

Estimating ammonium and nitrate load from septic systems to surface water bodies within ArcGIS environments



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SUMMARY

This paper presents a recently developed software, ArcGIS-based Nitrogen Load Estimation Toolkit (ArcNLET), for estimating nitrogen loading from septic systems to surface water bodies. The load estimation is important for managing nitrogen pollution, a world-wide challenge to water resources and environmental management. ArcNLET simulates coupled transport of ammonium and nitrate in both vadose zone and groundwater. This is a unique feature that cannot be found in other ArcGIS-based software for nitrogen modeling. ArcNLET is designed to be flexible for the following four simulating scenarios: (1) nitrate transport alone in groundwater; (2) ammonium and nitrate transport in groundwater; (3) ammonium and nitrate transport in vadose zone; and (4) ammonium and nitrate transport in both vadose zone and groundwater. With this flexibility, ArcNLET can be used as an efficient screening tool in a wide range of management projects related to nitrogen pollution. From the modeling perspective, this paper shows that in areas with high water table (e.g. river and lake shores), it may not be correct to assume a completed nitrification process that converts all ammonium to nitrate in the vadose zone, because observation data can indicate that substantial amount of ammonium enters groundwater. Therefore, in areas with high water table, simulating ammonium transport and estimating ammonium loading, in addition to nitrate transport and loading, are important for avoiding underestimation of nitrogen loading. This is demonstrated in the Eggleston Heights neighborhood in the City of Jacksonville, FL, USA, where monitoring well observations included a well with predominant ammonium concentrations. The ammonium loading given by the calibrated ArcNLET model can be 10–18% of the total nitrogen load, depending on various factors discussed in the paper.

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1. Introduction

Excessive nitrogen loading to surface water bodies has led to nutrient enrichment and eutrophication in watersheds and estuaries (Dodds and Welch, 2000; U.S. EPA, 2002; Sanderson and Coade, 2010), and nitrogen pollution has been considered as one of the most prevalent and challenging environmental problems worldwide (U.S. NRC, 2000; Bricker et al., 2007). Depending on land use, hydrology and wastewater management in a watershed, wastewater treatment using onsite sewage treatment and disposal systems (OSTDS) (a.k.a., septic systems) can be an important source of nitrogen (Burkart and James, 1999; Goolsby et al., 1999; Schilling and Zhang, 2004; Wood et al., 2015). In USA, approximately 25% of the population use septic systems (Hazen and Sawyer, 2009),

and septic systems are the second largest source of groundwater nitrogen contamination (Canter and Knox, 1985). In the state of Florida, about 2.5 million septic systems are in use by about 30% of the population (FDOH, 2014), and Badruzzaman et al. (2012) estimated that nitrogen input from septic systems into the Florida environment is $2.4\text{--}4.9 \times 10^{10}$ g N/year. This estimated input is less than the estimate of 1.4×10^{11} g N/year from fertilizer application, but more than the estimates of $1.2 \times 10^8\text{--}2.6 \times 10^{10}$ g N/year from reclaimed water and of $5.9\text{--}9.4 \times 10^9$ g N/year from atmospheric deposition. For management of nitrogen pollution, it is important to study nitrogen transport from septic systems through the vadose zone and shallow groundwater to surface waterbodies (Schilling, 2002; Schilling and Zhang, 2004; Maruyama et al., 2011).

The fate and transport of nitrogen from a septic system, consisting generally of a septic tank with a drain field from which the effluent percolates through the soil, includes several reactions and transformations. After ammonification (or mineralization) in

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the septic tank, nitrogen in the septic tank effluent is largely in the form of ammonium. As the effluent discharged into the drain field and travels from the drain field downwards through the vadose zone, the ammonium is nitrified when the environment is oxic. Some assessments have considered nitrate as the only nitrogen species of concern from septic (e.g., Hajhmad and Almasri, 2009; MACTEC, 2010; Rios et al., 2013; Wang et al., 2013a; Kazakis and Voudouris, 2015). However, complete conversion to nitrate may not occur due to anoxic conditions, especially when the water table is shallow (Heatwole and McCray, 2007), in which case both ammonium and nitrate can enter groundwater and, depending on further transformation, can travel to surface water bodies. Monitoring data collected in several neighborhoods in the city of Jacksonville, FL, where nitrogen contamination from septic systems is the suspected source (Leggette, Brashears, and Graham, Inc., 2004), were used to evaluate the speciation of nitrogen in groundwater. The analysis of the data by Ouyang and Zhang (2012) showed that the average concentrations in groundwater of organic nitrogen, ammonium, and NO_x (nitrate and nitrite) are 0.25 mg/L, 1.19 mg/L, and 5.67 mg/L, respectively. These values indicate that, while the organic nitrogen concentration is much smaller than the nitrate concentration, the ammonium concentration is of similar magnitude to the nitrate concentration. For improved understanding and effective management of nitrogen pollution it is beneficial to simulate transport of both ammonium and nitrate and to estimate ammonium and nitrate loading to surface water bodies.

Various computational codes have been developed to do so (Prommer et al., 2003; Almasri and Kaluarachchi, 2007; Peña-Haro et al., 2009; Bonton et al., 2012; Andersen et al., 2007; Lalehzari et al., 2013; Zhu et al., 2013). TOUGHREACT-N, a numerical code developed by Maggi et al. (2008), is viewed as the most sophisticated code to date for simulating coupled processes of advective and diffusive nutrient transport, multiple microbial biomass dynamics, and equilibrium and kinetic chemical reactions in soil and groundwater. TOUGHREACT-N has been used in nitrogen modeling of various cases (Ajami and Gu, 2010; Gu et al., 2012). However, codes of such complexity are mainly for fundamental research, and their uses for environmental management projects may be limited for the following reasons. First, using complex codes usually requires intensive input data (e.g., hydrologic and soil properties) and calibration data (e.g., nitrogen concentrations), but the data needs may not be satisfied in practice. In addition, the complexity may be a hurdle for general users to set up model runs; a trained professional is always required to operate the models and interpret modeling results for decision-makers of environmental management. At last, running complex codes always takes long execution time, which may not be computationally affordable in practice. For many projects of nitrate transport modeling and load estimation, including those related to environmental regulation such as Total Maximum Daily Load (TMDL), it may not be feasible to use the complex codes, and less complex screening models may be more practical and appropriate for many management projects that require loading estimates on a watershed scale (Yang et al., 2014).

The first generation of the ArcGIS-based Nitrate Load Estimation Toolkit (ArcNLET) was developed by Rios et al. (2013) as such a tool. ArcNLET is a GIS-embedded model in which all the flow and transport simulations and related pre- and post-processing are conducted within the ArcGIS environment. It thus fully utilizes the GIS capability of pre- and post-processing spatial features (e.g., topography and surface water bodies) involved in nitrogen modeling (Schilling and Wolter, 2007; Yang and Lin, 2011; Thorp and Bronson, 2013). ArcNLET considers the fundamental processes of groundwater flow, solute transport with advection and dispersion, and denitrification. ArcNLET was used for estimating nitrate

loads from thousands of septic systems to surface water bodies in several neighborhoods in the City of Jacksonville (Wang et al., 2013a) and in the St. Lucie River and Estuary Basin in Florida, USA (Ye et al., 2015). However, earlier use of the ArcNLET tool only focused on simulating nitrate transport in groundwater and estimating nitrate loading. At that time, the model could not simulate the transport and transformation of nitrate and ammonium in the vadose zone and it did not include transport of ammonium in the ground water. The new ArcNLET tool now allows the calculation of nitrogen transformation and transport in the vadose zone, which provides better estimates of nitrogen concentrations at the source plane in groundwater system. The new ArcNLET tool also includes ammonium reactive transport in groundwater and loading to surface water bodies, which allows better estimation of total nitrogen loading, especially in areas with shallow water table where nitrification may be incomplete.

The objective of this study was to enhance the modeling capability of ArcNLET to simulate transport of both ammonium and nitrate in not only vadose zone but also groundwater. The enhancement is necessary when ammonium is not completely nitrified in vadose zone and enters into groundwater. The enhancement is done with two major code development. First, in comparison with the previous ArcNLET (Rios et al., 2013) that simulates groundwater transport of nitrate only, the new ArcNLET has the capacity to simulate groundwater transport of both ammonium and nitrate. This was achieved by overhauling the previous ArcNLET to incorporate new algorithms for simulating simultaneous transport of ammonium and nitrate in groundwater. This new development is the focus of this study. The other enhancement is to develop a new capability of simulating unsaturated transport of both ammonium and nitrate in the vadose zone. This was achieved by integrating into ArcNLET another ArcGIS-based software, VZMOD (Vadose Zone Model), developed by Wang et al. (2012, 2013b) that estimates ammonium and nitrate concentrations in the vadose zone. The integration is seamless, and more details are given in Section 2. With the two new capabilities, ArcNLET now stands for ArcGIS-based Nitrogen (dissolved inorganic nitrogen including ammonium and nitrate) Load Estimation Toolkit, and it can simulate nitrogen reactive transport from septic drain fields to surface water bodies.

In the following, we summarize the conceptual and mathematical models of fate and transport of ammonium and nitrate in Section 2, followed by a description of the computational implementation and verification in Section 3. In Section 4, we illustrate the application of the new code to a neighborhood in the city of Jacksonville, FL. The application achieves agreement between results of the new ArcNLET code and observed concentrations of ammonium and nitrate, and shows that ignoring ammonium transport in groundwater can result in under-estimation of nitrogen loading to surface water bodies in areas where water table is shallow and nitrification is incomplete.

2. Conceptual and mathematical models

This section gives in Section 2.1 a brief description of the conceptual model of flow and nitrogen fate and transport in the vadose zone and groundwater. Its focus is on the development of the mathematical model for ammonium and nitrate reactive transport in groundwater (Section 2.2) and the estimation of ammonium and nitrate loading via groundwater transport (Section 2.3).

2.1. Conceptual model of ammonium and nitrate reactive transport

Fig. 1 shows the conceptual model of ammonium and nitrate transformation processes in the vadose zone and groundwater.

The conceptual and mathematical models of vadose zone processes in the new ArcNLET code are the same as those of VZMOD described previously by Wang et al. (2012, 2013b). VZMOD calculates saturation and concentration profiles between each drain field and the water table for steady-state, one-dimensional vertical transport with constant incoming water, ammonium, and nitrate fluxes. VZMOD also simulates the following geochemical reactions: linear adsorption of ammonium on soil particles, first-order kinetics of nitrification that transforms ammonium to nitrate, and first-order kinetics of denitrification that transforms nitrate to nitrogen gas. The first-order nitrification and denitrification rates are evaluated by multiplying potential rates with correction factors (between zero and one) due to impacts of temperature and saturation on nitrification and denitrification. Although aerobic conditions in unsaturated soils prevent optimal denitrification from happening (nitrification dominates over denitrification), denitrification in soils has long been reported (e.g., Kirda et al., 1974; Reed and Crites, 1984), and aerobic denitrifiers have been continuously isolated by the microbiology community (e.g., Takaya et al., 2003). In practice, an empirical threshold of degree of saturation is used, and denitrification occurs when the threshold is exceeded. As shown in Heinen (2006), the threshold varies between 0.5 and 0.9. Following McCray et al. (2010), the threshold of 0.6 is used in VZMOD.

