

Estimation of nitrate load from septic systems to surface water bodies using an ArcGIS-based software

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Abstract Nitrate, as a commonly identified groundwater and surface water pollutant, poses serious threats to human health and the environment. One important source of nitrate in the environment is due to wastewater treatment using Onsite Sewage Treatment and Disposal Systems (OSTDS) (a.k.a., septic systems). To facilitate water resources and environmental management, an ArcGIS-Based Nitrate Load Estimation Toolkit (ArcNLET) is developed to simulate nitrate transport and estimate nitrate load from septic systems and collocated fertilizer applications in groundwater to surface water bodies. It is a screening tool based on a simplified conceptual model of groundwater flow and nitrate transport. It is used in this study to estimate nitrate load from thousands of septic systems to surface water bodies in two neighborhoods located in Jacksonville, FL, USA, where nitrate due to septic systems is believed to be one of the reasons of nutrient enrichment and an isotope study indicates that denitrification is significant. A global sensitivity analysis is performed to identify critical parameters for model

calibration, and the most critical parameter is the first-order decay coefficient used to simulate the denitrification process. Hydraulic conductivities at different soil zones have different levels of influence on simulated nitrate concentrations at different locations. By manually adjusting model parameters, simulated shapes of water table and nitrate concentration agree reasonably with average field observations, suggesting that ArcNLET is able to simulate spatial variability of field observations. Estimated nitrate loads exhibit spatial variability, which is useful to facilitate decisions on the conversion of OSTDS into sewers in certain areas for reducing nitrate load from septic systems to surface water bodies.

Keywords GIS-based screening model · Nitrate transport · Denitrification · Nitrate loads · Sensitivity analysis · Morris method

Introduction

Nitrate (NO_3^-), as a commonly identified groundwater and surface water pollutant, is associated with a number of adverse health and environmental impacts. Nitrate concentration higher than 10 mg L^{-1} (measured as nitrogen, EPA drinking water primary standard) in drinking water may cause methemoglobinemia, also known as blue baby syndrome. Discharge of nitrate-rich groundwater to surface water bodies can lead to fish kills, algal growth, hypoxia, eutrophication, and outbreaks of toxic bacteria. One important source of nitrate in the environment 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; McCray et al. 2005). The nitrate contribution from septic

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systems to surface water bodies may be significant in areas where septic systems are located in close proximity to surface water bodies. Shallow groundwater in surficial aquifers is always vulnerable to nitrate contamination, because of direct discharge of effluent from septic systems into soil. This may pose a threat to public health if drinking water supply depends on shallow domestic wells (Hitt and Nolan 2005). In the U.S., approximately 25 % of the population and 30 % of all new development utilize septic systems (Hazen et al. 2009). In the state of Florida, nearly a third of households use septic systems and 92 % of drinking water supply is from groundwater (Ursin and Roeder 2008; Hazen et al. 2009). Therefore, for protection of the environment and public health, it is important to simulate nitrate transport in groundwater due to septic systems and to estimate corresponding nitrate load to surface water bodies.

Various numerical models with different levels of complexity have been developed to simulate nitrate fate and transport. A review of computational models developed to facilitate modeling assessment and decision-making associated with pollutants from septic systems is given in McCray et al. (2009), in which the models are categorized into six primary types: mass balance screening models, GIS-based screening models (GIS stands for Geographic Information System), surface water models, vadose zone models, groundwater models, and integrated watershed models. In the wide spectrum of nitrate models, one extreme is to consider, to the extent possible, all biogeochemical processes involved in nitrate/nitrogen fate and transport. For example, MacQuarrie et al. (2001a, b) developed a mechanistic flow and reactive transport model that includes the most relevant physical, geochemical, and biochemical processes associated with wastewater plume evolution in sandy aquifers. Recently, Maggi et al. (2008) developed a numerical code, TOUGHREACT-N, one of 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. While the complex models may yield results that can potentially agree well with field observations, their 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. In addition, to utilize sophisticated functions of the models, a large amount of model input and calibration data as well as long execution time may be needed, which may not be available or 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 models, and screening models, including some that are GIS-based, may have to suffice.

GIS-based models have gained popularity in nitrate (and other environmental) modeling, because a GIS is an efficient way to integrate regional/local spatial characteristics of a system (e.g., digital hydrologic and topographic data). Skills required for the application of GIS-based models are widely available. They can be used as a pre- and post-processor for preparing model input files for other modeling programs, as a modeling environment for simple conceptual models using analytical equations that can be implemented within a GIS, and for analyzing and visualizing modeling results by non-technical citizens (National Research Council 2010). The first use includes utilization of GIS as a front-end of the actual model, such as MODFLOW Analyst (Aquaveo, LLC) for MODFLOW 2000 (Harbough et al. 2000), and ArcAEM (Silavisesrith and Matott 2005) for the analytic element modeling software SPLIT (Bandilla et al. 2006). GIS-based models for the second use always have a simple conceptual model and use analytical equations that can be implemented within a GIS; examples of such models are PRO-GRADE (Lin et al. 2009) and uWATER-PA (Yang and Lin 2011; Rios et al. 2011a). In addition to the three GIS-based models reviewed by McCray et al. (2009), MANAGE (Kellogg et al. 1996), NLM (Valiela et al. 1997) and PLSM (Adamus and Bergman 1995), there are other models related to nitrate transport modeling. The topography-based model TNT2 (Beaujouan et al. 2002) considered nitrogen and nitrate transport at the catchment scale due to agricultural activities. Ye et al. (1996) presented a map-based subsurface flow modeling tool integrated directly with GIS. Romshoo and Muslin (2011) applied a GIS-based distributed modeling approach to assess the nutrient load to surface water bodies using geospatial data sets such as digital elevation models (DEM) and soil maps. Becker and Jiang (2007) developed a GIS-based groundwater contaminant transport model using the analytic element method. With a focus on nitrate pollution from agricultural sources, Schilling and Wolter (2007) developed a GIS-based model to estimate groundwater travel time using DEM data. The Watershed Analysis Risk Management Framework (WARMF) (Herr et al. 2001) is another GIS-based model for calculation of TMDLs for most conventional pollutants at the watershed scale.

Specifically for simulating nitrate transport in surficial aquifers due to septic systems and for estimating corresponding nitrate load to surface water bodies ArcNLET, an ArcGIS-Based Nitrate Load Estimation Toolkit (Rios et al. 2011b, 2013), has been developed. Similar to other GIS-based models, ArcNLET relies on a simple conceptual model and analytical equations describing nitrate transport. However, different from other GIS-based screening models that do not include hydrogeologic processes and/or data density necessary for site-specific modeling, ArcNLET

considers advection, hydrodynamic dispersion, and denitrification processes involved in nitrate transport; ArcNLET can also incorporate fully heterogeneous hydraulic parameters that vary by raster elements and partially heterogeneous transport parameters that vary by individual septic systems. Therefore, ArcNLET is able to simulate field observations at specific sites, as demonstrated below. However, ArcNLET should still be used as a screening model to provide quick estimates, because of a number of assumptions and simplifications involved in its conceptual model.

In the remainder of this paper, the conceptual model and its computational implementation in ArcNLET are described, followed by its applications to estimation of nitrate load from thousands of septic systems and fertilizer applications to surface water bodies in two neighborhoods of the Lower St. Johns River Basin (LSJRB) in Florida, USA, where nitrate due to septic systems is believed to be one of the causes for nutrient enrichment (Leggette and Graham 2004). The ArcNLET applications include global sensitivity analysis and trial-and-error model calibration against field observations of hydraulic head and nitrate concentration.

Simplified conceptual model

ArcNLET is based on a simple conceptual model of groundwater flow and nitrate transport. The model has three sub-models: groundwater flow model, nitrate transport model, and nitrate load estimation model. The results from the flow model are used by the transport model, whose results are in turn utilized by the nitrate load estimation model. By invoking assumptions and simplifications to the system being modeled, computational cost is significantly reduced, which enables ArcNLET to provide quick estimates of nitrate loads from septic systems to surface water bodies. The three sub-models are briefly described here; more details are described by Rios et al. (2011b, 2013).

