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In-situ Bioremediation modeling of organic contaminant

Sudheer Ch and Shashi Mathur
Department of Civil Engineering IIT Delhi, India.

***Abstract*— The contamination of groundwater has been a major challenge faced by environmentalists in the recent past. Organic contaminants can enter the groundwater environment from a variety of sources that include toxic waste disposal sites, accidental chemical spills and improperly designed or maintained chemical transportation and storage facilities. Groundwater contamination by the organic chemicals is of immense concern because of their widespread use and harmful effect even when present at very low concentrations. Though organic compounds are usually less soluble in groundwater than many inorganic contaminants of interest, they often dissolve to concentration values that far exceed levels considered acceptable for human consumption. Remediation efforts are normally resorted to at contaminated sites to contain the contaminant plume, to eliminate and finally to extract the contaminants during the restoration work. A Finite difference model is also developed to simulate the process of in-situ bioremediation using Alternate-Direction Implicit technique. This model (BIOFDM) yields the spatial and temporal distribution of contaminant concentration for predefined initial and boundary conditions. The simulated model is later validated by comparing the simulated results with those obtained using BIOPLUME III model of the case study of Shieh and Peralta (2005). The results are found to be in close agreement.**

***Keywords*—Ground water Modelling, In-situ Bio Remedaition, Finit Differnce technique.**

I. Introduction

Remediation of contaminated groundwater is an extremely expensive process [1] and the conventional pump-and-treat method has been one of the most commonly used methods for both large and small scale groundwater quality problems so far [2,3]. According to a study by the U.S. Environmental Protection Agency, the remediation cost for contaminated soil and groundwater in United States was estimated at 187 billion US dollars in 1996. An analysis of the costs involved at the pump-and-treat remediation sites show that annual capital costs per 1000 gallons of groundwater treated ranges from $ 2.9 to $1600 and the average annual operating cost per 1000 gallons of groundwater treated ranges from $ 0.21 to $ 170 [4].

Besides this, organic contaminants like pesticides, organochlorines, polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs) synthetic dyes, wood preservatives, munitions waste and synthetic polymers either degrade or are converted into less toxic forms through bioremediatio. Bioremediation could be mediated by bacteria, fungi, a cocktail of microorganisms or plants or even a combination of all of these

In-situ bioremediation for contaminated groundwater is considered as an efficient remedial alternative not only because of its cost-effectiveness but also due to it's ability to achieve complete destruction of organic contaminants in a stipulated duration of time [5]. Clearly, if the cost incurred by the existing and future remediation systems be reduced, significant economic benefits could be realized.

The design of an in-situ bioremediation program usually involves determination of the location and the pumping rates of the injection and extraction wells. Injection wells are also used to stimulate growth of a microbial population to accelerate the degradation of the pollutants by injecting an increased supply of electron acceptors or nutrients. Furthermore, the contaminant plume is also hydraulically contained to prevent further spread of the contaminant using these extraction wells. Provision of an up gradient injection well and a down gradient extraction well results in an increase in the hydraulic gradient that further accelerates the movement of the electron acceptors and nutrients through the containment plume thereby enhancing the transport of the injected substance. Moreover, injecting the extracted water back after treatment with electron acceptors and nutrients involves a substantial cost. Thus an optimal injection and extraction pumping rates that could result in an overall reduction in the cost can be determined through an optimization model.

In this study, a model which simulates the biodegradation of organic contaminants using oxygen as the electron acceptor is developed. The developed model is then used to study an in-situ bioremediation problem of Shieh and Peralta [7]. The model is validated by using BIOPLUME III. A review of literature shows that even though there are many popular softwares like BIOSCREEN, MT3ds, BIOPLUME available, it becomes very difficult to develop an interface between these existing softwares and the advanced computing softwares like MATLAB for addressing the complex search problems. In this study, a Finite difference model is solved by MATLAB to simulate the flow and contaminant transport of the substrate and oxygen.

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II. Description of the study area

The aquifer is assumed to be homogeneous with the west and the east sides of the domain taken as constant head boundaries with the head values of 30.5 m and 27.7 m respectively and the north and south side boundaries assumed to be impervious (Shieh and Peralta 2005). Consequently, the flow is assumed to be from west to east with an initial hydraulic gradient of 0.004. The groundwater flow simulation is assumed to be at steady state. The representative organic pollutant assumed is BTEX. Figure 1 depicts the initial contaminant concentration and a set of preselected injection and extraction well location for an in-situ bioremediation system .

