

Support of sustainable management of nitrogen contamination due to septic systems using numerical modeling methods

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Abstract Nitrogen contamination is a serious concern to sustainable environmental management, and one important source of nitrogen contaminant is due to wastewater treatment using onsite sewage treatment and disposal systems (OSTDS, a.k.a., septic systems). This paper presents a study in which numerical modeling is used to support sustainable decision-making and management of nitrogen contamination by utilizing a recently developed GIS-based software, VZMOD, a Vadose Zone MODEL for simulating nitrogen transformation and transport in vadose zone between drainfield of septic systems and water table. VZMOD is based on a physical model of unsaturated flow and nitrogen transformation and transport, and the model is solved numerically using the finite element methods. This is the major difference between VZMOD and other GIS-based software of nitrogen modeling. Using GIS techniques, VZMOD considers spatial variability of a number of hydrogeologic parameters such as hydraulic conductivity and porosity. A unique feature of VZMOD is that VZMOD addresses spatial variability of water table by using VZMOD together with ArcNLET, an ArcGIS-based software developed to simulate groundwater flow and nitrate load from septic systems to surface water bodies. VZMOD is designed to execute in different modes to be compatible with different levels of data availability in various management projects of nitrogen contamination. This paper presents an application of VZMOD at a

neighborhood with hundreds of septic systems and heterogeneous hydraulic conductivity, porosity, and water table depth. The modeling results indicate that using septic systems at the considered neighborhood is unsustainable and more management means are necessary.

Keywords Geographic information system · Python programming language · Spatial variability · Nitrification · Denitrification · Unsaturated flow · Depth to water table

1 Introduction

Nitrogen (nitrate NO_3^- , nitrite NO_2^- , and ammonium NH_4^+) contamination of groundwater and surface water is associated with a number of adverse health and environmental impacts (Walters 1983). For example, nitrate concentration higher than 10 mg/L (measured as nitrogen) in drinking water may cause methemoglobinemia, also known as blue baby syndrome. Discharge of nitrogen-rich groundwater to surface water bodies can lead to fish kills, algal growth, hypoxia, eutrophication, and outbreaks of toxic bacteria (Kumar et al. 2011). Among various nitrogen sources, an important source of nitrogen in the environment, especially in urban areas, is due to wastewater treatment using onsite sewage treatment and disposal systems (OSTDS) (a.k.a., septic systems) (U.S. Environmental Protection Agency (EPA) 1993, 2002; Umezawa et al. 2008). Approximately 25 % of the population and 30 % of all new development in USA utilize septic systems (Hazen and Sawyer 2009); in the state of Florida, nearly one-third of households use septic systems (Ursin and Roeder 2008; Hazen and Sawyer 2009). Septic systems are considered to be a major contamination source in more than 40 states in USA (Fetter 1999). Based on a study at the Virginia Coastal Plain,

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Ready (2004) estimated that, at Chesapeake Bay watershed, nitrogen loading from septic systems to shallow ground water is comparable to that from dominant row crop land use in the mid-Atlantic Coastal Plain. Shallow groundwater in surficial aquifers is vulnerable to nitrate contamination, and nitrate contribution from septic systems to surface water bodies may be significant in areas where septic systems are located in close proximity to surface water bodies. Valiela et al. (1997) showed that, in Butter-milk Bay, MA, 40 % of nitrogen entering watershed was from septic systems and 80 % of the nitrogen was transported through groundwater. Given the trends in population growth, nitrogen loads from septic systems are expected to increase. Therefore, sustainable decision-making and management of nitrogen contamination due to septic systems are urgently needed.

Sustainable management of nitrogen contamination can be achieved by multiple means, such as monitoring and mapping of the contamination, quantifying the amount of contamination through calculation of total maximum daily load (TMDL), connecting the contamination to human benefits and values, and/or analyzing nitrogen life cycle for science-informed decision-making. This paper is aimed at calculating nitrogen load from septic systems to groundwater and subsequently from groundwater to surface water bodies. The estimated load to surface water bodies is a key factor in TMDL analysis for protecting the environment and public health. Accurate load estimation entails understanding and quantifying nitrogen transformation and transport in subsurface environment including both vadose zone and groundwater. This is commonly done through numerical modeling of nitrogen reactive transport, which is cost-effective and particularly useful for scenario-based decision-making (Karvetski et al. 2011).

A large number of computer codes and software programs have been developed for simulation of nitrogen reactive transport (McCray et al. 2009). They are with different levels of complexity. Generally speaking, complex models can yield results that can potentially agree well with field observations, whereas high model complexity may be a hurdle for general users; a trained professional is always required to operate the models and interpret modeling results for decision-makers of environmental management. In addition, to utilize sophisticated functions of the models, a large amount of model input and calibration data as well as long execution time are needed, which may not be available or affordable in practice. On the other end of the spectrum of nitrogen models are simple models that are conceptually straightforward and easy to use. While the simple models gain their popularity in environmental management when data are scarce and project time and/or budget is limited, they are always based on a number of simplifications and

assumptions that may not be fully justified in real-world situations.

A computer program suitable for sustainable management of nitrogen (and other) contamination should be based on a physical model whose inputs and outputs have physical meaning and can be obtained from and verified by laboratory and/or field experiments. In addition, complexity of the models should be compatible with available data and information; in the situation of data scarcity, it is often necessary to reduce model complexity to a certain extent while maintaining validity of modeling results (Pachepsky et al. 2005). An example of such models for nitrogen modeling is the soil treatment unit model (STUMOD) developed by McCray et al. (2010). It considers a number of important processes in nitrogen transformation and transport, but does not require a large amount of data for running the model and conducting model analysis.

A computer program that effectively facilitates environmental management should also address spatial variability of quantities of interest at a site so that modeling results are site specific and thus useful to practical environment management. This has been embraced in many programs by using techniques of geographic information system (GIS), an efficient way to integrate regional/local spatial characteristics of a system (e.g., digital hydrologic and topographic data) and to analyze and visualize modeling results by non-technical citizens (National Research Council 2010; Yang and Lin 2011). Development of GIS-based programs for nutrient modeling started about two decades ago (e.g., MANAGE developed by Kellogg et al. 1996, NLM by Valiela et al. 1997, and PLSM by Adamus and Bergman 1995) and has become popular since skills required for the application of GIS-based models are widely available (McCray et al. 2009).

