

# Stochastic simulation of shallow aquifer heterogeneity and its using in contaminant transport modeling in Tianjin plains

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**Abstract:** Shallow aquifers of Tianjin Plain formed by alluvium, marine and lacustrine sedimentary sequences, and resulting complex structure impose challenges to modeling groundwater flow and contaminant transport in it. To solve the problem and prove its feasibility, this study utilizes TProGS (Transition Probability Geostatistical Software) to describe hydrogeological structure of engineering sites, and then simulates contaminant transport by integrated using MT3D (Modular Three-Dimensional Transport Model) with traditional layered assignment approach and transition probability geostatistical approach respectively. The results show that aquifer structure on local scale is effectively described by TProGS and there is a smaller plume distribution in modeling with transition geostatistical approach than that with traditional layered assignment approach, it's also more in line with the groundwater flow direction. It illustrates the advantages of stochastic simulation in detailed conceptualization of hydrogeological structure. Furthermore, it demonstrates that integrated utilizing stochastic simulations and MT3D is more practicable than traditional approach in engineering practice for both probabilistic estimation of hydraulic conductivities and probabilistic assessment of contaminant plume capture at a heterogeneous field site.

**Keywords:** Stochastic Simulation, Heterogeneity, TProGS, MT3D, Tianjin Plains

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## 1 Introduction

Constraints in accurate and realistic groundwater flow modeling are caused by the difficulty of characterizing the geological structure [1]. And the subsurface heterogeneity heavily influences the distribution of contaminants in the groundwater system [1]. However, the aquifer properties can vary as much as two orders of magnitude within a ten-foot radius and the scale of heterogeneity is often smaller than the data availability (e.g. Borehole spacing) [2]. Therefore, the selection of appropriate approach for accurate conceptualization of geological structure and description of aquifer heterogeneity is the critical work for modeling contaminant transport.

One approach for dealing with model heterogeneity is stochastic simulations based on multiple equally plausible candidate realizations of the site heterogeneity [3]. Stochastic simulations are particularly well-suited to local scale models since the resulting complex heterogeneity is more representative of actual stratigraphic deposition [3]. Among multiple methods of generating stochastic simulations of

hydraulic parameters, the transition probability approach of indicator geostatistics is the relatively robust and practical one for representing heterogeneity in 3-D aquifer stratigraphy. The powerful tool called TProGS (Transition Probability Geostatistical Software) developed by Carle operates on the basis of transition probabilities [3] and it has been successfully applied to simulate highly heterogeneous subsurface systems by constraining the simulation to borehole data [4].

Compared to the traditional indicator methods, the distinct strength of TProGS is the simple and direct incorporation of explicit facies manifestations like means lengths, volumetric proportions and juxtapositional tendencies into model [1]. In other words, the transition probability approach provides the conceptual framework to incorporate the geologic interpretation into the development of 3-D Markov chains models of spatial variability [5,6,7,8,9,10]. Furthermore, TProGS also provides the consideration for asymmetric tendencies such as fining-upwards, which is common in geological processes but not be captured by simply using a variogram model. Generally speaking, the transition probability approach couples geologic knowledge and

mathematical manipulations to overcome the shortcomings of the traditional indicator geostatistics methods.

The objectives of this paper are to prove that if it is more appropriate to conceptualize aquifer structure in detail by utilizing TProGS and then to illustrate the advantages and significances for the Environmental Impact Assessment of engineering project and groundwater pollution assessment with integrated utilization of stochastic simulations and MT3D.

## 2. Study Sites

Two sites we selected located at Tianjin urban, which is situated in northeast of North China Plain (see Fig.1). At present, with the rapid expansion of the city and population growing, extensive groundwater exploitation activities are taking place, and many new factories have been set up in research area, this process ultimately caused an unprecedented pollution risk to groundwater resources, especially the shallow aquifer that plays an important role in local ecological environment has been polluted seriously already. Accurate assessing the impacts of new factories to groundwater, and correct predicting contaminant transport in groundwater flow are big challenges for local government and scientists. The two sites we choose in this study are located in difference places, one is located in urban centre, at where the shallow groundwater have disturbed and contaminated. The other is located in core region of Binhai New Develop Area, this place is currently developing, many factories and buildings promise to erect in near future. In the traditional groundwater flow simulation, all these two places were conceptualized as the same aquifer structure except for geometry.

