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ORIGINAL ARTICLE

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Prediction of agriculture derived groundwater nitrate distribution in North China Plain with GIS-based BPNN

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Abstract In recent years, nitrate contamination of groundwater has become a growing concern for people in rural areas in North China Plain (NCP) where groundwater is used as drinking water. The objective of this study was to simulate agriculture derived groundwater nitrate pollution patterns with artificial neural network (ANN), which has been proved to be an effective tool for prediction in many branches of hydrology when data are not sufficient to understand the physical process of the systems but relative accurate predictions is needed. In our study, a back propagation neural network (BPNN) was developed to simulate spatial distribution of NO_3-N concentrations in groundwater with land use information and site-specific hydrogeological properties in Huantai County, a typical agriculture dominated region of NCP. Geographic information system (GIS) tools were used in preparing and processing input–output vectors data for the BPNN. The circular buffer zones centered on the sampling wells were designated so as to consider the nitrate contamination of groundwater due to neighboring field. The result showed that the GIS-based BPNN simulated groundwater NO_3-N concentration efficiently and captured the general trend of groundwater nitrate pollution patterns. The optimal result was obtained with a learning rate of 0.02, a 4-7-1 architecture and a buffer zone radius of 400 m. Nitrogen budget combined with GIS-based BPNN can serve as a cost-effective tool for prediction and management of groundwater nitrate pollution in an agriculture dominated regions in North China Plain.

Keywords Nitrate · Groundwater · Artificial neural network · Nitrogen budget · North China Plain

Introduction

North China Plain (NCP) contributes about 30% of China's total agricultural production. The annual chemical nitrogen fertilizer input is estimated as high as 400–600 kg hm^{-2}. High nitrogen fertilizer rates generally result in low nitrogen use efficiency (NUE) and high nitrogen loss. Loss of fertilizer nitrogen through leaching was estimated to be 8.5-28.7% of the applied rates (Li et al. 1999). Recently, much concern have been directed toward agriculture-derived groundwater nitrates pollution, which may cause algal blooms and eutrophication in aquifers, and can produce potential hazards to human health (Fan and Steinberg 1996; Gelberg and Church 1999; Gulis et al. 2002). Some studies conducted in the NCP areas showed that the NO_3–N concentrations had more than half exceeding the NO_3–N concentration limit of 10 mg L^{-1} (Zhang et al. 1996). In a recent survey, it is reported that nitrate contaminations have even increased in some local shallow groundwater in the NCP (Zhu and Chen 2002).

Several process-based models have been developed for simulating the fate and transport of nitrogen in soils and groundwater, and further details can be found in Ma and Shaffer (2001) and Chowdary et al. (2005). However, nitrate occurrence in groundwater, when related to land use distribution, agricultural management practices, and the physical and chemical processes in soil and groundwater, does not exhibit well behaved relationships. The process-based distributed models used to describe such relationships require complex mathematical equations, initial and boundary conditions, and detailed characterizations of the study area, including the physical, chemical, and biological processes, but such processes are not always understood (McGechan and Wu 2001). Furthermore, these models cannot estimate concentrations of nitrate in groundwater using easily measurable data such as nitrogen input and soil texture.

Thus, process-based models do have some practical limitation. When data are insufficient and obtaining accurate predictions is more important than understanding the nitrogen cycling process, black box and conceptual models with less data requirement and calibration time may be suitable alternatives. Artificial neural network (ANN) are 'black box' models with particular properties greatly suited to dynamic nonlinear system modeling and can overcome the difficulties of processed-based techniques used in simulating complex features of different relationships. ANN has been widely used for simulation and prediction of water quality (Aguilera et al. 2001; Kralisch et al. 2003; Daliakopoulos et al. 2005; Mohammad and Jagath 2005a). The advantages of ANN models over conventional simulation methods have been discussed in detail by French and Krajewski (1992). This paper is intended to predict groundwater pollution patterns in agriculture-dominated area with land use information and some easy obtained site-specific data, developing the potential of GIS and artificial neural network.

