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GIS-based nitrogen removal model for assessing Florida's surficial aquifer vulnerability

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Abstract Florida's aquifer system exhibits spatially variable hydrogeological characteristics including shallow depth to aquifer and karst features. These characteristics contribute to groundwater vulnerability to nitrogen contamination and thus warranting vulnerability studies that allow zonation of areas into different levels of susceptibility to contamination from land use practices. A geographic information system (GIS)-based nitrogen fate and transport model (GIS-N model) was developed to assess aquifer vulnerability to contamination by examining the fate and transport of ammonium and nitrate from onsite wastewater treatment systems (OWTS). The GIS-N model analyzes fate and transport of nitrogen through the unsaturated zone using a simplified advection-dispersion equation. Operational inputs considered in this model include wastewater effluent ammonium or nitrate concentration, hydraulic loading rates, and OWTS locations. The GIS-N model considers two different modeling approaches: single step and two step. The single-step model considers a denitrification process assuming all the ammonium is converted to nitrate before land application, while the two-step

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² Department of Civil and Environmental Engineering, Colorado School of Mines, 1500 Illinois St, Golden, CO 80401, USA model uses ammonium as an input and considers nitrification followed by denitrification. The resulting maps were classified into vulnerability zones based on the Jenks's natural breaks in the data histogram. It was revealed that groundwater vulnerability from OWTS is sensitive to the depth to water table, first-order reaction rates, and parameters controlling the time and amount of conversion. Nitrate concentration is highest in areas with shallow water table depth. The vulnerability maps produced in this study will facilitate planners in making informed decisions on placement of OWTS and on groundwater protection and management.

Keywords Onsite wastewater treatment system · Nitrogen fate and transport · Groundwater · Advection– dispersion · Aquifer vulnerability · Surficial aquifer system

Introduction

In the State of Florida, onsite wastewater treatment system (OWTS) has been a feasible and economical wastewater treatment option for about 30 % of the Florida's population according to the 2010 US Census. OWTS release nitrogen rich effluent mostly in the forms of ammonium and nitrate, negatively impacting human and environmental health. Groundwater contamination from OWTS may reach the surficial aquifer system (SAS) and surface water bodies via percolation and subsurface transport of nitrogen. The detrimental impact of excess nitrogen in the environment warrants vulnerability studies that allow the delineation of areas more or less susceptible to contamination from land use practices.

In this study, a regional scale geographic information system (GIS)-based nitrogen fate and transport model

(GIS-N model) has been developed to provide an alternative method in identifying aquifer vulnerability, utilizing a simplified advection-dispersion equation (ADE) for fate and transport of nitrogen. The simplified ADE assumes steady state and describes sorption, nitrification, and denitrification processes via sorption, first-order reaction processes, and operational inputs which includes effluent loading rate and concentrations. Those processes are determined from spatially variable parameters which include soil and hydrological data for the entire State of Florida. The GIS-N model is used to identify vulnerable areas based on site characteristics and operational parameters. The vulnerability maps produced from the model will assist planners in identifying areas sensitive to contamination from OWTS and making informed decisions in protection and management of surface and groundwater.

Study area

There are three main aquifer systems in the State of Florida: the surficial aquifer system (SAS), the intermediate aquifer system (IAS), and the Floridan aquifer system (FAS). The modeled study area is the entire State of Florida, focusing on the effects of nitrogen to the SAS. While the IAS and the FAS are mostly confined, the SAS is comprised of unconfined aquifers, including the sand and gravel aquifer and the Biscayne aquifer. Due to its proximity and connectedness to the land surface, the SAS is highly susceptible to direct infiltration of contaminants from OWTS (Arthur et al. 2007). The SAS consists of mostly beds of unconsolidated sand, shelly sand, and shell. Complex, interbedded, fine, and coarse-texture rocks are present throughout the state with prominent limestone beds in the south and confining layers formed from clay beds in a few areas in the north (Miller 1990; Copeland et al. 2009). Although the confined aquifers serve as the source of drinking water, they are connected to the SAS in some areas with the possibility that contaminant can enter the confined aquifer systems.

Previous studies

There have been previous studies that focused on developing vulnerability assessment models to address the susceptibility of aquifer systems to contamination. The DRASTIC model is a widely used model which determines vulnerability based on parameters significant in contaminant transport (Pathak et al. 2009; Rahman 2008; Rundquist et al. 1991). The DRASTIC model is based on seven parameters: depth to aquifer, net recharge, aquifer media, soil media, topography, impact of vadose zone, and hydraulic conductivity. The parameters define a composite description of major geological and hydrologic factors that affect and control groundwater movement (Aller et al. 1985). The DRASTIC model calculates an aquifer vulnerability index based on a system of rates and weights. Each of the seven parameters is assigned a rate on a scale of 1-10 based on their effect on aquifer vulnerability and a weight from 1 to 5 based on their relative importance (Babiker et al. 2005). The rates are assigned based on site characteristics as related to a specific parameter. Systems for rate and weight assignments have been studied to increase model correlation with groundwater quality data (Antonakos and Lambrakis 2007; Thirumalaivasan et al. 2003). The main advantages of the DRASTIC index model include its applicability to multiple contaminants, easily obtainable or interpolated data, and large number of parameters for good representation and reduced impact of errors (Babiker et al. 2005). However, there are a number of limitations, as described in Arthur et al. (2007) and Babiker et al. (2005), including high sensitivity to certain parameters, underweighting important parameters such as net recharge and hydraulic conductivity, a subjective ranking system, sharp transitions between data sets and vulnerability maps, generalization of site features (such as soil types and karst features), and over emphasizing effect of topography.

