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Simulation of Plume Behavior at the Macrodispersion Experiment (MADE1) Site by Applying the Coupled Markov Chain Model for Site Characterization

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Abstract: Numerical simulations of solute transport are performed in a highly heterogeneous field with a complex geological configuration at the Macrodispersion Experiment (MADE1) site, Columbus Air Force Base in northern Mississippi. The purpose of these simulations are two fold. The first is to illustrate how the coupled Markov chain model can be applied to delineate the complex geometrical configuration at the site. The second is to show how reliable this model is for predicting plume behavior in a highly heterogeneous subsurface. Although we adopted some assumptions like two-dimensional steady flow in confined aquifers, the results are quit satisfactory. The results emphasized that delineation of the geometrical configuration of the aquifer heterogeneity is the key to obtain accurate prediction of plume evolution in heterogeneous formations. The coupled Markov model is a powerful tool to characterize formation heterogeneity.

1. INTRODUCTION

The objective of this paper is to investigate how the coupled Markov chain (CMC) model, described in [1], can be applied to characterize heterogeneity at a well know tracer test site, Columbus Air Force Base in northeastern Mississippi, and moreover, on how CMC model is linked with flow and transport models to predict plume behavior at the site.

1.1 Site Description

A field tracer experiment, called the MADE1 site (first Macro-dispersion Experiment), is performed at Columbus Air Force Base in northeastern Mississippi [2]. The shallow unconfined aquifer that immediately underlines the site consists of an alluvial terrace deposit

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averaging approximately 11 m in thickness. The aquifer is composed of poorly sorted to well-sorted sandy gravel and gravelly sand with minor amounts of silt and clay. Soil mapping investigations adjacent to the site indicated that soil facies occur as irregular lenses and layers having horizontal dimensions ranging up to 8 m and vertical dimensions of less than 1 m. The spatial distribution of the hydraulic conductivity at the site was determined from 2187 measurements of conductivity obtained from borehole flowmeter tests conducted in 49 fully penetrating wells. For a full description of the site, reference is made to [2] and [3]. It is concluded from the site investigation that the Columbus site is distinct from previous natural gradient experiments in the literature because of the extreme heterogeneity of the aquifer, Its heterogeneity is at least an order of magnitude more than aquifers at other sites such as Borden landfill in Ontario, Canada [4] and Cape Cod, Massachusetts, USA [5]. It has also large-scale spatial variations in groundwater velocity and extensive set of hydraulic conductivity measurements for the aquifer.

The hydraulic head field at the site exhibits complex temporal and spatial variability that accounted for by the heterogeneity of the aquifer and large seasonal fluctuations of the water table. The flow field showed a converging groundwater flow towards a narrow zone of relatively high mean conductivity and an increasing groundwater velocity in the zone of convergence as shown in [6]. The converging groundwater flow field in the vicinity of the test site played an important role in the evolution of the tracer plume. General trends have been observed form the water table maps at the site. In the far-field region of the test site there is relatively high mean conductivity (i.e., of the order of 10^{-2}-10^{-1} cm/s corresponding to widely spaced contours whereas, the closely spaced contours in the near-field indicate relatively low mean conductivity (i.e., of the order of 10^{-3} cm/s). These trends are consistent with the borehole flowmeter measurements of hydraulic conductivity [3]. The specific yield estimates for the tests indicate that the aquifer is unconfined to semi-confined.