Methods and materials

Study area and data source

The study was conducted in Huantai County of the North China Plain (Fig. 1), covering an area of 509.5 km^2. It represents the transient zone from the mountain alluvial plain in central Shandong to the Yellow River plain in the north. The soil parent material mainly consists of mountain diluvium and Yellow River alluvial deposits, which formed the clay loam soils classified as Calcaric Fluvisols. The landscape of the study area is relatively flat with relative elevations of 6.5–29.5 m and gradient ratios of 1/800–1/3,500 (Liu et al. 2005). Both groundwater and surface water run roughly in the same direction as the land slopes from southwest down to northeast. The average groundwater table was 13.6 ± 8.2 m across the entire county in 2002.

The study area has been dominated by winter wheat and summer maize rotation system which account for 75% of all crops planted for decades. More than 15 t ha^{-1} of grain was produced across the entire area since 1990. Excessive amounts of fertilizer and water have been applied annually. *N* fertilizer was applied at 634 kg N ha^{-1} for the double cropping system in 2002. Under such an intensive farming practice, NO_3-N leaching from plant rooting zones was usually observed (Liu and Wu 2002, 2003).

Groundwater sampling

Water sampling was carried out in November 2002 and 2004 in shallow aquifers across the Huantai County to analyze the nitrate concentration. All sites were away from the influence of high-density housing. In total, 616 water samples were collected from irrigation wells. The location of the wells was precisely recorded with a global position system (GPS) receiver. Groundwater was sampled with portable pump for shallow and installed pump for relatively deep water. The continuous flowing analyzer was used to analyze NO_3-N concentration of the sampled water.

Data collection

Information on the yields and nitrogen inputs (fertilizer and manure) for various crop systems in the last 4 years

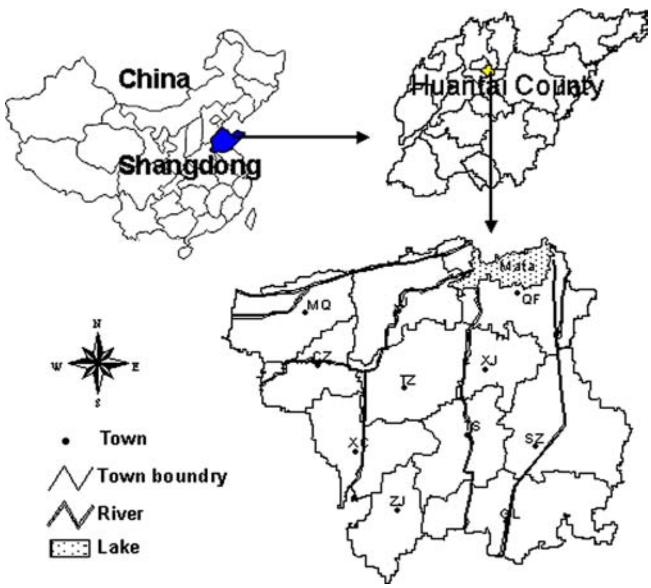

Fig. 1 Geographic location of the study area, Huantai County

Table 1 Hydrogeological properties of different agricultural land use types

Hydrogeological factors	Wheat–maize	Vegetables	Cotton	Fruit trees
Depth to groundwater (m)	2.1–34.5	7.5–27.2	3.7–29.3	6.3–33.5
Soil sand content at 30–60 depth (%)	4.5–45.2	12–29.6	8.8–31.6	14.5–30.2
Soil organic matter content (%)	1.08–2.36	1.28–1.77	1.13–1.69	1.12–1.58

were collected through farmer interviews with the 130 owners of randomly selected sampling wells. The cropping systems in the buffer zone of the sampling well were derived from Huantai Land Use Information System (LUIS, on a scale of 1:10,000), a land use database which was compiled and maintained in 2002 by the Huantai Land Resources Bureau. It was assumed that present land use patterns have never changed since it was developed for agriculture.

Soil sand content of various soil types in the study area was referenced to previous study (Liu 2004). Soil organic matter contents of the cropping horizon were monitored in 1996, 1999, and 2002. Depth to groundwater data was collected by local groundwater table monitoring stations. The annual data from 1996 to 2002 was averaged across observations at 5-day intervals from 32 monitored wells in the study area.

