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Prediction of Groundwater Arsenic Contamination using Geographic Information System and Artificial Neural Network

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Abstract

Ground water arsenic contamination is a well known health and environmental problem in in several countries including Bangladesh. Sources of this heavy metal are known to be geogenic, however, the processes of its release into groundwater are poorly understood phenomena. In quest for the mitigation of the problem, it is necessary to predict probable contamination before it causes any damage to human health. This research has been carried out to investiaget the factors affecting the mobility of the contaminant and develop the prediction model.

Researchers have generally agreed that the elevated concentration of arsenic is affected by several factors such as soil reaction (pH), organic matter content, geology, iron content, etc. However, the variability of concentration within short lateral and vertical intervals, and the inter-relationships of variables among themselves, make the statistical analyses highly non-linear and difficult to converge with a meaningful relationship. Artificial Neural Networks (ANN) comes in handy for such a black box type problem. This research uses Back propagation Neural Networks (BPNN) to train and validate the data derived from Geographic Information System (GIS) spatial distribution grids. The neural network architecture with (6-20-1) pattern was able to predict the arsenic concentration with reasonable accuracy.

Keywords: arsenic; contamination; groundwater; ANN; GIS; pH

1. Introduction

Elevated concentrations of arsenic in groundwater are reported from several countries including United States, Mexico, Argentina, Vietnam, China, India, Nepal and Bangladesh among others (Bhattacharya *et al*., 2004; Smedley and Kinniburgh, 2005; Bhattacharya *et al*., 2010). In Bangladesh, groundwater from shallow aquifers of Pleistocene to recent fluvial origin have been extensively used as the main sources of drinking and irrigation. The aquifers in unconsolidated and estuarine sediments are often contaminated with arsenic and pose a serious health and environmental concern in this country. According to a British Geological Survey report, a large part of Bangladesh groundwater is found to contain arsenic concentration beyond World Health Organization limit (≤10 μg/L) and national recommended standard (≤50 μg/L) (NERC/DPHE/DFID, 2001). It is estimated that around 57 million people drink water with arsenic levels exceeding the limits set by the WHO (Polizzotto *et al*., 2005).

It is generally accepted that the origin of arsenic is natural, and it is being released into the ground water through different processes, which are poorly understood. Two main processes on which the arsenic mobility in the groundwater depend are adsorption and desorption which are influenced by physicochemical conditions such as pH, occurrence of redox (reduction/oxidation) reactions, presence of competing anions, and solid-phase structural changes at the atomic level. Arsenate (As III) and arsenite (As V), the two forms of arsenic commonly found in ground water, are adsorbed to the surfaces of a variety of aquifer rock, including iron oxides, aluminum oxides, and clay minerals.

Groundwater arsenic concentration and distribution in the Bengal basin are not well understood. Variability of concentration within short lateral and vertical distances makes it further difficult to predict the level of arsenic of a given well, even when the concentration of the adjacent wells are known (Van *et al*., 2003). It is, however, essential to establish relationships between arsenic level with simple yet measurable and identifiable indices such as channel proximity, pH level, organic matter content etc. for long term engineering solution of the problem. When the relationship between the input and output is complicated or application of other available methods are cumbersome or expensive, Artificial Neural Networks (ANN) comes in handy as an alternative numerical analysis procedure.

ANNs are networks of highly interconnected neural computing elements that have the ability to respond to input stimuli and to learn to adapt to the environment. Using compiled historical data and the selected significant parameters, ANNs have already proven a powerful tool for various modeling requirements, including geotechnical engineering applications (Neaupane and Achet, 2004). ANN is now a well established tool, and details about it can be found elsewhere (Hayakin, 1998).

Backpropagation neural networks (BPNN) is a widely used algorithm for connectionist learning. Its rapid rise in popularity has been a major factor in the resurgence of neural networks. Developed by Rumelhart *et al*. (1988), backpropagation is a systematic method for training multi-layer neural networks. Despite its limitations, BPNN has dramatically expanded the range of problems to which artificial neural networks can be applied. This research uses Back Propagation Neural Networks (BPNN), a kind of multi-layered perceptron, to predict the arsenic concentration using input variables derived from GIS spatial analyses.

2. Materials and Methods

Causes of elevated arsenic concentration and factors affecting it were studied to select the variables/ indicators to include in the model. ArcGIS software was used to generate, process and analyze spatial data of the selected indicators.