This paper presents a recently developed GIS-based software, VZMOD, a Vadose Zone MODEL for simulating nitrogen transformation and transport in vadose zone between septic drainfield and groundwater water table. The vadose zone is of particular interest to this study, because biogeochemical processes (e.g., nitrification and denitrification) occurring in vadose zone are key factors determining nitrogen load to groundwater and subsequently to surface water bodies. Different from many GIS-based software of nitrogen modeling, VZMOD is based on a physical model that describes processes of unsaturated flow and nitrogen transformation and transport, and solves the model numerically using the finite element methods. As discussed below, the process-based model enables VZMOD users to better understand effects of various system components (e.g., soil types) on nitrogen transformation and transport, which cannot be provided by mass balance or rule-based models used by many GIS-based software of nitrogen modeling. Solving the model

numerically makes VZMOD to handle spatial variability of many quantities (e.g., source concentrations of nitrogen species, soil types, and water table) important to nitrogen modeling, a feature that is unavailable in analytical solutions used by other GIS-based software. While the physical model of VZMOD is similar to that of STUMOD (McCray et al. 2010), VZMOD solves the model numerically whereas STUMOD uses analytical solutions. A more important distinction between VZMOD and STUMOD is that STUMOD is an EXCEL-based program that considers only one septic system, whereas VZMOD is a GIS-based software that considers multiple septic systems and spatial variability of hydrogeologic variables in the system of interest.

VZMOD is designed to be used together with another GIS-based software, ArcNLET, an ArcGIS-based Nitrate Load Estimation Toolkit (Rios et al. 2013) for solving groundwater flow and estimating groundwater nitrate load. The coupling is implemented in the manner that VZMOD-estimated nitrate concentration at water table are used as an input source of ArcNLET for simulating nitrate transport in groundwater. On the other hand, the shape of water table given by the flow model of ArcNLET is directly used in VZMOD. It is demonstrated in Sect. 3 that the spatial variability of water table is important to simulated profiles of nitrogen in the vertical direction. Incorporating spatial variability of water table is a strength of VZMOD in comparison with other GIS-based software of vadose zone modeling that always assumes uniform water table. VZMOD and ArcNLET can be integrated into one framework in the manner of Jeong et al. (2011), which, however, is beyond the scope of this study.

In addition to the model development, this paper presents for the first time the VZMOD application for estimating nitrogen transformation and transport from hundreds of septic systems to groundwater in a neighborhood of the Lower St. Johns River Basin (LSJRB) in Florida, USA, where nitrogen due to septic systems is believed to be one of the causes for nutrient enrichment in surface water bodies (Leggette Brashears, and Graham, Inc. 2004). The current management scheme of septic-related nitrogen contamination does not appear to be sustainable, as evidenced by continuous deterioration of water quality in groundwater and surface water. State and local governments have spent a large amount of resources and are planning to spend more on environmental restoration and protection in LSJRB. This study demonstrates that VZMOD can be used to support the management and decision-making by providing vertical profiles of ammonium and nitrate concentrations between drainfield and water table for individual septic systems. However, it should be noted that the application of VZMOD in this paper is only for the purpose of demonstration. Since

vadose-zone measurements of moisture contents and concentrations of ammonium and nitrate were not available at the modeling site, the VZMOD model was not calibrated. As a result, the modeling results cannot be used directly for nitrogen management.

2 Conceptual and mathematical models

As shown in Fig. 1, a conventional septic system has four main components: a pipe from the home (wastewater source), a septic tank (pretreatment unit), a drainfield/leachfield, and the soil. Wastewater 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 (by gravity or a pump) into the drainfield and then percolates through the vadose zone down to groundwater. The soil provides final treatment by removing harmful bacteria, viruses, and nutrients. Suitable soil and vadose zone thickness are necessary for successful wastewater treatment. Understanding the soil treatment processes is critical to design of septic systems and environmental protection of nitrogen contamination to groundwater and surface water bodies (McCray et al. 2010).

VZMOD is focused on modeling the treatment processes and transport of nitrogen in the vadose zone. Since this software aims at simulating long-term, vertical migration of septic effluent from drainfield to groundwater, the vadose zone flow and nitrogen transport are assumed to be one-dimensional (1-D) in the vertical direction and in steady state. The simplified conceptual-mathematical model of vadose zone flow and transformation and transport of ammonium and nitrate are described in Sects. 2.1–2.3, followed by the algorithm of numerical solution, design of the software, and execution scenarios of VZMOD in Sects. 2.4–2.7.

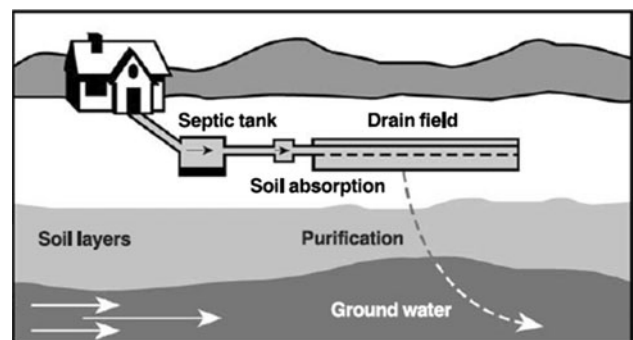


Fig. 1 Diagram of conventional onsite wastewater treatment system (from National Small Flows Clearinghouse 2000)

2.1 Unsaturated flow model

The steady-state, 1-D vertical water movement in unsaturated porous medium is described by the Darcy's law of unsaturated flow,

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

where h is water pressure head [L], z is spatial coordinate [L] (positive upward), q is hydraulic loading rate (HLR) 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:

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

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

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

where K_s is saturated hydraulic conductivity [LT^{-1}], S is degree of saturation [–], θ is volumetric water content [$\text{L}^3 \text{L}^{-3}$], 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 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 being zero. The depth to water table (DTW) varies for individual septic systems, and it is determined by digital elevation model (DEM) of land surface and smoothed DEM that is an output of ArcNLET (Rios et al. 2012); the detailed procedure of calculating DTW is given in Sect. 2.7. In VZMOD, HLR and soil hydraulic parameters (K_s , α , n , θ_r , and θ_s) are specified by the users in the block of “Hydraulic params” of the VZMOD graphic user interface (GUI) shown in Fig. 2. Numerical solution of Eqs. (1)–(4) in VZMOD gives the vertical profile of moisture content and degree of saturation; the latter is used below for simulating transformation and transport of ammonium and nitrate.

