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High-resolution 3D spatial modelling of complex geological structures for an environmental risk assessment of abundant mining and industrial megasites

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Abstract

Conceptual geological models of industrial and mining megasites are an essential task of groundwater investigations as well as environmental risk assessment studies. Therefore, the conceptualization process of the structural geological model has depended on the development of a set of 2D cross-sections to portray a 3D picture of groundwater flow. This attempt always includes some simplifications that require, only to some extent, the true 3D situation of heterogeneous aquifers. Consequently, the modelled predictions of the path flow and transport conditions of contaminated groundwater are not satisfying in terms of a flow-path and risk based modelling approach. A more structured approach to develop the hydrogeological framework for the conceptual model is advocated, using different 3D geological modelling software packages to assemble the data, working in three dimensions and using this platform for subsequent groundwater flow modelling. Attention is given to the capability of different 3D modelling approaches, indicated by geostatistically based versus constructive cross-section based interpolations of complex sedimentary successions, that are compared in their results and suitability for subsequent hydrogeological modelling requirements.

The paper describes the results, in high-resolution 3D modelling, of the complex geological environment of the Bitterfeld/Wolfen megasite in the eastern part of Germany. Identification, assessment, and remediation of large-scale groundwater contamination require a detailed knowledge of the heterogeneous geological structure to predict the fate and pathways of contaminants and their potential interaction with, e.g., surface water. An area of 16 km^2 of the model area of the Bitterfeld/Wolfen area was chosen to transfer the complex structural geological setting. The subsurface geology could be assigned to 31 lithostratigraphic units and depicted using a 10×10 m GIS grid. This constructive and "knowledge-driven" 3D modelling allows the prediction of vertical and horizontal sections, visualization purposes, volumetric calculations of distinct sedimentary units, GIS applications, and the use of the detailed digital information within the subsequent flow and transport groundwater modelling. The high-resolution digital 3D model improves the hydrogeological modelling results. It is considered a basic requirement for groundwater modelling and investigations on environmental risk and impact assessment by fate, and pathway exposure route analysis of the complex geological and groundwater situations.

Keywords: 3D geological modelling; Mining area; Groundwater flow modelling; Environmental risk assessment

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1. Introduction

Large-scale groundwater contamination sites in the eastern part of Germany are characterized by different environmental impacts caused by the former chemical industrial complexes and the extensive impact on aquifers by open-pit lignite mining for more than 100 years. The region around Bitterfeld/Wolfen located in the Federal State Saxony-Anhalt is one of the most investigated locations of a former mining and industrial megasite with regional groundwater contaminations. Due to the multi-source regional contamination of the upper and lower aquifers, risk assessment based investigations of distinct exposure routes of the contaminated groundwater have been made. The hydrochemical situation is characterized by a complex mixture of organic compounds (chlorinated aliphatic and aromatic hydrocarbons) comprising a high diversity of individual organic substances as well as a high regional variability of contaminants in the aquifers, respectively (Wycisk et al., 2003; Heidrich et al., 2004, Weiss et al., 2004a, b). The understanding of related transport and natural attenuation processes in the groundwater needs a detailed understanding of the complex hydro-stratigraphy in the subsurface, related to the groundwater flow and transport processes and resulting impacts on environmental receptors.

Besides the complex situation of mining-induced aquifer geology, the hydraulic regime of the aquifers has changed completely. During the past mining activities, the groundwater table was lowered tremendously, inducing a regional shift of the groundwater flow directions due to related water exploitation with extended extraction cones. After the re-unification of the two German States in 1989, the lignite open-pit mining and the groundwater extraction came to an end. Subsequently, the groundwater table of the Bitterfeld area was continuously rising and reached the former natural position when an exceptional flooding event of the Mulde River happened in August 2002. The exceptional flooding event filled up the remaining open-pit mining Lake Goitzsche within 2 days and raised the groundwater table more than 8 m (Geller et al., 2004; Wycisk et al., 2005).

The dynamic change of hydraulic conditions in a regionally contaminated area with a high complexity of geological structures needs very detailed and accurate subsurface information about the heterogeneous aquifers and their related hydraulic properties. The simulation and identification of flow-path lines within the regionally contaminated groundwater could only be done by numerical groundwater modelling. Environmental risk and impact assessment requires an appropriate true 3D structural geological model of high resolution for subsequent simulation to minimize the uncertainties of estimated exposure routes of groundwater contaminants within the heterogeneous and complex aquifer situation as well as the potential interaction with surface water and aquatic biocenosis.

Due to the fact that the availability and use of 3D models and GIS-based geological information is increasing, the major question arises: is it worth it to move from a "simplified" conceptual structural model of Fookes (1997) toward a "real" ground model of high resolution and accuracy as a platform for subsequent groundwater modelling? This attempt leads to ongoing challenges to subsurface characterization research posed by Rosenbaum (2003) and Culshaw (2005):

- To achieve better transitions between cognitive and computational representations and manipulations of geological information.
- To find ways of summarizing, modelling, and visualizing the differences between a digital representation and the real phenomenon.
- To respond to the increasing quantity of data and the different quality of information.
- To create simulations of geological phenomena in a digital form that are indistinguishable from their real counterparts.

The latter challenge is one of the main focuses of the paper, comparing different 3D modelling tools and modelling concepts by using the same geological data set of borehole information and their resulting variances. Therefore, the simulated results will be compared to the "real-world scenario" of the 3D spatial model of the investigated site as well as to the influence of the calculated results on subsequent groundwater modelling for environmental risk assessment studies.

2. Regional setting and site investigation

2.1. Historical background

The historical industrial region of Leipzig–Halle–Bitterfeld is characterized by overlapping environmental impacts of the former chemical industry, an extensive impact to the landscape, and a significant change of the groundwater table caused by lignite mining. Among the different tasks of land reclamation, the management of hazardous waste deposits and risk assessment of groundwater contaminants, as well as sustainable remediation strategies, are of general importance and were carried out during the last years. Underground and open-pit mining activities since 1830 have resulted in an extensive lowering of the groundwater table and in a change of the groundwater dynamics. Major parts of the industrial waste deposits of the former petrol–chemical industry, before and after World War II, are in contact with the groundwater. Therefore, an approx. 200 km^2 area of the Bitterfeld region is generally affected, of which an area of 25 km^2 shows a significant groundwater contamination, containing a volume of about 200 million m^3 (Heidrich et al., 2004; Weiss et al., 2004a, b). The regional setting of the Bitterfeld area is given in Fig. 1. To optimize the visualization, the model in the presented paper shows only a sub-area of 16 km^2 of the entire modelled area of 46 km^2.

The industrial landfill sites are located in a region with severely disturbed hydraulic groundwater conditions due to the abundant open-pit mining. Since the former industrial dumps were incompletely sealed, the contaminants affected the groundwater directly. During the last 100 years, the mean groundwater level was kept noticeably below the floor of the pits. The consequences of the currently rising groundwater level after closing the mines also clearly affects the groundwater flow directions and related pathway conditions of the groundwater contaminants in local and regional concerns.

2.2. GIS-based multi-source data management

To assess the complex environmental situation of the Bitterfeld megasite, a GIS-based spatial model that includes the heterogeneous aquifer setting in the third dimension and in as much detail as possible is required. The subsurface information