A bromide tracer, in a form of $CaBr_2$, was used as the primary tracer which performs conservative in field studies. The tracer is injected as a uniform pulse released into approximately the middle of the saturated zone with a minimal amount of disturbance to the natural flow field. 10.07 m^3 of groundwater containing 2500 mg/L of bromide was injected at a uniform rate over a period of 48.5 hours. The monitoring method is multilevel samplers to provide water samples from discrete zones in the aquifer. Concentration maps of vertically averaged bromide plumes and vertical cross-sections are presented in [6]. In the current study, a focus is made on plume presentation in vertical cross-sections. Snapshots of Bromide plumes at 49, 279 and 594 days since release are shown in Figure 1. The salient features of the bromide plumes can be summarized as: (1) Skewness of the concentration distribution in the longitudinal direction. This is due to the relatively low mean conductivity (i.e., approximately 10^{-3} cm/s) at the near-field where the main body of the plume is moving with relatively slow velocity (5-10m/year). (2) Most of the tracer stays close to the injection well. (3) Unexpectedly large vertical spreading of the plume. This is can be attributed to three reasons. Firstly, the artificial vertical gradient created by tracer injection. Secondly, the natural upward vertical gradients present in the vicinity of the injection site. Thirdly, the density difference since, the tracer solution is approximately 0.4% more dense than ambient groundwater so it may contribute to the downward spreading of the plume. (4) Maximum bromide concentrations of the bromide profile at 594 days were located in the upper part of the plume near the water table. (5) Reduction of the plume thickness that occurred between approximately 20 and 40 m down gradient from the injection point. This is due to natural channeling (preferential flow path) of the flow through a relatively permeable zone in this region. (6) Vertical extension of the plume down gradient after the observed convergent in (5). This is consistent with the downward gradient on the far-field region.

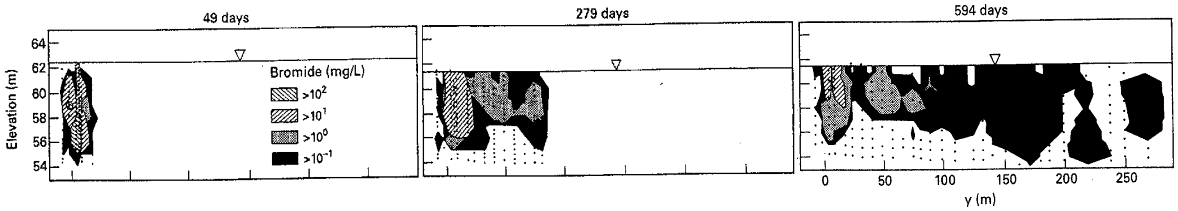

Figure 1. Three snapshots of the bromide plume at 49, 279 and 594 days [3].

2. APPLICATION OF THE 2D-COUPLED MARKOV CHAIN MODEL TO (MADE1) SITE

2.1 Coupled Markov chain model

The coupled Markov chain (CMC) model, developed by Elfeki [7] and extended by Elfeki and Dekking [1] to conditioning on multiple boreholes, is applied to MADE1 site. A brief description of the coupled Markov chain model is given below. The model is stochastic in nature that couples two chains. The first one is used to describe the sequence in lithology in the vertical direction, and the second chain describes the sequence of variation in the lithological structure in the horizontal direction. The two chains are coupled in the sense that a state of a cell in the domain is dependent on the state of two cells, the one on top and the other on the left of the current cell. This dependence is described in terms of transition probabilities from the two chains. An extension of the coupled Markov chain model to make conditioning on any number of boreholes possible is achieved [1]. The methodology is based on the concept of conditioning a Markov chain on future states. The conditioning is performed in an explicit way. This makes the methodology efficient in terms of computer time and storage in comparison with other techniques available in the literature.

2.2 Estimation of vertical direction transition probability matrix

In the MADE1 site, there are five different types of facies. The facies are described as open work gravel, fine gravel, sand, sandy gravel and sandy clayey gravel which are coded as 1, 2, 3, 4 and 5 respectively. It is assumed that the white space above the geological cross section of Figure1a is a hypothetical lithology coded with state number 6 and the space under the section is coded with state number 7. So, in total we deal with 7 states two of them are hypothetical. This is necessary to simulate the top and bottom boundaries of the geological section. The domain dimensions are 276×14.2 m. The vertical transition probability are calculated using a program called WELLLOG, which has been developed in the current study. Table 1 shows 7×7= 49 entries of the vertical direction transition probability matrix calculated from16 boreholes (shown in Figure 2b). These transitions are calculated in the vertical direction from top to bottom over a sampling interval of 0.1 m.