2.2 Transformation model of ammonium and nitrate

After being discharged to the soil, nitrogen in septic effluent is primarily inorganic (ammonium and nitrate); organic nitrogen is usually retained in the clogging zone at the infiltrative surface (Heatwole and McCray 2007). In the vadose zone transport process, ammonium and nitrate are subject to nitrification and denitrification, respectively. During nitrification ($\text{NH}_4^+ + 2\text{O}_2 \rightarrow \text{NO}_3^- + 2\text{H}^+ + \text{H}_2\text{O}$), 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 vadose zone, and complete nitrification usually occurs in the first 30 cm below the infiltrative surface (Fischer 1999; Beach 2001). Thus, nitrate is generally the pollutant of concern for septic systems, and VZMOD considers only nitrification from ammonium to nitrate.

As a mechanism of nitrogen removal in vadose zone, denitrification ($5\text{C} + 4\text{NO}_3^- + 2\text{H}_2\text{O} \rightarrow 2\text{N}_2 + 4\text{HCO}_3^- + \text{CO}_2$) is a microbially facilitated process of 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. Because denitrification rates are usually significantly smaller than nitrification rates in natural soils, denitrification is the limiting reaction for nitrogen removal in vadose zone. While complete denitrification in most vadose zone does not occur (Heatwole and McCray 2007), for simplicity, intermediate products of denitrification are not considered in VZMOD.

In VZMOD, the nitrification and denitrification processes are modeled as the first-order nitrogen transformation. Considering effects of temperature and soil saturation on the rates, the first-order reactions of nitrification and denitrification are as follows:

$$\frac{\partial [\text{NH}_4^+]}{\partial t} = k_{\text{nit}} f_{\text{t,nit}} f_{\text{sw,nit}} [\text{NH}_4^+] \quad (5)$$

$$\frac{\partial [\text{NO}_3^-]}{\partial t} = k_{\text{nit}} f_{\text{t,nit}} f_{\text{sw,nit}} [\text{NH}_4^+] - k_{\text{dnt}} f_{\text{t,dnt}} f_{\text{sw,dnt}} [\text{NO}_3^-] \quad (6)$$

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

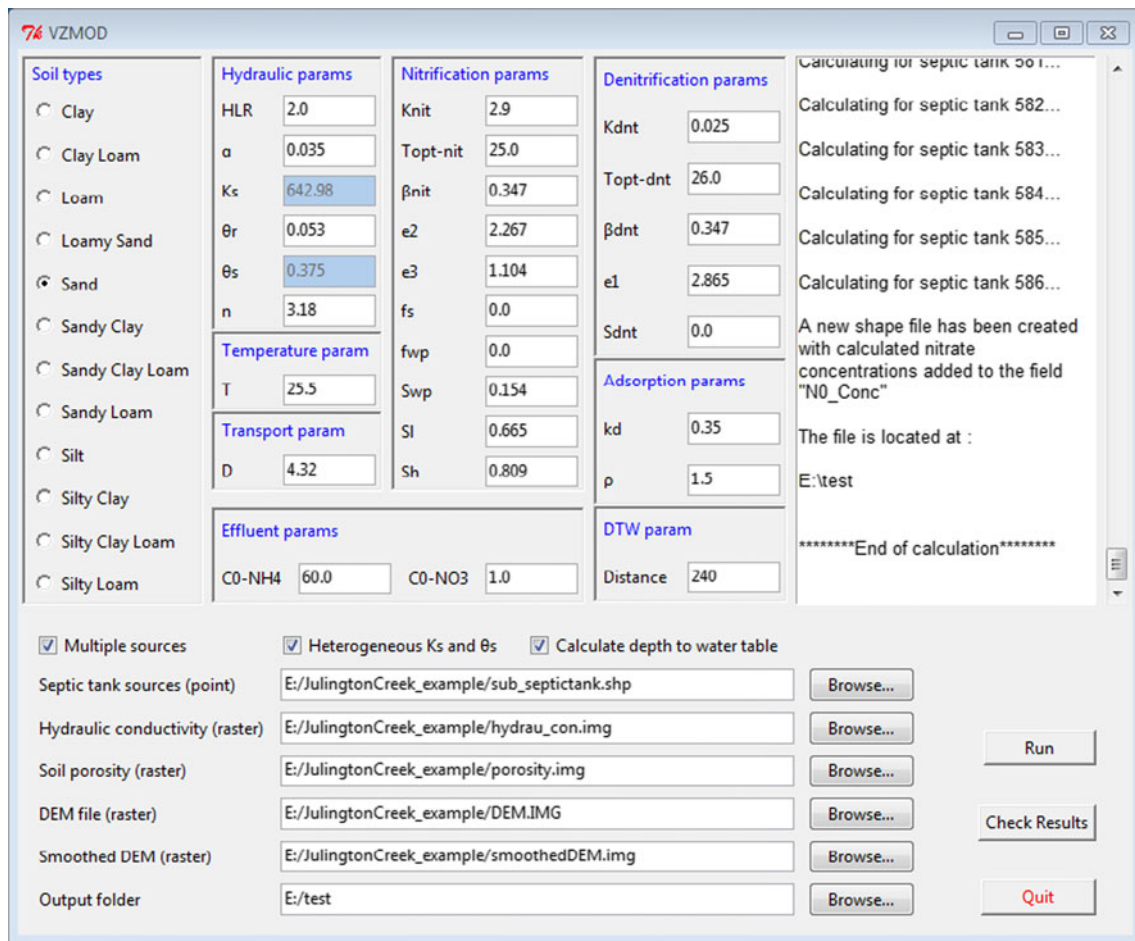


Fig. 2 Graphic user interface (GUI) of VZMOD and screen shot of the scenario of running the model for multiple septic systems located in sand soil with heterogeneous saturated hydraulic conductivity, porosity, and depth to water table

params” and “Denitrification params” of the VZMOD GUI (Fig. 2). 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. As suggested in Skaggs (1978), Youssef et al. (2005), and McCray et al. (2010), the temperature function, f_t (between 0 and 1), for nitrification and denitrification rates takes the same form,

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

where T is temperature, T_{opt} is the optimum temperature for nitrification or denitrification, and β is a fitting parameter. In VZMOD, the temperature functions, $f_{t,\text{nit}}$ for nitrification and $f_{t,\text{dnt}}$ for denitrification processes, are evaluated separately. The evaluation uses parameters $T_{\text{opt-nit}}$ and β_{nit} for nitrification and $T_{\text{opt-dnt}}$ and β_{dnt} for denitrification. Parameter T is specified in the block of “Temperature param” of the VZMOD GUI (Fig. 2); $T_{\text{opt-nit}}$ and β_{nit} are specified in the

block of “Nitrification params” and $T_{\text{opt-dnt}}$ 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. As nitrification is an aerobic process, it is unlikely that nitrification will occur in nearly saturated soils due to limited oxygen supply. On the other hand, when the degree of saturation is low, because connection of wetted soil pores is poor, diffusion of ammonium and dissolved oxygen between soil pores is limited. In other words, nitrification is limited or prohibited by low saturation limits. As a result, optimal nitrification occurs between the low and high degrees of saturation. The saturation function, $f_{sw,\text{nit}}$ (between 0 and 1), is defined as (McCray et al. 2010)

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

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 S 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 (Fig. 2). Unlike nitrification, denitrification takes place under anaerobic conditions. The saturation function of denitrification, $f_{sw,dnt}$ (between 0 and 1), is defined as (McCray et al. 2010)

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

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 (Fig. 2).