The groundwater flow model of ArcNLET is simplified by assuming that the water table is a subdued replica of the topography in the surficial aquifer. According to Haitjema and Mitchell-Bruker (2005), the assumption is valid if

$$\frac{RL^2}{mKHd} > 1, \tag{1}$$

where R [m day⁻¹] is recharge, L [m] is average distance between surface waters, m is a dimensionless factor accounting for the aquifer geometry, and is between 8 and 16 for aquifers that are strip-like or circular in shape, K [m day⁻¹] is hydraulic conductivity, H [m] average aquifer thickness, and d [m] is the maximum distance between the

average water level in surface water bodies and the elevation of the terrain. The criterion, as a rule of thumb, can be met in shallow aquifers in flat or gently rolling terrain. Therefore, the shape of water table can be obtained by smoothing land surface topography given by DEM of a study area. In ArcNLET, the smoothing is accomplished using moving-window average via a 7×7 averaging window. The smoothing process needs to be repeated for multiple times, depending on discrepancy between the shapes of topography and water table. The number of smoothing iterations is specified by ArcNLET users as an input parameter of ArcNLET. The smoothed DEM is assumed to have the same shape of the water table (not at the same elevation) so that hydraulic gradients can be estimated from the smoothed DEM. Because hydraulic gradients and water bodies are not hydraulically linked in the model, the modeler needs to evaluate if the resulting shape of the water table is consistent with the drainage network presented by the water bodies.

Additional assumptions and approximations are made as follows: (1) the Dupuit-Forchheimer assumption is used so that the vertical flow can be ignored and only two-dimensional (2-D) isotropic horizontal flow is simulated; (2) the steady-state flow condition is assumed, since this software is used for the purpose of long-term environmental planning; (3) the surficial aquifer does not include karsts or conduits so that Darcy's Law can be used; (4) mounding on water table due to recharge from septic systems and rainfall is not explicitly considered (but assumed to be reflected by the steady-state water table); (5) the flow field is obtained from the water table without consideration of a water balance. Consequently, the groundwater seepage velocity, v , can be obtained by applying Darcy's Law

$$v_x = -\frac{K}{\phi} \frac{\partial h}{\partial x} \approx -\frac{K}{\phi} \frac{\partial z}{\partial x}, \quad v_y = -\frac{K}{\phi} \frac{\partial h}{\partial y} \approx -\frac{K}{\phi} \frac{\partial z}{\partial y} \tag{2}$$

where K is hydraulic conductivity [LT⁻¹], ϕ is porosity, h is hydraulic head, hydraulic gradient ($\partial h/\partial x$ and $\partial h/\partial y$) is approximated by the gradient of the smoothed topography ($\partial z/\partial x$ and $\partial z/\partial y$). Implementing the groundwater flow model in a GIS environment yields the magnitude and direction of the flow velocity for every discrete cell of the modeling domain, which are used to estimate flow paths, originating from individual septic systems and ending in surface water bodies.

Figure 1 shows the conceptual model of nitrate transport in ArcNLET, which is similar to that of BIOSCREEN (Newell et al. 1996) and BIOCHLOR (Aziz et al. 2000) developed by the U.S. EPA. In the conceptual model, nitrate enters the groundwater zone with a uniform and steady flow in the direction indicated. The Y-Z plane in Fig. 1 is considered as a source plane (with a constant concentration C_0 [ML⁻³]) through which nitrate enters the

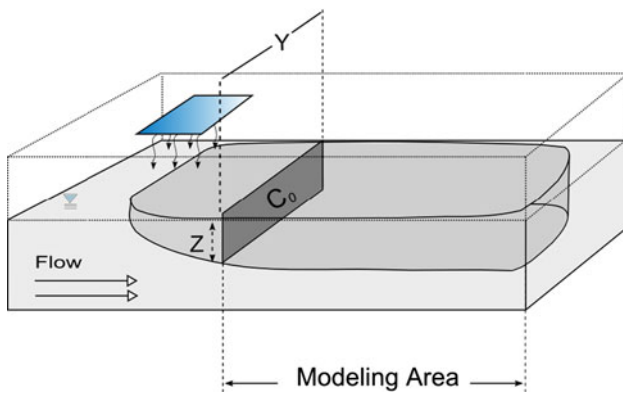


Fig. 1 Conceptual model of nitrate transport in groundwater adapted from Aziz et al. (2000). The unsaturated zone is bounded by the rectangular box delineated by the dotted lines; the groundwater zone is bounded by the box delineated by the solid lines

groundwater system. Two-dimensional (2-D) nitrate transport in groundwater is described using the advection–dispersion equation

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} - kC \quad (3)$$

where C is the nitrate concentration [ML^{-3}], t is time [T], D_x and D_y are the dispersion coefficients in the x and y directions, respectively [L^2T^{-1}], v is the constant seepage velocity in the x direction [L] and k is the first-order decay coefficient [T^{-1}]. This equation assumes homogeneity of parameters (e.g., dispersion coefficient) and uniform and steady flow in the x direction. The last term in Eq. 3 is to simulate the denitrification, in which nitrate is transformed into nitrogen gas through a series of biogeochemical reactions. Following McCray et al. (2005) and Heinen (2006), the denitrification process is modeled using first-order kinetics and included as the decay term, which can also be used to take into account other loss processes. The steady-state form, semi-analytical solution of Eq. 3 is derived based on that of West et al. (2007), which is of 3-D, steady-state form and similar to the work of Domenico (1987). The analytical solution used in this study is

$$C(x, y) = \frac{C_0}{2} F_1(x) F_2(y, x) \quad (4)$$

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

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

where α_x and α_y are the longitudinal and horizontal transverse dispersivity [L], Y and Z are the width and height of the source plane, respectively, [L] and C_0 is the constant source concentration at the source plane. A review of analytical solutions of this kind and errors due to

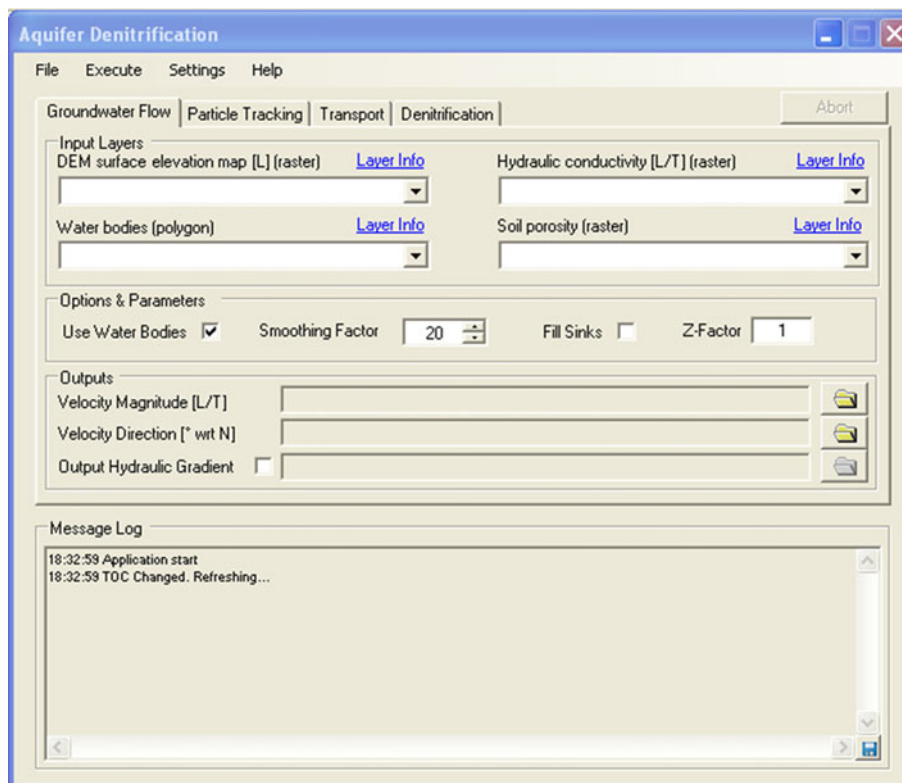
assumptions involved in their derivation are provided by Srinivasan et al. (2007).

