JOURNAL OF
ENVIRONMENTAL HYDROLOGY

The Electronic Journal of the International Association for Environmental Hydrology
On the World Wide Web at http://www.hydroweb.com

VOLUME 19 2011

MODELING BIOREMEDIATON AT ABANDONED WASTE DUMPING AND LANDFILL SITE USING MODFLOW AND RT3D PACKAGES

Noori M. Cata Saady | Civil and Environmental Engineering Department,
University of Windsor, Windsor, Ontario, Canada

This paper presents modeling of bioremediation of groundwater at an abandoned waste dumping and landfill site using MODFLOW and RT3D packages with Groundwater Modeling System (GMS) software interface. The objectives of the model were to predict the progress of bioremediation, contaminant concentrations and distribution over an assumed duration to get an idea about the cleanup time. The paper describes: (1) the problem at the site under consideration; (2) formulation of the model; (3) the conceptual model development and the assumptions involved; and (4) the results of MODFLOW and RT3D simulations. The models showed that bioremediation will be an effective treatment for groundwater contamination at the site, but it will need a relatively long time that extends to years. Two years of bioremediation would remove 3.5% of a typical aqueous phase organic contaminant. Heterogeneity of the geological formations decreased the degradation of the organic contaminant and resulted in a pool (unreachable confined zones) of high concentrations (98.5% of the original level) that remained after treatment in almost 20% of the area.

INTRODUCTION

In situ bioremediation techniques that utilize microbial activity to degrade organic substances in groundwater are a promising approach to cleanup contaminated aquifers (Gallo and Manzini, 1998). A decision-making process requires that the response of a contaminated groundwater system to the implementation of bioremediation methods be known before they are implemented (Bear et al., 1992). This paper presents an application of existing multidimensional packages into a model to simulate transport and biodegradation of an organic pollutant in saturated porous media. In addition, the model was used to predict the dynamics of subsurface pollutant plumes and the degradation rates of the given organic chemical under natural or enhanced conditions.

The bioremediation was considered because the polluting organic compound is aerobically biodegradable and the hydraulic conductivity of the geological formations at the site is amenable to in situ bioremediation.

The biodegradation is a biochemical reaction mediated by microorganisms where an organic compound is oxidized (loses hydrogen electrons) by an electron acceptor which itself is reduced (gains hydrogen electrons) (Rittmann and McCarty, 1980). Indigenous or extraneous bacteria and substrates (e.g., electron acceptor, electron donor, and nutrients) can be delivered to any location in the subsurface environment. Mathematically, the bioremediation model can be formulated in terms of a Darcy's law for single-phase groundwater flow in saturated soils, coupled with passive transport of a set of mutually interacting species, including bacterial biodegradation kinetics (Gallo and Manzini, 1998).

To design and implement an in situ bioremediation system properly, an accurate numerical model is needed to predict the concentration distributions of contaminants, microorganisms, electron donor and accepter, and other compounds involved in the biodegradation process. The model should describe the growth and decay of microorganisms as well as various mass exchanges between aqueous and solid phases (Sun, 2002). MODFLOW is a three-dimensional model, originally developed by the U.S. Geological Survey (McDonald and Harbaugh, 1988); it uses block-centered finite difference scheme for computing spatial and temporal variation in groundwater head distribution in saturated zone. RT3D is a model that simulates reactive transport of multiple mobile or immobile species in three dimensional saturated porous media. In order to preprocess (i.e., to develop the input files) and postprocess the outputs from MODFLOW and RT3D, Groundwater Modeling System (GMS) [v6.5 Aquaveo, LLC, Utah–USA] interface was used.

STUDY AREA

Description of the physical problem

The waste dumping and landfill site stretches on a triangular area of 3.4 km x 2.31 km x 2.03 km. The modeled area (semi trapezoidal shape with dimensions of 3.4 km x 5.0 km (average) x 3.0 km) covers the waste dumping site and extends to Dyala River, Baghdad-Iraq. Figure 1 is an aerial view and a schematic map. The mean ground surface elevation is about 34.3 m with an average slope of -0.0038% in the north-south direction, and an average slope of 0.06% in the east-west direction. The site was used as waste dumping and landfill facility for 15 years from 1979 to 1994. The abandoned waste dumping site is bounded by Dyala River from the south and a concrete lined drain from the west; the drain eventually discharges into the river almost 4 km southwest of the site. The site was enclosed later from the north by an extension of the drain; the purpose of the original drain and the extension at the time of construction was to supply proposed farms in the area with water