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 as follows:

$$D \frac{\partial^2 C_{NH_4}}{\partial z^2} - \frac{q}{\theta} \frac{\partial C_{NH_4}}{\partial z} - k_{nit} f_{t,nit} f_{sw,nit} \left(1 + \frac{\rho k_d}{\theta} \right) C_{NH_4} = 0 \quad (10)$$

$$\begin{aligned} D \frac{\partial^2 C_{NO_3}}{\partial z^2} - \frac{q}{\theta} \frac{\partial C_{NO_3}}{\partial z} - k_{nit} f_{t,nit} f_{sw,nit} \left(1 + \frac{\rho k_d}{\theta} \right) C_{NH_4} \\ - k_{dnt} f_{t,dnt} f_{sw,dnt} C_{NO_3} \\ = 0 \end{aligned} \quad (11)$$

where C_{NH_4} and C_{NO_3} are concentrations of ammonium and nitrate, respectively, D is dispersion coefficient [$L^2 T^{-1}$], ρ is soil bulk density [ML^{-3}], and k_d is distribution coefficient of linear adsorption [$M^{-1} L^3$]. The last term at the left-hand side of Eq. (10) indicates that nitrification occurs for the adsorbed ammonium; similarly, the last term at the left-hand side of Eq. (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 (Fig. 2).

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 concentrations in septic tank effluent by HLR. The

concentrations, denoted as C_0-NH_4 and C_0-NO_3 , are specified in the block of “Effluent params” of the VZMOD GUI (Fig. 2), and mass flux is calculated in the VZMOD code. VZMOD allows the effluent concentrations (C_{NH_4} and C_{NO_3}) to vary for different septic systems, and more details will be given in Sect. 2.6 below. The lower boundary of the vadose zone is the water table, and the boundary condition is zero concentration gradient for transport model.

2.4 Design of VZMOD

The above vadose zone flow and solute transport equations are solved numerically using the Galerkin finite element method utilized in the software HYDRUS-1D (Simunek et al. 2009). Details of the numerical scheme are provided in the manual of HYDRUS-1D.

Figure 3 is the flow chart of VZMOD, in which “source” is used to denote septic system for brevity. The first step is to read the parameters of flow and nitrogen transformation and transport from the VZMOD GUI (Fig. 2) for a given soil type. If VZMOD is used for a single septic system, these parameters are used to solve the flow and transport equations and the concentration profiles are saved for post-processing. If VZMOD is used for multiple septic systems at neighborhood scales, 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 Fig. 3, three ArcGIS layers of septic system locations, DEM raster, and Smoothed DEM Raster are used to calculate DTW in the procedure described in Sect. 2.7. 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 septic system. The heterogeneous data are extracted from the Hydraulic Conductivity Raster and Soil Porosity Raster to the locations of the multiple septic systems. After this, VZMOD solves the flow and transport model for each individual septic system.

Based on the flowchart, VZMOD is developed using the Python programming language, which is free and compatible of crossing different computer platforms. Therefore, VZMOD works on any personal computers with the Microsoft Windows operating system that meets the minimum requirements for ArcGIS 10.0 with Python 2.6.5 and Spatial Analyst extension. 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 for VZMOD to use ArcGIS data to address spatial variability of hydraulic parameters, septic tank locations, and water table.

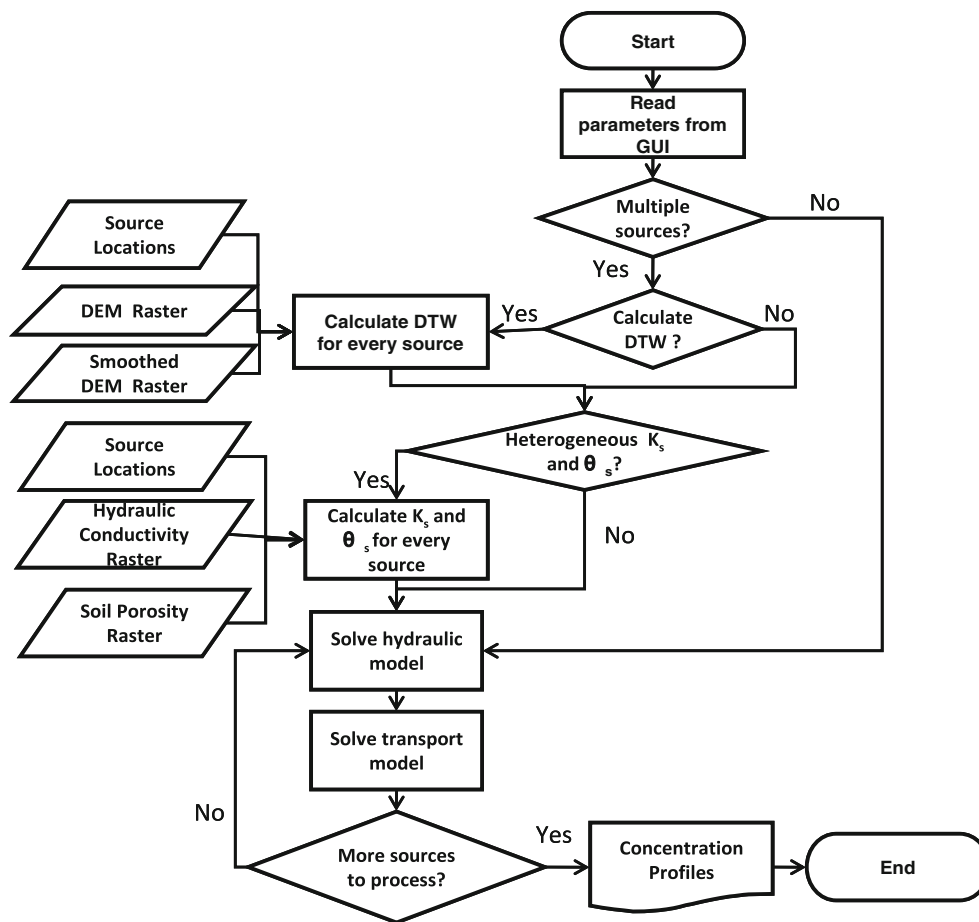


Fig. 3 Flowchart of VZMOD

2.5 VZMOD execution for a single septic system

VZMOD can be executed in different modes to be compatible with different levels of data availability in various projects of nitrogen environmental management. Detailed description of the execution modes and corresponding data requirements is provided in the VZMOD user manual (Wang et al. 2012). This paper provides only a brief description of two execution scenarios: for a single septic system and for multiple septic systems.