It is assumed in ArcNLET that nitrification is complete before septic effluent (or nitrogen from other sources) reaches groundwater and that there is no generation of nitrate in groundwater. In the vadose zone, ammonium is subject to nitrification and nitrate to denitrification. The nitrification process usually occurs relatively fast in the vadose zone, and complete nitrification usually occurs in the first 30 cm (Fischer 1999; Beach 2001). Because denitrification rates are usually significantly smaller than nitrification rates in natural soils, complete denitrification in most OSTDS does not occur (Heatwole and McCray 2007). Extent of nitrification and the fraction of nitrogen removed in the vadose zone is site specific (e.g., Aley IV et al. 2007 for three sites in central Florida). They can be estimated using a new model, VZMOD, developed by Wang et al. (2012) to simulate the fate and transport of nitrogen from septic systems in the vadose zone. When nitrification process is not completed in the vadose zone and ammonium enters groundwater, ArcNLET needs to be extended to simulate transport of both nitrate and ammonium in groundwater, which is warranted in future study.

The 2-D concentration plume is extended downwards to the depth Z of the source plane (Fig. 1); the pseudo three-dimensional (3-D) plume is the basis for estimating the amount of nitrate that enters into groundwater and loads to surface water bodies. While each individual septic system has its own source concentration, C_0 , drainfield width, Y , and average plume thickness, Z , when there is a lack of field data for these variables in a management project, it is not unreasonable to use constant values for the variables, as done in this study. However, each individual septic system has its own concentration plume, because flow velocity varies between the septic systems. Since the flow velocity estimated in the groundwater flow model is not uniform but varies in space, to use the analytical solution with uniform velocity, the harmonic mean of velocity (averaged along the flow path corresponding to the plume) is used for evaluating each individual plume. The plumes either end at surface water bodies or are truncated at a threshold concentration value (usually very small, e.g., 10^{-6}). After the plumes for all septic systems are estimated, by virtue of linearity of the advection–dispersion equation with respect to concentration, the individual plumes are added together to obtain the spatial distribution of nitrate in the modeling domain. The superposition, however, may result in higher and shallower concentrations than exist in the field unless the averaging depth is deep enough.

The nitrate load estimation model evaluates the amount of nitrate loaded to target surface water bodies. For the steady-state model, this is done using the mass balance equation $M_{out} = M_{in} - M_{dn}$, where M_{out} [MT^{-1}] is mass

Fig. 2 Main Graphic User Interface (GUI) of ArcNLET with four modules of groundwater flow, particle tracking, transport, and denitrification



load rate, M_{in} [MT^{-1}] is mass inflow rate from septic systems to groundwater, and M_{dn} [MT^{-1}] is the mass removal rate due to denitrification. The mass inflow rate, M_{in} , consists of inflow due to advection and dispersion, and is evaluated via

$$M_{in} = YZ\phi \left(vC_0 - \alpha_x v \frac{\partial C}{\partial x} \Big|_{x=0} \right) = YZ\phi v C_0 \frac{1 + \sqrt{1 + \frac{4ka_x}{v}}}{2} \tag{5}$$

The derivative, $\partial C/\partial x$, to calculate the dispersive flux is evaluated using an analytical expression based on the analytical expression of concentration in Eq. 4. The mass removal rate due to denitrification, M_{dn} , is estimated via

$$M_{dn} = \sum_i kC_i V_i \phi_i \tag{6}$$

where C_i and V_i are concentration and volume of the i -th cell of the modeling domain, and kC is denitrification rate assuming that denitrification is the first-order kinetic reaction (Heinen 2006). If a plume does not reach any surface water bodies, the corresponding nitrate load is theoretically zero. This is used to evaluate accuracy of numerical results by calculating mass balance error defined below, which should be small relative to the mass inflow rate and mass removal rate, e.g., less than 1 %.

The simplified groundwater flow and nitrate transport model are implemented as an extension of ArcGIS (both version 9.3 and 10.0) using the Visual Basic.NET

programming language. In keeping with the object-oriented paradigm, the code project is structured in a modular fashion. Development of the graphical user interface (GUI) elements is separated from that of the model elements; further modularization is kept within the development of GUI and model sub-modules. The main panel of the model GUI is shown in Fig. 2; there are four tabs, each of which represents a separate modeling component. For example, the tab of Groundwater Flow is for estimating magnitude and direction of groundwater flow velocity, and the tab of Particle Tracking for estimating flow path from each septic system. Each tab is designed to be a self-contained module and can be executed individually within ArcGIS. Five ArcGIS layers are needed for running ArcNLET; they are DEM, hydraulic conductivity, and porosity in raster form, septic system locations in point form, and surface water bodies in polygon form. These ArcGIS files need to be prepared outside ArcNLET. The output files are also ArcGIS layers that can be readily post-processed and visualized within ArcGIS. More details of the software development, including verification and validation, are described in Rios et al. (2011b, 2013).

Global sensitivity analyses

ArcNLET has a total of nine parameters: hydraulic conductivity (K), porosity (ϕ), longitudinal dispersivity (α_x), horizontal transverse dispersivity (α_y), first-order decay

coefficient (k), source nitrate concentration (C_0), smoothing factor ($SmthF$), the width (Y) and thickness (Z) of the source plane. Except for homogenous $SmthF$, ArcNLET supports heterogeneous K and ϕ that vary between raster elements and heterogeneous α_x , α_y , k , C_0 , Y , and Z that vary between septic systems. In this application, due to a lack of specific information on spatial variability of α_x , α_y , k , C_0 , Y , and Z , these parameters were considered to be homogenous for the whole modeling domain.

To identify the parameters most critical to the simulated nitrate concentration in the whole parameter space, global sensitivity analysis is performed using the Morris One-At-A-Time method (MOAT) (Morris 1991) implemented in software DAKOTA (Adams et al. 2011). The method is a screening tool to distinguish influential input variables (e.g., model parameters) to output of a computational model. The method is briefly described here and more details can be found in Morris (1991) and Adams et al. (2011). Use \mathbf{x} to denote the k -dimensional model inputs. For its component, x_i , specify its finite lower and upper bounds, scale the range to $[0, 1]$, and uniformly partitioned it into p levels and $p - 1$ segments. In other words, component x_i has p values in the set $\{0, 1/(p - 1), 2/(p - 1), \dots, 1\}$. Repeating this for all the k parameters creates a grid of p^k points; at each point, model evaluation takes place. During the sensitivity analysis, MOAT first randomly picks one out of the p^k points, and then varies one parameter at a time to create a sample of its elementary effects until all the parameters are varied. An elementary effect, d_i , of x_i is computed using forward difference via (Adams et al. 2011)

$$d_i(\mathbf{x}) = \frac{y(x_1, \dots, x_{i-1}, x_i + \Delta, x_{i+1}, \dots, x_k) - y(\mathbf{x})}{\Delta} \quad (7)$$

where Δ is a predetermined multiplier of $P/(2p - 2)$ for an scaled input variable, and y is the model output. In a particular application, the scaled input values are sampled and then subsequently rescaled to generate the actual values for model evaluation. After user-specified numbers of elementary effects are calculated for each parameter, the modified mean μ_i (calculated using the absolute values of the elementary effects) and standard deviation σ_i of the elementary effects are calculated and used as indicators to identify the influential parameters. A high mean value indicates large overall influence. A high standard deviation suggests that the parameter is either strongly interacting with other parameters or has a high nonlinear effect on the output.

Study areas and available data

ArcNLET is used to estimate nitrate load from septic systems to surface water bodies in LSJRB, where nutrient

enrichment with nitrogen and phosphorus is a serious environmental concern and septic systems are suspected as one important source of existing surface water body nitrate pollution (Leggette and Graham 2004). The targeted surface water bodies of nitrate load include rivers, creeks, lakes, ponds, ditches, swamps, and reservoirs. The Florida St. Johns River Water Management District (SJRWMD) has supported the collection of observations of water table levels and nitrate concentrations from 59 wells within 17 sites on a quarterly basis since 2003. However, there are no other site-specific data for characterizing site heterogeneity and understanding biogeochemical processes involved in nitrate transport at the sites. The data paucity is a hindrance for using sophisticated groundwater flow and transport models. On the other hand, environmental regulation and protection at the sites require a timely estimate of nitrate load. ArcNLET is a useful modeling tool in this circumstance.

