section 4.2 of the ArcNLET application manual. After the calibration, one needs to plot the measured water level and smoothed DEM as in Figure 3-3, which is adopted from Section 4.3 of Wang et al. (2011). By fitting a linear regression curve between the measured water level and smoothed DEM, the intercept of the linear curve is the value of A. In Figure 3-3, the A value is 2.86m.
- (2) Calculate the elevation of the infiltrative surface by subtracting the distance of the infiltrative surface to land surface (denoted as B) from the thickness of vadose zone, i.e., (DEM – B). One choice of B is 18 inches, because the drainfield is about 12 inches thick (for gravel) covered by 6 inches of soil (USEPA, 2002).
- (3) The distance from infiltrative surface to water table is calculated via $(DEM - B) - (Smoothed_DEM - A) = DEM - Smoothed_DEM + (A - B)$.

The user needs to input the value of A – B ([cm]) through the GUI in the box of “Distance”, which is at the same position of “DTW” in the GUI when VZMOD is used for a single septic system.

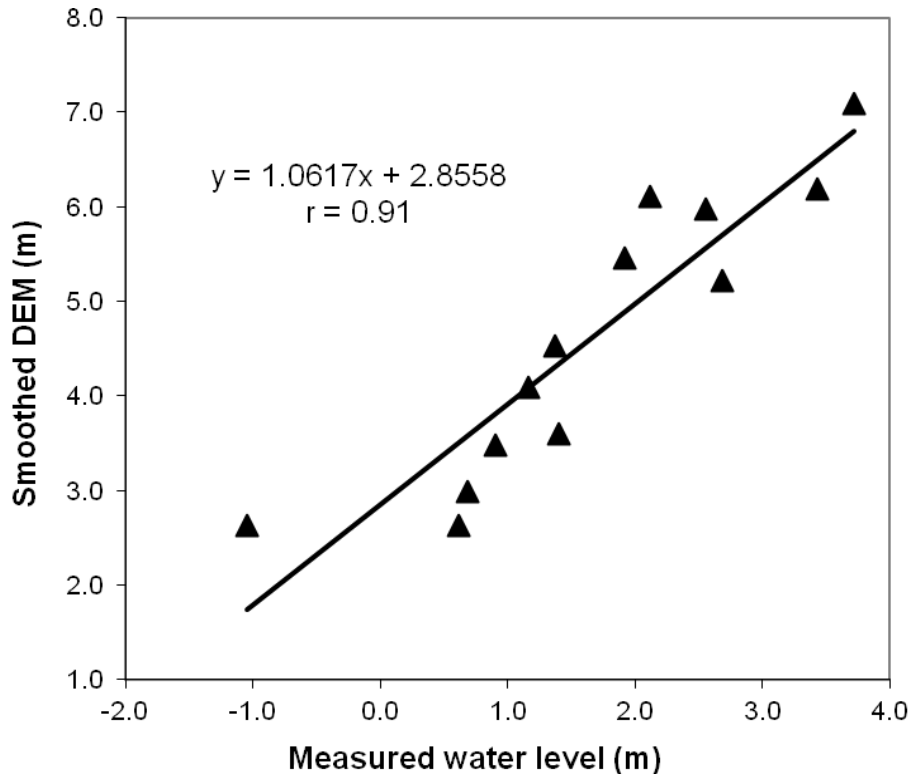


Figure 3-3. Linear regression curve between measured water level and smoothed DEM of Julington Creek neighborhood.

3.3.3 Model Outputs

The output files are saved in the folder specified by the users at the bottom of the GUI, in the box of “Output folder”. The output folder should already exist; otherwise VZMOD will raise an error and stop running. Note that the output file names are not specified by the users but hardwired by VZMOD. If the output folder is not empty, when a new simulation is completed, the old output files will be replaced by the new output files.

In addition to the plot of concentration profiles generated by clicking the “Check Results” button in the GUI, VZMOD outputs a text file called “result.txt”. First several lines of file are shown in Figure 3-4. The “Depth” column is the depth below bottom of the drainfield (cm); the “CNH4” and “CNO3” columns are the calculated concentrations of ammonium and nitrate, respectively. When VZMOD is used at the neighborhood scale with multiple septic systems, this concentration data will repeat for every septic system with a line that “Calculating for septic tank X...” added to the beginning of each data segment, where X is the FID of the septic systems starting with zero. This file is stored in the user specified output folder.