2.3 Estimation of horizontal direction transition probability matrix

Boreholes usually are insufficient to quantify spatial variability in the lateral directions, not only because of typically sparse lateral spacing but also unknown variations in depositional lateral directions. Trial-and-error procedure is adopted to find out the best estimate of the horizontal transition probability matrix. Table 2, 3 and 4 show three different forward (from left to right direction) horizontal transition probability matrices. The three matrices are diagonally dominant matrices (i.e. the diagonal elements are greater than the sum of the off-diagonal elements). The degree of diagonal dominancy increases from Table 2 to Table 4. It is also important to note that Table 3 is the vertical transition probability matrix. This was made on purpose to see if the vertical transition matrix could be used as an estimation for the horizontal one. The simulation results using the three matrices are presented in Figure 1 d, c and b that correspond to the horizontal transitions given in Table 2, 3 and 4 respectively. The results show that the increase in the degree of diagonal dominancy of the horizontal transitions improve the simulation results. However, the case of using the horizontal transition identical to the vertical transition still producing satisfactory results except for state 1 (appeared in yellow).

Table 1
Vertical transition probability matrix sampled over 0.1 m (Figure 1b).

State							
State	1	2	3	4	5	6	7
1	.879	.103	.009	.000	.009	.000	.000
2	.026	.911	.046	.009	.003	.000	.005
3	.003	.030	.897	.044	.010	.000	.016
4	.000	.006	.094	.869	.031	.000	.000
5	.000	.000	.003	.010	.961	.000	.026
6	.009	.014	.009	.005	.000	.963	.000
7	.001	.001	.001	.001	.001	.001	.994

Table 2
Forward horizontal transition probability (Figure 1c).

State							
State	1	2	3	4	5	6	7
1	.500	.100	.100	.100	.100	.100	.000
2	.100	.500	.100	.100	.100	.000	.100
3	.100	.100	.500	.100	.100	.000	.100
4	.100	.100	.100	.500	.100	.000	.100
5	.100	.100	.100	.100	.500	.100	.000
6	.001	.001	.001	.001	.001	.994	.001
7	.001	.001	.001	.001	.001	.001	.994

Table 3
Forward horizontal transition probability (Figure 1d).

State							
State	1	2	3	4	5	6	7
1	.879	.103	.009	.000	.009	.000	.000
2	.026	.911	.046	.009	.003	.000	.005
3	.003	.030	.897	.044	.010	.000	.016
4	.000	.006	.094	.869	.031	.000	.000
5	.000	.000	.003	.010	.961	.000	.026
6	.009	.014	.009	.005	.000	.963	.000
7	.001	.001	.001	.001	.001	.001	.994

Table 4
Forward horizontal transition probability (Figure 1e).

State							
State	1	2	3	4	5	6	7
1	.922	.015	.015	.015	.015	.015	.003
2	.015	.922	.015	.015	.015	.015	.003
3	.015	.015	.922	.015	.015	.015	.003
4	.015	.015	.015	.922	.015	.015	.003
5	.015	.015	.015	.015	.922	.015	.003
6	.015	.015	.015	.015	.015	.922	.003
7	.001	.001	.001	.001	.001	.001	.994

Influence of conditioning on different numbers of boreholes is investigated. Three scenarios are considered. These scenarios have been implemented by conditioning on 6, 9 and 16 boreholes as shown in Figure 2 (first row from left to right). The corresponding simulations are presented in Figure 2 (second row from left to right) respectively. The vertical and horizontal transition probability matrices used in the simulations are given in Table 1 and Table 4 respectively. In general, it is obvious that conditioning on less number of boreholes