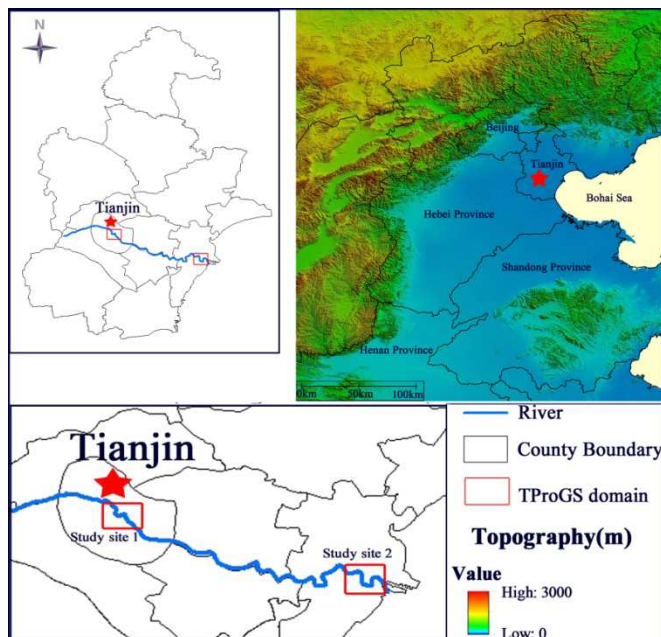


Fig 1. Location of two study sites in Tianjin plains

The problem of identify hydrogeologic structure on engineering site scale has not been well solved in local

environmental impact assessment. As stated in study objective, this study attempt to identify the differences of the hydrogeological structure between two sites not far from each other, and evaluate its effect on groundwater flow and contaminant transport prediction.

The hydrostratigraphy of the study site is characterized by the shallow aquifer system and the deeper fresh aquifer system, these two groundwater system hydraulically isolated with a thick impermeable clay layer. This study focuses on the shallow aquifer system which has a more sensitivity to anthropogenic activity. The shallow aquifer system composed of Holocene and late Pleistocene sedimentary sequences resulting from the deposition of continental alluvial, lacustrine, palustrine and marine sediments, which features by interbedded silt, clay, fine sand and sandstone. Two continuous transgressive sandy deposits are the main high permeability aquifers. Major marine transgressions and regressions and the resulting shifts of facies are the chief determinants of the sequences of high- and low-permeability sediments. Complicated sedimentary sequence causes difficulties to apply layered assignment parameters method for aquifer properties in this area, but it is an ideal place for stochastic simulation application.

## 3. Theoretical Backgrounds

TProGS (Transition Probability Geostatistical Software), included in the software Groundwater Modeling System (GMS), is a software package based upon the transition probability geostatistics approach to simulate spatial variability through the implementation of Markov Chains. It allows the simulation of multiple realizations through two mutually dependent steps: sequential indicator simulation (SIS)[11] and simulated quenching [6,12]. SIS algorithm establishes the initial configuration using transition probability-based co-kriging estimation [13]. And then the simulation quenching optimization algorithm will iteratively improve conditional simulation in terms of matching simulated and modeled transition probabilities, in other words, it will reshuffle the initial configuration[12]. The following steps are necessary to accomplish the TProGS implementation[3]: GAMEAS processes borehole data and calculates bivariate geologic characteristics (e.g., material proportions, transition probability, etc.). MCMOD develops one- and three- dimensional Markov chain models of spatial variability. TSIM generates three dimensional, cross correlated geological realizations.

### 3.1. Transition Probability

The transition probability is defined as

$$t_{j,k}(h_{\phi}) = \Pr\{k(x+h)|j(x)\}$$

where  $h_{\phi}$  represents the lag distance in direction  $\phi$ ;  $j, k$  are two categories, maybe  $j=k$ ;  $x$  is a location in space. As shown from above equation, the transition probability can be described as “the probability of category  $k$  occurs at the

location  $x+h$  based on the condition that category  $j$  occurs at location  $x$ ".

### 3.2. Markov Chain

Markov chain assumes that the future condition only depends on the current condition, not the past and the result of the  $n$  time only was impacted by the  $n-1$  result during the transition process of some factors in a system. 3-D Markov chain model simply but efficiently offers a mathematical method for the simulation of geostatistics spatial variability. Mathematically, the Markov transition probability matrix in primary direction  $\Phi$  was defined with the exponential matrix formal:

$$T(h_\Phi) = \exp(R_\Phi h_\Phi) = \begin{bmatrix} t_{11,\Phi} & \cdots & t_{1k,\Phi} \\ \vdots & \ddots & \vdots \\ t_{k1,\Phi} & \cdots & t_{kk,\Phi} \end{bmatrix}$$

where  $k$  is the number of categories;  $h_\Phi$  represents the lag distance in direction  $\Phi$ ;  $R_\Phi$  denotes the transition rate matrix in direction  $\Phi$ , it is defined as:

$$R_\Phi = \begin{bmatrix} r_{11,\Phi} & \cdots & r_{1k,\Phi} \\ \vdots & \ddots & \vdots \\ r_{k1,\Phi} & \cdots & r_{kk,\Phi} \end{bmatrix}$$

where  $r_{jk,\Phi}$  denotes the transition rate from category  $j$  to category  $k$  per unit length and  $j \neq k$ . It is obtained via the formula:

$$r_{jk,\Phi} = \frac{\partial t_{jk}(h \rightarrow 0)}{\partial h_\Phi}$$

And when category  $j=k$ , that is  $r_{jj,\Phi}$ , it denotes the self-transition rate of category  $j$ . It is defined through:

$$r_{jj,\Phi} = -\frac{1}{\overline{L}_{j,\Phi}}$$

where  $\overline{L}_{j,\Phi}$  represents the mean length of the category  $j$  in the direction  $\Phi$ , it is conceptually defined as

$$\overline{L}_{j,\Phi} = \frac{\text{total length of } j \text{ in direction } \Phi}{\text{number of embedded occurrences of } j}$$