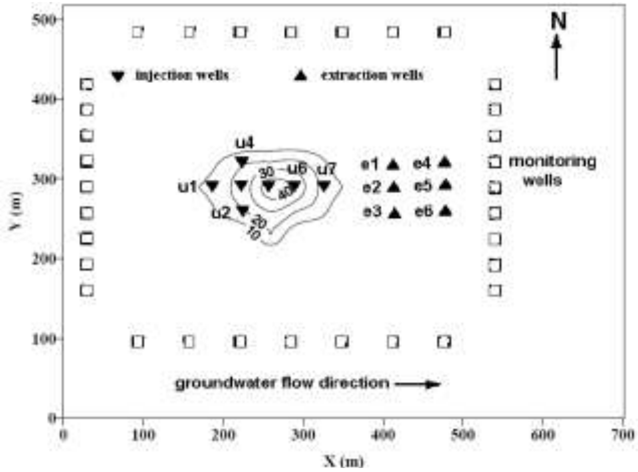

Figure 1: Initial concentration of contaminant and a set of preselected injection and extraction well locations for in-situ bioremediation system (Shieh and Peralta 2005)

III. Mathematical Formulation

The transport equations for contaminant and oxygen can be expressed (Rifai et al. 1997) as

$$\frac{\partial(bC_s)}{\partial t} = \frac{1}{R_s}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_s}{\partial x_j} - \frac{\partial b v_i C_s}{\partial x_i}\right)\right] - \frac{qC'_s}{\theta}$$

$$\frac{\partial(bC_o)}{\partial t} = \frac{1}{R_s}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C_o}{\partial x_j}\right) - \frac{\partial b v_i C_o}{\partial x_i}\right] - \frac{qC'_o}{\theta}$$

where C_s and C_o are the concentrations of contaminant (or substrate) and oxygen respectively (M/L3); Cs and C_o are the concentrations of contaminant and oxygen respectively in a source or sink fluid (M/L3); q is the volume flux per unit area (L/T); b is the saturated aquifer thickness (L); v_i is the average linear velocity in direction i (L/T); q is the effective aquifer porosity (dimensionless); Rs is the substrate retardation factor (dimensionless) defined using linear adsorption isotherm by equation

$$R_s = \left(1 + \frac{r\,b\,K_d}{q}\right)$$

where r_b is the soil bulk density and K_d is the solute partition coefficient. $D_{i\,j}$ is the hydrodynamic dispersion tensor (L2/T); i, j = 1,2 (principal coordinate directions (x and y)) and t is the time. Some assumptions have been made during the development of the simulation model. It is assumed that the hydrocarbons are generally simulated as a lumped organic matter comprising benzene, toluene, ethyl benzene or xylene (BTEX). Also, BTEX is treated as a single compound while the injected water is assumed to contain sufficient nutrients for growth and reproduction of microorganisms. Since the operating cost of pumping far exceeds the costs of adding nutrient and oxygen the injected nutrient and electron acceptor concentration is not considered as a decision variable in insitu bioremediation.

The decision variables thus are only a set of pumping locations of extraction and injection wells and their pumping rates respectively. Similarly, it is also often found that bioclogging (biological clogging) due to microbial growth reduces the porosity and hydraulic conductivity of a saturated porous medium. Since the biodegradation kinetics used in the study does not simulate microbial growth rate explicitly in the aquifer system, biological clogging in subsurface environment is thus neglected. In addition to the above, it is also assumed in the BIOFDM model that Darcy’s law is valid and the hydraulic gradient is the only driving mechanism for flow. Also, the porosity is spatially uniform whereas the hydraulic conductivity of the aquifer is constant with time. Further, it is assumed that fluid density, viscosity, and temperature does not affect the velocity distribution and that the vertical variation of head and concentration is negligible. Furthermore, it is also assumed that the fluid and aquifer properties donot change due to any chemical reaction and the entire domain is homogeneous and isotropic, thus $D_{xy} = D_{yx} = 0$