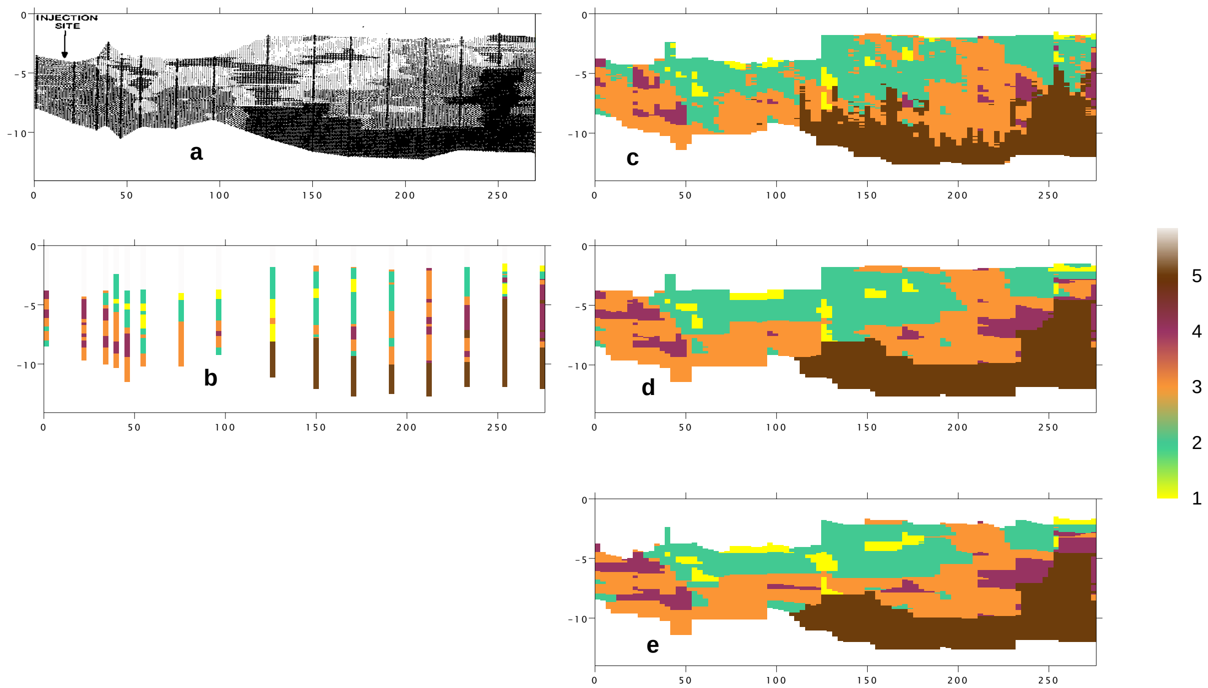

Figure 2. Comparison of different stochastic simulations of MADE1 site, shown in (a), using the calculated vertical transition probability matrix from 16 boreholes, shown in (Table 1) and assigning different horizontal transition probability matrices: (c) simulation by horizontal transition given in Table 2, (d) simulation by horizontal transition given in Table 3, (e) simulation by horizontal transition given in Table 4.

reduces details of the spatial heterogeneity of the aquifer. However, the main features and configurations are present in the results. The results by 9 boreholes still capturing the main features and configurations of the original geological sections.

3. NUMERICAL SIMULATIONS OF BROMIDE TRACER TEST AT MADE1 SITE

Data used in the simulation of the field experiment is collected from published literature about the site [2], [3] and [6]. These data are summarized in Table 5 and 6 together with simulation parameters. Computer codes developed by Elfeki [7] is used to perform the simulations. It is important to mention that the hypothetical states 6 and 7 in the domain are assigned a very low conductivity value 0.0001 m/day. The code is a finite difference model that solves the steady state saturated groundwater flow equation in heterogeneous medium under confined flow conditions with specified boundary conditions. The model considered the top and bottom of the domain as impermeable boundaries and the left and right sides as given head boundaries. The model calculates the hydraulic heads and the velocity field within the flow domain. A particle tracking random walk model has been developed to simulate solute transport in heterogeneous aquifers in saturated flow conditions. The random walk technique that is implemented in the code is based on the similarity of the transport equation and the Fokker-Planck equation [8].