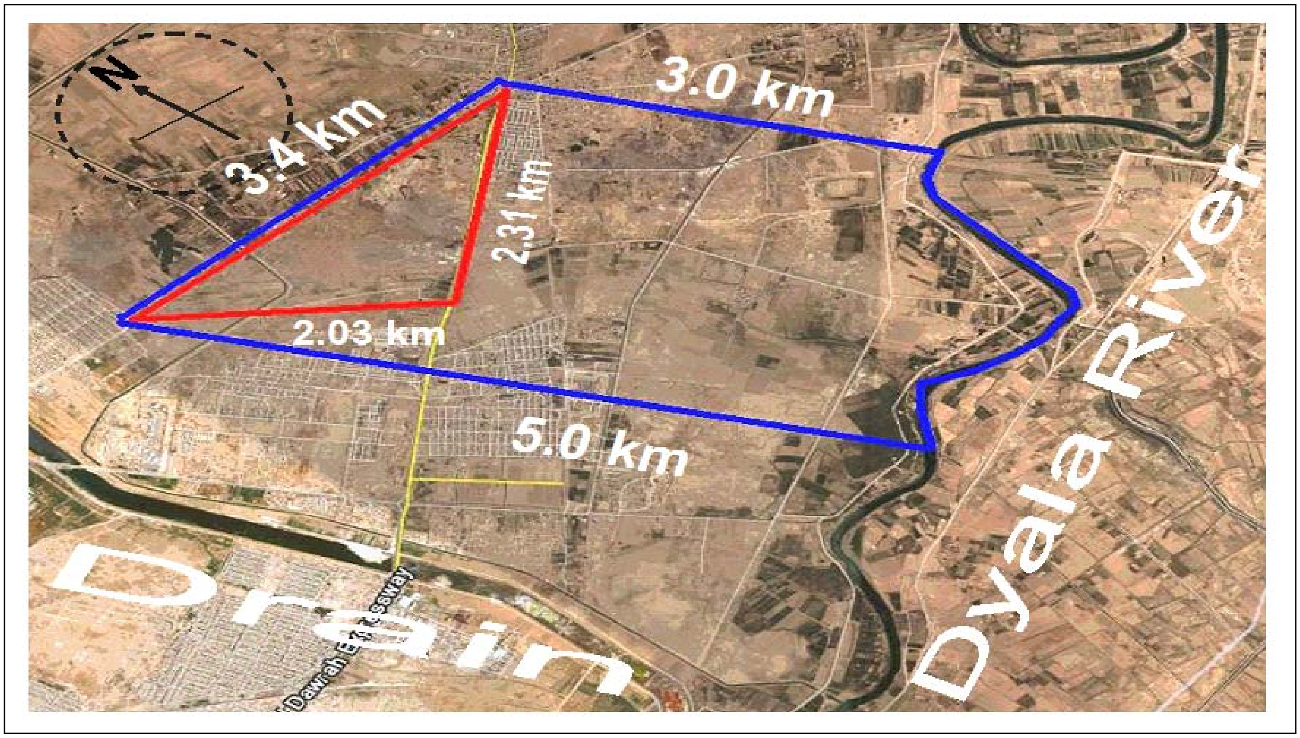

Figure 1. Aerial view of the waste dumping site and the surrounding. (Triangular area is the dumping site, whereas the semi-trapezoidal area is the scope of the model).

but both returned to work as drains later. The site is located at the southwestern corner of 2700 Km^2 catchment area which feeds Dyala River mainly and Tigris River ultimately. It can be seen in Figure (1) that the ground is almost not covered by any plantation especially at the site. The mean annual precipitation is 70 mm/yr.

Objectives of the model

There are no exact solutions which enable the prediction of the outcomes of applying the bioremediation techniques in the waste dumping site to remedy the contaminated groundwater; hence, a numerical model using MODFLOW would:

§ Quantify the contaminant biodegradation and predict the effectiveness of bioremediation to treat the groundwater contamination at the site by using a model which simulates physical, chemical, and biological processes.

§ Predict a scenario that may happen if a bioremediation technology is applied to the site and estimate contaminant concentrations and distribution in the modeled area during the course of bioremediation.

§ Determine the contaminant washout (leachate) from the unsaturated zone.

MODEL DEVELOPMENT

Conceptual model

The conceptual model aids in determining the modeling approach and which software to use. The conceptual model for the groundwater flow and contaminant transport took into account the significant features of the site and the relationships among them. Assumptions were made regarding the stratigraphy (the soil layers were assumed of constant thickness), but the actual average thicknesses of each layer as well as the followings were determined from site-specific data:

1- Boundaries of the flow system.

2- Aquifers and their hydraulic relationships with other geological units.