2.1. Causes of Elevated Arsenic in Bengal Basin

Groundwater arsenic concentration and distribution in Bengal basin is not uniform, and reconnaissance of well point data clearly indicates its strong correlation with surface geology. Higher levels of dissolved arsenic are generally found in low lying delta and flood plain areas of Bangladesh where water is produced generally from middle Holocene sediments. In this regard, several hypotheses are proposed to describe causes and processes of arsenic release into Bengal basin. Some of the most convincing and widely discussed causes of arsenic contamination in the basin are listed below:

Release of arsenic by oxidation of arsenic-minerals (e.g., diagenetic pyrite and arsenopyrite) in the alluvial sediments (Mallik and Rajagopal, 1996). Lowering of groundwater table draws in oxygen, which oxidizes sulfides releasing arsenic (Zahid *et al*., 2008). Reduction of iron-oxyhydroxides (FeOOHx) in anoxic conditions and release of sorbed arsenic to solution (Nickson *et al*., 2000; Bhattacharya *et al*., 2004). Arsenic species, in the form of As(V) and As(III), strongly adsorb on and/or co-precipitate with iron and manganese oxide/ hydroxides in the oxic environment and are released when anoxic conditions develop (Sullivan and Aller, 1996).

2.2. Factors Affecting Mobility of Arsenic

Experimental studies of arsenic movement in sediments are limited, consequently, the interactions between arsenic within a soil matrix are not well understood. It is generally believed that pH level, microbial activities, Dissolved Carbon Content (DOC) and competing ions play dominant roles in arsenic release adsorption and desorption into groundwater. However, the processes involved are complex, and often the factors interact among themselves as well as with the arsenic mobility.

2.2.1. pH level

pH conditions can result in a change in anionic charge which causes release of electro-statically bound arsenic. In saturated sediments under varying pH conditions, arsenic is most stable under neutral conditions (pH7); the arsenic becomes mobile under acidic (pH4) or alkaline (pH10) conditions, with greater mobility observed under acidic conditions (Shaw, 2006; Con *et al*., 2011). This is because the Arsenate (AS III) adsorbs strongly to iron-oxide surfaces at acidic and near-neutral-pH (Dzombak and Morel, 1990; Waychunas *et al*., 1993), but desorbs from iron-oxide surfaces under alkaline conditions (Waychunas *et al*., 1993; Fuller *et al*., 1993). The adsorption maximum for As (V) and As (III) on FeOOH lies approximately at pH 4 and pH 7-8.5, respectively (Fitz and Wenzel, 2002; Mahimairaja *et al*., 2005).

2.2.2. Iron Reducing Microbes

Reductive dissolution of iron(hydro)oxides (FeOOH) stimulated by microbial activity and organic materials is regarded as an important mechanism releasing arsenic into the aquifer (Islam *et al*., 2004; Ahmed *et al*., 2004; Mukherjee and Bhattacharya, 2001; Ravenscroft *et al*., 2001; Smedley *et al*., 2005). Under anaerobic conditions, FeOOH readily dissolves and arsenic is released into the soil solution (Takahashi *et al*., 2004). Nath *et al*. (2008) studied the mobility of arsenic in aquifer sediments from areas of low- and high-arsenic groundwater and found that occurrences of As-bearing redox traps, primarily formed of Fe- and Mn-oxides/ hydroxides, are important factors that control the release of arsenic into groundwater at their study site.

2.2.3. Organic Matter Content

It has been hypothesized that with increasing organic matter content the microbial activity is enhanced, which can impact the cycling of the elements. The concentrations of soluble As (V) as well as As (III) increase with an increase in soil organic matter content (Simona and Zagury, 2006). Dissolved Organic Carbon (DOC), in this connection, is a critical factor enhancing mobilization of both As (V) and As (III) in soil (Grafe, 2001). An increase in DOC content promotes both As (V) and As (III) solublisation in soils (Simona and Zagury, 2006). Harvey *et al*. (2002) studied detailed vertical profiles for groundwater arsenic and sediment properties from a study site in southern Bangladesh. He suggested that respiration of organic carbon plays a role in arsenic mobilization. As such, the Dissolved Organic Carbon (DOC) introduced into subsurface aquifers with groundwater recharge lead to reduction or dissolution of iron oxyhydroxides and the subsequent release of associated arsenic into groundwater.

2.2.4. Competing ions

Arsenic adsorption can also be affected by the presence of competing ions. In particular, phosphate and arsenate have similar geochemical behavior, and as such, both compete for sorption sites. Oxyanions of molybdenum, selenium, and vanadium, in addition to phosphate, may also compete for adsorption (Robertson, 1989).