Data-driven modeling approaches address some of the limitation of the DRASTIC model by employing methods like weight of evidence (WofE) to assess groundwater vulnerability (Masetti et al. 2007; Uhan et al. 2011). This approach examines natural and anthropogenic variables to make predictions based on spatial data. The modeling utilizes training points or areas of known occurrences to assess prior probability, weights of spatial data, and posterior probability of the results (Arthur et al. 2007). Training points can be locations of sampled concentrations of the contaminant. These training points are used to weigh spatial data and form evidential themes based on which areas of the evidence share a greater association with the location of training points. Different evidential themes are utilized and combined to predict occurrences of phenomenas or response themes (Uhan et al. 2011). The response themes show the probability that a unit area contains a training point based on the evidence. The probability is delineated to generate a final probability map illustrating aquifer vulnerability (Arthur et al. 2007). The main advantage of the WofE model is its updatable format, data driven analysis, selectable evidence of highest relevance, empirical calculation, and limited subjectivity. The limitations of this model are data time sensitivity (need for up-to-date data), low resolution (30 m).

To address aquifer vulnerability based on the vadose zone processes from OSWT, an alternative and new

modeling approach, the GIS-N model presented next, is developed in this study.

GIS-N model

The calculation for contaminant removal in the vadose zone in the GIS-N model is based on the simplified ADE implemented in similar models (Rao et al. 1985; Geza et al. 2014; McCray et al. 2010; Tonsberg 2014). The methods, effects of environmental factors on nitrogen transformation, data sources, model inputs, and GIS implementation of the GIS-N model are presented in below subsections.

Methods

The GIS-N model uses a simplified ADE incorporated into the GIS framework and accounts for spatial variability in inputs and site characteristics. The simplified ADE uses first-order reaction rates for nitrification and denitrification in contrast to the soil treatment Unit model (STUMOD) (Geza et al. 2014; McCray et al. 2010) that uses a Monod function. The GIS-N model also considers operational inputs (effluent concentration, effluent loading rates, porosity, and soil depth) in addition to sorption and reaction parameters (nitrification and denitrification) for nutrient transformation (Jury et al. 1987; McCray et al. 2010). The simplification ignores the effects of dispersion and assumes steady state conditions.

The simplified ADE is an exponential decay function, which calculates the concentration of ammonium and nitrate as a function of factors contributing to the removal, expressed as:

$$C(z) = C_0 \exp\left(\frac{-RK_{\rm r}}{V_{\rm z}}Z\right) \tag{1a}$$

Or

$$C(z) = C_0 \exp(-RK_r T)$$
(1b)

where C_0 is the initial concentration of ammonium or nitrate (mg/L) in the effluent applied to the infiltrative surface, Z is the soil depth or depth to water table (cm), V_z is the vertical water velocity evaluated as hydraulic loading rate divided by porosity (cm/day), K_r is the first-order reaction rate (nitrification rate for NH₄⁺ and denitrification rate for NO₃⁻), and R is the retardation factor. Note that Z/ V_z in Eq. (1a) was replaced by travel time (T) in Eq. (1b). The travel time is an important parameter in the ADE, controlling time available for reaction processes to remove the contaminant before reaching the water table. The simplified ADE includes reaction rates, retardation, applied effluent concentration; and the travel time for attenuation of contaminants which were not considered in the DRASTIC approach and the method implemented in WofE.

Effects of environmental factors on nitrogen transformation

Nitrogen transformation is a microbial facilitated process and is affected by environmental factors that influence soil microbial activity. Nitrification and denitrification reactions transform nitrogen into nitrate and nitrogen gas, respectively.

The GIS-N model considers the effect of environmental factors on biological reaction rates by adjusting the maximum reaction rate occurring at optimum environmental conditions for the effect of different factors affecting the reaction process such as degree of aeration, soil temperature, and organic carbon content. Aeration is an important factor for nitrification and denitrification since these processes are influenced by the aerobic and anaerobic conditions. Those factors, defined as response functions, are combined linearly and reflect the non-optimal conditions controlling the first-order biological reaction rates.

The first-order reaction rate, K_r , is defined as the actual reaction rate calculated from the maximum reaction rate (K_{rmax}) after adjustment for non-optimal biological activity. The optimal rate is adjusted for the effect of soil temperature, soil moisture, and soil organic carbon content. The effect of those processes on the first-order reaction rate are represented by empirical response functions for calculating empirical adjustment factors ranging from 0 to 1 accounting for non-optimal conditions, expressed as:

$$K_{\rm r} = K_{\rm max} f_{\rm t} f_{\rm sw} f_{\rm z} \tag{2}$$

where $K_{\rm rmax}$ is the maximum/optimal first-order reaction rate (day⁻¹), f_t is soil temperature response function, $f_{\rm sw}$ is the soil moisture response function, and f_z is the soil organic carbon response function.

The optimal conditions occur at 25 °C (Youssef 2003), intermediate saturation for nitrification (Fig. 1), complete saturation for denitrification (Fig. 2), and high organic carbon content for denitrification.