The agricultural land use was grouped into four categories: wheat–maize rotational systems, vegetables, and cotton and fruit trees. Table 1 shows the range of values for the collected data of different agricultural land use types.

Back propagation neural network development

The back propagation neural network (BPNN) was used as the exploratory model for our study. BPNN have performed well in simulating and predicting agricultural non-point pollution in stream water and groundwater (Mohammad and Jagath 2005a; Sahoo et al. 2005). Detailed descriptions of BPNN are provided by Sharma et al. (2003). An ANN learns the underlying different relationships of the system of interest from training samples, which are basically the cause-effects samples (Qu et al. 2004). Thus, the first step in the analysis is to conceptualize the cause-effect relationships for groundwater nitrate pollution and thus precisely identify input and output vectors of the ANN.

Conceptualization of groundwater nitrate pollution

In an agriculture-dominated region, nitrogen applied to cropped fields reaches the groundwater as nitrate dissolve in rainwater or irrigation water percolating out of the crop root zone. The nitrate concentration in groundwater depends on field nitrogen available for leaching and nitrogen transport through the soil with applied water.

The nitrogen available for leaching depends on agricultural land use and nitrogen management. In this study, field nitrogen surplus was used to measure the effect of land use. Aller et al. (1987) reported seven most important hydrogeological factors that control the groundwater pollution potential, i.e., *D* depth to aquifer, *R* recharge, *A* aquifer media, *S* soil media, *T* topography, *I* impact of vadose zone media, and *C* conductivity of the Aquifer. *A*, *T*, and *I* were considered to be spatial homogeneous at county scale in NCP. As such, only three hydrogeological factors including *D*, *R*, and *S* were considered in this study.

Field water percolates more easily through soils with less clay and higher sand content, and the sand contents at the 30–60 cm depth was found to be an accurate predictor of nitrate leaching risk (Assimakopoulos and Kalivas 2003). In addition, if a sufficient source of organic matter is present, bacterial systems are capable of denitrifying large amounts of NO_3-N in the soil zone, thus reducing the pool of nitrate available for leaching (Mujumdar and Sasikumar 2002).

Thus, field nitrogen surplus, groundwater depth, soil organic matter content, and soil sand content at 30–60 cm depth were identified as four indicators to reflect the impact of land use hydrogeological factors on groundwater nitrate pollution. They were used as input vectors of the artificial neural network, and the groundwater NO_3-N concentration as the output vectors.

It was reported that land use distribution in a greater catchment area may better reflect the effects of land use on groundwater nitrate concentrations than does the land use at the farm where the well is located (Kolpin 1997). Thus, circular-buffered zones, centered by the nitrate receptors, were designated, so that the effects of neighboring land uses and site properties on nitrate contamination of groundwater could be considered. Buffers with radii ranging from 200 to 2,000 m have been used in other studies (Kolpin 1997; McLay and Dragten 2001). We arbitrarily chose a radius of 200 m as the initial buffer zones radius, and used the trial and error method to obtain the most optimal one.

Preparation of training and validation data set

A soil surface budget was employed to calculate field nitrogen surplus for the present study, which records all nutrients that enter the soil via the surface and that leave the soil via crop's offtake (Oenema and Heinen 1999).

Nitrogen inputs via fertilizer and animal manure additions were adjusted for miscellaneous gaseous *N* losses from the soil and crops, which were estimated to be 20% of nitrogen input based on previous studies (Hu et al. 2004). Atmospheric deposition was estimated at 12 kg ha^{-1} year^{-1}, based on Lu (1998). The nitrogen output via crop offtake was calculated from crop yield and *N* content. The *N* content in plant parts was referred to Luo (2001).

Geographic information system (GIS) was used to manage the data. The values of the four input vectors for the water-sampling sites were estimated with interpolation of 12 neighboring values by using the inverse distance weighted (IDW) method (ArcView 3.3, ESRI), and then the input and output vectors data sets of the buffer zones of the sampling sites were computed. The 616 samples were divided into three subsets, of which approximately half of the samples were used for training the neural network, a quarter of the sample for model calibration, and the rest of the samples for model validation.