3- Relationships between groundwater and surface water: the groundwater is fed by precipitation and subsurface flow from the catchment areas.

4- Groundwater levels: measured groundwater heads were used to establish the groundwater contour map.

5- Groundwater flow directions: the measured groundwater heads were used to construct the contour map and determine the direction of groundwater flow. This was supported by field observation.

6- Groundwater sources (recharge) and sinks: the seepage of groundwater to Dyala River (the river works as a drain) is the only sink in the site.

Mathematical description of the problem

Biodegradation phenomenon in groundwater is composed of three processes (Gallo and Manzini, 1998): Groundwater flow, passive transport of reacting contaminants, and the degradation kinetics. Groundwater flow is described by Darcy's equations (Equations 1 and 2):

$$v = -T\,\nabla P \tag{1}$$

$$q = \nabla . v \tag{2}$$

where P is the hydraulic head, v is the Darcy velocity, T is the transmissivity, and q is a source/sink term. Passive transport of reacting contaminants is represented by advection-diffusion-reaction process:

$$\frac{\partial}{\partial t}(R_i n C_i) + \nabla.(vC_i) - \nabla.(D_i \nabla C_i) = C_m \Lambda_i \qquad i = 1,2,3,4 \tag{3}$$

where for the i species, R_i is the retardation factor, D_i is the diffusion-dispersion tensor, C_i concentration of the ith nutrient, C_m is the number of bacterial colonies per unit volume, n is the porosity, Λ_i is the reaction term. Equation 3 is written for any of the chemical constituents under consideration and for the microbial community. The degradation kinetics is usually represented by a suitable chemical and microbial kinetics. The formulation of reaction kinetics is site-specific. The Monod Kinetics expression is used to describe the specific growth rate (Bedient and Rifai, 1992). For dual substrates when the bioremediation requires the addition of electron acceptor, the Monod expression is:

$$\Lambda = \mu_{\max}\left(\frac{C_n}{K_s + C_n}\right)\left(\frac{A}{K_A + A}\right) \tag{4}$$

where Λ = is the specific growth rate. μ_{max} = the maximum growth rate when an excess nutrient is supplied. K_s = Monod constant which is specific for the electron donor (substrate C_n) and the microorganism; it is the concentration of the substrate at which the specific growth rate Λ is half its maximum value (Bailey and Ollis, 1986); hence, it indicates the affinity/sensitivity of microorganisms to the substrate. C_n = concentration of the substrate (organic contaminant) which serves as carbon source during the period of growth. A = concentration of the electron acceptor. K_A = Monod constant for the electron acceptor and the microorganism; it is the concentration of the electron acceptor at which the utilization rate is half the maximum.

Model requirements and code/software selection

The choice of models to be used for this site based on the characteristics of the groundwater systems, the distribution of contaminants, and the types of contaminants present.

A wide variety of contaminants are present at the site under consideration. Water is transporting these contaminants through the saturated zone, to the reach of Dyala River. The adverse effects of the contaminated groundwater that reaches Dyala River are very noticeable and converted this reach of the river into a dead zone.

The transport model is intended to simulate the instantaneous bioremediation of the contaminated groundwater during its movement from the contamination source area to Dyala River. Much of the site specific data required to develop defensible models of groundwater flow and contaminant transport at the waste dumping site have been obtained. Reasonable values were assumed for parameters for which no data are available.

GMS (v6.5 Aquaveo, LLC, Utah–USA) is well known industry standard software interface that was available and suitable for modeling this case. MODFLOW and MT3D and RT3D packages were used to produce the model.

Data requirements

Groundwater elevations or pressures (hydraulic heads) were obtained from recorded values at the site and its surroundings. Groundwater heads contour map and a 3D view are given in Figure 2 (A and B). A proper recharge rate was assumed. Hydraulic conductivities of the three layers modeled are given in Table 1.

Data required by contaminant transport models include: 1- Initial distribution and concentration of contaminants. The contaminant average concentration was 1800 mg L^{-1}, but decreases towards Dyala River. 2- Locations of contaminant sources: the cells in the waste dumping and landfill location (the triangular area, Figure 2B) were considered the source of the contaminant. Figure 3 shows source and distribution of the contaminant concentrations in the modeled area. The