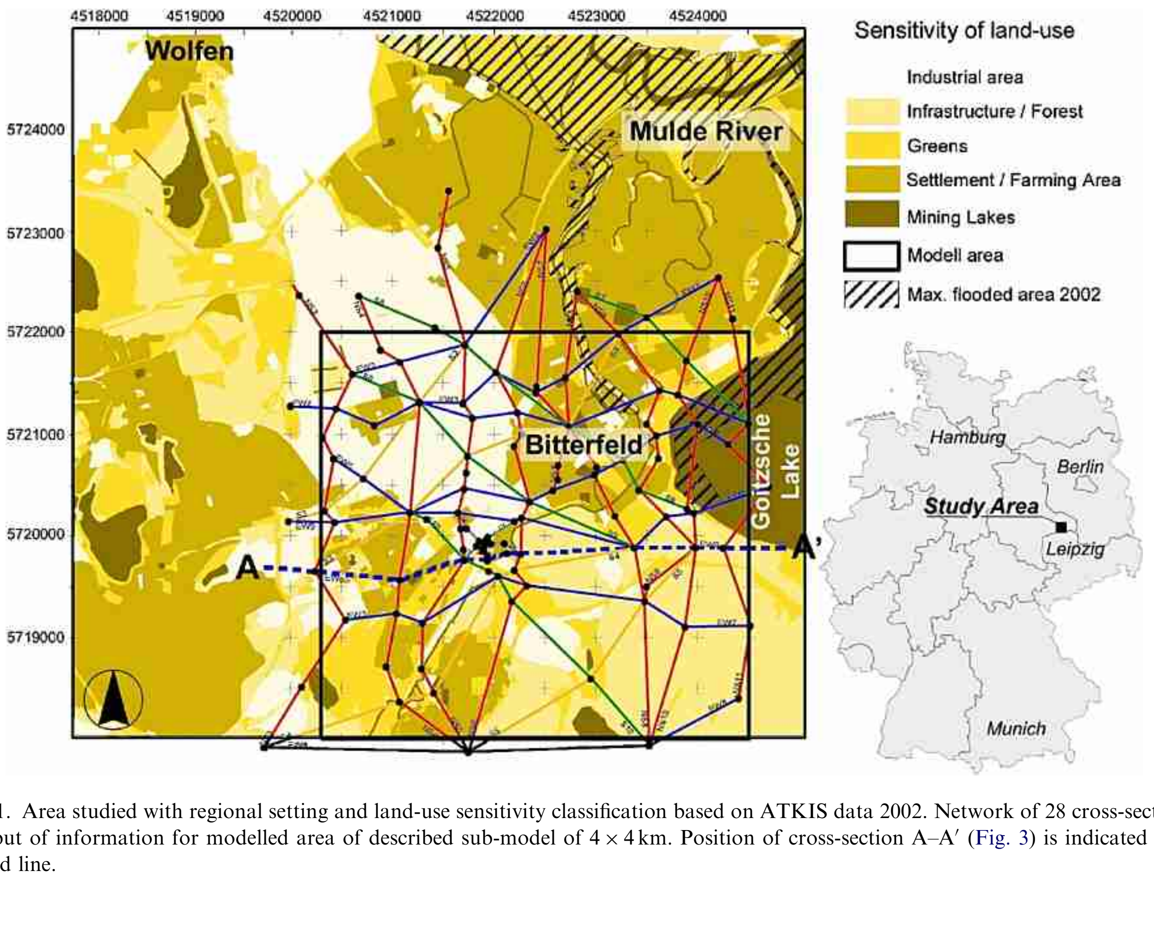

Fig. 1. Area studied with regional setting and land-use sensitivity classification based on ATKIS data 2002. Network of 28 cross-sections is input of information for modelled area of described sub-model of 4 × 4 km. Position of cross-section A–A′ (Fig. 3) is indicated by a dotted line.

has to be available for a GIS-based assessment and predictive calculations correlated to surface information of potential receptors. Therefore, the following major modules have to be integrated into the spatial model on a local scale, including the specific objectives and used modelling tools (Fig. 2):

- land-use classification,
- groundwater contaminants,
- hydrogeological data,
- 3D model of the subsurface geology.

The GIS data management for all hydrogeological and hydrochemical data was done with ArcView 3.x and ArcView 8.x (ESRI). The spatial model includes point data such as borehole data (lithology/stratigraphy), hydrochemistry (contaminants) monitoring data, line data such as rivers and creeks, and polygon data and surfaces such as the lignite open-pit mining areas. The geological cross-sections with their vertical 2D structure were held in a special tool for geological 3D models. The geological structure had to be held in a GIS database to obtain an interface to numerical groundwater modelling tools such as Feflow or Modflow. These data are stored in GRID or point formats in ArcView.

In order to characterize the regional groundwater pollution and to select parameters that should be further investigated, contamination profiles in which all substances are ranked according to their risk potential and with declining relevance for the contamination are needed. The available database comprises regional monitoring data of groundwater contaminants of nearly 10 years, approx. 3500 samples and up to 180 individual organic parameters (Wycisk et al., 2004). The criteria used to indicate a contamination profile were, e.g., the detection frequency and the average detected concentration per substance. Both criteria are normalized with assessment points, which are ranked in declining order of magnitude; the result is a contamination profile that can be completed by toxicological data. The most frequent substances are tetrachloroethene (PCE), trichloroethene (TCE), *cis*-1,2 dichloroethene (cis-1,2 DCE), vinylchloride (VC), 1,4-dichlorobenzene (1,4 DCB), 1,2-dichlorobenzene (1,2 DCB), monochlorobenzene (MCB), and benzene. The regional distribution of contaminants is not unique and reflects in general their different and multiple sources and pathway relations. Besides the specific problems of regionalization, a first attempt has been made by Thieken (2002), to classify the land-use areas (e.g., industry, mining, settlements, agricultural, and alluvial plains/meadows) in terms of average concentrations of the substances mentioned above.

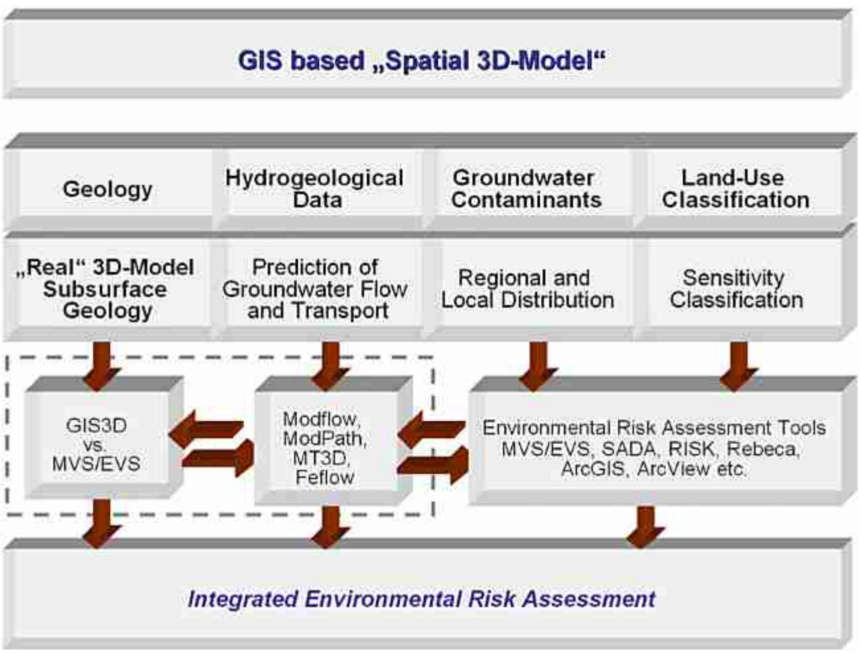

Fig. 2. Conceptual work flow of GIS-based “Spatial 3D-Model” with emphasis on 3D geological modelling and prediction of groundwater flow and transport for an integrated environmental risk assessment.

The identification of the sensitivity of land-use units has been done by recent digital topographic data and land-use classification (ATKIS). The ATKIS data set has been classified in terms of its sensitivity to groundwater contaminants and their potential exposure–receptor relations to selected land-use units (Wycisk et al., 2004, 2005). The sensitivity ranking is, to some extent, related to the normative concept of soil protection of Germany. The ranking of individual units comprises areas of increasing sensitivity: (i) industrial areas, (ii) forest and green land, (iii) meadows, (iv) agricultural use and open settlements, and (v) sensitive living areas and surface water, in relation to the selected objects of the ATKIS data set.

The contaminated area of the megasite Bitterfeld is located in the flood plain of the Mulde River and can be described by the following generalized geological and hydrogeological situations. As depicted in Fig. 3, the upper aquifer consists of Quaternary sands and gravel units. The Quaternary unit can be divided into a lower part, represented by lower terrace sediments of the Mulde River and overlying sediments, composed of braided river deposits of a smaller tributary stream. Both are separated by a hydraulically effective clay layer. The aquifer is in parts underlain by the remaining lignite seam of Miocene age, acting as a local aquitard (Wycisk et al., 2002). The lignite seam has been intensively mined in the southern part of Bitterfeld city. The lower aquifer consists of the Micaceous Sands with different hydraulic conductivity in the upper and lower parts. The bottom of this hydrogeological section is represented by clays (Rupelian Clay). The latter unit is considered to be the regional scale aquitard, hence corresponding to the bottom of the groundwater pollution. A detailed description of the hydro-stratigraphy and related hydraulic conductivities is given in Wycisk et al. (2002).

