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Two-dimensional Simulation of Nitrate Transport in an Agriculture-intensive Region

Morteza Mohsenipour, Hamid Asgari, Shamsuddin Shahid, Sahar Hadipuor and Peiman Roushenas

Department of Hydraulics and Hydrology, Faculty of Civil Engineering
Universiti Teknologi Malaysia (UTM), Skudai 81310, Johor, Malaysia
✉ mmorteza2@live.utm.my

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Abstract: A two-dimensional steady-state solute transport model is developed to simulate movement of non-point sources of pollution in anisotropic porous media. The migration of chemicals dissolved in groundwater is governed by advective-dispersive processes which are also affected by the velocity of the flowing groundwater. Therefore, groundwater flow equation is solved for hydraulic gradient and hydraulic conductivity to approximate the average linear velocity of the fluid. The advection-dispersion is used to approximate the spatial and temporal distribution of non-reactive dissolved chemical in a flowing groundwater. A computer code is developed in MATLAB to solve the groundwater flow and solute transports equations by finite difference methods. The developed program is verified with soil-tank experimental data. The solute transport model is used to simulate non-point source of nitrate pollution in an agriculture-intensive region. Finally, the model outputs are analyzed to understand the factors that influence the pollution transport in the study area.

Key words: Point and non-point sources of pollution, solute transportation, advective-dispersive processes, porous media, finite difference method.

Introduction

The demand for water has increased over the years across the world. This has led to water scarcity in many parts of the world. The situation is aggravated by gradual contamination of freshwater resources. Groundwater is one of the major sources of freshwater all over the world. Contamination of groundwater is a major concern in recent years especially in areas where it is used for drinking (Lin et al., 2010). Groundwater pollution may happen both through point and non-point sources. However, non-point source (NPS) of groundwater contamination poses problems that have significantly greater economic effects compared to point source of pollution (Duda, 1993; Loague et al., 1996). Anthropogenic activities such as urbanization, industrial development and unsustainable agricultural activities are the major sources of non-point pollution of groundwater (Martínez-Navarrete et al., 2011). Nitrate is the most common pollutant found in contaminated groundwater across the world (Keeney and Olson, 1986; Rivett et al., 2008; Burow et al., 2010). Groundwater nitrates are largely derived from fertilizer nitrogen and animal nitrogen applied in agricultural lands (Almasri and Kaluarachchi, 2007; Jiang and Somers, 2009; Mastrocicco, 2011). Nitrate is a colourless, odourless and tasteless chemical which is highly soluble and can move easily through the soil. In areas of high rainfall or over irrigation, nitrate is easily leached below the root zone to the groundwater (Jackson et al., 1973).

The increasing use of nitrogen-based fertilizers in agriculture has allowed global food production to stay ahead of rapid population growth, but at a potentially significant cost to current and future groundwater quality (Galloway et al., 2004). With the growth of world population, food demand will continue to increase and so the intensification of agriculture. Therefore, long-term pollution of groundwater from non-point sources, particularly in irrigated agricultural regions, is recognized as a critical threat to groundwater quality around the globe. Elevated nitrate concentration in groundwater can cause health hazards in the areas where groundwater is the major source of drinking water (Gulis et al., 2002; Wolfe and Patz, 2002).

Different management activities have been proposed so far for the protection of groundwater resources from unwanted contamination, such as land surface zoning, land use regulation, well head protection, in situ remediation measures, sources isolation, etc. (Fadlelmawla et al., 2011). However, in all the cases, it is important to know the fate of pollutant and their transportation through porous media. Groundwater modelling is an established tool to study the aquifer response for given input–output stress. Therefore, conceptual model for mass transport computation of dissolved chemical species in an aquifer at any specified time and space has been undertaken by several researchers in the recent years to propose mitigation measures to groundwater nitrate contamination (Lin et al., 2010; Tan and Zhou 2008; Jat et al., 2009; Ciftci et al., 2012; Elfeki et al., 2012; Zhang et al., 2012; Mousavi Nezhad et al., 2013). Zhang et al. (2012) used semi-analytical method for simulation of a conservative and non-reactive pollutant in steady state. Elfeki et al. (2012) analyzed the effects of temporal fluctuations and spatial heterogeneity on non-reactive pollution transport by simulating steady and unsteady flows.