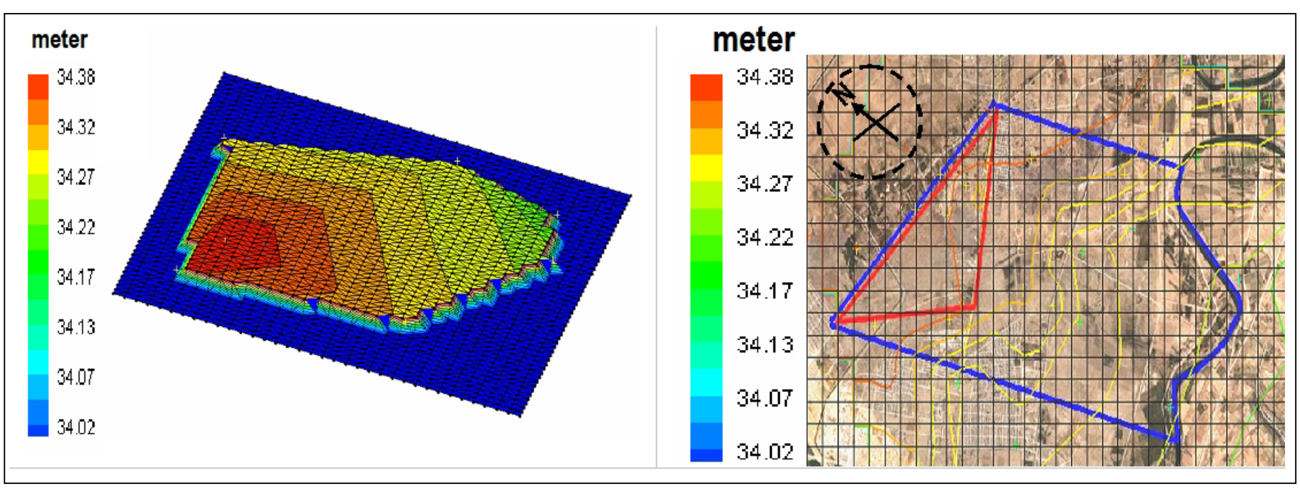

Figure 2. (A) 3D View of groundwater heads contour (B) contour map of groundwater heads.

Table 1. Characteristics of the geological formations.

Layer	Thickness (meter)	Hydraulic conductivity (m day^{-1})	Effective porosity
Clay	5.3	1.5	0.1
Clayey sand	4.7	2.0	0.29
Sand	7	5.0	0.37

biochemical parameters were selected within the range of those given in the literature (Rittmann and McCarty, 1980) and were not varied during the numerical experiments. The microbial parameters used in the reaction package are given in Table 2.

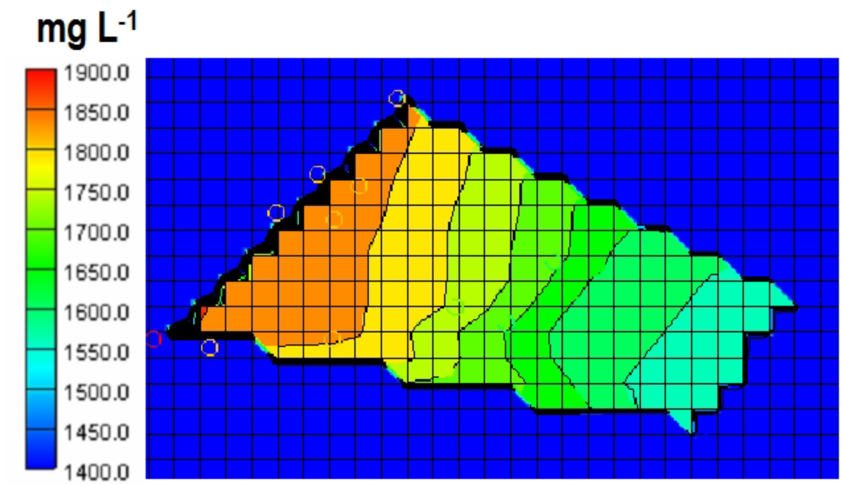

Figure 3. Distribution of the contaminant concentrations over the modeled area.

Table 2. Microbial parameters used in the model.

Parameter	Value
μ_{max}	0.1
k_{ed}	0.12
K_{ea}	0.1
$Y_{x/ed}$	0.005
$Y_{ea/ed}$	3.125
k_{decay}	0.001
k_{att}	70
K_{det}	1.0
Bulk density	1,600,000

MODEL SETUP

Boundary conditions

1- Constant head boundary (Dirichlet) and was determined by measured groundwater potential.

2- Drain (also constant head boundary by measuring the maximum head in Dyala River).

3- Constant flow boundary was assumed based on the experience with the site. The north and western boundaries were assumed constant flow.

The conceptual model for a contaminant transport addresses the major parameters and processes that affect contaminant concentrations and migration rates including:

1- Distributions of the major contaminant.

2- Contaminant sources.

