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ArcNLET: A GIS-based software to simulate groundwater nitrate load from septic systems to surface water bodies

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ABSTRACT

Onsite wastewater treatment systems (OWTS), or septic systems, can be a significant source of nitrates in groundwater and surface water. The adverse effects that nitrates have on human and environmental health have given rise to the need to estimate the actual or potential level of nitrate contamination. With the goal of reducing data collection and preparation costs, and decreasing the time required to produce an estimate compared to complex nitrate modeling tools, we developed the ArcGIS-based Nitrate Load Estimation Toolkit (ArcNLET) software. Leveraging the power of geographic information systems (GIS), ArcNLET is an easy-to-use software capable of simulating nitrate transport in groundwater and estimating long-term nitrate loads from groundwater to surface water bodies. Data requirements are reduced by using simplified models of groundwater flow and nitrate transport which consider nitrate attenuation mechanisms (subsurface dispersion and denitrification) as well as spatial variability in the hydraulic parameters and septic tank distribution. ArcNLET provides a spatial distribution of nitrate plumes from multiple septic systems and a load estimate to water bodies.

ArcNLET's conceptual model is divided into three sub-models: a groundwater flow model, a nitrate transport and fate model, and a load estimation model which are implemented as an extension to ArcGIS. The groundwater flow model uses a map of topography in order to generate a steady-state approximation of the water table. In a validation study, this approximation was found to correlate well with a water table produced by a calibrated numerical model although it was found that the degree to which the water table resembles the topography can vary greatly across the modeling domain. The transport model uses a semi-analytical solution to estimate the distribution of nitrate within groundwater, which is then used to estimate a nitrate load using a mass balance argument. The estimates given by ArcNLET are suitable for a screening-level analysis.

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1. Introduction

Estimating nitrate fate and transport in groundwater is an important task in water resources and environmental management because excess nitrate load on groundwater and surface water may cause negative impacts on human and environmental health. In humans, excessive nitrate-nitrogen becomes harmful due to its conversion to the more toxic nitrite-nitrogen. Elevated nitrate intake have been identified as a possible cause of gastric cancer (U.S. Environmental Protection Agency, 1993) and can cause methemoglobinemia in infants (blue baby syndrome) (U.S. Environmental Protection Agency, 1993). Elevated levels also harm livestock, fish and aquatic ecosystems. In aquatic ecosystems, high levels of nitrate can cause eutrophication of the water body, leading to algae blooms and excessive plant growth, the decay of which can cause anoxic conditions (Art, 1993). There are several sources of nitrogen contamination such as agriculture, wastewater treatment plants, industrial sources and natural sources, with the contribution of each source varying depending on the region of study. The contribution from Onsite Wastewater Treatment Systems (OWTS), also known as septic systems, may be especially important in areas where the OWTS are located in close proximity to a surface water body or where there is a dependence on shallow wells for drinking water.

The use of GIS in conjunction with hydrologic modeling began has become a well established concept due to the spatial nature of water models (Cesur, 2007; Maidment, 2002; Martin et al., 2005; Yang and Lin, 2011). As pointed out by Carrera-Hernández and Gaskin (2006), Lin et al. (2009), and Akbar et al. (2011), the versatility of GIS to act as a data pre- and post-processor as well

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as its ability to act as an effective data management platform and its capability to perform further spatial analyses makes it an ideal platform on which to base a groundwater modeling tool. GIS-embedded and GIS-linked nitrate models, both process-based (e.g., physically based) and non-process-based (e.g., empirical or statistical), have been previously developed (Hajhamad and Almasri, 2009; Lasserre et al., 1999; Schilling and Wolter, 2007). However, the focus has been on large-scale (regional), non-point sources (i.e., agricultural applications) and there have been few attempts to integrate more local point sources into these regional models (e.g. Bidwell and Good, 2007). Development of nitrate models focusing on smaller scale, point sources such as OWTS has not been seriously attempted, despite the fact of the importance of considering the effects of these sources on groundwater and surface water at local scales.

In order to support decision-making with regards to the effects of OWTS discharge on groundwater and surface water quality, the ArcGIS-Based Nitrate Load Estimation Toolkit (ArcNLET) was developed. ArcNLET functions as a screening model embedded within ArcGIS 9.3 (and 10.0) whose purpose is to estimate nitrate concentration distribution within groundwater and to estimate nitrate loads to surface water bodies from OWTS at neighborhood scales. This is achieved by using a simplified topography-based groundwater flow model and a semi-analytical approach to nitrate transport and fate. While sophisticated nitrogen transport models are available (e.g. Maggi et al., 2008; Valiela et al., 1997), the key driving force behind the development of the ArcNLET software is the need for a tool that is capable of providing quick, order-of-magnitude estimates of groundwater flow patterns and nitrate concentration distribution with the ultimate goal of estimating the nitrate loads to surface water bodies. Two important design criteria that define ArcNLET are (1) the ability to construct and run a model with a minimal amount of data while still providing scientifically defensible estimates and (2) the ability for less technical users use ArcNLET to construct and run a model within a time constrained scenario. These two characteristics, combined with the GUI-based interaction, render ArcNLET very easy to use with model runs that can be quickly set up, even by less technical users. Although the ArcNLET is developed using OWTS as the focus, it is applicable to any point source of nitrate (e.g., livestock facilities). The GIS-embedded model of Menezes and Inyang (2009) is similar in spirit to ArcNLET, but ArcNLET has more comprehensive groundwater flow modeling abilities and has the more ambitious goal of estimating actual contaminant loads. While ArcNLET does not simulate on-ground nitrogen loading and soil nitrogen dynamics, it can be coupled with software that simulates surface and vadose zone processes for comprehensive estimation of nitrate load from septic systems to surface water bodies. This is warranted in future study.