VZMOD is seamlessly integrated with ArcNLET in the following ways. First, the water table estimated from the ArcNLET groundwater modeling is used as the bottom boundary of the vadose zone modeling of VZMOD. The distance between drain field infiltrative surface and water table is estimated based on the digital elevation model (DEM) of the ground surface and an estimate for the water table. VZMOD assumes a constant depth of each drain field infiltrative surface below ground surface, 18 in. in this study (Wang et al., 2012). The water table elevation is estimated by subtracting a constant from the smoothed DEM given by ArcNLET as discussed below. This constant is the intercept of a linear regression between observed water table at monitoring wells and their corresponding smoothed DEM elevation. Examples of determining the constant can be found in Wang et al. (2012, 2013a, 2013b). When the estimated distance between the drain field and water table is negative near surface water bodies, VZMOD assumes a small distance (e.g., 0.1 cm), which corresponds to negligible nitrification. This distance could be modified to account for modern onsite systems, such as mounded drain fields, which maintain a water table separation. Second, the ammonium and nitrate concentrations, but not necessarily the mass flux, given by VZMOD at the water table, are used as the inputs to the modeling of ammonium and nitrate fate and transport in groundwater in the new ArcNLET code.

The conceptual and mathematical models of groundwater flow in the new ArcNLET code are the same as those described by Rios et al. (2013). To summarize, the steady-state flow field is represented in a two-dimensional raster field. This field is obtained by smoothing the topography obtained from a digital elevation model (DEM) and using it for the simulation of hydraulic gradients, based on the assumption that the water table is a subdued replica of topography (Haitjema and Mitchell-Bruker, 2005). The model relies on the gradients and surface water body information, along with soil information, to establish a flow path and travel time between each septic system and a surface water body. The model then estimates reactive advective–dispersive transport along each flow path at the average velocity and calculates the load to the surface water body. The conceptual and mathematical models of ammonium and nitrate reactive transport in groundwater are new, and they are the focus of this paper.

When septic tank effluent infiltrates downward from the drain field, if not all the ammonium is nitrified to nitrate in the vadose

zone, then both ammonium and nitrate enter the water table and travel in the groundwater. During the transport, ammonium adsorbs linearly and nitrate denitrifies following a first-order reaction. First-order nitrification continues for the adsorbed and dissolved ammonium, which increases nitrate concentrations. Although optimal nitrification generally does not occur within groundwater, nitrification in groundwater has been reported in literature of laboratory and field studies (e.g., Bjerg et al., 1995; Erskine, 2000; Smith et al., 2006), and reviewed by Buss et al. (2004) and McMahon and Chapelle (2008). The ideal way of simulating nitrification and denitrification in soil and ground is to explicit model redox conditions together with the species (e.g., carbon) related to nitrification and denitrification, as done in MacQuarrie and Sudicky (2001), Lee et al. (2006), and Maggi et al. (2008). This however is not pursued in this study in favor of developing a simplified model for practical use of environmental management. The simplified modeling of ammonium and nitrate reactive transport in this study is described below.

2.2. Mathematical model of ammonium and nitrate reactive transport in groundwater

The two-dimensional reactive transport of ammonium and nitrate is assumed to be steady state, and the governing equations are as follows:

$$0 = D_x \frac{\partial^2 c_{\text{NH}_4^+}}{\partial x^2} + D_y \frac{\partial^2 c_{\text{NH}_4^+}}{\partial y^2} - v \frac{\partial c_{\text{NH}_4^+}}{\partial x} - k_{\text{nit}} \left(1 + \frac{\rho k_d}{\theta} \right) c_{\text{NH}_4^+}, \quad (1)$$

$$0 = D_x \frac{\partial^2 c_{\text{NO}_3^-}}{\partial x^2} + D_y \frac{\partial^2 c_{\text{NO}_3^-}}{\partial y^2} - v \frac{\partial c_{\text{NO}_3^-}}{\partial x} + k_{\text{nit}} \left(1 + \frac{\rho k_d}{\theta} \right) c_{\text{NH}_4^+} - k_{\text{deni}} c_{\text{NO}_3^-}, \quad (2)$$

where D_x and D_y ($\text{L}^2 \text{T}^{-1}$) are the dispersivity coefficients in the longitudinal (x) and horizontal transverse (y) directions, respectively; $c_{\text{NH}_4^+}$ and $c_{\text{NO}_3^-}$ (M L^{-3}) are the concentrations of ammonium and nitrate, respectively; v (L T^{-1}) is linear groundwater velocity in the longitudinal direction; ρ (M L^{-3}) is bulk density; k_d ($\text{L}^3 \text{M}^{-1}$) is linear adsorption coefficient of ammonium; k_{nit} and k_{deni} (T^{-1}) are the first-order decay coefficients of nitrification and denitrification, respectively; and θ (–) is effective porosity. Eqs. (1) and (2) are based on the principle of mass conservation, and can be derived by following the standard procedure given in textbooks such as that of Zheng and Bennett (2002). The last term at the right hand side of Eq. (1) is the same as the second to the last term at the right hand side of Eq. (2) and considers nitrification of dissolved and adsorbed ammonium with first-order kinetics. The last term at the right hand side of Eq. (2) describes the denitrification of nitrate with first-order kinetics. The extents of nitrification and denitrification are controlled by the coefficients of nitrification and denitrification. The impact of redox conditions on nitrification and denitrification lead to the general expectation that nitrification reaction coefficients will be larger in the vadose zone than in groundwater while denitrification reaction coefficients will be larger in groundwater. Values for these coefficients should be chosen based on site specific conditions.

The boundary conditions for the ammonium and nitrate transport assume a vertical source plane underneath the drain field and are as follows:

$$c_{\text{NH}_4^+}(0, y) = \begin{cases} c_{\text{NH}_4^+,0} & -\frac{y}{2} < y < \frac{y}{2} \\ 0 & \text{elsewhere} \end{cases}; \lim_{x \rightarrow \pm\infty} \frac{\partial c_{\text{NH}_4^+}(x, y)}{\partial x} = 0; \lim_{y \rightarrow \pm\infty} \frac{\partial c_{\text{NH}_4^+}(x, y)}{\partial y} = 0, \quad (3)$$

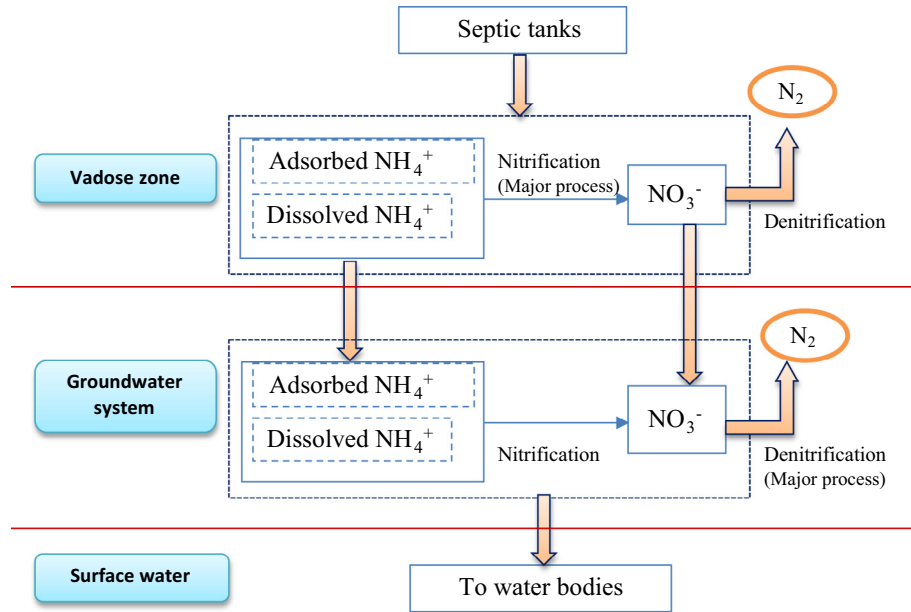


Fig. 1. Conceptual model of ammonium and nitrate transformation in the vadose zone and groundwater used for the new ArcNLET code.

$$c_{\text{NO}_3^-}(0, y) = \begin{cases} c_{\text{NO}_3^-,0} & -\frac{Y}{2} < y < \frac{Y}{2} \\ 0 & \text{elsewhere} \end{cases}; \lim_{x \rightarrow -\infty} \frac{\partial c_{\text{NO}_3^-}(x, y, t)}{\partial x} = 0; \lim_{y \rightarrow \pm\infty} \frac{\partial c_{\text{NO}_3^-}(x, y, t)}{\partial y} = 0, \quad (4)$$

where Y is the width of a source plane introduced for estimating the mass of ammonium and nitrate. By adopting the pseudo three-dimensional model used in EPA BIOCHLOR model (Aziz et al., 2000), it is assumed that contaminants from a septic drain field form a vertically oriented plane with the size of Y in the width and Z in the height. The Y - Z plane has a constant concentration, $c_{\text{NH}_4^+,0}$ for ammonium and $c_{\text{NO}_3^-,0}$ for nitrate, and the contaminants enter the shallow aquifer by advection and dispersion. The origin of the coordinate system is located at the center of the Y - Z plane with the positive x and y directions rightward and upward, respectively. While the source plane concentrations can be evaluated by using VZMOD, if the simulated concentrations of VZMOD are zero, a small value of 10^{-4} mg/L is assigned to $c_{\text{NH}_4^+,0}$ and $c_{\text{NO}_3^-,0}$ to avoid numerical instability. This small value does not affect the ultimate load estimation.

The analytical solutions of Eqs. (1) and (2) are obtained by using the method of Sun et al. (1999) that transforms the two coupled equations into two independent equations. This is done by defining the auxiliary variables,

$$a_{\text{NH}_4^+} = c_{\text{NH}_4^+}, \quad (5)$$

$$a_{\text{NO}_3^-} = c_{\text{NO}_3^-} + \frac{k_{\text{nit}}(1 + \rho k_d/\theta)}{k_{\text{nit}}(1 + \rho k_d/\theta) - k_{\text{deni}}} c_{\text{NH}_4^+}. \quad (6)$$

With the auxiliary variables, Eq. (1) does not change, except that $c_{\text{NH}_4^+}$ is replaced by $a_{\text{NH}_4^+}$; Eq. (2) is transformed to,

$$0 = D_x \frac{\partial^2 a_{\text{NO}_3^-}}{\partial x^2} + D_y \frac{\partial^2 a_{\text{NO}_3^-}}{\partial y^2} - v \frac{\partial a_{\text{NO}_3^-}}{\partial x} - k_{\text{deni}} a_{\text{NO}_3^-}. \quad (7)$$

Therefore, the two transformed equations have the same form below,

$$D_x \frac{\partial^2 a_i}{\partial x^2} + D_y \frac{\partial^2 a_i}{\partial y^2} - v \frac{\partial a_i}{\partial x} - k_i a_i = 0 \quad (i = \text{NH}_4^+, \text{NO}_3^-) \\ k_i = \begin{cases} k_{\text{nit}} \left(1 + \frac{\rho k_d}{\theta}\right) & i = \text{NH}_4^+ \\ k_{\text{deni}} & i = \text{NO}_3^- \end{cases}. \quad (8)$$

