Modular neural networks to predict the nitrate distribution in ground water using the on-ground nitrogen loading and recharge data

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Abstract

Artificial neural networks have proven to be an attractive mathematical tool to represent complex relationships in many branches of hydrology. Due to this attractive feature, neural networks are increasingly being applied in subsurface modeling where intricate physical processes and lack of detailed field data prevail. In this paper, a methodology using modular neural networks (MNN) is proposed to simulate the nitrate concentrations in an agriculture-dominated aquifer. The methodology relies on geographic information system (GIS) tools in the preparation and processing of the MNN input−output data. The basic premise followed in developing the MNN input−output response patterns is to designate the optimal radius of a specified circular-buffered zone centered by the nitrate receptor so that the input parameters at the upgradient areas correlate with nitrate concentrations in ground water. A three-step approach that integrates the on-ground nitrogen loadings, soil nitrogen dynamics, and fate and transport in ground water is described and the critical parameters to predict nitrate concentration using MNN are selected. The sensitivity of MNN performance to different MNN architecture is assessed. The applicability of MNN is considered for the Sumas-Blaine aquifer of Washington State using two scenarios corresponding to current land use practices and a proposed protection alternative. The results of MNN are further analyzed and compared to those obtained from a physically-based fate and transport model to evaluate the overall applicability of MNN.
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1. Introduction

Aquifers are vulnerable to contamination by residential, agricultural, and industrial pollutants. Sources of ground water contamination are widespread and include accidental spills, landfills, storage tanks, pipelines, and agricultural activities; among many other sources (Bedient et al., 1994). Of these sources, agriculture-related activities are well-known to cause non-point source pollution in small to large watersheds especially due to fertilizers and various carcinogenic substances found in pesticides (Jansen et al., 1999; Wolf et al., 2003; Tianhong et al., 2003). Nitrate (NO_3) is the most common pollutant found in shallow aquifers due to both point and non-point sources (Postma et al., 1991). Nitrate is the primary nitrogen species lost from soils by leaching due to its high mobility (Hubbard and Sheridan, 1994; Ling and El-Kadi, 1998; DeSimone and Howes, 1998; Tesoriero et al., 2000). Elevated nitrate concentrations in drinking water are linked to health problems such as methemoglobinemia in infants and stomach cancer in adults (Lee et al., 1991; Addiscott et al., 1991; Wolfe and Patz, 2002). As such, the U.S. Environmental Protection Agency (US EPA) has established a maximum contaminant level (MCL) of 10 mg l^{-1} as NO_3-N (U.S. Environmental Protection Agency, 2000).

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Many studies have shown that agricultural activities are the main source of elevated nitrate concentrations in ground water (Hudak, 2000; Spalding et al., 2001; Harter et al., 2002; Spruill et al., 2002; Johnsson et al., 2002; Mitchell et al., 2003; Lake et al., 2003). Agricultural practices can result in non-point source pollution of ground water (Sivertun and Prange, 2003). These agricultural activities include use of fertilizers, manure application, and leguminous crops. For instance, the extensive use of fertilizers on row crops is considered as a main source of nitrate leaching to ground water particularly in sandy soils (Hubbard and Sheridan, 1994; Tianhong et al., 2003). Elevated nitrate concentrations in ground water are common around dairy and poultry operations, barnyards, and feedlots (Hii et al., 1999; Carey, 2002). In addition to agricultural practices, non-point sources of nitrogen involve precipitation, irrigation with ground water containing nitrogen, and dry deposition (Cox and Kahle, 1999). Point sources of nitrogen are shown to contribute to nitrate pollution of ground water. The major point sources include septic tanks and dairy lagoons where many studies have shown high concentrations of nitrate in areas with septic tanks and dairy lagoons (Erickson, 1992; Arnade, 1999; MacQuarrie et al., 2001).

The assessment of ground water contamination by nitrate should account for on-ground nitrogen loading, nitrate leaching from soil, and fate and transport in the ground water. Regional assessment of ground water quality is complicated by the fact that nitrogen sources are spatially distributed (Tesoriero and Voss, 1997). Accurate quantification of nitrate leaching is difficult. Nitrate leaching from the soil zone is a complex interaction of many factors such as the land use, on-ground nitrogen loading, ground water recharge, soil nitrogen dynamics, soil characteristics, and the depth to water table. Several models have been developed for simulating the fate and transport of nitrogen in soils, and further details can be found in Ma and Shaffer (2001) and McGechan and Wu (2001). Once nitrate leaching is quantified, a fate and transport model of nitrate can be developed and used, in conjunction with a soil nitrogen model, to simulate the effectiveness of current and future agricultural practices on nitrate occurrences in ground water.

There are many fundamental difficulties associated with developing distributed models of fate and transport of nitrate for both soil and ground water. The key difficulties are: (1) the models need enormous data, which are generally difficult and costly to obtain; (2) the development of these models require detailed characterization of the study area including the physical, chemical, and biological processes when such processes are not fully known (McGrail, 2001); and (3) these models often use fine spatial and temporal discretization that require substantial computational resources to simulate multiple scenarios (Morshed and Kaluarachchi, 1998b; McGrail, 2001). To overcome these difficulties, many researchers have successfully used artificial neural networks (ANN). ANN are interconnections of simple processing elements called neurons that have the ability to identify the relationship between the input–output responses from given patterns (Beale and Jackson, 1991; Haykin, 1994). In this pattern recognition, ANN overcomes the difficulties of physically-based techniques used in simulating complex features of different relationships. As such, ANN is a powerful tool for representing the underlying relationships governing the input–output response patterns for different physical problems (Morshed and Kaluarachchi, 1998b).

Due to the capability of ANN in successfully handling large-scale physical problems, ANN has found use in a wide range of hydrologic applications (ASCE Task Committee on Application of Artificial Neural Networks in Hydrology, 2000). Ray and Klindworth (2000) used ANN to assess nitrate contamination of rural private wells. Input parameters were the thickness of the aquifer, sampling depth, distance to cropland, streams, disposal sites, and septic systems, topography around wells, season of sample collection, and time between the probable dates of nitrate application and the first flushing storms. The output of ANN was either *none, low, medium,* or *high* when the predicted nitrate concentration is $<10, 10–20, 20–30,$ or $>30 \, mg \, l^{-1}$, respectively. Kaluli et al. (1998) developed an ANN model that simulated nitrate leaching to ground water from a 4.2 ha site. ANN inputs included time of year, daily denitrification rate, cropping systems, water table depth, nitrogen fertilizer application rate, daily antecedent precipitation index, initial nitrate concentration, and the daily drain flow. They used ANN to simulate the impacts of different management options on nitrate leaching. In a different approach, many researchers used ANN as a proxy to a mathematical model of contaminant fate and transport (Ranjithan et al., 1993; Rogers and Dowla, 1994; Sawyer et al., 1995; Johnson and Rogers, 1995, 2000; Aly and Peralta, 1999; Morshed and Kaluarachchi, 1998a,b; Gumrah et al., 2000). Besides, ANN was utilized in simulating many environmental and water resources engineering systems (e.g. Bockreis and Jager, 1999; Maier and Dandy, 2000; Kralisch et al., 2003; Mas et al., 2004; Anctil et al., 2004).

This paper presents a simple, yet efficient approach using a special class of ANN known as modular neural networks (MNN) for simulating the spatial distribution of long-term nitrate concentration in agriculture-dominated aquifers. MNN utilizes high-order computational units to perform multifaceted tasks. These tasks were developed by dividing the physical problem into simpler subtasks via partitioning the input–output response patterns into regions of identical features. As such, MNN has the ability to understand the complex physical

problem better than a typical multilayer ANN (Haykin, 1994). Nitrate occurrences in ground water when related to the different on-ground nitrogen sources; land use distribution and practices, and the physical and chemical processes in soil and ground water do not exhibit well-behaved relationships. Therefore, MNN can be a potential analytical tool to simulate the spatial distribution of long-term nitrate concentrations in agriculture-dominated aquifers where well-behaved relationships do not exist. To the best of our knowledge, the applicability of MNN over ANN has not been studied previously in a similar physical problem. Since the long-term nitrate concentrations in large watersheds are controlled by many complex processes, we believe that the applicability of MNN should be evaluated for potential future use over ANN.

Degradation of ground water quality of the Sumas-Blaine aquifer located in the northwest corner of Washington State, mainly from nitrate, is of great concern to the residents of Whatcom County (Blake and Peterson, 2001). The Sumas-Blaine aquifer is the principal surficial unconfined aquifer in Whatcom County. High concentrations of nitrate have been detected in this aquifer since the early 1970s (Kaluarachchi et al., 2002). Many studies showed that agricultural practices and dairy farming are the probable causes of excessive nitrate levels in the shallow aquifer (Liebscher et al., 1992; Erickson, 1992, 1994; Garland and Erickson, 1994; Hulsman, 1998; Hii et al., 1999; Cox and Liebscher, 1999; Carey, 2002; Mitchell et al., 2003; Almasri and Kaluarachchi, in press). The issue of elevated nitrate concentrations in the Sumas-Blaine aquifer has called for urgent adoption of protection alternatives. In order to successfully strategize the proposed protection alternatives, a comprehensive study of ground water quantity and quality is needed. As part of the overall management plan, a study of nitrate pollution of ground water was undertaken, and the study included the analysis of long-term data of nitrate and the development of a comprehensive fate and transport model that can be used in assessing the effectiveness of various long-term management alternatives.

The overall MNN approach developed in this paper utilizes the National Land Cover Database (NLCD) grid of the U.S. Geological Survey to determine the spatial sources of nitrogen in the study area based on the land use distribution. A Geographic Information System (GIS) of ESRI (1999) is used to facilitate the MNN input and output processing and is integrated with the NLCD. The methodology enables the simulation of management alternatives that aim at reducing the on-ground nitrogen loading. The sensitivity of MNN to key concepts pertaining to input–output response pattern formulation is evaluated. The functionality of the proposed methodology is assessed by simulating the outcomes of the current practices and future proposed management alternatives on ground water quality and compares the output from MNN to that of a classical fate and transport model. The applicability of the developed approach is demonstrated for the Sumas-Blaine aquifer. The proposed MNN-based approach is distinctive as it considers a regional-scale aquifer where a broad spectrum of nitrogen sources and land cover classes interact in a complex manner to dictate the nitrate occurrences in ground water. Additionally, and to the best of our knowledge, this is the first study to evaluate the applicability and potential use of MNN in ground water quality management.

