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Construction of concentration fields of elements in 3D in groundwater of an industrial hub using GIS technologies☆

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ABSTRACT

Developing the scientific heritage of V.I. Vernadsky, the founder of hydrogeochemistry, and based on his research studies in the Tambov region (Russia) the authors have established a methodological approach to access information about hydrological, geochemical, and industrial objects located on the territory of an industrial hub using GIS technology. This approach allows (1) the generation of a spatial information model of an industrial hub, where all objects are geo-referenced, (2) the creation of retrievable data on water quality in an industrial hub, and (3) the presentation of data processing results in the form of concentration fields of elements or their compounds. The data for the model were obtained from several sources including raster maps of an industrial hub and attribute data about industrial and natural objects over a five year period. Typical components, which define the chemical composition of groundwater of the area, are increased hardness, excessive iron content and increased mineralization (dry residue). Analysis of operating conditions of observation wells located on the territory of an industrial hub and evaluation of contamination spread in the aquifer within the mining lease are carried out using the following models: a geo-filtration model, which allows obtaining pressure distribution values at the injection wells, and a geo-migratory model, which helps in forecasting the spread of industrial wastewater in the aquifer. These models allow estimating the size of contamination spread areas and validity of applied methods of industrial waste utilization.

1. Introduction

The quality of water used for water supply is one of the most important characteristics of its consumer properties. Chemical composition of water affects people's health and well-being. Stability of water quality parameters over time is of great importance for the society as a guarantee of their constancy in the foreseeable future.

Vladimir Ivanovich Vernadsky (1863–1945), a Russian geochemist and mineralogist who is considered to be one of the founders of geochemistry and biogeochemistry, has only recently become recognized internationally, despite being regarded in Russia as one of the greatest names in science of the 20th century. He paid much attention to the assessment of natural water quality in his works (Vernadsky, 1933, 1934, 1936, 2003). Field studies of soil gave him much data for scientific analysis and influenced his methodology and fundamental ideas that are still relevant today.

His research interests involved the geochemistry of soils, including natural waters (Vernadsky, 2003). The genetic approach in studying soils, minerals and nature as a whole led Vernadsky to geochemistry, which didn't possess a unified concept in the early twentieth century. Vernadsky has not only identified the patterns of concentration and dispersion of chemical elements during the evolution of the Earth establishing the concept of modern geochemistry, but also filled separate fields of this new science with content, and has much contributed to the development of the applied geochemistry, e.g. (Glazovskaya, 2002).

Resent publications such as Edmunds and Bogush (2013) are aimed to bring the most significant works of Vernadsky: "The biosphere" (Vernadsky, 1926), which was only fully translated into English in 1998 (Vernadsky, 1998) and "Essays on geochemistry" (Vernadsky, 1927) which have been translated partially into English in 2007 (Vernadsky, 2007), and "The history of natural waters" (Vernadsky, 1933, 1934, 1936, 2003) which was not translated into English to get further attention from the international geoscientific community. The latter explores many concepts in hydrogeology, geochemistry, and especially biology in which water is described as an integral part of the biosphere. Vernadsky also adopted the concept of the 'Noosphere' to emphasize man's role in the biosphere as well as a powerful geological agent. In relation to natural waters, Edmunds and Bogush (2012) conclude that Vernadsky's three main concerns – (i) a lack of integrated studies of various types of natural waters; (ii) a lack of parallel studies

☆ This article is dedicated to a special issue in honor of Vladimir Vernadsky.

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of water and minerals; and (iii) a lack of geochemical integration in hydrogeological studies – are now taken into the mainstream of research and practical application.

As pointed out by Shvartsev et al. (2006) and Chudaev et al. (2013), Vernadsky is not only the founder of hydrogeochemistry, but also the author of the concept of the geology of water and its geologic activity, which is based on the evolutionary development of the water–rock–gas–organic matter system and the special role of water as the most important component (medium) of the environment. The most important parts of this concept are the ubiquity of water, its unity, its perpetual geological mobility, water equilibrium in the Earth's crust, dissymmetry, water cycle, intensity of water exchange, and migration of chemical elements. These directions are being extensively developed in modern hydrological science.