For Eq. (8), the analytical solution of Domenico (1987) is used, and its simplification for the two-dimensional, steady-state condition is (Rios et al., 2013),

$$a(x, y) = \frac{a_0}{2} \times F_1(x) \times F_2(y, x), \quad (9)$$

$$F_1(x) = \exp \left[\frac{x}{2\alpha_x} \left(1 - \sqrt{1 + \frac{4k\alpha_x}{v}} \right) \right], \quad (10)$$

$$F_2(y, x) = \text{erf} \left(\frac{y + Y/2}{2\sqrt{\alpha_y x}} \right) - \text{erf} \left(\frac{y - Y/2}{2\sqrt{\alpha_y x}} \right), \quad (11)$$

where erf is the error function, and α_x and α_y (L) are longitudinal and horizontal transverse dispersivity, respectively. After solving Eq. (8) for the auxiliary variables a_i , the concentrations of ammonium and nitrate are obtained by back-transforming Eqs. (5) and (6) as follows,

$$c_{\text{NH}_4^+} = a_{\text{NH}_4^+}, \quad (12)$$

$$c_{\text{NO}_3^-} = a_{\text{NO}_3^-} - \frac{k_{\text{nit}}(1 + \rho k_d/\theta)}{k_{\text{nit}}(1 + \rho k_d/\theta) - k_{\text{deni}}} a_{\text{NH}_4^+}. \quad (13)$$

Using the method of Sun et al. (1999) enables using the analytical solution of the same form for a_i , and thus saves computational time and reducing complexity of the software development. However, a substantial effort of programming is needed for implementing the modifications to the ArcNLET code. In the ArcNLET numerical implementation of the analytical solutions, the modeling domain is discretized into a grid of uniform cells with the size of $\Delta x \times \Delta y$, and for a given plume the concentrations are evaluated for each cell. This approach of raster discretization allows capturing the effect of overlapping plumes (Rios et al., 2013).

2.3. Estimation of ammonium and nitrate loadings through groundwater

The loadings of ammonium and nitrate are estimated using a mass-balance approach for the final rasterized concentration field. The nitrogen mass entering the water bodies equals to the difference between nitrogen entering groundwater and nitrogen removal during the groundwater transport. Specifically speaking,

the ammonium and nitrate loadings for each plume are estimated via,

$$M_{\text{NH}_4^+, \text{out}} = M_{\text{NH}_4^+, \text{in}} - M_{\text{nit}}, \quad (14)$$

$$M_{\text{NO}_3^-, \text{out}} = M_{\text{NO}_3^-, \text{in}} + M_{\text{nit}} - M_{\text{deni}}, \quad (15)$$

where $M_{\text{NH}_4^+, \text{out}}$ and $M_{\text{NO}_3^-, \text{out}}$ (M T^{-1}) are the mass outflow rate (i.e., the loadings) of ammonium and nitrate, respectively, to surface water bodies; $M_{\text{NH}_4^+, \text{in}}$ and $M_{\text{NO}_3^-, \text{in}}$ (M T^{-1}) are the mass inflow rate of ammonium and nitrate, respectively, from septic systems to groundwater; M_{nit} (M T^{-1}) is the ammonium mass removal rate due to nitrification, and M_{deni} (M T^{-1}) is the nitrate mass removal rate due to denitrification. The mass removal rates caused by nitrification and denitrification are calculated as,

$$M_{\text{nit}} = \sum_j k_{\text{nit}}(1 + \rho k_d/\theta) \times c_{\text{NH}_4^+, j} \times V_j \times \theta, \quad (16)$$

$$M_{\text{deni}} = \sum_j k_{\text{deni}} \times c_{\text{NO}_3^-, j} \times V_j \times \theta, \quad (17)$$

where V_j (L^3) is the volume of the j -th cell of the ammonium and nitrate plumes. The volume is calculated as $\Delta x \times \Delta y \times Z$, where Z (L) is the height of source plane, and Δx and Δy (L) are the cell sizes in the x and y directions, respectively, determined by the ArcNLET users and input through ArcNLET user interface discussed in Section 3. The values of Z used in the calculation can be estimated in the two ways discussed below.

By considering advective and dispersive mass flux, the equation for estimating inflow mass rates were derived in Appendix A, and they are,

$$M_{\text{NH}_4^+, \text{in}} = c_{\text{NH}_4^+, 0} YZ\theta v \left(\frac{1 + \sqrt{1 + \frac{4k_{\text{nit}}(1 + \rho k_d/\theta)\alpha_x}{v}}}{2} \right), \quad (18)$$

$$M_{\text{NO}_3^-, \text{in}} = a_{\text{NO}_3^-, 0} YZ\theta v \left(\frac{1 + \sqrt{1 + \frac{4k_{\text{deni}}\alpha_x}{v}}}{2} \right) - \frac{k_{\text{nit}}(1 + \rho k_d/\theta)}{k_{\text{nit}}(1 + \rho k_d/\theta) - k_{\text{deni}}} \times M_{\text{NH}_4^+, \text{in}}, \quad (19)$$

where $a_{\text{NO}_3^-, 0}$ is the auxiliary variable of $c_{\text{NO}_3^-, 0}$ that is calculated according to Eq. (6).

The equations make it possible to handle the inflow mass rates in two ways. The first one is to directly estimate the rates using the equations given source concentrations and assuming dimensions Y (such as a drain field width) and Z (a harder to assess source zone depth). However, it requires specifying a uniform source plane height, Z , and results in inflow mass rates that vary for each septic system based on the specific estimate of the groundwater velocity for its flow path. When the height is difficult to estimate but the inflow mass rates can be estimated by other means (e.g., from literature or expert judgment), one can specify the nitrogen mass input rates M_{in} , the sum of $M_{\text{NH}_4^+, \text{in}}$ and $M_{\text{NO}_3^-, \text{in}}$, through ArcNLET user interface, and the code evaluates Z accordingly; the Z value is needed for estimating the cell volume used in Eqs. (16) and (17). According to Eqs. (18) and (19), M_{in} can be calculated for each plume as follows,

$$M_{\text{in}} = \left(Y\theta v c_{\text{NH}_4^+, 0} f_1 Z \right) + \left(Y\theta v a_{\text{NO}_3^-, 0} f_2 Z - \frac{k_1}{k_1 - k_2} \times Y\theta v c_{\text{NH}_4^+, 0} f_1 Z \right), \\ = \left(Y\theta v a_{\text{NO}_3^-, 0} f_2 + \frac{-k_2}{k_1 - k_2} Y\theta v c_{\text{NH}_4^+, 0} f_1 \right) Z, \quad (20)$$

where $k_2 = k_{\text{deni}}$, $k_1 = k_{\text{nit}}(1 + \rho k_d/\theta)$,

$$f_1 = \left(1 + \sqrt{1 + \frac{4k_{\text{nit}}(1 + \rho k_d/\theta)\alpha_x}{v}} \right) / 2, \quad (21)$$

and

$$f_2 = \left(1 + \sqrt{1 + \frac{4k_{\text{deni}}\alpha_x}{v}} \right) / 2. \quad (22)$$

The source plan height, Z , is then calculated as,

$$Z = M_{\text{in}}/Y\theta v \left(a_{\text{NO}_3^-, 0} f_2 + \frac{-k_2}{k_1 - k_2} c_{\text{NH}_4^+, 0} f_1 \right). \quad (23)$$

The two options are implemented in the new ArcNLET and allow users to choose.

3. Software implementation, structure, and verification

Following Rios et al. (2013), the new ArcNLET code of ammonium and nitrate reactive transport is written using Visual Basic .NET programming language. Since VZMOD is written in Python, it is called directly by the Visual Basic .NET programming language and included in the user interface of the new ArcNLET. The new ArcNLET code retains its modular structure with the four modules of Groundwater Flow, Particle Tracking, Transport, and Load Estimation (the name of the last module was changed from Denitrification of Rios et al. (2013) to Load Estimation) (Fig. 2).

The model inputs of the new ArcNLET code include three raster files (for DEM, hydraulic conductivity, and porosity), two shape files (for the locations and attributes of septic systems and surface water bodies), and a number of transport parameters that can be input through the software GUI. The output files include five raster files (for magnitude and direction of seepage velocity, shape of water table, and plumes of ammonium and nitrate), one shape file of flow paths, one text file of ammonium and nitrate concentrations at water table, and one CSV file of nitrogen load estimation that can be processed outside of ArcGIS. The outputs are highlighted in red boxes in Fig. 2.

While the modules of Groundwater Flow and Particle Tracking have not changed from the former ArcNLET code, the Transport module has been revised to accommodate ammonium. The graphical user interface (GUI) of the new Transport module is shown in Fig. 3. This module has the following four functions:

- (1) Simulating only *nitrate* transport in *groundwater*, which is the same as the one developed in the original version of ArcNLET by Rios et al. (2011, 2013). This function is used when ammonium is fully converted to nitrate in the vadose zone.
- (2) Simulating the transport of both *ammonium and nitrate* in *groundwater*. The function is used for the situation that ammonium is not fully converted to nitrate and both ammonium and nitrate enter groundwater. The ammonium transport modeling can be activated by checking the box of “NH4 Parameters”.
- (3) Simulating the transport of both *ammonium and nitrate* in *vadose zone* to produce ammonium and nitrate concentrations at water table. This function can be activated by clicking the “Click to Start VZMOD” button.
- (4) Simulating the transport of both *ammonium and nitrate* in *vadose zone* and in *groundwater*. This function is a combination of functions (2) and (3) above. The VZMOD-produced ammonium and nitrate concentrations at the water table are used automatically by the groundwater modeling.

The modeling procedure for using the new ArcNLET is as follows: (1) run Groundwater Flow and Particle Tracking to