Network architectures and efficiency evaluation

The MATLAB Toolbox (MathWorks, Inc., Natick, MA, USA) was used to develop the BPNN. It provides many training methods, of which the Levenberg-Marquardt training algorithm was selected, considering its fast convergence ability (Sahoo et al. 2005). A tangent sigmoid transfer function was used for hidden layers and a linear transfer function for the output layer according to Qu et al. (2004). The structure and learning rate of the network is determined using trial and error by varying learning rates, number of hidden layer, and nodes of the hidden neurons in the test scenarios.

Predictive efficiency of the BPNN was qualitatively assessed using the scatter plots of the predicted versus observed nitrate concentration, and quantitatively via R^2 efficiency criterion and root mean square error (RMSE). The R^2 efficiency criterion was defined as (Daliakopoulos et al. 2005):

$$R^2 = 1 - \frac{\sum_1^n (c_0 - c_\mathrm{p})^2}{\sum_1^n c_0^2 - \sum_1^n c_\mathrm{p}^2/n}$$

where R^2 represents the percentage of the initial variation explained by the model, n is the number of the testing patterns; c_0 and c_p are the observed and predicted nitrate concentrations, respectively. The RMSE indicates the discrepancy between the observed and calculated values. The best fit between observed and calculated values would have $R^2 = 1$ and $\mathrm{RMSE} = 0$. RMSE was calculated as:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_1^n (c_0 - c_\mathrm{p})^2}{n}}.$$

Results and discussion

Land use and groundwater nitrate pollution

Statistical data of the survey given in Table 2 shows the association of the field nitrogen surplus (FNS) and nitrate pollution in shallow groundwater. The vegetable systems showed the greatest FNS, with average values greater than 550 kg N ha^{-1} year^{-1}, and cotton had the lowest FNS, with average values close to 90 kg N ha^{-1} year^{-1}. It is generally believed that intensive farming with high nitrogen surplus would lead to more severe groundwater pollution. In our study, however, the vegetable cropping system with a FNS as high as 558.7 kg N ha^{-1} year^{-1} was acting similarly as the wheat–maize rotation system with a FNS of 194.8 kg N ha^{-1} year^{-1} in terms of NO_3-N concentration in groundwater. Moreover, the groundwater NO_3-N concentration beneath cotton fields with the lowest FNS have reached the highest lever, while the fruits tree fields with medium FNS had the lowest level of groundwater NO_3-N concentration. Careful analysis found that most of the water samples were taken from wheat–maize dominated areas where cotton and fruit trees were also commonly planted, which supports the assumption that the neighboring land use and site-specific properties may have played important role in shaping groundwater pollution patterns (Liu et al. 2005).

Table 2 NO_3-N concentration in shallow groundwater in relation to field nitrogen surpluses of aboveground cropping systems

Crop system	No of field samples	*N* input (kg ha^{-1} year^{-1})	Crop offtake (kg N ha^{-1} year^{-1})	*N* surplus (kg ha^{-1} year^{-1})	No of groundwater samples	NO_3-N concentration (mg L^{-1})
Wheat–maize	68	505.9 (43.2)	311.1 (12.2)	194.8 (33.2)	546	8.1 (8.6)
Vegetables	26	717.2 (81.8)	158.5 (34.7)	558.7 (93.1)	32	8.4 (9.3)
Cotton	20	157.6 (11.2)	69.7 (5.8)	87.9 (10.6)	28	9.1 (10.3)
Fruit trees	16	311.3 (33.4)	13.5 (3.7)	317.8 (29.7)	10	3.9 (2.8)

The values in parentheses are standard deviations.