3. High-resolution 3D geological modelling

3.1. Model concepts and requirements

With the advances in 3D modelling software and visualization tools during the last few years, as well

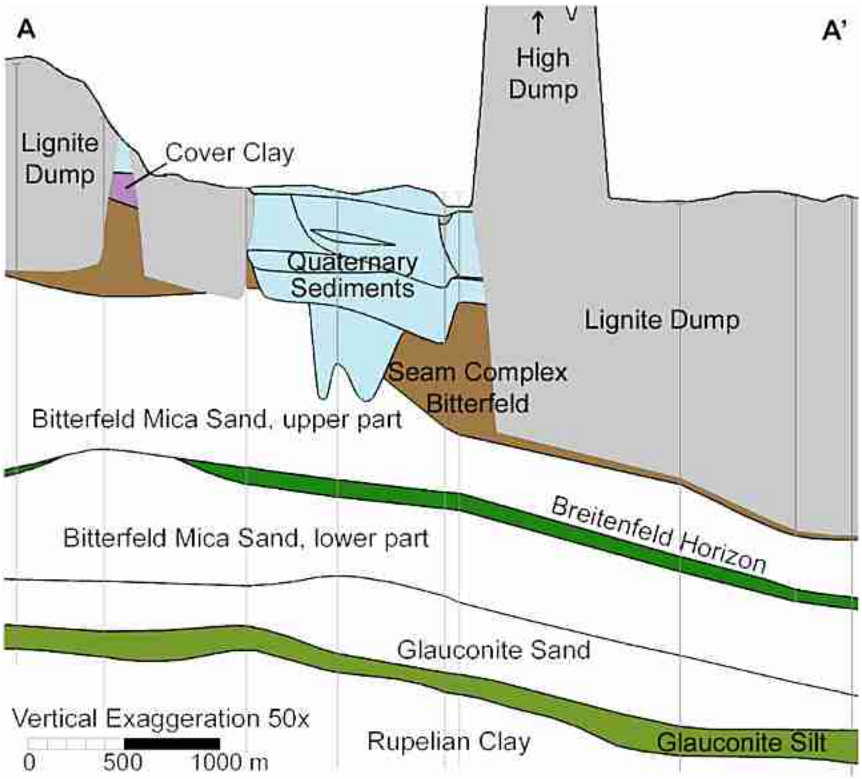

Fig. 3. Characteristic geological cross-section of modelled area. Note extension and geometry of hydraulic relevant Quaternary channel fill structures, remaining lignite and mining dumps of upper aquifer, as well as undisturbed Tertiary succession of lower aquifer.

as increasing 2,5D and 3D GIS applications, digital subsurface information of local to regional scales became more and more applicable and present (Culshaw, 2005; Wycisk et al., 2002). The development is additionally facilitated by the increasing availability of precise and sophisticated digital terrain models (DTM). This course goes in line with the increasing needs of conceptual and structural geological models in the broad field of groundwater simulation. Therefore, the quality of the subsurface model in terms of attributed hydrostratigraphical model layers, as well as "true" 3D volume models, are of increasing significance for future groundwater flow and transport modelling applications, respectively.

Depending on the local or regional scale and specific regional geological settings, different questions arise concerning the appropriate type of modelling, e.g.:

1. Which type of software tools represents the suitable "philosophy" of 3D modelling and is applicable?
2. What quotations should be solved?
3. Which capability of the software tools is essential to obtain an adequate true 3D model due to the specific regional geological situation?

Due to the complexity of 3D modelling software tools and the specific situation of regional geology, users might be not aware of the differences in their models or resulting limitations and disadvantages. 3D modelling software and visualization tools are available using geostatistical algorithms; e.g., Environmental Visualization System and Mining Visualization System (EVS/MVS), Rockworks, etc. are working completely differently from the TIN-based (triangulated irregular net) interpretation using intersected cross-sections like geological surveying and investigation in 3 dimensions (GSI3D). In the present paper, attention is given to the discussion of the quality and uncertainty of the modelled results. This depends on the different model concepts using the same data set of drilling information, especially related to Quaternary sediments and mining-effected artificial deposits.

Until now, "true" 3D modelling of geological structures had not been very common in regional hydrogeology and environmental assessment studies. On the one hand, the required coverage of geological drilling information, related to increasing aquifer heterogeneity, is not always available as a rule on a local to regional scale. On the other hand, the highly time-consuming modelling work and the not always realistic results are hampering the application of 3D subsurface models. The importance of sufficient geological subsurface information is applied, and hydrogeological modelling has been pointed out by different authors in the past: Houlding (1994), Rosenbaum (2003), Sobisch and Bombien (2003), Ozmutlu and Hack (2003), and Turner (2003).

The major obstacles in regional 3D modelling have been summarized by Berg and Keefer (2004) and can be confirmed by our experience from different regional models. The data verification of geology is very time consuming, and many projects requiring groundwater flow investigations have not had sufficient time or money to obtain the detailed geologic interpretations they really need. The interpretation of complex geological sequences, especially in the Quaternary, needs a specific experience in regional stratigraphy. Without the knowledge of lithostratigraphy and facies relations, any 3D modelling will be incomplete or will fail.

3.2. Cross-section net-based interpolation

GSI3D was developed by H.G. Sobisch and is currently intended for use in the near-surface modelling of superficial and Quaternary sediments (Sobisch, 1998; Sobisch and Bombien, 2003). The software is used by the British Geological Survey on different mapping scales and in combination with GoCAD for deep subsurface investigations and geological modelling (Culshaw, 2005) and for regional investigations of groundwater-contaminated megasites (Wycisk et al., 2002, 2004, 2005).

The modelling process with GSI3D is based on the creation of a series of intersecting user-defined cross-sections. The entire "stacking" order of all deposits in the study area has to be defined by the stratigraphers and sedimentologists, and a so-called generalized vertical section has to be created. In Quaternary deposits that underlie urban or abundant industrial and mining areas, this is less easy than it seems at first, due to inaccessibility or limited geological information; however, the lithostratigraphic classification of the sedimentary succession within a consistent regional stratigraphic framework is for modelling reasons much more helpful than a pure grain-size or lithology-based approach. The software allows the input of geological 2D mapping or surface information, especially from areas with a less dense borehole record. The uneven and spotty distribution of geological drilling information is one of the major obstacles in regional modelling with automatically contoured distribution and thickness. GSI3D allows the modelling of the distribution and geometry of sedimentary layers by knowledge-based control of the modeller, which is highly needed for heterogeneous aquifer systems and/or artificially formed lithological units of abundant open-pit lignite mining areas to bridge the partial lack of drilling information and involve the additional 2D information from different types of maps and technical mining documents.

The procedure for producing a local 3D model with GSI3D can be summarized as follows. Additional descriptions are given in Wycisk et al. (2002) and Culshaw (2005):

- DTM of appropriate resolution is loaded (10×10 m, up to 40×40 m).
- Sediment distribution maps of the Quaternary units, geological maps, and historical and recent maps from mining areas (e.g., distribution of mining dumps) are digitized.
- Borehole log data are stratigraphically, lithologically, and geophysically coded at the base of a generalized vertical section.
- Boreholes for cross-sectioning are selected.
- Starting with the shallowest, geologically realistic lines are digitized to connect the geological units.
- A series of regularly spaced cross-sections is created. Intersecting sections should cover local variations and anomalies and incorporate linear bodies (cut-and-fill structures, not adequately included in the major cross-sections). The positions of geological boundaries at cross-section intersections are checked and modified as necessary (Fig. 1).
- These generated surfaces are then spatially combined to produce the 3D geological model stack by attributing to each surface by reference to the DTM.
- The model can be checked for mis-correlations by creating a rectangular grid across the whole