Jiang and Somers (2009) developed a numerical model to simulate non-reactive non-point sources of pollution from agricultural lands in Prince Edward Island of Canada. Almasri and Kaluarachchi (2007) developed a model in order to evaluate the impact of land use on groundwater nitrate pollution in agricultural watersheds and propose alternatives for groundwater preservation. Mastrocicco et al. (2011) studied fate and transport of pollutant due to fertilizers in an unconfined shallow aquifer and concluded that recharge is a primary mechanism in nitrate remediation. Anayah and Almasri (2009) investigated the nitrate concentrations in an aquifer located in the West Bank of Palestine. Mousavi Nezhad et al. (2013) used numerical analysis in order to develop a model for simulation of solute transport in groundwater. The studies reveal that simulation is an effective method to understand the transportation of pollution through a porous media for effective control of groundwater pollution as well as groundwater resources management.

The partial differential equations describing groundwater flow and transport can be solved mathematically by using either analytical solutions or numerical solutions (Tan and Zhou, 2008). In recent years, numerical models have become indispensable in groundwater simulations, mainly for making predictions and improving process understanding (Abriola, 1997). One of the most widely used numerical methods for modelling groundwater flow is the finite difference method (Wang and Anderson, 1995). In recent years, number of research have been carried out on pollution transportation modelling by using finite difference methods (Lin et al., 2010; Jat et al., 2009; Ciftci et al., 2012; Göbel et al., 2004).

In the present study, finite difference method is used to solve partial differential equations of groundwater flow and solute transport in order to model transportation of nitrate through groundwater in a shallow unconfined aquifer of northwest Bangladesh where nitrate contamination of groundwater due to intensive agricultural activities is a growing concern.

The Study Area

The study area is located in northwest Bangladesh (latitudes 20°34’N and 26°38’N and longitudes 88°0l’E and 92°41’E). The location of the study area in the map of Bangladesh is shown in Figure 1. Irrigated agriculture is the lifeline of economy and people’s livelihood in the area (Shahid, 2008). Unlike other regions of the country, most part of the study area is free from flood. Groundwater in the area is mainly recharged by rainwater.

The topography of the area is mainly flat with an average elevation of 25 m above the mean sea level. The surface geology in the area comprises up-faulted terraces of Pleistocene sediments called Barind Tracts which are more strongly weathered than the surrounding alluvium. The sediments within the Barind Tracts and surrounding areas underlie much of the younger alluvial sediment at depths of the order of 150–200 m or more (British Geological Survey and Department of Public Health Engineering, 2001). A number of hydro geological studies have been carried out in the area (Rahman and Shahid, 2004; Islam and Kanumgoe, 2005; Faisal et al., 2005; Asaduzzaman and Rushton, 2006; Shahid and Hazarika, 2010; Shahid, 2011). The studies show that upper aquifers in the region are unconfined in nature. The thickness of the exploitable aquifer ranges from 10 m to 40 m (United Nation Development