Soil temperature regulates organic carbon decomposition and nitrogen transformation processes. The temperature response function accounts for the influence of temperature deviation from the optimum temperature (25 °C) for a biological process. The temperature response function used for both nitrification and denitrification which describes the temperature effect on both and accounts for temperature sensitivity is based on the van't Hoff equation (1874):

$$f_{\rm t} = \exp\left[-0.5\beta T_{\rm opt} + \beta T \left(1 - \frac{0.5T}{T_{\rm opt}}\right)\right]$$
(3)







Fig. 2 Distribution of f_{sw} versus relative saturation for denitrification

where *T* is actual soil temperature (°C), T_{opt} is the optimum temperature (°C) at which f_t equals unity, and β is an empirical coefficient set at 0.186 (Youssef 2003). The temperature response function results in values between 0 and 1, with the value of 1 at the optimum temperature and less than 1 at soil temperatures below or above the optimum (Youssef 2003).

Soil moisture content affects the diffusivity of gases into the soil, controlling oxygen availability to nitrifying microbes. Nitrification and denitrification processes are favored under aerobic and anaerobic conditions, respectively. The degree of saturation or soil moisture content is used as a substitute for the aeration conditions in the nitrification and denitrification processes. Nitrification rates significantly decrease when soil moisture content exceeds an optimum amount and may cease at saturation. In low soil moisture conditions, ammonium and aqueous CO_2 diffusion into to the pores is limited because of poor connectedness of pores leading to limited nitrification. Denitrification conditions are optimal as the relative soil moisture content reaches its maximum at complete saturation (Barton et al. 1999; Youssef 2003). The soil moisture response for denitrification, f_{sw} , is expressed as:

$$f_{\rm sw,dn} \begin{cases} 0 & s < s_{\rm dn} \\ \left(\frac{s - s_{\rm dn}}{1 - s_{\rm dn}}\right)^{e_1} & s \le s_{\rm dn} \end{cases}$$
(4)

where *s* is the relative saturation defined as the ratio of actual moisture content to moisture content at saturation ranging from 0 to 1, s_{dn} is a threshold relative saturation

below which denitrification does not occur, and e_1 is an empirical exponent.

The soil moisture response function for nitrification is expressed as:

$$f_{\rm sw} \begin{cases} f_{\rm s} + (1 - f_{\rm s}) \left(\frac{1 - s}{1 - s_{\rm h}}\right)^{e_2} & s_{\rm h} < s \le 1 \\ 1 & s_1 \le s \le s_{\rm h} \\ f_{\rm wp} + (1 - f_{\rm wp}) \left(\frac{s - s_{\rm wp}}{1 - s_{\rm wp}}\right)^{e_2} & s_{\rm wp} \le s < s_1 \end{cases}$$
(5)

where *s* is the relative saturation, s_h and s_l are the upper and lower limits of the relative saturation range within which nitrification proceeds at optimum rate, s_{wp} is the relative saturation at permanent wilting point, f_s and f_{wp} are the values of the soil water function at saturation and permanent wilting point, respectively, and e_2 is an empirical exponent (Youssef 2003).

Another factor controlling the first-order rate process equation is the organic carbon content represented by the response function for carbon content, f_z . During denitrification, microbes use soil organic carbon as an electron donor to obtain energy through oxidation (Rivett et al. 2008). The soil organic carbon content in soil varies with depth. The rate adjustment factor for the organic carbon response function (f_z) is set to 1 assuming organic carbon is not limiting. In this study, organic carbon is considered as non-limiting, assuming organic matter is continuously supplied from the applied wastewater effluent (McCray et al. 2010). Furthermore, for nitrification, carbon dioxide gas is the main energy source for the microorganisms. Soil gas is known to have high concentrations of CO₂ (Jury and Horton 2004), it is assumed that sufficient carbon will always be present for nitrification, providing that gas diffusion was not inhibited due to high soil water contents.

An additional process of retardation, represented by R in Eq. (6) is defined as:

$$R = 1 + \frac{K_{\rm d}}{\theta}\rho \tag{6}$$

where ρ is the bulk density of the soil (g/cm³), K_d is the distribution coefficient (L/kg), and θ is the soil moisture content (%). K_d , the distribution coefficient, is dependent on soil types and independent on water content (McCray et al. 2005). Retardation is considered for ammonium adsorbing onto negatively charged soils. On the other hand, nitrate is considered to not sorb and thus has a retardation factor of 1.

Data sources

GIS data for the required input data layers are acquired from the Natural Resources Conservation Service (NRCS) soil survey, Florida Department of Environmental Protection, and Florida Geographic Data Library (FGDL). The NRCS provides soil data for the entire State of Florida from the Gridded Soil Survey Geographic (gSSURGO) database in the format of an Environmental Systems Research Institute, Inc. (ESRI) file geodatabase. This format includes a 10-m raster of the map unit soil polygons feature class. The soil map unit links to table attributes created between 2012 and 2010 which includes: soil organic carbon, soil water content at field capacity, density, soil temperature, and soil texture. Map units are typically made up of one or more soils which defines the composition. 2009 locations of OWTS, effluent concentration, and loading rates were obtained from the Florida Department of Health. Florida land cover data were obtained through the Florida Fish and Wildlife Conservation Commission. Other parameters used in the contaminant removal calculation are from literature and reports. Nitrification, denitrification and sorption rates were obtained from peer reviewed literature.

