Simulation of hydraulic heterogeneity and upscaling permeability and dispersivity in heterogeneous sandy-clay formation

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**Abstract.** Radioactive waste has been injected in deep artesian aquifers of Cretaceous terrigenous deposits in Western Siberia since 1963. It is well known that for unconsolidated formations geologic heterogeneity strongly affects contaminant transport. The goal of this work is estimation of effective hydraulic and macrodispersion parameters on the basis of three-dimensional (3D) high spatially resolution lithological heterogeneity model of the injection site. The data set includes detailed geologic core description from 295 wells. 3D Markov chain model in combination with a conditional stochastic simulation was used to simulate 3D hydrofacies distributions at a resolution of 25 m x 25 m x 0.5 m for 18.5 km2 study area. Hydraulic conductivity was assigned to each cell corresponding to the simulated hydrofacies. For the modeled domain the numerical estimation of effective hydraulic and dispersion properties was performed. A three-dimensional steady state modeling approach was used to simulate groundwater flow with MODFLOW 2005. 3D advective solute transport was simulated with a particle tracking technique using PMPATH. The mean seepage velocity and the effective longitudinal macrodispersion from temporal moments of observed breakthrough curves for conservative tracer were calculated.

The results of this study show that for the studied medium: (1) the horizontal mean lengths exceed the vertical lengths more than 30 times and as the result the vertical effective hydraulic conductivity is two orders of magnitude less than the horizontal effective conductivity; (2) BTCs exhibit longer late tails and they are looks like non-Fickian; (3) the estimated effective longitudinal macrodispersivity in the vertical direction is one order of magnitude less than longitudinal macrodispersivity in the horizontal direction, that means for using Fickian framework for dispersion modeling in regional transport simulation one need to apply at least anisotropic-media dispersion model [Voss, Provost, 2002].

**Keywords.** Geostatistics, hydrogeology, stochastic simulations, heterogeneous media, Markov chain, T-PROGS, stochastic, groundwater, dispersion.

**1 Introduction**

Radioactive waste has been injected in deep artesian aquifers of Cretaceous terrigenous deposits in Western Siberia since 1963. The studied geologic formation includes the injection aquifers and the overlaying semipermeable layers that represent heterogeneous sand-clay strata formed in a continental near-sea border environment [Shestakov et al., 2002]. The regional scale flow and transport models for long-term waste migration forecast in groundwater is based on simplified geospatial description of natural heterogeneity of studied formation as layered system of permeable and semipermeable layers. Lithological study of well cores shows that each aquifer and each semipermeable layer marked at studied area has complex internal architecture consisting of succession of relatively high and relatively low permeable units.

Complex three-dimensional (3D) subsurface architecture of the aquifer may result in a highly heterogeneous spatial distribution of hydrogeological parameter values in porous media at different scales and may consequently significantly influence subsurface fluid flow and solute migration [Fogg, Carl, Green, 2000; Feehley, Zheng, Molz, 2000; Zinn, Harvey, 2003; Zheng, Gorelick, 2003;De Marsilyet al., *2005*, Engdahl, Weissmann, 2010; Dell’Arciprete et al., 2014]. Previous studies have shown that the problem of selection of the best model for prediction of long-term and regional scale waste transport at this site exists, because high-resolution 3D model cannot be applied for regional scale transport modeling and upcsaling to parameter of simplified model should be done [Pozdniakov et al., 2003; Pozdniakov et al., 2005]. The objectives of this work are: (1) study of transport in this heterogeneous media; (2) search of effective hydraulic and macrodispersion parameters on the basis of 3D high spatially resolution lithological heterogeneity model of the injection site for future long-term regional scale radioactive waste migration prediction. The modeling approach has three steps: (1) development of 3D high resolution model the heterogeneity of injection area through application of transition probability geostatistics; (2) simulation steady state groundwater flow and advective transport using obtained 3D spatial lithological heterogeneity model of the site, (3) estimation of effective hydraulic conductivity and effective macrodispersion parameters using a temporal moments of observed breakthrough curves.

