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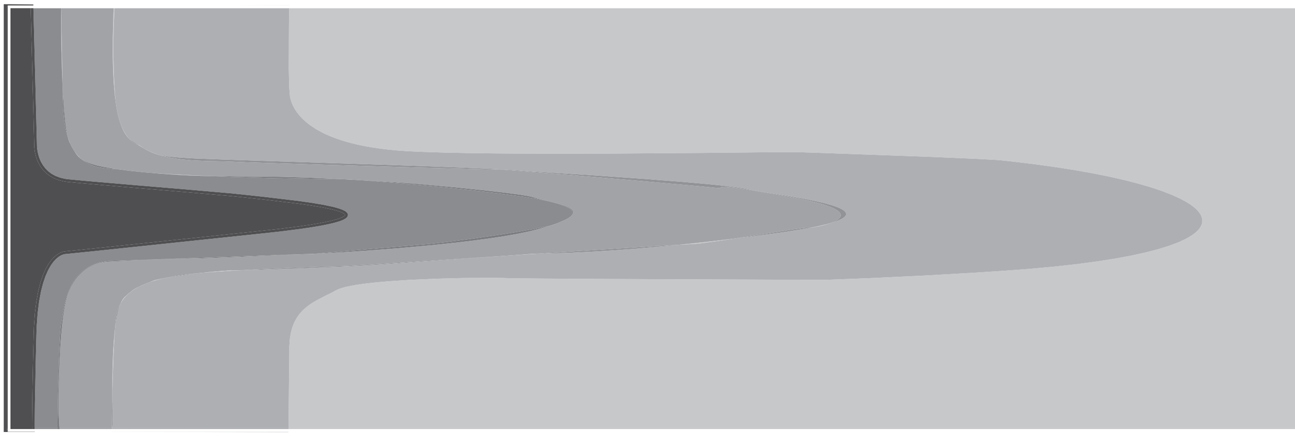

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3D Modeling of Injected Waste Transport in Sandy-Clay Formation

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A 3D high-spatial-resolution model of Injection Area 18 of the Siberian Chemical Complex disposal site was developed to simulate underground spreading of injected waste. Unlike previous models developed for this site, this new model provides a detailed description of the internal 3D structure of the formation. For the description and modeling of lithologic heterogeneity, a binary model of facies spatial succession was adopted. In this model, the Cretaceous terrigenous deposits are represented by a 3D sequence of clay and sand units; the proportion of each unit in the modeled medium is about 0.5. Using data from 210 wells with lithological logs, a 3D Markov's chain of transition probabilities was computed and vertical/horizontal correlation scales of sand and clay facies were estimated. The estimated correlation scales of both lithological units are similar in each direction; these scales are about 5 m vertically and about 350 m horizontally. Using TSIM tools that simulate lithologic heterogeneity by co-kriging with a transition probabilities algorithm, the 3D heterogeneity model of Injection Area 18 was created. The planar size of the model is 4,200 m × 4,200 m with a 33 m step; vertical size is 250 m with a 1 m step. Thus, the total number of blocks representing spatial heterogeneity is about 4 million.

A numerical estimation of effective hydraulic properties of the modeled formation, using a characteristic value of clay hydraulic conductivity at 10^{-4} m/day and sand conductivity at 1 m/day, shows essential hydraulic anisotropy of medium effective conductivity: The vertical effective conductivity is three orders of magnitude less than horizontal hydraulic conductivity; this phenomenon relates to obtained anisotropy of correlation scales of sand/clay facies, and it prevents vertical migration of injected waste.

A 3D flow and transport model of the injection area was developed by MODFLOW2000/ MT3DMS codes using a 3D spatial lithological heterogeneity model. To optimize computer time and the numerical convergence of solution methods, the step of the vertical numerical grid was increased five times. Thus, the total number of flow/transport model blocks was about 800,000. Calibration of the flow model was done by modeling an injection cycle during one year. Data on groundwater heads in the monitoring well, screened for the injection interval and overlying formation, was used for calibration of hydraulic conductivities and elastic storage of the clay. For verification of the calibrated model, monitoring data for another year were used. The results of calibration and verification indicate that the model well reproduces changes of hydraulic heads during injection. The calibration results give the following values of calibrated horizontal parameters: hydraulic conductivity of sand is 0.86 m/day, vertical hydraulic conductivity of sand is 0.009 m/day, isotropic hydraulic conductivity of clay is 4×10^{-5} m/day, and clay elastic storage is 8.4×10^{-7} m^{-1}. The obtained values fall within acceptable intervals of hydraulic parameters for these lithological units in the studied region.

Long-term transport of waste from an instantaneous small source placed within the modeled medium was simulated to study the possibility of using an effective macrodispersive approach for this medium. Two sets of simulation runs, with different mean flow directions, were performed: horizontal and vertical flows. In the first case, the simulated situation represents natural groundwater flow from injection site to discharge zone, with flow direction coinciding with the largest correlation scale of sand and clay bodies. In the second case, the upward flow within the discharge zone, with flow direction along the smallest correlation scale of lithological units, was simulated. For both cases, using the method of moments, the temporal changes during 3,000 years of the main diagonal terms of macrodispersivity tensor were estimated. The results of these numerical experiments show that for the studied medium, effective longitudinal macrodispersivity increases up to approximately 2,000 years after the transport process begins. The macrodispersivity tensor depends very strongly on flow direction. For horizontal flow, horizontal and vertical transverse dispersion terms are much less than the longitudinal term, while vertical flow transverse terms exceed the longitudinal term by two orders of magnitude. These numerical experiments generally show that a problem still exists regarding the selection of the best model for predicting long-term and regional scale waste transport at this site. Dispersion parameters of an effective macrodispersive model are time- and space-dependent, while a high-resolution 3D model cannot be applied to regional scale transport modeling.

The last step of the reported study was a simulation of 40 years of injection history to obtain an up-to-date 3D distribution of injected neutral species of the wastes within the formation. For this, the 3D flow and transport model, with estimated hydraulic parameters and local-scale mixing and diffusion, was used. The resulting complex irregular shape of a waste plume depends on changes in wells used for injection, their injection rate, and the influence of 3D topology of clay and sand facies. Analysis of modeled waste distribution shows that today the main mass of waste is predominantly distributed within the sand. The processes of clay filling due to diffusion and advection still play a small role in the overall waste transport. More important is the 3D clay/sand topology that affects the velocity field within highly permeable units of the studied formation.

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