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EXPOSURE ROUTE ASSESSMENT OF GROUNDWATER POLLUTANTS FROM MULTI-SOURCE CONTAMINATED MEGA SITES – A CASE STUDY

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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 their resulting waste dumps, as well as 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 (Germany) is one of the most investigated locations of a former mining and an industrial megasite with regional groundwater contaminations. It forms one of the earliest industrial sites in the world. Industrial production of chlorinated chemicals that make up the main contamination source started at the end of the 19th century with the chloro-alkali electrolysis. Due to the multi-source regional contamination of the upper and lower aquifers, risk assessment-based investigations of distinct exposure routes of the contaminated ground water 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[1,7,9]. The understanding of related transport and natural attenuation processes of the contaminated ground water needs a detailed understanding of the complex hydrostratigraphy in the subsurface, related to the groundwater flow and transport processes and resulting impacts on environmental receptors. Northwest of Bitterfeld, several former open-cast lignite mines have been used as landfills for industrial chemical waste during the former GDR time. Hydrogeologically the waste sites are situated in a region with severely disturbed groundwater conditions due to the lignite mining activities. Since the industrial dumps are incompletely sealed, the ground water was affected directly by prevailing chlorinated aliphatic and aromatic hydrocarbons. The long-term regional monitoring of the contaminated ground water comprises approximately 180 individual organic substances. The abandoned „Antonie“ landfill, e.g., contains about 6 million tons of various industrial residues, including waste material from pesticide production of Lindane (gamma-HCH) and DDT isomers.[2,5] The dynamic change of hydraulic conditions in a regionally contaminated area with a high complexity of the geological structures needs very detailed and accurate subsurface information about the heterogeneous aquifers and their related hydraulic properties. The simulation and identification of groundwater flow path lines within the regionally contaminated aquifer was possible only by numerical groundwater modelling. The exposure assessment of contaminant pathways requires an appropriate GIS-based 3D spatial model 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 their aquatic biocenoses.

Materials and Methods

GIS-based spatial 3D Model Bitterfeld: To assess the complex environmental situation of the Bitterfeld mega site, a GIS-based spatial 3D model that includes the heterogeneous aquifer setting in the third dimension is as much as possible required. The subsurface information has to be available for a GIS-based assessment and predictive calculations correlated to surface information of potential receptors.

Therefore, the following major topics have to be integrated into the spatial model on a local scale, including the specific objectives and used modelling tools:
a) Regionalization of groundwater contaminants,
b) Predicted groundwater flow directions and transport modelling,
c) High resolution 3D subsurface models of aquifer stratigraphy, and
d) Land-use sensitivity classification.

GSI3D (former GeoObject) has been used to model the underground in 3D.

Results and discussion

Groundwater contaminants: 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 within the SAFIRA Project comprises regional monitoring data of groundwater contaminants of more than 10 years, app. 3,500 samples and up to 180 individual organic parameters from nearly 250 observation wells[10,7]. The most frequent groundwater contaminants and their related concentration ranges are out of app. 65 priority contaminats e.g.: Tetrachloromethane (TCM 680-77000 µg/L), Trichloroethene (TCE 350 – 21 000 µg/L), cis-Dichloroethene (cis-DCE 220-23000 µg/L), Vinylchloride (VC 30-41000 µg/L), Monochlorobenzene (MCB 40-23000 µg/L), and Benzene (130-8200 µg/L).[1,3]

HCH isomers as well as DDT/D/E isomers are observed due to the former manufacturing activities and landfill deposits on a lower concentration level. A first attempt some years ago has been made to classify the land-use areas along a source-receptor path line downstream direction. The average detected concentration for the sampling campaign 1998 was given for 222 readings for HCH and 166 for DDT/D/E.[3,8,9]

a) Industry and Mining areas (HCH 2.6 µg/L; DDT/D/E 0.3 µg /L),
b) Urban areas, (HCH 2.0 µg/L; DDT/D/E 0.2 µg/L),
c) Agricultural areas (HCH not detected, DDT/D/E not detected), and
d) Alluvial plain Mulde River (HCH 1.8 µg/L; DDT/D/E 0.2 µg/L).