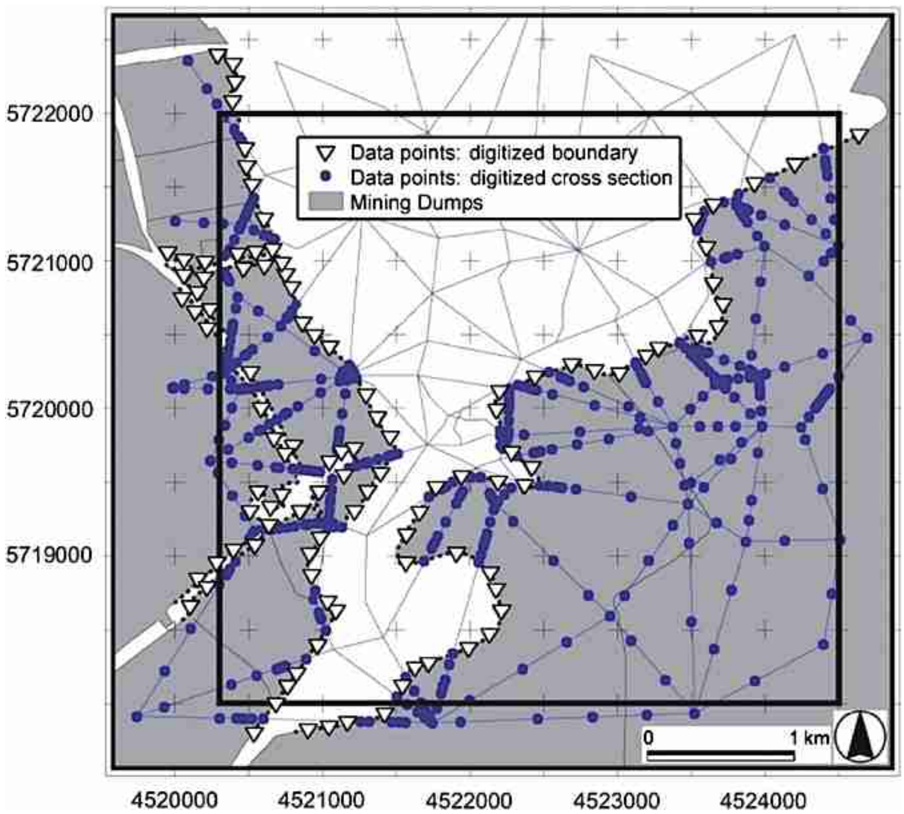

Fig. 4. Information input by cross-sections and hierarchical data points for 3D modelling of lignite mining dumps for software GSI3D. Lateral extension of mining dumps is defined by digitized boundaries from 2D mining maps. Modelled area is 4×4 km in all subsequent figures.

area, manually viewing the "synthetic" cross-sections, and correcting as necessary.

GSI3D is based on a "constructive method" and allows the implementation of different additional geological 2D information. This "knowledge-driven" approach is based on the detailed information of the sedimentological and stratigraphical situation as well as the history of the complex lignite mining activity over nearly 100 years. The 3D modelling of the Bitterfeld South sub-model (Fig. 1) comprises $16\,km^2$ and is based on a construction of 28 networked cross-sections that are constructed by 125 borehole records. Following the previous information, the hydraulically relevant small-scale lithological and structural heterogeneities, in particular of the Quaternary layers, could be assigned to 31 lithostratigraphic units and depicted using a $10\,m \times 10\,m$ GIS grid. This 3D information is available for the regional scale of $46\,km^2$. An assignment of hydraulic parameters to individual sedimentary bodies allows a combination with flow and transport models.

The challenge to model the artificial complex geometry of the lignite mining dumps is shown in Figs. 4–6. Fig. 4 depicts the different types of data points and their distribution. The geometry of the lignite-mining dump is characterized by the primary data sets of drilling information and related networked cross-sections indicated in Fig. 1. The second-order hierarchy data points consist of the digitized data points from the network cross-sections, and the spacing depends on the vertical gradient of the bottom surface. If necessary, a third-order set of additional data points can be inserted by interpolating cross-sections to optimize the geometry of the mining dumps. The required information of the horizontal distribution of the mining dumps is taken from technical maps, indicated as digitized boundary information in Fig. 4.

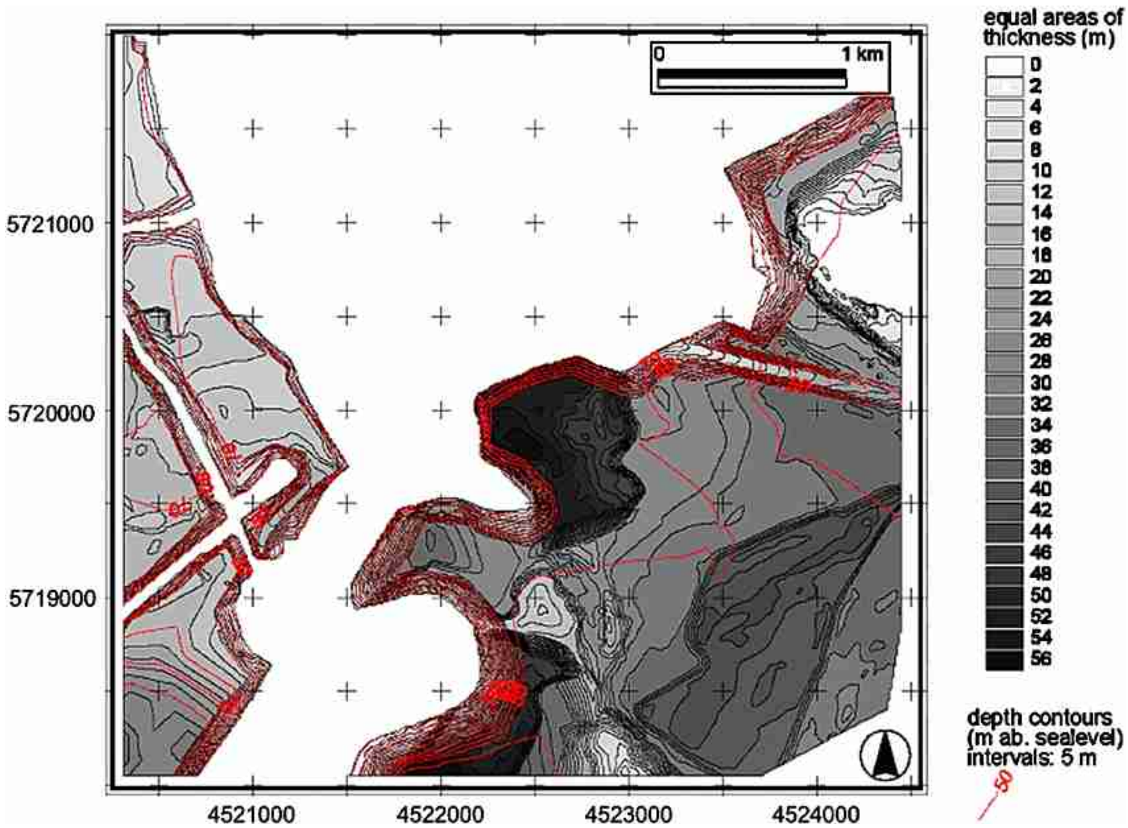

Fig. 5. Resulting contours of thickness of modelled mining dumps. Note steep gradient slopes and remaining street dams at western part of area and small-scale geometry.

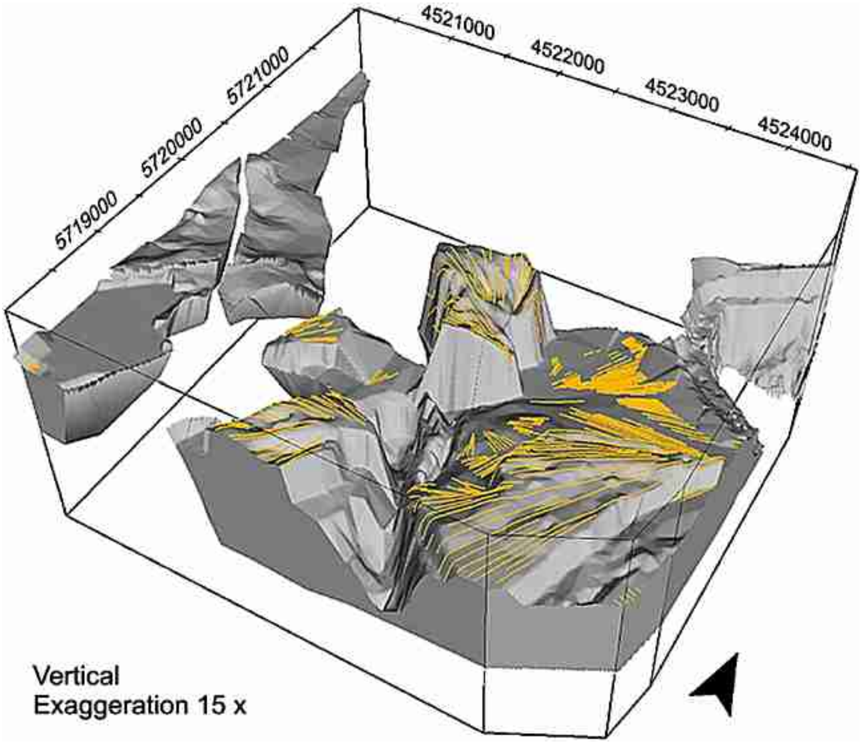

Fig. 6. Visualization of 3D high-resolution model of mining dumps with internal anisotropic structures.