2. Modular neural network

2.1. ANN versus MNN

ANN consists of an information-processing paradigm and a pattern recognition tool inspired by how the biological nervous systems process information (McCulloch and Pitts, 1943). ANN uses input–output response patterns to map a function approximation to the underlying governing rules of the output responses corresponding to specific inputs in a convoluted physical space (Morshed and Kaluarachchi, 1998b). Generally, ANN consists of three layers. The first is the input layer that receives the input and processes it to the hidden layer. The nodes of the hidden layer enhance the ability of ANN to model complex relationships (Zealand et al., 1999). The number of hidden nodes depends on the number of training patterns, the amount of data noise, and the complexity of the function that ANN is approximating (Hecht-Nielsen, 1987). The output layer presents ANN predicted output. Each hidden or output neuron is associated with an activation function for limiting the amplitude of the output of the neuron depending on the activity level at its input (Christodoulou and Georgiopoulos, 2001). For a detailed illustration on ANN functionality, the interested reader may refer to Beale and Jackson (1991), Haykin (1994), and Maier and Dandy (2000). In the following, a brief description of MNN functionality is provided along with the incentives for using MNN in this work.

In general, modularity allows for the use of high-order computational units to perform complex tasks by dividing the problem into simpler subtasks; this division is achieved via partitioning the input space into regions of identical governing rules and then combining their individual solutions. As such, MNN has the ability to learn a disintegrated convoluted function faster than a typical multilayer ANN (Haykin, 1994). Since the input–output response patterns between the distribution of nitrate concentration in ground water and the relevant processes are not well behaved, MNN is expected to be more suitable for such problems. For

instance, one expects high nitrate concentration in ground water with high on-ground nitrogen loading and vice versa. Nevertheless, in areas of high on-ground nitrogen loading and low ground water recharge, nitrate concentration is different from the case of low on-ground nitrogen loading and high ground water recharge (Nolan and Stoner, 2000). Also in agricultural areas, soil is rich with nitrogen constituents whereas in residential areas this is not the case. Therefore, agricultural land classes have embedded unique characteristics related to nitrate concentrations that are different from other land use classes. MNN automatically detects these relationships and can allocate the input vector into the expert modules.

2.2. Description of MNN

MNN consists of modules called *expert networks* that compete to learn different aspects of a problem. In addition, MNN has an integrating unit called a *gating network* that assigns different features of the input space to the different expert networks (NeuralWare, 2000). Fig. 1 depicts a typical MNN. The expert and gating networks receive the input. The gating network has output nodes equal to the number of expert networks. Each expert module produces a response corresponding to the input vector and the output of MNN is the weighted sum of these responses with the weights equals to the gating network output. Therefore, the gating network output at an expert module can be viewed as the prior probability that this module will be used for a given input vector (Zhang and Govindaraju, 2000; NeuralWare, 2000). In Fig. 1, $[X]$ represents the input vector and $[Y]$ represents the corresponding MNN output vector. In general, the notation I-J-K is used to define MNN of a vector of I input variables, a vector of J hidden nodes, and a vector of K output variables.

In order for MNN to map the relationship between $[X]$ and $[Y]$, it should be trained. The training of the MNN occurs concurrently for the expert and gating networks. In this work, the training is attained using the back propagation algorithm (BPA). A detailed mathematical description of BPA is provided by Rumelhart et al. (1986) and Maier and Dandy (1998). During the process of MNN training, the desired output is utilized to develop the posterior probabilities. The error at the gating network output is the difference between the posterior and prior probabilities. The gating network is trained via back propagation. In training the expert modules, the output errors are mitigated by the prior probabilities from the gating network and these errors are back propagated as well (NeuralWare, 2000). This learning approach tends to promote competition among the expert modules. If a specific module begins to take responsibility for a particular region of the input space, then the gating network will assist this module over the others. A detailed description of MNNs can be found in Haykin (1994), NeuralWare (2000), and Zhang and Govindaraju (2000). After MNN is trained, it should be tested. The main intent of MNN testing is to evaluate its efficiency in the prediction of patterns that have not been used in the training phase. MNN is said to generalize well if the predicted output matches closely the actual values (Beale and Jackson, 1991).

3. Conceptualization of nitrogen transport

The overall conceptual model of fate and transport of nitrate in ground water consists of the following three integrated phases as depicted in Fig. 2 (Almasri and Kaluarachchi, 2004): (a) *estimation of the spatial distribution of on-ground nitrogen loadings*; (b) *estimation of*
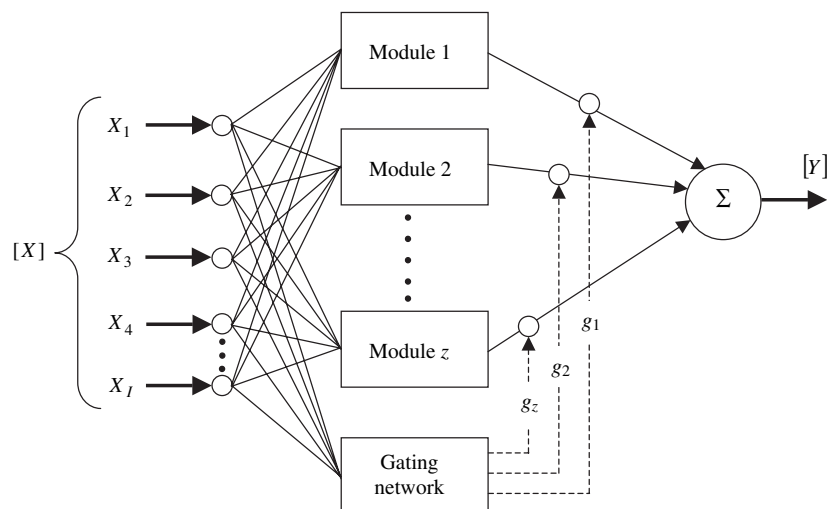

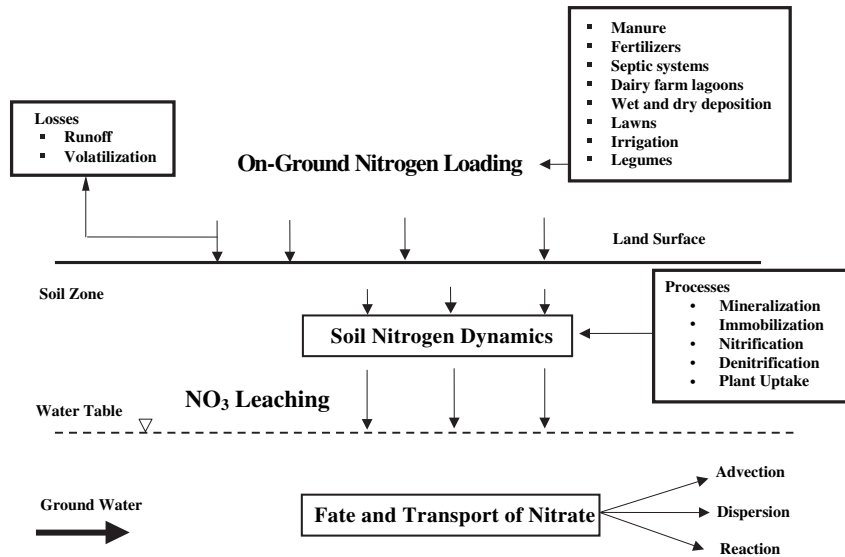Fig. 1. Architecture of a modular neural network (MNN).

Fig. 2. A schematic describing the integrated three-process approach to conceptualize the on-ground nitrogen loading, soil nitrogen transformations, and fate and transport of nitrate in ground water.

net nitrate leaching to ground water after allowing for soil nitrogen transformations; and (c) *modeling the fate and transport of nitrate in ground water*. In the next sections, a general description of the three integrated sub-systems is provided.

3.1. On-ground nitrogen loading

A major step in calculating the nitrate leaching to ground water is the estimation of the on-ground nitrogen loadings from different nitrogen sources. There are many sources of nitrogen, natural and anthropogenic, which can contribute to ground water contamination (Hallberg and Keeney, 1993). To differentiate between the different land application categories in order to assign the appropriate nitrogen loadings, the NLCD grid was utilized in this study. The NLCD grid is a 21-class land cover classification scheme applied consistently over the United States. The spatial distribution of the on-ground nitrogen loadings is a function of the spatial distribution of the NLCD classes and the nitrogen loadings contributing to each NLCD class. Therefore, the spatial distribution of on-ground nitrogen loading can be expressed as in the following relationship:

$$\Phi = f(\delta, \tau) \tag{1}$$

where Φ is the spatial distribution of net on-ground nitrogen loading after accounting for nitrogen losses due to volatilization and runoff; δ is the spatial distribution of the NLCD classes; and τ represents the nitrogen source loadings contributing to each NLCD class, simultaneously. The NLCD classes, δ, dictate the allocation of on-ground nitrogen sources. Apparently, the

nitrogen source determines whether the nitrogen is in a form that can be volatilized like organic nitrogen or ammonia; and if so, what are the volatilization rates associated with these nitrogen forms. For example, nitrogen from manure is allotted to the dairy farm cover class and is mainly in the organic form and, therefore, part of it will volatilize. The nitrogen loading, τ, is comprised of three nitrogen constituents; namely organic-nitrogen, ammonia, and nitrate which in effect have different volatilization rates. In addition, nitrogen sources like legumes, septic systems, and dairy lagoons are not subject to runoff losses.

3.2. Soil nitrogen dynamics

The amount of nitrate found at any point in ground water is the product of various physical, chemical, and biological processes that are taking place in the soil zone and ground water (Johnsson et al., 2002). The major soil transformation processes that greatly affect nitrate leaching are mineralization-immobilization, nitrification, denitrification, and plant uptake (Addiscott et al., 1991). In addition, the soil organic matter and crop residues influence the soil nitrogen content. Thus, nitrate available for leaching is a function of soil kinetics. Nitrate available for leaching can be expressed as in the following relationship:

$$O = f(\Omega, \upsilon, \Delta, \mu, \Phi, \varepsilon, \tilde{N}) \tag{2}$$

where O is nitrate available for leaching; Ω is the change in the nitrate mass in the soil due to mineralization-immobilization; υ is the change in the nitrate mass in the soil due to nitrification; Δ is the change in the nitrate

mass in the soil due to denitrification; μ is the change in the nitrate mass in the soil due to plant uptake; ε is the soil organic matter and crop residues; and $\tilde{N}$ is the soil residues of nitrogen constituents.