**2 Development of 3D model of heterogeneity**

The key step in this study is to generate a highly resolved and realistic model of the heterogeneity the studied geologic formation. To take into account the essential features of heterogeneity, lithological data of 295 wells placed irregularly within the area approximately 4 by 4 kilometers of area are processed. This dataset includes about 46 kilometers of lithological logs obtained in characterization, monitoring and injection wells, which were drilled during past forty years within the site. The vertical resolution of logs is 0.5 m. Core descriptions were categorized into the four hydrofacies units, defined as sand, sandy clay, clay sand and clay. The lithologic data were used to develop an indicator database representing the presence or absence of each hydrofacies at each point of observation with a vertical spacing of 0.5 m. The distributions of mean thickness of all hydrofacies look like an exponential distribution. The volumetric proportion, the effective range and the mean length of the four hydrofacies were estimated from the indicator data using GSLIB [Deutsch, Journel, 1992] and T-PROGS software [Carl, 1998] (Tab. 1). The results of analysis indicate that (1) the vertical range significantly smaller than the lateral (horizontal) range and (2) the horizontal mean length of hydrofacies exceeds the vertical scale more than 30 times (Tab. 1). Also we computed variograms and transition probabilities along the azimuths: the effective ranges and mean lengths in the horizontal plane appear to have no directional tendencies. The hydrofacies units serve as the basis for defining the aquifer system-scale heterogeneity of hydraulic properties, which enables litilogic descriptions of core obtained from vertical boreholes to serve as conditioning data for the geostatistical simulations. For modelling purposes, these hydrofacies were used, based on the analysis of conductivity values: least permeable (k=0.0001m/day, clay), poorly permeable (k=0.001m/day, sandy clay), permeable (k=0.03m/day, clay sand) and most permeable (k=1m/day, sand).

Table 1: Hydrofacies properties

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Hydrofacies category | Mean thickness (m)\* | Mean length (m)\*\* | | Range (m) | | Proportion (-) |
|  |  | vertical | horizontal | vertical | horizontal |  |
| Sand | 4.99 | 4.5 | 243 | 9.6 | 81 | 0.42 |
| Clay sand | 4.30 | 3.8 | 109 | 15 | 72 | 0.15 |
| Sandy clay | 3.20 | 2.7 | 87 | 10.2 | 93 | 0.03 |
| Clay | 5.50 | 6.1 | 287 | 15,3 | 411 | 0.40 |

\* - mean thickness is computed from borehole records; \*\* - mean length is inferred from transition probabilities.

This study uses the transition probability/ Markov chain (TP/MC) geostatistical approach described by Carl and Fogg [1996, 1997], Weissmann and Fogg [1999]. The TP/MC method is widely applied to model the geological heterogeneity [Weismann, Fogg, 1999; Fogg et al., 2000; Sun et al., 2008; Engdahl et al., 2010]. The TP/MC can better represent connections of hydrofacies than some conventional geostatistical methods [Maji et al., 2006, Lee et al., 2007, Ye and Khaleel, 2008]. Geostatistical simulations were produced using Transition Probability Geostatistics (T-PROGS) software [Carl, 1998]. 3D high spatially resolution model was developed using records of 295 wells with lithological logs. The model parameters (hydrofacies proportion, hydrofacies mean lengths and juxtapositional preference among hydrofacies) are inferred from available quantitative data, and the model realizations are generated and conditioned to these data. Its geostatistical parameters were estimated through direct measurement of transition probabilities from well logs (Fig. 1).

