Advective and diffusive contaminant transport through heterogeneous sandy-clay formation

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Problem and objectives

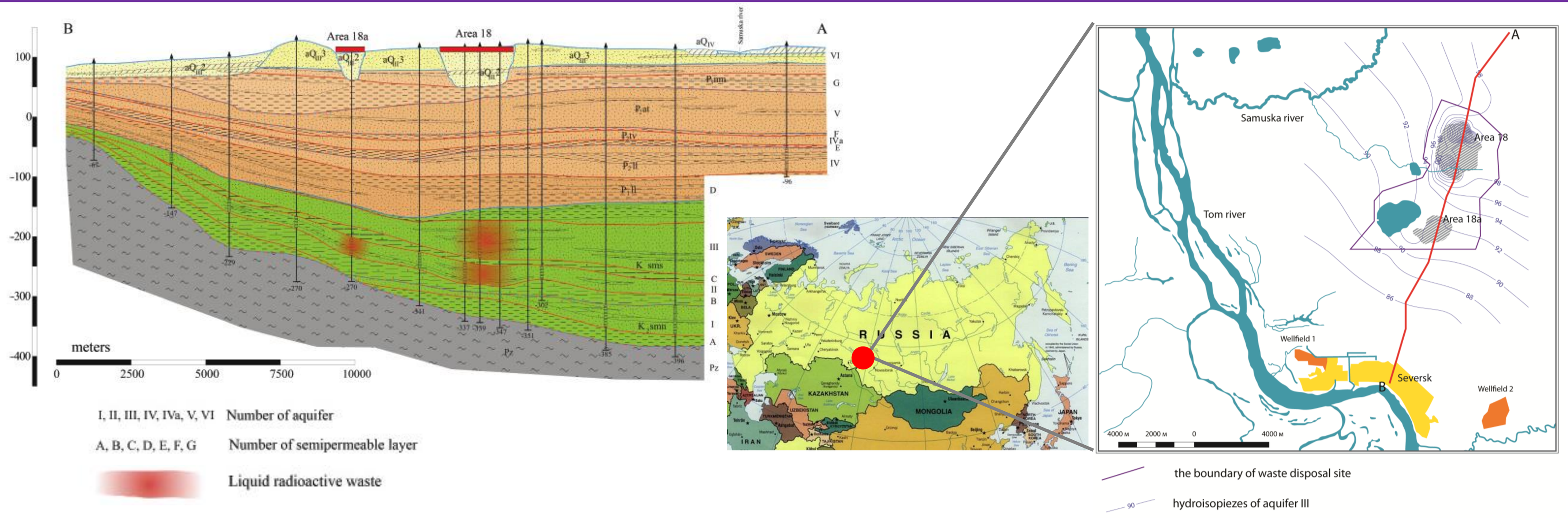
Characterization of local-scale hydraulic and transport parameters of aquifers with complex internal architecture is still a challenger. For low permeable units (facies) the uncertainty of estimated of hydraulic conductivity, distribution coefficient and diffusion coefficient values typically could be within an order of magnitude and even more, while the responsibility of these units for long-term subsurface migration could be very important in overall contaminant spreading.

The specific goal of this work is analysis of flow and transport within the waste injection zone that includes about 40% of discontinuous clay hydrofacies and estimation of protective role of low permeable units against contaminant transport to shallow aquifer.

To quantify the role of low permeable units on migration processes we:

a. estimated diffusion coefficient and hydraulic conductivity of clay samples taken from the injection zone;
b. developed high-resolution lithological models of injection aquifers and overlaying zone using 3-D TP/MC;
c. performed analytical and numerical analysis of flow and advective, advective-diffusion transport simulating upward injected waste spreading due to natural hydraulic gradient;
d. performed advective simulation transport with and without sorption in low permeable units.