2. Conceptual model

The conceptual model behind ArcNLET is composed of three separate sub-models: the flow, transport, and nitrate load estimation models. Each of these models is independent allowing for a modular approach to implementation and use. The implementation of the conceptual models is discussed in Section 3.

2.1. Flow model

The aim of the flow model is to generate a map of groundwater flow velocity (direction and magnitude) using a minimal amount of data by making several simplifications. Although these simplifications restrict the types of scenarios that the model can be applied to, they are necessary in order to achieve the goal of reducing data demands.

The simplifying assumptions made in the flow model are: (a) The water table is assumed to be a subdued replica of the topography. As a result, the water table can be approximated by smoothing the topography. This assumption is commonly employed to reduce the burden of collecting detailed data and to simplify modeling (Beven and Kirkby, 1979; Desbarats et al., 2002; Stieglitz et al., 1997; Sepúlveda, 2002; Schilling and Wolter, 2007). Whether it is justified or not depends on the general hydrologic characteristics of a particular study area (Haitjema and Mitchell-Bruker, 2005; Shahbazi et al., 1968). (b) Steady-state flow conditions. Because only long term estimates are desired, recharge and its transient effect on the shape of the water table is not directly considered (long term recharge is indirectly considered by how much the shape of the water table simulated by ArcNLET resembles the topography). (c) Only saturated flow in porous media is considered. (d) Flow occurs under Dupuit conditions. That is, flow lines are assumed to be horizontal and equipotentials vertical. In addition, the hydraulic gradient is assumed to be equal to the gradient of the water table and is invariant with depth. The Dupuit approximation is valid when the slope of the water table is small and the average aquifer thickness is small compared to the aquifer extent (Freeze and Cherry, 1979). In essence, the Dupuit approximation considers three-dimensional flow as two-dimensional.

Applying a two-dimensional form of Darcy's law

$$\vec{v} = -\frac{K}{\theta}\vec{\nabla}h \tag{1}$$

where $\vec{v}$ [L/T] is the groundwater seepage velocity, hydraulic gradient ($\vec{\nabla}h$ [–]) is approximated by the gradient of a subdued replica of the topography which is generated by processing a digital elevation model (DEM). Heterogeneous fields of hydraulic conductivity (K [L/T]) and the porosity (θ [–]) can be used in ArcNLET and such fields can be obtained from existing databases such as the Soil Survey Geographic database (SSURGO).

When using topographical maps for hydrologic models, the presence of sinks (depressions in the topography) and flat areas (areas with a gradient magnitude of zero) is problematic because if flow enters these areas, it will never escape. Sinks are treated by filling them. Sink filling is common when using DEM data for surface hydrologic models (Martz and Garbrecht, 1998; Pan et al., 2004) and was used in the context of groundwater flow in the simplified groundwater travel time model of Schilling and Wolter (2007). Due to the use of the topographical gradient to approximate the hydraulic gradient, flat areas present in the topography may result in areas of zero hydraulic gradient. In this model, flat areas are considered to be spurious. There can be several causes of flat areas, including limited vertical DEM resolution, rounding or truncation of elevation values, and sink filling (Martz and Garbrecht, 1998).

Once the seepage velocity is calculated using Eq. (1) for the entire study area, flow lines originating from one or more OWTS locations are calculated. Flow line generation follows a particle tracking approach: an imaginary particle is released from a given origin and allowed to move within the velocity field in a discretized manner. The particle advances with a user-defined step size according to the magnitude and direction of flow at the particle's current location. The flow line terminates when it reaches a water body or a maximum number of steps have been taken. In addition to serving as a visualization of the velocity field, information from these flow lines is used by the transport model (see following section).

2.2. Transport model

The transport model's objective is to calculate the nitrate concentration distribution, taking into account denitrification, originating from one or more OWTS by making use of a semi-analytical solution. The semi-analytical solution developed by

Domenico and Robbins (1985) and further refined by Domenico (1987) and Martin-Hayden and Robbins (1997) considers a three-dimensional plume undergoing first-order decay, emanating from a vertically oriented, constant concentration source plane centered at (0, 0, 0) having dimensions Y and Z. The full governing equation and the corresponding solution is given in Section S1 of Supplementary material and is hereafter referred to as the Domenico solution. In the Domenico solution, groundwater flow is exclusively in the longitudinal (positive x) direction and dispersion occurs in all three directions.

ArcNLET adopts a two-dimensional, steady-state version of the full Domenico solution (see Section S1 in Supplementary material for a derivation). By adopting this reduced solution, a significant savings in memory and an increase in computation speed is realized while at the same time reducing input data demands. The solution used by ArcNLET is

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

with

$$F_1 = \exp\left[\frac{x}{2\alpha_x}\left(1-\sqrt{1+\frac{4k\alpha_x}{v}}\right)\right] \tag{3a}$$

$$F_2 = erf\left(\frac{y+Y/2}{2\sqrt{\alpha_y x}}\right) - erf\left(\frac{y-Y/2}{2\sqrt{\alpha_y x}}\right) \tag{3b}$$

where $C(x,y)$ [M/L^3] is the concentration at location x,y, C_0 [M/L^3] is the concentration of the source plane, Y [L] is the width of the source plane, α_x and α_y [L] are the longitudinal and transverse dispersivities, v [L/T] is the constant seepage velocity in the longitudinal direction, and k [T^{-1}] is the first-order decay constant. Domenico-type solutions have been previously used in the U.S. EPA models BIOSCREEN (Newell et al., 1996) and BIOCHLOR (Aziz et al., 2000). BIOSCREEN aimed to model the biodegradation of petroleum hydrocarbons in groundwater while in BIOCHLOR, the target compounds were chlorinated solvents.