Depth	CNH4	CNO3
0.00	58.271	2.709
1.50	55.682	5.255
3.00	53.208	7.667
4.50	50.844	9.952
6.00	48.585	12.115
7.50	46.426	14.162
9.00	44.363	16.099
10.50	42.392	17.929
12.00	40.509	19.659
13.50	38.709	21.292
15.00	36.990	22.833
16.50	35.347	24.287
.	.	.
.	.	.
.	.	.

Figure 3-4. Illustration of first several lines of model output file “result.txt” generated for clay soil with default parameters and a single septic tank.

If “Multiple sources” is checked, a new ArcGIS point layer will be output. The name of the layer file is hardwired as “Septictank”. These new files are the same as the input “Septic tank source (point)” file except that a new field named “NO_Conc” is added to the attribute table. This “NO_Conc” field stores the simulated nitrate concentration at groundwater table for every septic system. This updated septic tank source file can be used directly as input of ArcNLET. The new GIS point layer will also be stored in the user specified output folder.

If “Heterogeneous Ks and θs” is checked, the program outputs a table of .dbf format named “table1” in the user specified output folder. As shown in Figure 3-5, the table stores the x- and y-coordinate of each septic tank as well as hydraulic conductivity and porosity in fields “HYDRAU_CON” and “POROSITY”, respectively. The data of hydraulic conductivity and porosity are read from the input “Hydraulic conductivity (raster)” file and “Soil porosity (raster)” file. This table is an intermediate output file and can be used by the user to analyze modeling results if needed. For example, this table reveals directly which septic systems are associates with high or low hydraulic conductivity.

If “Calculate depth to water table” is checked, the program outputs a table of .dbf format named “table2” in the user specified output folder. As shown in Figure 3-6, the table stores the x- and y-coordinate of each septic tank as well as DEM and smoothed DEM values in fields “DEM” and “SMOOTHEDDEM”, respectively. The values are read from the input “DEM (raster)” file and “Smoothed DEM (raster)” file. This table is an intermediate output file and can be used by the user to analyze modeling results if needed, because the concentration profile is a function of water depth and vadose zone thickness.

Rowid	MASK	X	Y	HYDRAU_CON	POROSITY
1	0	445250.818374	3334112.399259	18.934	0.41
2	1	445817.924663	3334112.728585	18.934	0.41
3	2	445758.598272	3334109.743748	18.934	0.41
4	3	445447.696886	3334102.273309	18.934	0.41
5	4	445717.586986	3334108.073562	18.934	0.41
6	5	445613.558862	3334093.962628	18.934	0.41
7	6	445409.950621	3334095.368386	18.934	0.41
8	7	446025.069374	3334093.55842	18.934	0.41
9	8	445818.744467	3334094.498816	18.934	0.41
10	9	445310.606538	3334092.388541	18.934	0.41
11	10	445353.48364	3334090.03053	18.934	0.41
12	11	445759.156925	3334091.532543	18.934	0.41
13	12	445433.66489	3334019.046067	18.934	0.41
14	13	445659.504109	3334030.83846	18.934	0.41
15	14	445188.343185	3334021.358057	18.934	0.41
16	15	445105.372103	3334018.548725	18.934	0.41
17	16	444996.411581	3334018.043113	18.934	0.41
18	17	444969.299686	3334017.178536	18.934	0.41
19	18	445042.831393	3333847.892412	8.48558	0.41
20	19	445213.585832	3333849.404566	8.48558	0.41
21	20	445768.332808	3333854.530723	18.934	0.41
22	21	445504.289762	3334093.8333	18.934	0.41

Figure 3-5. Illustration of “table1”, an intermediate output file of VZMOD.

Rowid	MASK	X	Y	SMOOTHEDDEM	DEM
1	0	445250.818374	3334112.399259	7.120416	8.185451
2	1	445817.924663	3334112.728585	5.992364	6.935652
3	2	445758.598272	3334109.743748	6.363541	7.5381
4	3	445447.696886	3334102.273309	7.238687	8.458047
5	4	445717.586986	3334108.073562	6.657873	7.306192
6	5	445613.558862	3334093.962628	6.943382	7.980749
7	6	445409.950621	3334095.368386	7.24467	8.314847
8	7	446025.069374	3334093.55842	3.607407	4.162064
9	8	445818.744467	3334094.498816	5.784418	6.888103
10	9	445310.606538	3334092.388541	7.147075	8.017777
11	10	445353.48364	3334090.03053	7.184652	8.123905
12	11	445759.156925	3334091.532543	6.245862	7.356498
13	12	445433.66489	3334019.046067	6.82016	8.143971
14	13	445659.504109	3334030.83846	6.417183	7.628976
15	14	445188.343185	3334021.358057	6.499188	8.054298
16	15	445105.372103	3334018.548725	6.187036	8.095702
17	16	444996.411581	3334018.043113	5.640224	7.882704
18	17	444969.299686	3334017.178536	5.534324	7.603837
19	18	445042.831393	3333847.892412	4.322984	5.250447
20	19	445213.585832	3333849.404566	5.030952	6.815746
21	20	445768.332808	3333854.530723	4.454371	5.503631
22	21	445504.289762	3334093.8333	7.150463	7.026293