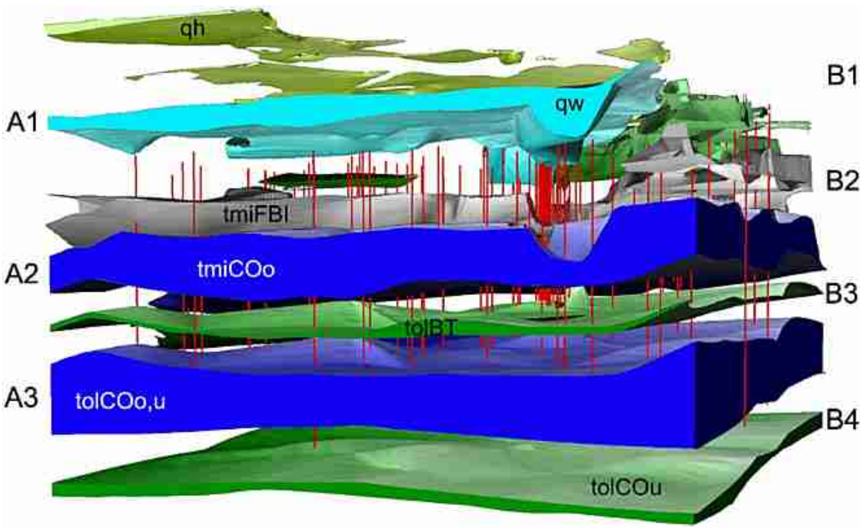

Fig. 7. High-resolution 3D model of distinct aquifers (A1–A3) and corresponding aquicludes (B1–B4) in an ''explosive view'' processed with GSI3D with a view from the northwest. For stratigraphical abbreviations refer to explanations in Fig. 9.

The structural complexity of the aquifer system is specifically increased by the impact of refilling from open-pit mining, which in turn covers up to 30% of the modelled area. One of the specific problems that have to be solved additionally was the modelling of the steep geometric inclination of the open-pit slopes. Fig. 5 illustrates the calculated contours depicting the small-scale geometry and variability of thickness of the mining dumps reflecting their different slope gradients. Corrections of the calculated contours have to be made manually by knowledge-based decisions.

The final 3D high-resolution geometry of the mining dumps is depicted in Fig. 6. The horizontal resolution of the Digital Terrain Model is 10 m × 10 m, and the topographic structures of the artificial sediments were mapped by airborne laser scanning DTM of 1 m × 1 m. Knowledge of the internal structure of such an artificial sedimentary layer is required for the calculation of anisotropy and hydraulic conductivity of the resulting aquifer conditions.

The architecture of the aquifer system is shown in Fig. 7. This "explosive view" of the 3D high-resolution model classifies the sub-aquifers (A1–A3) and the related aquicludes (B1–B4) within the Quaternary and Tertiary sedimentary succession. The individually modelled units can be classified and clustered according to their hydro-stratigraphical parameters as well as their calculated volume. A predominant hydraulic subsurface structure is the channel filling within aquifer A1, which is of regional hydraulic importance, as described in the following chapters.

Apart from hydraulic modelling, the high-resolution 3D models can be used for predictive application in the field of environmental and geotechnical investigations. This not only focuses on different types of visualization and predictive 3D mapping but also provides all types of virtual cross-sectioning and predictive calculations of hydro-stratigraphical units and plausibility inspections. Virtual sections can be calculated in highly variable positions and combined with subsurface and surface topographic information as well as groundwater contour lines. The processing of such horizontal and vertical virtual sections gives a very precise positioning of distinct units or structures within the spatial model, especially of geotechnical and remediation applications. The accuracy of positioning is defined by the used gridding space of 10 m × 10 m.

4. Modelling concepts and resulting simulations

After the modelling work described before with GSI3D using a "constructive" and knowledge-driven approach, first experience in 3D modelling based on a geostatistical interpolation with the modelling system EVS/MVS using the identical data set from above was already done (Hubert, 2005). One of the reasons for the comparison is to some extent the more time-consuming interactive remodelling process described before. Therefore, EVS/MVS is strictly based on the geostatistical interpolation between boreholes and calculates the contouring more or less automatically. To obtain comparable results, the same boreholes as in the system GSI3D were given as input data.

EVS/MVS (C Tech Development Corp. Kaneohe, HI) provides true 3D volumetric modelling and 2D and 3D kriging algorithms with best fit of variograms to analyze and visualize geoscientific and environmental data. EVS/MVS allows the seamless integration with ArcView GIS, as well as, e.g., Modflow and MT3D. The 3D modelling of the subsurface geology with EVS/MVS is exclusively based on selected drilling information and the geostatistical interpolation of the individual layers. This procedure can lead to some different results in cut-and-fill structures of Quaternary sedimentary channel-fills as well as artificial mining dumps with steep slopes of the former open-pit lignite mines in our case.

Fig. 8 shows the difference of stacking model layers of an erosive cut-and-fill structure and the

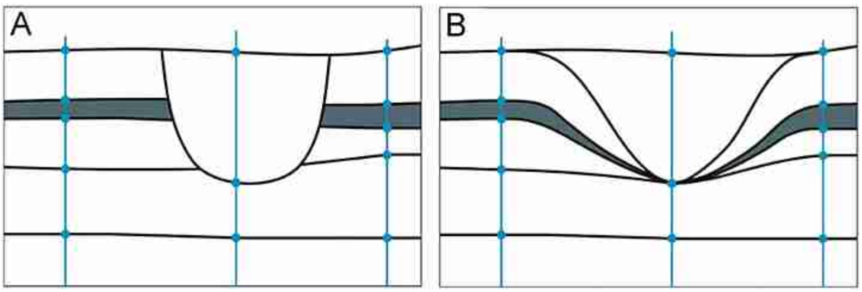

Fig. 8. Diagrammatic sketch of cut-and-fill structures: (A) depicts original position of strata and modelled result by GSI3D; (B) shows bring it down effect by geostatistical interpolation of cut-off layers under erosional fill-in structure.

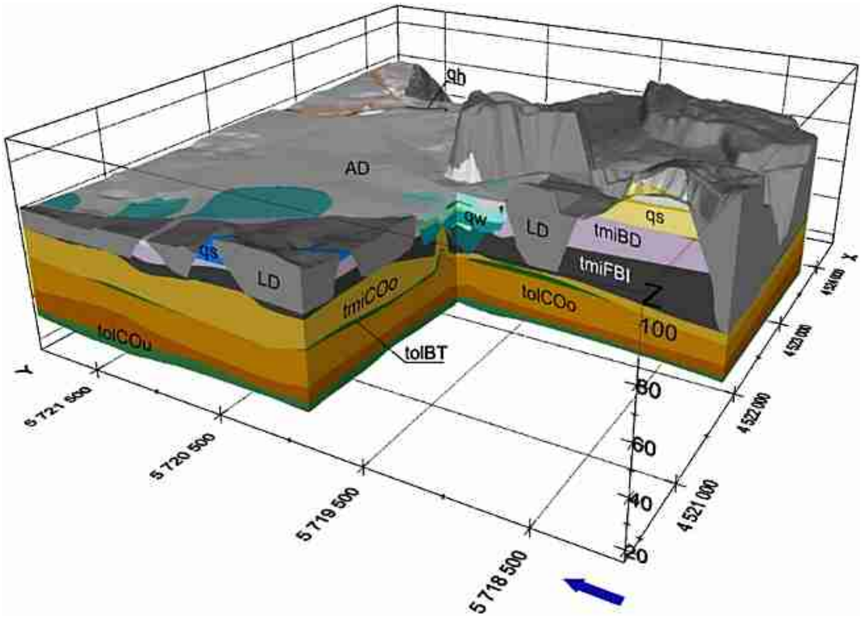

Fig. 9. Example of the real 3D model of the area studied simulated with GSI3D (vertical scale in m, vertical exaggeration 15 ×). Note the large number of mining dumps cut-in the remaining lignite seam as well as Quaternary layers. See Fig. 10 for comparison. Abbreviations: Quaternary: LD — lignite dumps, AD — artificial deposits, qh — Holocene, qw — Weichselian deposits, qs — Saalenian deposits; Tertiary: tmiBD — Bitterfeld Cover Clay, tmiFBI — seam complex Bitterfeld, tmiCOo — Bitterfeld Mica Sand (upper part), tolBT — Breitenfeld Horizon, tolCOo — Bitterfeld Mica Sand (lower part), tolCOu — glauconitic sand and glauconitic silt.