It is worthwhile to mention that the nitrogen dynamics are highly dependent on parameters such as pH, temperature, soil water content, soil biological characteristics, soil carbon content, crop residues, and cation exchange capacity. Shaffer et al. (1991) showed that the mass of nitrate leaching depends mainly on nitrate available for leaching and ground water recharge. Nitrate leaching, $\bar{O}$, is computed using the exponential relationship (Shaffer et al., 1991)

$$\bar{O} = O\left[1 - \exp\left(\frac{-\alpha \times \Re}{\omega}\right)\right] \tag{3}$$

where α is a dimensionless leaching coefficient; $\Re$ is the water available for leaching and can be coarsely approximated as ground water recharge; and ω is the volume of water in the top soil. As such, $\bar{O}$ can be approximated, after substituting Eq. (2) in (3) as in the following relationship:

$$\bar{O} = f(\Omega, v, \Delta, \mu, \Re, \alpha, \omega, \varepsilon, \tilde{N}, \delta, \tau) \tag{4}$$

3.3. Fate and transport in ground water

Many processes, including advection, dispersion, and decay can control the fate and transport of nitrate in ground water. Denitrification is the dominant chemical reaction that affects nitrate concentration in the ground water under anaerobic conditions (Frind et al., 1990; Postma et al., 1991; Korom, 1992; Tesoriero et al., 2000; Shamrukh et al., 2001). Denitrification can be expressed using first-order kinetics with a first-order decay coefficient, λ (Frind et al., 1990; Shamrukh et al., 2001). Nitrate is rarely sorbed by minerals because it is negatively charged. As a result, it is highly mobile in mineral soils (Shamrukh et al., 2001). Therefore, the long-term steady state nitrate concentration distribution in ground water can be expressed as in the following relationship:

$$C = f(\Gamma, D, v, q_s, C_s, \lambda) \tag{5}$$

where Γ is the vector of spatial coordinates; D is the dispersion coefficient vector; v is the pore water velocity; q_s is the steady-state fluid flux due to boundary conditions and sources and sinks; and C_s is the corresponding nitrate concentration can be expressed as in the following relationship:

$$C_s = f(\bar{O}, \varphi) \tag{6}$$

where φ is the vector of all nitrate concentrations of sources other than nitrate leaching from the soil zone.

Substituting Eqs. (4) and (5) in Eq. (6) yields the following relationship:

$$C = f(\Gamma, D, v, q_s, \lambda, \Omega, v, \Delta, \mu, \Re, \alpha, \omega, \varepsilon, \tilde{N}, \varphi, \delta, \tau) \tag{7}$$

Eq. (7) demonstrates the diversity of the soil and ground water properties and other parameters that concurrently influence the nitrate concentration in ground water, spatially and temporarily. Again, Eq. (7) confirms the fundamental difficulty in the accurate modeling of fate and transport of nitrate in ground water especially at regional-scale.

4. Methodology

The development of MNN requires the precise identification of the input and output vectors. Since the objective is to simulate the effect of current and future land use practices on nitrate occurrences in the ground water, the distribution of the long-term average nitrate concentration will be the output from the MNN. In order to categorize MNN input parameters, Eq. (7) was considered. Except for δ, τ, and $\Re$, the remaining parameters cannot be obtained without conducting a rigorous field data collection program. In some studies, literature-based values may be used and these values need to be improved through model calibration. Due to the difficulty of obtaining some of the properties listed in Eq. (7), the long-term steady state nitrate concentration C was reduced to the following simple formulation:

$$C = f(\Gamma, \delta, \tau, \Re) \tag{8}$$

In this work, MNN is used to predict the two-dimensional ground water concentration distribution of nitrate due to on-ground nitrogen loading, NLCD classes, and ground water recharge. Although Eq. (8) does not include all the applicable soil and ground water properties and parameters, many studies have attempted to predict the nitrate contamination of ground water due to neighboring land uses and nitrogen loadings (e.g. Tesoriero and Voss, 1997; Nolan et al., 2002; Mitchell et al., 2003). It should be noted that the ground water recharge is a function of many factors including the soil type, antecedent soil water content, precipitation, and land cover. Mapping the relationship between the nitrate concentration and ground water recharge provides an initial understanding of these soil factors.

To develop the input–output response patterns based on Eq. (8), we need to specify the spatial locations of nitrate receptors, Γ, and the corresponding nitrate concentrations, C; the spatial distributions of the NLCD classes, δ; on-ground nitrogen loading, τ; and ground water recharge, $\Re$.

5. Description of Sumas-Blaine aquifer

The Sumas-Blaine aquifer (see Fig. 3) is the principal surficial unconfined aquifer in the Nooksack Watershed in Whatcom County located in the northwest corner of Washington State. The extended Sumas-Blaine aquifer is used for domestic, agricultural, and industrial purposes and occupies an area of about 370 square miles (Tooley and Erickson, 1996). Most of the soils in the area are categorized as well-drained. The water table is shallow, typically less than 10 feet, but exceptions occur near the City of Sumas where the depth exceeds 50 feet and depths exceed 25 feet near the eastern part of the aquifer (Tooley and Erickson, 1996). Precipitation ranges from over 60 inches per year in the northern uplands to about 40 inches per year in the lowlands. Recharge to the aquifer is largely due to the infiltration of precipitation and irrigation. Evapotranspiration is highest during the June-to-August period (Cox and Kahle, 1999). The study area includes parts of Canada because of substantial poultry manure applications in berry plantations located in the Canadian side. Since the ground water flow is from north to south towards the Nooksack River, the nitrogen-rich manure application in the Canadian side has a major influence on ground water quality in the south (Stasney, 2000; Nanus, 2000; Mitchell et al., 2003). There are 39 drainages in the study area.

Due to the intensive agricultural activities in the study area, ground water quality in the aquifer has been continuously degrading and nitrate concentration is increasing (Erickson, 1998; Kaluarachchi et al., 2002; Almasri and Kaluarachchi, 2004). This degradation in water quality and the population growth have led to an increased demand of potable water while ensuring acceptable water quality (Nanus, 2000). Whatcom County is second in Washington State and eighth for the entire United States in dairy production (Stasney, 2000). The persistent elevated nitrate concentrations in ground water are found close to the locations of dairies (Morgan, 1999). Whatcom County produces more than 59% of the nation's red raspberries, ranking fifth in world raspberry production (Stasney, 2000; Gelinas, 2000). Since raspberries have a low nutrient requirement, high nitrogen addition to raspberries can result in substantial nitrate accumulations in the soil. The aquifer readily interacts with surface water and serves as an important source of summer streamflows for different rivers and creeks in the study area (Tooley and Erickson, 1996). The study area supports a variety of fish species important to the cultural heritage, economy, and the ecology of the area (Blake and Peterson, 2001). Since the role of nitrate in *eutrophication* is well recognized (Wolfe and Patz, 2002), nitrate contamination of surface water of the study area is a concern as it greatly affects the fish habitat. In general, the transport of nitrate to surface water occurs mainly via discharge of ground water during baseflow conditions (Hubbard and Sheridan, 1994; Devlin et al., 2000; Schilling and Wolter,
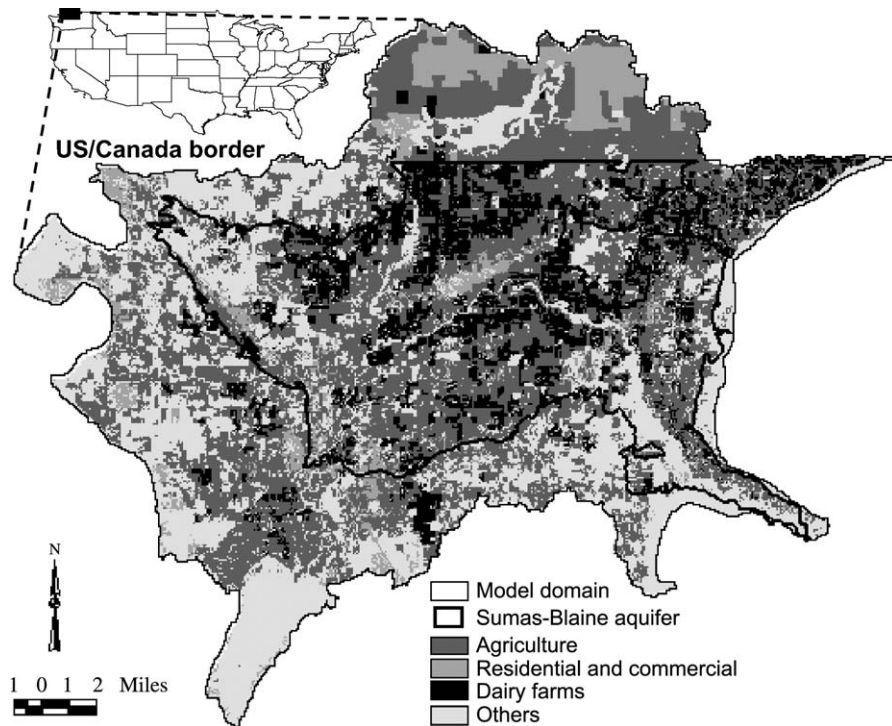

Fig. 3. A schematic of the Sumas-Blaine aquifer describing the different land use classes. The land use classes are summarized to four classes for ease of presentation.

2001; Bachman et al., 2002). Therefore, the prevention of ground water contamination from nitrate also protects surface water quality.

Kaluarachchi et al. (2002) analyzed nitrate occurrences in the study area for the period from 1990 to 2000. They found that the nitrate concentrations in the ground water are increasing. In addition, the findings show an increase in the number of wells with nitrate concentration exceeding the MCL. The nitrate concentration distributions in the ground water with land use classes were estimated and are shown in Fig. 4. The results indicate that areas with dairy farming have the highest median nitrate concentrations. In addition, Fig. 4 shows different nitrate trends within the agricultural land use classes. For the forest areas denoted by the code 42, the conspicuous outliers in Fig. 4 are because these areas are fragmented and scattered around and between agricultural areas and dairy farms. Apparently, the outliers that signify high nitrate concentrations are due to the transport of nitrate from the neighboring agricultural areas.