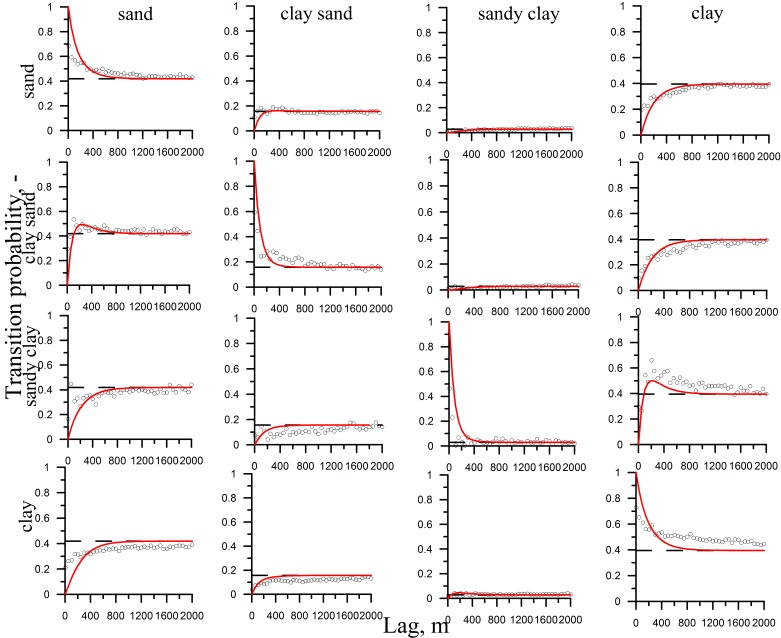
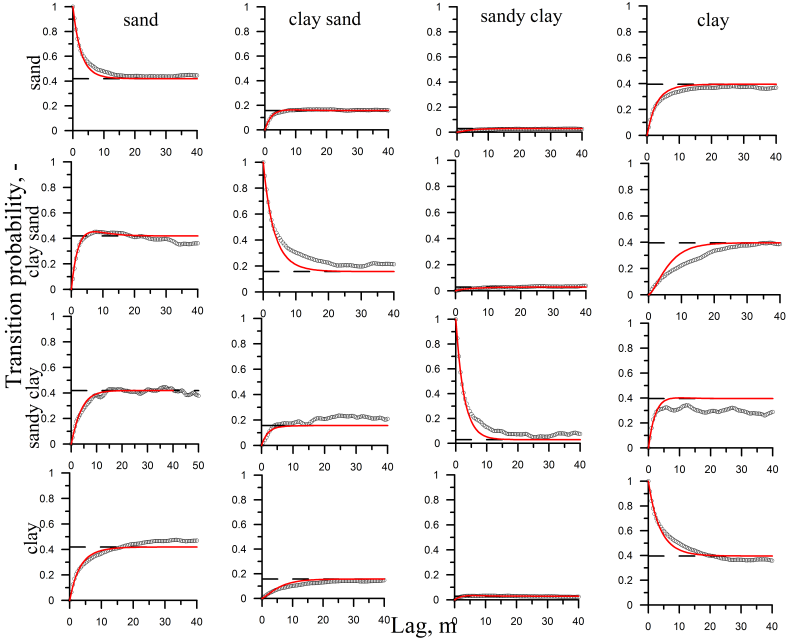
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Figure 1: Transition probability matrix in vertical (left) and horizontal (right) directions: core data measurements (dots), Markov chain model (solid line) and proportions (dashed line).

We generated 10 equally probable geostatistical realizations of the formation of the dimensions of 4300 m x 4300 m x 130 m (one example is shown at Fig. 2). The cell size is 25 m x 25 m x 0.5 m resulting in a total of about 6260800 nodes. The same grid and domain sizes were used in the ground water flow and solute transport simulations.

