COMPREHENSIVE APPROACH FOR 3D SIMULATION BY MATHEMATICAL MODELING OF GROUNDWATER CONTAMINATION

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ABSTRACT

Development of precise models for predicting and managing processes of groundwater contamination as a result of a number of natural and technogenic factors (mining activity, industry, agriculture, sanitary landfills, etc.) requires more detailed knowledge on the structure and morphology of aquifers. Some of the aquifers are located in sediments and sedimentary rocks of significant heterogeneity of the lithological properties, causing a rather high heterogeneity of porous medium. Past practice of mathematical modeling has not considered realistically enough the rate and specifics of this heterogeneity.

In recent years, sedimentology of aquifers acquires higher importance in the compilation of 3D prediction models. This comparatively new approach allows the application of a set of direct and indirect "in situ" and laboratory sedimentological, stratigraphic and geophysical methods, which allow the correct differentiation and definition of lithofacial and architectural-element units of different rank and scale. Each of them is characterized by relative inner homogeneity of hydrodynamic and migration properties. Thus, the differentiation of zones and layers simulating the correct hydrogeological conditions is allowed easily and precisely enough by compilation of numerical 3D models.

The comprehensive approach was successfully tested at the Plovdiv sanitary landfill.

INTRODUCTION

Groundwater is the main object of technogenic contamination and potential carrier of different contaminants. Hydrogeological conditions in the area of potential (or real) source of contamination are the major factor, limiting the behaviour of contaminants within the underground hydrosphere. For that reason good recognition and correct simulation of particular hydrogeologic medium is so important.

HETEROGENEITY OF POROUS MEDIUM AND OPPORTUNITES FOR ITS CORRECT SIMULATION

Aquifers (groundwater reservoirs) are often formed in non-homogeneous sediments and sedimentary rocks. Lithologic heterogeneity determines the significant variety in dimensions and geometry of porous medium and regularly brings to area variation of hydraulic and migration characteristics of water-bearing (saturated) medium. Unfortunately, simulation approaches for compilation of flow and mass-transport models has not considered yet the rate and specifics of this heterogeneity realistically enough. This fact predetermines the inaccuracy of prediction models and subsequent efforts for their elimination.

Recent practice widely applies several approaches for modeling the movement of contaminants in aquifers: simplified, stochastic and deterministric.

The simplified approach is based on the adoption that saturated medium is relatively homogeneous (quazihomogeneous) in the aspect of hydrogeological parameters. Each of the water-bearing layers, consisting of several aquifers and aquitards is considered quazihomogeneous and horizontal. In the simplified approach the distribution of conservatives (inert) contaminants in the aquifers is described well by the convection-disperse equation (Bear, 1972). Behaviour of contaminants with water-bearing medium is modeled by mathematical dependencies, describing the kinetics of processes of reversable and non-reversable elimmination (Bear, 1979; Freeze and Cherry, 1979). The reversible elimination (sorption-desorption) is described by the linear isoterm of Henry and is characterized by the coefficient of distribution K_d, with sorptional porosity n_s, respectively. Non-reversible elimination (hydraulitic decay and precipitation) is determined by the reaction of non-reversible elimination of first order and by the elimination constant γ. It is worth mentioning that this approach, widely applied in the past, may be used (with a sufficient precision) in a very limited number of cases and significant schematization of the hydrogeological background. It is valid within a local scale and a homogeneous media only.

The stochastic approach is developed and widely used in practice in the last 20 years. Movement of contaminants in the non-homogeneous medium is described by area correlation of random fields (Dagan, 1989; Gelhar, 1993) or by fractal distribution, laid over homogeneous or slightly varying trends (Wheatcraft and Tylor, 1988). Considerations are based on the adoption that area variation is small. This brings to the negligence of real existence of lithofacial and architectural-element units of different rank and size, which in fact determine the inner and outer boundary conditions in the flow area and strictly frame the possible ways for distribution of contaminants. No doubt, possible movement of contaminants is correctly modeled mathematically only after precise determination of sedi-

mentologic interconnection of different scale.

The deterministic approach pretends to simulate the real heterogeneity of natural objects with a maximum reliability. 3-D objects, homogeneous with respect to hydraulic and migration characteristics (layers and zones) are differentiated and described in the subsurface area. Objects, determined by this approach are treated as main architectural elements of the water-bearing structures. Movement of contaminants is described precisely enough by the mathematical means, applied by the simplified approach within each quazihomogeneous object. In the compilation of regional mathematical models for prediction of groundwater contamination, each element is included as a 3-D object with established geometry and properties (hydraulic conductivity k, dispersivity α, effective and sorptional porosity n_0 and n_S, elimination constant γ etc.). In this case software packages MODFLOW and MT3D, standardized by USGS and EPA and widely applied in the world practice may be used (Andersen, 1993; McDonald и Harbaugh, 1988; Zheng, 1990 et al.).

