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The Influence of Conceptual Model of Sedimentary Formation Hydraulic Heterogeneity on Contaminant Transport Simulation

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Abstract—Development of heterogeneity model of layered sandy-clay formation and impact of this model on transport is considered. The lithological data of more than 250 wells that captured 300 meters formation at the investigated area of 40 km² are used for model of heterogeneity construction. Two models of heterogeneity were developed with using these well data: TP/MC model based on 3D Markov chain simulation for four hydrofacies and 2D kriging interpolation of thicknesses of elementary lithological layers. Simulation of conservative transport by particle tracking algorithm shows that horizontal transport along layers is similar for both models. The main difference is in vertical transport cross formation bedding. The kriging interpolation model gives more conservative results than TP/MC model due to larger characteristic horizontal length of layers in the kriging model. As the result vertical effective hydraulic conductivity of formation is in two times larger and the first particle arriving time is in four times faster in TP/MC model.

Keywords: heterogeneity, Markov chains, kriging, anisotropy, effective parameters, contaminant transport.

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INTRODUCTION

Sections of exploration, operation and monitoring wells drilled in the Siberian Chemical Combine (SCC) in the last 50 years were used as research facilities. Liquid radioactive wastes (LRW) have been buried since 1963 in aquifers with heterogeneous lithologies at the SCC, which is located in Tomsk. The geological cross section of the area has a clear two-tiered structure: the lower tier is the Paleozoic basement and the top one is the Mesozoic–Cenozoic cover. Mesozoic–Cenozoic sediments of the cover are presented as a complex alternation of sandy and clay layers. The layers form more sandy (aquifers) and more clayey (aquitard) rhythms. Seven aquifers, which are separated by waterproof layers, were allocated in the cross section of the covers with a total length of about 400 m in the SCC area. The LRW repository was located at landfills of deep disposal with aquifers located at depths of 270–390 m from the surface (Rybal'chenko et al.,

1994) and are composed of assorted sands mixed with clay material (Chernyaev et al., 2002). The sediments used for waste disposals have Late Cretaceous–early Paleocene ages (the Santonian Danian stage) and belong to the Sym retinue (Podobina, 2009); their formation occurred in continental and coastal–marine environments (a coastal lowland plain that was occasionally flooded by the sea) (Podobina, 2009; Gol'bert, 1987; Bulynnikova and Surkov, 1962).

Justification of geofiltration and geomigration predictive modeling in such heterogeneous environments depends on the detailed characteristics of the geofiltration heterogeneity. According to the results of the geostatistical analysis of the spatial distribution of patterns of lithological varieties that were conducted on the basis of lithological cuts through well sections in the area of the industrial sites at the SCC, a three-dimensional binary model of the spatial heterogeneity of well and impermeability differences was con-

structed previously (Pozdniakov et al., 2005). The aim of this research was to build a model that includes heterogeneity with a more detailed characterization of sediments of the Mesozoic and Cenozoic cover that comprise four hydrofacies taking the non-horizontal bedding of Paleozoic rocks in the area into account. As well, a comparison of the results of modeling migration with this model with results that were obtained on a simplified model based on the kriging interpolation of individual layers was performed.

MATERIALS AND METHODS

Geostatistical methods were used to construct models of spatial heterogeneity.

To create models of the spatial heterogeneity of sediments geostatistical modeling techniques are widely used. These can be divided into two main groups process-imitating and structure-imitating methods (Koltermann and Gorelick, 1996). The first group is based on the direct mathematical modeling of physical processes that control erosion, transport, and sediment accumulation. The main drawback of the construction of geofiltration and geomigratory models of specific objects is that the resulting models are not based on well data.

The second group of methods is based on statistical characteristics and probabilistic laws and numerically reproduces spatial structures without direct consideration of sedimentation. This group of methods includes statistical grid methods for reconstruction and modeling hydrofacies (HRM) using a wide range of input data and providing a detailed three-dimensional image of hydrofacies allocation in space (Falivene et al., 2007). Depending on their results, all HRMs can be divided into two groups: deterministic and stochastic (Falivene et al., 2007). Deterministic methods, such as the kriging method and the method of inverse distance weighting, give only one model as a result of interpolation algorithms; this model provides a smoothed estimate of parameters, especially as we move away from points of sampling. Stochastic methods provide a set of equiprobable models based on well data; each model reproduces the original geostatistical characteristics as well (the distribution law and spatial parameter correlation) (Dubrule, 2002).