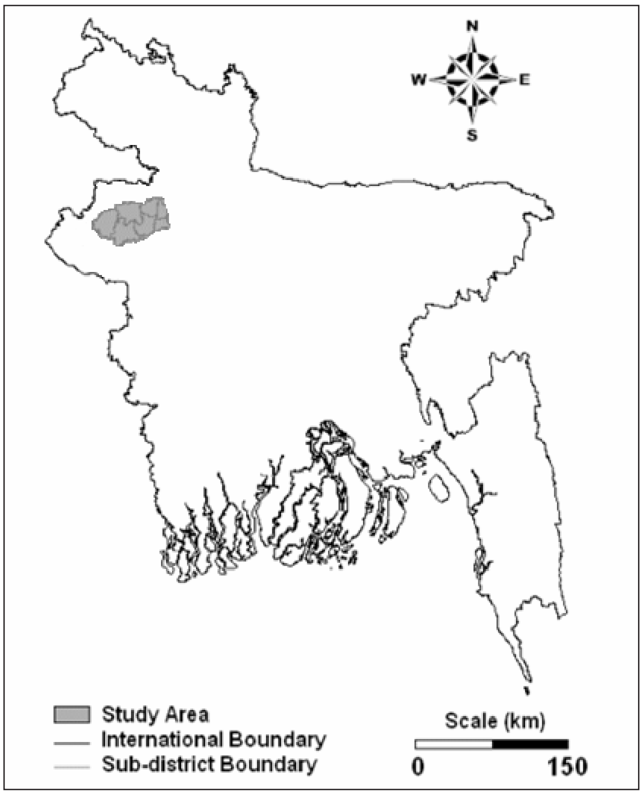

Figure 1: Location of study area in the map of Bangladesh.

Programme, 1982). The maximum depth to groundwater table from land surface is approximately 7 m. During monsoon, groundwater table comes very near to surface and make it highly vulnerable to pollution.

Methodology

The advection-dispersion equation to describe the transport of solute in saturated zone can be written as (Wang and Anderson, 1995),

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x_i}(cv_i) + \frac{\partial}{\partial x_i}\left[D_{ij}\frac{\partial v}{\partial x_i}\right] + R_c; i, j = 1, 2, 3 \quad (1)$$

where c is concentration of the solute; R_c is sources or sinks, D_{ij} is dispersion coefficient tensor and v_i is velocity tensor. The spreading of the solute in the direction of bulk flow is known as longitudinal dispersion. Spreading in directions perpendicular to the flow is called transverse dispersion. Longitudinal dispersion is normally much stronger than lateral dispersion. Longitudinal dispersion is calculated by using the following equation:

$$\frac{K_l}{D_0} = \frac{1}{f\varphi} + 0.5\frac{U\sigma dp}{D_0};\ \frac{U\sigma dp}{D_0} < 50 \quad (2)$$

where K_l is longitudinal dispersion coefficient (cm^2/sec), D_0 is the molecular diffusion coefficient (cm/sec), F is formation electrical resistivity factor, ϕ represents porosity, U is average interstitial velocity (cm/sec), σ is a measure of the inhomogeneity of the porous pack and dp is particle diameter (cm) (Perkins and Johnston, 1963). Transverse dispersion is considered 10% of longitudinal dispersion in model development (Hill, 1984). Diffusion coefficient for nitrate ranges between 0.53×10^{-6} and 3.2×10^{-6} cm^2/s. In the present study, diffusion coefficient of nitrate is considered as 1.52×10^{-6} cm^2/s.

Estimation of particle diameter (dp) is required for the calculation of longitudinal dispersion in different geological media. Different classification systems use different grain sizes to demarcate the soil types. A classification system known as MIT system is used in the present study for the classification of geological media from litholog data (Kaniraj and Kaniraj, 1988). Porosity of different materials is estimated by using the prescribed values proposed by Freeze and Cherry (Freeze and Cherry, 1979).

The Formation Resistivity Factor, F, is an intrinsic property of a porous insulating medium, required for the calculation of longitudinal dispersion. In the present study formation resistivity factor is obtained by using following equation:

$$F = \frac{1}{\phi_t^m} \quad (3)$$

where ϕ_t is total porosity and m in its simplest form is equal to 1 (Perkins and Johnston, 1963).

Hydraulic conductivity of different materials are estimated from the prescribed values proposed by Das (1994). If the criteria ($U\sigma dp/D_0 < 50$) is not met in equation (2), dispersion coefficient is obtained by using a curve proposed by Perkins and Johnston (1963).