However,  $t_{jk,\Phi}$ , the element in transition probability matrix  $T(h_\Phi)$ , cannot be directly calculated by  $t_{jk,\Phi}(h_\Phi) = \exp(r_{jk,\Phi} h_\Phi)$ . The eigenvalue analysis of the transition probability matrix, as the following equation shows, is essential.

$$\exp(Rh) = T(h) = \sum_{i=1}^k \exp(\lambda_i h) Z_i$$

$\lambda_i, Z_i$  denote the eigenvalue and eigenvector of the transition rate matrix respectively.

So for the current system composed of four categories, the transition rate elements are calculated by:

$$t_{jk}(h) = p_k + z_{jk,2} \exp(\lambda_2 h) + z_{jk,3} \exp(\lambda_3 h) + z_{jk,4} \exp(\lambda_4 h)$$

where  $p_k$  is limiting probability of category  $k$ .

Once the transition probability curve for the vertical direction was accomplished, the combination of Walther's Law and geologic knowledge is indispensable for the development of the transition probability curves in lateral ( $x$  and  $y$ ) directions. It is because that rarely is the quantity of data adequate to develop an accurate model in lateral directions. And Walther's Law states that vertical successions of deposited facies represent the lateral succession of environments of deposition. However, one issue will arise when applying vertical transition trends to lateral directions is how to work out asymmetric vertical trends like fining upwards. Take a typical condition in fluvial deposition for instance, sand tends to deposit on gravel. The transition rate of gravel to sand is greater than sand to gravel because of the fining upward trend. Therefore, in order to determine a transition rate for lateral conditions, the transition rate between the two categories should be equivalent or symmetric as defined via:

$$r_{jk} = \frac{p_k}{p_j} r_{kj}$$

When finish the calculation of Markov chains in three primary directions, the MCMOD will be utilized to enable the generation of 3-D Markov chain model. So the transition rate in faculative direction is defined as:

$$|r_{jk,\Phi}| = \sqrt{\left(\frac{h_x}{h_\Phi} r_{jk,x}\right)^2 + \left(\frac{h_y}{h_\Phi} r_{jk,y}\right)^2 + \left(\frac{h_z}{h_\Phi} r_{jk,z}\right)^2} \quad \forall j, k \neq \beta$$

where  $\beta$  is the background material and  $h_x, h_y, h_z$  is the lag distance of the  $x, y, z$  direction respectively, they are the components of the lag length in faculative direction:

$$h_\Phi = \sqrt{h_x^2 + h_y^2 + h_z^2}$$

And the last required is that the discrete-lag distance Markov chains should be transferred into the continuous-lag distance Markov chains by:

$$R_\Phi = \frac{\ln[T(\Delta h_\Phi)]}{\Delta h_\Phi}$$

### 3.3 Sequential Indicator Simulation and Simulated Quenching

The initialization step utilizes the sequential indicator simulation (SIS) algorithm described by Deutsch and Journel [13], except that a transition probability-based indicator cokriging estimate is used to approximate local conditional probabilities by

$$\Pr\{k \text{ occurs at } x_0 | i_j(x_\alpha); \alpha = 1, \dots, N; j = 1, \dots, K\} \\ \approx \sum_{\alpha=1}^N \sum_{j=1}^K i_j(x_\alpha) w_{jk,\alpha}$$

where  $N$  is the number of data,  $K$  is the number of categories,  $w_{jk,\alpha}$  represent a weighting coefficient, and  $i_j(x_\alpha)$  represents the value of an indicator variable

$$i_j(x_\alpha) = \begin{cases} 1, & \text{if category } j \text{ occurs at } x_\alpha \\ 0, & \text{otherwise} \end{cases} \quad j = 1, \dots, K$$

The transition probability-based cokriging system of equations [5,14] for computing the weighting coefficients is

$$\begin{bmatrix} T(x_1 - x_1) & \cdots & T(x_N - x_1) \\ \vdots & \ddots & \vdots \\ T(x_1 - x_N) & \cdots & T(x_N - x_N) \end{bmatrix} \begin{bmatrix} W_1 \\ \vdots \\ W_N \end{bmatrix} = \begin{bmatrix} T(x_0 - x_1) \\ \vdots \\ T(x_0 - x_N) \end{bmatrix}$$

where,

$$W_\alpha = \begin{bmatrix} w_{11,\alpha} & \cdots & w_{1K,\alpha} \\ \vdots & \ddots & \vdots \\ w_{K1,\alpha} & \cdots & w_{KK,\alpha} \end{bmatrix}$$

The quenching step attempts to solve the optimization problem of

$$\min \left\{ 0 = \sum_{i=1}^M \sum_{j=1}^K \sum_{k=1}^K [t_{jk}(h_i)_{\text{MEAS}} - t_{jk}(h_i)_{\text{SIM}}]^2 \right\}$$

where “0” denotes an objective function, the  $h_i$  denotes  $l = 1, \dots, M$  specified lag vectors, and “MEAS” and “SIM” distinguish measured and simulated (measured from the realization) transition probabilities, respectively [6,12,13,15].