The application of traditional hydrogeological means and vehicles to the deterministic approach most often brings to difficulties. The attempts to determine 3-D objects based on statistical processing of results from "in situ" and laboratory filtration (hydraulic) tests (Боревский и др., 1973, Мироненко и Шестаков 1976, etc.) showed that investigations of that kind might have only theoretical importance and did not reveal any specific meaning for practice as statistical methods required performing of numerous tests in different points of the subsurface area which would bring to unreasonably high financial cost.

A modification of the deterministic approach, new for hydrogeological practice and recognized in specialized references as aquifer sedimentology (Huggenberger and Aigner, 1999) has recently shown its advantages. This sedimentological approach comprises a set of direct and indirect "in situ" and laboratory sedimentological, stratigraphic and geophysical methods, which allow the direct determination of lithofacial and architectural-element units of different rank and scale (size). Each of those units is characterized with relative homogeneity of hydrogeological characteristics. The approach allows compilation of a good and rather precise 3D model, showing the natural heterogeneity of medium by a limited number of laboratory and field hydrogeological tests. Reliability of prediction model depends much on precise correlation between hydraulic and migration characteristics and existing 3D variation. However, cost efficiency and other practical concerns usually limit the number of exploratory and hydrogeological tests, which reduces the precision of simulation. This fact may not decrease the importance of suggested approach as the ratio of (financial cost)/(precision of prediction) may be optimized for each specific object depending on its significance. In some cases, below suggested dependence of correlation between hydraulic conductivity and size of grains of prevailing fraction and rate of sorting may be used purposefully for preliminary assessments and predictions.

SEDIMENTOLOGY OF WATER-BEARING STRUCTURES

As it has already been mentioned, the sedimentological approach has been successfully applied to hydrogeological issues. Often, especially when located in fluvial deposits, aquifers reveal a wide spectrum of lithological and lithofacial variability, which significantly predestinates the hydraulical and migration properties of medium. Recently many attempts to characterize and systematize qualitatively and quantitatively those heterogeneity by the form of a hierarchic system have been done (for example van de Graaff and Ealey, 1989; Dreyer, 1993). According to Huggenberger and Aigner (1999), within such hierarchic scheme of the degree of the lithological heterogeneity, the individual subdivisions could be treated as both genetic sedimentologic units and hydrogeologic units, for exapmle:

❑ Giga-scale lithological heterogeneity, determined by development of sedimentary basin. It controls the confinements and inner structure of entire water-bearing basins;
❑ Mega-scale lithological heterogeneity, determined by the type of sedimentary environment. It characterizes the area interrelations of aquifers and complexes in the water-bearing basins;
❑ Macro-scale lithological heterogeneity, determined by local facial dynamics of sedimentary accumulation. It determines the morphology and inner structure of individual aquifers and aquitards;
❑ Meso-scale structural and textural variations, related to sedimantary dynamics. It subdivides aquifers into zones of different hydrogeologic characteristics;
❑ Micro-scale differences in petrology, porosity and permeability, related provenance and diagenesis. They control the processes of filtration and mass-transport at a micro level (in the pore channels).

The architectural-element analysis is among the main tools for implementation of macro- and mezo-scale investigations in sedimentology of aquifers, located in fluvial sequences. The method is based on the comprehension that fluvial sedimentary sequences are composed of eight constructive units, nominated as "architectural elements" (Allen, 1983; Miall, 1985, 1988). Their identification and characterization is possible in large two- and three-dimensional outcrops. The definition of these architectural elements is based on both their outer morphology, determined by the character of their confining surfaces, and organization of their inner structure. Those features reveal the different style and dynamics of sedimentary body generation and in most cases are related to morphologic features of dimensions of the complex sedimentary macroforms. Despite of some variations in their characteristic, it is accepted that most fluvial depositions are composed of those eight elements in different proportions.

The architectural element description and definition comprise:
❑ Nature and morphology of confining surfaces;
❑ Unit scale: thickness, lateral (parallel and perpendicular to the direction of the sedimentation paelotransport) development;
❑ Outer unit geometry;

❑ Inner structure of the unit: lateral and vertical lithofacial assemblages and sequences, presence and orientation of low-rank erosion surfaces, orientation of the indicators of the sedi-

mentary paleotranspot, interaction of bedding in respect of the limiting surfaces.