Model inputs

Model input required in the ADE include the operation parameters (effluent concentration and hydraulic loading rates), first-order reaction rate for nitrification and denitrification, and sorption. Other site specific parameters include soil moisture, and soil temperature, and depth to water table. Model inputs were defined as raster layers and are discussed in the subsequent sections.

OWTS location

The Florida Department of Health maintains a statewide inventory of onsite sewage treatment and disposal systems for the State of Florida. The 2009 wastewater inventory database is a record of wastewater treatment methods for all parcels of land compiled from the integration of data from the Department of Environmental Protection permitted wastewater treatment facilities, Environmental Health Database, and County Health Departments. For parcels with an unknown wastewater treatment method, a logistic regression model was used to estimate the probability of the parcel being on an active OWTS based on parcels with a known wastewater treatment method (EarthSTEPS, LLC and GlobalMinda 2009). The 2009 wastewater inventory database estimated 2,559,757 parcels with an active OWTS. The parcels were used as contaminant input location after conversion from a polygon feature class to a point feature class using the centroid of each polygon for spatially variable contaminant input in the existing OWTS application scenario. The 2,559,757 parcel data represented in polygon features were converted to a point feature class.

Seepage velocity

The seepage velocity determines the travel time for the applied effluent to reach the groundwater table and is dependent on the effluent hydraulic loading rate and the porosity for corresponding USDA soil textures. A hydraulic loading rate (HLR) of 2 cm/day applied to subsurface trenches was used as a representative value (McCray et al. 2010). The porosity values from Rawls et al. (1982) were used for the seepage velocity calculation and assigned to the corresponding USDA soil textures in the NRCS map unit attribute table. Calculated seepage velocity ranged from 4.65 to 3.99 cm/day. The values corresponded well with literature on low seepage velocity in areas of clay rich soil texture and higher seepage velocity in coarser soil textures (Witheetrirong et al. 2011).

Maximum first-order reaction rates

The first-order maximum nitrification and denitrification rate coefficients used in the simplified ADE were obtained from the cumulative frequency diagram (CFD) of reaction rates developed by McCray et al. (2005). The CFDs in McCray et al. (2005) were developed based on literature review of nitrification and denitrification rates observed for natural soils under both saturated and unsaturated conditions.

Prior to choosing the nitrification rate for our GIS-N model, we assessed model performance in comparison to removal rates observed in the field. Our goal in the vulnerability assessment was to obtain relative differences among sites in the amount of nitrogen reaching the groundwater table. This relative difference among sites is not affected by the absolute concentration values and yet, we attempted to obtain concentration values that were close to observed data in the field. Thus, nitrification and denitrification rates were selected with the range found in the CFD and at the same time, produce values that reflect measured concentration in the field. The CFD distribution for nitrification rates has a higher standard deviation and fewer data points compared to the denitrification CFD. The maximum nitrification rate from the CFD was exceptionally high (221 day^{-1}) . This value resulted in very fast conversion of ammonium to nitrate, within 5 cm in most cases, while field data showed nitrification may persist to 30 cm below a drain field infiltrative surface, provided that the water table is not present and the soil zone is unsaturated (Brown 2003). Given that nitrification rate data is limited and soil conditions in Florida is based on the usually wet and humid conditions, $K_{\rm rmax}$ for nitrification was specified at the median value of 3.25 day^{-1} in the development of the vulnerability maps. Using the median nitrification rate of 3.25 day^{-1} , ammonium removal rates correspond best to the literature values. Other literatures have also indicated that ammonium persisted in the subsurface to a depth of 30 cm and most of the ammonium is removed within 5 cm, as determined from Heatwole and McCray (2007) for loam soil group.

Anderson and Otis (2000) reported that nitrate removal under Florida's conditions ranged from 10 to 50 %. Denitrification rates provided in the CFD ranges from 0.004 to 2.27 day^{-1} . A median denitrification rate of 0.025 day $^{-1}$ underestimated nitrate removal relative to field data. As with the nitrification rate, the denitrification rate was selected to result in percent removal within the range reported in literature. The upper quartile denitrification rate of 0.27 day⁻¹ better reflected field observed nitrate removal ranges of 10–50 % observed under Florida conditions (Anderson and Otis 2000).

The first-order reaction rate after adjustment for soil temperature, moisture, and organic carbon content for the nitrification and denitrification reaction ranges from 3.25-0.36 to 0.27-0.0046 day⁻¹, respectively, with a $K_{\rm rmax}$ value at 3.25 and 0.27 day⁻¹, respectively.

Soil temperature

The USDA divides the contiguous US territory to five subregions based on soil annual average soil temperatures; frigid, cryic, mesi, thermic and hyperthermic. Florida is divided into the two soil temperature zones, the hyperthermic and thermic, based on the USDA soil annual average temperature map. In this study, areas are assigned the annual mean soil temperature of 25.5 and 18.5 °C for the hyperthermic zone and thermic zone, respectively, by adding the field in the NRCS map unit attribute table.