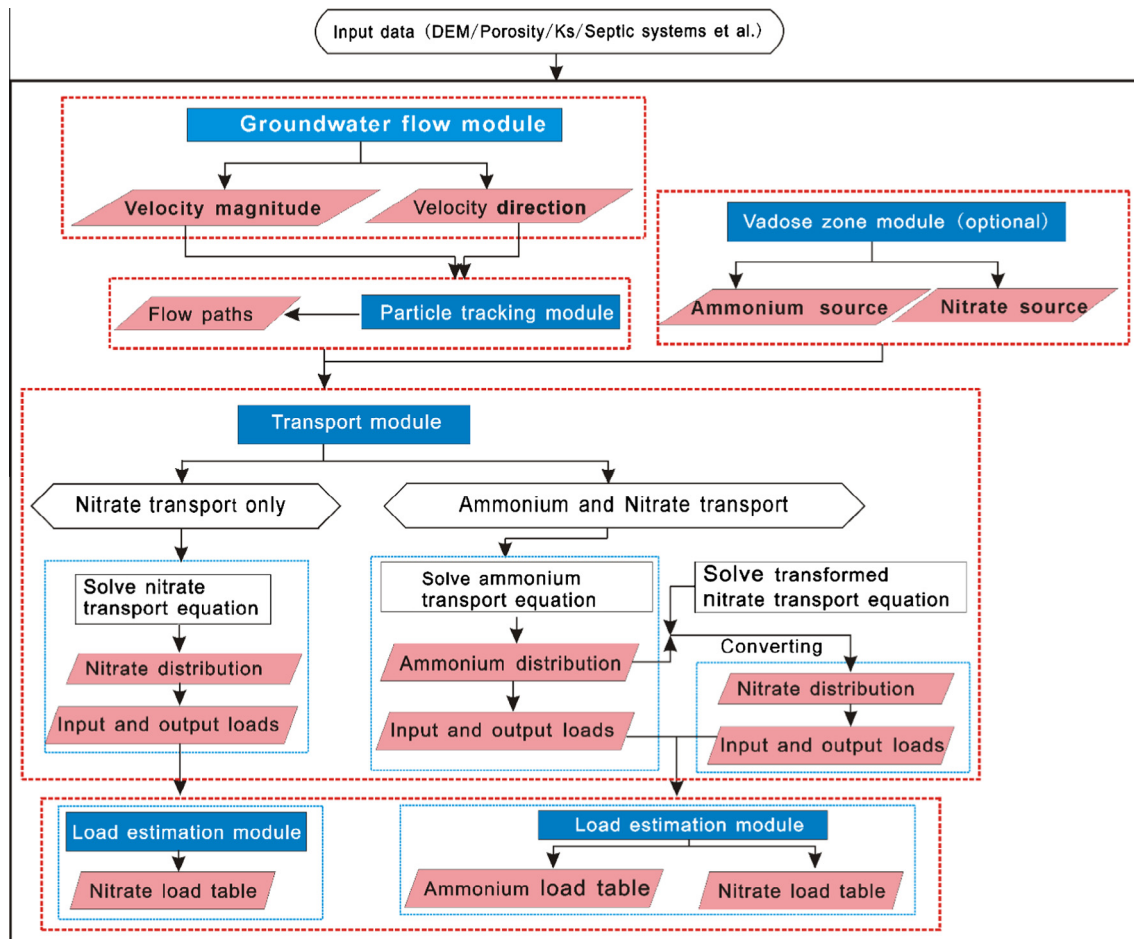


Fig. 2. Overview of the structure of the new ArcNLET code for ammonium and nitrate reactive transport in both vadose zone and groundwater system. The five modules are in the blue boxes, and model outputs are in the red boxes. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

generate the shape of water table and flow paths from septic systems to surface water bodies; (2) run VZMOD to produce ammonium and nitrate concentrations at water table; and (3) run the Transport module for both ammonium and nitrate in groundwater. The design of the Load Estimation module is similar to the Transport module in the way it estimates the separate loadings of ammonium and nitrate to surface water bodies (the GUI of this module is not shown).

Since Rios et al. (2013) and Wang et al. (2013b) have verified the former ArcNLET code and VZMOD, respectively, this paper reports only verification of the new ArcNLET function of simulating ammonium and nitrate transport in groundwater. Code verification is used here in the sense of ensuring that the mathematical equations are correctly programmed. This is done by comparing the ArcNLET results with those obtained using the EPA BIOCHLOR code (Aziz et al., 2000). BIOCHLOR was selected for two reasons. The first reason is that it uses the same analytical solution of Domenico (1987) and the method of Sun et al. (1999) to solve multi-species solute transport. The other reason is that the FORTRAN code of BIOCHLOR is available in its user manual to make transparent the numerical comparison between the results of BIOCHLOR and ArcNLET. Table 1 lists the variable values used to run ArcNLET and BIOCHLOR for the verification. Fig. 4 shows that the plumes simulated by ArcNLET are visually identical to those simulated by BIOCHLOR, which verifies the new ArcNLET code. To illustrate the use of the screening tool and to validate it to some extent by comparison to field data, we present next an example of an application.

4. Software application example

The new ArcNLET is used to estimate the loading of ammonium and nitrate from septic systems to surface water bodies in the Eggleston Heights neighborhood located in Jacksonville, Florida, USA. In the residential neighborhood with few signs of residential fertilizer use, nitrogen from septic systems is believed to be one of the important sources of existing nutrient enrichment in a receiving stream system (Leggette, Brashears, and Graham, Inc., 2004). Eggleston Heights is one of 17 neighborhoods where water table elevation and nitrogen concentrations were routinely monitored during the period of 2005–2010. Eggleston Heights is selected for this study because it has more frequent observations than the other sites do. For the observations at Eggleston Heights, there are more observations in 2005 and 2006 than in other years, with at least one observation in each month from March to December in 2005 and 2006. The Eggleston Heights neighborhood has four monitoring wells installed by Leggette, Brashears, and Graham, Inc. (2004). As shown in Fig. 5, well AM-MW-1 is located at the shore of the Red Bay Branch, and the other three wells are located farther from the water body. Because their depth to water table varies, such well locations are well suited for understanding the impact of water table elevation (depth to ground water) on ammonium and nitrate transport in the vadose zone. Wang et al. (2013a) estimated the nitrate load of Eggleston Heights with the previous version of ArcNLET. However, monitoring data of groundwater quality in this neighborhood suggest that ammonium load should

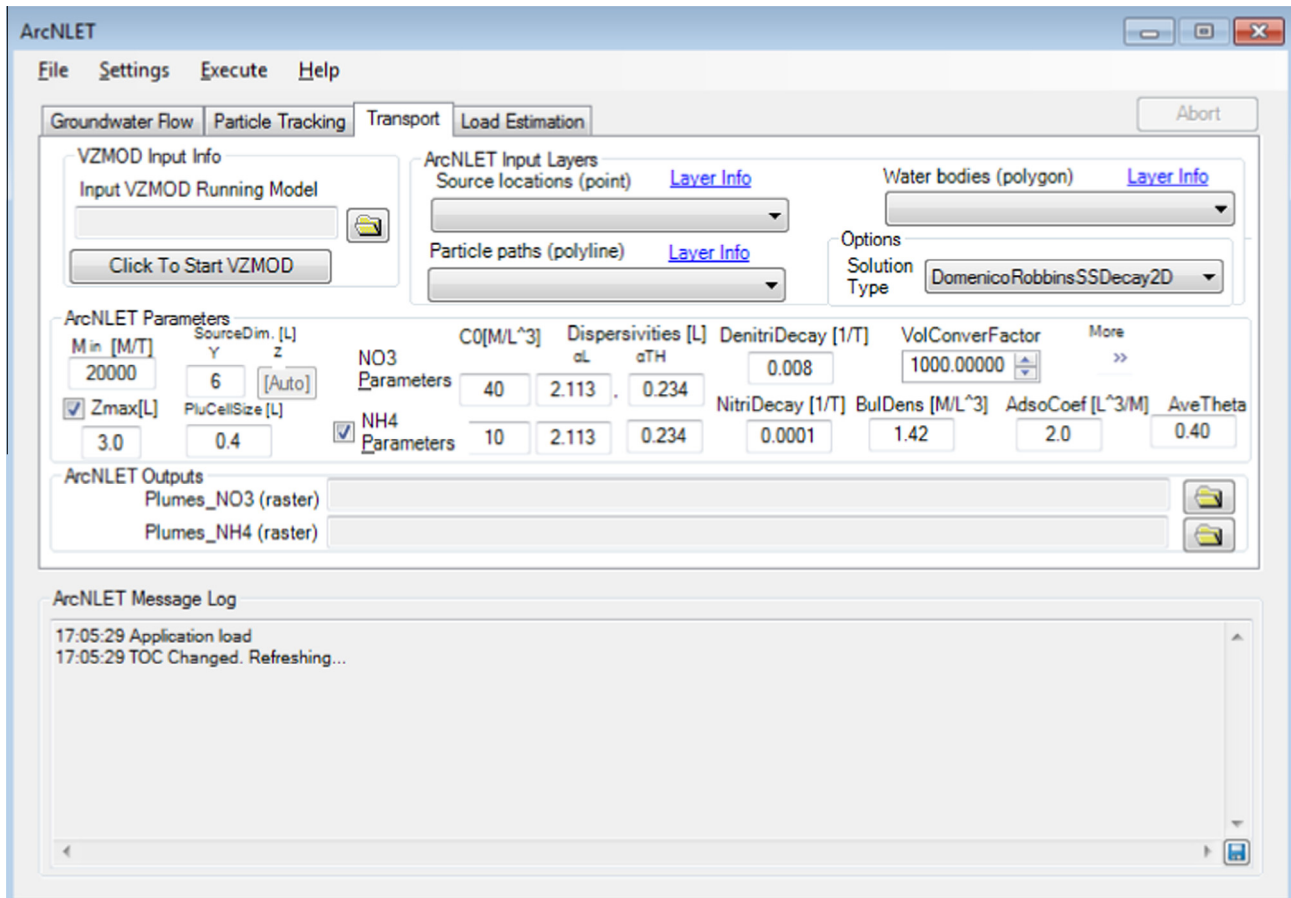


Fig. 3. Graphic user interface (GUI) of the new Transport module that simulates the reactive transport of ammonium and nitrate in groundwater. The reactive transport of ammonium and nitrate in the vadose zone is carried out independently by running VZMOD.

Table 1

Values of the variables used for running ArcNLET and BIOCHLOR to verify the new ArcNLET code.

Variable	Description	Value	Unit
Δx	Cell size in the x direction	0.4	m
Δy	Cell size in the y direction	0.4	m
$C_{NO_3,0}$	Nitrate concentration of the source plane	40	$g\ m^{-3}$
$C_{NH_4,0}$	Ammonium concentration of the source plane	5	$g\ m^{-3}$
v	Seepage velocity in the x -direction	0.078657	$m\ d^{-1}$
α_x	Dispersivity in the x -direction	2.113	m
α_y	Dispersivity in the y -direction	0.234	m
Y	Source plane width in the y direction	6.0	m
Z	Source plane width in the z direction	1.0	m
k_{nit}	First-order nitrification rate	0.0008	d^{-1}
k_{deni}	First-order denitrification rate	0.008	d^{-1}
k_d	Adsorption coefficient of ammonium	4.0	$m^3\ g^{-1}$
ρ	Bulk density	1.42	$g\ m^{-3}$

not be ignored in areas near surface water bodies. The observed water table elevation and concentrations of ammonium and nitrate are plotted in Fig. 6. Among the four monitoring wells, well AM-MW-1 (with shallow water table) has negligible nitrate concentration but consistent ammonium concentration. This indicates incomplete nitrification in the flow paths to well AM-MW-1. Fig. 6 also shows that, at the other three wells where the water table is deeper, the ammonium concentrations are negligible compared to the nitrate concentrations, suggesting complete nitrification along the flow path to these three wells.

To evaluate the steady-state assumption involved in the groundwater flow and nitrogen reactive transport models, linear

trend lines are added to the observations shown in Fig. 6. For the head observations (Fig. 6a), while temporal variability exists, the trend horizontal lines justify the use of steady-state flow model. This is also confirmed by the flow modeling results of Zhu et al. (2015), who used a transient-state, variably saturated flow model with time-varying precipitation and evapotranspiration. The modeling results showed that simulated water table varies slightly over time, not only at the monitoring well locations but over the entire Eggleston Heights neighborhood. Concentrations showed more variability without a clear seasonal pattern. Overall, a decreasing trend is observed in the observations of ammonium concentration at well AM-MW-1, and an increasing trend is observed in the observations of nitrate concentration at wells AM-MW-3 and AM-MW-4. Therefore, the steady-state assumption may affect accuracy of the load estimation, and the limitation is discussed in Section 5.