Depending on the algorithm used all, HRMs can be divided into two groups: object-based and pixel-based methods (Falivene et al., 2007).

In the object-based method, lithologic bodies are modeled as distributed in space simple forms that are typical for sediments. When using object modeling in practice adequate results can be obtained only in cases where the layers have a high net sand coefficient (Pinus and Pairazy, 2008). Pixel-based methods fill each grid cell with hydrofacies in accordance with the calculated probability distribution function. Depending on the types of variables used, pixel methods can be continuous (porosity and permeability coefficients)

and indicator (for categorical variables, such as geological facies and lithological types of rocks). In both approaches, a description of the geological structures is implemented with the indicator variogram or indicator covariance function, but in the first approach, assessment of spatial structural models is problematic because of the small quantity of data on permeability and their distance in space (Weissmann, Carle, and Fogg, 1999). Indicator methods use more lithological data, allow one to simulate individual lithotypes, and do not depend on the type of distribution. The most frequently used pixel methods include the Truncated Gaussian simulation method (Truncated Gaussian simulation TGS) and Sequential indicator simulation method (Sequential indicator simulation, SIS).

The TGS method is used for continuous variables and is suitable for sediments that suggest a highly ordered model, while the SIS method is used for categorical variables and is used for a variety of environments of deposition (Falivene et al., 2007).

One important variety of traditional indicator geostatistics is the method of transition probabilities, which is based on Markov chains (TP/MC method) (Carle and Fogg, 1996, 1997; Weissmann and Fogg, 1999). Markov chains are used to predict preferred lithofacial sequences (Koltermann and Gorelick, 1996). The parameters that are used (number of categories, their proportions and mean lengths in the lateral and vertical directions, as well as juxtapositional tendencies) can be estimated empirically through direct measurements or by means of qualitative geologic interpretation (Weissmann, Carle, and Fogg, 1999; Weissmann and Fogg, 1999). Major advantages of the TP/MC method include the union of all available geological information for building a geologically plausible and realistic three-dimensional model of the spatial variability of sediments (this is especially important in nonvertical directions); the ability to include the average values of the thickness and proportion of categorical variables, along with the ability to simulate asymmetrical facies sequences (e.g., an increase or decrease in grains upward in the section; lithotype contacts can be both stepped and sharp as well); and the ease of geological interpretation of the transition probabilities compared with variograms or autocovariance functions (Elfeki and Dekking, 2001). There are many examples of the use of the TP/MC method for models creating lithologic heterogeneity in alluvial deposits (Weissmann and Fogg, 1999; Sivakumar, Harter, and Zhang, 2005; Dai et al., 2007; Sun, Ritzi, and Sims, 2008; Engdahl, Vogler, and Weissmann, 2010), glaciofluvial drifts (Ritzi et al., 2000; Proce et al., 2004), water-bearing sediments, and in marine (Yong and Fogg, 2003), lacustrine, and deltaic deposits (Bishop, Wallace, and Lowe, 2007).

Analysis of the Initial Data

On the basis of the detailed lithological subdivision of the sections of 261 wells (more than 50 km in total)

that were located within the ranges of deep burial of the SCC, 17 lithological types were determined in the studied interval (Table 1). The minimum output layers that were selected in the cross sections had sizes of 0.5 meters. Sand and clay predominate in the context of the total thickness (41% and 35%, respectively), followed by kaolin clay, clay breccia, clayey sand, sandy clay, conglomerate. The other encountered lithological differences made up less than 1% (Table 1).

Some of the differences were not typical of mesozoic–kainozoic cover, which appears to be due to the fact that individual wells revealed the weathering crust of the Paleozoic basement.

Depending on the characteristic values of the relative permeability of rocks all lithologic types that were encountered in the section were assigned to one type of hydrofacies: sand, clayey sand, sandy clay, and clay (Table 1). Thus, all strata of sediments were presented as four hydrofacies.

GEOSTATISTICAL MODELING

The thickness analysis showed that the distribution of thickness values of layers for each hydrofacies is described well by an exponential law, which corresponds to a simple Markov chain model; therefore, model construction of the lithologic heterogeneity was based on the TP/MC method. Building a model of heterogeneity was carried out using the T-PROGS software package (Carle, 1998).

The first step in modeling heterogeneity was to construct empirical curves of the transition probabilities of each hydrofacies compared to itself and to other hydrofacies, for which model (theoretical) curves of the transition probabilities were selected. For the vertical direction, the empirical and modeling curves are in good agreement (Fig. 1) and the resulting characteristic dimensions of the layers correspond to the calculated average values of the thickness layers (Table 2).