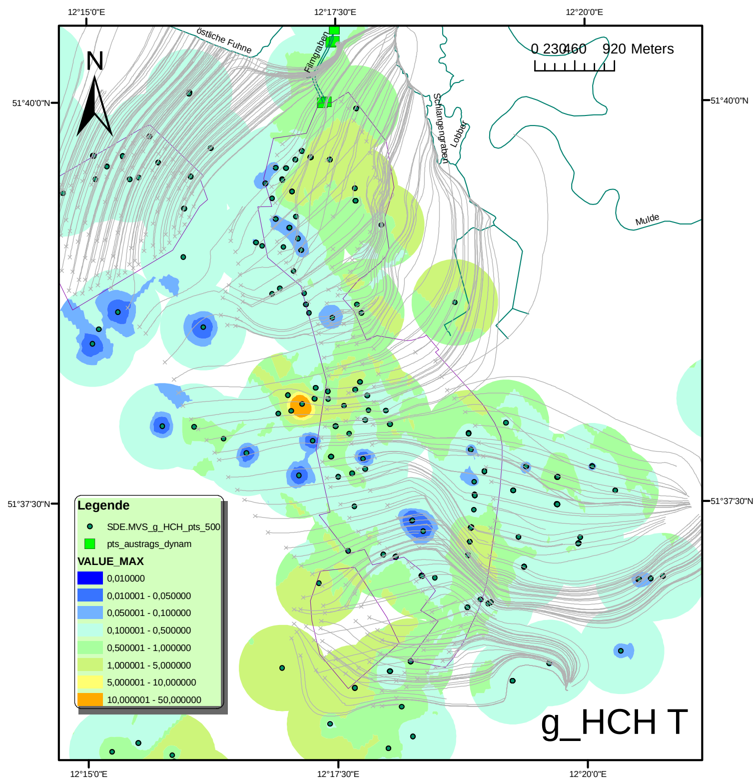

Figure 1: Regionalized lindane concentrations in the Tertiary aquifer with pathlines overlayed (ground water flow situation 2000).

Tab. 1: Descriptive statistics of samples (surface water) and mean values (groundwater) of observation wells. Where multiple measurements were available at a single well, mean values have been calculated.

Schlangengraben Surf .W.	***a-HCH***	***b-HCH***	***g-HCH***	***d-HCH***	***o,p-DDT***	***o,p-DDD***	***o,p-DDE***
Samples	27	11	9	8	2	4	1
Max	0.035	0.389	0.034	0.061	0.004	0.002	0.000
Median	0.010	0.074	0.009	0.021	0.002	0.001	0.000
Std. Dev.	0.008	0.124	0.011	0.020	0.002	0.001	0.000
Lobber Surface Water							
Samples	26	10	8	7	0	4	1
Max	0.087	0.130	0.129	0.085	n.d.	0,002	0,000
Median	0.013	0.049	0.012	0.013	n.d.	0,001	0,000
Std. Dev.	0.019	0.039	0.054	0.028	n.d.	0,001	n.d.
Groundwater Quaternary							
Count	171	171	171	171	123	127	127
Max	345.750	124.000	414.390	348.330	13.35	0.590	0.47
Median	0.265	0.130	0.175	0.240	0.025	0.021	0.0165
Std. Dev.	35.126	13.000	42.439	34.120	1.6075	0.064	0.051
Groundwater Tertiary							
Count	165	165	165	165	134	152	152
Max	525.000	91.500	125.000	545.000	528.000	71.400	4.052
Median	0.320	0.055	0.174	0.430	0.025	0.025	0.025
Std. Dev.	40.824	7.125	9.752	42.471	45.607	5.800	0.330

To assess the environmental risk on a local to regional scale, it is very important to review the individual analytical data on a statistical base. The regional long term monitoring during the last years allows some insights of reported concentration values of e.g. HCH and DDT/D/E isomers and leads to a more realistic evaluation of the data. Tab. 1 shows the descriptive statistical data for the a, b, g, d-HCH isomers and the DDT/D/E isomers for the upper and lower aquifer. The HCH mean values show to some extent higher levels compared with the set of comparable data from 1998 described below. The DDT/D/E mean values of Tab. 1 are quite similar to the set of 1998.