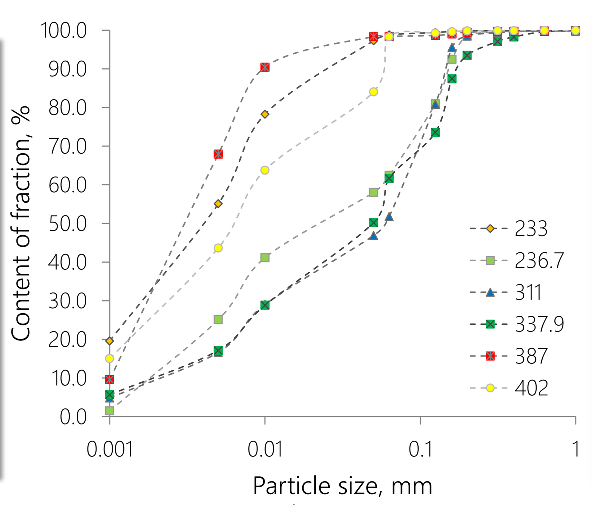
1. The site description

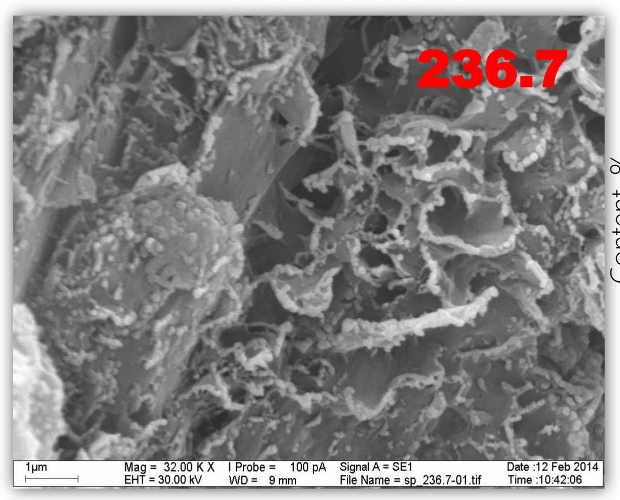


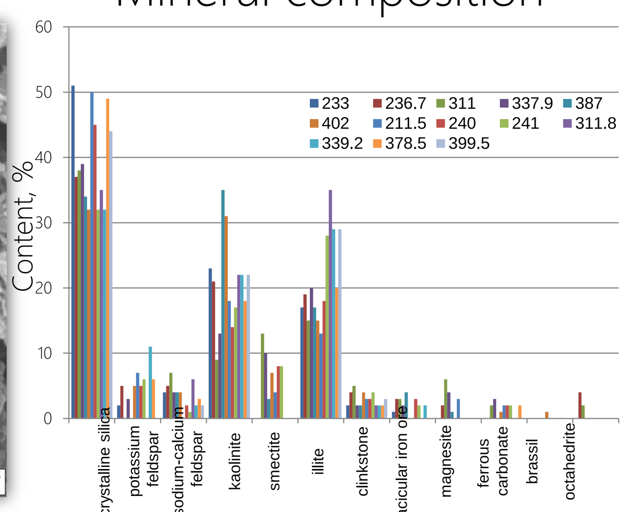
The waste disposal site of Siberian Chemical Combine is located 20 km to the north of the city Tomsk, and is the largest nuclear waste injection site in Russia. Since 1960's more than 45 million m3 of liquid radioactive wastes were injected by wells to the depth of 270 - 400 m.

Injection and overlaying zones are sandy-clay formation with complex internal architecture. The injected wastes now are vertically inside the injection zone and the planar extend of the plume still is within the site area.