6. Data synthesis

6.1. Estimation of on-ground nitrogen loading

A major step in developing the input—output response patterns is the estimation of the on-ground
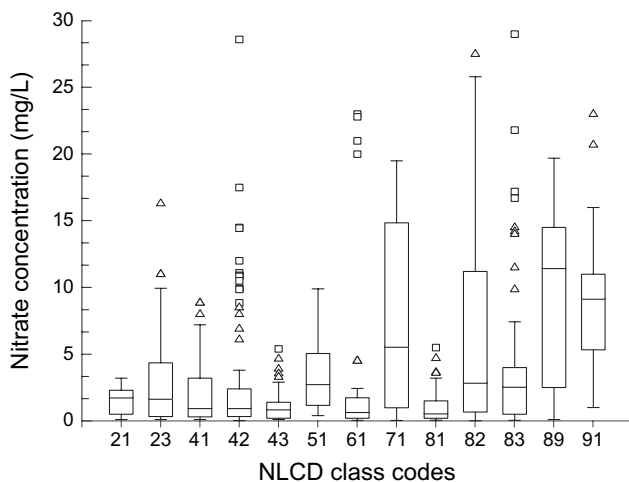

Fig. 4. Box plots of nitrate concentration from 1990 to 1998 for the main NLCD classes present in the study area. Box upper and lower bounds represent the 25th and 75th percentiles or the interquartile (IQR). The line in the middle of the box is the 50th percentile (the median). The upper and lower adjacent values represent the IQR plus and minus 1.5 times the IQR, respectively. The triangles and squares represent concentration outliers below and beyond three IQRs from the 25th and 75th, respectively. NLCD codes are: 21, low intensity residential; 23, commercial/industrial/transport; 41, 42, and 43, forest; 51, shrubland; 61, orchards; 71, grasslands; 81, pasture; 82, row crops; 83, grains; 89, dairy farms; 91, wetlands.

nitrogen loadings. The NLCD grid (Fig. 3) is utilized to designate the spatial distribution of on-ground nitrogen loadings (Nolan et al., 2002; Almasri and Kaluarachchi, 2004) that enabled the use of simultaneous sources for a given land use. The computations were performed at drainage-scale resolution across the 39 drainages. To facilitate the computations of on-ground nitrogen loadings and to make possible the development of the input—output response patterns that are necessary for the construction of MNN, the study area was divided into a uniform finite difference grid of 100×100 m^2 cell size.

The nitrogen sources in the study area include dairy and poultry manure, dairy lagoons, applications of fertilizers on agricultural fields and lawns, atmospheric deposition, irrigation with nitrogen-contaminated ground water, septic tanks, and nitrogen fixed by legumes (Almasri and Kaluarachchi, 2004, in press). Septic tanks and dairy farm lagoons were treated as point sources and their nitrogen loadings were estimated independently from the NLCD grid using GIS point shapefiles. Table 1 shows the different nitrogen sources that concurrently contribute to each NLCD class (Almasri and Kaluarachchi, 2004). Table 1 was utilized in the allocations and computations of the on-ground nitrogen loadings for the study area.

Manure application to agricultural fields has been identified as a significant source of nitrate in the study area (Cox and Kahle, 1999; Stasney, 2000; Nanus, 2000) where there are approximately 53 000 milking cows; 7500 dry cows; 12 800 heifers; and 7600 calves (Almasri and Kaluarachchi, 2004). The ranges of annual production of nitrogen per head from milking cows, dry cows, heifers, and calves were obtained from Meisinger and Randall (1991). Using the animal distribution for the dairy class category and the individual nitrogen production rates, the total nitrogen from dairy manure was computed. Estimates of the poultry manure application in the Canadian portion of the study area were obtained from Brisbin (1995). Typically, dairy lagoons tend to leak if not properly sealed. Cox and Kahle (1999) reported an annual average of 1880 lbs of nitrogen loading per lagoon for the study area.

The total nitrogen applied from agricultural fertilizers per crop per drainage was obtained by multiplying the fertilizer application rate with the actual fertilized area for the given crop. This amount of nitrogen was then distributed uniformly over the agricultural NLCD classes; for instance, *orchards, row crops, grasslands/herbaceous, fallow, pasture/hay*, and *small grains* (Almasri and Kaluarachchi, 2004). Nitrogen loading from lawn fertilizers was calculated by multiplying the application rate (Morton et al., 1988) with the areas of the *residential* and *urban/recreational/grasses* NLCD classes. The average nitrogen concentration in rainfall in western Washington is 0.26 mg l^{-1} (Cox and Kahle,

Table 1
The contribution of different nitrogen sources for each land cover class

NLCD class	Dairy manure	Wet deposition	Dry deposition (regional)	Dry deposition (dairy)	Irrigation	Fertilizer	Lawns	Legumes
Open water	×	×	×	×	×	×	×	×
Perennial ice/snow	×	×	×	×	×	×	×	×
Low intensity residential	×	✓	✓	×	×	×	✓	×
High intensity residential	×	✓	✓	×	×	×	✓	×
Commercial/industrial/transportation	×	×	×	×	×	×	×	×
Bare rock/sand/clay	×	✓	✓	×	×	×	×	×
Quarries/strip mines/gravel pits	×	✓	✓	×	×	×	×	×
Transitional	×	✓	✓	×	✓	✓	×	×
Deciduous forest	×	✓	✓	×	×	×	×	×
Evergreen forest	×	✓	✓	×	×	×	×	×
Mixed forest	×	✓	✓	×	×	×	×	×
Shrubland	×	✓	✓	×	×	×	×	×
Orchards/vineyards/other	×	✓	✓	×	✓	✓	×	×
Grasslands/herbaceous	×	✓	✓	×	✓	✓	×	×
Pasture/hay	×	✓	✓	×	✓	✓	×	✓
Row crops	×	✓	✓	×	✓	✓	×	×
Small grains	×	✓	✓	×	✓	✓	×	×
Fallow	×	✓	✓	×	✓	✓	×	×
Urban/recreational/grasses	×	✓	✓	×	×	×	✓	×
Dairy farms	✓	✓	✓	✓	✓	×	×	×
Woody wetlands	×	✓	✓	×	×	×	×	×
Emergent herbaceous wetlands	×	✓	✓	×	×	×	×	×

1999). The nitrogen loading from precipitation was calculated by multiplying this concentration with the yearly precipitation volume for each drainage. The regional annual dry nitrogen deposition for western Washington is about 1 lb acre^{-1}. The annual rate of dry redeposition of nitrogen volatilized from manure is 15 lbs acre^{-1} (Cox and Kahle, 1999). The total nitrogen loading from dry depositions equals the deposition rate multiplied by the corresponding areas of the NLCD classes.

Nitrogen addition to the subsurface from irrigation water was calculated by multiplying the average concentrations of nitrate, ammonium, and organic-N for each drainage with drainage irrigation volumes assuming that 60% of agricultural use of ground water was for irrigation. The computed nitrogen loadings were then assigned to the agricultural NLCD classes. The nitrogen loading from septic tanks is 10 lbs per capita per year (Cox and Kahle, 1999). The annual contribution of 5 lbs acre^{-1} of NO_3-N from legumes for the study area was considered based on the work of Cox and Kahle (1999), and this nitrogen loading was assigned to the *pasture/hay* class. The detailed calculations related to on-ground nitrogen loadings are given in Kaluarachchi and Almasri (2003) and Almasri and Kaluarachchi (2004).

6.2. Input−output response patterns

After estimating the distribution of on-ground nitrogen loadings for the study area, the distribution of ground water recharge has to be obtained. The annual ground water recharge distribution was described by a GIS polygon shapefile for the study area using data from Vaccaro et al. (1998). The data are classified into seven intervals ranging from 0 to greater than 50 inches per year. Vaccaro et al. (1998) estimated recharge values for Puget Sound aquifer system, which encompasses the study area, using a liner regression between precipitation and ground water recharge. Data for estimating the regression equations were from precipitation and recharge estimates of 26 small basins or areas within the Puget Sound aquifer. The recharge estimates were obtained from previous studies in the area that used a deep percolation model and the Hydrogeological Simulation Program-FORTRAN (HSPF).

The nitrate concentration data used in this study were obtained mainly from four agencies, U.S. Geological Survey, Whatcom County Department of Health, Washington State Department of Health, and Washington State Department of Ecology (Kaluarachchi et al., 2002). A GIS point shapefile of the spatial locations of the monitoring wells and the corresponding nitrate concentrations were developed from 1990 to 1998 and used in the formulation of the input−output response patterns. The nitrate concentration data are observations sampled from the monitoring wells in the study area by the abovementioned agencies.

The next step is to spatially join the input vectors to the output vectors according to Eq. (8). The basic premise followed in preparing the input−output response patterns was to designate the optimal radius of a specific circular-buffered zone centered by the nitrate receptor. In doing so, the input parameters, δ, τ, and $\Re$ at the

upgradient areas of each receptor are optimally correlated with the nitrate occurrences in the ground water. For each well, the upgradient direction of ground water flow was obtained from the potentiometric head distribution of the study area developed by Kemblowski and Asefa (2003). By considering the upgradient areas, the vector of the input parameters in Eq. (8) for the contributing neighboring areas, $[\beta_{x,y}^{\eta}]$, to the monitoring well at (x,y) within a specified zone of radius, η, is considered. In other words, $[\beta_{x,y}^{\eta}]$ for a monitoring well located at (x,y) is the vector of the total on-ground nitrogen loading, fractions of NLCD classes, and the total ground water recharge as estimated based on a specific optimal radius, η, assigned for each input parameter. Fig. 5 presents a flow chart that depicts the abovementioned approach for the development of the input–output response patterns.

In order to develop the optimal radius, η, for each input parameter, the correlation coefficients for the parameters of Eq. (8) and the corresponding nitrate concentrations were calculated for 50 different radii ranging from 0.1 to 5 km as shown in Fig. 6. The results show that the nitrate concentration in ground water is highly correlated with the on-ground nitrogen loading at an optimal radius of 2.2 km. In addition, the results indicate that no conclusive relationships exist between other parameters and the nitrate concentration distri-

bution, suggesting the necessity of combining more than one parameter at once. The results are in agreement with the conclusions made by Nolan et al. (2002) who showed that in poorly drained soils, ground water contamination was low even for moderate nitrogen loading. Nevertheless, the correlation coefficient is a linear association between a single input and an output parameter and the introduction of the spatial location of the nitrate receptors in MNN training will increase the uniqueness of the input–output response patterns. The intention of using the correlation coefficient at this stage was merely to obtain a preliminary estimate for the optimal radii so that MNN patterns can be developed accordingly.