2.2.5. Surface Geology

Since the origin of arsenic is geogenic and processes of release into the groundwater is geochemical, it is supposed to have relation with surface geology as well as physicochemical properties of the surface soil. The present study attempts geospatial analysis of arsenic status data in relation to some soil properties to predict the relation.

2.2.6. Drainage and surface elevation

In general, if there is no impermeable layer, groundwater follows the hydraulic gradient like surface water but at a relatively low pace. Most of shallow aquifers of Bangladesh have similar flow gradient as that of the rivers, and in the dry season the aquifers discharge into drainage channels. In anoxic condition, arsenic releases into the groundwater, and possible carried down the gradient towards drainage channels. This is evident by the pattern of distribution of arsenic in the Bengal basin. Higher concentration of arsenic, in general, is found near the channels, which increases with decreasing surface elevation.

2.3. Data generation using GIS technology

Based on the review of available literature as described above, variables affecting the release of arsenic into groundwater including arsenic concentration, surface elevation, soil reaction (pH), organic matter, iron content, surface geology and proximity to channels, were selected to predict the level of arsenic concentration. *ArcGIS* 9.2 was used to generate process and analyze spatial data from the study area, Bangladesh. Digital maps of rivers and drainage networks, and sample location maps of soil reaction, organic matter content and iron content were collected from Soil Resource Development Institute (SRDI), Dhaka, Bangladesh. Likewise, the digital elevation model and surface geology map of the country were received from Center for Environmental and Geographic Information Services (CEGIS) and Geological Survey of Bangladesh respectively. The point map of arsenic concentration, generated by Department of Public Health and Engineering as shown in Fig. 1, was used to create arsenic distribution surface, analyze the geospatial relationship of arsenic and validate degree and distribution pattern of arsenic in the predicted spatial data (NERC/DPHE/DFID, 2001). Surface geology maps of Bangladesh were generalized into eight geological units on the basis of similarity in origin, deposits and age of deposition (Fig. 2). Point maps of pH, organic matter content and iron content were created by adding attribute data from soil survey reports to the sample location map. From a limited number of points or sample values, GIS software was used to produce continuous surface where the values to the surface, between the measured values, are assigned by interpolation. Triangulated Irregular Network (TIN) surfaces of organic matter, pH and iron concentration were created from the respective point maps (Figs. 3-5).

Digital Elevation Model (DEM), a single-band raster dataset, contains continuous elevation values over a topographic surface by a regular array of *z values* representing surface elevation. A DEM data of Bangladesh of 300 m spatial resolution were used to study the relation of surface elevation to arsenic concentration (Fig. 6).

The ‘Proximity toolset’ in the ‘Analysis toolbox’ of ArcGIS was used to establish proximity relationships with feature data. The toolset can produce output information with buffer features. Multiring buffer tool was employed to create a cover of channel proximity classifying the area into ten units, ranging from 1□10 km distance from the nearest river, was created from the river system cover.

To make a homogeneous dataset for spatial analysis all the surfaces created were converted into grid surfaces of equal sized cells 100 m×100 m. Sample tool of