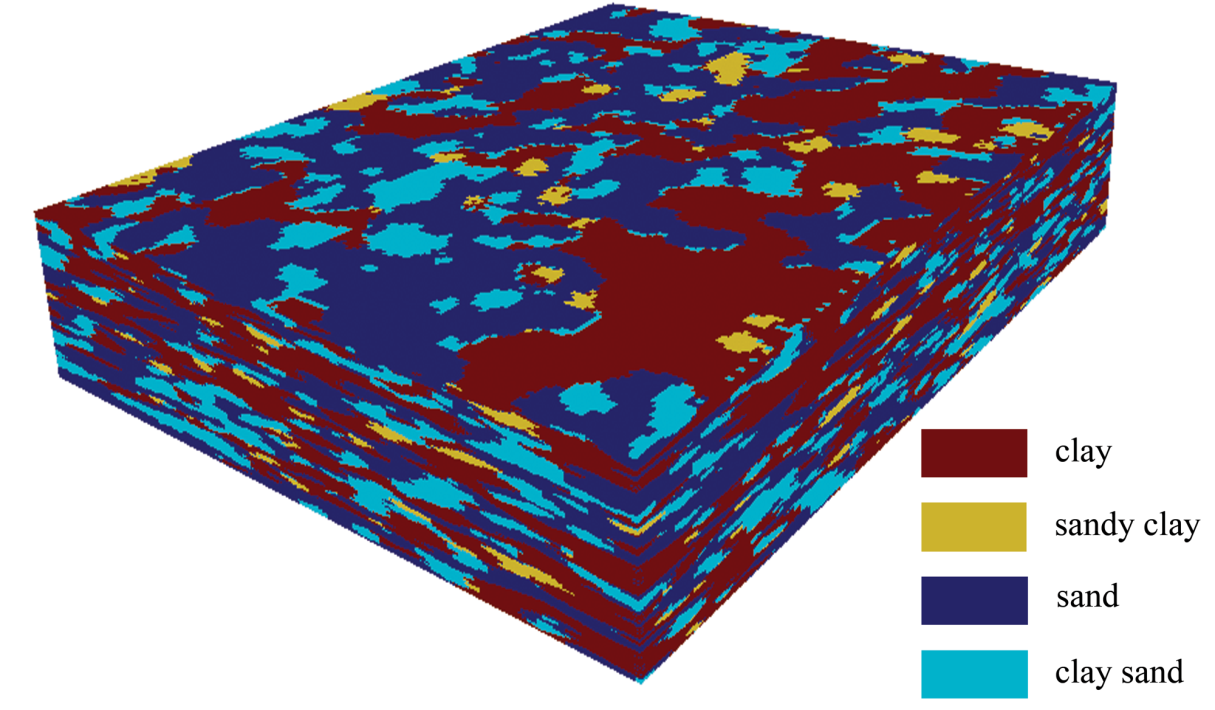


Figure *2*: The three-dimensional view of the heterogeneous model for the realization 1.

The simulated length of the domain in each direction is several times larger than the mean lengths (or correlation lengths) of the hydrofacies in this direction. The block size was chosen from two opposing needs: the block size in horizontal and vertical directions is less than the mean lengths of the hydrofacies and computational limitations of the groundwater flow modeling. The comparison of vertical average distribution of hydrofacies found from well data and simulation result is used for validation of simulation results.

**3 Simulation of flow and transport**

Hydraulic conductivity (K) was assigned to each cell based on the simulated hydrofacies determined by the geostatistical realization. Values used for K of each hydrofacies were estimated from literature estimates, empirical formulations based on grain-size distributions of samples of the sediments, field hydraulic tests, calibrating mathematical model of aquifers.

For purpose of development long-term predictive models with simplified heterogeneity structure the effective hydraulic and macrodispersion properties of modeled medium were studied. Flow and transport was simulated for heterogeneous realizations. The porosity is assumed to be spatially homogeneous with a value of 0.2. Transition probabilities in the horizontal plane are assumed isotropic. Two sets of simulation runs with different mean flow direction were performed: horizontal and vertical flows. The constant head boundaries were set on two opposite sides of the domain and no-flow boundaries on all other sides. Simulations of the steady state flow problem for each realization were conducted with the finite difference code MODFLOW-2000-2005 [Harbaugh et al., 2000]. The differences of heads between opposite boundary for horizontal and vertical flows were selected to reproduce natural lateral and vertical mean flow gradient for the given environments [Shestakov et al., 2002]. The velocity field is then used in a particle tracking transport code that simulated the solute advective transport by portioning the solute mass into a large number of representative particles. Particle tracking simulations was performed using PMPATH [Chiang, Kinzelbach, 2001]. A total of 4500 particles are used in the horizontal and vertical direction. The particles were placed in high-permeable cells, i.e. the cells with hydraulic conductivity more than 0.001 m/day.