Soil moisture

Soil moisture content data were needed to account for the degree of aeration provided by soil types. Actual moisture content data were not continuously available for the entire state. As a result, field capacity from the NRCS soil database was used to reflect potential differences in soil moisture content among soil types. Since field capacity represents soil moisture content after drainage of a saturated soil, field capacity was assumed to represent relative difference in moisture content among soil types. Therefore, locations with sandy soil textures which have a lower moisture content at field capacity will favor higher nitrification and lower denitrification and the vice versa for locations where clayey texture is dominant. This allowed assessment of spatial variability of vulnerability based on soil types in relative terms. For a sensitivity analysis as represented in this study, the assumption would be sufficient to compare performance differences among soil types. The other necessary parameters including porosity and coefficients presented in Eqs. (4) and (5) are from literature and are listed in Table 1.

Depth to water table

The depth to water table controls the distance available for contaminant transformation through microbial activity in the vadose zone as described by the travel time in Eq. (1a, 1b). The NRCS map unit attribute of annual minimum water table depth is measured as the shallowest depth to a wet soil layer (water table) at any time during the year expressed in centimeters from the soil surface. The depth is estimated based on the observation of the water table at selected sites or on the physical characteristics of the soil that are considered evident of a saturated zone. The observed water table for each map unit must be observed for at least 2 weeks before recording. A high, representative, and low value is provided as a range to account for variability. There are observed differences leading to abrupt change in depth to water table measurements between counties that are due to the different time of measurement, people performing the measurement, and updates to sampling concepts (Leach 2014, personal communication). The depth to water table layer using the recorded representative value is depicted in Fig. 3, with a range of 0-203 cm.

Retardation factor

Ammonium sorption is dependent on soil type due to differences among soil types in cation exchange capacity or amount of charged ions a soil can hold. Clay-rich groups have a slight excess of negatively charged sites, resulting in a high cation exchange capacity (Ramesh Reddy and Delaune 2008). Thus, the distribution coefficient (K_d) values are defined for clay-rich and clay-poor groups. The median K_d values from literature were 0.35 L/kg for claypoor groups (less than 30 % clay) and 1.46 L/kg for clay-

Table 1 Coefficient values used for soil moisture function	Para
	S_{dn}
	е
	e_1
	e_2

Parameter	Value
S _{dn}	0
е	1.4
e_1	1
<i>e</i> ₂	1
S _h	0.85
S_1	0.5
Swp	0
F _s	0
$F_{\rm wp}$	0

USDA Annual Minimum Water Table Depth



Fig. 3 Depth to groundwater table for the State of Florida with values from 0 to 203 cm $\,$

rich soil groups (more than 30 % clay) (McCray et al. 2010). These values were assigned to the different USDA map unit attribute of soil textures for the State of Florida. The clay-poor soil textures include: sand, loamy sand, sandy loam, loam, silt loam, and silt. All other soil textures were assigned the clay-rich soil group K_d value of 1.46 L/kg. Additional parameters for the calculation of the retardation factor; bulk density (ρ) and soil moisture content (θ) were obtained from the NRCS soil database and literature, respectively. The soil moisture content is assumed to equal porosity, which represent the saturated water content. The calculated retardation values based on Eq. (6) ranged from 1.72 to 7.38.

GIS implementation

The GIS-N model used to assess Florida's surficial aquifer vulnerability is implemented in a GIS platform. GIS allows the integration of spatially heterogeneous data to represent spatially variable events by relating a series of data layers or thematic maps (Bonham-Carter 1996). In this study, ArcGIS 10.1 developed by ESRI is used to process and manage spatial data through the input of data layers stored in a customized geodatabase. Each data layer represents a variable in the contaminant fate and transport equation. All input layers were combined to produce zonation maps illustrating Florida's surficial aquifer vulnerability in the form of outputs of nitrogen concentrations at the water table. Performing the fate and transport calculations in a GIS platform with the map algebra tool allows the raster display of spatially variable inputs and outputs and a side by side visual comparison of site features used as inputs and corresponding model outputs.

The GIS-N model is applied to four different scenarios: a single-step model with uniform input (single-step uniform input), a two-step model with uniform input (two-step uniform input), a single-step with variable input (singlestep variable input), and a two-step model with variable input (two-step variable input). The single-step model assumes all the ammonium is converted to nitrate before land application and considers the denitrification process only. The two-step model uses ammonium as input and considers nitrification followed by denitrification. The uniform input assumes uniform application of nitrogen to the entire study area and the variable input assumes variable spatial input based on existing OWTS locations.

Single-step uniform input model

Nitrogen released from a septic tank is mainly in the form of ammonium. It is estimated that the concentration of ammonium discharged into the subsurface is about 60 mg/ L, after conversion from organic nitrogen via decomposition by bacteria in the septic tank (Crites and Tchobanoglous 1998). However, the single-step uniform input model assumes all the ammonium is nitrified before it is applied to the soil and considers only the denitrification. This represents a scenario where ammonium is nitrified using aerobic treatment units before it is applied to the soil (McCray et al. 2010). Map algebra was used to combine data layers representing parameters in the simplified ADE (Eq. 1a or 1b); an approach used for other scenarios as well. A uniform input of 60 mg-N/L as nitrate was applied to the entire State of Florida and nitrate concentration reaching the water table was calculated to generate a vulnerability map. The effluent input concentration from aerobic treatment units is usually less than the 60 mg-N/L value used here. The values used in this study represent the worst case scenario since the vulnerability maps are based on relative differences among sites.