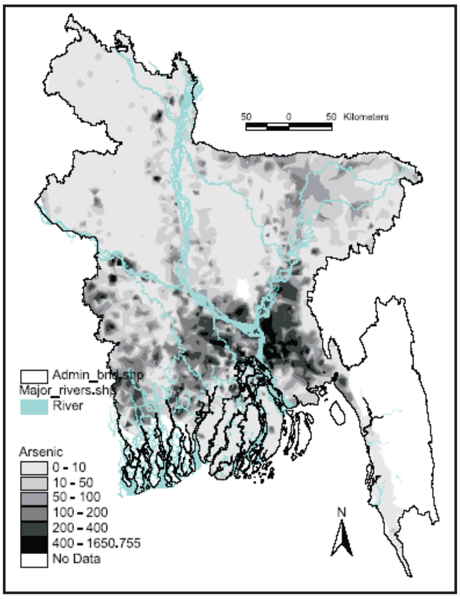

Figure 1. Point map of arsenic concentration

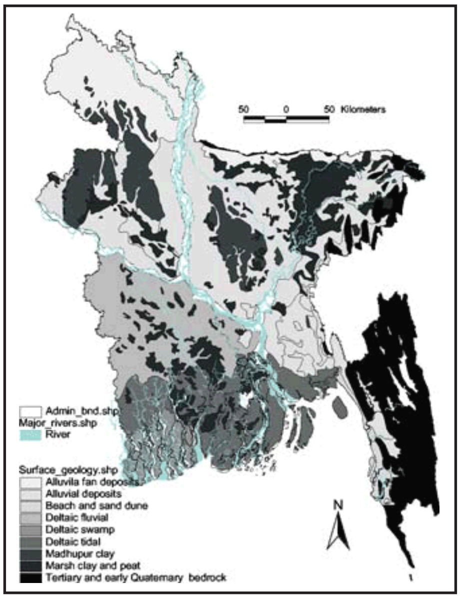

Figure 2. Geology of Bangladesh

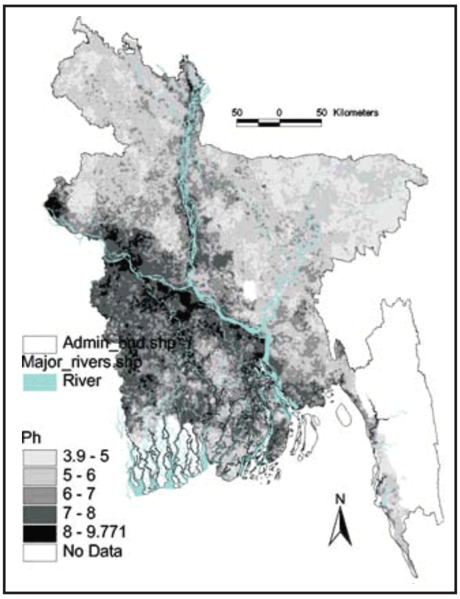

Figure 3. Soil pH map of Bangladesh

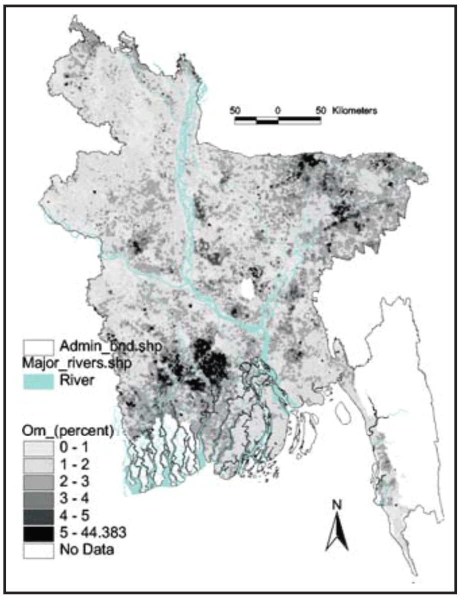

Figure 4. Organic matter content map of Bangladesh

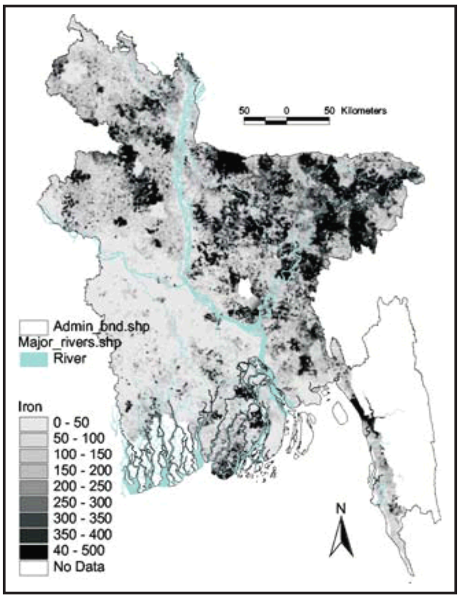

Figure 5. Iron content (in ppm) map of Bangladesh

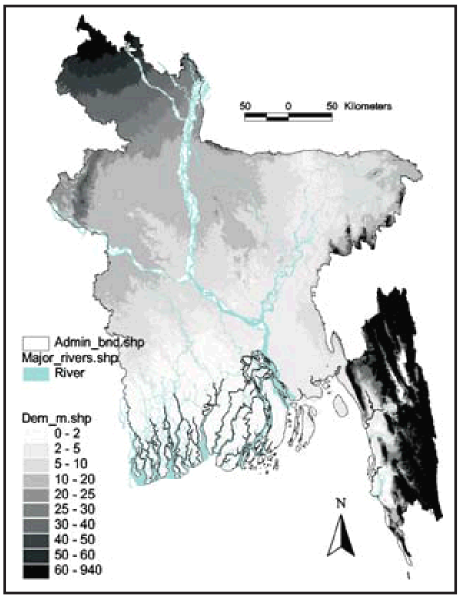

Figure 6. DEM map of Bangladesh

Table 1. Range of values used for training and recall

Parameters	Range of Values
Soil organic contents (µg/L)	0.056 – 12.279
Iron content (µg/L)	1.273 – 500.00
Arsenic concentration (µg/L)	0.000 – 1078.2
Soil pH	4.197 – 8.5640
Channel proximity (km)	0.000 – 10.000
Ground elevation (m)	0.000 – 67.350
Geology (units)*	1 – 8