When running VZMOD for a single septic system, spatial variability is not considered and all variables are constant, not varying in space. Their values are read through the VZMOD GUI (Fig. 2). Since the hydraulic parameters, the coefficient, e_1 , of saturation function of denitrification, and the coefficient, k_d , of adsorption are specific to soil types, one needs to select soil type before inputting these parameter values. If site-specific parameter values are not available, one can use literature values compiled in McCray et al. (2005, 2010), which are referred to as default values in the rest of the paper. Note that the default parameters are merely reference values and users

of VZMOD are responsible for determining appropriate values for their project of nitrogen modeling. In addition, the values of dispersion coefficient (D), temperature (T), and depth to water table (DTW) are site specific, and the users need to specify the values appropriate to their sites of interest. During the execution for a single septic system, simulated concentrations of ammonium and nitrate in the vertical direction are displayed in the window above the “Run” button at the rightmost block of the GUI. The simulation results are saved in a text file and can be visualized within VZMOD by clicking the “Check Results” button, which activates a pop-up window to plot the calculated concentration profiles of ammonium and nitrate. Example plots are shown in Sect. 3 for different soil zones of the demonstration case.

2.6 VZMOD execution for multiple septic systems

Running VZMOD for multiple septic systems requires multiple ArcGIS files to address spatial variability of hydraulic conductivity, soil porosity, and depth to water table. Details of preparing these files are provided in the

user manual of VZMOD (Wang et al. 2012) and ArcNLET (Rios et al. 2011, 2013; Wang et al. 2013). Executing VZMOD in this scenario starts from checking the box of “Multiple sources” in the GUI (Fig. 2), which activates the file input box of “Septic tank source (point)” to select a GIS point layer for the drainfield locations. If effluent concentrations of ammonium and nitrate are available for every septic system, they are saved in the attribute table of the ArcGIS file. VZMOD extracts the concentrations (the parameters $C_0\text{-NH}_4$ and $C_0\text{-NO}_3$ in the block of “Effluent params” will be disabled) and uses them to evaluate concentrations of ammonium and nitrate between drainfield and water table for each septic system. This allows VZMOD to consider spatial variability of effluent concentrations of ammonium and nitrate. However, it is difficult, if not impossible, to obtain these concentrations for each septic system, and using uniform values for all septic systems is a common practice.

When running VZMOD for multiple septic systems, in addition to the default text file that saves simulated concentrations of ammonium and nitrate, a new ArcGIS point layer is generated with default name “Septictank”. It is revised from the input “Septic tank source (point)” file by adding a new field named “NO_Conc” to the attribute table for storing the simulated nitrate concentration at water table for individual septic systems. This output point file of VZMOD can be used directly as input of ArcNLET.

Checking the box of “Multiple sources” also activates the options of “Heterogeneous K_s and θ_s ” and “Calculate depth to water table”. The two options can be used either separately or jointly, depending on availability of the two kinds of data. This makes VZMOD runs flexible. 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 (Fig. 2) and the two file input boxes of “Hydraulic conductivity (raster)” and “Soil porosity (raster)” will be activated to input ArcGIS raster layers of heterogeneous saturated hydraulic conductivity and soil porosity. If “Calculate depth to water table” is checked, the distance between drainfield and water table will be calculated using two raster files to consider spatial variability of surface elevation and water table. Details of the raster files and the procedure of calculation are given below.

2.7 Calculation of distance between infiltrative surface and water table

If “Calculate depth to water table” is checked, the distance between infiltrative surface and water table is calculated for individual septic systems. The calculation needs two GIS raster layers loaded through the boxes of “DEM (raster)” and “Smoothed DEM (raster)”. The

DEM raster file is conventional, and the smoothed DEM is the output raster file of running the groundwater flow module of ArcNLET. The smoothed DEM is expected to have the same shape of groundwater table, because water table can be viewed as a subdued replica of topography, which has been validated at the study area (Rios et al. 2013; Wang et al. 2013).

With the two DEM files, the distance is calculated for each individual septic system in the following procedure. The first step is to calculate the elevation of water table by subtracting a constant (denoted as A) from the smoothed DEM, that is, $\text{Smoothed_DEM} - A$. This constant is the distance between the smoothed DEM and the water table, and it can be estimated from field measurements of water level in monitoring wells as described in Wang et al. (2013). While A is assumed to be a constant, because Smoothed_DEM varies in space, $\text{Smoothed_DEM} - A$ (e.g., water table elevation) varies in space. The next step is to calculate the elevation of the infiltrative surface by subtracting the distance (denoted as B) between the infiltrative surface and land surface from the thickness of vadose zone, that is, $\text{DEM} - B$. One choice of B is 18 inches, because drainfield is about 12 inches thick (for gravel) covered by 6 inches of soil (USEPA, 2002). The distance from infiltrative surface to water table is thus calculated via $(\text{DEM} - B) - (\text{Smoothed_DEM} - A) = \text{DEM} - \text{Smoothed_DEM} + (A - B)$. The user needs to input the value of $A - B$ through the GUI in the box of “Distance” in the block of “DTW param” (Fig. 2). While the value of $A - B$ is a constant, the difference between DEM and Smoothed_DEM varies between septic systems. Therefore, the distance from infiltrative surface to water table varies between septic systems. As shown in the next section, the vertical distributions of ammonium and nitrate concentrations are different for individual septic systems when the systems have different depths to water table.