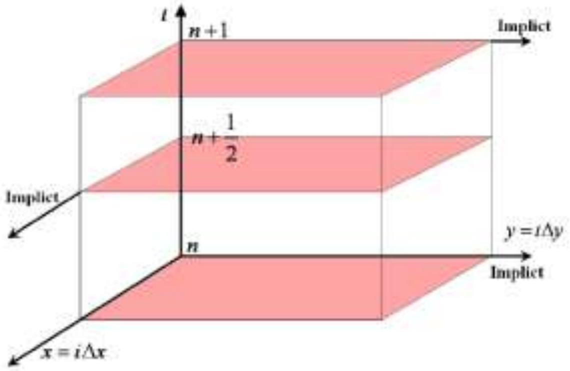

Figure 2: ADI calculation procedure

The contaminant transport equation is first discretized numerically in time and space using an Alternate Direction Implicit Finite Difference Method coupled with the Gauss sidel iteration scheme. The ADI method is a two step scheme. A tridiagonal matrix is solved for each j row of the grid in step

1 whereas during step 2, a tridiagonal matrix is solved for each i row of the grid. As a result of this 'splitting' in the algorithm a tridiagonal system of linear algebraic equations is obtained. This procedure is also illustrated in figure 2. The ADI method is second order accurate.

The study domain is discretized into a grid which is a network of points defined by taking increments of length dx and breadth dy. Figure 3 depicts this gird drawn for the aquifer where the index along the abscissa is denoted by i and that along the breadth ordinate is j.

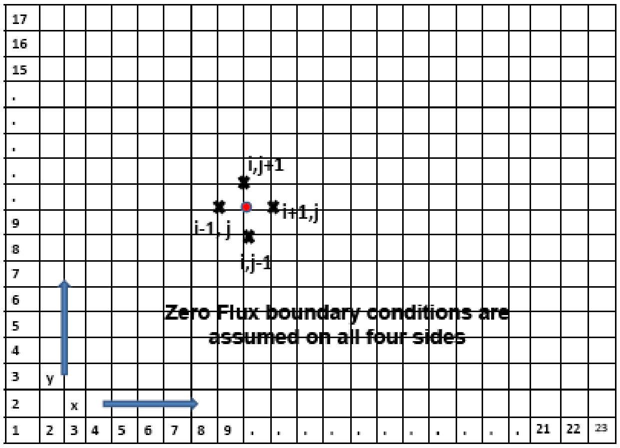

Figure 3: A schematic representation of grid discretization

IV. Model Validation

Figure 1 depicts the layout and the initial concentration profile of the contaminated plume studied by Shieh and Peralta (2005), the data of which is adopted in this study as well. Zero flux boundary conditions are assumed on all the four sides of the aquifer. Table 1 highlights the input parameters used in the BIOFDM model for the study area of 701.5 m × 518.5 m.

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Input Parameter	Value
Grid Size	19 X 25
Cell Size	30.5 X 30.5
Hydraulic Conductivity	6×10^{-5}
Longitudanal Dispersivity	10 m
Effective Pororsity	0.3
Retardation factor	1
Anisotropy Factor	1
Back ground Concentration of Oxygen	5 ppm
Remediation Period	3 Years

The developed model BIOFDM is validated by comparing the simulated finite difference results with those obtained by using BIOPLUME III for the hypothetical site of Shieh and Peralta (2005).

Initially, the model was compared without incorporating the biodegradation process. Later, the effect of bio degradation was also included while comparing the simulated models. Both, the spatial and temporal variations of the plume concentrations were compared. The BIOPLUME III program is a two-dimensional, finite difference model that simulates natural attenuation of organic contaminants in ground water due to advection, dispersion, sorption, and biodegradation. The model simulates the biodegradation of organic contaminants using a number of aerobic and anaerobic electron acceptors (oxygen, nitrate, iron (III), sulfate, and carbon dioxide).

BIOPLUME III is a very popular software and is thoroughly tested for many field applications by U.S EPA (Environmental Protection Agency). The spatial and temporal variations of concentration profiles were generated by BIOLUME and BIOFDM for the problem defined by Shieh and Peralta [7]. The results obtained by using both the models are compared as shown in figures 4, 5 and 6. Figure 4 depicts the comparison of concentration plumes after 5 years. Figure 4 also shows the plume configuration after 5 years in the absence of any remediation work. It can be seen from Figure 4 that the contaminated plume eventually reaches the monitoring wells after 5 years under the prevailing conditions. An in-situ bioremediation is therefore required to contain the plume and enhance the contaminant biodegradation process.