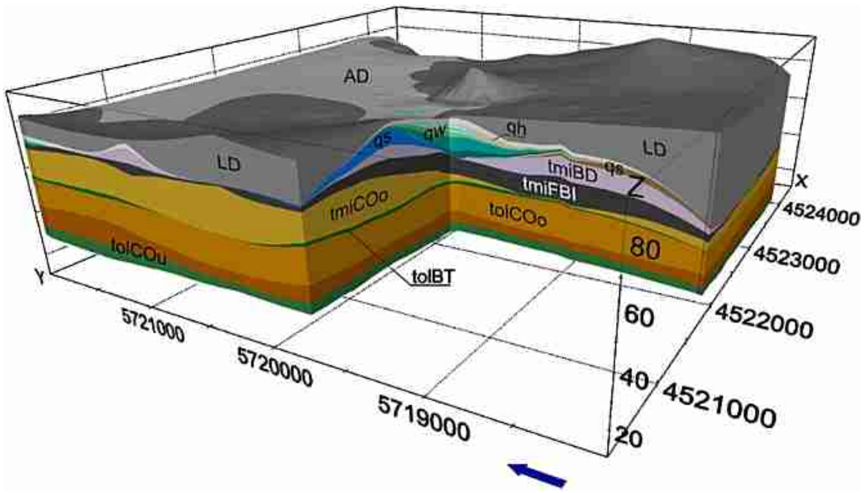

Fig. 10. Example of the ''real'' 3D model of the area studied simulated with EVS/MVS by a geostatistical approach (vertical scale in m, vertical exaggeration 15 ×). Compare Fig. 9, and see text for further explanation. Stratigraphical abbreviations explained in Fig. 9.

effect of ''automatically'' geostatistically based contouring processes. Geostatistical modifications can be made concerning the individual layers, but not within the entire stacked structural geological model. Due to the fact that erosive structures of natural and anthropogenic origin are quite common in the near surface Quaternary record, the geostatistically based simulation of true 3D subsurface models has to be taken into account with the knowledge that there could be some limitations.

The comparison of the modelling results by using an identical set of drilling information shows very clear effects for cut-and-fill structures in near-surface sediments. The geostatistically based interpolation of geological layers requires sufficient statistical borehole coverage. Due to local variations of the Quaternary sediments and the artificial mining activities, the coverage of borehole information is not sufficient to simulate a ''real'' scenario of the geological setting. The geostatistically oriented approach is based on the configuration of individual layers, continuously spread over the model area. This leads to an unrealistic predicted scenario explained in Figs. 9 and 10. It is obvious that if these results will be transferred as a structural base to local groundwater models, the results could be misinterpreted and will affect the subsequent groundwater flow modelling.

To simulate the regional hydraulic impact of the identified Quaternary channel-fill structure, the contouring of the thickness of the upper Bitterfeld Mica Sand was modelled with GSI3D and EVS/MVS. The modelling results with GIS3D shows a distinct erosive channel morphology, based on drilling data and paleogeographical and hydrogeological indications (Figs. 11 and 12), and the result with EVS/MVS, exclusively based on drilling information and geostatistical interpolation, gives

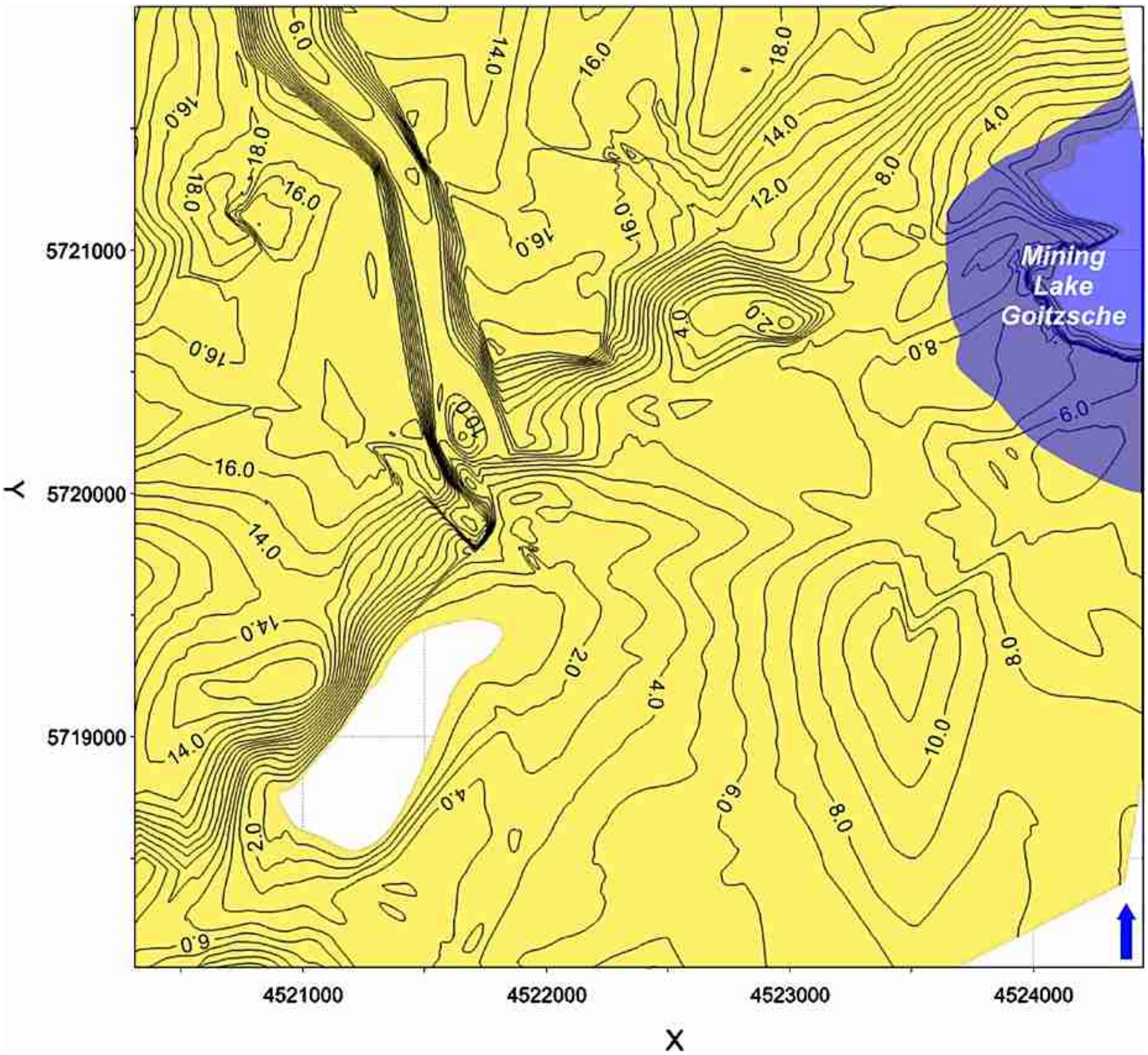

Fig. 11. Thickness contours in m of the Bitterfeld Mica Sand (upper part) processed with GSI3D. Note the predominant feature of the northward striking channel-fill structure.

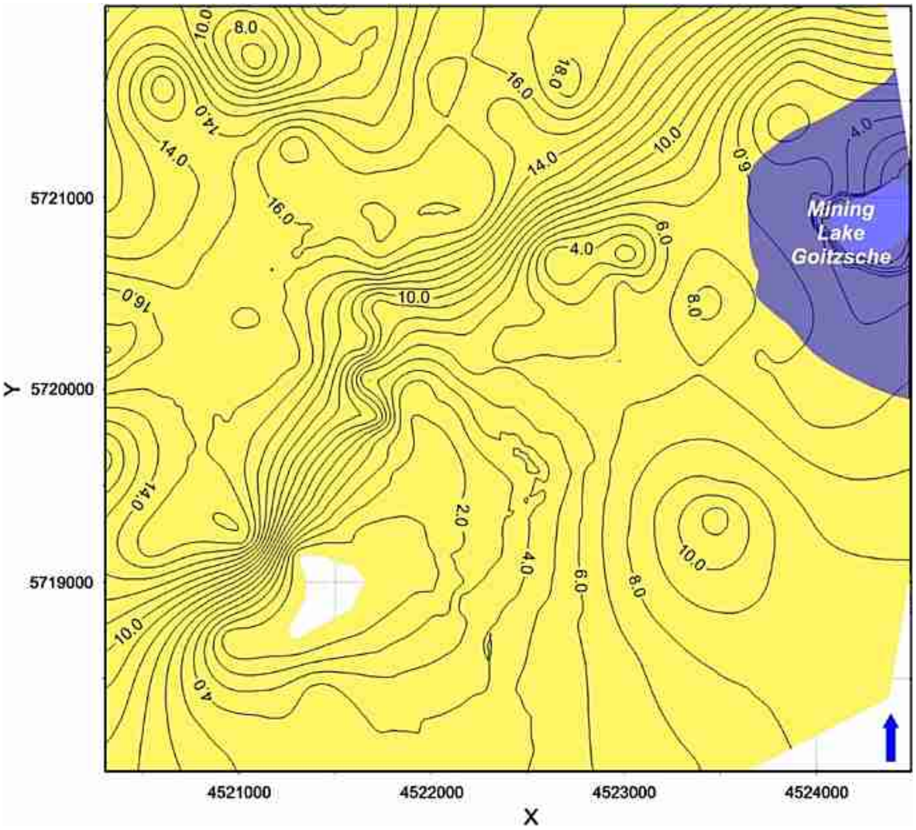

Fig. 12. Thickness contours in m of Bitterfeld Mica Sand (upper part) processed with EVS/MVS. Note the missing feature of the northward striking channel-fill structure, indicated in Fig. 11. See text for further explanation.

no clear indication for such a predominant hydraulic structure.