Finite difference method is used to approximate the above equations. A finite-difference model is constructed by dividing the model domain into square regions called blocks or cells. Concentration is computed at discrete points within the model (Wang and Anderson, 1995). Partial differential equation of advection-dispersion with each component of dispersion coefficient tensor and velocity components yields:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial x}\left(D_{xy}\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial x}\left(D_{xz}\frac{\partial c}{\partial z}\right)$$
$$+ \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yz}\frac{\partial c}{\partial z}\right) +$$

$$\frac{\partial}{\partial z}\left(D_{zz}\frac{\partial c}{\partial z}\right)+\frac{\partial}{\partial z}\left(D_{zx}\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial z}\left(D_{zy}\frac{\partial c}{\partial y}\right)$$

$$-\frac{\partial}{\partial x}(V_x C)-\frac{\partial}{\partial y}(V_y C)-\frac{\partial}{\partial z}(V_z C) \quad (4)$$

Finite difference method substitutes the derivatives in a partial differential equation (PDE) system with finite difference schemes. The PDE then becomes a system of algebraic equations. For the derivation of the equation, forward difference approximation in time and central difference approximation in space have been implemented. Soil-tank experimental data is used to calibrate the model. Sensitivity analysis is carried out by varying model input parameters over a reasonable range and observing the relative changes in model response.

Finally, the developed model is applied in an anisotropic porous media to simulate transportation of non-point sources of nitrate pollution through groundwater system. Hydrological and hydro-geological data of northwest Bangladesh is used in the study. The model is used to simulate nitrate transportation through a single layered shallow unconfined aquifer. As the shallow aquifer is used for groundwater exploitation of drinking and irrigation in the area, pollution of this aquifer has significant impacts on socio-economy of the area. Transportation of pollution through a media depends on many factors. Therefore, model outputs are analyzed to identify the geological factors that influence the pollution transportation in the groundwater system in the study area.

Result and Discussion

Three experiments are carried out to simulate the pollution flow. First two experiments are carried out to simulate pollution flow in a sand tank so that the model parameters can be calibrated by using the results obtained through physical simulation of pollution flow in the sand tank. The third experiment is carried out to simulate pollution flow in an intensive agriculture zone located in northwest of Bangladesh. The results obtained through the experiments are discussed below.

Experiment 1

The first experiment is carried out to simulate pollution transportation from a point source. The experiment is carried out to simulate the data obtained through an experimental sand tank. The objective was to calibrate the model parameters. The physical experiment was carried out by Dwi (2001) in a soil tank with dimension of 240 cm × 220 cm × 110 cm. The type of porous media, the properties of the porous media and the properties of the pollutant used in the experiment are also used to simulate the flow of the pollution. The model output is given in Figure 2.

Finite difference grid size and model parameters are calibrated to match the computer simulated flow with that obtained through the soil-tank experiment. After calibration, it was observed that simulated pollutant front has reached same lateral and vertical extents as the experimented one after 72 hours.

Experiment 2

The calibrated model is then used to simulate non-point sources of pollution in the experimental sand tank. The result is shown in Figure 3. The results show that level and spread of pollution will be much higher in case of non-point sources of pollution compared to point sources of pollution.

The experiment is repeated for various geological materials, groundwater velocity conditions, pollution concentrations, and grid sizes. The study shows that pollution transportation in groundwater depends mainly on: (1) geology of the media, (2) velocity of groundwater, and (3) concentration and type of pollutant. The model is also found variable to grid size of finite difference model and dimension of the model.

Experiment 3

Finally, the model is used to simulate the pollution transportation in a non-isotropic media. Borehole litholog data collected from 21 locations in the study area located in northwest Bangladesh is used to develop the geological structure of the area. The geological structure used for the simulation is shown in Figure 4. The aim of the study was to show how pollution will flow if it is released at surface when the subsurface medium is saturated with water. This often happens in northwest region of Bangladesh. Aquifers in the region are mainly unconfined in nature. Groundwater level reaches ground surface during monsoon in the region. Monsoon rain fed agricultural activities are very common in the area. Fertilizers are widely used in the flooded crop land for higher food production.

Outputs of the simulation model are presented in Figure 5. The figure 5 shows the movement of solute in porous media in the study area.