3- Contaminant sinks.

4- Potential contaminant receptors.

5- Pathways from contaminant sources to receptors.

6- Processes that affect contaminant transport (e.g., biodegradation).

MODEL CONSTRUCTION IN GMS SOFTWARE

Constructing a model using GMS software consists of several steps which include selection of the packages to be used and defining all the required parameters. The main steps in the model construction in GMS were:

1. Determining the 3D grid (model grid size and spacing).

2. Determining the hydraulic conductivity/transmissivity, recharge, any additional model input.

3. Input of the hydraulic heads data and producing the groundwater heads contour map.

4. Specifying transient or steady state modeling.

5. Determining dispersion coefficients, degradation rate coefficients, etc.

6. Defining the boundary conditions.

7. Defining the elevations of the top three layers and input of their hydraulic and geological characteristics.

8. Building MODFLOW model and selecting the package required for this model like the drain, recharge, source/sink packages and setting up types of cells.

9. Building the MT3D model and run the RT3D simulation; this step includes selecting the bioreaction model and defining the parameters such as concentration of the contaminant, concentration of bacteria in the aqueous and soil phases, and concentration of the electron acceptor.

RESULTS AND DISCUSSION

The output of the MODFLOW and RT3D models were given in the form of graphs of contour map and cross sections that show the distribution of the contaminant at different times during the course of bioremediation. Figure 4 shows the progression of the treatment with the time. The local concentrations of contaminant decreased sequentially from 1800 mg L^{-1} to 1300 mg L^{-1} in some spots at the southern boundary. The average removal was approximately 100 mg L^{-1}. The presence of the swamps on the western boundary of the site is explained in Figure 4; for some geological reason the groundwater discharge to Dyala River seems to be less than the base flow that appears in the form of swamps. This phenomenon adds complexity to the site and impaired the reach of Dyala River in this region. Mass balance (Figure 5) showed that two years of bioremediation would remove only 10 Kg of the contaminant (out of total of 298 Kg) assuming that it is in the aqueous phase. This slow rate of removal is one of the major limitations of bioremediation, thus treating the groundwater contamination at the site would take very long time.

The concentration of the contaminant decreased more in the third and second layers in comparison to the top layer (Figures 6 and 7) likely because of the higher hydraulic conductivity and porosity which means faster and larger flow of groundwater.