The assessment of the relative uncertainty can be given for the upper surface of the Bitterfeld Mica Sand, calculated by EVS/MVS in Fig. 13. The relative uncertainty is given in relation to the borehole coverage and the spatial variability of z values of the upper surface of the modelled layer. The statistic analysis of the relative uncertainty with GSI3D cannot be done inside the software package. Due to the plausibility checked cross-section network, as well as additional information from 2D mapping and expert-driven interactive remodelling, the statistically based uncertainty of information is therefore difficult to estimate.

5. 3D models — a platform for groundwater modelling

To support the investigations of an integrated environmental risk assessment of contaminated megasites on a local scale, the high-resolution 3D structural model was enlarged to about 46 km^2 for the entire region and its downstream areas. The structural model was generated by combining point information of about 250 boreholes that were implemented in about 62 cross-sections in total. This model allows — beyond visualization purposes — volumetric calculations of partial or distinct sedimentary units, like the remaining lignite, which are relevant for assessing the natural attenuation potential and retardation processes.

The digital data set of the true 3D structural geology was used with reference to their hydraulic characterization for subsequent flow and transport models. The numerical groundwater model was carried out with two objectives:

- Description of the hydrodynamic system and the path line prediction of the post-mining time.
- Predictive calculations of the changed hydraulic situation after the flooding of the Goitzsche Lake and raising the groundwater level of approx. 8 m after August 2002.

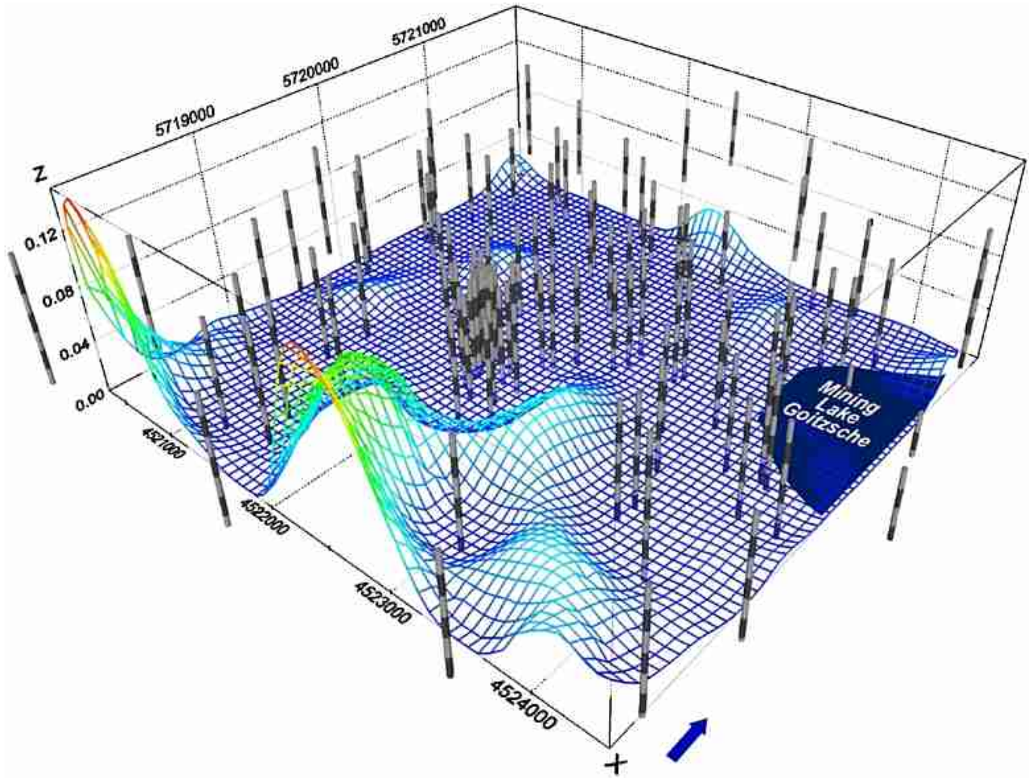

Fig. 13. Colour-classified mesh of the uncertainties of the upper surface of the Bitterfeld Mica Sand (shown in Fig. 12). The uncertainty interpolation (red mesh — high uncertainty, dark blue mesh — low uncertainty) is based on the borehole data (black-grey columns) and on the spatial variability of the z values, calculated by EVS/MVS. The units of the z-axis are uncertainties, varying between 0 and 1.

The numerical model consists of two parts: a groundwater flow model and a transport model based on the flow model. The modelling systems Modflow, ModPath, and MT3D with the Visual Modflow 3.0 pre- and postprocessors were used for the studied area. The general stratigraphic succession was clustered by condensing geological layers according to their hydrogeological properties: i.e., hydraulic conductivities and porosities. Most important for the numerical hydrogeological model is the completion of geological layers that are fading out. The 31 geological layers were reduced to 10 layers of the numerical groundwater model that have to be sustained across the whole model area. This part of the modelling process could only be done by working with a GIS database. The hydraulic parameterization and structural setting was described by Wycisk et al. (2002, 2004). The main structure of the model is composed of Quaternary and Tertiary aquifers. Both distinct aquifers are separated by a clay layer and also by the lignite seam and are subdivided by several less conductive layers. Boundary conditions of the models were taken from the water levels measured in surrounding lakes and piezometers. The values were taken as mean groundwater levels and regionalized for the boundaries of the model area and also held in a GIS structure.

To evaluate the hydraulic conditions before and after the flooding, two steady-state groundwater flow models were calculated. The numerical groundwater model after August 2002 has to incorporate two hydrological events. On the one hand, a heavy rainfall with precipitation rates of more than 100 mm within 3 days led to an increased groundwater recharge in the entire catchment area; on the other hand, the exceptional flooding event of the former lignite-mining pit Goitzsche by the River Mulde raised the downstream boundary condition in the east of the model area by about 8 m.

The groundwater flow models were calibrated to the measured water levels of the observation points and the groundwater contours that were also held in a GIS database. Calibration of the groundwater models was supported by the GIS database handling. By this, not only the water

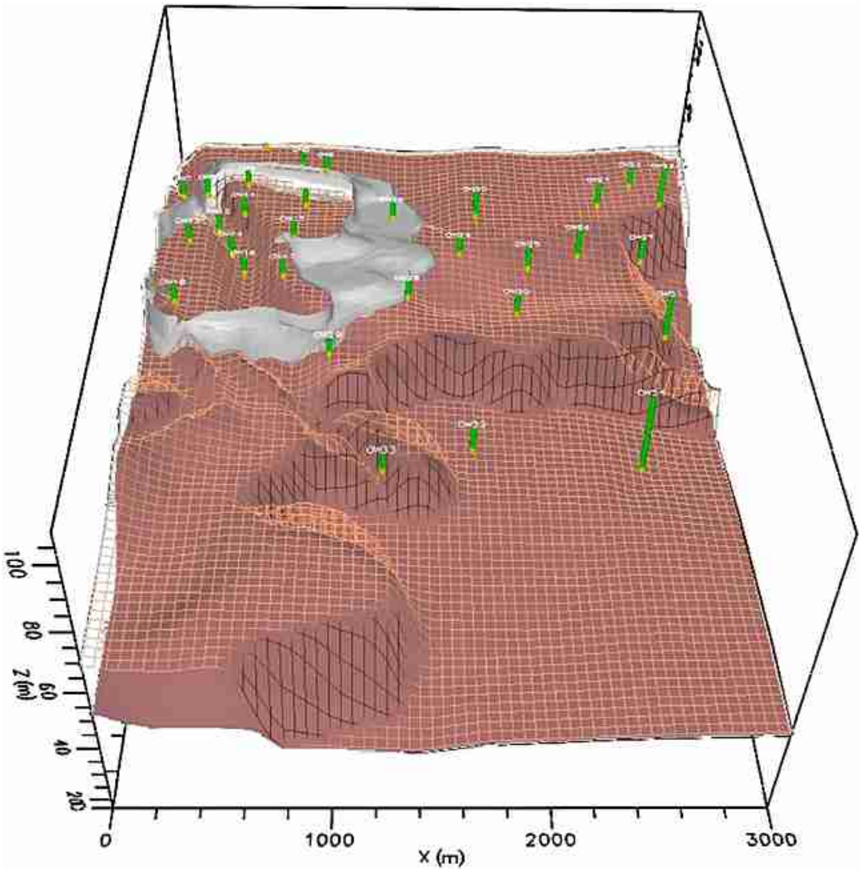

Fig. 14. Isosurface of a non-reactive tracer after 10 years of transport. Morphology net has been transferred from 3D geological model and indicates boundary of upper and lower aquifer. Note the approx. N–S striking channel structure.

levels at piezometers, but also the overall flow pattern, shown by groundwater contours, could be compared.