Since the previous ArcNLET version cannot estimate the ammonium transport and loading, the new ArcNLET modeling used at this site is helpful to evaluate importance of the ammonium loading relative to the nitrate loading. Fig. 5 shows the DEM of the modeling area, the estimated location of 287 septic systems, and soil zones of hydraulic conductivity and porosity aggregated from the Soil Survey Geographic database (SSURGO) by following the procedure described in Wang et al. (2012). There are two soil zones, which are sand and sandy loam, and their hydraulic conductivity values are 7.9 m/d and 0.69 m/d, respectively. The soil porosity has little variability, with values ranging from 0.35 to 0.42. The smoothing factor of 60 is used here.

Fig. 7a shows a constant difference between the smoothed DEM and the measured water table. The agreement between the shapes

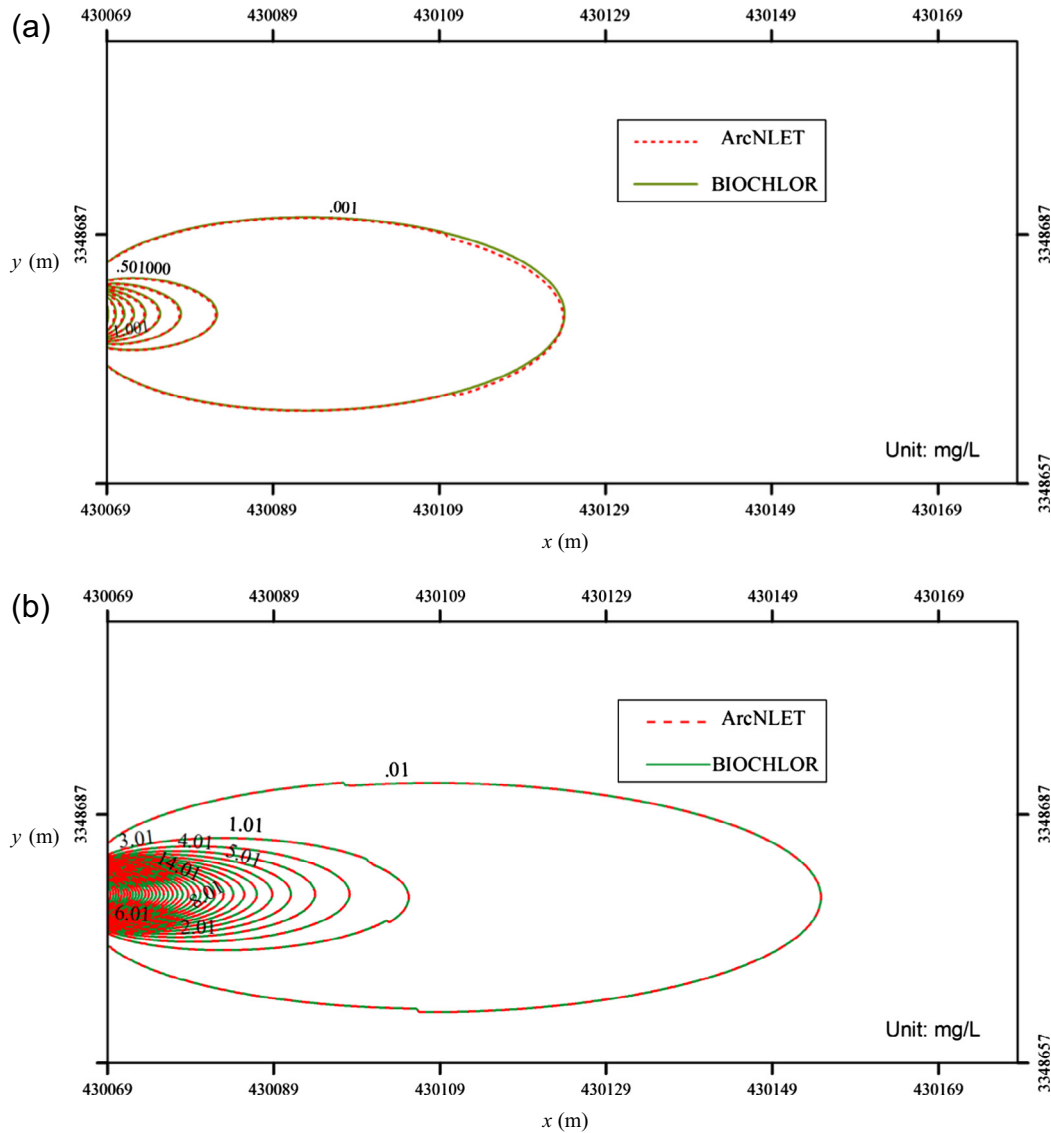


Fig. 4. Contours of (a) ammonium and (b) nitrate concentrations simulated by ArcNLET and BIOCHLOR.

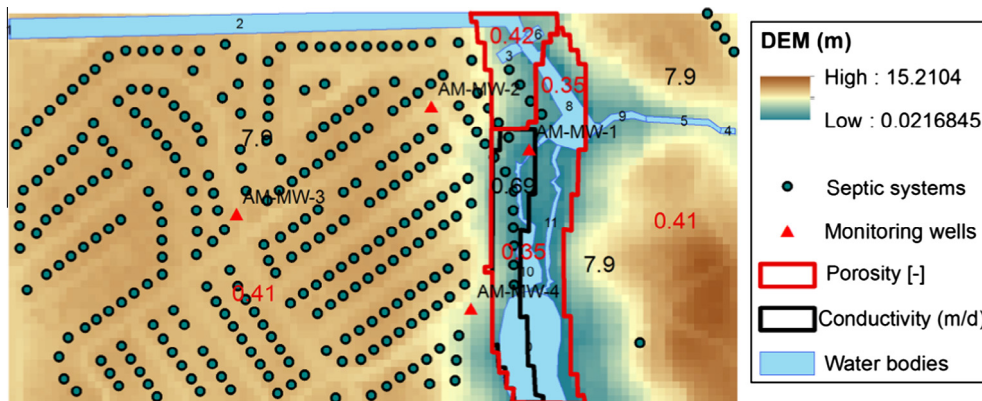


Fig. 5. Locations of four monitoring wells (red triangle) and septic systems (blue circles, at centroid of parcels) in the Eggleston Heights neighborhood of Jacksonville, FL, USA. The background color is DEM. FID of the surface water bodies are labeled in small font within the water bodies. Soil zones of hydraulic conductivity and porosity are delineated in black and red, respectively. The values of hydraulic conductivity and porosity are also labeled in black and red, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 6. Time series for observations of (a) water table elevation, (b) ammonium concentration, and (c) nitrate concentration at four monitoring wells. Linear trend lines are added to all water table data, ammonium concentration at well AM-MW-1, and nitrate concentration at wells AM-MW-2, AM-MW-3, and AM-MW-4.

of the smoothed DEM and measured water table suggests that the directional orientation of the flow field will be acceptable. The high $R^2 = 0.9$ value shown in Fig. 7b for the linear regression between the measured water table and smoothed DEM indicates that the smoothed DEM is a satisfactory approximation to the water table shape. These results suggest that the assumption of water table being a subdued replica of topography is valid in the study area. This is confirmed by using the rule of thumb developed by Haitjema and Mitchell-Bruker (2005), i.e., $\Phi = RL^2/mkHd$, where R (m/d) is recharge, L (m) is average distance between two surface waterbodies, m is a dimensionless factor accounting for the aquifer geometry, K (m/d) is hydraulic conductivity for the area between the two surface waterbodies, H (m) is average aquifer thickness, and d (m) is the maximum terrain rise as the difference between the average water level in surface water bodies and the elevation of the terrain between the two waterbodies. According to Haitjema and Mitchell-Bruker (2005), for one-dimensional flow between two parallel surface water boundaries, $m = 8$; for radial flow with diameter, $L, m = 16$. When Φ is larger than one, water

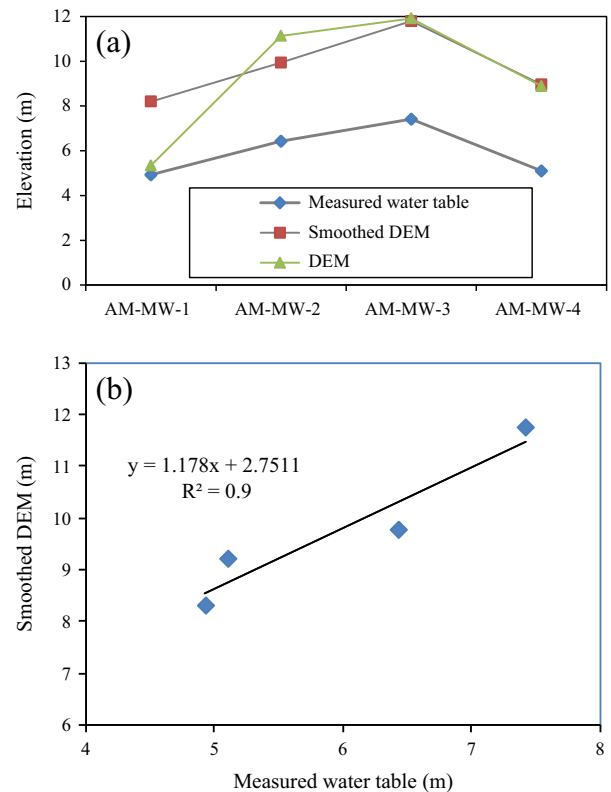


Fig. 7. (a) Comparison of the elevations of measured water table, smoothed DEM, and DEM at the four monitoring wells. (b) Linear regression line between the smoothed DEM and the measured water table.

table is topography controlled; otherwise, water table is recharge controlled. The Φ value is evaluated for the Eggleston Heights neighborhood. The left and right boundaries of the neighborhood are the St. Johns River and Red Bay Branch, respectively, marked in green¹ in Fig. 11. By using the value of $R = 6.986E-4$ m/d, $L = 2957$ m, $m = 8$, $K = 1.52$ m/d, $H = 19$ m, and $d = 6.1$ m specific to the neighborhood, the Φ value is 4.33, indicating that the water table is topography controlled. This is consistent with the conclusion made by Rios et al. (2013), who investigated the relation between water table and topography at a nearby site located in the City of Jacksonville.

Different from Wang et al. (2013a) who used the previous ArcN-LET and calibrated the source plane concentration of nitrate, $c_{NO_3^-,0}$, this study does not calibrate $c_{NO_3^-,0}$, but estimates $c_{NO_3^-,0}$ and $c_{NH_4^+,0}$ using VZMOD. Constant ammonium and nitrate concentrations of 60 mg L^{-1} and 1.0 mg L^{-1} , respectively, in the septic effluent are used for all the individual septic systems; these values are selected based on the literature data given in McCray et al. (2005). The source plane size is set as $Y = 6$ m in width and $Z = 1$ m in height. The first-order nitrification and denitrification coefficients are set as 2.9 d^{-1} and 0.025 d^{-1} according to McCray et al. (2005). The values of other parameters used in VZMOD are set as the literature values given in McCray et al. (2010) specific to the two soil types (sand and sandy loam) of the study area given in the SSURGO database. Fig. 8 plots the VZMOD-estimated concentrations of ammonium ($c_{NH_4^+,0}$) and nitrate ($c_{NO_3^-,0}$) at the water table. Generally, one or the other predominates, and the spatial variability of the concentrations is largely controlled by water table elevation.