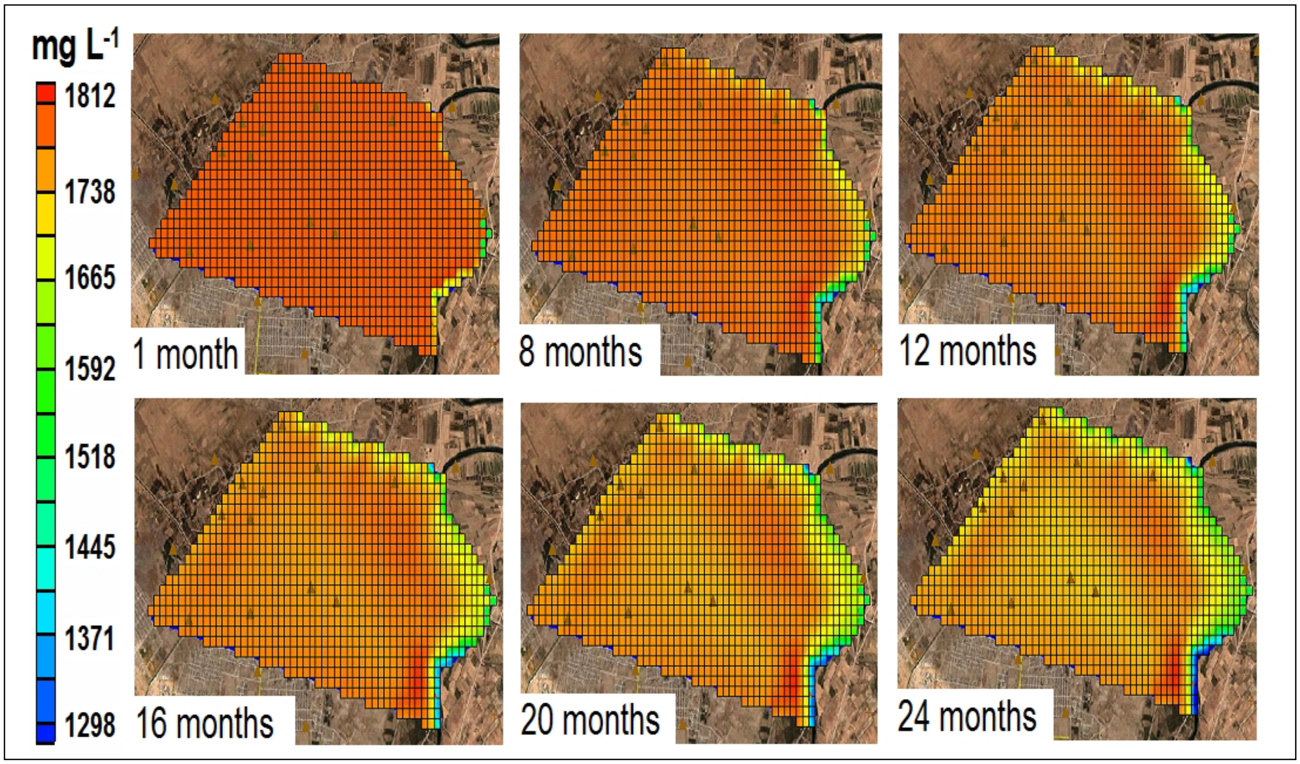

Figure 4. Distribution of the contaminant during bioremediation.

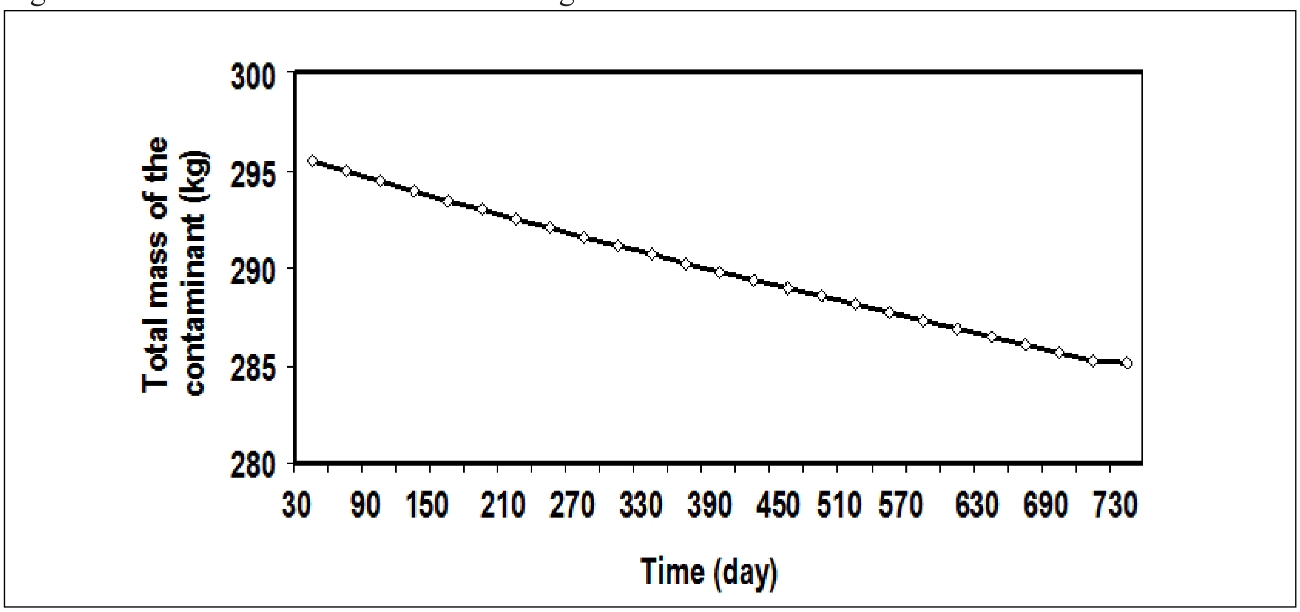

Figure 5. Change in contaminants mass during two years of bioremediation.

A pool of high concentrations of the contaminant (98.5% of the original level) remained after treatment in almost 20% of the area at the southwestern corner likely because of heterogeneity of the geological formations which decreased the degradation of the organic contaminant and created unreachable confined zone.

Simulation results suggested that in situ bioremediation occurred at the site, but with a low efficiency. Only 3.5% of the contaminant was degraded during two years, this indicates that most of the electron acceptor was consumed by inorganic reductants. Approximately 20% of the contaminated area showed the highest reduction (33%) in the contaminant concentration while 50% of the area showed modest reduction (12%).