Figure 3-6. Illustration of “table 2”, an intermediate output file of VZMOD.

The modeling scenarios of VZMOD are summarized in Table 3-3 with inputs and outputs in different scenarios. This table can be used as a quick reference for the reader for “Run”ning VZMOD.

Table 3-3. Model inputs and outputs for different modeling scenarios of VZMOD.

Modeling Scenarios		Options	Inputs	Outputs
Single septic system			All parameters in the user interface	result.txt
Multiple septic systems	Heterogeneous hydraulic conductivity and soil porosity	(1) Multiple source (2) Heterogeneous K_s and θ_s	(1) All the parameters in the user interface except for K_s and θ_s ; (2) Source location; (3) Hydraulic conductivity; (4) soil porosity;	(1) result.txt; (2) source location with “N0_Conc” field; (3) table1.dbf
	Heterogeneous depth to water table	(1) Multiple source (2) Calculate depth to water table	(1) All the parameters in the user interface except for changing <i>DTW</i> to <i>Distance</i> (2) Source location; (3) DEM; (4) smoothed DEM;	(1) result.txt; (2) Source location with “N0_Conc” field; (3) table2.dbf
	Heterogeneous hydraulic conductivity, soil porosity, and depth to water table	(1) Multiple source (2) Heterogeneous K_s and θ_s (3) Calculate depth to water table	(1) All the parameters in the user interface except for K_s and θ_s and changing DTW to Distance (2) Source location; (3) Hydraulic conductivity; (4) Soil porosity; (5) DEM; (6) Smoothed DEM;	(1) result.txt; (2) Source location with “N0_Conc” field; (3) table1.dbf (4) table2.dbf

3.3.4 “Run” VZMOD for Multiple Soil Types

When multiple soil types exist for a modeling domain, the users need to “Run” VZMOD for each soil type separately in the following procedure:

- (1) Prepare ArcGIS files of septic tank sources for each soil type outside of VZMOD. The soil types can be obtained from the SSURGO database, and an example is given in the next chapter.
- (2) Generate ArcGIS files of hydraulic conductivity, soil porosity, DEM, and Smoothed DEM for the entire modeling domain. This needs to be done outside of VZMOD.

- (3) “Run” VZMOD for each soil type using the septic tank sources file of the corresponding soil type and the other ArcGIS files prepared for the modeling domain.

Since each “Run” generates output files of the same names and the original files are replaced, which is hardwired in the code, the users need to change the file names to save the original files after each “Run”. These files may be post-processed to meet the project needs. The most useful post-processing is to generate the septic tank source file needed for “Run”ning ArcNLET. This can be done by merging the multiple shape file generated from the separate “Run”s of VZMOD for different soil types.

4 EXAMPLE

This section presents an example of using VZMOD for a representative neighborhood-scale modeling with 587 septic tanks and heterogeneous hydraulic conductivity, porosity, and water table depth. The selected example modeling site is a subarea of the Julington Creek neighborhood of Jacksonville, Florida (Figure 4-1). The data files used in the example simulation are included in the “JulingtonCreek_example” package which can be downloaded from the software release website. The data package can be uncompressed at any disk location, independent of VZMOD file locations.

4.1 Description of Input Data and Files

The first step of “Run”ning VZMOD is to determine soil texture of the modeling domain. Like hydraulic conductivity and porosity, soil texture information can be extracted from the SSURGO database. In this example, the clay, silt, and sand contents of horizons are first aggregated to the component level before components are aggregated to the map unit level. Thickness of horizons and percentage of components are used as weights during the aggregation. Then based on the clay, silt and sand percentages, the soil texture is determined for every map unit. More details of this procedure are referred to Section 2.3 of the ArcNLET application manual (Wang et al., 2011). The soil texture in Jacksonville is mainly sand with small areas of sandy loam, loamy sand, sandy clay loam and clay. As shown in Figure 4-1, the soil type is sand for almost all the septic systems at the modeling area, except that the soil type is sandy loam for three septic systems. VZMOD is thus “Run” twice for the two soil types, and the procedure will be given in the next section.