The Domenico system considered by ArcNLET can be conceptualized as shown in Fig. 1. As shown in the figure, contaminants exit the OWTS drainfield, percolate through the unsaturated zone (bounded by the rectangular box indicated by the dotted lines), and enter the saturated zone (bounded by the box indicated by the solid lines) which has a uniform and steady flow in the direction indicated. Once the nitrate reaches the saturated zone, the evolution of the contaminant plume is approximated using Eq. (2). Denitrification is commonly considered to be a first-order decay process (McCray et al., 2005) and is modeled here using the first-order decay term in Eq. (3a). Evaluation of Eq. (2) occurs over a discretized domain where the size of each evaluation cell is specified by the user.

Eq. (2) is applied to each septic tank substituting the velocity information calculated by the flow model for the v variable in Eq. (3a). Heterogeneous v is considered via averaging along the flow path and warping of the plume (see Section 3.2 for details). In regions where two or more plumes overlap, concentration values are summed using the principle of superposition made possible by the linearity of the governing equation (Ibaraki, 2001).

2.3. Nitrate load estimation

Nitrate load estimates are obtained from the steady-state transport model using a simple mass-balance approach. The output of the load estimation model is not a map but is instead a list of values giving the nitrate load corresponding to each affected water body. By giving the nitrate load on a water body-by-water body basis rather than a lumped sum, it allows for the identification of nitrate contamination hotspots.

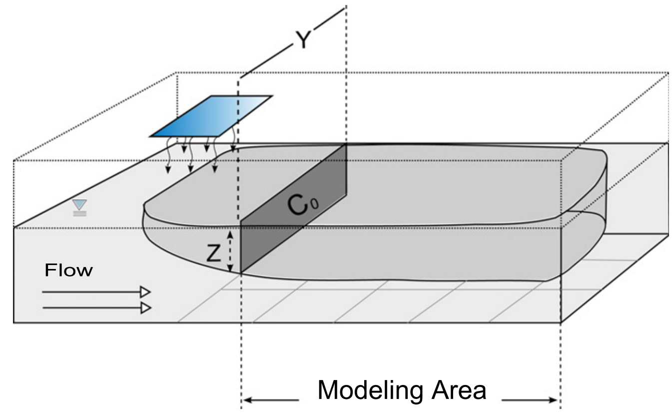

Fig. 1. Conceptualization of the application of the Domenico solution in the transport model of ArcNLET. Contaminants from a septic tank drain field enter groundwater and form a contaminant plume. For modeling purposes, the plume is considered to emanate from a vertically oriented plane ($Y-Z$) having a constant concentration C_0 after which the plume is advected with the flow of groundwater while undergoing dispersion in the longitudinal and transverse directions. The origin of the coordinate system is located at the center of the $Y-Z$ plane with the positive x direction towards the right. Adapted from Aziz et al. (2000).

In the steady-state, the mass output rate, M_{out} [M/T], can be calculated via

$$M_{out} = M_{in} - M_{dn} \tag{4}$$

if the mass input rate, M_{in}, and the mass lost due to denitrification, M_{dn} are known (or can be calculated).

Similar to BIOCHLOR, nitrate mass is calculated by converting the plume calculated by Eq. (2) into a pseudo-three-dimensional (pseudo-3D) form by extending the two dimensional plume vertically downwards to a depth Z (this Z is equivalent to the Z dimension of the source plane in Fig. 1). This Z is then multiplied by the length and width of a cell yielding the volume of a cell, V_i. Mass is then calculated on a cell-by-cell basis by multiplying the concentration in each cell by the pore volume. With this pseudo-3D plume, the $Y-Z$ plane can still be thought of as the constant concentration plane of the 3D Domenico solution, however the plume concentration at any point in the domain becomes invariant in the z direction. This pseudo-3D approximation is considered to be valid when the vertical dispersivity of the aquifer is small or the seepage velocity is relatively high. Under most circumstances, the vertical dispersivity can be considered small since it is normally two orders of magnitude smaller than the longitudinal dispersivity and an order of magnitude smaller than the horizontal transverse dispersivity (Gelhar et al., 1992). Additionally, very low vertical dispersivities have been observed in field measurements (Gelhar et al., 1992).

Because denitrification is modeled as a first-order decay process, we can use the definition of first-order decay to calculate the rate of denitrification for every cell in the plume. The rate is multiplied by the mass of solute to obtain the mass rate of denitrification

$$M_{dn} = \sum_i k C_i V_i \theta \tag{5}$$

where k [T^{-1}] is the first-order rate constant for the plume, C_i [M/L^3] is the concentration in cell i, V_i [L^3] is the volume of cell i, and θ [–] is the soil porosity. The rate constant is assumed homogeneous over the entire domain. Similar to the treatment of spatially heterogeneous velocity in Eq. (2), the porosity is averaged along the flow line (arithmetic mean).

The M_{in} term in Eq. (4) corresponds to the mass input rate from the constant concentration source plane of Eq. (2). The input load calculation accounts not only for mass input due to advection but