## 4. Simulation Processing and Results

### 4.1. Collection and Collation of Borehole Data

Table 1. The hydrogeological parameters of the materials

Property	Material			
	Silt clay	Muddy clay	Silt	Silt sand
Horizontal hydraulic conductivity (m/d)	0.2	0.5	0.9	1.2
Vertical hydraulic conductivity (m/d)	0.06	0.2	0.3	0.36
Porosity	0.3			
Longitudinal dispersivity(m)	20			
Recharge concentration(mg/l)	20000			

### 4.2. Development of Geological Structure Model

The collated borehole data will be firstly passed to a utility within TProGS called GAMEAS to compute a set of transition probability curves with a given sampling interval. When it completed a successful run, the results will be read into the corresponding data fields in the “Vertical Markov Chain” dialog to develop a Markov chain model for vertical direction.

There are totally 49 borehole logs with varying depths utilized to describe the spatial variability in study sites and the two sites with size of 52 km<sup>2</sup> and 78 km<sup>2</sup> respectively occupy 28 and 21 borehole numbers. In order to gratify for the software’s limitation which is imposed to keep data processing at a reasonable level, the totally eight geological formations has been grouped into four categories based on the similar grain size and hydraulic conductivity: muddy clay, silt clay, silt and silt sand.

Among the above four categories, the most repeated material which is “silt clay” was designed as the background material that fills in the remaining areas not occupied by other units. Fig.2 presents the locations of the borehole logging and the material textural distribution over the defined grid frame of the first study site according to the previous categorization.

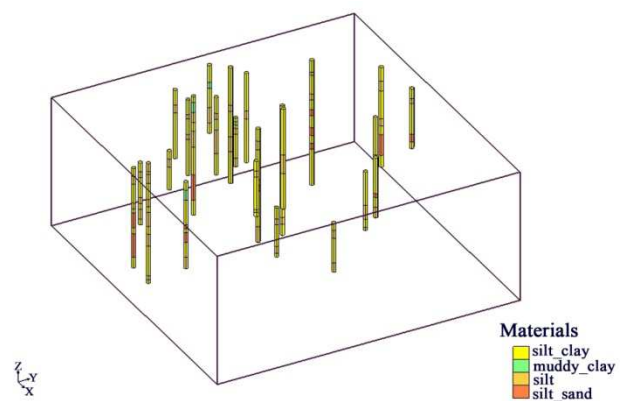


Fig 2. Borehole cross-section distributions in oblique view

In order to match the vertical grid spacing more closely to the thicknesses of the actual layers, the vertical thickness of the grid cells, determined by the user, must be as small as possible. So the two study sites were respectively conditioned on two 73×71×32/93×84×35 cell grids with the same discretization of 100m×100m×2m. And Table 1 shows their hydrogeological parameters obtained on the basis of geological exploration data.

Amongst the five alternative methods of generating Markov Chains, the “Edit the embedded transition probabilities” was selected for that it is a more intuitive method of generating Markov chains and is conducive to sites with data because embedded occurrences can be easily tallied from borehole data[2]. The computation result of transition probability matrixes in vertical direction of both study sites were respectively constituted as



$$t_{jk,z} = \begin{bmatrix} 3.675 & 1 & 0 & 0 \\ 0.048 & 11.246 & 0.762 & 1.190 \\ 0.021 & 0.979 & 4.512 & 0 \\ 0 & 0.917 & 0.083 & 5.750 \end{bmatrix}$$

$$t'_{jk,z} = \begin{bmatrix} 7.862 & 0.923 & 0.077 & 0 \\ 0.311 & 8.295 & 0.551 & 0.138 \\ 0.235 & 0.735 & 3.319 & 0.030 \\ 0 & 0.889 & 0.111 & 7.164 \end{bmatrix}$$

The diagonal elements represent self-transitions, that is, the transition probabilities from one category to itself. They coincide with corresponding vertical lens lengths (see Table 2) since the stacked beds of the same category are assumed not distinguishable from a single bed. And the off-diagonal elements per line satisfy