* Geological units are assigned unique values ranging from 1 to 8

ArcGIS spatial analyst creates a table that shows the values of a raster, or several rasters, at a set of sample point locations. A sample point cover of 1,000 random samples spreading all over the country was created to extract data from same location points of all grid covers. Sample data for training and testing the neural network (ANN) were extracted from the created grid data set using the generated sample point cover as described above.

2.4. BPNN Model

Fig. 7 illustrates the NN architecture used in this study. An input layer and a hidden layer were used to generate the output with the linear transfer function (also known as activation function). For the hidden layer, the 'TanSig' nonlinear activation function was used. In this study, trial and error method was used to determine the number of neurons in the hidden layer. The range of data used for training/testing is presented in Table 1.

3. Results and Discussion

The final network architecture consists of 6 inputs, a hidden layer with 20 neurons and an output layer with single neuron. The network architecture is shown in Fig. 7. A number of trial runs were performed with a learning rate of 0.001, 0.05 and 0.01. From these trials a learning rate of 0.05 was found stable. Interestingly, the network converged in 10,000 epochs with mean squared error of 0.01.

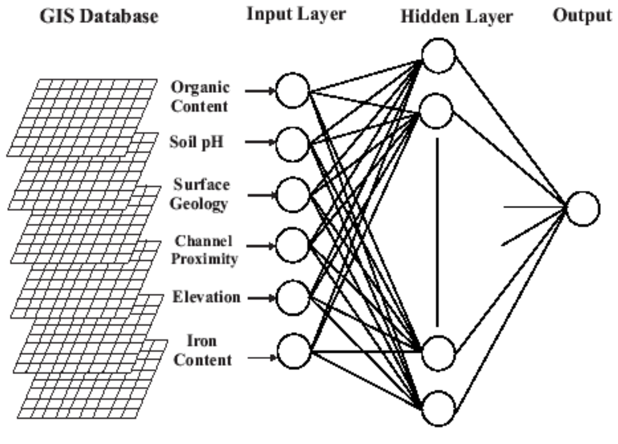

Figure 7. Neural Networks Architecture

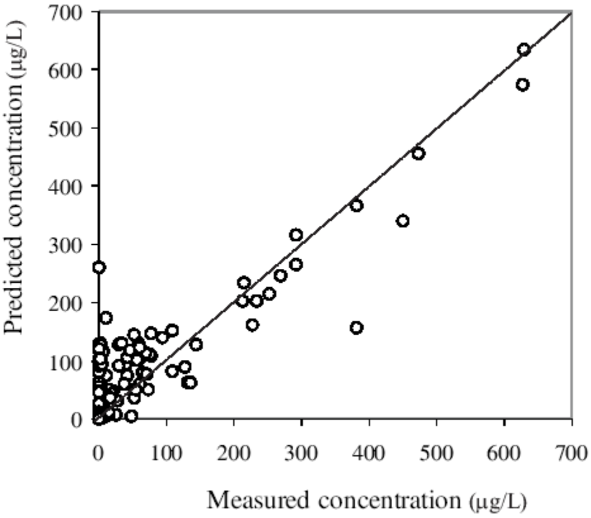

Figure 8. Measured versus predicted concentration of arsenic

Fig. 8 illustrates the predicted arsenic level in µg/L versus the observed one obtained from British Geological Survey data (NERC/DPHE/DFID, 2001). The scatter of the predicted concentrations was assessed using regression analysis. The coefficient of correlation of 0.5 was obtained. The diagonal line in the figure represents perfect goodness of fit as it is equidistant from both the axes. The results indicate that the neural network was successful in learning the relationship between the input and output variables.

5. Conclusions

Geographic Information System (GIS) has become an indispensable analysis and modeling tool for many real-world problems involving spatial data distribution. In this study, the GIS capabilities were used to extract data from various cover maps, namely: arsenic, iron content, pH, organic matter content, drainage and DEM maps, and fed into a three layered BPNN to predict the level of arsenic values. The multi-layered perceptron predicted the level of contaminant with reasonable accuracy. However, the successful prediction of a phenomenon not only depends on the accuracy of the developed model but also relies greatly on the availability of quality data from field observation. Despite limited geotechnical information, the BPNN model demonstrated a promising result.

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