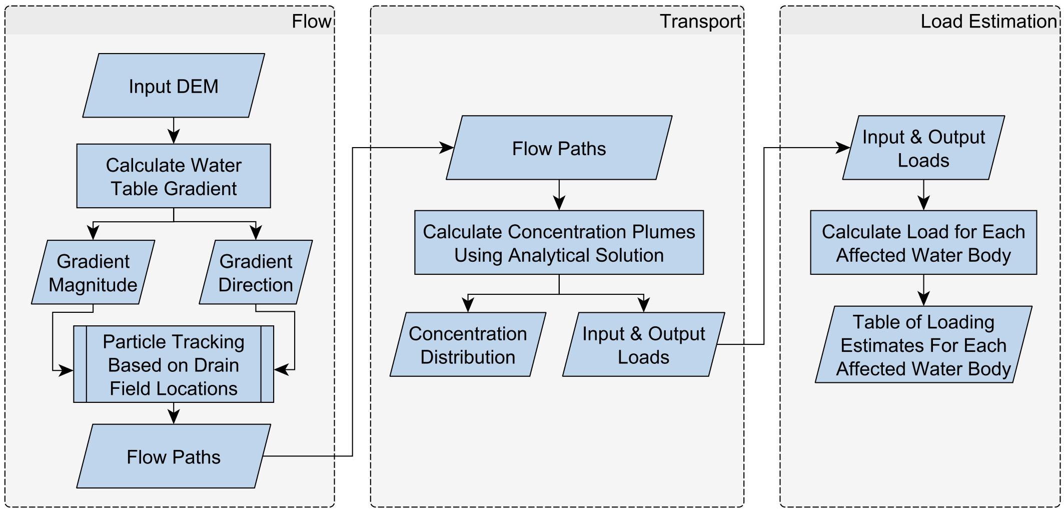

Fig. 2. An overview of the structure of ArcNLET. The workflow of a typical run begins with the Flow module and the flow path calculation. Subsequently, the Transport module calculates the nitrate concentration distribution and load for each OWTS. Finally, the total load for each affected water body is calculated by the Load Estimation module.

also through dispersion. M_{in} consists of two terms

$$M_{in} = M_{adv} + M_{dsp} \tag{6}$$

where M_{adv} is the advective component and M_{dsp} is the dispersive flux resulting from the concentration gradient across the boundary.

The advective term is calculated via

$$M_{adv} = C_0 YZ\theta v \tag{7}$$

The dispersion term is calculated by assuming dispersion is governed by Fick's law via

$$M_{dsp} = -D_x YZ\theta \frac{\partial C}{\partial x} \tag{8}$$

where D_x [L^2/T] is the hydrodynamic dispersion coefficient along the longitudinal direction; the remaining parameters are the same ones from Eq. (7). Disregarding molecular diffusion, the dispersion coefficient is calculated as (Freeze and Cherry, 1979)

$$D_x = \alpha_x v \tag{9}$$

where α_x [L] is the medium's dispersivity in the longitudinal direction. Substituting Eqs. (7)–(9) into Eq. (6) leads to

$$M_{in} = C_0 YZ\theta v - \alpha_x v YZ\theta \frac{\partial C}{\partial x} \tag{10}$$

Using Eq. (2) to calculate the partial derivative of C, M_{in} can be expressed analytically as

$$M_{in} = C_0 YZ\theta v \left(\frac{1+\sqrt{1+\frac{4k\alpha_x}{v}}}{2} \right) \tag{11}$$

The derivation for Eq. (11) is provided in Section S2 of Supplementary material. If the value of Z is difficult to estimate for certain sites but M_{in} is known, ArcNLET can estimate the Z value from M_{in} using Eq. (11). This equation shows that the mass input rate is independent of the nitrate concentration of the plume but dependent on the source plane concentration.

3. Implementation

ArcNLET is implemented as an extension to ArcGIS using the Visual Basic .NET programming language. In keeping with the object-oriented paradigm, the program is structured in a modular fashion based on the distinct sub-models of Section 2. In this paper, we make the distinction between a *model* and a *module*. A *model* refers to the conceptual models used in the software while a *module* refers to the software implementation of one or more models. Fig. 2 presents an overview of the Flow, Transport, and Load Estimation modules and a brief description of each module's inputs, algorithm, and outputs is provided below. Additional details are given in Section S3 of Supplementary material. For demonstration purposes, a complete model run is described in Section S4 of Supplementary material.

3.1. Flow module

The purpose of the Flow module is to generate a map of groundwater flow velocity and direction in the surficial aquifer using a DEM and heterogeneous maps of hydraulic conductivity and porosity by applying Darcy's law on a cell-by-cell basis. The output of the flow module consists of two raster files, representing the magnitude and direction of seepage velocity, respectively. These are generated by applying a smoothing filter to the DEM, and calculating flow magnitude and direction based on a Sobel filter, while taking into account the presence of sinks and flat areas in the smoothed DEM. These rasters are then used by the particle tracking functionality to calculate flow paths.

3.2. Transport module

This module applies Eq. (2) to a set of OWTS locations (provided by the user in the form of a shapefile) in concert with the groundwater flow paths (which contain velocity and direction information) calculated by the Flow module. A plume is calculated individually for each OWTS. Once all plumes have been calculated, they are combined into a single raster, summing the concentration values where plumes overlap. Heterogeneity in the groundwater flow field is considered by averaging the flow velocity along the flow path using the harmonic mean, combined with a transformation (thin-plate spline or polynomial) of the plume such that its centerline conforms to the flow path. The output of the Transport module is a raster containing the combined nitrate concentration plumes of all sources in the input shapefile along with an auxiliary shapefile containing information (e.g., load to groundwater) about each individual plume.

3.3. Nitrate load estimation module

The Nitrate Load Estimation module estimates the load using Eq. (4). The values of M_{in} and M_{dn} for each septic tank are read from the auxiliary file generated by the Transport module. For each affected water body, a value of M_{out} is produced. An affected water body is one where one or more nitrate plumes reach that water body. Unlike the Groundwater Flow and Transport modules, the Nitrate Load Estimation module does not output a shapefile or raster. Instead, the output is a single number corresponding to the load to each affected water body. If there are multiple affected water bodies, a list of such numbers is output. This list can then be exported to a spreadsheet software for further analysis.

4. Verification

In order to test the validity of the assumptions and the accuracy of the approximations involved in the software, several test cases are examined. Each model is tested in isolation by comparing the model results with a numerical model of the same test case. In the case of the flow model, the comparison is made to a numerical model based on a previously studied real-world location. On the other hand, the transport and load estimation calculations are compared to hypothetical scenarios.

4.1. Flow module

The fundamental simplification made by the flow model is that the water table is a subdued replica of the topography. In order to evaluate the effectiveness of this approximation, ArcNLET's results are compared to a steady-state, two-dimensional model of the U.S. Naval Air Station (NAS) located in Jacksonville, Florida constructed by the USGS (Davis et al., 1996). The comparison serves to demonstrate that the degree to which the water table resembles the topography can be highly variable over regions as large as the NAS.