Among the 17 sites, the Eggleston Heights, Julington Forest, Manor Del Rio, and Siesta Del Rio neighborhoods are chosen in this study, because these sites have more observations available than other sites. The latter three neighborhoods are connected and thus combined into one, called Julington Creek, in this study. Mixed nitrate sources, such as septic systems and lawn fertilizer, are common in urban areas, posing a challenge to applying ArcNLET in many neighborhoods of Jacksonville. To deal with this situation, a simplified solution is proposed in this study, which is to account for fertilizer effects by factoring them into the source plane concentration (C_0). This simplified solution may deteriorate accuracy of modeling results since extra assumptions are required, including that the fertilized areas are located at the same places of septic systems and limited to the extent of the drainfields. However, when there is no information about the lawn/gardens locations, areas and fertilizer applications to eliminate its impact from field measurements, this simplified solution is useful to give a screening level estimation of nitrate load due to the mixed sources. On the other hand, since the estimated load is approximately a linear function of C_0 (Wang et al. 2012), the actual nitrate load from septic systems can be estimated by comparison with a separately determined C_0 from septic systems only area (e.g., by field measurements or VZMOD) (not the C_0 obtained from model calibration). Based on isotope studies in the study areas, while little fertilizer application occurs in Eggleston Heights, both the septic systems and lawn fertilization are the major nitrate sources in Julington Creek. These contrasting sites allow an illustration of the simplified accounting of different nitrate sources. For the two sites, the goal of the numerical simulation using ArcNLET is to match the smoothed DEM to the observed shape of water table and simulated concentrations to corresponding field observations at the monitoring wells.

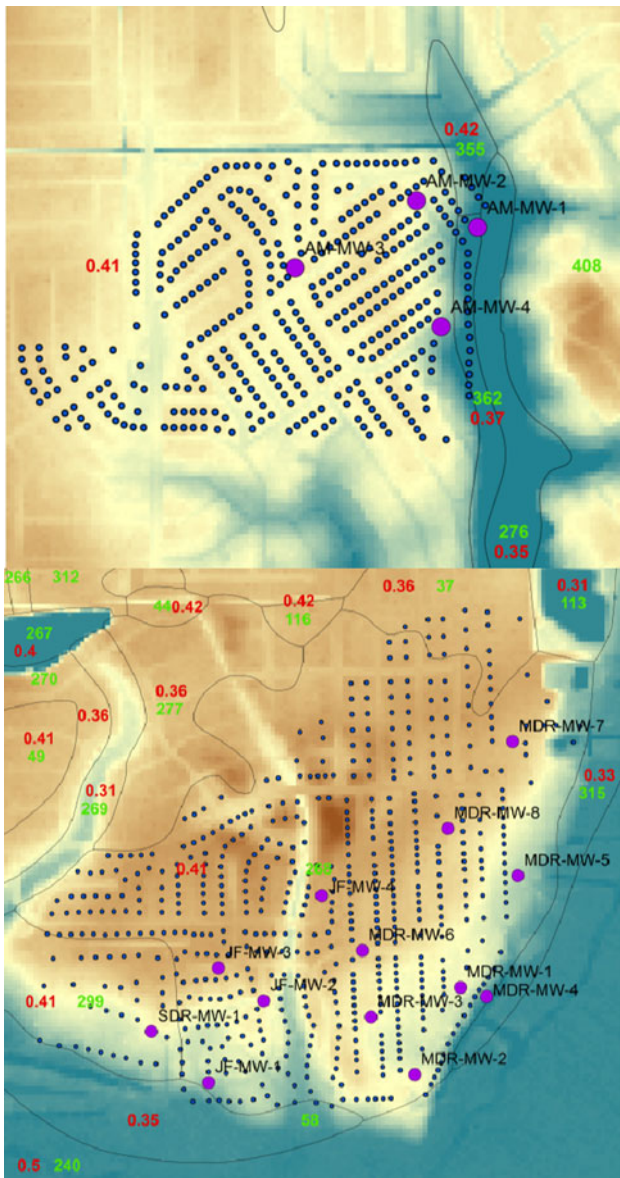


Fig. 3 Locations of monitoring wells (purple circles) and septic tanks (blue points) in Eggleston Heights (upper) and Julington Creek (lower) Neighborhoods of Jacksonville, FL, USA. FID of each soil unit is labeled in green, and porosity value of each zone is highlighted in red

There are four monitoring wells in Eggleston Heights and 13 wells in Julington Creek, and their locations are shown in Fig. 3. Depths of well screens relative to top of well casing are obtained from Leggette and Graham (2004) and listed in Table 1. Figure 3 also plots the locations of a portion of septic systems installed in the neighborhoods and the LiDAR DEM (with a horizontal resolution of $5 \times 5 \text{ ft}^2$) as background; the septic system locations are assumed to be the centroid of properties. While it would be ideal if the locations represent the centroid of drainfields, such information is not available. The GIS layers of

Table 1 Depths (m) of screens and averages of measured water table relative to the depths of TOP of casing below ground level at four monitoring wells (the first four wells in the table) in Eggleston Heights and 13 monitoring wells in Julington Creek

Well name	Screen depth (below TOP) (m)	Water table depth (below TOP) (m)	TOP (m)
AM-MW-1	0.49–3.54	0.42	0.08
AM-MW-2	3.51–6.55	4.71	0.10
AM-MW-3	3.47–6.52	4.50	0.11
AM-MW-4	3.20–6.25	3.79	0.10
MDR-MW-1	3.23–6.28	4.11	0.10
MDR-MW-2	3.08–6.13	4.48	0.12
MDR-MW-3	3.14–6.19	4.07	0.12
MDR-MW-4	0.46–3.51	0.72	0.10
MDR-MW-5	1.71–4.75	2.03	0.07
MDR-MW-6	4.15–7.19	4.38	0.06
MDR-MW-7	3.44–6.49	4.44	0.10
MDR-MW-8	3.51–6.55	3.62	0.09
SDR-MW-1	3.60–6.64	3.95	0.07
JF-MW-1	1.34–4.39	2.09	0.09
JF-MW-2	2.90–5.94	3.66	0.09
JF-MW-3	4.42–7.47	4.79	0.08
JF-MW-4	2.87–5.91	4.00	0.11

monitoring wells, septic system locations, and LiDAR DEM are obtained from the database of the Florida Department Environmental Protection (FDEP). The water body layer is generated based on data downloaded from the USGS National Hydrography Dataset (NHD).

In Eggleston Heights, a total of 3,517 septic tanks had been installed by 2008. The number of septic systems is 1,978 in Julington Creek. A total of 136 observations of hydraulic head and 143 observations of nitrate concentration have been collected from the four monitoring wells within Eggleston Heights during the period of 2005–2010. For the Julington Creek neighborhood, a total of 451 observations of water level depth and 484 observations of nitrate concentration have been collected from the 13 monitoring wells during the period of 2003–2010. Average measured water level depth for each monitoring wells are listed in Table 1. Time series of the data are plotted in Fig. 4; for a better illustration, only the data from four monitoring wells are shown in Fig. 4c, d for Julington Creek. The head observations (Fig. 4a, c) are relatively stable over time (despite of some fluctuations), indicating that it is reasonable to assume the steady-state flow. While the concentration observations (Fig. 4b, d) have more significant fluctuations, there is no trend observed. During the model calibration, the mean value of the head and concentration observations are used as the calibration targets. For the concentration, minimum and maximum as well as lower and upper quartile