Two-step uniform input model

The two-step uniform input model in contrast to the singlestep model considers two separate steps. In this case it is assumed that the ammonium is applied to the subsurface directly. The two-step model assumes ammonium is nitrified first and followed by a denitrification process converting the nitrate to gaseous nitrogen. The first step simulates the nitrification process with a uniform input concentration of 60 mg-N/L as ammonium. Nitrification was assumed to occur at the first top 30 cm depth from the point of application (Brown 2003; Fischer 1999; Beach 2001). By assigning part of the vadose to the nitrification process, the method provides a conservative estimate (a higher concentration) of nitrate reaching the water table compared to a single step model. Our study also demonstrated that most of ammonium was converted within the first 30 cm. For the second step, the layer below the 30 cm mark and above the water table was used as a denitrification layer to calculate nitrate removal with an input nitrate concentration obtained from the first (nitrification) step. If the water table was shallow (less than 30 cm), it is assumed that the denitrification layer is not present and the nitrate concentration reaching the water table is equivalent to the amount of ammonium converted to nitrate in the first step. The remaining nitrate concentration reaching the water table from the two processes provides final results of nitrate-nitrogen reaching the water table.

Single-step variable input model

The single-step variable input is similar to the single-step uniform input except the spatially variable input, varied based on the distribution of existing locations of active OWTS put in as point features in the GIS-N model. An initial 60 mg-N/L of nitrate nitrogen is applied to the centroid of the parcels influenced by OWTS. Parameters from the developed map layers are converted to point features for the output calculation, with 1,612,305 OWTS points corresponding to locations with data. The calculated nitrate concentration reaching the water table from the single-step variable input model provides information on areas currently affected by OWTS. The resulting nitrate concentration calculated for each location was used for interpolation with the indicator kriging method to provide a probability of nitrate exceeding a predefined threshold and areal extent of contaminant influence from OWTS effluent loading. Indicator kriging assumes that points closer together are more alike. Indicator kriging is a transformed binary data set. The binary data were created through the use of a user-defined threshold for continuous data with values less than the threshold as zeros and values greater than or equal to the threshold as ones. Indicator kriging is modeled by:

$$I(s) = \mu + \varepsilon(s) \tag{7}$$

where μ is an unknown constant and I(s) is a binary variable (a value of 0 or 1). Using binary variables, indicator kriging proceeds the same as ordinary kriging. Because the

indicator variables are 0 or 1, the interpolations will be between 0 and 1, and predictions from indicator kriging can be interpreted as probabilities of the variable being 1 or being in the class that is indicated by 1. If a threshold was used to create the indicator variable, the resulting interpolation map would show the probabilities of exceeding (or being below) the threshold (Johnston et al. 2001).

Two-step variable input model

The two-step variable input model follows the same idea where contaminant input is spatially varied based on existing locations of active OWTS. The two-step approach is used to calculate remaining nitrate concentrations. Areas of OWTS influence is also determined by indicator kriging with the threshold set based on the distribution of remaining nitrate from the two-step approach.

A different threshold is set between the single-step and two-step model (discussed below) based on the output distribution of remaining nitrate concentration reaching the water table determined from the geometric interval.

Results and discussion

Florida surficial aquifer vulnerability maps are produced using the GIS-N model with single-step and two-step uniform input and single-step and two-step variable input approaches. The models indicate the likelihood of areas susceptible to nitrate contamination based on nitrate concentrations reaching the water table calculated using the contaminant fate and transport equation.

Single-step and two-step uniform input approach results

The vulnerability maps of nitrate reaching the water table from the single-step uniform input approach provide distribution of concentrations reaching the water table and thereby the sensitivity of the model to site characteristics. The remaining NH₄–N concentration distribution after nitrification is less than 1 mg/L for most regions. Higher ammonium concentration regions are due to shallow depth to water table and/or low nitrification rates, resulting in incomplete conversion of ammonium to nitrate. Regions with an NH₄–N concentration of 60 mg/L correlate with a value of zero depth (e.g. lakes or rivers) between the soil surface and the water table. This correlation is also seen when 60 mg-N/L of nitrate reaches the water table during the denitrification step.

The denitrification process is highly sensitive to shallow water table depth. A uniform input of 60 mg-N/

L as nitrate to the entire state resulted in the calculated NO_3 -N concentration in the range of 35–60 mg/L, with most of the values between 50 and 60 mg/L. While nitrate concentration reaching the water table is also sensitive to the first-order denitrification rate, little spatial variation between the denitrification rates exists for the State of Florida. The calculated actual denitrification rates adjusted for environmental factors for the State range from 0.0046 to 0.27 day⁻¹, where a denitrification rate less than 0.03 day⁻¹ constitutes a majority of the study area.