¹ For interpretation of color in Fig. 11, the reader is referred to the web version of this article.

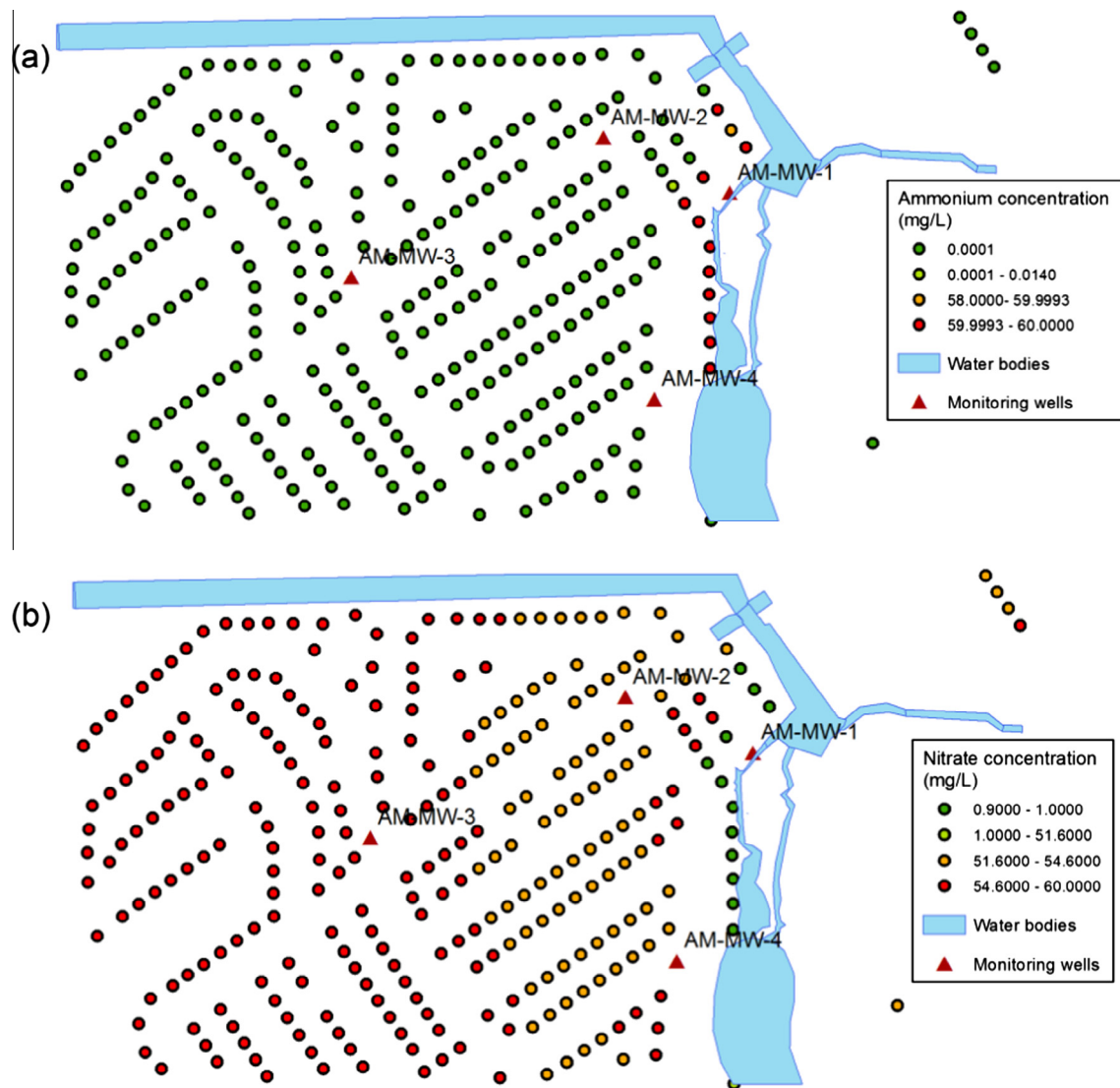


Fig. 8. VZMOD-simulated concentrations of (a) ammonium and (b) nitrate at the water table in the modeling domain.

Fig. 8a shows that, along Red Bay Branch, the simulated ammonium concentrations at the water table for 12 septic systems are close to 60 mg/L. This is attributed to the high water table conditions near the stream (negligible nitrification occurs when water table is close to the drainfield). The simulated ammonium concentrations are low far from Red Bay Branch, where water table becomes deep and nitrification may be complete. The nitrate concentrations at water table plotted in Fig. 8b exhibit an opposite pattern of spatial variability, because nitrate is transformed from ammonium by nitrification. For example, smaller nitrate concentrations are shown in the high groundwater table area close to Red Bay Branch.

While the spatial variability of the simulated ammonium and nitrate concentrations at the water table is expected, it should be noted that VZMOD is not calibrated, because there are no observations for the vadose zone in the modeling domain. The lack of observations makes it difficult to validate/invalidate the conceptual model of VZMOD, and indirect evaluation of the conceptual model is necessary. This is done by using the VZMOD-simulated ammonium and nitrate concentrations as the input for the groundwater transport modeling. If the simulated groundwater concentrations of ammonium and nitrate match the corresponding field observations, one may conclude that the VZMOD simulations are

not unreasonable. However, vadose zone observations are still needed to further evaluate the conceptual model of VZMOD.

The groundwater transport model was calibrated by trial and error to estimate the transport parameter values by matching simulated ammonium and nitrate concentrations to the observations. The calibrated values of $\alpha_x = 10.0$ m, $\alpha_y = 1.0$ m are identical to those obtained by Wang et al. (2013a). The calibrated value of $k_{deni} = 0.008$ d⁻¹ is used. The calibrated value of $k_{nit} = 0.00025$ d⁻¹ reflects limited oxygen availability. The calibrated k_d value is 2.0 m³ g⁻¹, which is within the range of 0.025–8.7 L kg⁻¹ given by McCray et al. (2010). Fig. 9 shows that the simulated groundwater concentrations of ammonium and nitrate are close to the mean of the observed concentrations at the four monitoring wells, and all of the simulated concentrations fall within the range of the observations. The root mean square errors (RMSEs) for ammonium and nitrate concentrations are 0.009 mg L⁻¹ and 2.823 mg L⁻¹, respectively. The simulated ammonium and nitrate plumes are plotted in Fig. 10. The ammonium plumes are concentrated along the shore of the Red Bay Branch, where nitrate concentrations are small. Concentrations are occasionally higher than the source plane concentration due to the addition of concentrations from multiple plumes in the raster file. Monitoring wells are located in the plume of one to a very few septic systems, indicating that uncertainty in

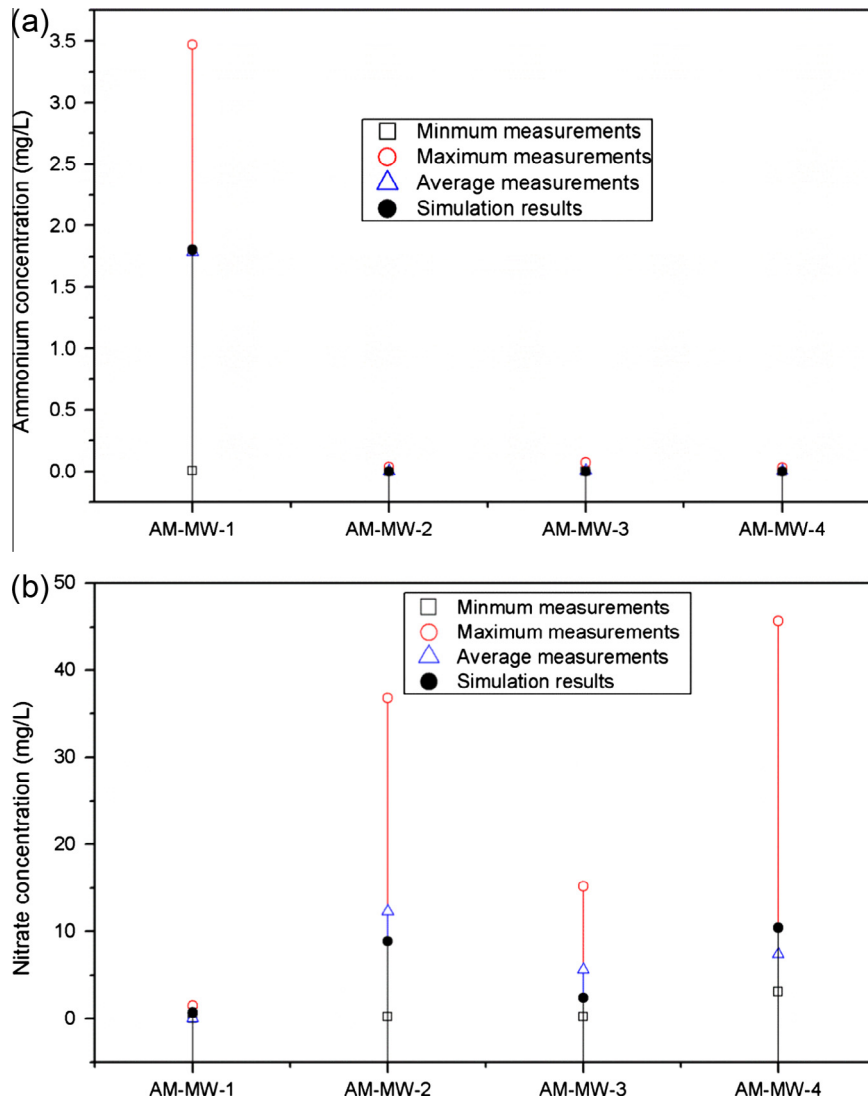


Fig. 9. Simulated concentrations and average, minimum and maximum observed concentrations of (a) ammonium and (b) nitrate in groundwater at the four monitoring wells.

the relative location of these feature could influence parameter estimates and results. The results suggest that the new ArcNLET code is capable of simulating both ammonium and nitrate transport in the domain.

The calibrated model is used to estimate ammonium and nitrate loading to the surface water bodies from the 287 septic systems. The accuracy of the load estimates cannot be evaluated directly, because there are no observations of the loading. An indirect way of evaluating the estimates is to compare the estimated average load to groundwater (i.e., M_{in}) per septic system with literature data. One such estimate for the average total nitrogen contribution to septic systems is 11.2 g of nitrogen per person per day (U.S. EPA, 2002). Multiplying it with 2.58 persons per household in Duval County (<http://quickfacts.census.gov/qfd/states/12/12031.html>) gives an average of 28.9 g nitrogen discharge per household per day. A 10% nitrogen reduction through volatilization of ammonia and removal of solids is estimated by Anderson (2006), who also estimated a 25% reduction of nitrogen due to denitrification as the wastewater percolates through the unsaturated zone. Therefore, about 19 g nitrogen per septic system per day enters groundwater. At the modeling domain, the calculated total inflow mass rate (including ammonium and nitrate) to groundwater is 7.0 kg d⁻¹ (Table 2), resulting in an average nitrogen load for each

septic system of 24.4 g d⁻¹, close to the estimated comparison value of 19 g d⁻¹. A large part of the difference is due to the VZMOD estimate of less than 25% reduction of nitrogen in the vadose zone (Fig. 8).