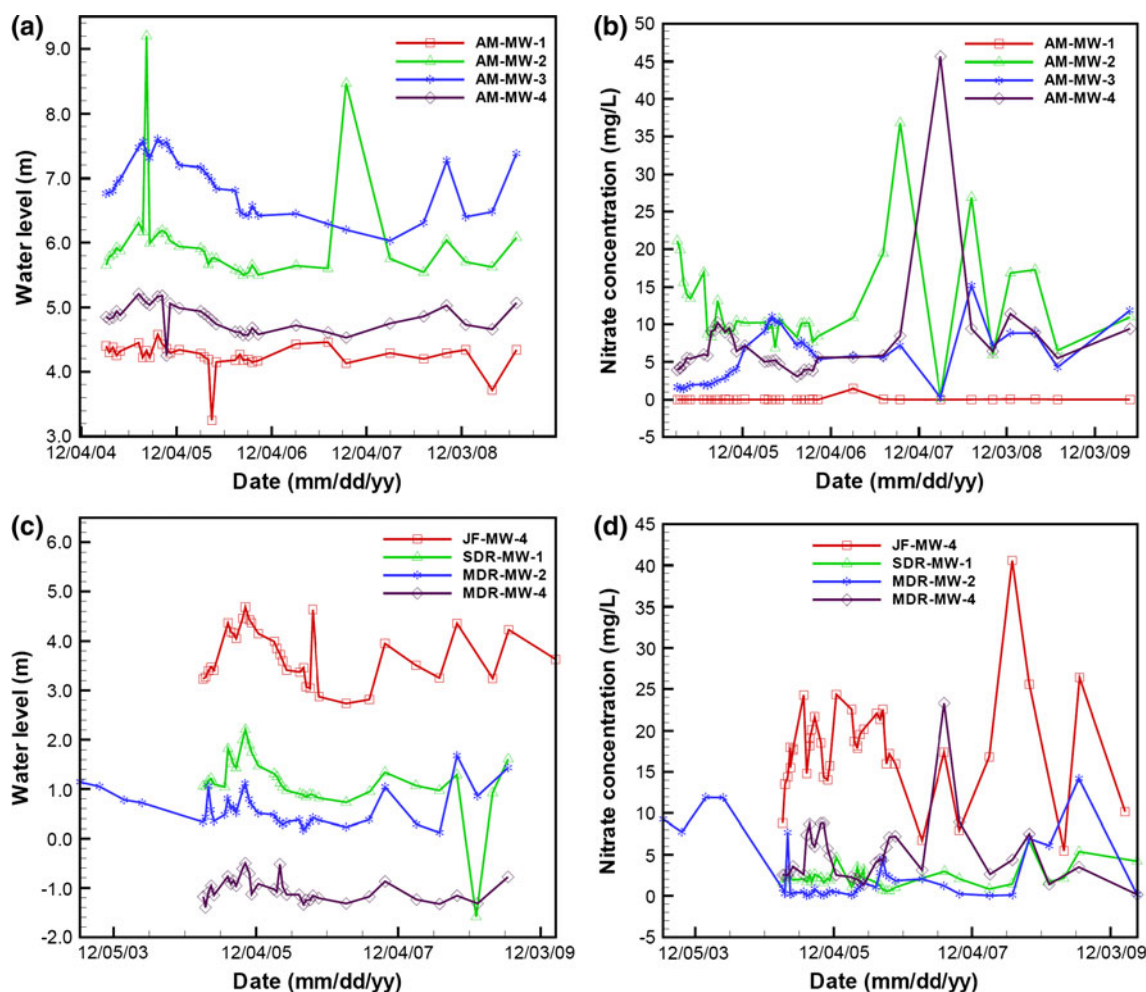


Fig. 4 Time series of observations of **a** hydraulic head, **b** nitrate concentration at Eggleston Heights, **c** hydraulic head, and **d** nitrate concentration at Julington Creek

of the observations are also used to evaluate the calibration results.

Hydraulic conductivity and porosity of the surficial aquifer are approximated using those available in the Soil Survey Geographic (SSURGO) database. SSURGO indicates that there are four soil map units in Eggleston Heights and seven units in Julington Creek, which are delineated by the grey polygons shown in Fig. 3. The FID of each soil zone is labeled in green and porosity values in red. Using the SSURGO database, heterogeneous hydraulic conductivity and porosity values corresponding to the soil map units are incorporated into the ArcNLET modeling (including sensitivity analysis, model calibration, and load estimation discussed below). Hydraulic conductivity used in this study are horizon attributes listed in columns “ksat_l” (low value), “ksat_r” (representative value), and “ksat_h” (high value) in the SSURGO “chorizon” table, which is defined as “the amount of water that would move vertically through a unit area of saturated soil in unit time

under unit hydraulic gradient” in the SSURGO Table Column Descriptions report. Porosity used in this study are horizon attribute listed in column “wsatiated_r” (representative value) in the same table, and is described as “the estimated volumetric soil water content at or near zero bar tension, expressed as a percentage of the whole soil”; low and high values of porosity are unavailable. In this study, hydraulic conductivity and porosity are aggregated from horizon to component levels by choosing the value of the deepest horizon available for each component. The parameter values are then aggregated to the map unit level by calculating the average value of the major components. The resulting values are listed in Table 2. For most of the units, the base of the deepest horizon is 2.03 m below the soil top, which is not deep enough to reach the groundwater table for most of the monitoring wells (Table 1). Therefore, hydraulic conductivity and porosity values of these horizons are only considered as approximations, and model calibration is necessary to achieve satisfactory match

Table 2 Representative (ksat_r), low (ksat_l), and high (ksat_h) values of hydraulic conductivity (m day⁻¹) obtained from SSURGO database for soil zones (FID shown in Fig. 3) at the listed horizon depths (cm) in Julington Creek and Eggleston Heights

Soil zone FID	Horizon depth	ksat_l	ksat_r	ksat_h
Julington Creek				
37	173–203	2.190	7.194	12.198
58	36–203	3.659	7.949	12.198
113	0–203	12.182	21.341	30.499
240	0–203	3.659	7.949	12.198
268	13–203	7.540	20.948	34.340
299	13–208	3.659	7.949	12.198
315	89–203	3.659	7.949	12.198
Eggleston Heights				
276	36–203	3.659	7.949	12.198
355	114–203	0.083	0.416	0.721
362	99–203	0.037	0.086	0.122
408	13–203	7.540	20.948	34.341

between simulated and observed concentrations. During the sensitivity analysis and model calibration, the representative values of hydraulic conductivity for each soil map unit are used as initial values, and the low and high values are used as lower and upper bounds. The soil porosity for each soil map unit is used as constant due to its relatively small variability in space.

Isotope data collected at the two sites show strong evidence of denitrification. From September to October, 2010, isotope data were collected from 21 water samples within Julington Creek and 7 samples within Eggleston Heights. Figure 5 plots the $\delta^{15}\text{N}$ values against $\delta^{18}\text{O}$ and shows a linear relationship between the measurements with linear regression slopes of 0.55 and 0.45 for the Eggleston Heights and Julington Creek, respectively. The linear relationship and the slope values indicate occurrence of denitrification, according to the theoretical and experimental studies of (Chen and MacQuarrie 2005; Bottcher

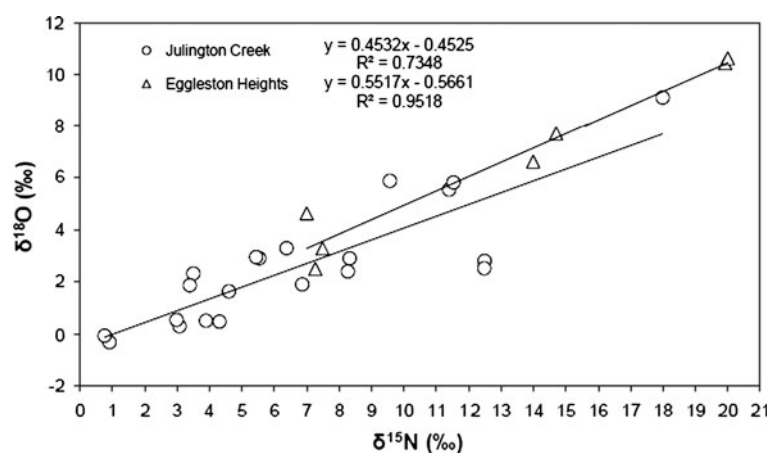
et al. 1990; Aravena and Robertson 1998; Cey et al. 1999; Mengis et al. 1999). Chen and MacQuarrie (2005) suggested that the slope is 0.51 if denitrification is described using the first-order kinetics as in this study. The nitrate isotope data are also used to determine the nitrate sources. According to Tihansky and Sacks (1997) and consistent with earlier work by Kreitler (1975), $\delta^{15}\text{N}$ less than 4 ‰ suggests inorganic nitrate sources such as fertilizer, $\delta^{15}\text{N}$ larger than 9 ‰ suggests organic nitrate sources such as human waste from septic tanks, and values in between suggest organic nitrate sources or fractionated inorganic sources. As shown in Fig. 5, the lower $\delta^{15}\text{N}$ values of the Julington Creek, compared to the relatively higher $\delta^{15}\text{N}$ values of the Eggleston Heights suggests a higher proportion of fertilizer in the nitrate load of Julington Creek. This is consistent with the lawn maintenance status observed during field visits of the two sites. More isotope data and analysis are needed to better distinguish between different nitrate sources.