The era of extensive use of modern information technologies allows the application of an integrated approach to the investigation of water resources involving geological, geochemical, biological and sociological dimensions. A growing interest in the potential for integrating GIS technology and groundwater simulation models was revealed in a simultaneous use of GIS-based hydrogeological databases and groundwater modeling done by Gogu et al. (2001) in Belgium for the Walloon region, which include data from five river basins, chosen for their contrasting hydrogeological characteristics. A “loose-coupling” tool was created between the spatial-database scheme and the groundwater numerical model interface which provides a powerful tool for hydrogeological studies.

Another successful attempt for 3D geologic framework models for regional hydrogeology and land-use management in the St. Lawrence Lowlands, Canada was made by Ross et al. (2005). The detailed stratigraphic reconstruction using gOcad allows improving understanding of subsurface conditions above the regional aquifer and provision of a common stratigraphic framework for hydrogeologic applications.

McCarthy and Graniero (2006) from the University of Windsor, Canada have developed a GIS-based borehole data management and 3D visualization system (BoreIS) as an extension to ESRI's® ArcScene ™ three-dimensional (3D) GIS environment, which uses borehole or well data supplied by the user. By matching table elements to spatially and geologically significant terms through the interactive setup a 3D GIS representation can be queried, visualized, and analyzed and as a result it allows automating many high-level GIS functions so that an inexperienced GIS user can still use the system.

A watershed characterization and modeling system was developed by Strager et al. (2010) to support decision making and the management of water resources at a statewide level in West Virginia by providing consistent technical information related to natural watershed processes and prediction of the impacts of alternative management scenarios for decision makers. Components of the current system include: an overland flow path model that indicates optimum water quality sampling locations, flow estimation for all streams in an identified area, an instream water quality and loading model for pollutant levels, and a ranking model to prioritize treatment alternatives based on user defined criteria and preferences.

Chesnaux et al. (2011) present an approach for the development of an exhaustive and comprehensive groundwater database through (1) the gathering of relevant sources of information related to groundwater, and (2) the application of a quality control process in order to screen the data for accuracy and quality. A unified compatible combination of “Relational Database Management System–ArcGIS®–Arc Hydro Groundwater” technologies was used for the 3D structural representation of aquifers (groundwater reservoirs) of the Saguenay Lac-Saint-Jean region, Quebec (Canada).

In this paper, which pursues and develops the scientific heritage of Vernadsky, we established a spatial information model based on the example of an industrial hub in the Tambov region, Russia, using ArcGIS®. As a result we are able to obtain objective information about water resources of an industrial hub and to present data processing results about groundwater quality parameters in the form of concentration fields of elements or their compounds.

2. Methodological background of the approach

Nowadays, obtaining reliable information about the quantity and quality of water in a convenient form cannot be done without modern information technology (Malygin et al., 2001; Nemtinov, 2005a,b).

Authors used the ArcGIS® system of the ESRI® (Environmental Systems Research Institute) as the base for the study (DeMers, 2009). A system comprising Intel® Core™2 Quad processors (Q6600, 4 cores, running at 2.4 GHz) and 8 GB RAM was used.

The current scheme of water supply for large consumers within the Tambov region, which was formed in the first decades after the World War II (1941–1945) initially utilized the simplest way of water extraction from surface sources, i.e. rivers. Nowadays this approach is less suitable as surface waters are heavily polluted. Water treatment and post-treatment aiming on the improvement of drinking water quality both require constant and substantial investments, which are available only for very large customer groups.

There are currently unsolved problems such as comparative evaluation of groundwater and surface water for domestic water supply, impact of polluted river water on groundwater, etc. As a consequence, the following regional objectives gain high priority:

- assessment of the capability for using groundwater aquifers in the valleys of the river Tsna, which flows through Tambov industrial hub, and its tributaries by mathematical modeling of depression cone development and possible interaction of groundwater and surface water;
- choosing aquifers as water supplies for large customers;