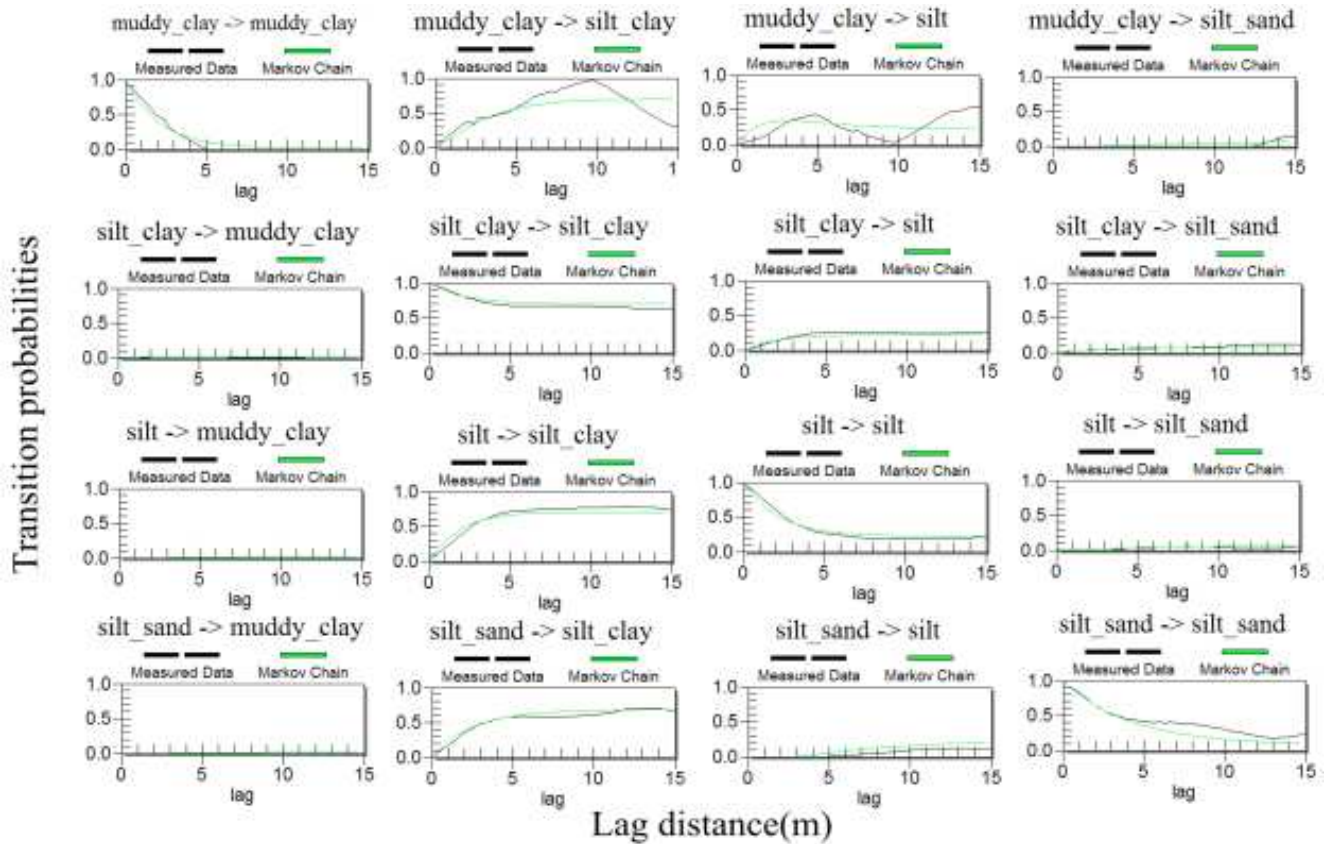
$$\sum_{k=1}^K t_{jk,z} = 1, \quad j \neq k$$