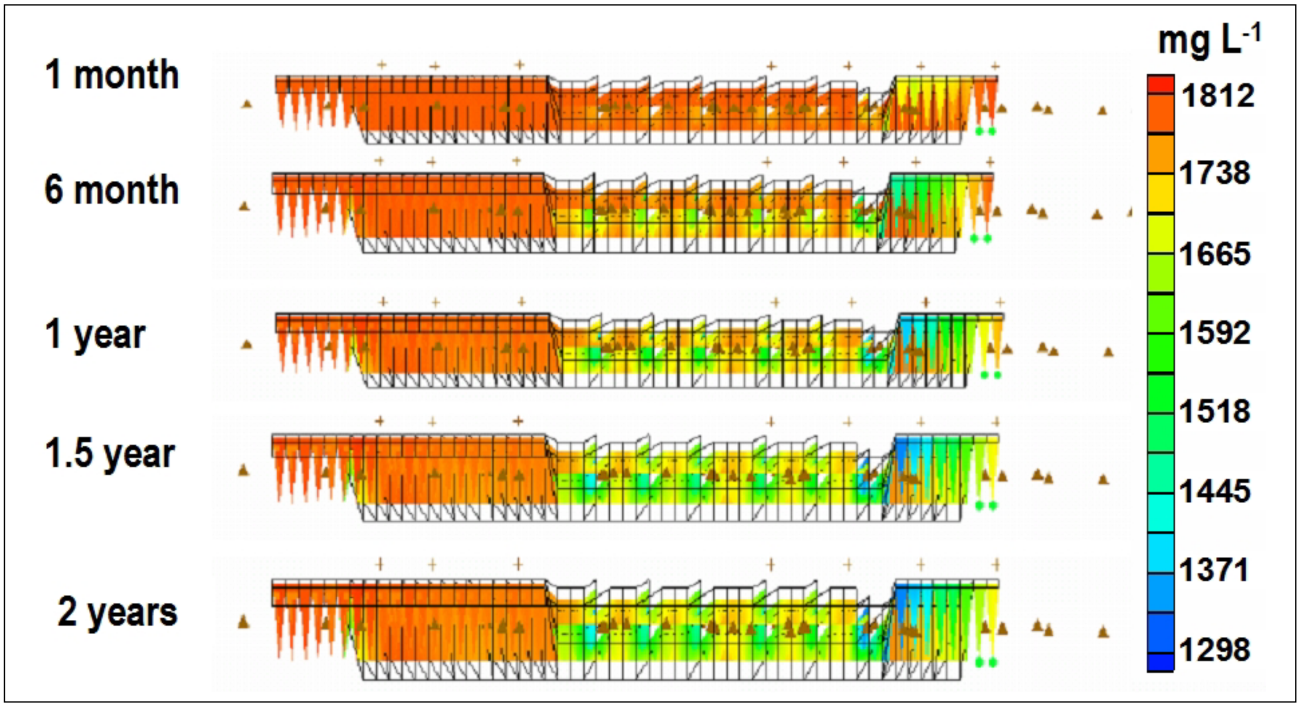

Figure 6. North-South contaminant distribution during the bioremediation period.