The result shows that due to the unconfined nature of aquifer system in the study area, groundwater may be

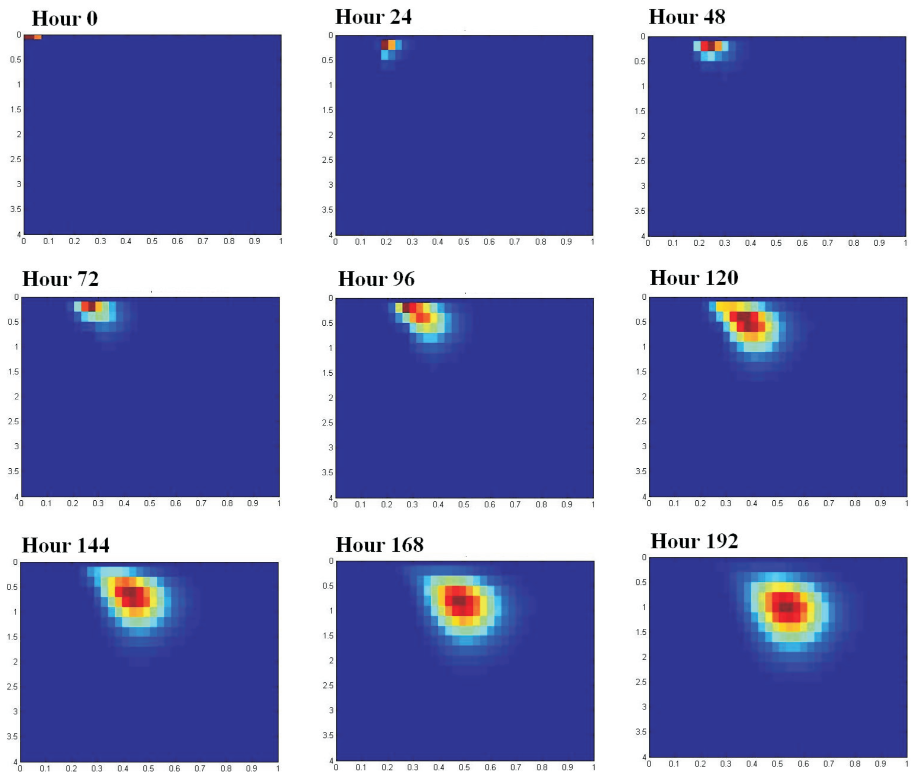

Figure 2: Output of finite difference pollution transportation model for point source of pollution at different time interval.