For the horizontal direction, the model curves describe the empirical data (Fig. 2). Therefore, selection of the typical lateral dimensions of layers was carried out using controlled repeated modeling of the three-dimensional structure of the medium heterogeneity. Then the option was chosen that coincided best with the curve of the fraction of each hydrofacies in the section, which was constructed according to the empirical data from the strip logs of wells, with the curve constructed using the modeling results (Fig. 3). Figure 3 shows that modeling of the proportions of each hydrofacies in a section presents the same trends as curves that were averaged according to wells. Here, the smoother form of the model results compared to the averaging of the wells is due to the large number of points used for this averaging. The typical model sizes of hydrofacies in the horizontal direction that were chosen as a result of this selection are given in Table 2.

The second step was the modeling of the three-dimensional distribution of hydrofacies by the SIS

Table 1. Proportions of the lithologic types in the section

Lithologic type	Total thickness, m	Proportions, %	Hydrofacies
Sand	21 492.4	40.63	sand
Gravelly sand	12.5	0.02	
Clay	18 393	34.77	clay
Kaolin clay	4059	7.67	
Clay breccia	3367	6.36	clayey sand
Clayey sand	3176.5	6.00	
Conglomerate	683.5	1.29	
Sandy clay	1375.6	2.60	sandy clay
Weathered shale	143.6	0.27	
Mudstone	64.5	0.12	
Lignite	46	0.09	
Weathered intrusion	30	0.06	
Siltstone	27.9	0.05	
Shale	10	0.02	
Sandstone	12	0.02	
Aleurolite	10	0.02	
Amount	52903.5	99.99	—

method on the basis of the selected model curves of the transition probabilities in the horizontal and vertical directions. During the modeling the fact that the surface of Paleozoic deposits is non-horizontal was taken into account by giving its real topography.

In plan view the sizes of the modeled area were 5000×8025 m (the grid size on the axes was 25 m), the vertical size was 350 m with a grid size of 1 m.

Thus, a model of the lithological heterogeneity of the studied area was obtained based on the TP/MC method (hereafter, model number 1). An alternative model of the lithological heterogeneity of the studied area was developed in the laboratory of geotechnological SCC monitoring; this model was created on the basis of geological interpretations of the same lithologic data (up to 261 wells) and in the same boundaries of the interpolated area in the plan view, but here another approach to data interpolation was used.

In the SCC model (hereinafter, model number 2) 159 elementary geological layers were allocated on the basis of informal analysis in the studied section. Using a two-dimensional kriging interpolation the boundaries of the top and bottom of each layer for all of the modeled area were then interpolated. The obtained