The red diamonds shown in Figure 4-1 represent septic system locations. The corresponding septic tank source file is “sub_septic_tank.shp”. The ArcGIS layer is provided by the Florida Department of Environmental Protection (FDEP), and the septic tank locations are assumed to be at the center of the properties.

Figure 4-1 also depicts the zones of hydraulic conductivity and soil porosity. The two parameters are homogeneous within each zone but heterogeneous in different zones. The raster files (“hydrau_con.img” for hydraulic conductivity and “porosity.img” for porosity) are generated from the Soil Survey Geographic (SSURGO) database available at <http://soildatamart.nrcs.usda.gov/>. Instructions of generating the raster files can be found in Section 2.3 of the ArcNLET application (Wang et al., 2011).

The DEM and smoothed DEM raster files are “DEM.IMG” and “smoothedDEM.img”. The LiDAR DEM, plotted in Figure 4-1, is provided by FDEP and has a horizontal resolution of 5×5 ft². If LiDAR DEM is not available, alternative DEM raster files can be used. For example, the DEM raster file with horizontal resolution of 1/3 arc seconds can be obtained from the NED service maintained by the USGS. The procedure of preparing such a raster file is described in Section 4.3 of the User’s Manual of ArcNLET (Rios et al., 2011). The smoothed DEM is an intermediate output file of the flow module of ArcNLET and instructions of generating it can be found in Section 4.4 of Rios et al. (2011).

Note that the ArcGIS layer files used in VZMOD are independent to soil types. Except that the smoothed DEM is an output file of ArcNLET, the other four ArcGIS layer files are also input files of ArcNLET. This makes it efficient to use VZMOD together with ArcNLET.