Some assumptions have been made to perform the flow and transport simulations at the MADE1 site: (1) The groundwater aquifer is assumed confined which is not the case in the site. Therefore, we expect that the flow is faster in the simulation in comparison with the site. (2) Flow and transport is assumed to take place in two-dimensional domain, however it is three-dimensional in the site. Therefore, the conclusions are made in qualitative sense rather than in quantitative sense. (3) Temporal variability in the hydraulic gradient is negligible. Therefore, the flow field is assumed steady.

Table 5. Hydraulic conductivity values assigned to facies

Facies	Measured Conductivity (m/day)
1. Open work gravel	864.
2. Fine gravel	86.4
3. Sand	8.64
4. Sandy gravel	0.864
5. Sandy clayey gravel	0.0864

Table 6. Numerical values used in the simulation of the tracer experiment.

Parameter	Numerical Value
Domain dimensions	Lx=276. m, Ly=14.2 m
Domain discretezation	DX=3 m, DY=0.1 m
Average head difference at the site	0.7 m
Mean flow direction	Left to right, under gradient =0.0025
Injected tracer mass of bromide	2.5 kg
Number of particles	1000,000 Particles
Time step in calculations	0.5 Day
Longitudinal pore-scale dispersivity	0.10 m
Transverse pore-scale dispersivity	0.01 m
Effective porosity	0.35
Average aquifer thickness	10.m
X-coordinate of injection	12.m
Molecular diffusion coefficient	0.0

4. DISSCUSION OF SIMULATION RESULTS

Figure 2 shows the plume data and simulation results conditioned on 6, 9 and 16 boreholes in terms of plume concentrations at specified times 49, 279 and 594 days respectively since release. The simulation results reproduced many features of the flow field and the plume behavior such as:

1. Closely spaced contours in the near-field indicate relatively low mean conductivity at the injection site.
2. In the far-field region of the test site there is widely spaced contours that correspond to relatively high conductivity.
3. Skewness of the concentration distribution in the longitudinal direction. Most of the tracer stays close to the injection well. This is due to the relatively low conductivity zone in the near-field.
4. Large vertical spreading of the plume at the vicinity of the injection well. The simulation starts with an initial vertical dimension of the plume with about 4 m.

While, this vertical dimension increases very much when it evolves in time although lateral dispersivity is very small (0.01 m). This is due to natural upward vertical gradients present in the vicinity of the injection site.

5. Maximum bromide concentrations of the bromide profile at 594 days were located in the upper part of the plume.
6. Reduction of the plume thickness that occurred between approximately 20 and 40 m down gradient from the injection point. This is due to natural channeling (preferential flow path) of the flow through a relatively permeable zone in this region.

Vertical extension of the plume down gradient after the observed convergent in (6). This is consistent with the downward gradient on the far-field region.