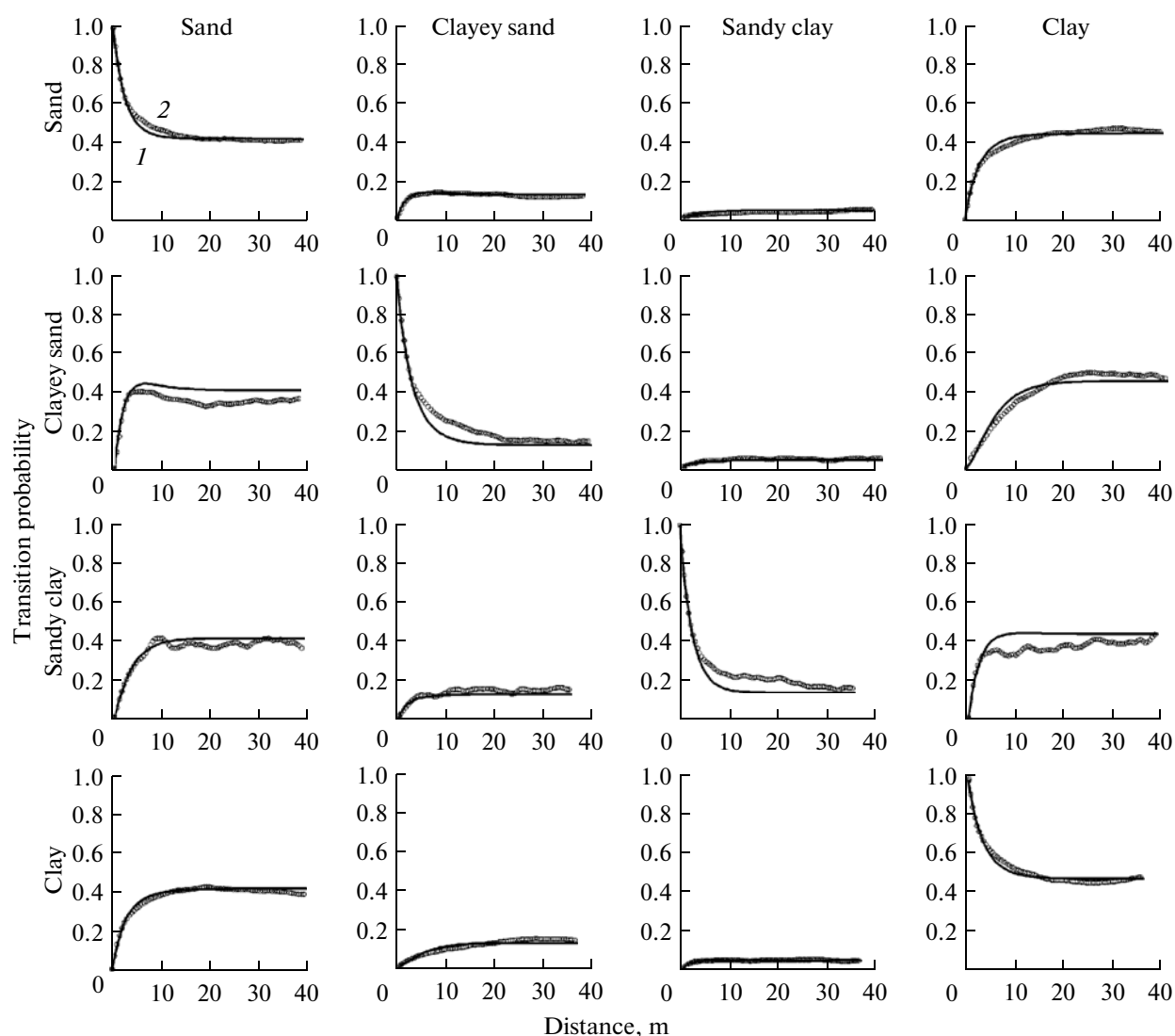


Fig. 1. Matrix of vertical-direction transition probabilities showing empirical data (2) and the Markov chain model (1).

result was corrected by testing the lack of cross layers and negative values of the thickness of each layer. Depositional termination was assumed.

Thus, at the first stage we obtained two models of the lithologic heterogeneity of the studied area: model number 1 on the basis of the TP/MC approach and

model number 2 using the kriging interpolation of the thickness of the elementary geological layers that were allocated in the section. Figure 4 shows a section along the western boundary of the modeled area for both models. For each lithologic heterogeneity model a representative sub-area stood out in the area of the

Table 2. The mean lengths and the proportions of the allocated hydrofacies in the studied section

Hydrofacies	Mean thickness, calculated from the wells, m	Model of the transition probabilities		Proportions, %
		Vertical mean lengths, m	Horizontal mean lengths, m	
Sand	5.7	4.6	400	45.8
Clayey sand	4.2	4	203	11.8
Sandy clay	2.9	2.9	100	3.3
Clay	4.9	4.9	349	39.1