However, there is no measurement of decay coefficient (or denitrification rate) at the two sites. Reviews of Anderson (1998) and Fernandes (2011) found that there is a positive, linear relationship between the natural denitrification rate and soil organic content. A site-specific investigation of Belanger et al. (2011) shows that the average particulate organic carbon (POC) content is 0.35 and 1.08 % at Eggleston Heights and Julington Creek, respectively. Therefore, a higher value of the decay coefficient should be used at Julington Creek.

Results of global sensitivity analysis

The global sensitivity analysis is conducted to determine the influential parameters to simulate nitrate concentration at the locations of monitoring wells. Among the nine ArcNLET parameters, zonal hydraulic conductivity is considered in the sensitivity analysis, and the parameter

Fig. 5 Measured $\delta^{15}\text{N}$ and $\delta^{18}\text{O}$ values for Julington Creek and Eggleston Heights neighborhoods. The linear relationship and slope close to 0.5 indicate significant denitrification at the sites



ranges of each zone are adopted from the SSURGO database. Porosity does not vary because of its relatively small effect on the nitrate concentration. Due to lack of information, the longitudinal dispersivity (α_x), horizontal transverse dispersivity (α_y), first-order decay coefficient (k), and source nitrate concentration (C_0) are considered to be homogenous over the whole modeling domain to avoid over-parameterization. Following Davis (2000) and Gelhar et al. (1992), the range of 0.21–21.34 m is determined for α_x , since the longitudinal dispersivity typically ranges over 2–3 orders of magnitude, and α_y is set to be 10 % of α_x and change with it simultaneously. According to McCray et al. (2005), the ranges of the k and C_0 are determined to be 0.004–2.27 day⁻¹ and 25–80 mg L⁻¹, respectively. The smoothing factor (*SmthF*) is also constant over the domain by virtue of the simplified conceptual model, and its range is determined to be 40–120 based on our experience. Note that the Morris method only requires users specifying parameter ranges and parameter probability distributions are not needed.

The source plane dimension parameters, Y and Z , are not included in the sensitivity analysis or calibration. According to the conceptual model of ArcNLET, Y is the width of the drainfield perpendicular to the flow direction. While this depends on the dimensions of the drainfield, which in turn depend on house size, soil condition, drainfield construction, and its orientation relative to the direction of flow, a value of 6 m corresponding to a square 400 ft² drainfield was assumed. Z is the average thickness of the plume and only used to calculate nitrate loads (Eqs. 5, 6). In this study, this value is assumed to be 1 m. This is smaller than what is indicated by well screen depths and average water table depths (listed in Table 1). These suggest that the measured concentrations represent about the upper two meters of groundwater. The value is also smaller than the results from a more comprehensive study conducted in Wekiva River Basin, which showed that the plume thickness is around 3–4.5 m (Aley IV et al. 2007).

Figure 6 plots the mean and variance of the elementary effects for all the parameters at the 13 monitoring well locations in Julington Creek (results for Eggleston Heights are not shown). It shows that ranking order of the mean and variance is the same at all the well locations except at well MDR-MW-4. Parameters k , C_0 , α_x and hy_con268 (hydraulic conductivity at soil zone 268 delineated in Fig. 3; the naming convention applies to hydraulic conductivity of other soil zones) are determined to be most critical parameters. Importance of k , C_0 , and α_x is physically reasonable according to Eq. 4. Parameter hy_con268 is important because it is for the largest soil zone at Julington Creek. For the heterogeneous hydraulic conductivity, the sensitivity analysis can reveal which hydraulic conductivity is important at which monitoring well

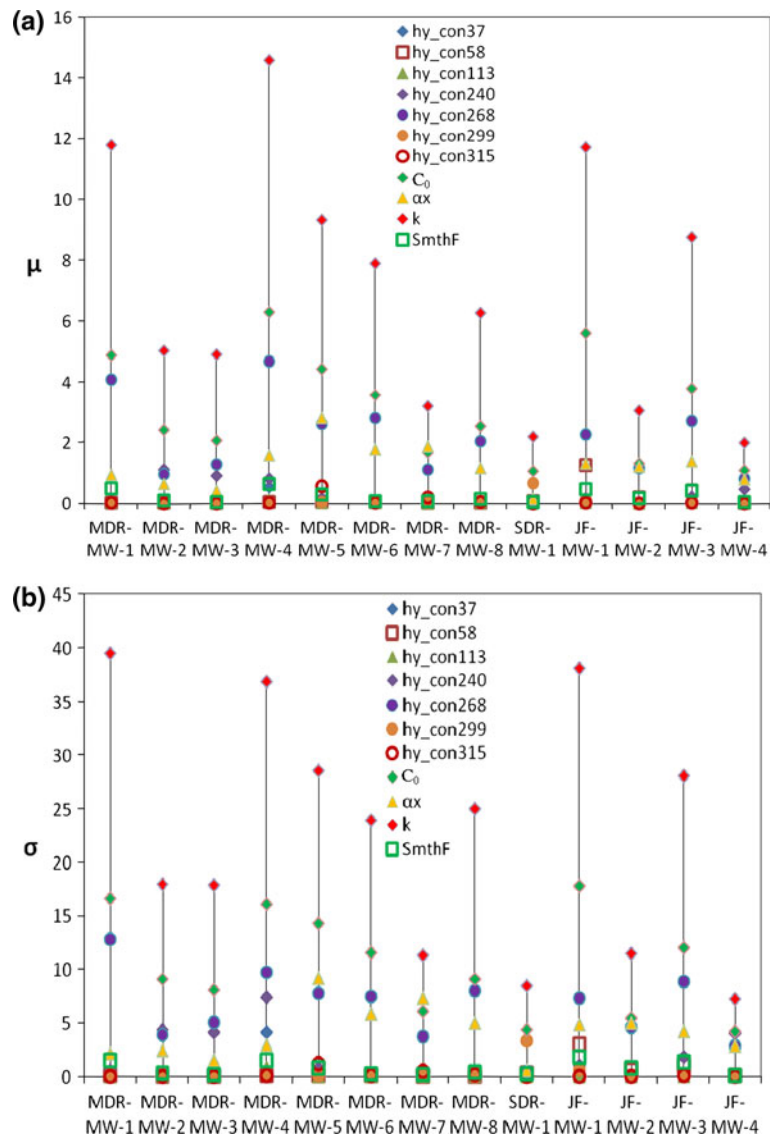
location. For example, parameter hy_con240 is critical to simulated nitrate concentration at well MDR-MW-2 and MDR-MW-3, hy_con299 to SDR-MW-1, and hy_con58 to JF-MW-1. These results are used as guidelines for the trial-and-error based model calibration discussed in the following section to match simulated nitrate concentrations to observed values.

Calibration results and load estimates

The model calibration is conducted using the trial-and-error method to match the simulated hydraulic gradients and nitrate concentrations with corresponding field observations by adjusting the critical parameters identified in the sensitivity analyses. The smoothing factor is first adjusted to match the simulated elevation gradient (calculated from the smoothed DEM) to the observed hydraulic gradient and then remains constant during the transport calibration. Following Davis (2000), the initial values of α_x is taken as 2.134 m. Based on McCray et al. (2005), the initial values of C_0 and k are 40 mg L⁻¹ and 0.025 L day⁻¹, respectively. The initial values of hydraulic conductivity are representative values of the SSURGO database listed in Table 2. During the adjusting, the parameter ranges discussed in the sections of sensitivity analyses are considered as constraints in that the adjusted parameter values are within the ranges to be physically reasonable.