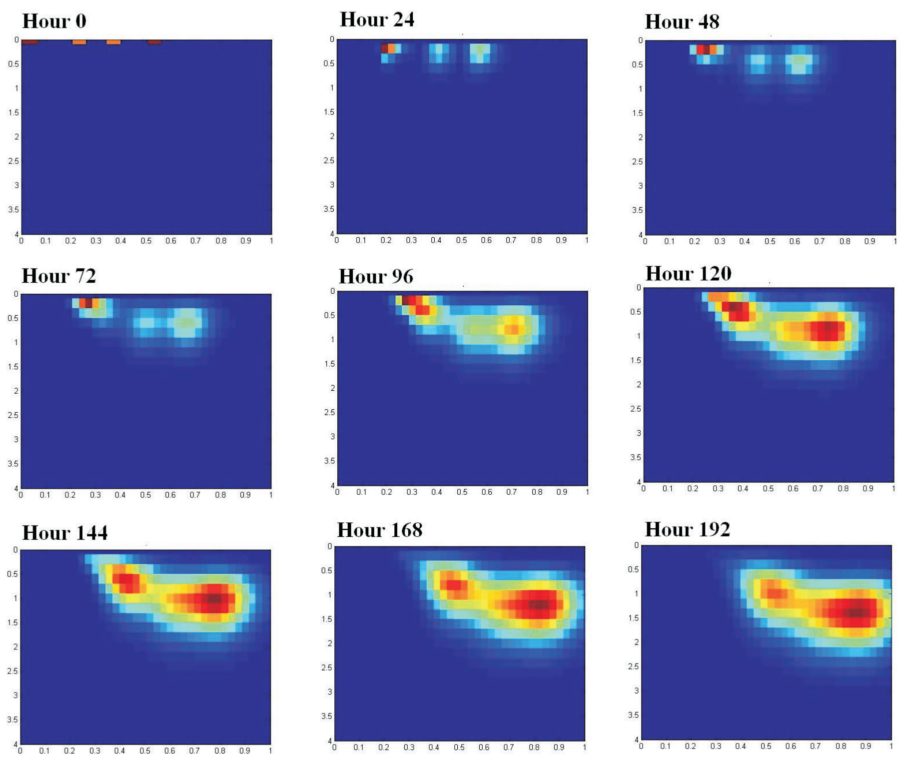

Figure 3: Output of finite difference pollution transportation model for non-point source of pollution at different time interval.

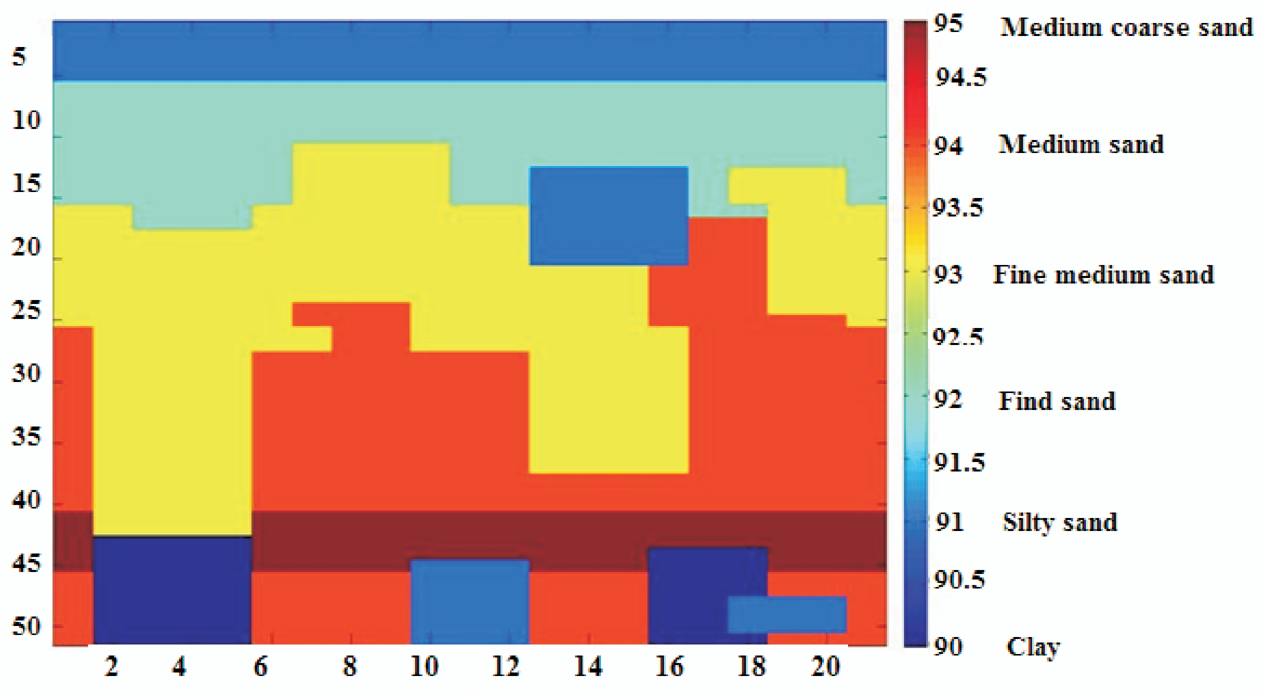

Figure 4: Geological structure of the study area used for the simulation of transport flow in a non-isotropic heterogeneous media.