**Table 2.** The material proportions and lens lengths of two study areas

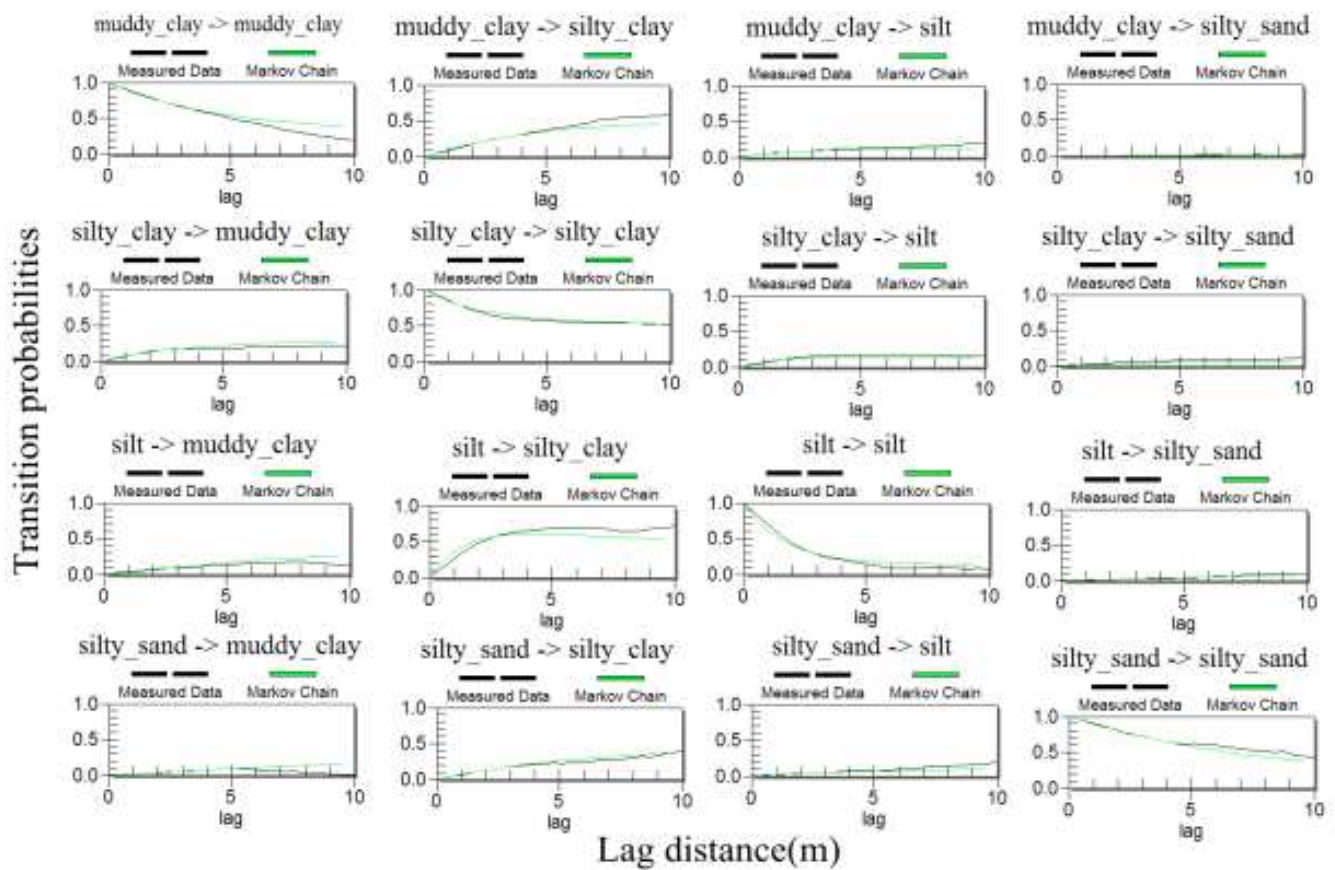
Material	Proportion		Lens length	
	Site 1	Site 2	Site 1	Site 2
Muddy clay	0.015	0.238	3.675	7.862
Silt clay	0.699	0.555	11.246	8.295
Silt	0.218	0.127	4.512	3.319
Silt sand	0.068	0.080	5.750	7.617

The values in Table 2 show the proportions and lens lengths of four categories in both study sites. The material proportion is represented by the probability corresponding to the flat part of the diagonal curve shown in Fig. 3. And the lens length of material is expressed as the point where a tangent line from the early part of the curves on the diagonal intersects the horizontal (lag distance) axis on each curve. And it should be

noted that lens length value of silt clay in site 1 is larger than site 2 (11.246 > 8.295), but the value of muddy clay is smaller (3.675 < 7.862). This indicates that the silt clay is more continuous in vertical direction in site 1 but muddy clay in more continuous in site 2. The phenomenon is displayed in Fig. 4 obviously.