**4 Estimation of effective parameters**

The effective (equivalent) upscaled hydraulic conductivity was determined from simulations of steady-state groundwater flow and was calculated with the following formula:

|  |  |
| --- | --- |
|  | (1) |

[m3/day] is the total flow rate, *l* [m] is the length of the domain (the distance along primary direction of flow), и [m] are the constant heads, *ω* [m2] is the cross sectional flow area.

We used evaluation of observed breakthrough curves (BTCs) of flux concentration which computed from the distribution of particle arrival times at control planes. Simulations show that the transport of conservative tracer in studying geologic formation is non-Fickian because the BTSs contain a heavy late tails and thus deviates significantly from Gaussian plum (Fig. 3). Also we evaluate the non-Gaussian features of the BTCs obtained at the control planes based on the coefficient of skewness (Tab. 2).

The moment method used to obtain transport parameters. Using temporal moments of BTCs the mean seepage velocity and the effective longitudinal macrodispersion for conservative tracers can be calculated with the following equations [Jury, 1990; Yu et al., 1999]:

|  |  |
| --- | --- |
|  | (2) |
|  | (3) |
|  | (4) |

where *x* is the distance between the plane of initial particle positions and the control plane of particle sampling, и are the first and second order normalized moments, *С(x,t)* is the concentration, t is time.

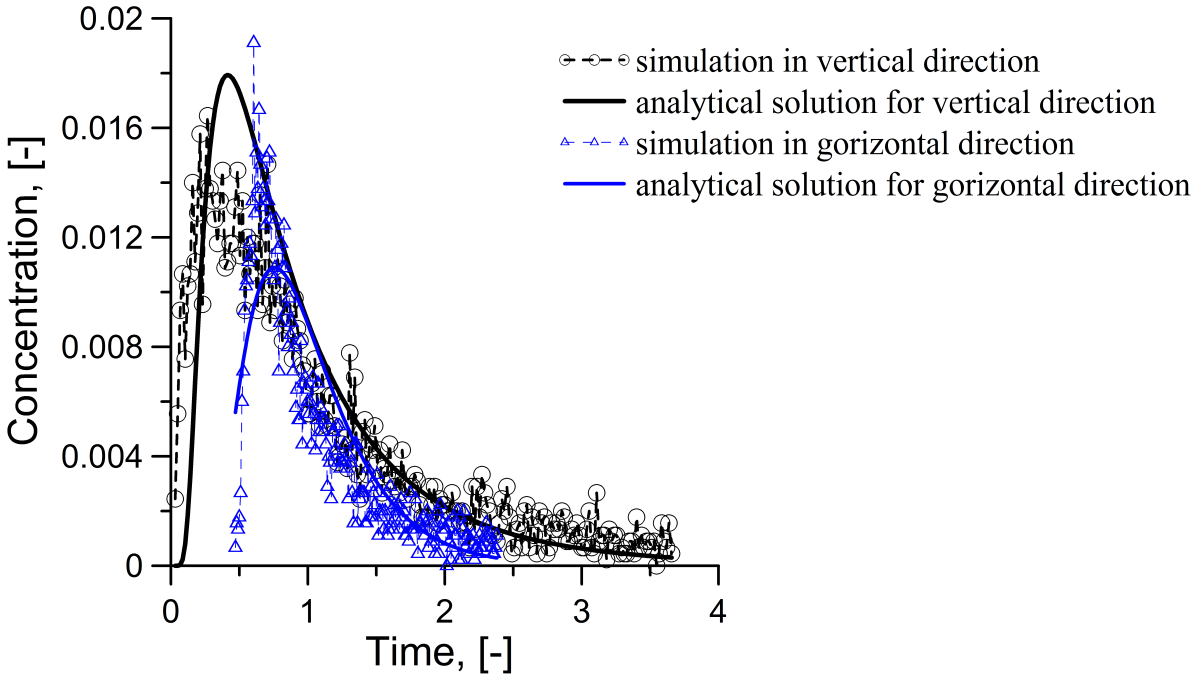


Figure 3: Breakthrough curves in horizontal and vertical directions for the realization 1. Normalized time is calculated as , where t is the particle arrival time.

