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# Predictive modelling of dump water impact on the surroundings of the lignite dump site Jänschwalde (Eastern Germany)

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## Abstract

Open cast mining of lignite leads to dumps containing highly mineralised pore waters. To predict the impact of the dump waters on the undisturbed aquifers two steps are necessary. (1) The prediction of dump water quality at times when steady state flow conditions will be established. (2) The simulation of the dump ground water migration with a model that is able to handle the complexity of the homogeneous and heterogeneous interactions of the migration process.

For the investigated site Jänschwalde, which is still dewatered, a chemical mass balance was performed. The predicted alkalinity potentials exceed acidity potentials for the dump as a whole. The distribution of these parameters show high alkalinity potentials for the northern part.

In order to model the migration process the transport code PCGEOFIM® [Anwenderdokumentaion, IBGW Leipzig, (in German)] was coupled with the geochemical equilibrium code PHREEQC [USGS, Water-Resources Investigations Report]. This was done to simulate redox reactions, mineral dissolution and precipitation, and cation exchange in the ground water zone. The model is verified by a column flow test. The results of the simulations show a small effect of the migrating dump waters on the quartenary aquifer with respect to acidity changes. This results from calcite buffering and cation exchange. The impact on the quartenary aquifer by sulphate is much higher. © 2001 Elsevier Science B.V. All rights reserved.

*Keywords*: acid mine drainage; contaminant transport; lignite mining; reactive transport modelling

## 1. Introduction

Open cast mining of lignite creates dumps containing highly mineralised pore waters. This is caused by oxygen exposure to reduced sulphur compounds within the tertiary layers. The dump water quality is influenced by hydrogeochemical reactions. After that, the mine will be closed, a natural flow system will be reestablished and the ground water will flow from the dump into the undisturbed aquifer. This scenario was simulated to predict possible future hazards. The work was carried out in two steps:

- Prediction of pore water quality within the dump for the times when steady state flow conditions have been re-established.
- Modelling hydrogeochemical interactions as ground water migrates from the mine.

### 1.1. Location and geological deposit conditions

Investigations were carried out at Jänschwalde mine, which has been active since the seventies. The

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## Nomenclature

| | |
|---|---|
| $C$ | volume concentration of a contaminant in the fluid (kg $m^{-3}$). |
| $C_t$ | content of total carbon within sediment (wt% C) |
| CEC | cation exchange capacity (meq/100 g sediment) |
| $D$ | dispersion coefficient ($m^2s^{-1}$). |
| $I$ | hydraulic gradient (–) |
| $n$ | porosity (–). |
| $Pe$ | grid Peclet number, $Pe \approx (\Delta x/\delta L)$ |
| $q$ | source strength of the transport equation (kg $s^{-1}$ $m^{-3}$). |
| $R$ | retardation factor (–). |
| $S_t$ | content of total sulphur (wt% S) |
| $t$ | time (s). |
| $w$ | Darcy velocity (m $s^{-1}$). |
| $\delta$ | dispersivity (m). |
| $\lambda$ | decay (degradation) coefficient ($s^{-1}$). |
| | |
| | Indices |
| k | species. |

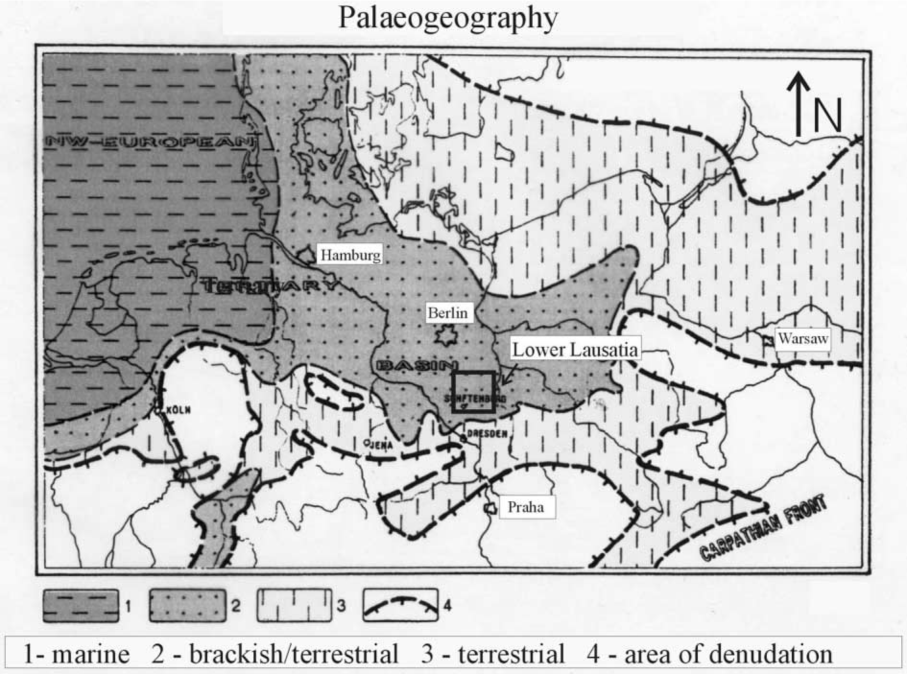

Fig. 1. Palaeogeography Lower/Middle Miocene — northern part of Central Europe (after Standke and Suhr, 1992).