The Florida surficial aquifer vulnerability map for single-step approach is developed based on the removal of nitrate via the denitrification process as nitrogen percolates to the groundwater. The classification of vulnerability is based on nitrate concentrations reaching the water table, categorized into less vulnerable, vulnerable, and more vulnerable based on Jenks' Natural Breaks algorithm. Natural breaks classification identifies groups with similar values and maximizes the difference between classes (Jenks 1967). The histogram for nitrate concentration reaching the water table with the natural breaks used for delineation of the vulnerability zones is shown in Fig. 4. Of those classes, only in a small percentage of the zones does nitrate concentration reaching the water table fall below 10 mg/L. The EPA maximum contaminant level (MCL) for nitrate in drinking water is 10 mg/L. However, the Florida surficial aquifer is not the source of drinking water. It is possible that nitrate becomes diluted as it travels laterally through the saturated zone further decreasing concentration. Even when concentrations reaching the water table are higher than the MCL, it is possible that the MCL standards are met in the drinking water aquifer, which is beyond the scope of this study. The assessment done using the GIS-N model cannot be applied directly to assess whether drinking water requirement are met but provides a general understanding of vulnerability of a site to groundwater pollution in relative terms as related to site characteristics. Thus, MCL was not used as natural break for the vulnerability maps. Based on natural breaks classification for nitrate concentration reaching the water table, the result in Fig. 5 illustrates that the most vulnerable areas are along the borders of water bodies and areas in southern Florida. The vulnerable areas are mostly grouped around central Florida and less vulnerable areas in the sand and gravel aquifer. Certain zones within the sand and gravel aquifer system are classified as less vulnerable due to a greater depth to water table and interbedded layers of low permeability. Furthermore, interbedded layers of silt and clay can also hold the contaminant for the nitrification and denitrification processes, resulting in zones with less permeable sands and clays correlating with lower vulnerability





Florida Surficial Aquifer Vulnerability



Fig. 5 Florida surficial aquifer vulnerability map based on the singlestep uniform input nitrogen removal model, showing remaining NO_3 -N concentrations in mg/L

and zones with high permeability being classified as vulnerable.

The high vulnerability areas correlate with the spatial distribution of shallow depth to water table. The trend is observed when comparing the aquifer vulnerability map (Fig. 5) with the water table depth layer in Fig. 3. Water table was found to be the most important factor followed by the first-order reaction rate because water table depth largely influences the time available for the nitrification and denitrification processes as the nitrogen percolates through the unsaturated zone. Shallow water tables result in

limited conversion of nitrate into nitrogen gas and therefore corresponding to higher vulnerability observed along the water bodies with shallow water table depth.

Florida surficial aquifer vulnerability map based on the two-step uniform input model considers both nitrification and denitrification processes. The nitrate input for the second step in the two-step approach is nitrate converted from ammonium distribution from the first nitrification step in the top nitrification layer. The resulting nitrate concentration reaching the water table is then classified into three aquifer vulnerability groups based on the natural breaks calculated in ArcGIS. The two-step model predicts more vulnerable areas in southern Florida and vulnerable areas in northern and central Florida (Fig. 6).

Single-step and two-step spatially variable input approach results

Nitrogen inputs in these scenarios are varied based on existing OWTS location. Nitrate removal was then calculated for points with active OWTS, limiting the amount of area with data points. Aquifer vulnerability for the single and two-step approaches with spatially varied inputs were depicted as the probability of nitrate exceeding a threshold determined by the geometric interval from the remaining nitrate concentration distribution. The concentration of remaining nitrogen results were classified into vulnerability classes based on the natural breaks in the distribution of count versus probability of exceeding the predefined threshold as shown in Fig. 7, presenting areas currently influenced by nitrogen input from OWTS. However, the radial extent of the contaminant transport was estimated by kriging over a large range and does not represent actual flow patterns. The spatially variable input approaches



Fig. 6 Florida surficial aquifer vulnerability map based on the twostep uniform input nitrogen removal model, showing remaining NO_{3} -N concentrations in mg/L

predict probability of vulnerability based on the indicator kriging interpolation from output point data. Vulnerability is low at locations further away from OWTS and vulnerability at a point with an OWTS is based on the soil parameters considered in the contaminant fate and transport equation.

The aquifer vulnerability for the single-step variable input approach depicts areas being less vulnerable in northern and central Florida (Fig. 8). Vulnerable areas border the outer parameter of less vulnerable areas, and more vulnerable areas surround costal water bodies.

The aquifer vulnerability for the two-step variable input model also depicts areas being less vulnerable in northern and central Florida, with vulnerable areas bordering the outer parameter of less vulnerable and more vulnerable areas surround costal water bodies (Fig. 9).

Comparison of the four scenarios/approaches of the GIS-N model

Each of the four nitrogen removal scenarios/approaches have pros and cons. For the uniform input scenarios, the two-step approach predicts a higher overall trend in aquifer vulnerability for the sand and gravel aquifer compared to the single-step approach, but more localized areas of less vulnerable zones within different regions were observed (Fig. 10). This is due to the relatively small distance for the denitrification process because part of the unsaturated zone is used for the nitrification. Nitrifying ammonium before application to soils in areas with shallow depth to water table can help reduce vulnerability.