3 Demonstration of VZMOD Application

This section demonstrates the use of VZMOD for a representative neighborhood-scale modeling with 587 septic systems and heterogeneous hydraulic conductivity, porosity, and water table depth. The study site is a subarea of the Julington Creek neighborhood in the LSJRB, Florida (Fig. 4). The soil texture of the study site is sand for almost all the septic systems, except for three septic systems that are located in sandy loam soil (Fig. 4). Considering that nitrification and denitrification parameters are constant for each soil type, VZMOD runs twice for the two soil types, and the results are aggregated together in post-processing within ArcGIS. The zonal soil units and their corresponding values of hydraulic conductivity and porosity (shown in

Fig. 4 Digital elevation model (DEM) of Julington Creek neighborhood with multiple septic systems (red diamond). Soils units are delineated by polygons. For each unit, soil texture is labeled in *black*, hydraulic conductivity in *red*, and soil porosity in *purple*. Locations of monitoring wells of hydraulic heads are marked with *circles*. *Blue squares* denoted selected locations of six septic systems whose concentration profiles are plotted in Fig. 7; the numbers labeled at the locations are FID of the septic systems (Color figure online)

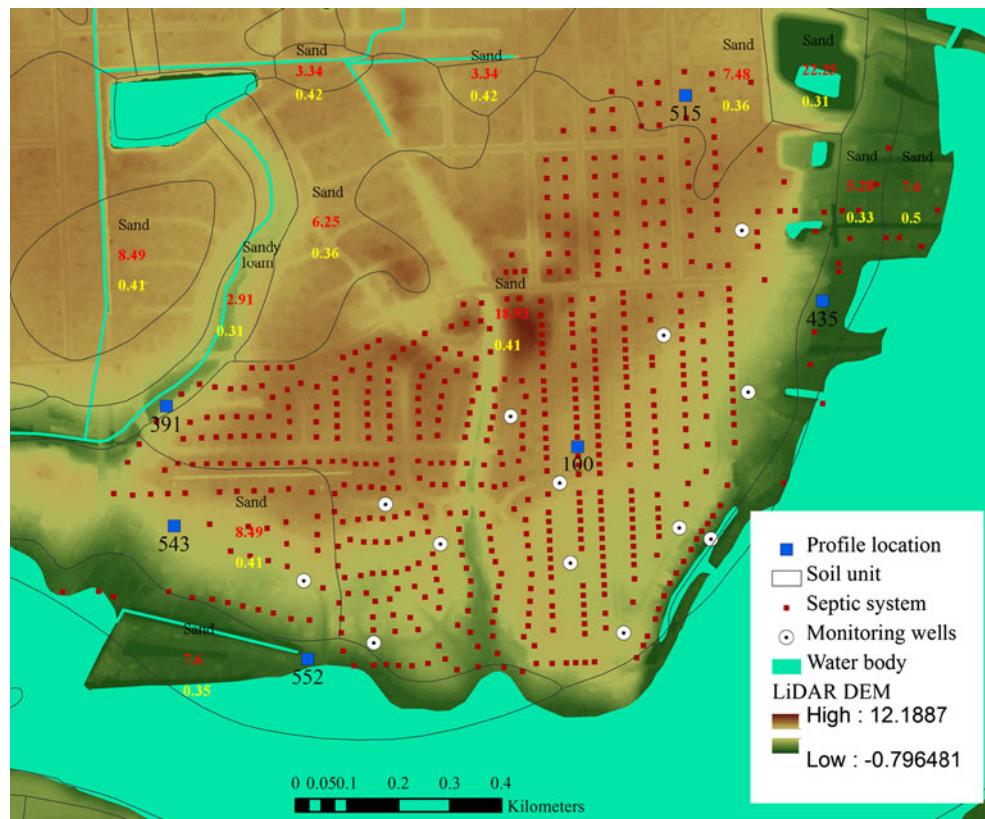


Fig. 4) are obtained from the SSURGO database. The parameters are homogeneous within each unit, but vary between units. The LiDAR DEM and smoothed DEM raster files have a horizontal resolution of $5 \times 5 \text{ ft}^2$. The smoothed DEM used for calculating the distance between infiltrative surface and water table is adapted from Wang et al. (2013), generated by calibrating ArcNLET flow model against average water table elevation at 13 monitoring wells shown in Fig. 4. The comparison between smoothed DEM and measured water table in Fig. 5 shows that the smoothed DEM and water table have similar shape (the slope of the linear regression curve is close to one). The intercept of 2.86 m is used for variable A defined in Sect. 2.7 for calculating the water table elevation. Since the smoothed DEM varies in space, the water table elevation and subsequently the distance between infiltrative surface and water table also vary in space.

Data are extremely scarce at the modeling site. Except the data described above, there are no measurements of other model parameters, moisture contents, and concentrations of ammonium and nitrate in the vadose zone. Lack of monitoring data makes model calibration impossible. While this is common in many management projects of nitrogen contamination, decision-making is always needed in a timely manner before extensive scientific investigation is conducted. An order-of-magnitude estimation is needed for decision-making, and VZMOD is

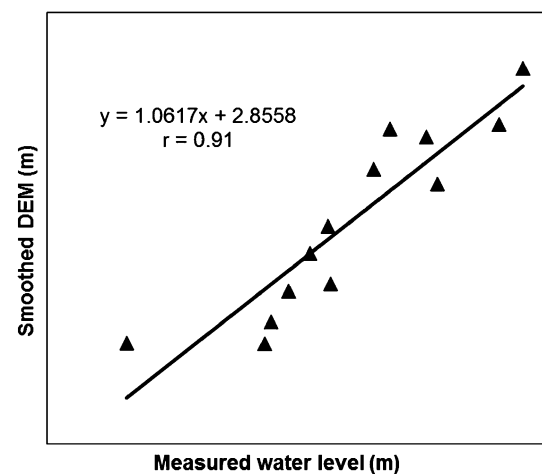


Fig. 5 Linear regression curve between measured water level and smoothed DEM at Julington Creek neighborhood