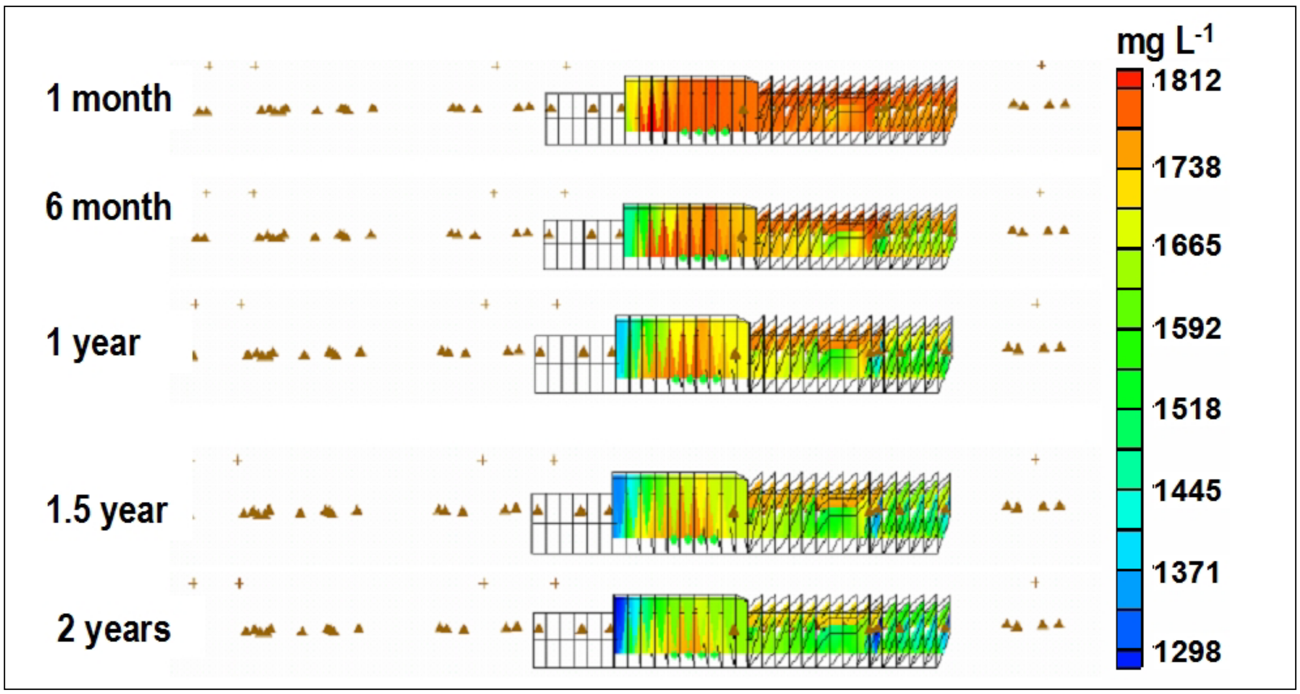

Figure 7. East-West contaminant distribution during the bioremediation period.

The results of this model demonstrated the usefulness of GMS software in comparison with other models developed to simulate flow, transport, and biodegradation of a monoaromatic hydrocarbon (such as benzene, toluene, etc.) in heterogeneous saturated aquifers. For example, Gallo and Manzini (1988) developed the mixed-hybrid finite element/finite volume numerical model and used it in a similar case. Their model showed that 16 years were not sufficient to obtain an acceptable degree of pollutant degradation and the concentration distributions computed showed highly irregular patterns, due to the heterogeneity of the domain. Gallo and Manzini (1988) concluded that heterogeneity affected the bioremediation by creating many unreachable spots which were observed as isolated pools of contaminant in the final concentration patterns.

CONCLUSION

MODFLOW and RT3D models (with GMS interface) were used to simulate bioremediation for an abandoned waste dumping and landfill site. The modeling study indicated that bioremediation occurred and gave a good prediction to what may happen. The model indicated that bioremediation will be helpful though it requires a relatively long time to treat groundwater contamination at the waste dumping site. Over two years bioremediation it is possible to remove 3.5% (10 kg) of the aqueous phase contaminant. Heterogeneity in the geological formations at the site resulted in a non-uniform distribution of the contaminant after bioremediation in some zones.

ACKNOWLEDGMENT

This paper was reviewed by Dr. Tirupati Bolisetti, Assistant professor, University of Windsor, Ontario, Canada, and Dr. Subba Rao Chaganti, Great Lakes Institute for Environmental Research (GLIER), Windsor, Ontario, Canada. The software of Groundwater Modeling System (GMS) v6.5 was kindly provided by Aquaveo, LLC, Utah - USA.

REFERENCES

Bailey, J.E., and D.F. Ollis. 1986. Biochemical Engineering Fundamentals, 2nd edition, McGraw Hill Book Company.

Bear, J., M.S. Beljin, and R.R. Ross. 1992. Fundamentals of ground-water modeling. EPA: Ground Water Issue. EPA/540/S-92/005. April 1992.

Bedient, P.B., and H.S. Rifai. 1992. Ground water contaminant modeling for biodegradation: a review, Journal of Hazardous Materials, Vol. 32, p. 225-243.

Brigham Young University. 2005. Groundwater Modeling System Software Version 6.5 Tutorial, Vol. I, II, III and IV. Brigham Young University-Environmental Modeling Research Laboratory.

Gallo, C., and G. Manzini. 1998. 2-D numerical modeling of bioremediation in heterogeneous saturated soils, Transport in porous media, Vol. 31, pp. 67-88.

Kresic, N. 1997. Quantitative solutions in hydrogeology and groundwater modeling. CRC Press; Lewis Publishers.

Rittmann, B.E., and P.L. McCarty. 1980. Model of steady-state biofilm kinetics. Biotechnol. Bioeng., Vol. 22, pp. 2359-2373.

Sun, N-Z. 2002. Modeling biodegradation processes in porous media by the finite cell method. Water Resources Research, Vol. 38, No. 3, 1029.

ADDRESS FOR CORRESPONDENCE
Noori M. Cata Saady
Department of Civil and Environmental Engineering
University of Windsor
Essex Hall – 205G,
401 Sunset Ave., Windsor, ON, N9B 3P4
Canada.

Email: saady@uwindsor.ca