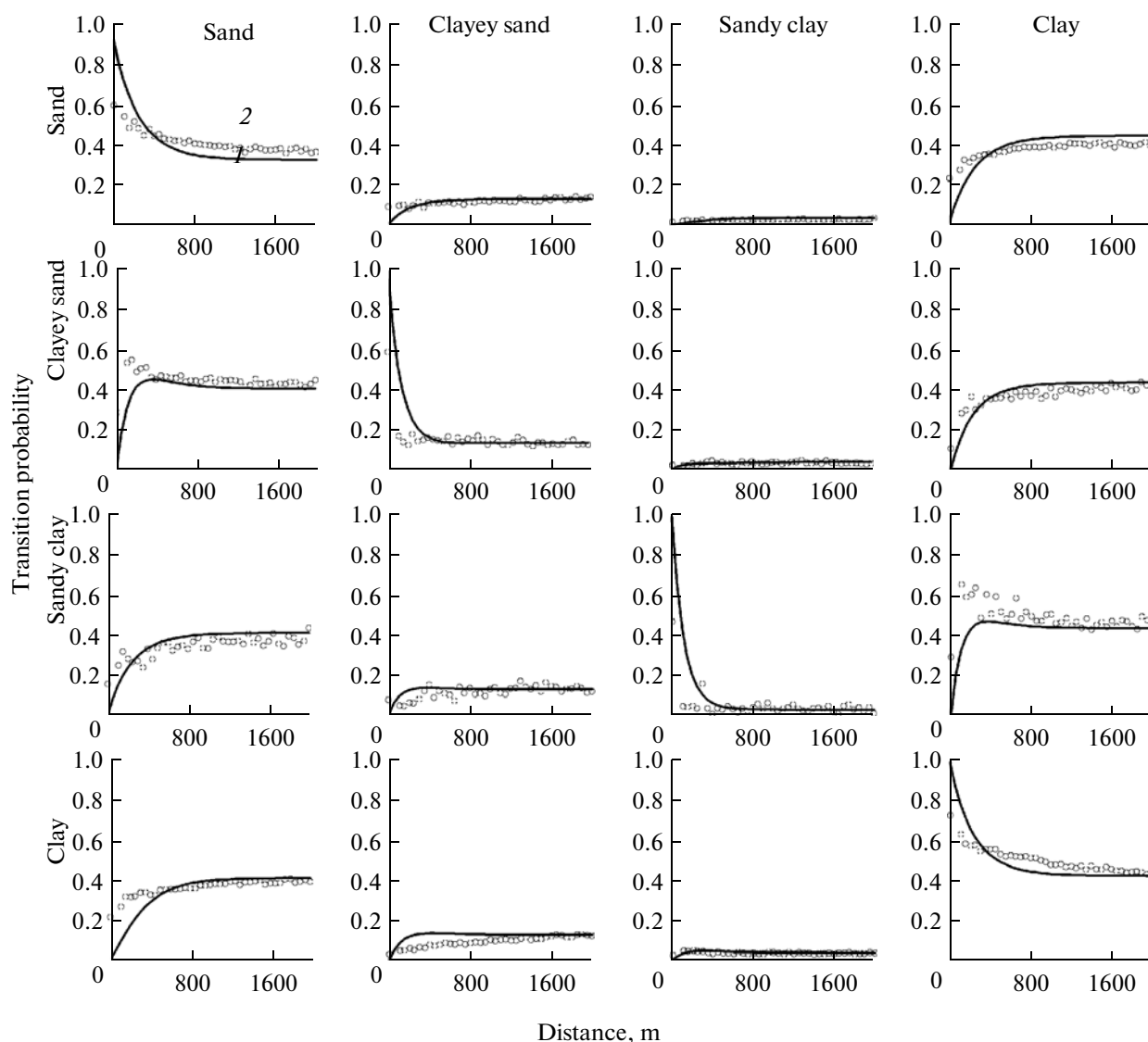


Fig. 2. Matrix of horizontal – direction transition probabilities showing empirical data (2) and the Markov chain model (1).

landfill of deep SCC disposal (with an interval of absolute boundaries from 100 m up to 200 m) with dimensions of $2500 \times 2500 \times 100$ m, including a million estimated units ($100 \times 100 \times 100$), which was used for further geofiltration and geomigratory modeling. The selected area is covered with a dense network of wells; thus, only one implementation of lithologic heterogeneity modeling was used by the TP/MC method.

GEOFILTRATION AND GEOMIGRATORY MODELING

At the second stage, the lithologic models were converted into models of geofiltration heterogeneity. Transformation of lithological model number 1 was performed by setting the value of the hydraulic conductivity (m/day) for each hydrofacies (sand, 1; clayey sand, 0.01; sandy clay, 0.001; clay, 0.0001). It should be

noted that these values of the hydraulic conductivity are quite typical for the studied strata (Rybal'chenko et al, 1994; Pozdniakov et al, 2005).

For model number 2, hydraulic conductivities were used, which were calculated by the level weighing formula:

$$k_{ef} = \left[\frac{\sum_{i=1}^4 N_i k_i^n}{\sum_{i=1}^4 N_i} \right]^{1/n},$$

where k_{ef} is the effective hydraulic conductivity, k_i indicates the characteristic values of the hydraulic conductivity hydrofacies (the same ones that were used in model number 1), N_i is the number of wells