Table 2 lists the amount (kg d⁻¹) of ammonium and nitrate entering groundwater (M_{in}) and surface water bodies (M_{out}) as well as the amount of ammonium nitrification and nitrate denitrification during nitrogen transport in groundwater. The ammonium loading is mainly to water bodies 8 and 10 along the Red Bay Branch (Fig. 5), adjoining the septic systems for which VZMOD estimated high ammonium concentrations at the water table. The ammonium loading is 18% of the total nitrogen loading. Because of the small value of nitrification rate used in this study, only 16% of the ammonium entering groundwater is nitrified to nitrate. The remaining 84% of ammonium entering groundwater is loaded to the surface water bodies. In contrast, 84% of nitrate entering groundwater is denitrified, and only 16% of groundwater nitrate is loaded to surface water bodies. The results illustrate the potential importance of ammonium to estimating nitrogen loading to surface water bodies.

The modeling exercise was repeated for the entire Eggleston Heights neighborhood with a greater number of septic systems (3516 septic systems) within a larger modeled area to further

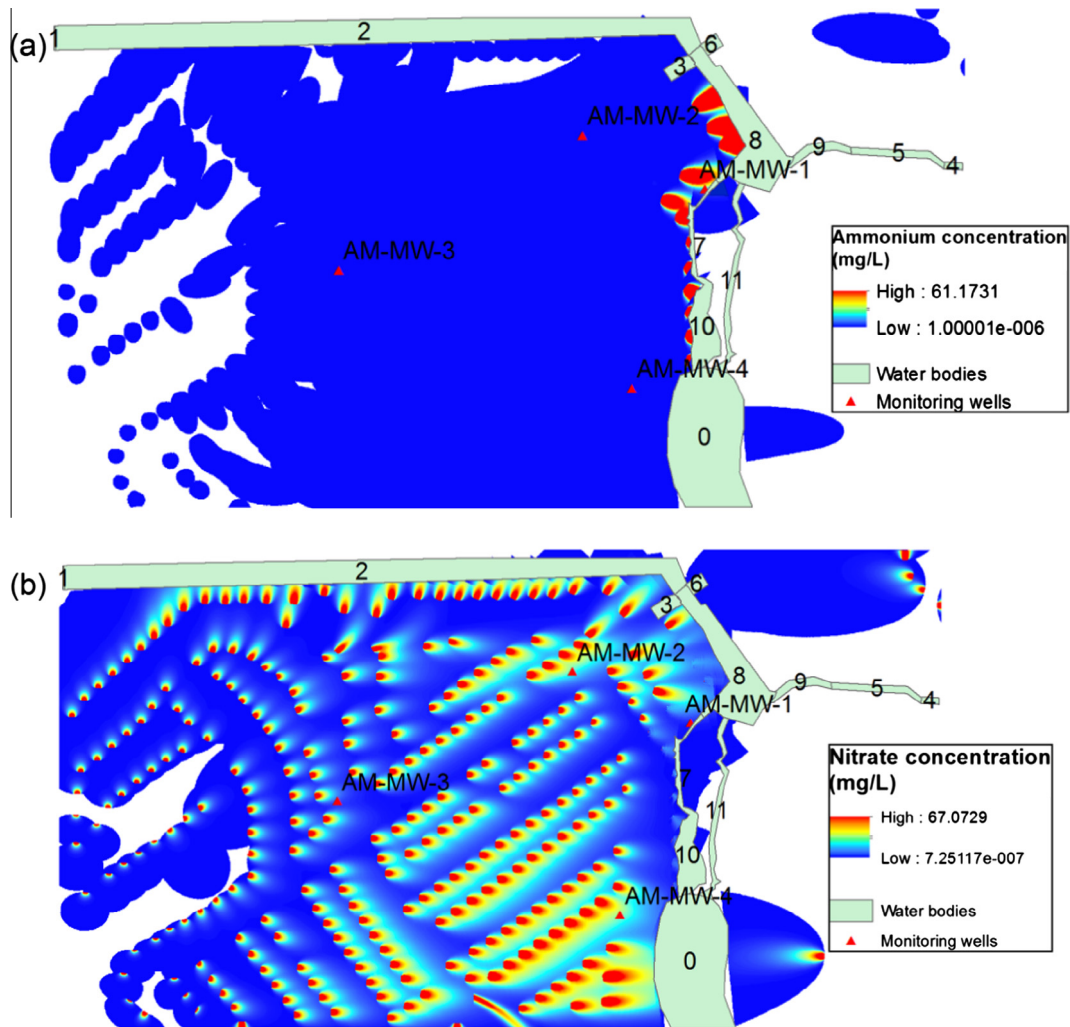


Fig. 10. Simulated plumes of (a) ammonium and (b) nitrate in groundwater from 287 septic systems.

Table 2

Nitrogen loading to groundwater and surface water bodies from 287 septic systems (Fig. 5) located in the Eggleston Height neighborhood. Ammonium and nitrate removal in groundwater is due to nitrification and denitrification, respectively.

	Ammonium	Nitrate	Total
Loading to groundwater (kg d^{-1})	0.30	6.69	6.99
Loading to surface water bodies (kg d^{-1})	0.25	1.10	1.35
Percentage of removal (%)	15.88	83.54	80.67
Percentage of loading to water bodies (%)	18.46	81.54	100.00

evaluate the importance of ammonium loading to total nitrogen loading. Using the calibrated parameters, ammonium and nitrate plumes in groundwater were simulated. The average load per system is 23.9 g d^{-1} , which is very close to the estimate of 24.4 g d^{-1} for the smaller domain. Fig. 11a shows that ammonium concentrations are close to zero in most of the modeling domain, except near Red Bay Branch and ditches north to it where groundwater table is shallow. Table 3 lists the loadings of ammonium and nitrate to groundwater and surface water bodies under this scenario. The percentage of ammonium removal due to nitrification is again very small (16%), indicating that most of the ammonium enters into the surface water bodies. The percentage of nitrate removal due to denitrification is 86%, a little higher than the value of 84% for the smaller modeling domain. Because of the large amount of nitrate

loading, the ammonium loading for the large modeling domain is 10%, which is less than the 18% of the total nitrogen loading for the small modeling domain. This percentage is still significant, indicating importance of the ammonium modeling for estimating nitrogen load from septic systems to surface water bodies.

5. Conclusions and discussion

This paper presents a recently developed software, ArcGIS-based Nitrogen Load Estimation Toolkit (ArcNLET). In comparison with its previous version that only simulated nitrate transport in groundwater, the new code simulates both ammonium and nitrate transport in both the vadose zone and in groundwater. In other words, the new ArcNLET can estimate ammonium and nitrate loading from septic drain fields to surface water bodies. This is a unique feature that cannot be found in other ArcGIS-based software for nitrogen modeling. The new code development consisted of two major efforts to: (1) integrate VZMOD into ArcNLET for simulating ammonium and nitrate transport in vadose zone, and (2) overhaul the ArcNLET transport module to allow simulation of both ammonium and nitrate transport in groundwater. The software is designed to be flexible for simulating (1) nitrate transport alone in groundwater, (2) ammonium and nitrate transport in groundwater, (3) ammonium and nitrate transport in vadose zone, and/or (4) ammonium and nitrate transport in vadose zone and groundwater. This is another unique feature that makes ArcNLET

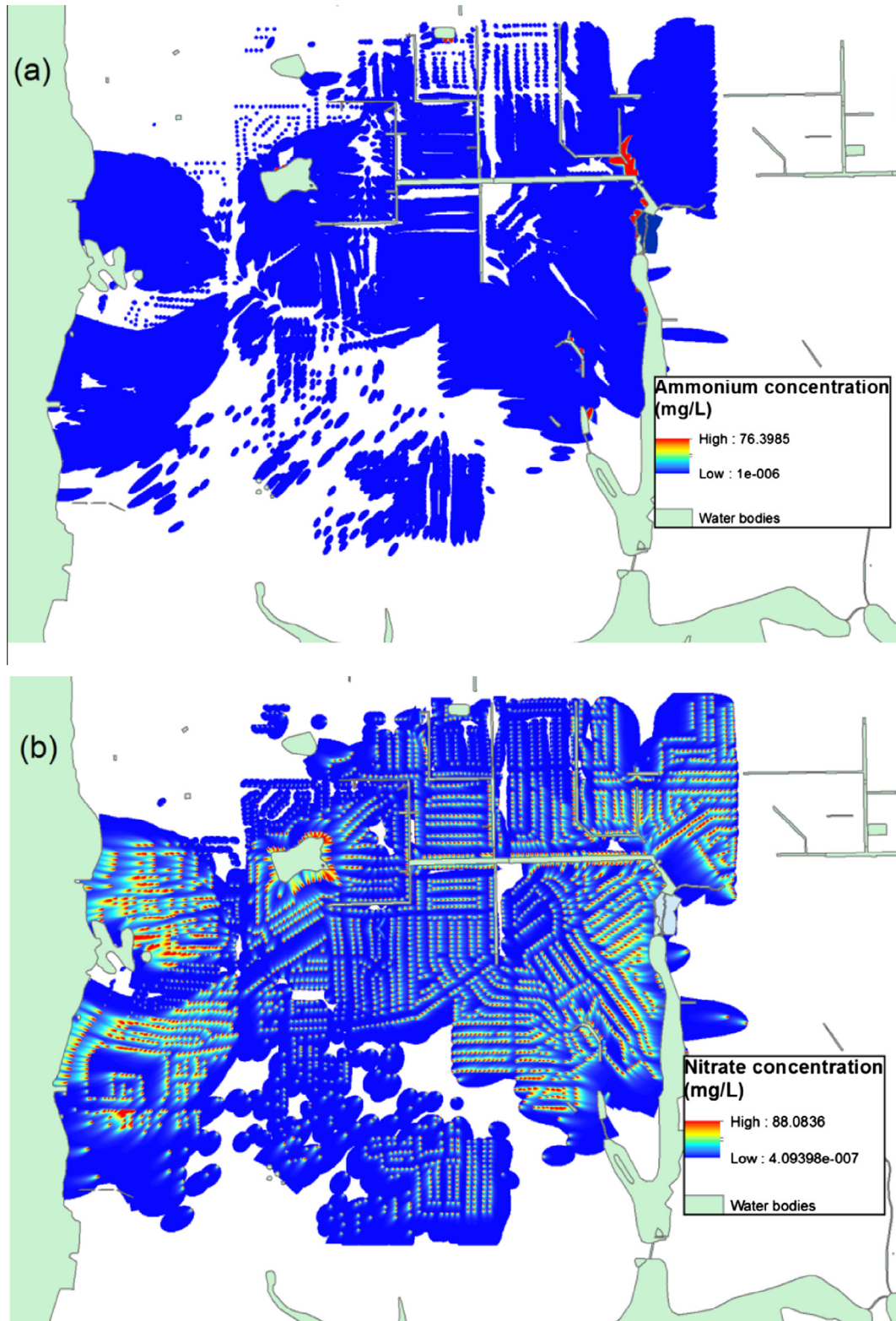


Fig. 11. Simulated plumes of (a) ammonium and (b) nitrate in groundwater from 3516 septic systems of the entire Eggleston Height neighborhood.

useful to different projects with different needs for management of nitrogen pollution.