7. Modular neural network development

To develop a reliable MNN that can be used with full confidence, internal parameters of the MNN should be optimally designated. The main step in MNN development is the designation of the training and testing sets. A data set, Đ, of input–output response patterns based on Eq. (8) and the approach depicted in Fig. 5 was developed. A total of 665 patterns were allotted into Đ. Thereafter, Đ was divided into training and testing sets, $Đ_R$ and $Đ_T$, respectively. In allocating $Đ_R$ and $Đ_T$, a simple procedure based on a user-defined expected
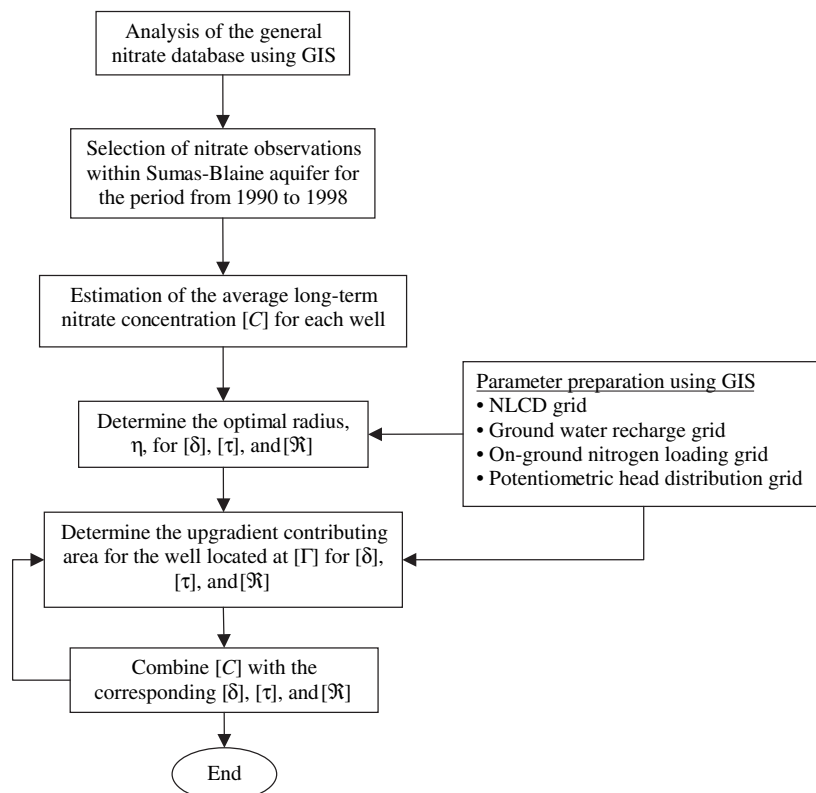

Fig. 5. A flow chart depicts the steps for the development of the input–output response patterns.
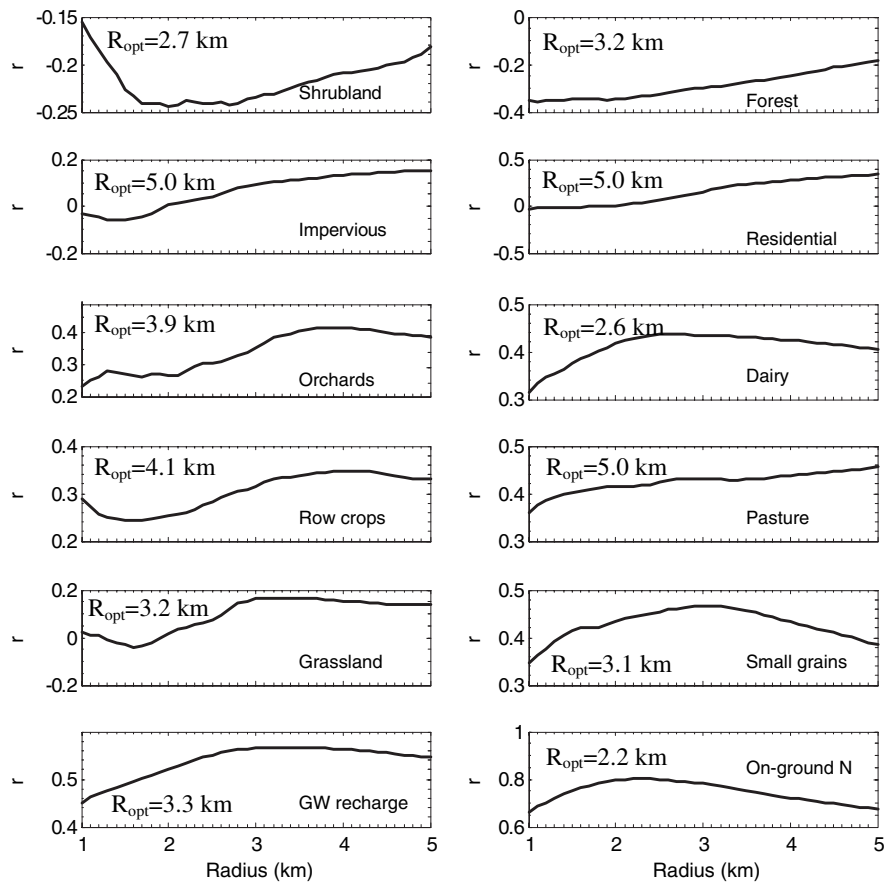
Fig. 6. Correlation coefficients (*r*) between the average long-term nitrate concentration from 1990 to 1998 and a selected set of major parameters presented for different radii of the upgradient areas surrounding each sampling well.

fraction, ξ, was followed (Morshed and Kaluarachchi, 1998b). A number, $\varnothing$, is randomly generated within the interval [0, 1] for each pattern. If $\varnothing \leq \xi$, then the pattern is assigned to Ð$_R$ otherwise to Ð$_T$. This method is expected to allocate ξ and $(1-\xi)$ fractions of Ð to Ð$_R$ and Ð$_T$, respectively. As there are no guidelines for allocating Ð$_R$ and Ð$_T$, $\xi \in [0.1, 0.90]$ was used.

MNN was developed using the Neural Works Professional II/Plus$^{\circledR}$ (NeuralWare, 2000). The internal parameters of MNN include learning count; L, learning rate for the output and hidden layer, momentum, seed, activation function, epoch, scaling intervals, and learning rule. In addition, MNN functionality depends on the number of hidden nodes; J. Scaling intervals follow the type of the activation function used. Morshed and Kaluarachchi (1998b) showed that the hyperbolic function, $\tanh(\cdot)$, improved ANN performance when compared to the sigmoidal function, sgm$(\cdot)$. Therefore, $\tanh(\cdot)$ was used in MNN development and the input and the output parameters were linearly scaled in the intervals $[-1,+1]$ and $[-0.8,+0.8]$, respectively. The scaling was performed using the minimum and maximum values for both the input and the output of Ð$_R$ and Ð$_T$. The learning rule used was the extended

delta-bar-delta. MNN development was performed using the default values in the package (see Table 2) except for L.

MNN performance is assessed qualitatively using the scatterplots of the predicted versus observed nitrate concentrations and quantitatively via using the

Table 2
Summary of MNN parameters and corresponding values

Parameter	Value
No. of input nodes	13
No. of output nodes	1
No. of hidden nodes	14
No. of hidden layers	1
Learning rate	
Hidden layer	0.30
Output layer	0.15
Momentum	0.40
Random seed	257
Epoch	16
Activation function	$\tanh(\cdot)$
Scaling interval	
Input vector	$[-1,+1]$
Output vector	$[-0.8,+0.8]$
Learning count	194 850
Learning rule	Extended delta-bar-delta

correlation coefficient, root mean squared error, and the mean relative error as defined in the following equations:

$$r = \frac{\sum_1^n (C_O - \bar{C}_O)(C_P - \bar{C}_P)}{\sum_1^n (C_O - \bar{C}_O)^2 \sum_1^n (C_P - \bar{C}_P)^2} \qquad (9)$$

$$\text{RMSE} = \sqrt{\frac{\sum_1^n (C_O - C_P)^2}{n}} \qquad (10)$$

$$\text{MRE} = \frac{\text{RMSE}}{\gamma} \qquad (11)$$

where r is the correlation coefficient (L^0); RMSE is the root mean squared error (mg l^{-1}); MRE is the mean relative error (L^0); n is the number of the testing patterns; C_O and C_P are the observed and predicted nitrate concentrations, respectively; $\bar{C}_P$ and $\bar{C}_O$ are the mean values of C_P and C_O, respectively; and γ is the range of the observed concentrations and equals the difference between the maximum and minimum observed nitrate concentrations.

The proposed MNN predicts the $[C]$ given $[I]$, $[\tau]$, $[\delta]$, and $[\Re]$ where $[I]$ is the vector of the spatial coordinates; $[\delta]$ represents the vector of the *agricultural, residential, impervious*, and *forest* NLCD classes; $[\tau]$ represents the on-ground nitrogen loading vector; and $[\Re]$ is the ground water recharge vector. Agricultural NLCD classes include *orchards, row crops, fallow, pasture, grasslands/herbaceous*, and *small grains* (Almasri and Kaluarachchi, 2004a). There are 13 inputs, $I = 13$, equivalent to two inputs for well spatial coordinates, one input for $[\tau]$, one input for $[\Re]$, nine inputs for $[\delta]$, and one output, $K = 1$, corresponding to $[C]$.