The application of architectural-element analyses to the study of fluvial sequences simplifies significantly their sedimentological modeling thus increasing precision and sustainability of prediction mathematical model.

COMPREHENSIVE APPROACH FOR SIMULATION OF 3D MEDIUM IN THE MATHEMATICAL MODEL OF GROUND-WATER CONTAMINATION IN THE AREA OF PLOVDIV SANITARY LANDFILL

The sanitary landfill of Plovdiv is developed in Quaternary and partially Neogene loose, mainly alluvial sediments. The uppermost part of the sedimentary section in and around the landfill is represented of four fluvial cycles, located one above the other. The thickness of the separate cycles is within the range of 8-13 m showing lateral variations. Only the uppermost of these cycles outcrop on the surface, however, due to the character of sediments its exposure is rather limited. That is the reason, instead of the standard approach for architectural-element analysis, in a larger part of the area the acquiring of the necessary for the analysis data to be reduced to:
- Studying the vertical lithofacial sequences;
- Systematic measuring of all types of indicators in the direction of sedimentary paleotransport;
- Detailed study of morphology and orientation of limiting surfaces of individual lithofacial units.

As a result 10 lithofacial varieties and 6 types architectural elements are identified and characterized. The description of architectural elements in the present study is based on the proposed by Miall (1996) scheme with some changes and additions.

Groups of carefully correlated outcrops, located in a cross and longitudinal direction of dominating paleotransport trends are studied for achieving of correct model of the fluvial depositions. The acquired data have been used for interpreting the results of numerous exploratory boreholes in the area. A network of profiles, which illustrate the area distribution of separate fluvial cycles and comprise the entire territory of the landfill, is developed. Within each fluvial cycle the spatial interrelations of constructing architectural-elementary units are illustrated.

Based on numerous grain-size analyses, the degree of sorting of the sediments in each separate lithofacial unit is determined, and hence – in the architectural-elementary units that they compose. The representation and analysis of grain size data in standard phi-scale allows hydraulic and genetic interpretation of the studied sedimentary bodies.

A correlation diagram (Fig. 1) is compiled on the base of the relations between granular characteristics and rate of sorting of sediments, on one hand and hydraulic conductivity on the other, which many authors have obtained, (according to Виссмен, и др., 1979; Де Уист, 1969; Daly, 1982; Davis and DeWiest, 1966; Morris and Johnson, 1967,etc). It allows interpreting of lithofacial and architectural-elementary units as hydrogeological units (aquifers and zones of particular geome-

try and characteristics). At first approximation, two aquifers and one aquiclude are determined in the subsurface area of the Plovdiv sanitary landfill area. Zones of different penetration are differentiated in the aquifers, and a number of interruptions, so called hydrogeological windows, are localized in the clayey aquiclude.
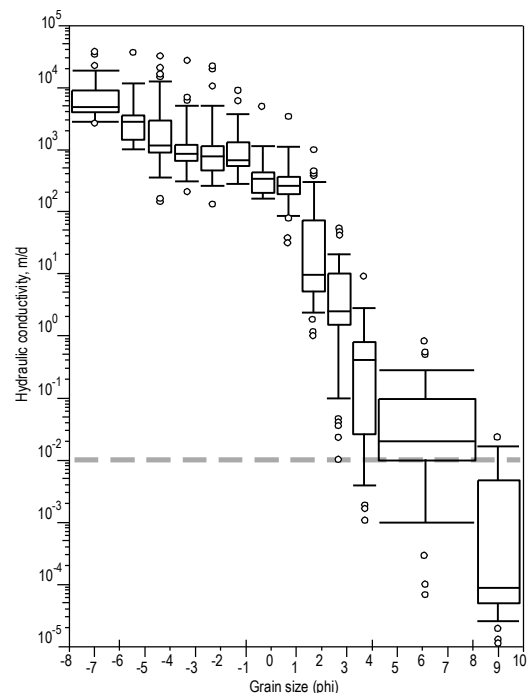

Figure 1. Correlation box-diagram of the type of sediments and hydraulic conductivity. Dotted line shows the boundary between permeable and practically impermeable sediments. Circles show the values, typical for well-sorted and poorly sorted varieties.

Each layer and zone acquires values of characterizing hydraulic and migration parameters based on data from laboratory and "in situ" filtration and traser tests. Thus, a rather precise 3-D model of subsurface area in the region of Plovdiv sanitary landfill is compiled. This model is successfully applied by the authors for precise simulation of aquifers and zones (potential medium for distribution of contaminants) in the filtration field for compilation of mathematical models for prediction of processes of groundwater contamination in the landfill.

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