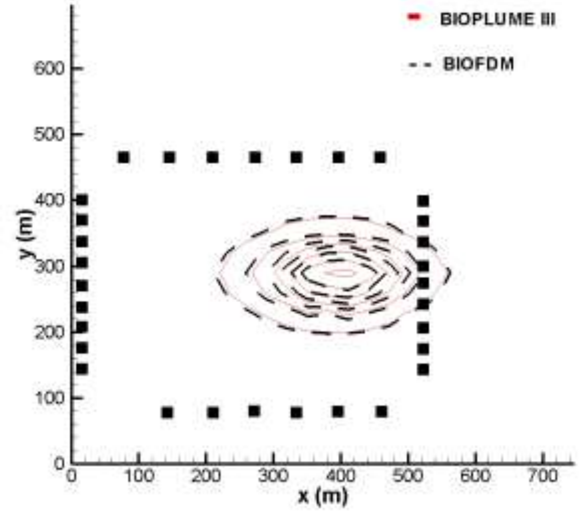

Figure 4: Comparison of concentration plumes after 5 years

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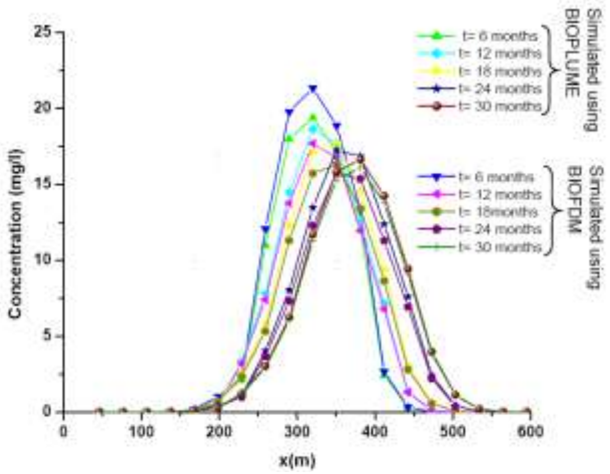

Figure 5: Temporal Variation of concentration along centerline of plume intervals without biodegradation

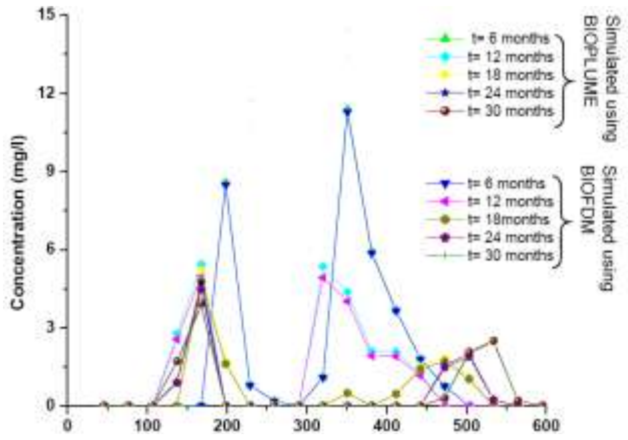

Figure 6: Temporal Variation of concentration along centerline of plume intervals with biodegradation.

Thus the process of bioremediation is simulated in the model by using the instantaneous reaction model BIOFDM developed in this study. Furthermore, the maximum allowable concentration C_{max} is assumed to be 5 ppm for the entire study area. The upper and lower bounds on hydraulic heads are also taken as 31.4 m and 27.7 m (the constant head boundary values at the west and east sides of the aquifer) respectively. From figure 4 one can observe that a good match of spatial variation of plume concentration after 5 years is obtained. Further, the concentration profile along the central plume line is plotted for both the models (BIOFDM and BIOPLUME) at different time steps as shown in figure 5. The results obtained indicate a good agreement between BIOFDM and BIOPLUME. Later on, the effect of biodegradation is also included and the concentration variation along the central plume line is compared as shown in figure 6. Again the results show a good match between the developed model and BIOPLUME results.

V. Conclusions

A finite difference model BIOFDM is developed to study an in-situ bioremediation problem of Shieh and Peralta (2005). The model is validated by comparing the model results with the simulated results of Shieh and Peralta (2005) using BIOPLUME III. A close agreement is found between the two. The model is developed using MATLAB® hence it can be integrated with the advanced optimization tools which thus helps in designing the optimal in-situ bio remediation system.

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About Author (s):

Shashi Mathur is Professor at Civil Engineerng Department IIT Delhi. He did his Phd from Delaware University. His research interest include Groundwater Contamination, Bioremedation of soils, flow through porous media, phyto remeidation etc.

Sudheer Ch. received his PhD in Water resources from Indian Institute of Technology Delhi. Currently he is a Senior Project Scientist in Civil engineering Department at IITDelhi. His research interests include Groundwater Contamination, Bioremediation of Soils, Design of landfills, Developing mathematical models for Malaria transmission.