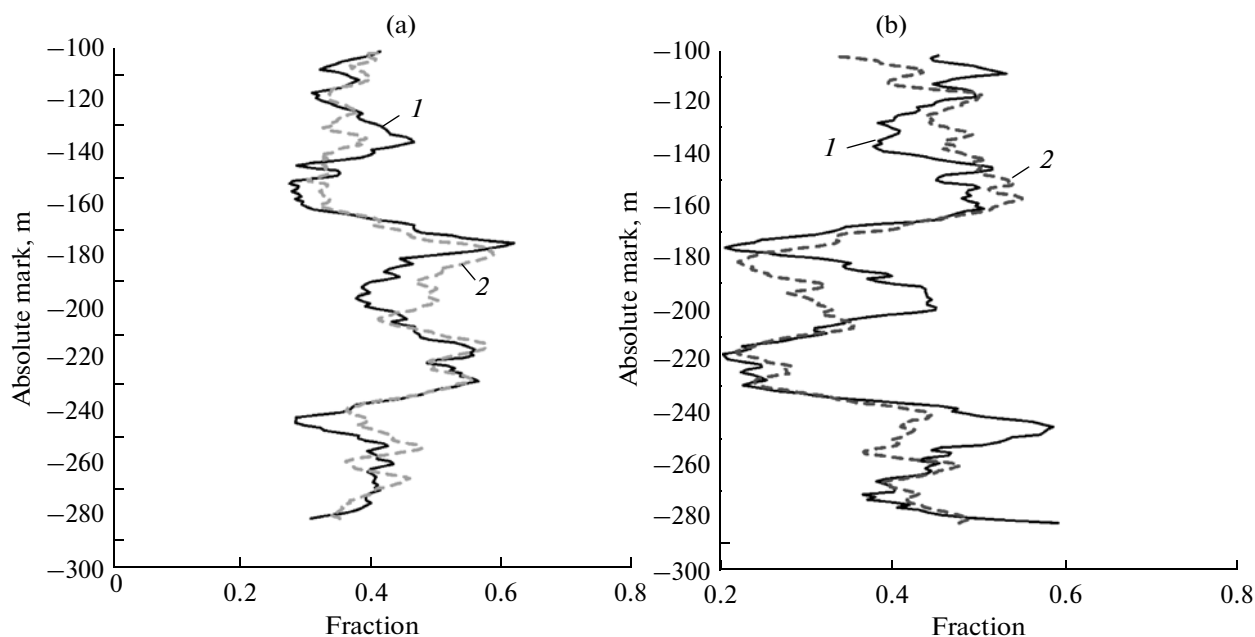


Fig. 3. Comparison of averaged over all wells (1) vertical distribution of sand (a) and clay (b) fractions in vertical section with modeling result (2) used fitted probabilities.

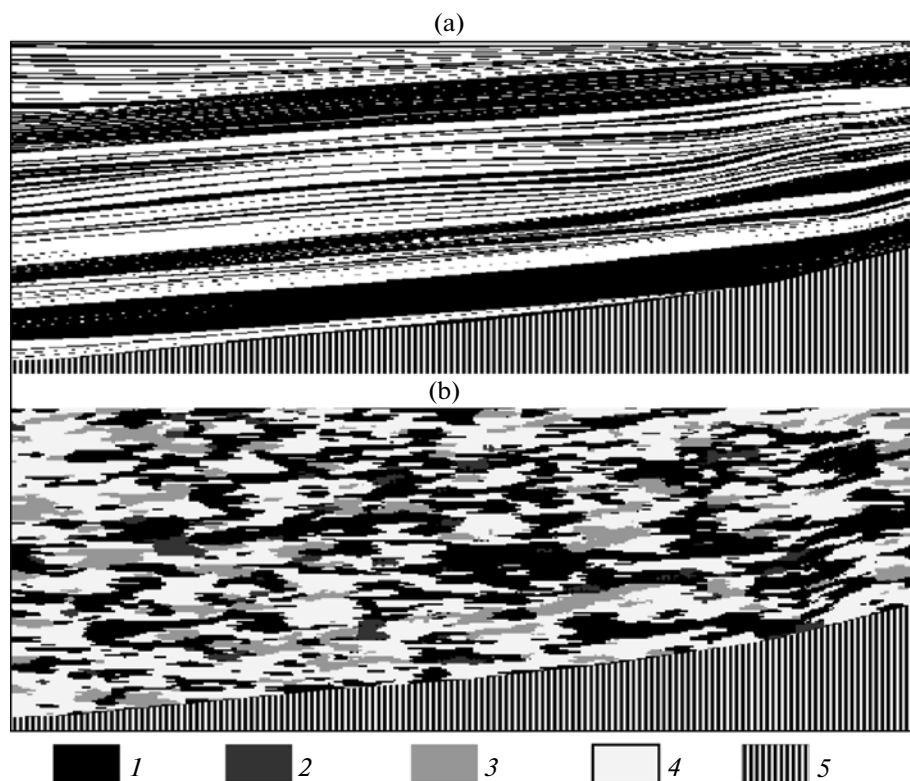


Fig. 4. The north-south section along the western boundary of the lithological models (at the top, model number 2; at the bottom, model number 1). Dimensions: vertical, 350 m, horizontal, 8025 m: 1, clay; 2, sandy clay; 3, clayey sand; 4, sand; 5, paleozoic basement.

that penetrated i hydrofacies in this layer, and n is a parameter of level weighting equal to $1/3$ (Pozdniakov and Tsang, 1996). The porosity for the entire modeling area was equal to 0.2.