The NAS is located in Jacksonville, Florida along the banks of the St. Johns River and is bounded to the west by the Ortega River (Fig. 3). The composition of the surficial aquifer in the vicinity of the NAS consists of medium to fine-grained unconsolidated sands with interspersed local sandy clay beds. The base of the aquifer corresponds to the top of the Hawthorn group which is a confining clay layer separating the surficial aquifer from the Upper Floridian aquifer (Davis et al., 1996). The depth to the Hawthorn group is variable but ranges between 3 and 30 m and the aquifer rises to approximately 9 m (up to 20 m in areas) above sea level.

The model by Davis et al. (1996) was constructed using the numerical package MODFLOW (Harbaugh et al., 2000) as a single-layer, steady-state model of groundwater flow and was calibrated against 128 well measurements (locations shown in Fig. 3). The simulated hydraulic head in 121 of the 128 wells fell within the 2.5 ft calibration criterion.

Over the area of the entire NAS, the water table generally follows the topography, as demonstrated by a correlation coefficient of 0.87 ($R^2=0.76$) between the water table and the topography shown in the upper plot of Fig. 4. However there is much variation on smaller scales as evidenced by the spread of the data points in the plot. In the lower plot of Fig. 4, a subdued replica of the topography was generated by the algorithm discussed in Section 3.1 using 50 smoothing iterations (determined by trial-and-error). The subdued replica of the topography has a correlation coefficient of 0.92 ($R^2=0.85$), indicating that ArcNLET's smoothing algorithm provides a better approximation to the water table compared to using the unprocessed topography alone. The variation in the data points around the best-fit line in the lower plot of Fig. 4 again shows that the degree to which the water table resembles a subdued replica of the topography varies in space. Because of this variation in the water table–topography relationship over the entire domain of the NAS, a smaller sub-area

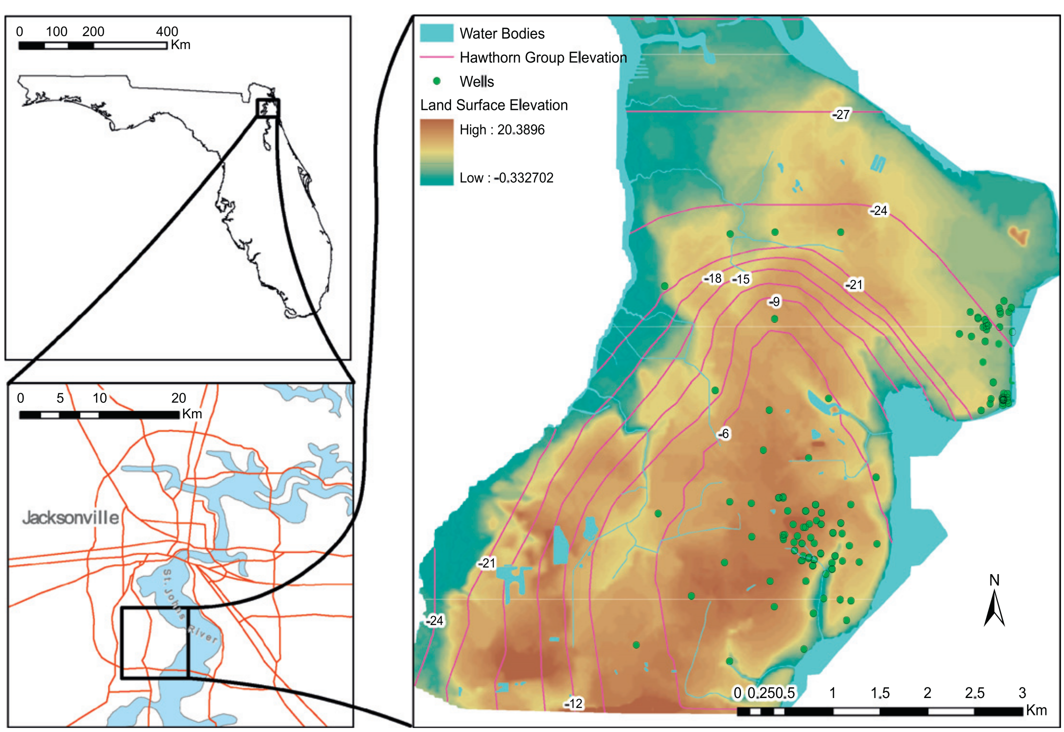

Fig. 3. U.S. Naval Air Station (NAS) Jacksonville, Florida. The NAS is used to evaluate the flow model used by ArcNLET by comparing it to a calibrated numerical model constructed by the USGS. The location of the calibration wells is shown as the small circles on the map. Elevation values are in meters.

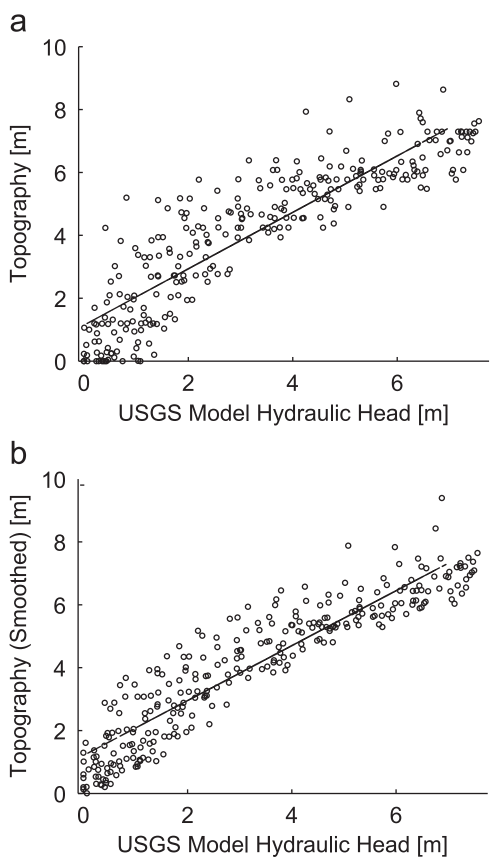

Fig. 4. Relationship between the water table and the topography in the NAS (a) and relationship between the water table and a subdued replica of the topography (b). Pearson's correlation coefficient is 0.87 and 0.92 respectively. Overall, this shows a good relationship in both cases however the spread of points suggests local variation.