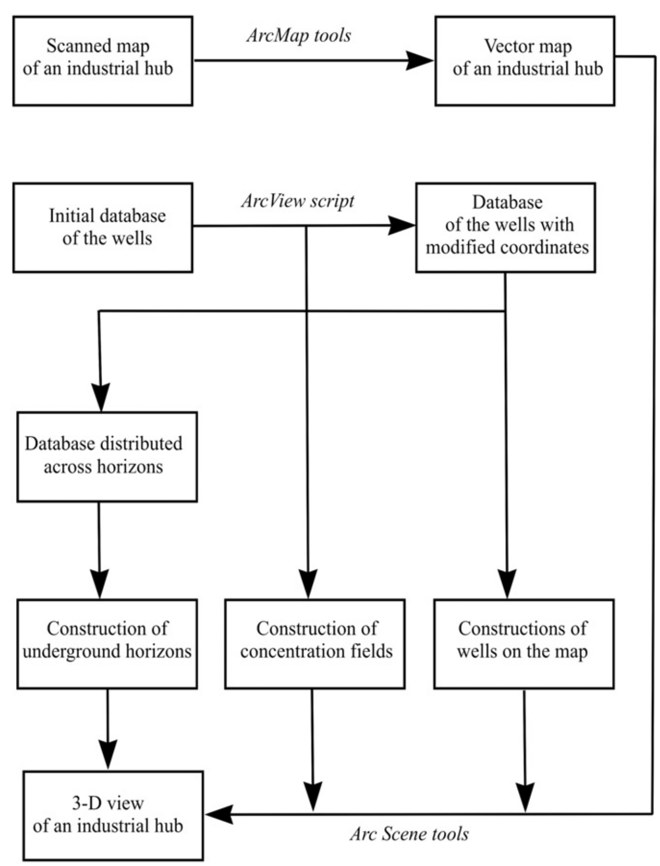

Fig. 1. Construction flowchart of surface relief, underground horizons and concentration fields of element in water.