At the third stage for each flow model the heterogeneity was modeled for stationary flow using MODFLOW-2000 within the selected sub-area. To compare the modeling results of the stationary geofil-

Table 3. Effective hydraulic conductivity and typical time of particle motion

Parameter	Horizontal flow		Vertical flow	
	Model number 1	Model number 2	Model number 1	Model number 2
Effective hydraulic conductivity k_{ef} , m/day	0.244	0.221	7.2×10^{-4}	4.5×10^{-4}
Average speed of the particles $U = k_{ef} \frac{H_1 - H_0}{Ln}$, m/year	0.9	0.815	0.066	0.0415
Average time of convective transfer, $t = \frac{L}{U}$, years	2750	3040	1490	2380
The time of arrival of the first particles, year	700	860	156	650
The time of arrival of 50% of the particles, years	5600	5460	3700	2900

tration for the two heterogeneity models we used the value of the effective hydraulic conductivity for the selected sub-area, which was defined according to the formula:

$$k_{ef} = \frac{QL}{\omega(H_1 - H_2)},$$

where Q is the rate of flow, L is the length of the filtration path, H_1 and H_2 are the given pressures on the boundaries of the model, and ω is the area that is open to flow.

Thus, for both analyzed flow models the effective permeabilities in the horizontal direction (differential pressures between the eastern and western boundaries of the modeled area were made) and the vertical direction (differential pressures were stated between the upper and lower boundaries) were determined. In all variants the differential pressure was 5 meters, which, under the assumed sizes of the sub-areas, corresponds to approximately horizontal and vertical flow gradients in the SCC area (Rybal'chenko et al, 1994).

At the fourth stage the convective transport of the neutral component from one boundary of the modeled sub-area to the other was modeled. To assess the impact of heterogeneity on the transfer of the neutral component of a contaminant in the modeled flow at a border with a large value of pressure labeled particles were placed in blocks with hydraulic conductivity of 0.01 m/day or more.

Upon knowing the filtration velocity in all nodes of the model, the expected time of arrival of each particle at the opposite boundary was found. This calculation was performed using the PMPATH program (Chiang, Kinzelbach, 2001) for tracking the trajectories of the motion and movement time of tagged particles in a convective flow. In this formulation, the time distribution of particle arrival depends only on the distribution of the values of the hydraulic conductivity in the modeled area.

RESULTS AND DISCUSSION

The results of the geofiltration modeling showed that the effective horizontal hydraulic conductivity was practically identical for both models, while the vertical coefficient of filtration was 2 times lower for model number 2 (Table 3), for which the extent of layers is much higher, which prevents vertical filtration. According to the results of modeling, the particle motion diagrams of the distribution of the arrival times of the particles were obtained, which for horizontal filtration proved to be virtually identical for both models. This suggests that horizontal convective transport occurs in permeable layers and weakly depends on the model of heterogeneity. Despite the fact that all the particles were placed in only permeable blocks, in the foreseeable time in both models only about 65% of the particles reached the opposite side, that is about 35% of the particles were found in blind zones, where permeable sediments are screened by impermeable sediments.

A different picture is obtained by modeling the vertical flow, in which the arrival curves of the time distribution differ significantly (Fig. 5). In model number 1, the first particles arrive much earlier than in model number 2. It is due to the phenomenon mentioned above that the greater length of the layers in the model leads to a significant shielding of the flow during vertical filtration. In model number 1 areas exist in which more rapid movement of particles occur due to the lower extent of the layers. Typical values of time movement of the particles are shown in Table 3, which shows that on average the first particles arrive 3–4 times faster than the typical time of convective transport for all variants, except for vertical migration in model number 1, when the first particles arrive up to 10 times faster than the average time of convective transport. Figure 6 shows the distribution curves of the dimensionless time of the arrival of the particles (the time ratio of the arrival of the particles to the average time of convective transport) for the vertical and horizontal filtration to models number 1 and 2. Since the use of