Based on both steady-state flow models, before and after the flooding event of August 2002, two transient transport models were run as study models for ideal, non-reactive tracers (Fig. 14). The figure shows the boundary of the upper and lower aquifers from the 3D structural model. The aquifer/aquifer contact is clearly marked by the morphology of the excavated lignite seam and the erosive Quaternary channel-fill structure striking approx. N–S. To understand the local hydraulic and transport conditions, only diffusion and dispersion for the simulation were implemented because sufficient sorption and biological degradation data are still not available. Thus, the GIS data structure is important for several stages in numerical groundwater modelling: building the database of hydrogeological parameters and boundary conditions, calibration of the groundwater model by comparison of modelling results with measured data, and visualization of the scenario results. Therefore, it is necessary to realize a safe data exchange between the 3D geological modelling system and the GIS database that also allows further data processing to adapt the geological model to the structure of a numerical groundwater model.

The integration of simulated results from high-resolution 3D geology as well as from flow and transport modelling is depicted in Fig. 15. The 3D geology model shows the subsurface topography of the geological strata with removed mining dumps. In addition, the simulation of the transport modelling (non-reactive tracers) running time of 30 years and the path line distribution from flow modelling are integrated by GIS. It is very clearly shown that the predominant hydrological impact of the highly conductive Quaternary channel-fill structure is evident and leads to a NE-ward spreading of the

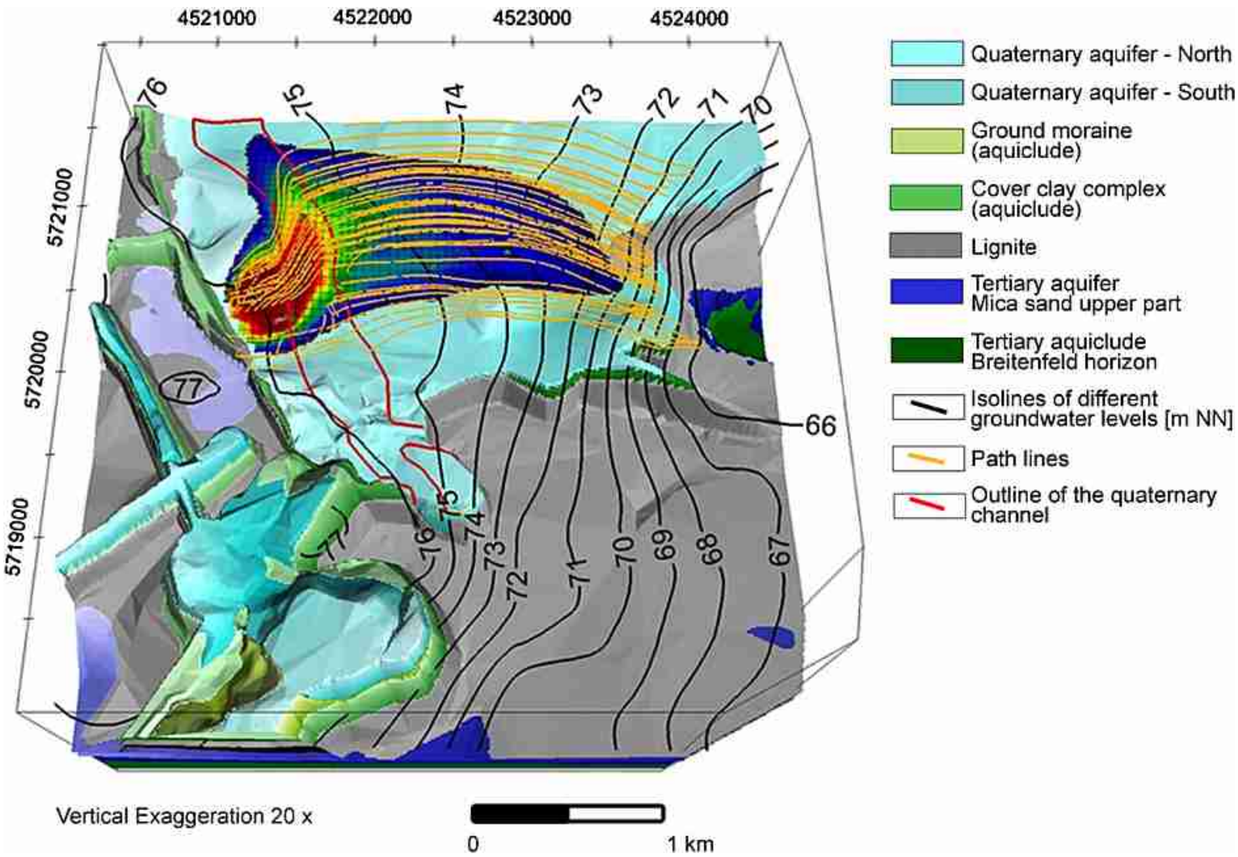

Fig. 15. Integrated results of the numerical groundwater model, visualized in the 3D geological model for further interpretation: groundwater contours, path lines and fringes of non-reactive tracer after 20 years of transport (red — 100% non-reactive tracer, blue — 10% non-reactive tracer). Mining dumps layers are removed.

contaminant plume before August 2002 (Wycisk et al., 2005). The impact of the predominant channel-fill is also evident after the flooding event and results in a more focused straight northward groundwater flow direction. The simulation of path lines is of great importance for any source receptor-related environmental assessment studies.

6. Conclusion and discussion

The steps from a conceptual model to a "true" 3D geological model correspond to scaling effects density of availability of information as well as suitable modelling concepts and algorithms. It was clearly shown that the complexity and specific situation of regional structural and facies situation needs adequate processing methods.

Using 3D structural models for any subsequent groundwater modelling, it is obvious that the differences between a digital representation and the real phenomenon of structural setting will also influence the resolution of numerical groundwater models from 2D to 3D models with low resolution and afterwards to highly discredited numerical 3D groundwater models. The comparison of different modelling approaches by using the identical set of data, as far as possible, indicates differences in the representation or simulation of 3D geology, depending on the specific structural situation of the modelled area. Therefore, the strengths and weaknesses of adequate 3D modelling software tools and their related concepts need to develop further.

To generate a detailed environmental impact scenario, it is necessary to gather not only high-resolution land-use information in terms of source and receptors and morphological data, but also a model of the aquifer systems corresponding to the real-world scenario of the geological setting, as well as the "true" regionalization of contamination data. The lithostratigraphic approach in construction of

3D geological models gives better results than only a pure grain-size or lithological-based automatically contoured approach. This statement is valid for most Quaternary sediments and artificial cut-and-fill structures. It must be stated very clearly that the mentioned restriction depends on the specific geological situation. The advantages of geostatistically based modelling are high if the coverage of borehole data is sufficient. The insufficient density of borehole data is a function of the complexity of the subsurface. Therefore, the application of 3D subsurface models, on local or regional scale, has to be completed by knowledge-based control, as much as possible.

The 3D geological model also serves as a database for a numerical groundwater model, although the detailed structure must be simplified in a hydrogeological sense. The adaptation of the 3D geological model data to a 3D numerical groundwater model is possible, but it has to be corrected to avoid structures with fading out layers and to aggregate geological units with similar hydrogeological characteristics. On the other hand, additional information such as hydraulic conductivities, porosities, and boundary conditions are necessary to set up the complete model. The modelling results can also be exploited in GIS as well as in the 3D geological model to obtain detailed information about contaminated layers, potential traps of dense non-aqueous phase liquids, and additional adsorption facilities. From these points of view, the detailed true 3D geological model carries a greater significance than to serve only as a basis for a structural hydrogeological model in the investigations of environmental risk assessment.

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