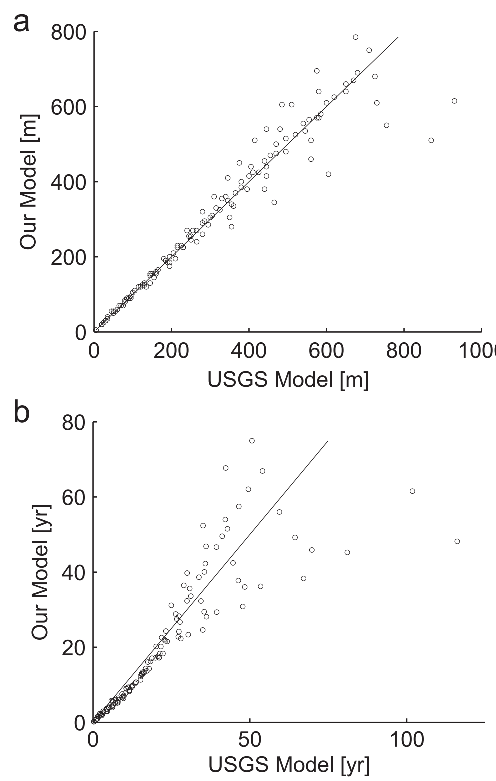

Fig. 5. Correlation of travel distance (a) and time (b) estimates between ArcNLET and the USGS model of Davis et al. (1996). The correlation coefficients are 0.96 and 0.86 respectively and the line represents the ideal 1:1 correspondence between estimates.

with less variation, located in the mid-northern part of the NAS, was selected for comparison to ArcNLET.

The Flow module was executed for the NAS sub-area using a 10 m by 10 m resolution DEM of the NAS obtained from the National Elevation Dataset (NED) and a map of water bodies obtained from the National Hydrography Dataset (NHD). Homogeneous hydraulic conductivity and porosity parameters were set to the same values as the USGS model (2.28 m/day and 0.25 respectively). The smoothing factor parameter was set to 50. Fig. 5 shows the correlation between travel time and distance estimates (used as a proxy for velocity) produced by ArcNLET with those produced by the USGS model. There is strong correlation in both time and distance estimates (0.86 and 0.96 respectively), especially in short time and small distances. As flow times and distances increase, the estimates produced by ArcNLET become less accurate due to the accumulation of error stemming from ArcNLET's simplifications. Travel time estimates are more variable because there exists multiple flow paths having the same flow distance with each path having a different flow velocity (and therefore travel time).

4.2. Transport module

Despite its inexact nature, the Domenico solution itself has previously been shown to be a useful tool for predicting the transport and fate of contaminant plumes (Aziz et al., 2000; Gutierrez-Neri et al., 2009; Newell et al., 1996; Pennsylvania Department of Environmental Protection, 2002; Srinivasan et al., 2007; West et al., 2007). In this section we show that using the Domenico solution, ArcNLET is capable of providing screening-level estimates of nitrate concentration distributions in two-dimensions if the assumptions under which the Domenico solution was derived are met. Additionally, the advantages and limitations of the velocity averaging and plume warping approaches taken by ArcNLET to handle heterogeneous domains are discussed.

The Domenico solution in the form of Eq. (2) as implemented by ArcNLET is compared to a numerical model of a hypothetical test case constructed using MODFLOW (Harbaugh et al., 2000) and MT3DMS (Zheng and Wang, 1999). A steady-state flow system consisting of a single layer of depth 2 m and a grid size of 4 m $\times$ 4 m was constructed such that the constant head boundary conditions resulted in a flow field with a constant magnitude and direction. Using a constant hydraulic conductivity and porosity of 2.113 m/day and 0.25 respectively, the resulting hydraulic gradient produced a flow field of magnitude of 0.0212 m/day in a west-to-east direction over the entire domain. A Domenico-type contaminant source was simulated using MT3DMS by placing three adjacent constant concentration cells (40 mg/l each) within the domain such that the axis of the aligned cells was perpendicular to the flow. The longitudinal dispersivity was set to 2.113 m and the horizontal transverse to 0.234 m while the decay constant was set to 0.008 1/day. The equivalent Domenico plume was calculated and the results compared with the MT3DMS plume. For this set of parameters, the Domenico solution underestimates the concentration along the plume centerline, ranging from 3% near the source and increasing with distance to an underestimation of over 60% near the end of the plume (defined as the location along the centerline where the concentration of the MT3DMS plume drops below 0.001 mg/l). A 60% difference corresponds to an absolute difference of 0.0006 mg/l. This result agrees with the studies by Srinivasan et al. (2007) and West et al. (2007) who, by numerically solving