2.1 Lab study of properties

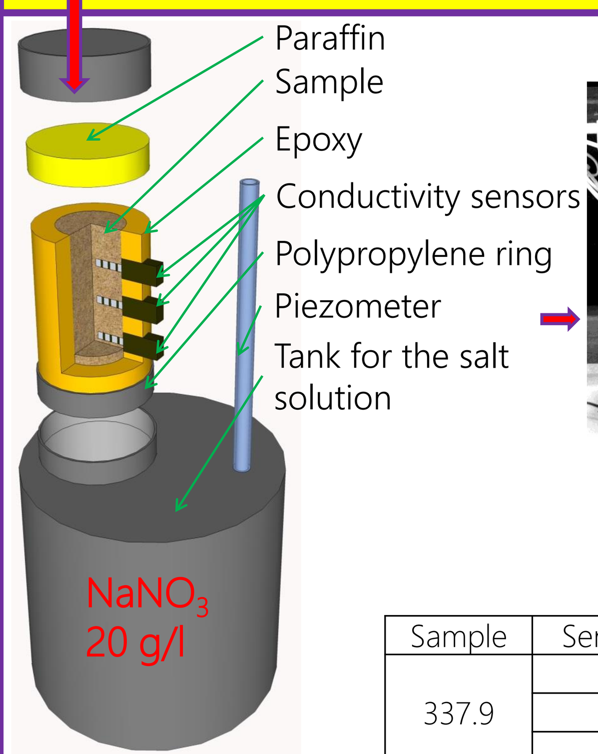






According to mineralogical analysis, the samples are aleurite-clay of continental origin. The content of primary minerals in the average of 50% is indicating unfinished transformation into the clay and remaining 35 to 50% (among which mainly kaolinite and hydromica, smectites) indicates a low CEC.

2.2 Lab study of diffusion coefficient



The experimental installation for determining the diffusion properties

Differential equation of diffusion mass transfer

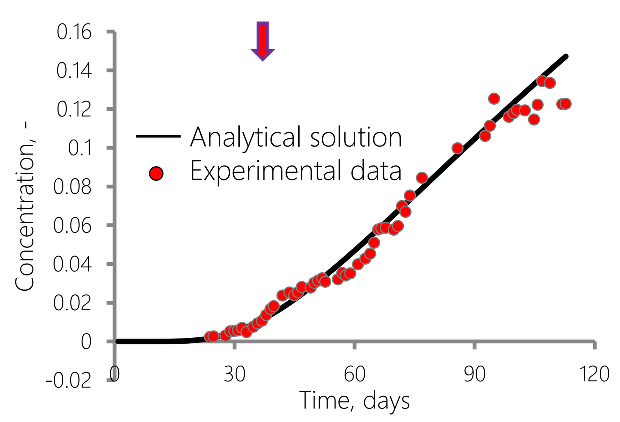
$$D\frac{\partial^2 C}{\partial x^2} = n_e \frac{\partial C}{\partial t}$$

where D is diffusion coefficient, n_e is effective porosity

The solution for a sample of finite length

$$\frac{c-c^0}{c_0-c^0} = \sum_{s=1}^{\infty} \frac{2}{p_s}(-1)^{s+1}\cos p_s \frac{L-x}{L}\exp\left(-p_s^2\frac{Dt}{nL^2}\right);\ p_s=(2s-1)\frac{\pi}{2}$$

where C is concentration at a given time, C^0 is concentration on the initial time, C_0 is concentration on the final time, L is length of the sample, x is distance to the boundary with a constant concentration, t is time.



Sample	Sensor	D/n, m²/day	n, -	D, m²/day
337.9	1	$1{,}02\times10^{-6}$	0,24	$3{,}57\times10^{-7}$
	2	$3{,}40\times10^{-6}$		$1{,}19\times10^{-6}$
	3	$3{,}86\times10^{-6}$		$1{,}35\times10^{-6}$
211.5	1	$4{,}94\times10^{-6}$	0,35	$1{,}73\times10^{-6}$
	2	$6{,}25\times10^{-6}$		$2{,}18\times10^{-6}$
378.5	1	$1{,}22\times10^{-6}$	0,25	$4{,}27\times10^{-7}$
	2	$4{,}00\times10^{-6}$		$1{,}40\times10^{-6}$

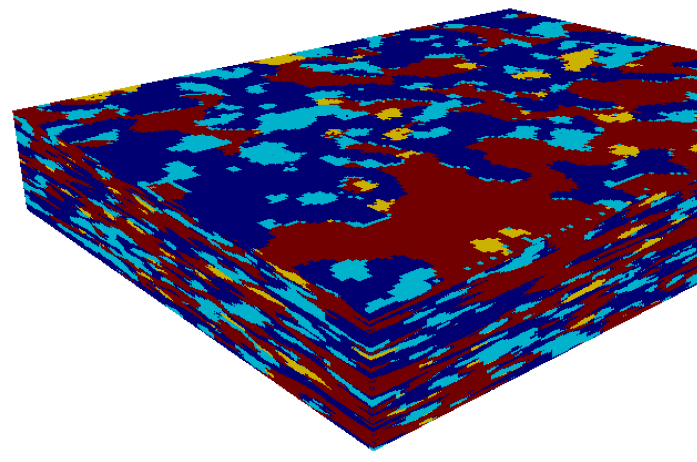
The composition of the diffusion solution was made similar to the composition of the injected waste with replacing the radioactive isotopes by their stable counterparts. Diffusion experiments used 1.5-liter tank of prepared solution with known concentration of each species.