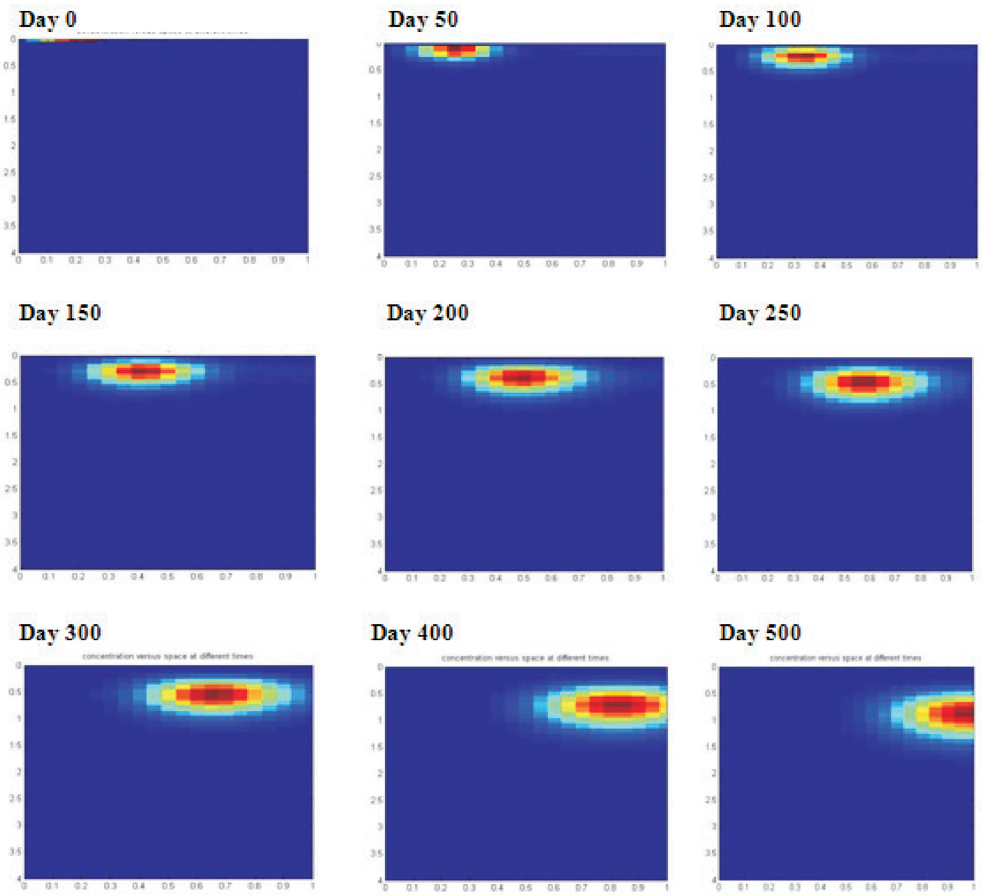

Figure 5: Finite difference pollution transportation model for the study area.

easily polluted. Nitrate pollution can travel up to five kilometres horizontally in the direction of groundwater flow and 25 metres vertically down in a single year.

Conclusion

Finite difference approach has been used in the present study to simulate two-dimensional flow of non-reactive non-point sources of pollution in a non-isotropic porous media. Simulation of groundwater pollution is a complex process which needs accurate model parameters. Those can only be obtained through laboratory test. As all the parameters could not be obtained through laboratory simulation, empirical equations were used to calculate some model parameters. The study reveals that pollution transportation in a groundwater system heavily depends on the geology of the media, velocity of groundwater flow and pollution concentration. Specially, near surface geology is highly sensitive to pollution transportation. The simulation shows that presence of a porous media near the surface can spread the pollution at a higher rate. The study also shows that appropriate grid size is necessary to identify for accurate simulation of groundwater pollution as the model output is sensitive to grid size. The present study considered that the pollutants are non-reactive and non-decaying. Further research can be carried out in future to simulate fate by considering the reactive characteristics of pollutants.

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