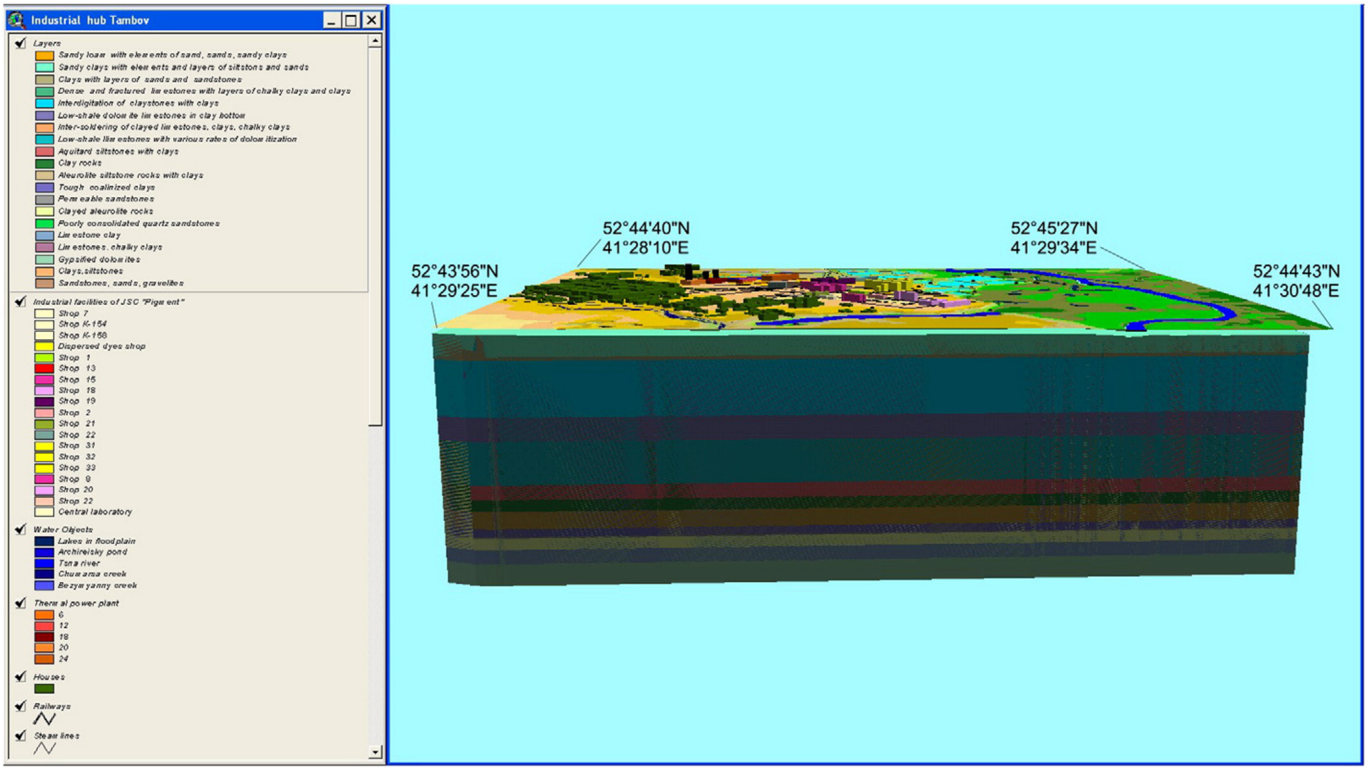

Fig. 2. General 3D-view of a spatial information model of an industrial hub.

- economic feasibility assessment of using remotely located aquifers and small aquifers containing water which do not comply with accepted quality standards, etc.

In order to resolve these issues it is necessary to develop an appropriate spatial information model of the Tambov industrial hub which includes: a map of terrain relief and of aquifers (with their geologic

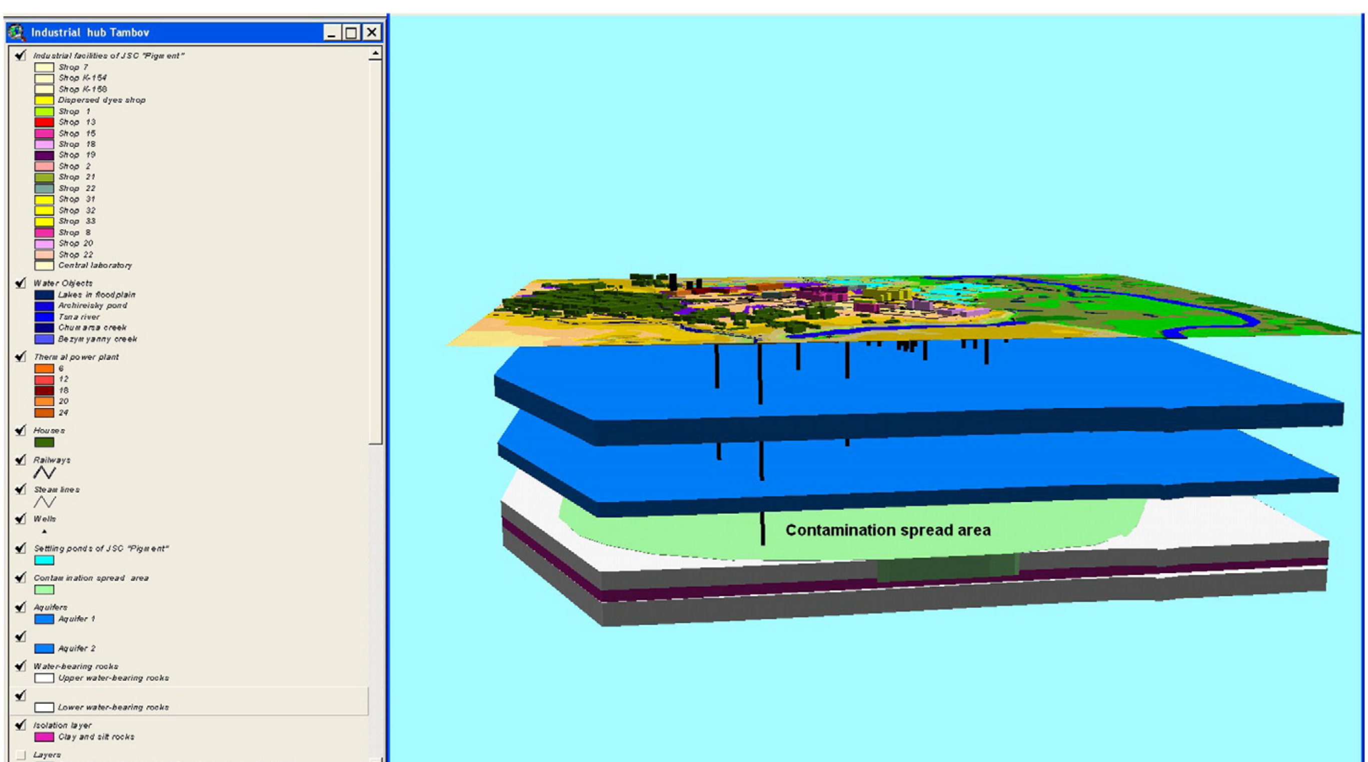

Fig. 3. 3D-view of a spatial information model of an industrial hub with underground aquifers and contamination spread area.