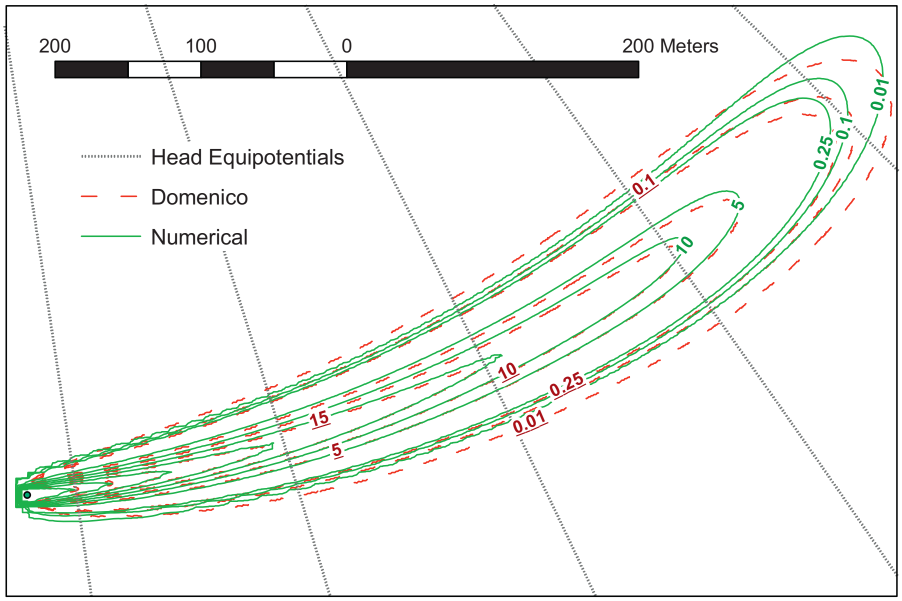

Fig. 6. Concentration contours showing the effect of applying ArcNLET's warping on the Domenico plume. Compared to the numerically calculated plume, the differences are minor.

an exact solution by Wexler (1992), found that the Domenico solution can underestimate concentration near the centerline. Regarding parameter sensitivity, it has been previously determined that the most sensitive parameters affecting the shape of Domenico plumes are (in order of decreasing sensitivity) the first-order decay coefficient, flow velocity, and horizontal transverse dispersivity (Wang et al., 2011). Although it is known that the Domenico solution (and its various forms) is only an approximate solution to the governing equation (Domenico and Schwartz, 1998; Guyonnet and Neville, 2004; Srinivasan et al., 2007; West et al., 2007), it is still recognized as a useful method for screening level analyses, with accuracy improving as the longitudinal dispersivity is decreased relative to the flow velocity (Srinivasan et al., 2007; U.S. Environmental Protection Agency, 2008).

In order to test the effect of velocity averaging (see Section 3.2) on the Domenico solution, the MODFLOW model described above is modified so that a linearly increasing velocity gradient is present in the west-to-east direction with a 65% difference between the minimum and maximum velocity values. The minimum concentration difference between ArcNLET and the numerical model along the centerline is 0.2% (occurs near the source) while the greatest difference is an overestimation of the concentration by 160% at a distance of approximately 1900 m from the source along the plume centerline (plume length is approximately 2500 m). A 160% difference corresponds to an absolute difference of approximately 4 mg/l, which is well within an order-of-magnitude estimation. Averaging velocity has little effect on plume width, producing behavior similar to the constant velocity case.

The effect of applying ArcNLET's warping algorithm so that the Domenico plume conforms to the flow path is examined by comparing to a MODFLOW/MT3DMS model constructed such that curved flow lines are produced (Fig. 6). The velocity magnitude is constant along each flow line. In order to highlight the effects of warping, a 50 year plume with no decay was generated. As shown in Fig. 6, the concentration contours of the warped Domenico solution are slightly shifted to the southeast and have a slightly different shape compared to the numerically calculated ones. The shift across a concentration profile taken perpendicular to the flow at a distance of 500 m along the flow path averages 4% and results from the inability of the warping algorithm to take into account the fact that velocity increases across the profile from southeast to northwest (this can be seen from the closer spacing of the head equipotentials in the northwest-southeast direction in Fig. 6).

4.3. Nitrate load estimation module

M_{in} and M_{dn} are calculated with Eqs. (10) and (5) respectively and the resulting values are compared to the MODFLOW/MT3DMS constant velocity model with decay (0.008 1/day) used in the Transport module comparison, discussed in Section 4.2.

Table 1 shows the load values for the test model as calculated by MT3DMS and by ArcNLET. In addition to the results obtained using a 4 m grid resolution, a 1 m grid was calculated for both MT3DMS and ArcNLET (recall that Eq. (2) is evaluated over a discretized domain) so as to demonstrate the effect of discretization error on both models. Looking at the Input Load column of Table 1, the value represents the rate at which nitrate is entering groundwater via the constant concentration source plane. From the table, the discretization error in the input load value calculated by MT3DMS is apparent. When the grid size is decreased, the MT3DMS result moves closer to the one calculated by ArcNLET using the analytical expression of Eq. (10). In the 4 m resolution case, the MT3DMS and the ArcNLET input loads differ by 17% and in the 1 m case, the results differ by 4%. This highlights an advantage of using an analytical expression to calculate the input load: the input load is independent of the grid resolution.

Turning now to the denitrification mass, our model predicts a lower value than the MT3DMS results. For the 4 m resolution case, the denitrification mass rate is underestimated by 30% however for the 1 m case ArcNLET and MT3DMS differ by 8%, a marked improvement. The improvement is attributed to the reduction of discretization error in both models. The remaining 8% discrepancy is attributed to the underestimation of plume concentrations by the Domenico solution as well as further discretization error of both solutions. Because concentration takes on the largest values in the vicinity of the plume centerline, combined with the fact that concentrations along the centerline are underestimated, this likely results in the observed underestimation of the denitrification mass rate by ArcNLET (see Eq. (5)).

The final two columns of Table 1 show that ArcNLET produces a lower than expected estimate of nitrate removed. For both test

Table 1
Load values calculated directly from MT3DMS and with ArcNLET for two test runs using a decay constant of $k=8E-3$ 1/day. Load and rate values are in kg/day. Grid resolution is in meters.