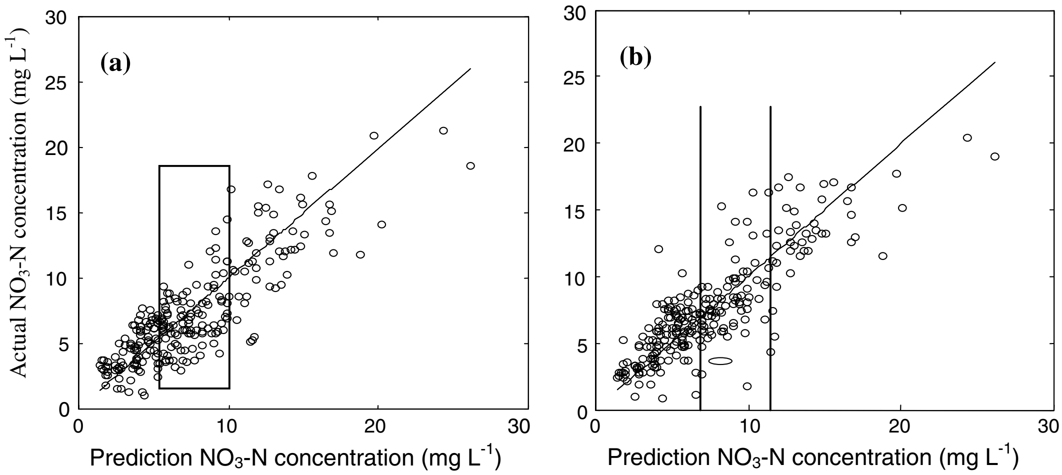

Fig. 2 Scatter plots of the observed versus BPNN-predicted NO_3-N concentration for circular zoned buffer areas with radii of (**a**) 200 m and (**b**) 400 m

Model training and verification

The configurations of the BPNN, such as the learning rate and the size of the hidden layer and neurons, were determined by trial and error. The learning rate varied from 0.01 to 0.2, with the hidden layer kept at 1 with 10 neurons. This low learning rate was chosen because high fluctuations in error were observed at higher learning rates. Analysis of these results led to an optimum learning rate of 0.02.

The model was then tested by varying the size of the hidden layer and neurons. The number of hidden layers was set to one and two, and then neurons ranging from 4 to 15 in each layer were used to test the BPNN model according to Qu et al. (2004). The correlation coefficients were all greater than 0.85 in the training phase, but most were less than 0.75 in the validation phase, indicating that the BPNN model was trained well but lost some of its generalization ability. The architecture 4–7–1 (four neurons in the input layer, seven neurons in the hidden layer, and one in the output layer) produced the optimum results with $R^2 = 0.77$ and RMSE = 2.93 mg L^{-1} in the validation phase. Scatter plots of the observed versus BPNN-predicted NO_3-N concentrations were given in Fig. 2b, which showed higher predictive efficiency for groundwater NO_3-N concentration ranging from 5 to 10 mg L^{-1} and relatively lower efficiency for other ranges. The lower efficiency was assumed to be affected by relatively small data set to train the BPNN.

The sensibility of predictive efficiency to the radius of the well buffer zone is also examined. The optimal BPNN developed above was tested with the radius ranging from 100 to 2,000 km with 50-m intervals. The best performance was obtained at the radius of 400 m with $R^2 = 0.81$ and RMSE = 2.37 mg L^{-1} in the validation phase. Scatter plots of the observed versus BPNN-predicted NO_3-N concentrations at this radius were given in Fig. 2b. The results were similar to Kolpin (1997) which showed that a 500-m radius provided the best correlation with NO_3-N in groundwater across a wide range of soil types and land uses in the Unite States. In comparison to Fig. 2a, Fig. 2b showed higher predictive efficiency for ranges of 6–11 mg L^{-1}. Predictive efficiency increasing due to buffer zone designation indicates that land use patterns and site-specific properties of neighboring field play important role in shaping groundwater nitrate pollution in an agriculture dominated region.

Simulation of groundwater NO_3-N concentration distribution

The NO_3-N concentrations in groundwater were classified into four groups defined by Liu (2004). The four concentration ranges are: clean (0–3 mg L^{-1}), lightly polluted (3–6 mg L^{-1}), polluted (6–10 mg L^{-1}), and severely polluted (> 10 mg L^{-1}). Figure 3a shows the observed distribution of NO_3-N concentration interpolated from the groundwater sampling data using the IDW method.