The effective (equivalent, apparent) longitudinal macrodispersivity , the apparent porosity , and the mean flow velocity were calculated as:

|  |  |
| --- | --- |
|  | (5) |
|  | (6) |

|  |  |
| --- | --- |
|  | (7) |

*I* [-] is gradient.

Table 2 summarizes the results of the analysis.

Table 2: Estimated parameters for ten 3D high-resolution geostatistical realizations

|  |  |  |
| --- | --- | --- |
| Parameter | Value for the direction of flow (minimum – maximum (mean)) | |
|  | vertical | horizontal |
| Effective conductivity *keff*, m/day | 0.298 – 0.305 (0.302) | 0.0013 – 0. 0018 (0.0015) |
| Effective longitudinal macrodispersion D, m2/day | 0,004 – 0,007 (0,005) | 0,99 -1,09 (1,04) |
| Apparent porosity , - | 0,45 – 0,52 (0,49) | 0,13 - 0,14 (0,14) |
| Longitudinal macrodispersivity αL , m | 39 – 54 (43) | 388 – 412 (402) |
| Transport connectivity indicators CT1\* | 6,77-9,94 (8,12) | 1,75-1,84 (1,78) |
| Transport connectivity indicators CT2\*\* | 1 – 1,38 (1,18) | 1,18 – 1,41 (1,29) |

\*CT1= tave/t5, where tave is the average arrival time, t5is the time at which 5% of the solute has arrived at the control plane;\*\*CT2 is the coefficient of skewness [Knudby, Carrera, 2005].

These dispersivity estimates (Tab. 2) can be ultimately used as input parameters in transport models that commonly solve the advection-dispersion equation. Apparent parameters as calculated in Eqs. (1), (2), (5) are viewed as equivalent values in homogeneous porous media that, when used the classic convection-dispersion equation, lead to the same spatial moments of the plume as observed in the simulations for heterogeneous porous media.

The numerical results are compared (Fig. 3) with analytical solutions (the convection-dispersion equation for narrow pulse input of conservative solute for the case of steady state water flow, one-dimensional transport) [Jury, 1990]:

|  |  |
| --- | --- |
|  | (8) |

где – the flux concentration, –the probably density function of the travel time.

**5 Summary and conclusions**

In this paper the 3D high spatially resolution model of injected area of disposal site was developed. The geological realizations were constructed using Markov chain geostatistics and conditional simulations using the TPROGS model. The results of this study show approximately equals volume fraction of high and low permeable hydrofacies within the studied formation and its anisotropy: the horizontal mean length of hydrofacies exceeds the vertical mean length more than 30 times. For the modeled domain numerical estimation of effective hydraulic properties and effective longitudinal macrodispersivity were performed. Analysis of effective hydraulic properties shows essential hydraulic anisotropy of the medium: the vertical effective conductivity is two orders of magnitude less than horizontal effective hydraulic conductivity.

For the studied medium BTCs exhibit longer late tails and they are looks like non-Fickian. Using temporal moments of observed breakthrough curves the longitudinal macrodispersion and the mean seepage velocity have been calculated. The present study shows that for the studied heterogeneous medium, the rate of transport and effective longitudinal macrodispersivity depend on the direction of flow relative to bedding. We can note that our results are consistent with results Engdahl and Weissmann, 2010. Numerical studies of transport show that the estimated effective longitudinal macrodispersivity in the vertical direction is one order of magnitude less than longitudinal macrodispersivity in the horizontal direction, that means for using Fickian framework for dispersion modeling in regional transport simulation one need to apply at least anisotropic-media dispersion model [Voss, Provost, 2002].

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