The two-step model is more sensitive to the depth to water table value and soil moisture content. For the twostep model, the available water table depth for denitrification is reduced because only part of the unsaturated zone (below the ~ 30 cm) was available for denitrification process since the top layer was the zone where nitrification occurred. For water table depths shallower than 30 cm, no depth is available for the denitrification process. However, very shallow water table depths and limited or high soil saturations will result in incomplete conversion of ammonium to nitrate, resulting in a lower initial nitrate concentration available for denitrification, which means that most



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Fig. 8 Florida surficial aquifer vulnerability map based on the singlestep OWTS nitrogen removal model with vulnerability classification based on the natural break in the predicted probability of exceedance

180 Miles



Fig. 9 Florida surficial aquifer vulnerability map based on the twostep OWTS nitrogen removal model with vulnerability classification based on the natural break in the predicted probability of exceedance

of nitrogen was in the form of ammonium. Thus, areas with very shallow water table depth (less than 5 cm), depicted as less vulnerable, do not necessarily reflect better conditions because the total nitrogen reaching the water table (ammonium plus nitrogen in this case) was still high. The total nitrogen levels represented as remaining ammonium plus nitrate is provided in Fig. 11. Total nitrogen values are important in assessing the impacts of aquifer vulnerability from remaining levels of unconverted ammonium. Overall, the total nitrogen distribution pattern follows that of the water table depth layer, resulting in higher total nitrogen in areas of shallow water table depths.

When compared to the single-step existing OWTS nitrogen removal model, the two-step model shows northern Florida with higher vulnerability zones and central Florida with greater areas of less vulnerability. These differences correlate with the reduced available water table depth for nitrogen removal and bias at shallow water table depth locations.

Model comparisons

The GIS-N model examines the vadose zone processes which includes the surficial aquifer system, while the DRASTIC and Flordia Aquifer Vulnerability Assessment (FAVA) model is applied broadly to the three main aquifer systems. When compared to the DRASTIC model approach, the GIS-N model developed in this study includes an unsaturated zone model specified to include parameters affecting nitrogen fate and transport. This model offers a more detailed approach based on a simplification of the ADE that considers reaction and sorption of contaminants as they percolate to the water table. The GIS-N model differs from the DRASTIC model in that it includes actual processes including sorption and nitrification of ammonium and denitrification processes. The effect of the degree of saturation is included as a surrogate to account for the impact of aeration on nitrification and denitrification processes. In contrast to a more generalized DRASTIC model which is based on weights and rates that are subjective, the GIS-N model is more specific to nitrogen transformation processes expected to produce relatively more accurate vulnerability maps. The GIS-N model is also more dynamic and applicable to current and futures impact from OWTS than the data-driven FAVA model. The FAVA model is based on the use of training points from past well data, which may not be applicable to the current distribution of concentration in the field because the FAVA model does not allow a general sensitivity map from current measured levels of nitrate concentration from a mixture of anthropogenic and natural sources as the development of the maps was based on past concentration measurements. On the other hand, the GIS-N model allows the user to define the source location and concentration, adjusting the initial input concentration to forecast future vulnerability.

The main advantages of the GIS-N model include: consideration of parameters influencing the fate and





Fig. 11 Total nitrogen levels based on the combination of remaining ammonium and nitrate from the two-step OWTS nitrogen removal model

transport of nitrogen in the vadose zone, more detailed depiction of the bio-chemical processes and based on the application of the ADE, updatable and flexible in adjusting contaminant input concentration and location, utilizes anthropogenic sources of contamination from OWTS, 10-m resolution for raster map format, mostly data driven analysis, and indirectly accounts for karst features with the depth to water table layer.

The limitations of the GIS-N model include: applicable to removal in the vadose zone only and represents the surficial aquifer system only, some NRCS soil parameters (soil temperature, depth to water table, and soil moisture) are data time sensitive, the model is sensitive to water table depth and first-order biological reaction rate, and uncertainty in the first-order biological reaction rates.

Summary and conclusion

Florida's surficial aquifer system relative vulnerability to contamination from anthropogenic sources stemming from land use practices particularly from OWTS was assessed. In Florida, OWTSs contribute to nitrogen loading into the vadose zone and aquifer system. This study modeled the fate and transport of nitrogen in the vadose zone based on a simplified groundwater flow equation implemented within GIS. The resulting aquifer vulnerability maps produced with spatially variable soil data will facilitate efforts of land management in protecting water resources for better human and environmental health.

The key findings in this study are listed below:

- Depth to water table in Florida is generally shallow, ranging from 0 to 203 cm with 24.3 % the area ≤5 cm. Most vulnerable areas reflect shallow depth to water table measurements, site characteristics, and estimates of nitrogen reaching the water table at different location.
- The lower vulnerability areas, with greater depth to water table are present within zones of the gravel and sand aquifer. The lower vulnerability areas contain known occurrences of silt and clay confining lenses, holding the contaminant for conversion.

• Streams near OWTS are of concern due to the discharge of the groundwater as baseflow. Groundwater from the surficial aquifer system moves along quick and short flow paths, which can prevent any additional denitrification in the groundwater.

The following recommendation for future research addresses the limitations in data availability and options to improve modeling efforts for the end user:

- Addition data can help validate and calibrate model. Measured nitrate levels in the vadose zone at USDA water table depths could provide field observations to obtain a more accurate parameter value through calibration and could improve the accuracy of the outputs.
- Incorporating Florida Department of Health data on OWTS technologies can adjust initial concentration input released from performance based OWTS.
- Updating the data to address new data collection methods, standardization and smoothing of boundary layers between measurement locations, and any changes to observed patterns. When the new data is available, the maps could be updated to reflect most up-to-date data.
- A higher resolution study can be conducted for a smaller study area of interest, such as a county in Florida, where collection of nitrogen samples is more feasible and GIS-based calculations are less intensive.
- GIS model builder can automate the workflow to streamline updates to the vulnerability maps.

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