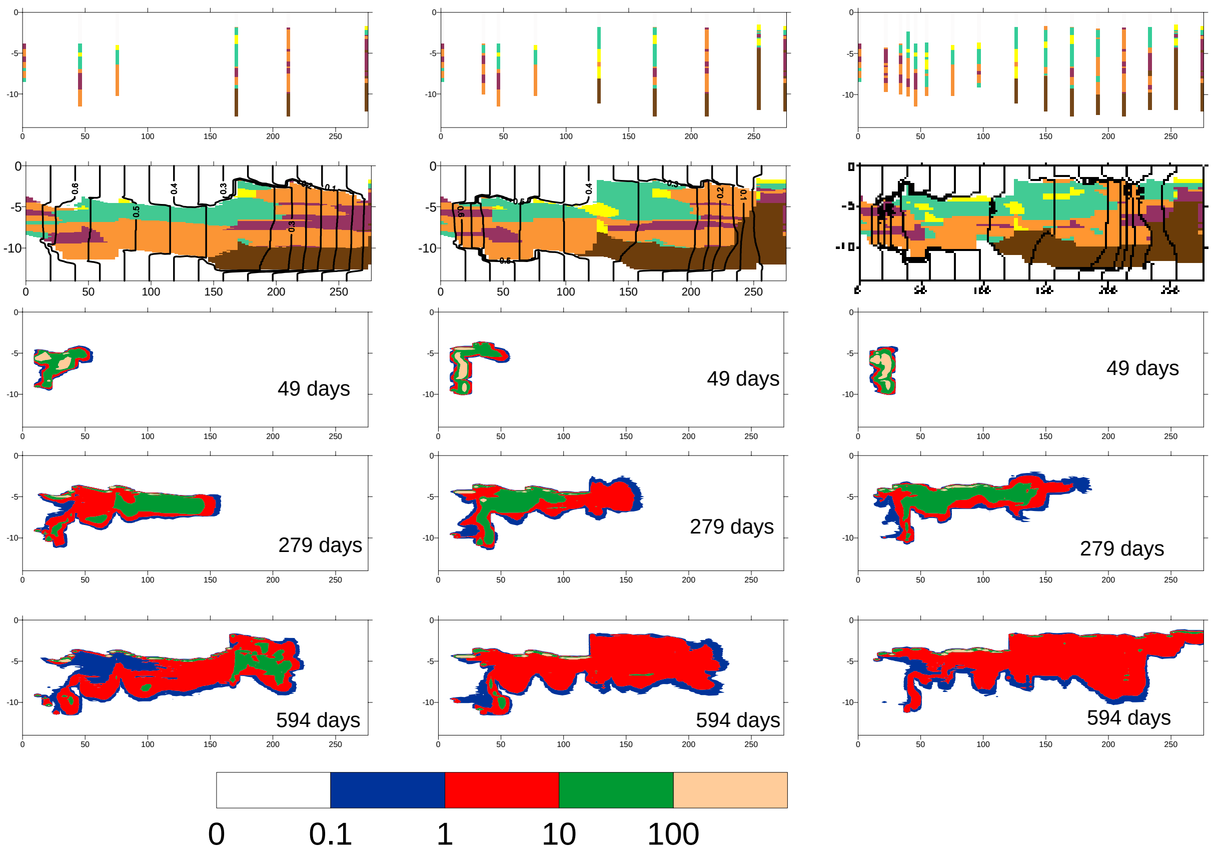

Figure 3. Comparison of numerical flow and transport simulations conditioned on number of boreholes. Left most column is a geological simulation of the aquifer conditioned on 6 boreholes with the corresponding plume evolution at 49, 279 and 594 days respecivley. Second and third columns from the left side are similar to left most column but conditioned on 9 and 16 boreholes respectively. The concentration scale is in (mg/L).

5. CONCLUSIONS

Some conclusions can be drawn from this study:

1. The coupled Markov chain model has shown successful results in delinating the complex geological configuration of the aquifer at the MADE1 site.

2. Forward horizontal transition probability matrix given in Table 4 is capable of capturing the main features of the Columbus site when conditioned on the given 16 boreholes. Values of the diagonal elements of the horizontal transition probability matrix which have been taken equal to 0.922 for the facies are sufficient to produce the main heterogeneous features in the site.
3. Flow and transport simulations capture the salient features of the flow field and the large scale plume behavior at the site, although some assumptions are made regarding dimensionality of the problem, steady state and confined flow conditions. This means that delineation of the large scale geological configuration is crucial to obtain satisfactory simulation results in terms of plume shape.
4. Conditional simulations on 16, 9 and 6 boreholes show reasonably the same plume behavior in terms of average longitudinal and vertical extensions specially in the far-field. This gives more reliability on the use of the coupled Markov chain model for subsurface characterization.

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