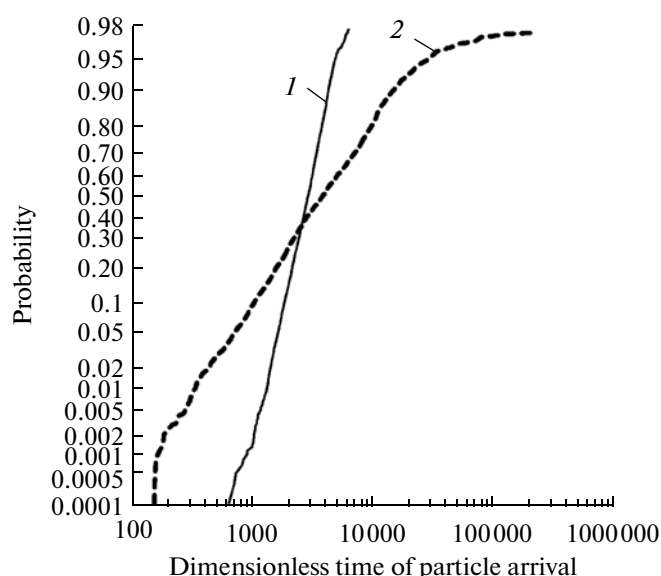


Fig. 5. The distribution of the time of particle arrival during vertical flow: 1, model number 2; 2, model number 1.

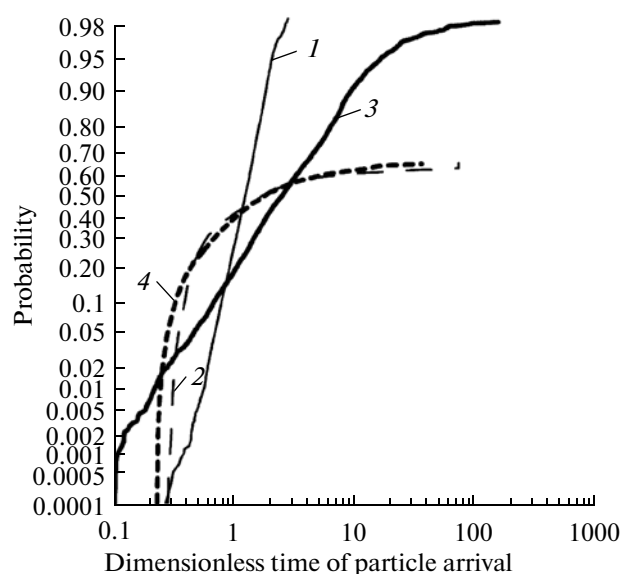


Fig. 6. Distribution of the dimensionless time of particles arrival: 1, model number 2 vertical; 2, model number 2 horizontal; 3, model number 1 vertical; 4, model number 1 horizontal.

dimensionless time removes the dependence of the results from the differential pressures and length of the filtration path, Figure 6 reflects the general patterns of convective transport in the investigated conditions with horizontal and vertical flow. Great differences are observed in vertical flow; moreover, model number 1 indicates the possibility of faster vertical transport of the first portions of contaminants than model number 2.

CONCLUSIONS

Using the method of geostatistical modeling based on Markov chains (TP/MC method) a model of the lithologic heterogeneity in an area of deep disposal landfills at the SCC was developed. The model is based on analysis of the lithological sections of 261 wells and presents the spatial alternation of the four major lithologic types in the section.

This model was compared with a model that was developed in the laboratory of geotechnological monitoring at the SCC and in terms of the same data, but is based on informal allocation of the elementary geological layers in the section with their subsequent kriging interpolation. In order to compare them, the two models were transformed into a model of geofiltration heterogeneities; for the deep burial area around the landfill modeling of stationary filtration and calculation of the convective motion of the particles of a conventional non-sorbing contaminant were performed.

The results of the comparison show that the main differences between the models occur in the vertical flow and convective vertical transport of particles. The model based on kriging interpolation of thickness values of geological layers is more conservative due to the larger characteristic horizontal length of the layers in the horizontal direction. Therefore, the vertical effective hydraulic conductivity of this model is 2 times lower than in the model based on the TP/MC method and the first particle arriving time is more than 4 times longer than in the model that was constructed on the basis of the TP/MC method.

Taking the great conservatism of the model based on the kriging interpolation of values of the thickness of layers into account, it is appropriate to use models that are based on the TP/MC method for the analysis of hypothetical accidents.

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