Regionalization of Contaminants: The long term discharge of contaminants into the upper and lower aquifer, and changing groundwater flow directions due to the regional open-pit mining activities during the last 100 years, creates a regional pattern of contaminant distribution, which in term is not always very clear and cannot be compared with most well known single source contaminant plumes. Furthermore, the range of contaminant concentrations differs to a large extent within the aquifers vertically as well as regionally due to the multiple sources and pathway relations. Therefore, special attention has been given recently to the statistical and geostatistical evaluation of the regional monitoring data of distinct contaminants within the SAFIRA Project. The regionalizations of the HCH isomers as well as the DDT/D/E isomers have been processed by different statistical regionalization algorithms and the best results have been obtained from the ordinary kriging geostatistical calculation. Due to the regional variability of the horizontal change of concentrations, a buffer of 500 m radius has been placed around each individual sampling point of the approximately 200 groundwater observation wells. The regional contamination patterns for the HCH (a, b, g, d) and DDT/D/E isomers show a different pattern within the upper and lower aquifer due to the different hydraulic conductivity. The regional distribution of the individual isomers shows only to some extent a clear downstream oriented decreasing concentration pattern. Areas of higher concentration as hot spots are found only very locally and the major part of the area is represented by concentrations around the detections limits. The assessment of the interpolated g-HCH concentration in the upper aquifer is shown by the subsequent figures which demonstrate the narrow original source area as well as the widespread contamination range of distal areas. The GIS-based classification indicates the increasing max. value of detected g-HCH concentration and related impact of the area within the total 34.00 km^2: Class 1: 0.1 µg/L 15 km^2; Class 2: 0.5 µg/L 14 km^2; Class 3: 2.0 µg/L 3 km^2; Class 4: 10.0 µg/L 0,6 km^2; Class 5: 410 µg/L 0.4 km^2. To understand the given complex groundwater flow and transport situation of the regional contaminated aquifer system, additional information of local modeled groundwater flow and path line prediction is needed for a deeper understanding and plausible interpretation of the long-term regional contamination patterns.

Surface water contamination: Due to the regional contamination in the Bitterfeld – Wolfen area a new investigation of the interaction of ground water related contaminates and surface water impact has been carried out. Therefore, run-off measurements as well as water samples have been taken monthly from the small creeks Schlangengraben und Lobber, which are tributaries to the Spittelwasser and Mulde River for more than one year. The impact of the contaminated effluent groundwater is depicted in Tab. 1. The max. values of the HCH isomers from the Schlangengraben location are in the range of 0.03 - 0.39 µg/L, but are recorded only during a few months within the year. The detailed discharge processes are under investigation. The related HCH values of the upper aquifer (Quaternary) and the lower aquifer (Tertiary) are shown in Tab. 1. The sampling locations of Schlangengraben und Lobber are in a downstream position of the Bitterfeld-Wolfen area presenting a lateral distance to the major contamination sites of app. 3-4 km. The effluent of DDT/D/E isomers from the groundwater to the surface water sampling locations is close to the analytical detection limits. The groundwater / surface water interaction has been controlled by the subsequently described groundwater flow and transport modeling.

Geological and Hydrogeological 3D Modeling: To support the investigations of an integrated environmental risk assessment of contaminated megasites on a local scale, a spatial geological subsurface model of 45 km^2 have been built for the entire region and downstream areas. This model allows, beyond visualization purposes, volumetric calculations of partial or distinct sedimentary units (aquifer/aquiclude) like the remaining lignite in the subsurface, which is relevant for assessing the natural attenuation potential and retardation processes as well as the flow and transport processes due to the distinct hydraulic conductivity. The subsequent numerical groundwater model was carried out with the major objectives:

a) Description of the hydrodynamic system and the path line prediction of the post-mining time to identify the detailed exposure routes of contaminants parallel of the groundwater flow lines reaching observation wells and surface water bodies.

b) Predictive calculations of the meanwhile changed hydraulic situation after the flooding of the Goitzsche Lake and raising the groundwater level of app. 8 m after August 2002.

The numerical groundwater model consists of two parts: A groundwater flow model and a transport model based on the flow model. The modeling systems *Feflow, Modflow, ModPath, and MT3D* with the *Visual Modflow 3.0* pre- and postprocessors were used for the studied area. 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 held also in a GIS structure 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. To understand the local hydraulic and transport conditions, only diffusion and dispersion for the simulation were implemented at a first step. Thus, the GIS data structure is important for several stages in numerical groundwater modeling: building the database of hydrogeological parameters and boundary conditions, calibration of the groundwater model by comparison of modeling results with measured data, and visualization of the scenario results. The integration of simulated results from high-resolution 3D geology as well as from flow and transport modelling has been done. The impact of the predominant Quaternary channel-fill structures in the subsurface is evident and results in a more focused straight northward groundwater flow direction after the flooding event of August 2002. The simulation of the groundwater flow is of great importance for any source receptor-related contaminant transport and environmental assessment studies to understand the groundwater driven transport processes before and after the flooding event 2002.

Conclusions

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 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 modeling results can also be exploited in GIS as well as in the 3D geological model to get 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 lot more importance than only to serve as a base for the structural hydrogeological model in the environmental risk assessment. Regional "real world scenarios" of contaminated megasites with heterogeneous aquifers and groundwater contaminants require a model based approach for prediction and assessment which is able to integrate the spatial information within an information system and use the results for a reliable process-orientated environmental assessment.

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