According to preliminary calculations only 1,2% mass of species from this volume can diffuse into sample, so we can ignore mass loss in the tank and consider it as the upper boundary with constant concentration.

The installed piezometers maintained a zero hydraulic gradient to avoid advective transport. The concentration along a sample was measured by four contact conductivity sensors, based on the audio Jack 2.5 mm connector measured.

3.1 Transport simulation

1. The 3D view of the heterogeneous model (The overall dimensions of the simulated region are 4300 m x 3500 m x 130 m, the cell size is 25 m x 25 m x 0.5 m)



Model	Average horizontal length of clay L, m	Average thickness of clay M, m	Simulation vertical gradient	Porosity	K clay, m/day	D, m²/day	K_{eff}, m/day
Short	283	6,6	0.038	0,2	0,0001	3×10^{-6}	0,0015
Long	430	6,9	0.038	0,2	0,00055	3×10^{-6}	0,00074
Perfectly-layered	Infinite	6.9	0.038	0,2	0,00055	3×10^{-6}	0,00014

4. Define of the local number's Pe for clay facies

$$Pe = \frac{v\cdot M}{D}$$

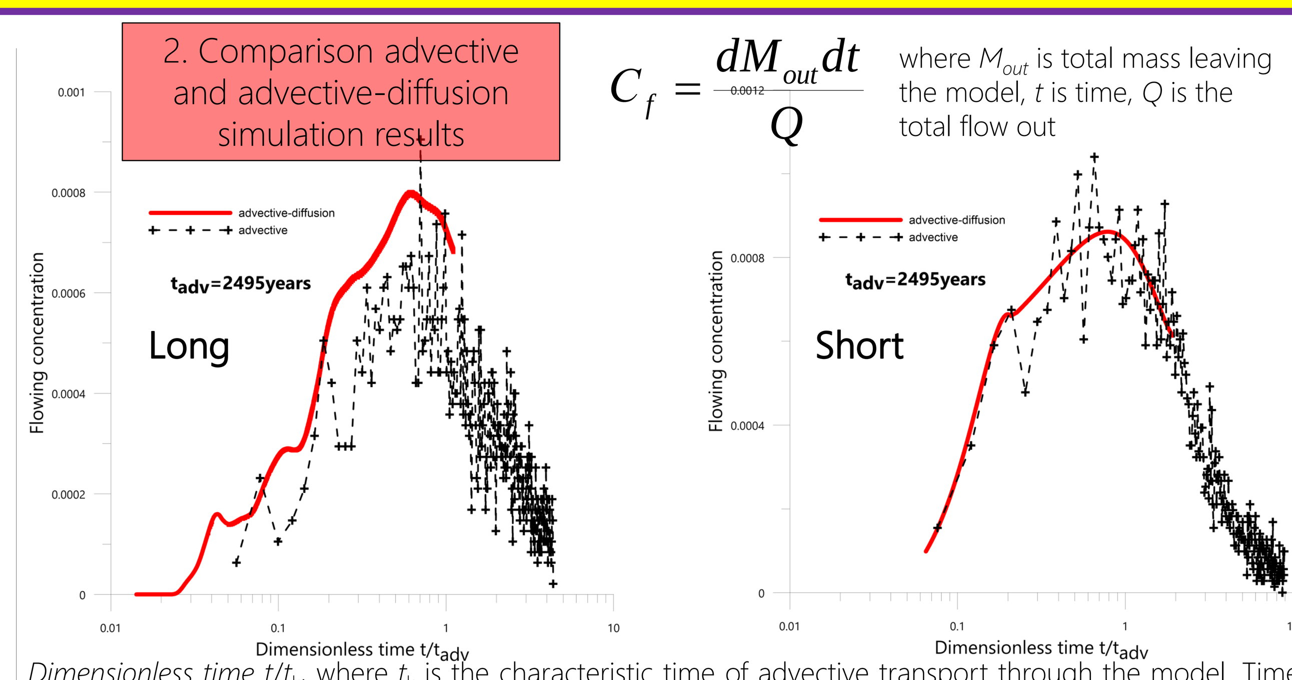
where v is average velocity in facies, M is typical thickness of facies, D is diffusion coefficient