To illustrate the approach followed in the utilization of the optimal radius, η, of each input parameter in developing the input−output response patterns, Fig. 7 was prepared for two selected nitrate wells. Three input parameters pertaining to three NLCD classes, namely dairy farms, pasture, and residential area, were considered. The optimal radii for these three NLCD classes are 2.6, 5.0, and 5.0 km, respectively as can be concluded from Fig. 6. In order to designate the contributing areas for the two wells, the upgradient area for each well was delineated up to the optimal radius of each input parameter of interest. Afterward, the fraction of each NLCD class is computed considering the area occupied by each class and the corresponding total area within the upgradient area of that well. For instance, for well (a) in Fig. 7, dairy farms occupy an area of 2.16 km^2 and the total area of the upgradient zone is 6.01 km^2. Therefore, the input to MNN considering the dairy farms for well

(a) is the fraction of dairy farms from the upgradient zone area and equals 0.36. The same concept is considered when developing the inputs that pertain to the different NLCD classes. It is worth mentioning that across all the nitrate wells, the upgradient areas differ in shape, the relative location to the well, and the total area as can be concluded from Fig. 7 for wells (a) and (b). Fig. 8 is similar to Fig. 7 except that one nitrate well is considered but for two different input parameters pertaining to on-ground nitrogen loading, $[\tau]$, and ground water recharge, $[\Re]$. For cases (a) and (b) in Fig. 8, the values of the input parameters $[\tau]$ and $[\Re]$ are taken respectively as the total on-ground nitrogen loading and the volume of ground water recharge contained within the upgradient area of the well. For instance, $[\tau]$ is taken as the summation of all on-ground nitrogen loading values assigned to the finite-difference cells contained within the upgradient area of the well.

In reference to Eq. (8) and Fig. 1, the input vector $[X]$ is comprised of the following input parameters: X_1 and X_2 for the spatial coordinates, X_3 for the on-ground nitrogen loading, X_4 for the ground water recharge volume, and X_5 to X_{13} for the abovementioned nine NLCD classes. The number of the hidden nodes, J, was taken as the summation of the numbers of the input and output nodes, I and K, respectively. As such, a hidden layer of 14 neurons, $J = 14$, was considered and a 13-14-1 network was developed. A total of 13 expert modules were considered, and a 13-14-13 gating network was used in the MNN. Depending on the input features, 13 gating networks were used to consider low, medium, and high on-ground nitrogen loadings; agricultural, residential/impervious, and forest classes; and the ground water recharge values.

Optimal MNN performance was found at $L = 194\,850$ and $\xi = 0.65$. When $\xi \in [0.1, 0.6]$, MNN performance was inferior due to the insufficiency of training patterns to map the search space and to provide a good understanding of the governing relationships. Although MNN was well trained and its performance sufficiently improved for $\xi \in [0.60, 0.95]$, MNN did not test well for some extreme input−output response patterns. Fig. 9 shows the scatterplots of MNN predictions with $r = 0.87$; RMSE = 2.18 mg l^{-1}; and MRE = 6.57%. MNN performance shows some inferior predictions at different concentrations. The outliers in Fig. 9 signify the possible impacts of soil and ground water properties and processes on nitrate mass and distribution. Such processes and properties include, but are not limited to, chemical reactions in soil and ground water and transport processes such as advection and dispersion.

The sensitivity of MNN performance to the number of hidden nodes, the type of activation function, and the learning rule was investigated. Two values of $J \in \{4, 28\}$ were considered. $J = 4$ corresponds to the geometric
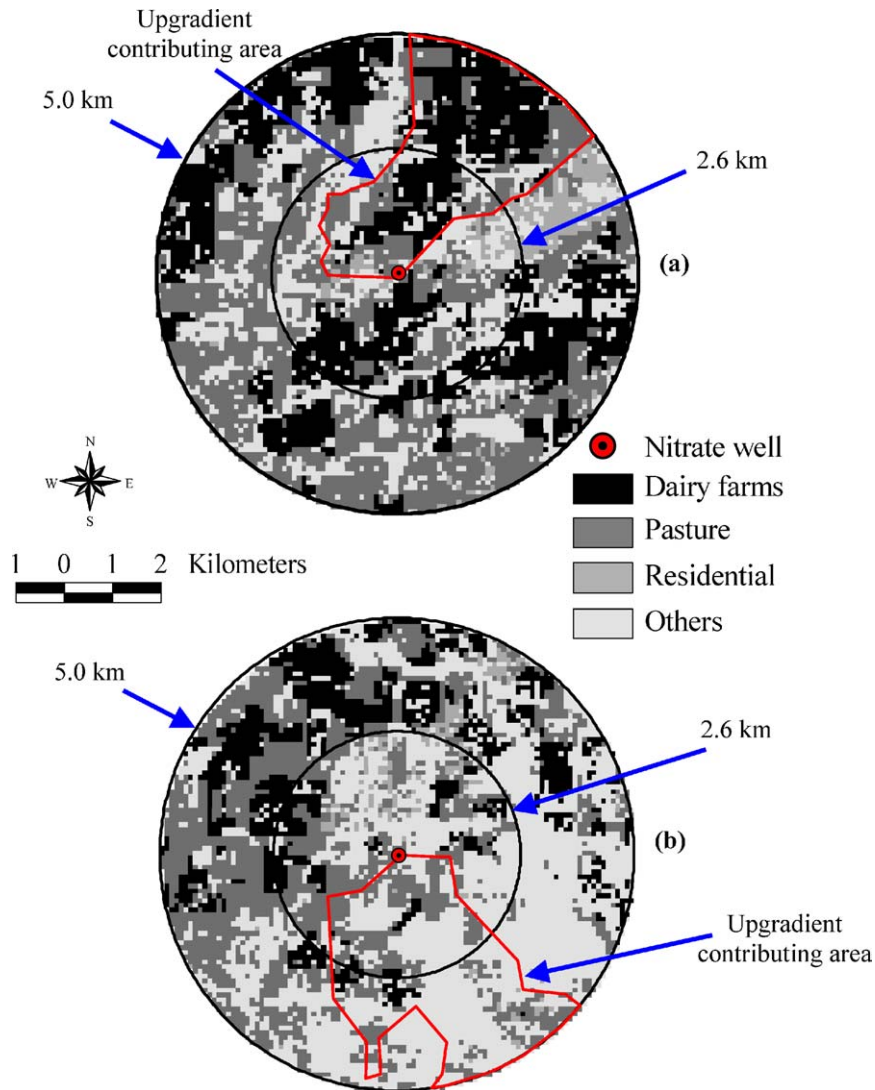
Fig. 7. A schematic for the upgradient contributing areas for two different wells for different input parameters pertaining to the NLCD classes of dairy farms, pasture, and residential. The land use classes are summarized to four classes for ease of presentation.

mean of the input and output nodes as recommended by Pachepsky et al. (1996). For $J = 4$, MNN performance was inferior with $r = 0.76$; RMSE = 2.75 mg l^{-1}; and MRE = 7.91%0. For $J = 28$, MNN performance was found to be sufficiently insensitive. Apparently, using the summation of MNN input and output nodes as the number of the hidden nodes yielded the optimal MNN performance in addition to minimizing the training time. To evaluate MNN sensitivity to the type of the activation function, the sgm(·) was used instead of the tan$h$(·). MNN performance was inferior with $r = 0.71$; RMSE = 2.98 mg l^{-1}; and MRE = 8.9%. The delta-rule learning rule was used instead of the extended delta-bar-delta rule, and the results were $r = 0.81$; RMSE = 2.42 mg l^{-1}; and MRE = 6.67%. The results of the MNN parameter sensitivity analysis are summa-rized in Table 3. In order to perform a comparative analysis between ANN and MNN, a single 13-14-1 ANN was used; and the results are summarized in Table 3. Apparently, MNN performed well in all the predictions compared to ANN. For instance, upon using tan$h$(·), 14 hidden nodes, and the EDBD as a learning rule, MNN performed extremely better than ANN. For instance, the correlation coefficient did increase by 16% while the RMSE and MRE decreased by more than 70%. As such, MNN is preferable over ANN in this current application for the prediction of nitrate concentration distribution in ground water. MNN is appealing since it automatically allocates the input vector into the expert modules based on the different relationships embedded within the input–output response patterns.
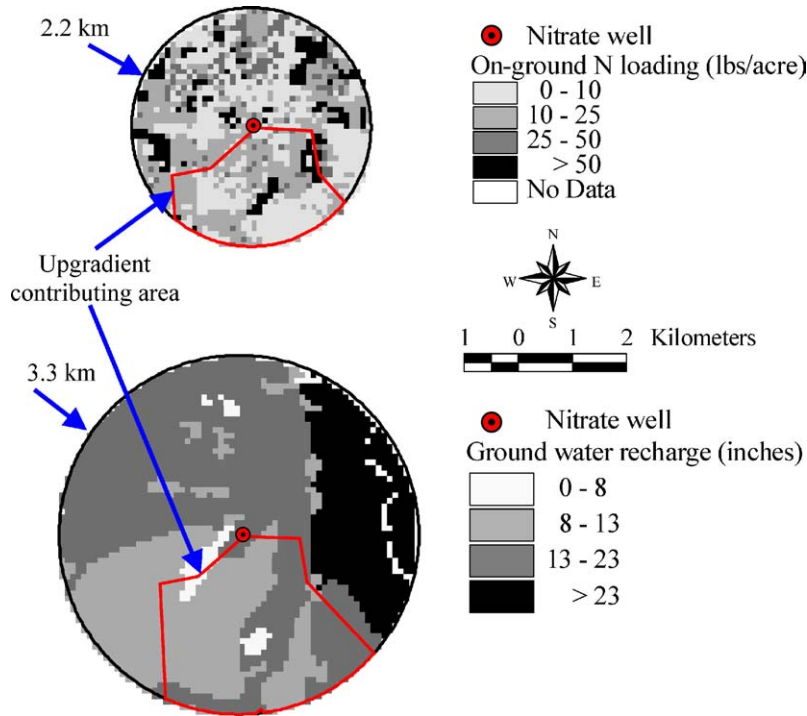
Fig. 8. A schematic for the upgradient contributing areas for a nitrate well for two different input parameters pertaining to (a) on-ground nitrogen loading, and (b) ground water recharge. Parameter categories are summarized to four classes for ease of presentation.