and hydro-geologic characteristics including reservoirs for injection of highly contaminated industrial wastewater); industrial facilities used for various purposes (enterprises, stations of biological treatment of wastewater, etc.); natural objects (lakes, part of the river Tsna and its tributaries, which flow through the Tambov industrial hub); sources of surface water and groundwater contamination; water wells and barrage wells of large chemical enterprises with data on volumes of injection of wastewater into a deeper watertight stratum and barrage water diversion; water wells with data on water diversion for different purposes; observation wells and their characteristics; river stations and other units (points) of surface water sampling; data on field studies of groundwater and surface water at the hub, etc. (Nemtinov and Nemtinova, 2005; Nemtinov et al., 2008).

The data were obtained from the following data sources:

- raster maps of the industrial hub;
- attribute data about various objects collected by the authors together with the employees of the territorial center of state monitoring of geologic environment of Tambov region over a five year period. Fig. 1 shows the procedure for constructing surface topography, aquifers and concentration field using the main components of ArcGIS®: ArcMap™, ArcView® and ArcScene™.

The flowchart shows that a scanned map of an industrial hub is first converted to a 2D-model and then to a 3D-model using ArcGIS® tools. Background information containing the results of long-term observations on wells is converted by applying a software module developed by the authors so that it can be used by ArcGIS® tools to build surface topography, subsurface horizons and concentration fields of various elements in the water.

3. Spatial information model of an industrial hub

The research resulted in the development of an information model; examples of it are illustrated in Figs. 2–5. An overview of the 3D-model of the Tambov industrial hub is shown in Fig. 2. It comprises industrial sites of the north-eastern part of the city of Tambov.

Fig. 3 depicts a more detailed view of the underground aquifers and layers used by a chemical company for injection of industrial wastewater. For the purposes of better visualization, linear dimensions of wells in Fig. 3 have been increased tenfold compared with their actual sizes.

For wastewater injection in two aquifers of Givetian stage of the Middle Devonian age (more than 700 m below the surface). Water-bearing rocks are formed by fine-grained quartz sandstone. Minable seams are separated by a layer of impermeable clays and silts.

Analysis of observation well functioning and evaluation of injected wastewater spread into the aquifer within the mining lease are conducted by using a geo-filtration model, which allows obtaining pressure