The model calibration is first conducted for the Eggleston Heights neighborhood. Figure 7a plots the mean head observations and smoothed LiDAR DEM at the four observation wells. The smoothed DEM is obtained using the smoothing factor of 60, i.e., the smoothing (through spatial average) is performed 60 times for the entire modeling domain. Figure 7a shows that the smoothed DEM data agree well with the observed water table with a linear correlation coefficient of 0.93 and slope of the linear regression close to 1.0. The slope of regression close to 1 is critical, since it ensures that the shape of the smoothed DEM mimics the shape of water table. The smoothed DEM is higher than the water table, and the distance between them is the intercept of the linear regression equation shown in Fig. 7a. After adjusting the hydraulic conductivity of the soil zones identified in the sensitivity analysis and changing α_x to 10.0 m, α_y to 1.0 m, source concentration C_0 to 80 mg L⁻¹, and k to 0.005 L day⁻¹, the simulated nitrate concentrations are close to the mean observations at the four monitoring wells, at three of which the simulated concentrations fall within the inter-quartile of the observations (Fig. 7b). In this sense, the calibration results are considered acceptable, and it suggests that ArcNLET is able to simulate field observations and spatial distribution of nitrate concentrations. The simulated nitrate

Fig. 6 Modified mean (a) and variance (b) of elementary effects of every parameter at the 13 locations of monitoring wells



plumes for the entire Eggleston Heights neighborhood are plotted in Fig. 8 for illustration. It should be noted that the monitoring wells are located at the far east end of the study area.

Using the calibrated parameters of the Eggleston Heights neighborhood as the starting values, the model calibration is performed for the Julington Creek neighborhood. Using a smoothing factor of 100, the smoothed DEM data agree well with the observed water table with a linear correlation coefficient of 0.91 and slope of the linear regression close to 1.0 (Fig. 7c). The value of C_0 is increased to 100 mg L⁻¹ to empirically account for nitrate contribution from fertilizer use; the value of k is increased to 0.012 L day⁻¹, because of higher POC at the Julington Creek. The dispersivities are the same as those used for Eggleston Heights because the scales and hydrogeological properties of the two sites are considered to be similar. The calibration results in Fig. 7d show that, at 7 out of 13

observation wells, the simulated nitrate concentrations are close to the mean observations; at 11 wells, the simulated concentrations are within the range of maximum and minimum observations. In this sense, the modeling results are considered as acceptable, despite that overestimation occurs at several wells such as MDR-MW-4 and MDR-MW-5 (the overestimation of concentration may result in overprediction of load to the river). The calibration results at Julington Creek are less satisfactory than those at Eggleston Heights, which may be due to the effect of fertilizer use that is not explicitly incorporated in the simulation or heterogeneity of transport parameters that are assumed to be constant during the calibration.

Accuracy of the numerical results is evaluated using the mass budget error calculated for the plumes that do not reach the surface water bodies. For such plumes, the inflow mass rate M_{in} should be equal to the denitrification mass

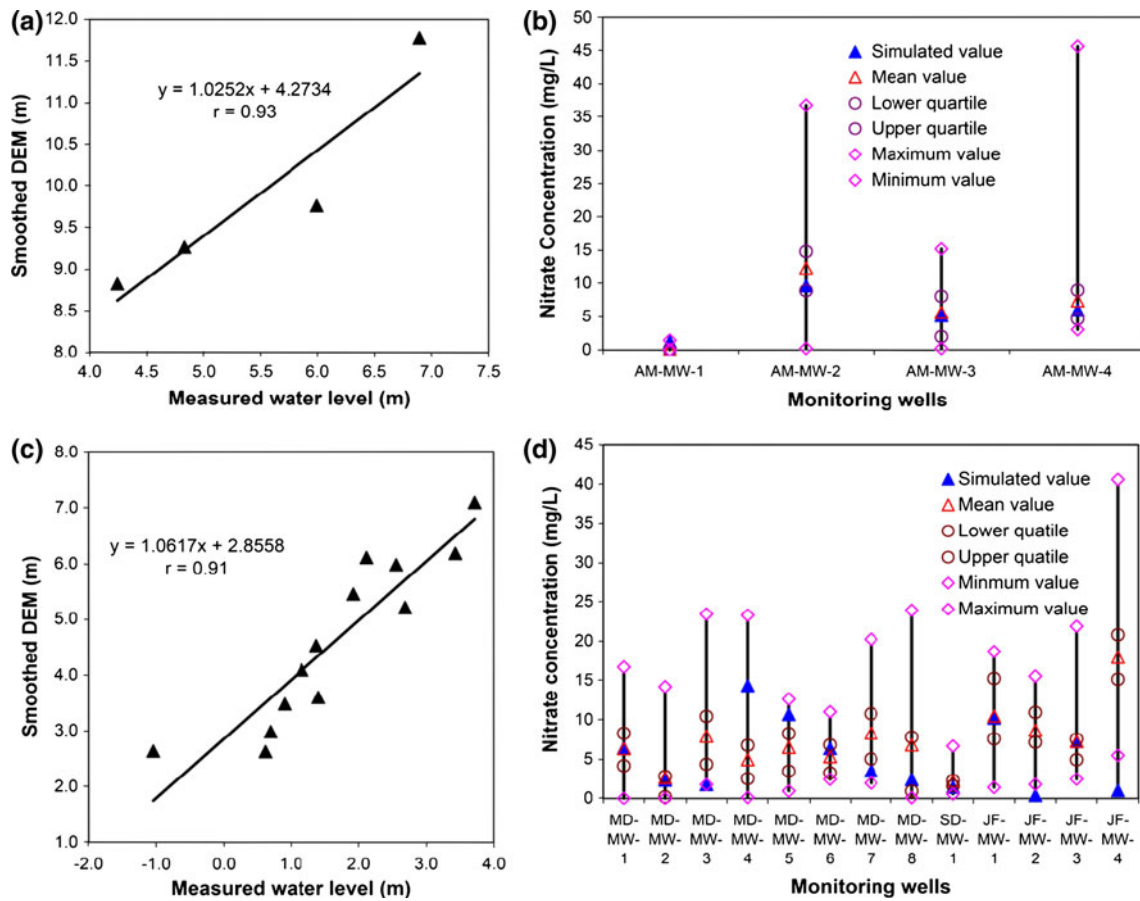
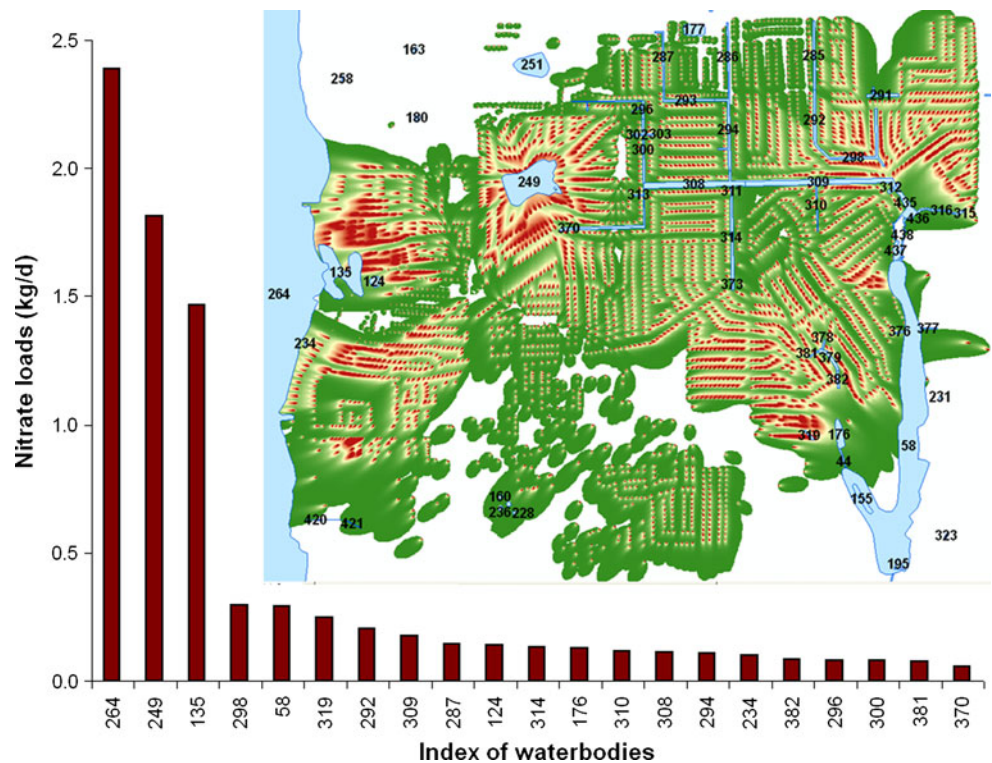


Fig. 7 Calibration results of **a** hydraulic head, **b** nitrate concentration for Eggleston Heights neighborhood, **c** hydraulic gradient, and **d** nitrate concentration for Julington Creek neighborhood

Fig. 8 Simulated nitrate plumes and nitrate loads to target water bodies at Eggleston neighborhood. The load estimates less than 0.05 kg day^{-1} are not shown



rate M_{dn} ; the discrepancy between them serves as an indicator of mass balance error. The difference between M_{in} and M_{dn} is calculated as a percent error, via

$$\text{Discrepancy (\%)} = \frac{M_{in} - M_{dn}}{0.5(M_{in} + M_{dn})} \times 100 \quad (8)$$

The discrepancy is 0.9 % for Eggleston Heights and 2.2 % for Julington Creek, indicating satisfactory mass balance in the numerical evaluation.