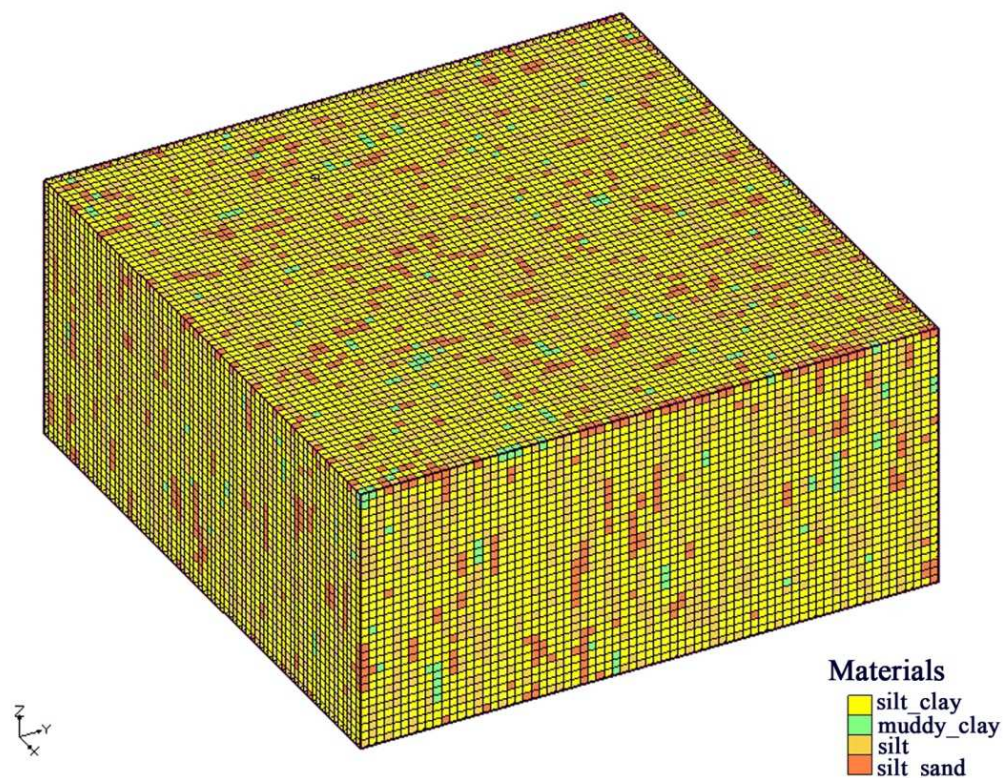


(a)



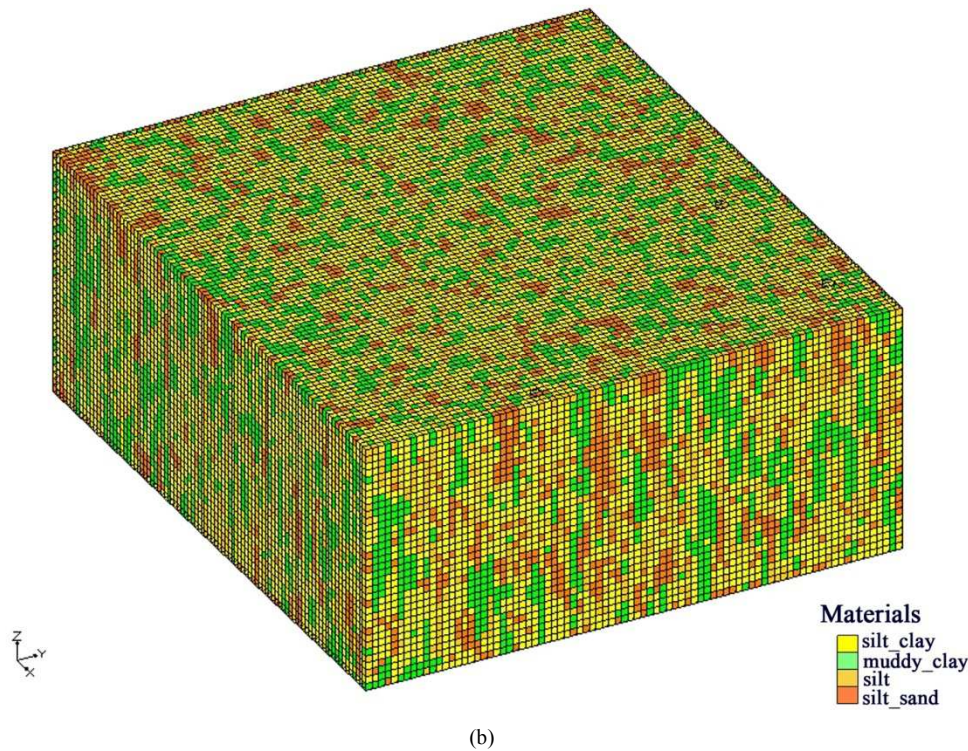
(b)

**Fig 3.** Measured transition probabilities curves (black lines) and Markov chain model (green lines) for a set of borehole data with four categories: a represents the result of site 1; b represents result of site 2



(a)





**Fig 4.** 3-D illustration of TProGS realization #1 filled with material colors: a represents the result of site 1; b represents result of site 2

With the utility of MCMOD, the measured vertical transition probability curves associated with above transition probabilities of both study sites are shown by the black lines in Fig.3. The diagonal self-transitional curves start at a probability of 1.0 decreasing with distance and the off-diagonal transition probability curves start at zero probability increasing with distance and they are eventually flatten out at some distance.

Finally the TSIM algorithm finished the generation of three-dimensional, cross correlated conditional simulations. Figure 4 shows one of the realizations of stochastically generated geologic units that honor known data.

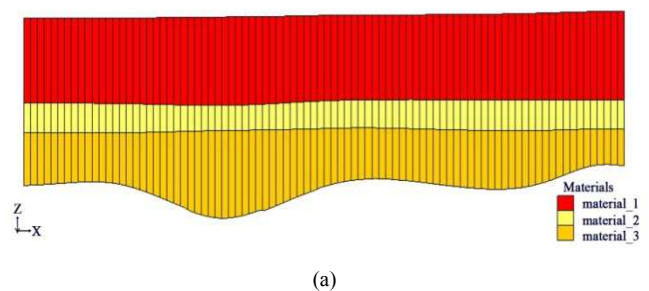
#### 4.3. Simulations of Contaminant Transport