8. Sensitivity analysis

8.1. Sensitivity to the well zone radius

The proposed MNN design, the procedure followed in developing the input–output response patterns, and the results listed earlier were obtained using the concept furnished in Figs. 5, 7, and 8 for the different optimal well zone radii shown in Fig. 6. Although this plot,
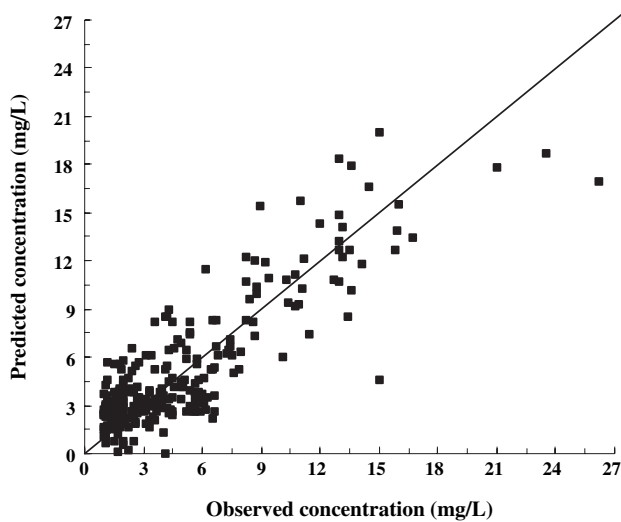

Fig. 9. Scatterplot between the observed versus MNN predicted nitrate concentrations.

Fig. 6, shows the existence of different optimal radii, yet, the calculation of the optimal radius for each input parameter is a time-consuming process that may be viewed as impractical in many instances. As such, the sensitivity of MNN performance to a uniform well zone radius across all input parameters is interesting to investigate. In this analysis, MNN predicted $[C]$ for $[\Gamma]$, $[\delta]$, $[\tau]$ and $[\Re]$ using a uniform well radius for the upgradient contributing areas and the results are shown in Fig. 10. It can be concluded that the best performance of MNN was obtained at a uniform radius of 1.9 km with $r = 0.74$ and RMSE $= 3$ mg 1^{-1}. However, the approach that utilized the non-uniform optimal well zone radii to develop the input parameters had produced better MNN performance over using a uniform radius value across all input parameters.

8.2. Sensitivity to the contributing area of the receptor

In this work so far, the upgradient area within the circular zone of the receptor was considered in developing the input–output response patterns. Although researchers showed definite impacts of agricultural practices and manure applications in the upgradient areas on the downgradient nitrate concentrations (Erickson, 1992; Stasney, 2000; Nanus, 2000; Mitchell et al., 2003), many studies considered the total area within a well zone as a contributing area without

Table 3
Summary of MNN and ANN prediction statistics

Activation function	Hidden nodes	Learning rule[a]	MNN				ANN			
			L	r	RMSE (mg l^{-1})	MRE (%)	L	r	RMSE (mg l^{-1})	MRE (%)
$\tan h(\cdot)$	14	EDBD	194850	0.87	2.2	6.6	195400	0.75	3.8	11.5
$\tan h(\cdot)$	4	EDBD	142500	0.76	2.7	7.9	20400	0.71	2.9	8.5
$\tan h(\cdot)$	28	EDBD	84350	0.84	2.3	6.9	182250	0.75	3.1	8.6
$\text{sgm}(\cdot)$	14	EDBD	195950	0.71	2.9	8.9	8250	0.70	3.0	9.1
$\tan h(\cdot)$	14	DB	139450	0.81	2.4	6.7	4450	0.72	3.2	8.6

[a] EDBD, extended delta-bar-delta rule; DB, delta-bar rule.

distinguishing between the upgradient and downgradient areas (Tesoriero and Voss, 1997; Nolan et al., 2002). MNN performance was assessed again when considering the total area within a given receptor zone that corresponds to the optimal radius. For instance, when considering the on-ground nitrogen loading, the contributing area for the nitrate well in case (a) of Fig. 8 is the entire circular area defined by a radius of 2.2 km. The results for this case produced $r = 0.78$, RMSE $= 2.73$ mg l^{-1}, and MRE $= 7.73\%$ signifying an inferior MNN performance compared to the case using the upgradient area only. In essence, the prediction results indicate that the nitrate concentration at a well is highly correlated with the upgradient area for that specific well rather than the entire area.

8.3. Sensitivity to noisy input data

Sensitivity of MNN to noisy input data was assessed by introducing a noise to the testing patterns. The following multiplicative error function was utilized to introduce the noise (Skaggs and Kabala, 1994):

$$I_{NE} = I_N + \kappa \vartheta I_N \qquad (12)$$

where I_{NE} is the vector of the noisy input parameters; I_N is the vector of the exact input parameters; κ is the

magnitude of the noise; and ϑ is the random deviate. Normally distributed random deviates of mean $= 0$ and variance $= 1$ were generated and added to the input in the testing set. The noise was assumed to follow a uniform distribution. A total of 600 Monte Carlo simulations were utilized in the assessment of MNN performance. Five uniform distributions of noise were considered where $\kappa \in \{[0, 10\%], [0, 20\%], [0, 30\%], [0, 40\%], \text{ and } [0, 50\%]\}$. Such distributions may account for the large uncertainty in the input parameters such as manure loading, fertilizer application rate, land use changes, and inaccuracy in field observations. Fig. 11 shows the percentages of relative change in the correlation coefficient and root mean squared error for the five noise distributions compared to the base case with zero-noise. The results show that with increasing the magnitude of noise, higher prediction errors are expected. It is worthwhile to note that RMSE is more sensitive to the noisy data than the correlation coefficient, signifying the necessity to use different statistical measures to assess the MNN performance.

9. Application of MNN in water quality management

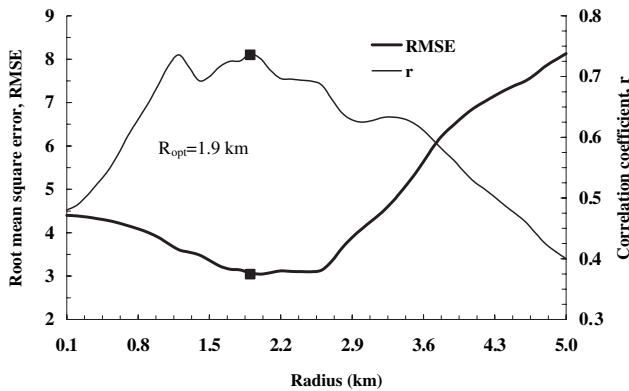The need to introduce management options to protect the ground water quality of the Sumas-Blaine

Fig. 10. MNN performance described from correlation coefficient (r), and the RMSE for different uniform well zone radii $\in [0.1, 5]$ km across all the input parameters. The solid squares represent best MNN performance.
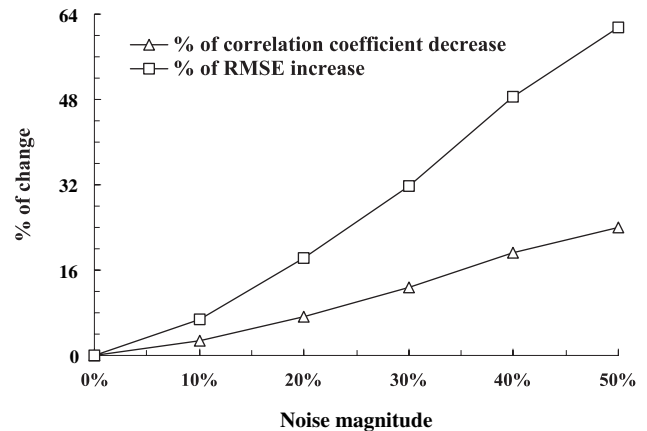

Fig. 11. Percentage of change in the correlation coefficient (r), and the root mean square error for different noise magnitudes introduced to the input vectors in the testing patterns.

aquifer is of critical importance to the residents of Whatcom County (Almasri and Kaluarachchi, 2004, in press). In order to assess the practicability and reliability of the MNN-based approach, the impacts of proposed protection alternatives on the nitrate contamination were evaluated using the developed MNN model. The assessment was performed by comparing the prediction results of the MNN model with that of the fate and transport model of nitrate developed for the area. The integrated conceptual model, shown in Fig. 2, was used in developing the fate and transport model using MODFLOW (Harbaugh and McDonald, 1996) for the steady-state ground water flow model and MT3D (Zheng and Wang, 1999) for nitrate fate and transport. Interested readers are referred to Kemblowski and Asefa (2003) and Kaluarachchi and Almasri (2003) for details on the model development.

9.1. Scenario 1: simulation of current land use practices

MNN was utilized to predict the nitrate distribution in the Sumas-Blaine aquifer under existing conditions. To assess the probable anthropogenic effects on ground water quality, nitrate concentrations across the Sumas-Blaine aquifer were classified into four groups based on the work of Madison and Brunett (1985) and Cox and Kahle (1999). The four concentration ranges are: $0-1$ mg l^{-1} to indicate the most likely background concentration, $1-3$ mg l^{-1} to indicate a possible human influence, $3-10$ mg l^{-1} to indicate pollution due to human influence, and greater than 10 mg l^{-1} to indicate that the MCL was exceeded as a result of extensive human activities.

The study area was divided into a uniform finite difference grid of 100×100 m^2 cell size for the fate and transport model. The same grid was used with the MNN simulation where MNN predicted the concentration at each cell of 38 695 locations. Fig. 12 shows the comparison between the distribution of nitrate concentration predicted by MNN and that simulated by the fate and transport model. It is seen that MNN overestimated the concentrations in the northernmost area of the aquifer. Nevertheless, the areas predicted to exceed the MCL by the MNN are coinciding to a good extent with those of MT3D predictions. These areas consist of berry plantations with substantial manure applications. Although there is a discrepancy between the MNN and MT3D predictions, it can be said that MNN captured the general trend of [C] in most parts of the aquifer. However, [C] as simulated by MT3D shows higher spatial variability due to model's ability to take into account local effects due to actual processes such as
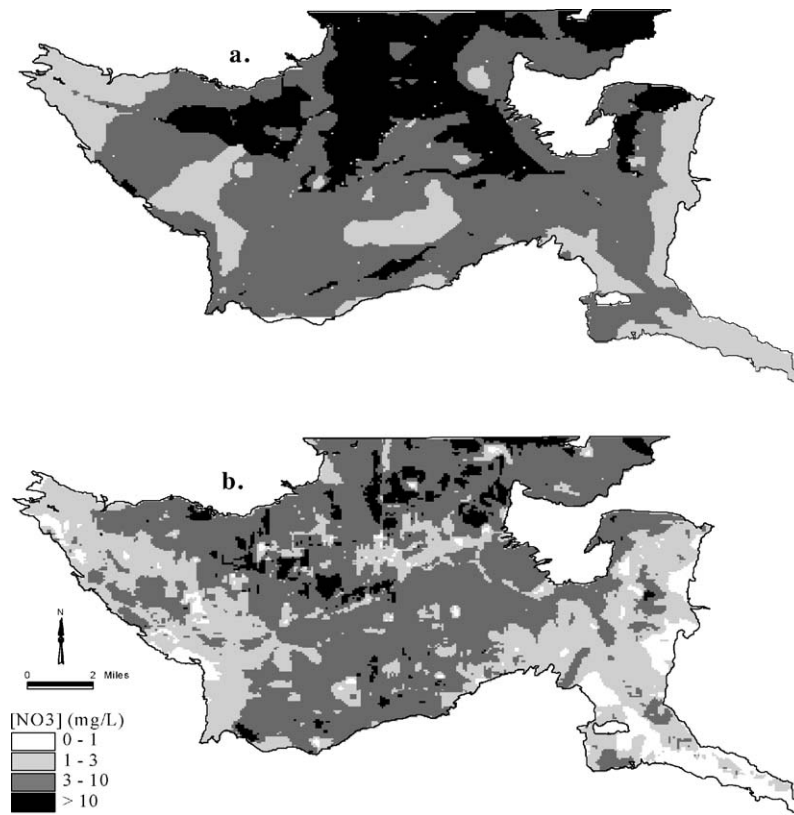