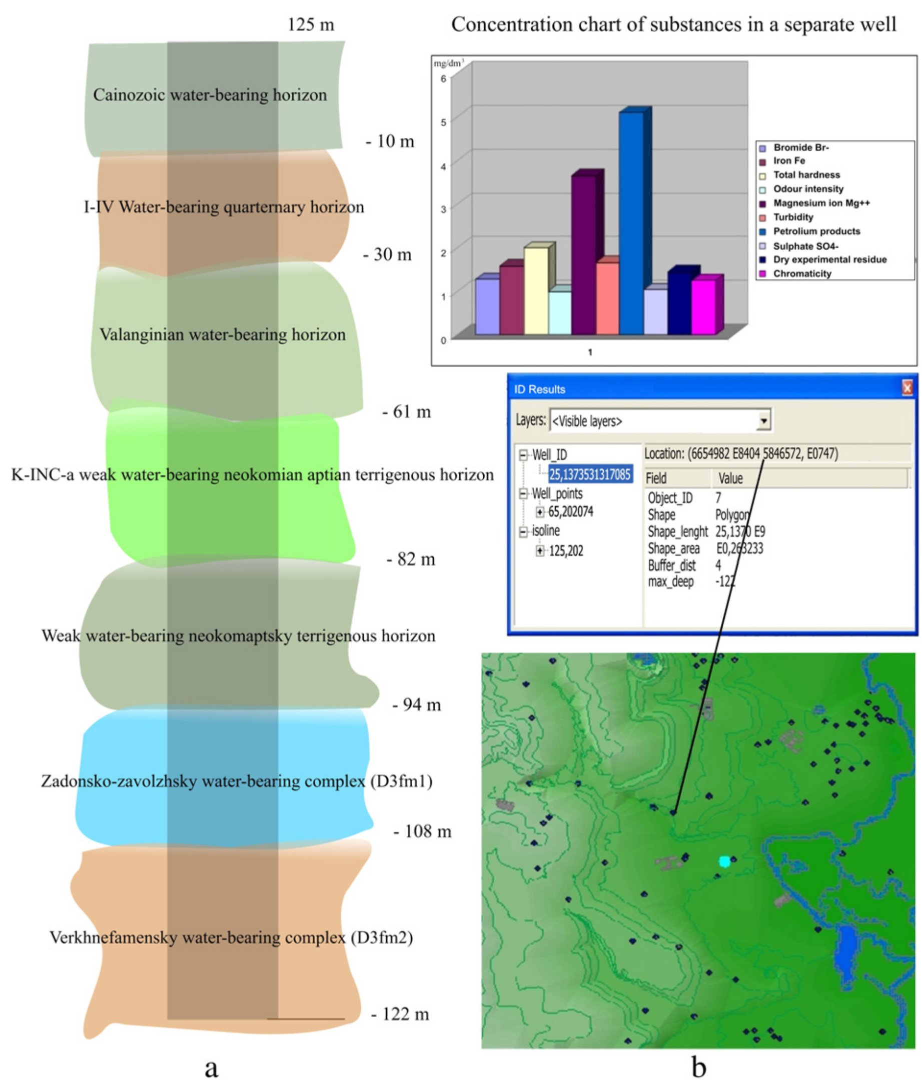

Fig. 4. Data on chemical composition parameters of water in a single well.