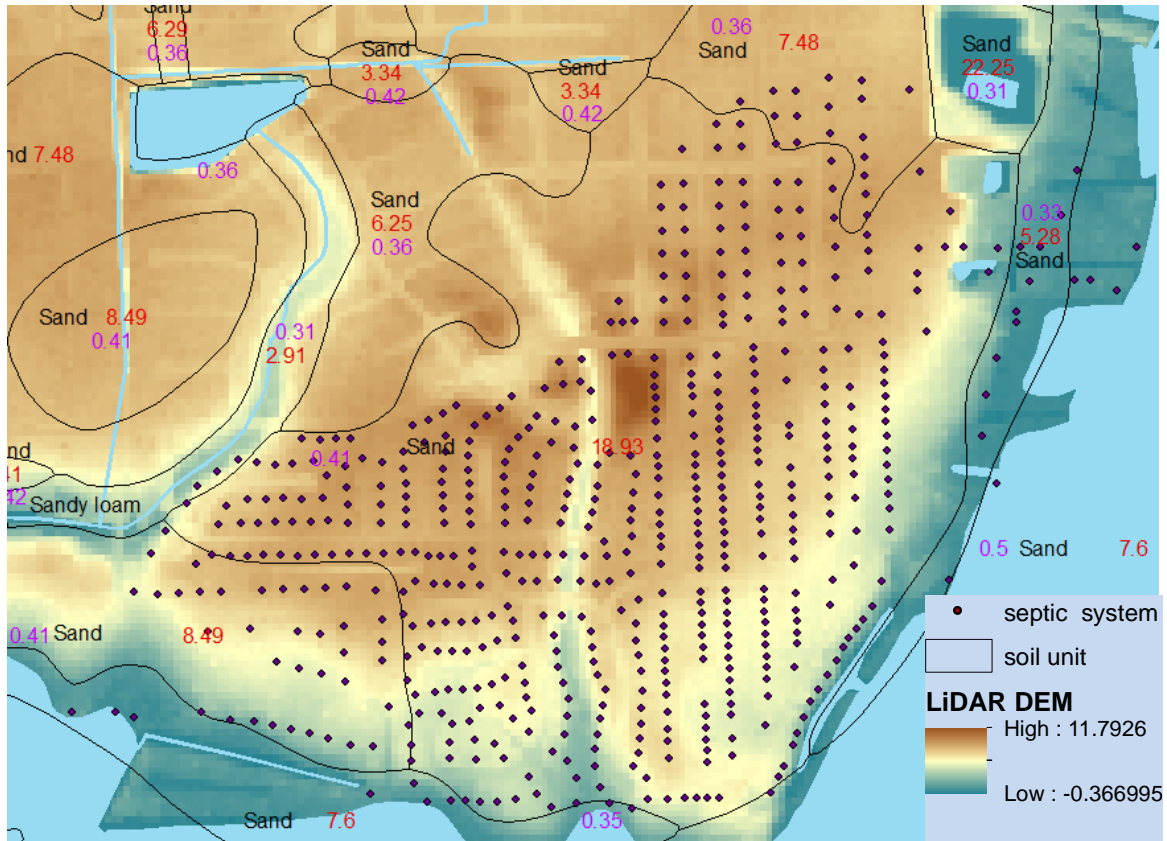


Figure 4-1. DEM of Interested site (a.k.a part of Julington Creek neighborhood) with septic system locations, soil texture (black), and hydraulic conductivity (red) and soil porosity (purple) values labeled

4.2 Modeling Procedure

Because the modeling domain has two soil types, VZMOD needs to “Run” twice for the two soil types. This can be done using the formal procedure described in Section 3.5. However, since there are only three septic systems located in sandy loam soil, we ran the example problem in a less formal way. Instead of generating two ArcGIS layers for septic tank sources corresponding to the two soil types, VZMOD is first “Run” by using the ArcGIS layer file “sub_septic tank.shp” for sand soil, and then for sandy loam soil. Figure 4-2 shows the screen shot of the first “Run”. After the two “Run”s, the attribute table of the shape file of septic tank sources generated the first “Run” is edited by changing the “NO_Conc” values of the three septic systems located in sandy loam sand to the corresponding values of the second “Run”.