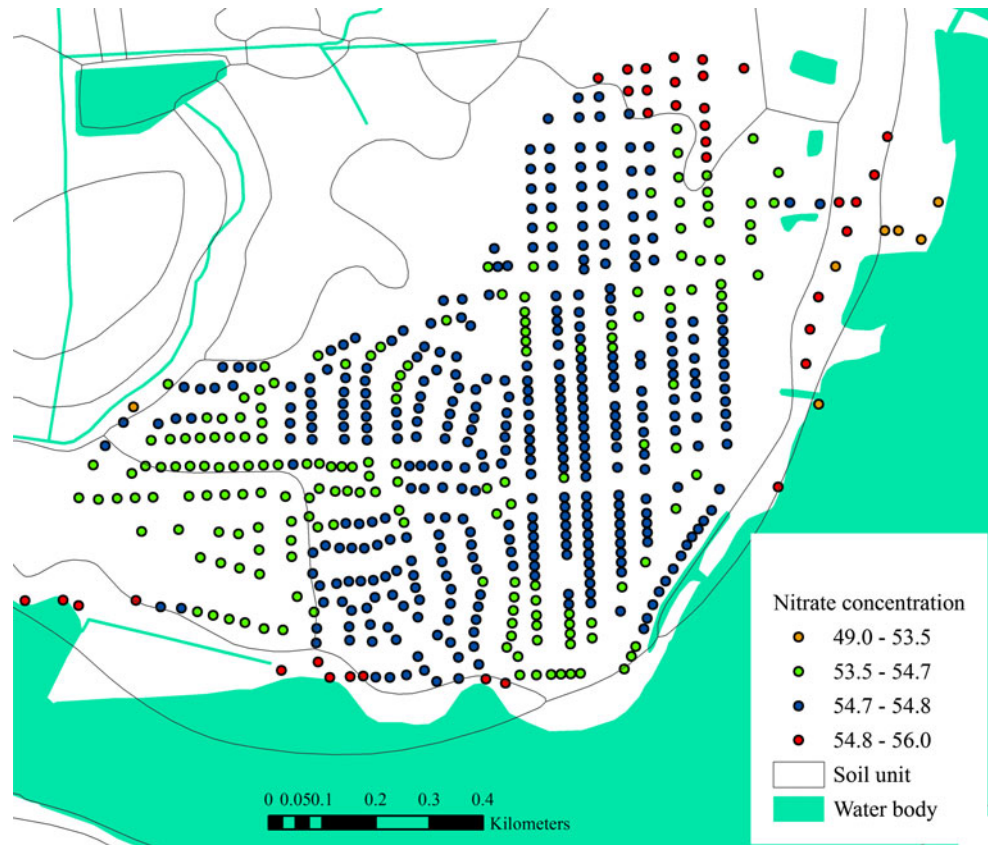
able to provide such an estimate by using literature values of model parameters. The model parameters used in this study are adapted from McCray et al. (2010) obtained from a thorough literature review. In particular, constant effluent concentrations of ammonium and nitrate (also adapted from McCray et al. 2010) are used for all septic systems, although VZMOD can handle the situation that each septic system has its own effluent concentration.

The simulated nitrate concentrations at water table for the individual septic systems are shown in Fig. 6. This figure indicates a relatively uniform distribution of nitrate concentration over the domain within a range from 49 to 56 mg/L. Since the concentration is higher than 10 mg/L, it suggests that current management of septic systems is not sustainable and that more management means are needed. Despite the relatively small range of nitrate concentrations at water table, spatial variability of the simulated nitrate concentrations is observed in Fig. 6, with high nitrate concentrations in the north end of the domain and close to river. Since the concentrations of ammonium and nitrate at the infiltrative surface are the same for all septic systems, spatial variability of nitrate concentrations at water table is determined by the following factors: (1) soil types (because of different nitrification and denitrification parameters for different soil types), (2) soil units (because of different hydraulic conductivity and porosity for different soil units), (3) distances between infiltrative surface and water table (because of different moisture content distributions for different distances). Since the soil type is the same for almost all (except 3) septic systems, the second factor explains spatial variability of nitrate concentrations between different soil units. Spatial variability of nitrate concentration within the same unit (e.g., the largest one in Fig. 6) is attributed to the third factor. This is the reason

that nitrogen dynamics is closely related to hydrologic factors such as moisture content dynamics.

The distance between infiltrative surface and water table varies significantly between soil units, and its effect on nitrogen transformation and transport is investigated. Figure 7 plots the concentration profiles of six septic systems with FID 100, 391, 435, 515, 543, and 552. As shown in Fig. 4, the six septic systems are located in different soil units. Figure 7 shows that the depth to water table is dramatically different at different septic systems, resulting in significantly different shapes of the concentration profiles. It suggests importance of considering spatial variability of the depth to water table. Ammonium concentration in Fig. 7 decreases while nitrate concentration increases during their downward transport, because ammonium becomes nitrate due to nitrification. The ammonium concentration continues decreasing until all ammonium is transformed into nitrate if water table is deep enough. If water table is shallow (e.g., near surface water bodies such as rivers and streams), the transformation process may not be completed and ammonium concentration is significant at water table. The rate of transformation is different for different septic systems, depending on maximum nitrification rate and the functions of temperature and saturation as described in Sect. 2. In this demonstration, since the maximum nitrification rate and temperature function are

Fig. 6 Calculated nitrate concentration (mg/L) at water table for individual septic systems