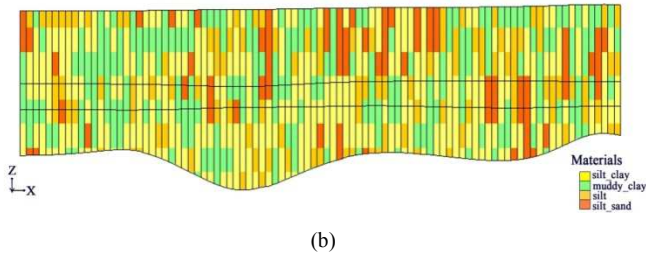
MT3D, developed by Zheng [16], is a 3-dimensional finite-difference calculation program that was used to model contaminant transport in groundwater systems. It combines the advection, dispersion and chemical reactions of contaminants comprehensively and it is able to deal with the complex sources and sinks and boundary conditions. For that, it can accurately model the contaminant transport process in confined, unconfined and leaky aquifers. Thereby, in recent years, Zheng and Wang[17] and Clement[18] proposed the improvement based on the previous program. It has been widely accepted in research of hydrogeology and water environment modeling.

On the basis of previous experience of the impact assessment of groundwater environment, we presume that there is a refuse landfill with area of 500m×500m in site 2 and the leachate permeates into underground with a fixed concentration. We utilize two different conceptual methods to

describe the geological structure of local site, in other words, different approaches for getting aquifer properties will be used in MT3D. Finally, contamination transport results of them will be compared intuitively to illustrate the advantages of the combination of TProGS with MT3D.

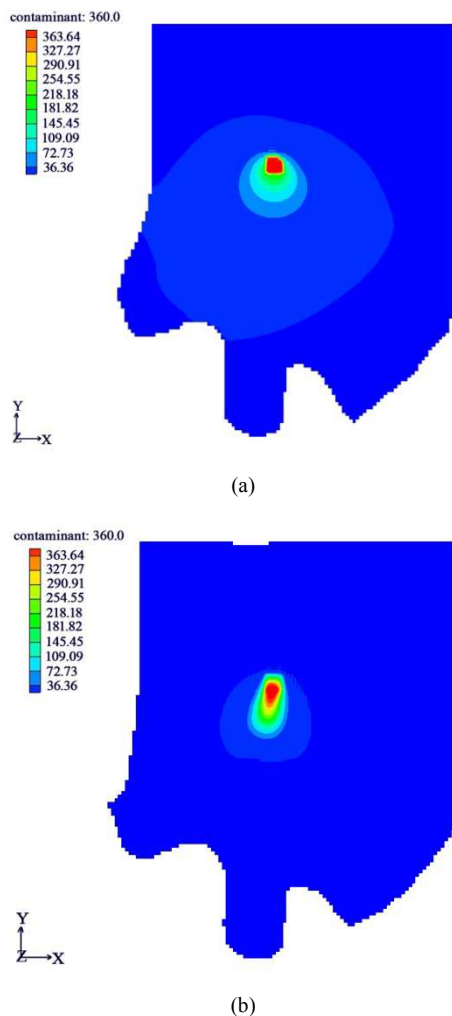
Fig.5 shows the side view of a MODFLOW grid with three curvilinear layers interpolated by elevations of true layers obtained through the borehole data. Fig.5 (a) is the result obtained through layered assignment method. On the basis of local lithology characteristic and experiences of previous numerical modeling, the model is conceptualized three layers and respectively assigned the aquifer properties (permeability coefficients, porosity, long dispersion, etc.). And Fig.5 (b) shows the result obtained through the combination of transition probability geostatistical approach with HUF (Hydrogeologic Unit Flow) package [19] in MODFLOW. The grid used in it is the same with upper one, but stochastic simulation program calculates the detail geological structure in a background grid which has a large number of layers.





**Fig 5.** Side view of geological structure of site 2 with two different conceptual methods: a represents the result with layered assignment method; b represents result of combination of transition probability geostatistical approach with HUF package

And then the geological conceptualization results and aquifer properties are utilized in MT3D simulations with the same boundary and starting conditions. The values of hydrogeological parameters are obtained based on the values shown in Table 1. The results of contaminant transport modeling with two methods are respectively shown in Fig.6(a) and Fig.6(b). Obviously, the pollution plume distribution in second condition is smaller and the movement direction of contaminant in it is consistent with the flowing direction of groundwater.



**Fig 6.** Plan view results of MT3D simulations with layered assignment approach (a) and transition probability geostatistic approach (b)

## 5. Conclusions

Hydrogeological structure differences on local scale between two engineering sites were identified by TProGS accurately. And compared with the pollution plume distribution of layered assignment approach, the affected area of contaminant with stochastic simulation method is smaller, and the movement direction of contaminant is consistent with the flowing direction of groundwater. Therefore, the modeling results with stochastic simulations have more realistic representation to the local situation. It illustrates that the application of stochastic simulations and its combination with MT3D is more practicable than traditional approach in engineering practice for both probabilistic estimation of hydraulic conductivities and probabilistic assessment of contaminant plume capture at a heterogeneous field site.

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