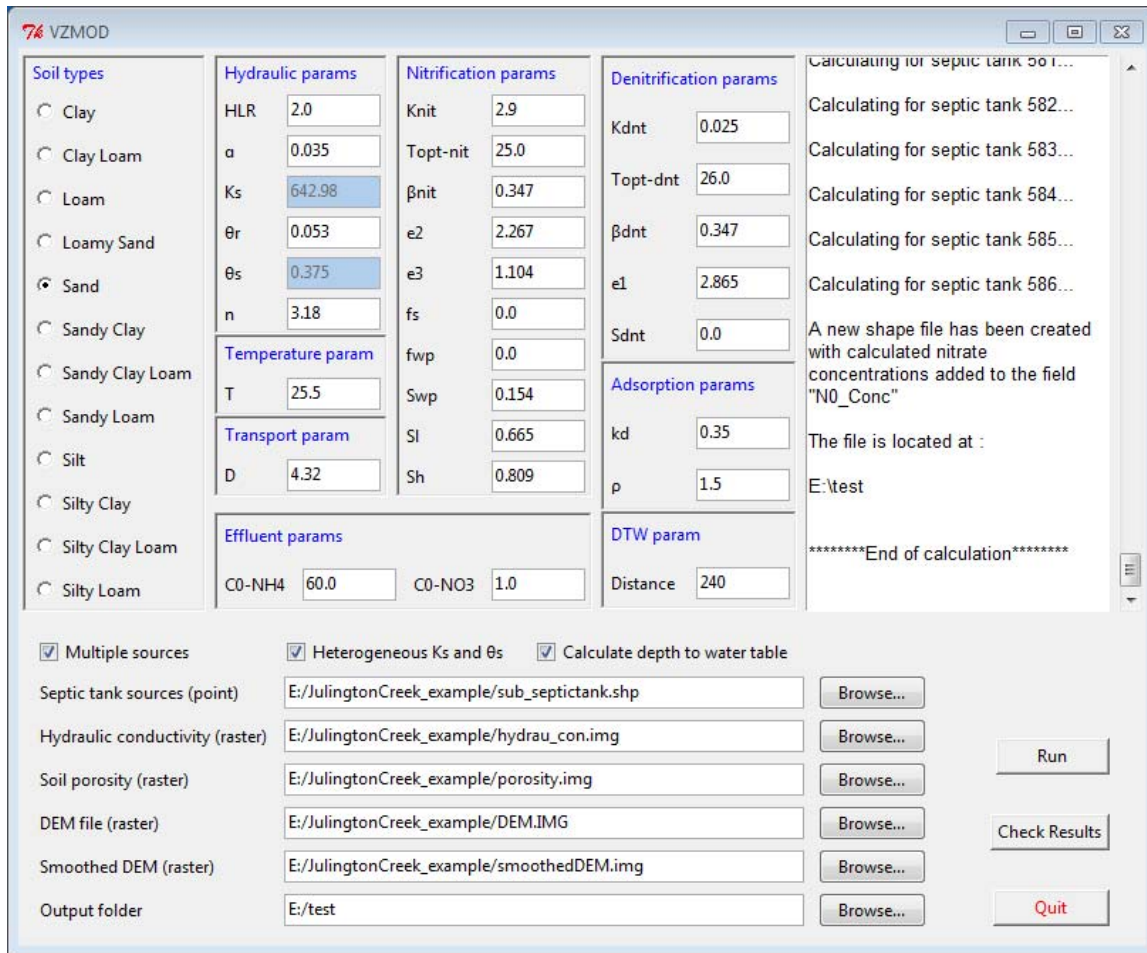


Figure 4-2. Screen shot of the model “Run” for sand soil.

4.3 Modeling Results

The simulated nitrate concentrations at water table for the individual septic systems are labeled in Figure 4-3. This figure indicates a relatively uniform distribution of nitrate concentration over the domain within a range from 51 to 56 mg/L. Figure 4-4 plots the concentration profiles of six septic systems with FID 100, 391, 435, 515, 543, and 552, selected for the six soil units. The locations of the six septic systems are shown in Figure 4-5. Except that septic system 391 is located in sandy loam soil, the other five septic systems are located in sand soil.

The profiles plotted in Figure 4-4 show that, during the downward transport, ammonium concentration decreases while nitrate concentration increases. This indicates that ammonium becomes nitrate due to nitrification. The ammonium concentration continues decreasing until all ammonium is transformed into nitrate. However, the transformation process may not be completed if water table is shallow, which is not the case in this example problem. Figure 4-4 shows that, for all the selected septic systems, ammonium concentration becomes zero eventually. However, the rate of transformation is different for different septic systems, depending on maximum nitrification rate and the functions of temperature and saturation described in Section 2.2. For this example

problem, since the maximum nitrification rate and temperature function are the same for all septic systems, the actual nitrification rate is determined solely by saturation. Figure 4-4 shows that the process of nitrification is faster in sandy loam (FID 391) than in sand (FID 100, 435, 515, 543, and 552).

The profiles of nitrate are more complicated than those of ammonium. For all the profiles, the nitrate concentration first increases due to nitrification of ammonium. When the nitrate concentration reaches the maximum, the nitrate concentration starts decreasing for septic systems with FID 100, 391, and 435. The decrease is caused by denitrification. While denitrification also occurs before the nitrate concentration reaches the maximum, it is negligible because the maximum concentration is close to 61 mg/L, the total nitrogen of the system given the input data shown in Figure 4-2. The rate of denitrification increases when the profile approaches the water table, because the saturation function increases with saturation (Figure 2-3), which increases toward the water table. For septic systems with FID 515, 543, and 552, after reaching the maximum, the nitrate concentration remains constant (or visually unnoticeable) for a distance and then decreases. The reason of the constant concentration is that the denitrification rate is negligible due to the value of saturation. When the saturation is large near the water table, denitrification process become strong and causes decrease of nitrate concentration, which is also observed for the septic systems with FID 100, 391, and 435. Because denitrification only affects nitrate concentration near the water table, the simulated nitrate concentrations are more or less uniform (Figure 4-3), despite of heterogeneity in the depth to water table, hydraulic conductivity, and soil porosity.