	Grid Resolution	Input load	Denitrification mass rate	Output load	Percent nitrate removal
MT3DMS	4	6.6247E−3	6.6247E−3	1.0480E−10	100
	1	7.4718E−3	7.4718E−3	4.6082E−11	100
ArcNLET	4	7.7620E−3	4.5451E−3	3.2169E−3	59
	1	7.7620E−3	6.8415E−3	9.2050E−4	88

cases presented in the table, the plume should be completely denitrified meaning that in theory, the output load should be zero (corresponding to a percent nitrate removal of 100%). With a four meter resolution, ArcNLET predicts a 59% removal of nitrate compared to the $\sim 100\%$ predicted by MT3DMS. As expected, decreasing the size of the grid cells over which Eq. (2) is evaluated yields a more accurate result: ArcNLET now predicts an 88% removal, a marked improvement. From Eq. (4), the output load depends on the estimated nitrate concentration only through Eq. (5) therefore an underestimation of the concentration will produce an overestimation of the load. This means that an underestimation of concentration produces a conservative (higher than expected) output load estimate.

4.4. Computational savings

ArcNLET is computationally more efficient than its MODFLOW/MT3DMS counterpart due to ArcNLET's use of an analytical solution and ArcGIS-aided model setup. In order to highlight the potential computational savings that ArcNLET can provide, the creation of Fig. 6 is used as an example. The MODFLOW/MT3DMS-generated plume in Fig. 6 exists in a domain of size 500×500 cells at a resolution of 4 m per cell. ArcNLET generated the plume shown in Fig. 6 and calculated the load in less than 30 s (counting from the time the Transport module was executed to the time the load value was displayed, including time spent interacting with the user interface). MT3DMS took several hours in its calculation.

A larger benefit is perhaps the time saved setting up complex models. Because ArcNLET is able to directly make use of pre-existing GIS datasets, a significant savings, possibly on the order of days to weeks, are realized. This carries over to the analysis and display of results. Because ArcNLET's outputs can be read directly by a GIS, the full suite of GIS functionality is immediately available to carry out further processing.

5. Conclusions

ArcNLET is a GIS-based tool for estimating nitrate loads from localized sources to surface water bodies under steady-state conditions. The primary focus is to provide an easy-to-use software capable of providing quick, screening-level load estimates using commonly available data. This is achieved by developing simplified models of groundwater flow and nitrate fate and transport and by implementing the models along with an easy-to-use point and click interface as an extension to ArcGIS. ArcNLET provides workflow flexibility by separating functionality into modules where each module represents a specific part of the simulation: groundwater flow/particle tracking, transport, and load estimation.

The fundamental assumption of the groundwater flow model is that the water table is a subdued replica of the topography (a common assumption in many studies). If this assumption holds, and flow is considered to occur under the Dupuit conditions, then ArcNLET is capable of providing flow velocity estimates that compare favorably to a numerical model. Areas with different topographical and hydrological features may have a water table that locally resembles the topography to varying degrees. Because of this, if it is required to model such an region with ArcNLET, it is recommended to break up the domain into smaller areas where there is less variation in the water table–topography relationship.

ArcNLET estimates nitrate concentration by making use of a commonly used semi-analytical solution to the advection–dispersion equation (i.e., the Domenico solution). It is found that in the presented test case, the Domenico solution tends to underestimate concentration values, from 3% to over 60% compared to the equivalent MT3DMS numerical model. This underestimation effect agrees with studies by other authors. The underestimation of concentration may result in an *overestimation* of nitrate load, calculated via Eq. (4), since the amount of denitrification, M_{dn}, depends on the estimated nitrate concentration. A low M_{dn} value results in a higher than expected M_{out} since M_{in} does not depend on the estimated concentration. Although not originally designed to handle heterogeneous flow velocities, the utility of the analytical solution is improved by taking into account the spatial variability in the velocity field. This is achieved by a combination of velocity averaging along flow lines and warping the resulting contaminant plume to conform to the flow path. Modifying the plume in this way results in a acceptable (order-of-magnitude) estimate of concentration values when compared to a numerical model. If there is not a large variation in the flow field, averaging and warping provide a good way to handle flow heterogeneity.

It is shown that for a test case with a 1 m resolution, ArcNLET predicts a nitrate removal of 88% while a numerical model predicts a value of $\sim 100\%$, with the discrepancy being attributed to discretization error in the MT3DMS and in the ArcNLET solution as well as the underestimation of nitrate concentration by the Domenico solution. The result is satisfactory for screening level analyses because the under-prediction of nitrate removal results in a conservative estimate of nitrate load.

ArcNLET consolidates previously developed ideas, such as the topography–water table assumption and the geometry of the contaminant transport problem as posed by BIOSCREEN and BIOCHLOR, into an integrated, easy-to-use, GIS-based tool. In addition, ArcNLET addresses several issues not considered by previous models. For example, when using the topography to approximate the water table, ArcNLET explicitly considers the presence of both sinks and flat areas, which are problematic because flow entering these regions will never escape. Furthermore, ArcNLET extends the capability of Domenico-type solutions by allowing for the partial consideration of spatially heterogeneous domains (Domenico-type solutions can only handle homogeneous parameters).

As with any model, there are limitations to what can be accomplished. For example, future improvements include the quantification and reduction of uncertainty of the load estimate via automated optimization methods (as opposed to trial-and-error methods) and modeling nitrate transport in vadose zone and groundwater as a whole (as opposed to estimating the nitrate load to groundwater from literature or model calibration). These new features, once developed, can be readily integrated into the software due to its modular structure thereby will render the software more robust in water resources and environmental management. The tool presented here is not meant to replace advanced numerical solvers like MT3DMS. Instead, because of its low data requirements, it can be used to obtain a “first estimate” of actual or potential contamination in a given area, thereby fulfilling a need for an easy-to-use screening level tool that is capable of leveraging the power of GIS for data management and spatial analysis.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.cageo.2012.10.003.

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