The calibrated models are used to estimate nitrate load to the surface water bodies from 3,495 septic systems in Eggleston Heights and 1,924 in Julington Creek. However, the accuracy of the load estimates cannot be evaluated directly, since there is no on-site observation of the load. An indirect way of evaluating the load estimate is to compare the estimated average load to the groundwater per septic system with other estimates in literature. The U.S. EPA Onsite Wastewater Treatment Systems Manual (Table 3–8, U.S. EPA, 2002) estimated that the average total nitrogen contribution to septic systems is 11.2 g of nitrogen per person per day. According to the census data available at http://en.wikipedia.org/wiki/Duval_County,_Florida, the average household size is approximately 2.51 persons per household in Duval County. This equates to an average of 28.11 g nitrogen per home per day discharged to septic systems. A 10 % reduction of nitrogen through volatilization of ammonia and removal of solids as septage 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 (mainly nitrate) per septic system per day is discharged to the groundwater. At Eggleston Heights, the estimated source input load to groundwater from 3,495 septic systems is $115.4 \text{ kg day}^{-1}$; the average nitrate load for every septic system is about 33 g day^{-1} . At Julington Creek, the estimated source input load to groundwater from 1,924 septic systems is about 59.4 kg day^{-1} ; the average load is 31 g day^{-1} per septic system. While the average value at Eggleston Heights is higher than the estimated 19 g based on literature data, it appears to be in a reasonable range, considering the variability of household size, different drainage conditions, and heterogeneous hydrogeologic properties. Since the estimated source input load at Julington Creek includes fertilizer applications, it should not be directly compared with this literature data of 19 g. However, if assuming that C_0 contributed by septic tank effluent is the same at Julington Creek and Eggleston Heights (i.e., 80 mg L^{-1}), then by virtue of the linear relationship between source input load and C_0 (Eq. 5), the load at Julington Creek due to septic systems can be estimated easily. The estimated average load is 24.8 g day^{-1} per septic system, which is close to the literature value of 19 g.

A unique feature of ArcNLET is that it can estimate nitrate loads to different water body components identified by the FID of polygon features of the surface water bodies input layer. This is demonstrated in Fig. 8, which plots the estimated loads to 21 water bodies within or around the Eggleston Heights neighborhood. The three largest loads (in the descending order) are to the water bodies with indices of 264, 249, and 135; they receive about 66 % of the total load. Water body 264 is the St. Johns River. The flow paths indicate that it is the target of 776 septic systems, more than 1/5 of the total number of the septic systems in the neighborhood. In addition, the hydraulic conductivity is significantly larger in part of the areas around this water body, which leads to high source input due to fast flow. Receiving nitrate from a large number of septic systems and high hydraulic conductivity in the vicinity of the water body are believed to be the major reasons for the large nitrate load estimate. This is also true for water body 249 (Lake Lucina), which is the target of 430 septic systems and surrounded by a zone of relatively large hydraulic conductivity (about 12.0 m day^{-1}). Water body 135 is a swamp, the target of 97 septic systems. It receives the third largest nitrate load, because of its low elevation; larger hydraulic gradient exists and results in higher simulated flow velocity. These analyses suggest that the loads estimates are reasonable as they are consistent with the hydrogeologic information of the area. Since ArcNLET is capable of identifying whether a plume reaches surface water bodies, the software can be used to evaluate a setback distance beyond which septic systems have no or negligible effect on the surface water body, which is useful to environmental management such as facilitating decision-making on converting OSTDS into sewers.

At Julington Creek, the total nitrate load to the surface water bodies is about 1.4 kg day^{-1} , much smaller than that of 8.6 kg day^{-1} at Eggleston Heights. This is not surprising considering the smaller number of septic systems and larger denitrification rate at Julington Creek. The results of load estimation suggest high nitrate removal effectiveness of the shallow groundwater systems (93 % for Eggleston Heights and 98 % for Julington Creek).

Conclusion and discussion

ArcNLET, an ArcGIS-Based Nitrate Load Estimation Toolkit, is developed as a screening tool for estimating nitrate load from septic systems to surface water bodies. The software is based on a simplified groundwater flow and nitrate fate and transport model, and is developed as an ArcGIS extension using the Visual Basic.NET programming language. The model execution as well as pre- and

post-processing are performed within ArcGIS. The software is user friendly and can be used by non-technical users (including decision-makers) for water resources and environmental management. However, when the load estimate is used for decision-making, simplifications and assumptions embedded in the conceptual model and handling of fertilizer use should be considered.

ArcNLET is used in this study to demonstrate how to estimate nitrate load from thousands of septic systems to surface water bodies in two neighborhoods of Jacksonville, FL, USA, where nitrate due to septic systems is believed to be one of the reasons of nutrient enrichment and an isotope study suggests that denitrification is significant. The global sensitivity analyses are performed using real data at Julington Creek to identify the parameters critical to simulated nitrate concentration for model calibration. The global sensitivity varies in space and is different for different parameters. The homogeneous parameters k , C_0 , and α_x are influential to simulated nitrate concentrations at all monitoring well locations. For the zonal hydraulic conductivity, its values at different zones have different level of influence at different locations. Overall, hydraulic conductivity (hy_con268) at soil zone 268 has the most prominent effect, because this soil zone is the largest at Julington Creek. By manually adjusting model parameters, approximated hydraulic gradients and simulated nitrate concentrations agree reasonably with average field observations. This indicates that ArcNLET is able to simulate spatial variability of nitrate concentration, which cannot be achieved by other ArcGIS-based screening models. The reason is that the conceptual model of ArcNLET considers key hydrogeologic processes of nitrate transport. Estimated nitrate loads to surface water bodies exhibit spatial variability, which is useful to facilitate decisions on converting OSTDS into sewers at certain areas for reducing nitrate load from septic systems to surface water bodies. However, there are various sources of uncertainty in the nitrate load estimation, including unknown model parameter values, variation in the load from individual households, measurement errors, extrapolation from the area around a few monitoring wells to large areas, and inadequacy of the simplified conceptual model. Quantification of uncertainty of the load estimates is warranted in future study, as the uncertainty analysis provides more information for science-based decision-making. The uncertainty can be reduced by validating model assumptions and calibrating the model with more field data.

The load estimates in this study have not been directly validated against field load measurements due to the lack of the measurements. Although the flow and transport models were calibrated against field measurements of hydraulic heads and nitrate concentrations, there is no guarantee that the load estimation given by the calibrated model is the

true field value. One concern is the use of the pseudo 3-D model, which requires using the average plume thickness, Z , the average plume thickness. The value of Z used in this study has not been validated due to lacking information on vertical concentration profiles. Since the Z value is directly related to the load estimation, it may result in over- or under-estimation of the load, depending on whether the plumes are shallower or thicker than the Z value. Another concern relates to the calibration of the source plane concentration, C_0 , that determines the input load to groundwater. Although the input load is comparable with literature data, it is unknown whether the calibrated C_0 value agrees with field observations. It is expected that these concerns of model validation can be addressed by collecting more field data. A sensitivity analysis to identify the most influential parameters to the load estimation may be the first step in future study. In addition, the ditches in the two neighborhoods are not considered in the load estimation, which may affect the load estimate through the groundwater flow model.

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