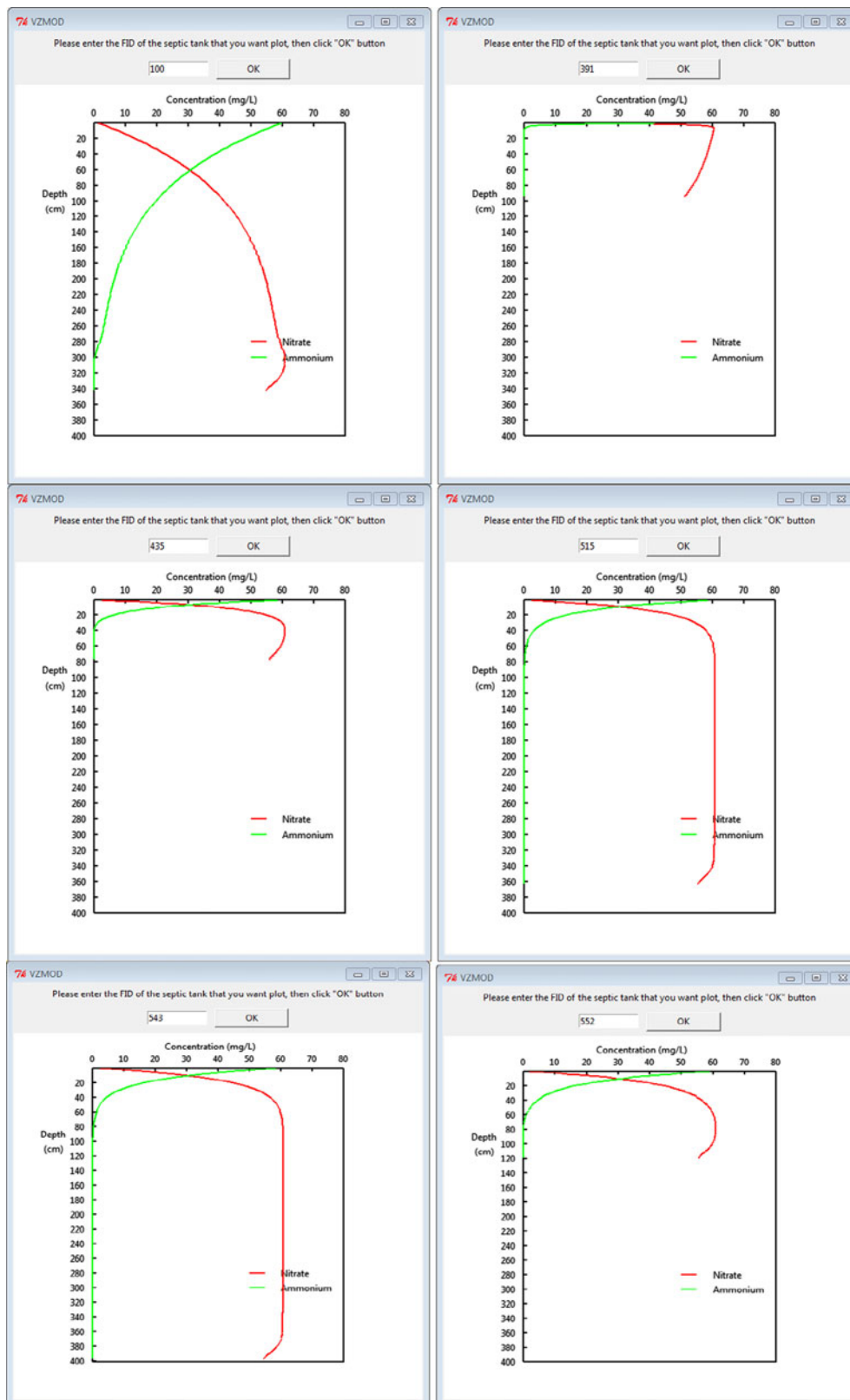


Fig. 7 Vertical profiles of ammonium and nitrate concentrations from infiltrative surface to water table for septic systems with FID 100, 391, 435, 515, 543, and 552, whose locations are shown in Fig. 4

the same for all the septic systems, the actual nitrification rate is determined solely by saturation following Eq. (8). Due to higher saturation in sandy loam soil, 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, it starts decreasing for septic systems with FID 100, 391, 435, and 552, due to denitrification. While denitrification also occurs before the nitrate concentration reaches the maximum, it is negligible because the maximum concentration is high, close to 61 mg/L, the total nitrogen into the system as specified in the “Effluent params” block of Fig. 2. The rate of denitrification increases when the profile approaches the water table, because the saturation function increases with saturation according to Eq. (9) and saturation increases toward the water table. For septic systems with FID 515 and 543, after reaching the maximum, the nitrate concentration has negligible change for a distance and then decreases. The reason for the near constant concentration is that the denitrification rate is negligible due to the value of saturation. When the saturation is large near the water table, the denitrification process becomes strong and causes decrease in nitrate concentration.

The VZMOD-simulated ammonium and nitrate profiles help better understand the nitrogen transformation and transport for sustainable management of nitrogen contamination. The profiles in Fig. 7 indicate that, with the default parameter values, ammonium is transformed to nitrate quickly after septic effluent leaves drainfields at Julington Creek. Due to relatively insignificant denitrification in the vadose zone, nitrate concentration at water table always exceeds the regulation criterion of 10 mg/L. Since new septic design techniques may reduce the amount of ammonium entering vadose zone but cannot enhance the denitrification process, converting septic systems to centralized sewage appears to be a necessary management approach for sustainable protection of groundwater and surface water bodies.

4 Summary and conclusions

To support sustainable environmental management and protection of public health from nitrogen contamination due to septic systems, VZMOD is developed to simulate vertical distributions of ammonium and nitrate in vadose zone between drainfield of septic system and groundwater. This software is based on a physical model and its numerical solutions of unsaturated flow and nitrogen transformation and transport, which is the major difference

between VZMOD and other GIS-based software for nitrogen modeling. While the physical model is similar to that of STUMOD developed by McCray et al. (2010), VZMOD differs from STUMOD in that VZMOD solves the model numerically using the finite element method, but STUMOD relies on analytical solutions. The numerical solution is more flexible and subject to less assumption than the analytical solution. More importantly, STUMOD is an EXCEL-based software that considers only one septic system, whereas VZMOD is an ArcGIS-based software that can consider either one or multiple septic systems as well as spatial variability of hydraulic conductivity, porosity, and/or water table. VZMOD is designed to execute in different modes to be compatible with different levels of data availability in various projects of nitrogen environmental management. For example, spatial variability of hydraulic conductivity and water table can be addressed either together or separately in VZMOD. The application of VZMOD at Julington Creek exhibits importance of the spatial variability of water table to the vertical transport of ammonium and nitrate.

VZMOD is designed to be used together with ArcNLET, a software simulating nitrate transport in groundwater and estimating nitrate load from septic systems to surface water bodies. The two software programs share some common ArcGIS files such as the point file for septic locations and raster files for hydraulic conductivity and porosity. In addition, the two softwares are coupled in two ways. First, the smooth DEM generated by the ArcNLET's flow module mimics the shape of water table and is used by VZMOD to address spatial variability of depth to water table. On the other hand, the nitrate concentrations at water table simulated by VZMOD can be used as a direct input to the transport module of ArcNLET for its groundwater modeling.

While VZMOD has been applied at nitrogen modeling at Julington Creek neighborhood, it has not been thoroughly verified and validated. In the future study, comprehensive code verification and model validation will be conducted using numerical, laboratory, and field experiments. The code verification is straightforward, and it can be carried out by comparing VZMOD results with analytical solutions or numerical solutions of well-benchmarked programs such as TOUGHREACT-N. However, model validation is more challenging. As shown in Ajami and Gu (2010), due to complexity of nitrogen transformation and transport, even TOUGHREACT-N cannot fully capture spatial and temporal patterns of nitrogen concentrations. On the other hand, although the transformation and transport model of VZMOD is simplified, there is still lack of site-specific values of the model parameters. It is critical to conduct field investigation to collect necessary data for gaining insights into the model parameters through model

calibration or model abstraction. These are warranted in future study.

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