Then the BPNN was used to predict the NO_3-N distribution in the aquifer across Huantai County under present land use conditions. GIS was used to divide the area into homogenous zones in accordance with four input vectors layers including field nitrogen surplus, soil sand content at 30–60 depth, soil organic matter content, and depth to groundwater. A new map of 2,326 basic simulation units (BSU) were generated by overlaying these layers and the attributes data were prepared for running the BPNN model.

As show in Table 3, the BPNN underestimated the clean and slighted polluted areas, which was assumed to be affected by relatively small data set ranging from 0 to 6 mg L^{-1} of NO_3-N concentration to train the BPNN.

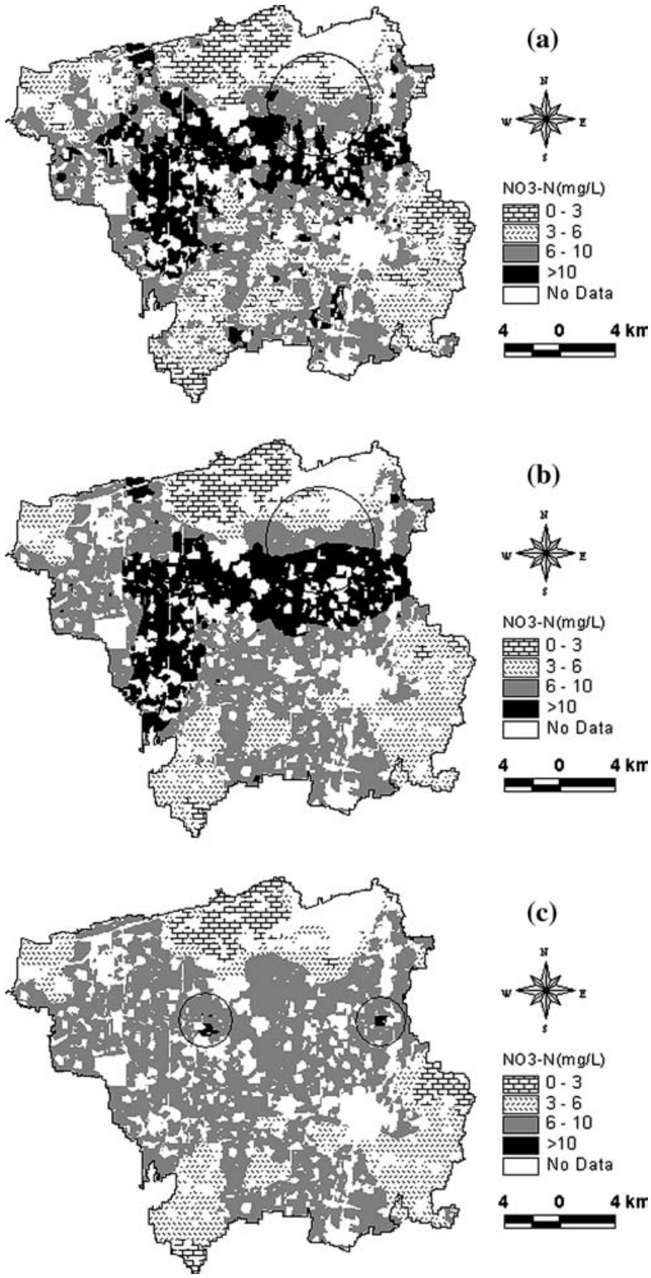

Fig. 3 Distributions of NO_3-N concentrations in the study area: **a**estimation by interpolation of the sampling data; **b** BPNN prediction under current land use conditions; **c** BPNN prediction with the FNS reduction of 35% in the severely polluted areas

In addition, the simulation result overestimated the polluted and the severely polluted areas by 9.60 and 13.23%, respectively. Figure 3b shows the NO_3-N concentration distribution simulated by the BPNN model. The overestimated severely polluted areas are mainly distributed in the northeast corner of the county, where the Mata Lake was supposed to dominantly shape the NO_3-N distribution patterns. In comparison to grid form of output data generated by IDW method, the GIS-based BPNN exported vector data in shape form. As such, landscapes were more concentrated in Fig. 3b, while Fig. 3a showed more fragmentation for different ranges of groundwater NO_3-N concentrations. However, comparison between Fig. 3a and b clearly demonstrated that the BPNN model captured the general trend of nitrate distribution in most parts of the study area.