Fig. 12. Distributions of nitrate concentration for the current land use practices for Sumas-Blaine aquifer; (a) MNN prediction and (b) MT3D simulation.

denitrification, dispersion, and advection as well as nitrate leaching to ground water.

It should also be noted that MNN simulations were 180 times faster than MT3D while requiring much less data. Table 4 further shows the accuracy of MNN predictions as compared to those of MT3D using different statistical indices. Details of these statistical indices can be found in Anderson and Woessner (1992) and Legates and McCabe (1999). On the whole, the statistics show less accuracy in the MNN predictions, especially in the correlation-based measures, whereas the overall RMSE is 4.83 mg 1^{-1}. Nevertheless, the mean relative error shows an acceptable value of 16%.

9.2. Scenario 2: simulation of the protection alternatives

In general, management alternatives for protecting ground water quality are practices designed to prevent further pollution or to reduce the existing pollution to acceptable levels (Jansen et al., 1999). In the context of nitrate contamination, management alternatives are intended to reduce the nitrate concentration in ground water below the MCL. This goal is achieved via minimizing nitrate leaching to ground water through the reduction of on-ground nitrogen loadings and/or using nitrification inhibitors. Since MNN does not account for soil parameters, the applicability of the MNN framework was used here with key nitrogen sources; namely, manure and fertilizers.

Table 4
Key statistics for MNN performance in comparison to the MT3D results

Statistics	Scenario 1		Scenario 2	
	MT3D	MNN	MT3D	MNN
Mean (mg 1^{-1})	4.51	6.89	3.61	5.46
Median (mg 1^{-1})	3.88	5.20	3.14	4.20
Standard deviation (mg 1^{-1})	3.11	4.45	2.45	3.25
Range (mg 1^{-1})	29.99	17.90	22.71	16.80
Root mean squared error (mg 1^{-1})		4.83		3.79
Mean absolute error (mg 1^{-1})		3.55		2.82
Mean relative error (%)		16.09		16.67
Correlation coefficient (−)		0.43		0.36
Coefficient of efficiency[a] (−)		−1.41		−1.39
Index of agreement[a] (−)		0.57		0.53
Modified coefficient of efficiency[a] (−)		−0.46		−0.45
Modified index of agreement[a] (−)		0.41		0.37

Scenario 1 is for current land uses and Scenario 2 is for the proposed protection alternative.

[a] The coefficient of efficiency ranges from −∞ to 1 and the index of agreement ranges from 0 to 1. Higher values signify better match.

Manure is one of the main sources of nitrogen in the study area and a reduction in manure loading is expected to lower the nitrate leaching to ground water (Almasri and Kaluarachchi, 2004, in press). Manure loading rate is largely reduced by downsizing the dairy herds, increasing the manure spreading area, considering manure composting and exporting, and/or adopting a herd feeding strategy that minimizes manure nitrogen content while maintaining high milk production levels (Davis et al., 1999). Assigning a percentage reduction of manure loading is difficult without considering the economic implications, which are beyond the scope of this work. On the other hand, simulating a percentage reduction of dairy manure loading helps in understanding and mapping the relationship between [C] and [τ]. Such information is crucial in management decision-making processes. To predict the impact of the protection alternatives, a 50% reduction in manure loading is considered in this simulation.

In addition to manure application reduction, agricultural fertilizers are an important source of nitrogen in the study area, especially in berry plantations (Almasri and Kaluarachchi, 2004, in press); and many studies in the literature recommended the reduction of fertilizer application to minimize nitrate leaching to ground water (Wolf et al., 2003; Tianhong et al., 2003). Puckett et al. (1999) cited many studies that estimated a fertilizer application rate that is 24−38% higher than the crop demand. As such, a 40% reduction in fertilizer application is considered in the simulation. Fig. 13 shows [C] predicted by MNN and MT3D using 50% and 40% reductions in manure and fertilizer loadings, respectively.

By comparing Fig. 13 with Fig. 12, it can be concluded that the MCL exceeding areas predicted by MNN became smaller. [C] as predicted by MNN showed higher MCL exceedance areas compared to those simulated by MT3D. Additionally, [C] was reduced in the northern portion of the aquifer with intensive agricultural activities and MNN predictions in this area are acceptable. The key statistics for this scenario are also summarized in Table 4. The overall RMSE is 3.79 mg 1^{-1} indicating better performance by MNN compared to the previous scenario.

10. Summary and conclusions

In this paper, a MNN-based nitrogen simulation model was proposed and tested for applicability with the aid of GIS tools to predict the nitrate concentration in an agriculture-dominated aquifer. The selection of MNN for this work was motivated by the fact that different processes simultaneously dictate nitrate concentration in ground water and MNN has the ability to understand these complex behaviors. The MNN-based model was applied to the Sumas-Blaine aquifer; a heavily
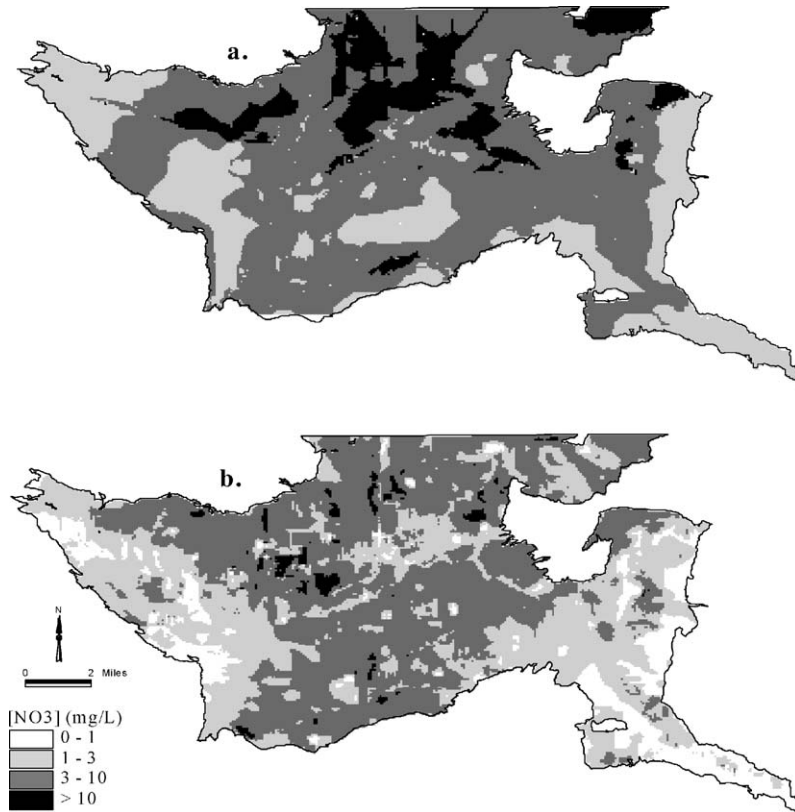
Fig. 13. Distributions of nitrate concentration due to the proposed protection alternative Sumas-Blaine aquifer; (a) MNN prediction and (b) MT3D simulation.

agricultural area in northwest Washington State. The physical and chemical processes that impact nitrate occurrences in ground water were studied to designate the input–output response patterns. In order to achieve the optimal MNN performance, MNN was developed for different combinations of internal parameters. The sensitivity of MNN for different concepts pertaining to the formulation of the input–output response patterns was evaluated. The applicability of MNN was assessed using the data from the Sumas-Blaine aquifer under current and future management options. The results from the MNN model were compared to those obtained from a classical fate and transport model. The following conclusions can be made from the MNN prediction results:

1. The MNN-based approach is simple and utilizes the available data from local agencies and different studies and reports. This approach is economical since process-based physical models require extensive data gathering and monitoring plans.
2. The development of MNN did not require the entire input space of the influential parameters. A sub-vector of this input space was sufficient for MNN to efficiently predict the distribution of nitrate concentration.
3. The approach followed throughout this paper was in the utilization of non-uniform optimal well zone

radii as opposed to a uniform radius produced better MNN performance.
4. MNN performance proved to be superior when considering the upgradient contributing areas of nitrate receptors in formulating the input–output response patterns. The use of both upgradient and downgradient areas gave inferior predictions.
5. The performance of MNN deteriorated with noisy data indicating that MNN is sensitive to errors in the input data.
6. ANN was less accurate than MNN in predicting the spatial distribution of nitrate concentration. It should be kept in mind that this conclusion cannot be generalized since the performance of ANN or MNN relies mainly on the physical phenomenon in hand and the input parameters that were considered in the formulation of the training and testing sets.
7. Long-term simulations performed by MNN to assess the effectiveness of future management alternatives rationally predicted the areas of potentially high nitrate concentrations.
8. The MNN-based approach to predict nitrate contamination should be viewed as a preliminary assessment for regional agriculture-dominated aquifers and a good tool in delineating areas of high priority for further action.

9. Although MNN performed less robustly compared to the simulations of a classical fate and transport model, the results showed that MNN is promising for a complex physical system analyzed here and future work should focus on including more subsurface-specific parameters to improve MNN performance.

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