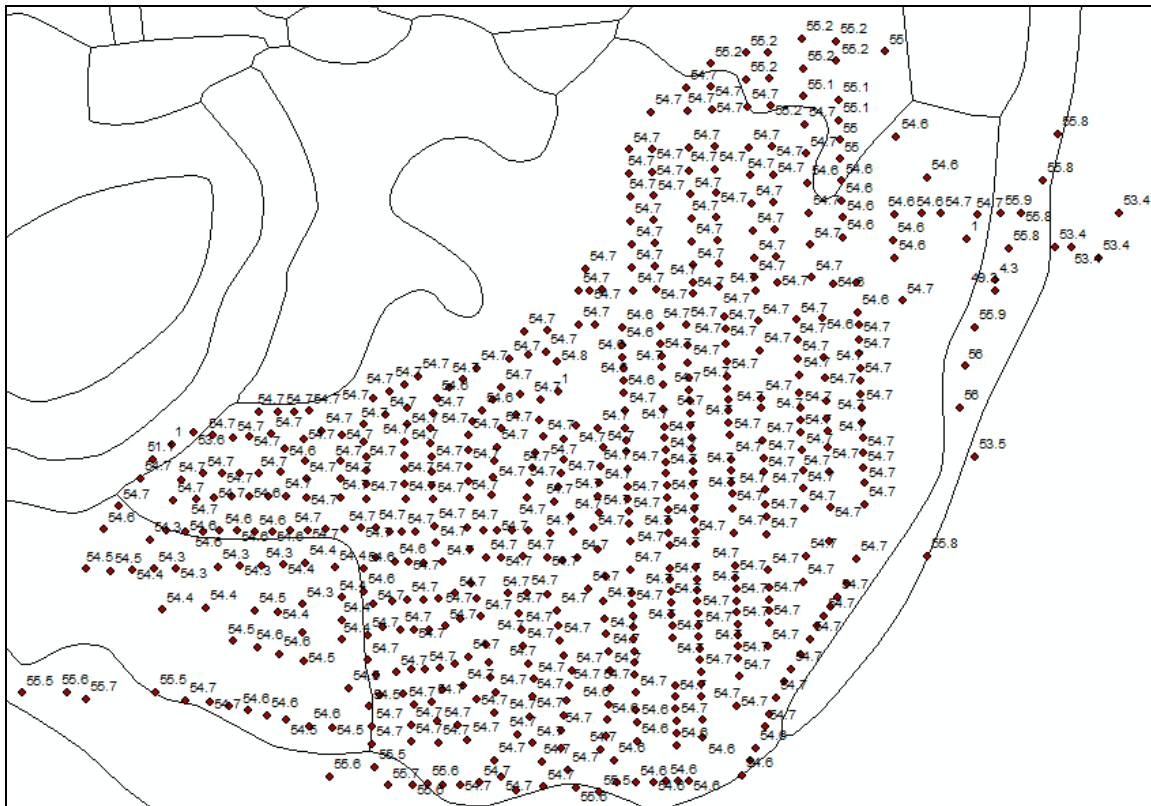


Figure 4-3. Calculated nitrate concentration (mg/L) at water table for individual septic systems.