Model	Pe	Type of mass transport
Short	$27<Pe<1100$	Advective
Long	$1<Pe<115$	Advective
Perfectly-layered	12	Advective

2. Comparison advective and advective-diffusion simulation results

$$C_f = \frac{dM_{out}dt}{Q}$$

where M_{out} is total mass leaving the model, t is time, Q is the total flow out

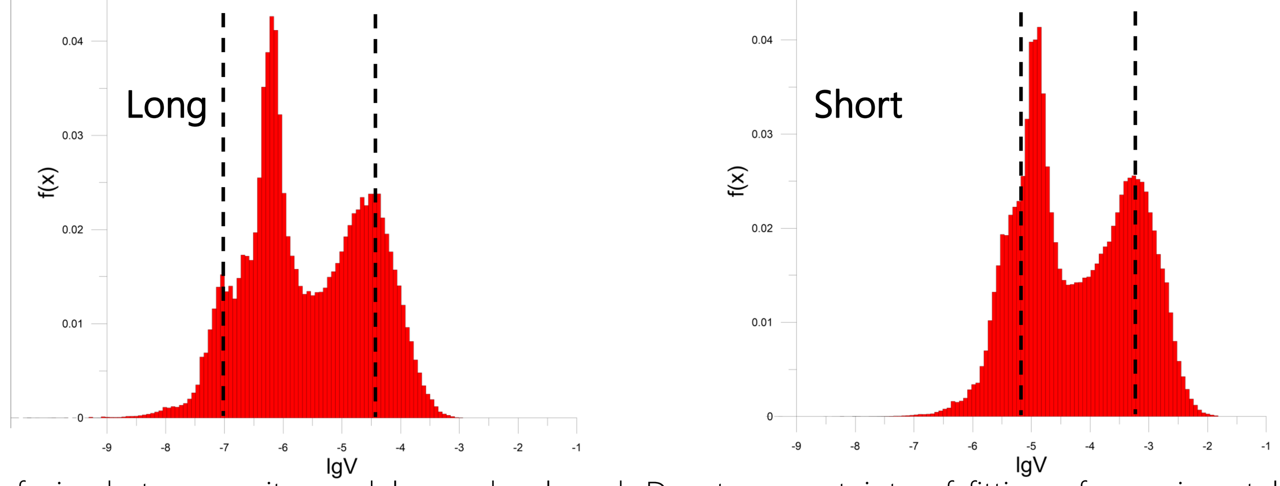


Dimensionless time t/t_k, where t_k is the characteristic time of advective transport through the model. Time of advective transport is calculated according to the formula $t_k=(S\cdot n)/v$, where S is the height of the model, n is porosity