Table 3 BPNN simulation results in comparison to observed results

Range of NO_3-N concentration (mg L^{-1})	Areas (km^2)	
	IDW method	BPNN
0–3	28.65	44.86
3–5	85.42	95.64
5–10	159.54	140.89
> 10	88.79	81.01

Application in groundwater quality management

The increasing evidence of the nitrate contamination of groundwater in agriculture-dominated areas required protection alternatives. Due to the presence of the nitrogen surplus in soil-crop systems that provide nitrate to groundwater, it is assumed that there is a sustainable nitrogen surplus (SNS) that soil-crop systems can handle without providing too much nitrate available for leaching (Mohammad and Jagath 2005b). Thus, agriculture-derived nitrate pollution can be controlled by maintaining the nitrogen surplus of the crop fields under the SNS. SNS is a goal-oriented rather than means-oriented indicator, leaving government and farmers the more freedom to select proper measures to control agriculture derived groundwater pollution and keep the groundwater NO_3-N concentration lower than 10 mg L^{-1}. Consequently, the severely polluted area can be reduced. So, we investigated the practicability of the GIS-based BPNN by simulating the sensibility of severely polluted area to FNS change and recommending the SNS.

Under current agricultural land use conditions, the severely polluted area simulated by the BPNN is 88.79 km^2, where the average field nitrogen surplus is 224 kg ha^{-1} $year^{-1}$. The reductions of field nitrogen surplus ranging from 5 to 50% at intervals of 5% were simulated by the BPNN model. The result shows that decrease of FNS would notably reduce the severely polluted area. A 35% decrease of FNS resulted in 84.7% reduction of the severely polluted area. Further decrease of the filed nitrogen surplus results in much less reduction of the severely polluted areas. Figure 3c showed the simulation results of NO_3-N concentration distribution with the FNS reduction by 35% (reduced to

146 kg ha^{-1} $year^{-1}$) only in the severely polluted areas. The remained severely polluted areas is 12.41 km^2, where soil sand content at depth of 30–60 cm was greater than 40% and the nitrate concentration reduction was supposed to be more sensitive to rain fall and irrigation. Thus, the FNS of 146 kg ha^{-1} $year^{-1}$ can be recommended as the SNS in the severely polluted areas. However, a uniform SNS for the whole severely polluted areas may be arbitrary because of spatial heterogeneity of groundwater NO_3-N concentration. So, it may lead to economic loss as a result of unnecessary reductions of nitrogen input in some area. Therefore, the spatial pattern of the sustainable FNS in the severely polluted areas requires further research.

Conclusion

To predict the nitrate concentration distribution in an agriculture-dominated region, a GIS-based BPNN model was developed. Field nitrogen surplus and three easily obtained site-specific hydrogeological properties were selected as input vectors to simulate the NO_3-N concentration in groundwater. The buffer zones were designated so that the effects of the land use patterns on groundwater nitrate pollution distribution can be considered. Modeling efficiency increases because buffer zone designation supports the assumption that the land use patterns and site-specific properties of neighboring field play important roles in shaping groundwater nitrate pollution patterns.

The optimal performance of the BPNN was obtained with a learning rate of 0.02, a 4–7–1 architecture, and a buffer radius of 400 m. Although the BPNN underestimated the clean and slightly polluted areas and overestimated the severely polluted areas in comparison to observed results, it did capture the general trend of the nitrate distribution in the study area under current agricultural land use conditions. It was assumed that there is a sustainable nitrogen surplus that soil-crop systems can handle without too much nitrate available for leaching. The sustainable FNS in the severely polluted areas was recommended by running the BPNN with various FNS progressively. The severely polluted area was observed to be sensitive to reduction of the FNS.

A simple combination of nitrogen budget with GIS-based BPNN can be constituted as a cost-effective tool for prediction and management of groundwater nitrate pollution in an agriculture dominated region in the NCP. The significant advantage of BPNN method should be the easily obtained data supports and such an analytical tool is more practical for policy-making.

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