The new ArcNLET model was applied to estimate concentrations and loads of ammonium and nitrate at the Eggleston Heights neighborhood in Jacksonville, FL, USA. In this neighborhood, ammonium was the predominant form of nitrogen found in samples from one monitoring well located in a high water table area

near surface water bodies, and nitrate was the predominant form of nitrogen in three other wells. Limited changes to literature values for parameters achieved a satisfactory match between the simulated and observed ammonium and nitrate concentrations in the groundwater near these wells. This suggests that ArcNLET is useful as an assessment model for evaluating nitrogen loading to surface waters and as a planning tool for managing nitrogen pollution.

Table 3

Nitrogen loading to groundwater and surface water bodies from 3516 septic systems of the entire Eggleston Height neighborhood. Ammonium and nitrate removal in groundwater is due to nitrification and denitrification, respectively.

	Ammonium	Nitrate	Total
Loading to groundwater (kg d ⁻¹)	1.54	82.34	83.87
Loading to surface water bodies (kg d ⁻¹)	1.30	11.13	12.43
Percentage of removal (%)	15.52	86.48	85.18
Percentage of the loading to water bodies (%)	10.45	89.55	100.00

The corroborated ArcNLET model was used to estimate nitrogen loading to surface water bodies at the Eggleston Heights neighborhood. This exercise illustrates to what extent nitrogen loading is underestimated when ignoring ammonium loading. Two estimates were obtained, for a portion of the neighborhood and the entire neighborhood. For the small modeling domain, ammonium loading is 18% of the total nitrogen loading. The percentage decreases to 10%, when the modeling domain is extended to the entire neighborhood. In either case, ignoring ammonium transport in groundwater can lead to significant underestimation of nitrogen loading. Qualitatively speaking, for a given number of septic systems, the importance of ammonium loading to nitrogen loading depends on the following factors:

- (1) Nitrification in vadose zone. When nitrification is high and all ammonium is converted into nitrate, there is no need to simulate ammonium transport in groundwater.
- (2) Water table depth. When the water table is shallow, it is likely that nitrification is incomplete and that ammonium could enter groundwater. Modern construction standards for septic systems address this concern by elevating the drain field in high water table areas. Depending on the conditions of the existing infrastructure, it may be necessary to simulate ammonium transport in groundwater.
- (3) Area of shallow water table. If a domain has a larger area of shallow water table, more ammonium enters groundwater, and this increases ammonium loading. In such situations, effort is needed to ensure an accurate representation of the water table in ArcNLET.
- (4) Nitrification rate and denitrification rate in groundwater. Ammonium loading is important to nitrogen loading when nitrification rate is low and denitrification rate is high, because low nitrification rate means small amount of ammonium removal and high denitrification rate means large amount of nitrate removal. The combined effect increases the fraction of ammonium loading in total nitrogen loading.

With the above understanding, the authors suggest first running VZMOD to estimate ammonium and nitrate concentrations at the water table and then examining whether the ammonium concentration is high enough to warrant the modeling of ammonium transport in groundwater.

Because ArcNLET is based on a simplified model of nitrogen reactive transport, its modeling results are subject to the following limitations. First, the nitrification and denitrification processes are not controlled explicitly by redox conditions but implicitly by the empirical nitrification and denitrification rates. To determine the rate values, model calibration is needed, and this in turn requires field measurements of ammonium and nitrate concentrations in both vadose zone and groundwater. In this study, the rate values specific to vadose zone are not well calibrated, due to the lack of ammonium and nitrate data in the vadose zone. In addition, although the assumption that the water table is a subdued replica of topography is valid in this study, the assumption may not be

valid for other areas. When measurements of hydraulic head are unavailable, it is necessary to examine the smoothed DEM and simulated groundwater flow paths to ensure that they are physically reasonable. Lastly, the steady-state models of groundwater flow and nitrogen reactive transport cannot capture temporary variation of the areas of interest, especially when strong rainfall events occur. Therefore, ArcNLET should be used as a screening tool for estimating long-term nitrogen load from septic tanks to surface waterbodies.

Acknowledgements

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Appendix A. Derivation of inflow mass rate given by Eqs. (18) and (19)

The ammonium inflow mass rate, $M_{\text{NH}_4^+, \text{in}}$ (M T⁻¹) from the source plan on the boundary of modeling domain (Eqs. (3) and (4)) can be written as,

$$M_{\text{NH}_4^+, \text{in}} = M_{\text{NH}_4^+, \text{adv}} + M_{\text{NH}_4^+, \text{dis}}, \quad (\text{A.1})$$

where $M_{\text{NH}_4^+, \text{adv}}$ (M T⁻¹) is advective mass inflow rate of ammonium and $M_{\text{NH}_4^+, \text{dis}}$ (M T⁻¹) is dispersive mass inflow rate of ammonium. $M_{\text{NH}_4^+, \text{adv}}$ can be calculated by

$$M_{\text{NH}_4^+, \text{adv}} = c_{\text{NH}_4^+, 0} YZ \theta v, \quad (\text{A.2})$$

and $M_{\text{NH}_4^+, \text{dis}}$ by Fick's law as

$$M_{\text{NH}_4^+, \text{dis}} = -D_x YZ \theta \left. \frac{\partial c_{\text{NH}_4^+}}{\partial x} \right|_{x=0}, \quad (\text{A.3})$$

where Y (L) and Z (L) are the width and height of the source plane, respectively, D_x (L² T⁻¹) is the longitudinal dispersivity coefficient in the x direction, $c_{\text{NH}_4^+}$ (M L⁻³) is ammonium concentration, v (L T⁻¹) is uniform seepage velocity in the longitudinal direction, and θ (-) is effective porosity. Evaluating (A.3) requires the analytical expression of $c_{\text{NH}_4^+}$. It is

$$c_{\text{NH}_4^+}(x, y) = \frac{c_{\text{NH}_4^+, 0}}{2} \times F_1(x) \times F_2(y, x), \quad (\text{A.4})$$

according to the two-dimensional, steady-state Domenico solution of ammonium given in Eqs. (9)–(11). Substituting (A.4) into (A.3) gives

$$M_{\text{NH}_4^+, \text{dis}} = -D_{xx} YZ \theta \left. \frac{\partial c_{\text{NH}_4^+}}{\partial x} \right|_{x=0} = -\frac{c_{\text{NH}_4^+, 0}}{2} D_x YZ \theta \left[F_2(y, x) \times \left. \frac{\partial F_1(x)}{\partial x} \right|_{x=0} + F_1(x) \times \left. \frac{\partial F_2(y, x)}{\partial x} \right|_{x=0} \right]. \quad (\text{A.5})$$

Using the analytical expressions of $F_1(x)$ and $F_2(y,x)$ given in Eqs. (10) and (11) and denoting $k = k_{nit}(1 + \rho k_d/\theta)$ leads to

$$\frac{\partial F_1(x)}{\partial x} \Big|_{x=0} = \frac{(1 - \sqrt{1 + \frac{4k\alpha_x}{v}})}{2\alpha_x} \tag{A.6}$$

$$\begin{aligned} \frac{\partial F_2(y,x)}{\partial x} \Big|_{x=0} &= \\ &= \frac{\partial}{\partial x} \left(\frac{2}{\sqrt{\pi}} \int_0^{\frac{y+Y/2}{2\sqrt{\alpha_y x}}} e^{-t^2} dt \right) \Big|_{x=0} \\ &\quad - \frac{\partial}{\partial x} \left(\frac{2}{\sqrt{\pi}} \int_0^{\frac{y-Y/2}{2\sqrt{\alpha_y x}}} e^{-t^2} dt \right) \Big|_{x=0} \\ &= -\frac{1}{\sqrt{\pi}} \\ &\quad \times \exp \left[-\frac{(y+Y/2)^2}{4\alpha_y x} \right] \left[-\frac{y+Y/2}{2\sqrt{\alpha_y}} \frac{1}{x^{3/2}} \right] \Big|_{x=0} \\ &\quad - \left\{ -\frac{1}{\sqrt{\pi}} \exp \left[-\frac{(y-Y/2)^2}{4\alpha_y x} \right] \left[-\frac{y-Y/2}{2\sqrt{\alpha_y}} \frac{1}{x^{3/2}} \right] \right\} \Big|_{x=0} \\ &= 0, \end{aligned} \tag{A.7}$$

$$F_2(y,x) \Big|_{x=0} = 2. \tag{A.8}$$

Substituting Eqs. (A.6)–(A.8) into Eq. (A.5) gives

$$\begin{aligned} M_{NH_4^+,dis} &= -D_x YZ \theta \frac{\partial c_{NH_4^+}}{\partial x} \Big|_{x=0} \\ &= -\frac{c_{NH_4^+,0}}{2} D_x YZ \theta \left[F_2(y,x) \times \frac{\partial F_1(x)}{\partial x} \Big|_{x=0} \right] \\ &= -\frac{c_{NH_4^+,0}}{2} YZ \theta v \times \left(1 - \sqrt{1 + \frac{4k\alpha_x}{v}} \right). \end{aligned} \tag{A.9}$$

Substituting Eqs. (A.2) and (A.9) into Eq. (A.1) leads to Eq. (18) directly.

Similar to Eq. (A.1), the nitrate inflow mass rate ($M_{NO_3^-,in}$) is expressed as

$$\begin{aligned} M_{NO_3^-,in} &= M_{NO_3^-,adv} + M_{NO_3^-,dis} \\ &= c_{NO_3^-,0} YZ \theta v - D_x YZ \theta \frac{\partial c_{NO_3^-}}{\partial x} \Big|_{x=0}. \end{aligned} \tag{A.10}$$

Substituting the expression of $c_{NO_3^-}$ given in Eq. (6) into Eq. (A.10) gives

$$\begin{aligned} M_{NO_3^-,in} &= \left(a_{NO_3^-,0} - \frac{k}{k - k_{deni}} c_{NH_4^+,0} \right) YZ \theta v \\ &\quad - D_x YZ \theta \frac{\partial}{\partial x} \left(a_{NO_3^-} - \frac{k}{k - k_{deni}} c_{NH_4^+} \right) \Big|_{x=0} \\ &= \left(a_{NO_3^-,0} YZ \theta v - D_x YZ \theta \frac{\partial a_{NO_3^-}}{\partial x} \Big|_{x=0} \right) \\ &\quad - \frac{k}{k - k_{deni}} \left(c_{NH_4^+,0} YZ \theta v - D_x YZ \theta \frac{\partial c_{NH_4^+}}{\partial x} \Big|_{x=0} \right). \end{aligned} \tag{A.11}$$

The expression in the first parenthesis at the right hand side of (A.11) is symbolically the inflow mass rate of $a_{NO_3^-}$, i.e.,

$$\begin{aligned} a_{NO_3^-,0} YZ \theta v - D_x YZ \theta \frac{\partial a_{NO_3^-}}{\partial x} \Big|_{x=0} &= \frac{a_{NO_3^-,0}}{2} YZ \theta v \\ &\quad \times \left(1 + \sqrt{1 + \frac{4k_{deni}\alpha_x}{v}} \right) \end{aligned} \tag{A.12}$$

The expression in the second parenthesis at the right hand side of (A.11) is $M_{NH_4^+,in}$. Considering these and $k = k_{nit}(1 + \rho k_d/\theta)$, deriving Eq. (19) is straightforward.

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