3. Flow velocity statistics

$$|V| = \sqrt{V_x^2+V_y^2+V_z^2}$$

where V_x, V_y and V_z are flow velocity in the directions X, Y and Z



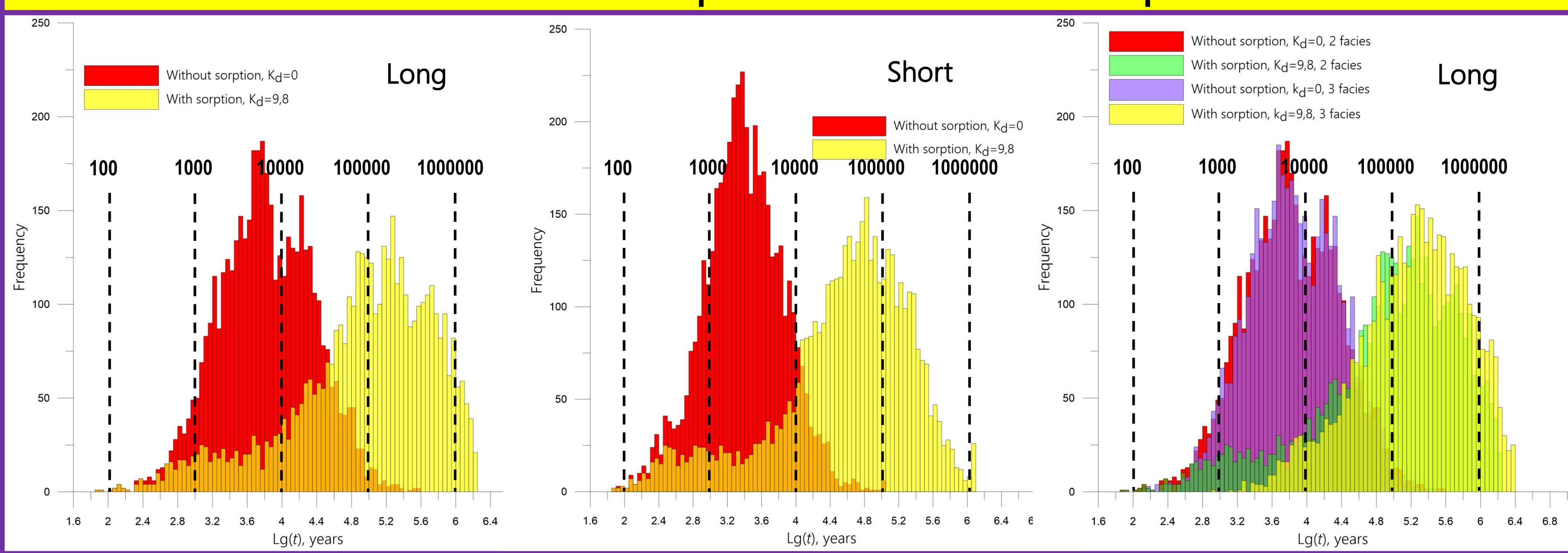
Based on lithological logs of 200 wells and with the use of TP/MC method four-facies heterogeneity model was developed. Due to uncertainty of fitting of experimental transition probabilities in horizontal direction two models conditioned on these wells were used for future transport simulation: "short" and "long" clay facies models. For comparative study, the third "perfectly-layered" model is also considered.

Advective (by particle tracking with PMPATH) and advective-diffusive (with MT3Dms) transport within the injection zone of 130 m thickness was simulated for the important practical case – upward flow due to natural vertical hydraulic gradient with a simulation period of 2300 years.

Modflow 2005 simulated the flow field used for the transport calculation and effective hydraulic conductivity estimation.

Transport of contamination from the instant source distributed along the bottom plane of the model was analyzed. The breakthrough curves of flowing concentration at upper boundary and temporal distribution of concentration between blocks (i.e. low permeable facies) and canals (i.e. high permeable facies) was considered. For local Peclet number calculation the statistic of 3-D flow velocities field was calculated.

3.2 Transport simulation with sorption



Advective transport simulation with linear sorption have been done by particle tracking with PMPATH. To take into account the sorption we have used effective porosity value $n_a=n+K_d$. Here K_d is dimensionless sorption constant.

The non zero Kd value in different model runs was applied for the two and three low permeable facies. Comparing the arriving time of particles distribution for runs without sorption and with sorption, we evaluated the delay due to sorption.

Conclusions

1. Molecular diffusion coefficient obtained in the experiments (average value $2\cdot10^{-6}$ m²/day) turned out to be less than expected for this clay and generally this value is smaller than reported in literature for similar soils at the similar depth.
2. For both "short" and "long" facies model the used upward hydraulic gradient 0.038 that characterizes flow in the discharge zone shows that advection is the main transport agent in this medium. Even perfectly layered model is predominantly advective.
3. For the zone of smaller vertical gradient and sublateral flow the diffusion to low permeable units will play more important role.
4. The arrival time of the first particles does not change if only clay (i.e. 40% of medium) are sorbent material, but the average time of arrival of the particles is slowed down in comparison with the medium without sorption.
5. In the case where only sand is not sorbed unit (i.e. 60% of the medium absorbs contamination) arrival time of the first particles s increased by more than 900 years. This bear witness of the poor vertical connectivity of sand bodies.
6. Thus, studies have shown that long-term predictions for the vertical migration of contamination, in the sediments of the type studied the key issues is the development of a detailed model of heterogeneity and evaluation of the sorption properties of different facies that formed this heterogeneity.

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