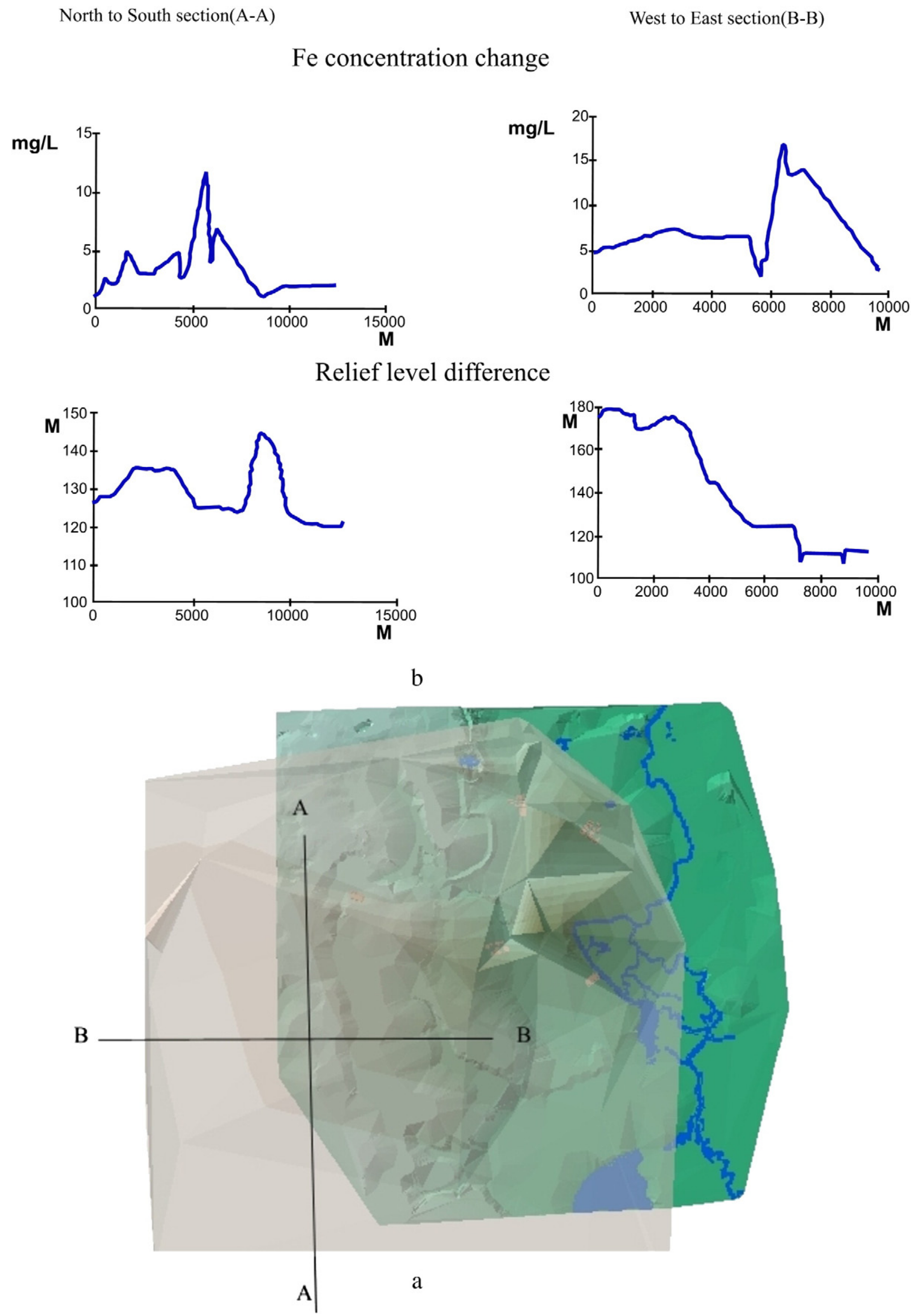

Fig. 5. Graphs of iron concentration fields (Fe) based on geochemical analysis of water (macFe = 0.3 Mg/l).

distribution in injection wells, and a geo-migratory model, which helps in forecasting propagation of industrial wastewater into an aquifer (Fetter, 1994; Shestakov, 1995). These models allow conclusions to be drawn about the size of contaminated areas (see Fig. 3) and prospects of using suitable method of industrial waste recycling within the allocated mining lease.

Data about the depth of soil horizons obtained during drilling allowed the mapping of surfaces of each horizon within the industrial hub of Tambov using subsystem ArcScene™. Data from more than 400 wells was used. For example, Fig. 4a shows surface fragments in the vicinity of a separate well. This well is 122 m deep and the surface level is located 125 m above the sea level.

A database of water quality indicators for each well was developed over a long period of their operation. Typical components, which define the chemical composition of groundwater of the area, are high hardness, excessive iron content and increased mineralization (dry residue). Average values of water quality (iron, hardness, sulfate, etc.) in a single well are shown in Fig. 4b.

In order to obtain summary data about groundwater quality in different places of an industrial hub, surfaces of concentration fields for each indicator (bromide, iron, total hardness, odor intensity, magnesium ion, turbidity, petroleum products, sulfate, dry experimental residue, chromaticity) were mapped by the means of ArcScene™ subsystem. As an example, Fig. 5a shows concentration field of iron in water. By imposing these surfaces with planes, which characterize the values of maximum allowable concentrations, areas with elemental concentrations exceeding permitted levels can be identified.

In order to obtain more detailed information, there is an option of building timing diagrams of concentrations at any cross section of fields. Fig. 5b shows graphs of iron concentration changes in two directions: from north to south and from west to east.

In these cross-sections a significant excess of iron content compared to the maximum allowable concentration of 0.3 Mg/l can be observed. Similar information can be also obtained for other elements and their compounds contained in the underground water.

4. Conclusions

Developing scientific heritage of Vernadsky the authors have implemented a methodological approach in accessing information about different objects of an industrial hub using GIS technologies, which allow:

- creating a spatial information model of an industrial hub, where all objects are geo-referenced;
- retrieving data on water quality in an industrial hub;
- presentation of data processing results in the form of concentration fields of elements or their compounds.

The empirical results of this research for the Tambov industrial hub (Russia) can be also used in water quality assessment at similar territories.

In the future the proposed approach will be applied for water quality assessment of natural water reservoirs, for example, at water quality monitoring station with small water outflow.

Appendix A. Supplementary data

Supplementary data associated with this article can be found in the online version, at http://dx.doi.org/10.1016/j.gexplo.2014.04.007. These data include Google maps of the most important areas described in this article.

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