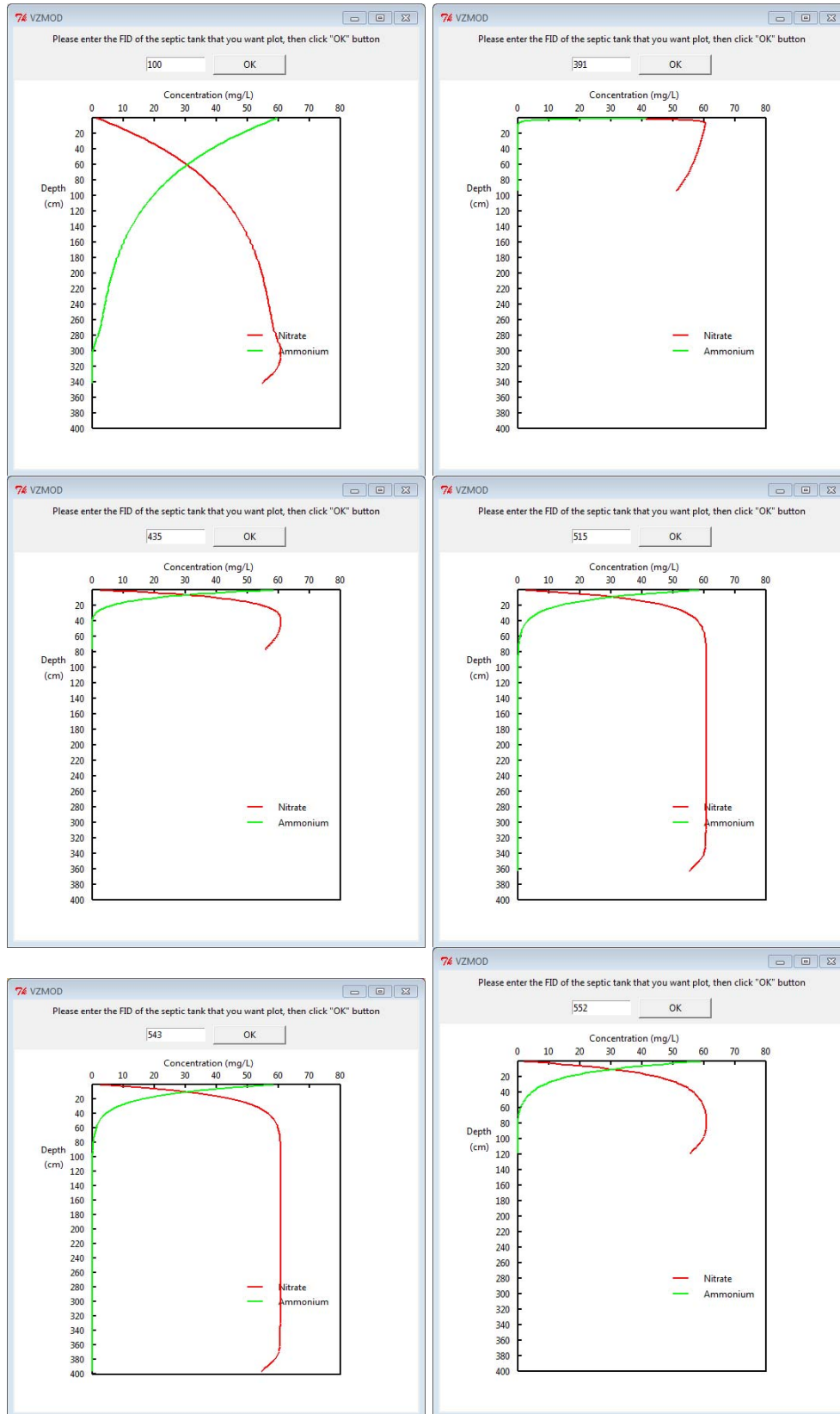


Figure 4-4. Vertical profiles of nitrate and ammonium concentrations for septic systems with FID 100, 391, 435, 515, 543, and 552, whose locations are shown in Figure 4-5.

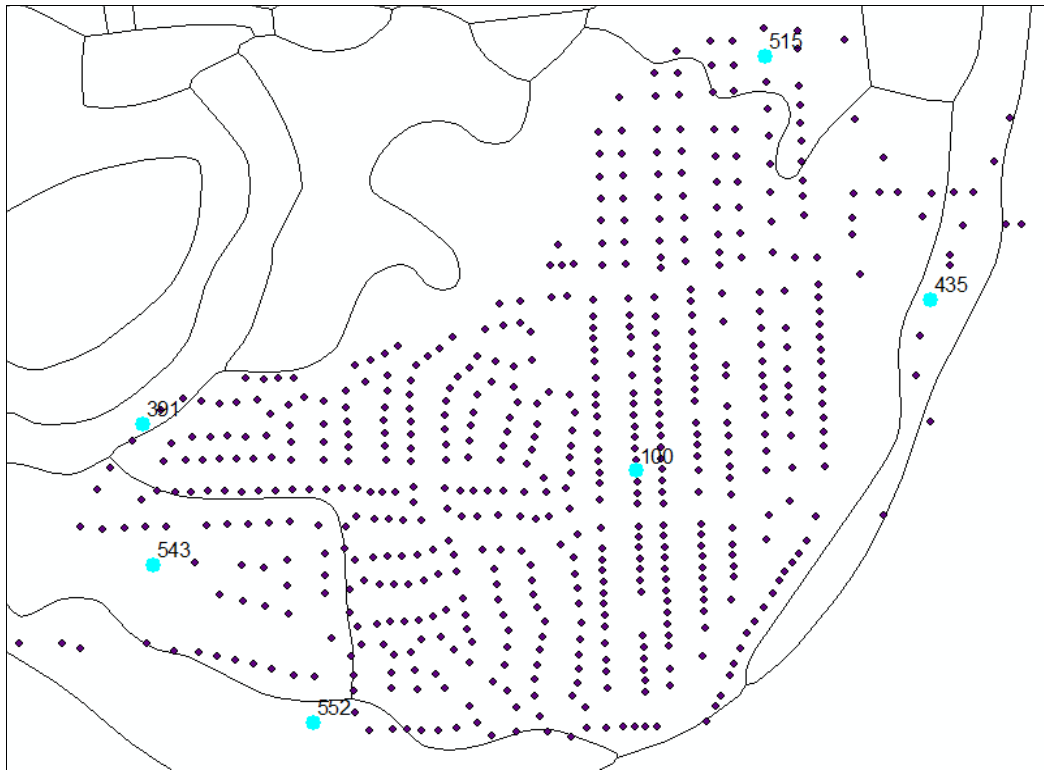


Figure 4-5. Locations of selected individual septic systems. The blue circles highlight the locations the six septic systems whose profiles of nitrate and ammonium are plotted in Figure 4-4. The numbers are FID of the septic systems.

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