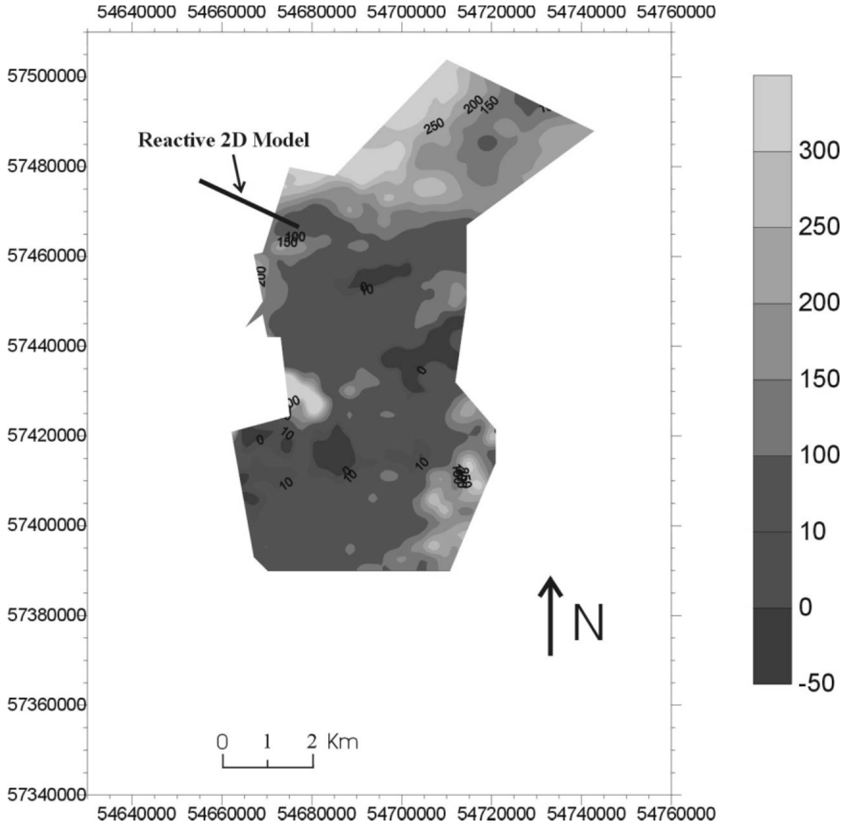

Fig. 2. Predicted ’Simplified acid–base balance‘ of the main dump body (mmol/l).

mine will be active up to 2019. It is situated near the border having Poland and represents the northernmost open cast mine of the Lower Lausatian Lignite District. The Tertiary strata series of Lower Lausatia is built up in regular sequences of coal, silt to clay and sand layers. This results from the palaeogeographic location of this district. Fig. 1 shows the marginal position of Lower Lausatia in the NW European Tertiary Basin during Lower/Middle Miocene. In the coal field Jänschwalde the thickness of the overburden varies between 40 and 90 m above the mined Miocene seam. The pyrite containing, carbonate free Tertiary layers represent 20–40% of these overburden. The remaining part being quaternary layers (glaciofluviatile sands, boulder clay and glacilimnic sediments).

### *1.2. Mining technology*

In the open cast mine Jänschwalde the overburden is removed using ‘conveying bridge‘ technology. Quaternary and Tertiary sediments are simultaneously cut from the highwall. They are transported to the dump by means of a large band conveyor, which spans the whole open cast mine. Due to technology of the mine, the dump can be vertically divided into different parts (compare Fig. 4). The resulting main dump body is heterogeneous in micro scale (up to 10 m) but in a hydrogeological scale (>100 m) it is a well mixture of the whole coal hanging layers.

## 2. Prediction of dump water quality

The following key aspects were considered:

- Distribution of disulphide content within the Tertiary layers.
- Kinetic of pyrite weathering within the open cast

mine (‘primary weathering’) and after displacement within the water unsaturated dump (‘secondary weathering’).

- Investigation of the main buffering potentials (calcite content, cation exchange capacity — CEC and feldspar weathering) of the different layers.

A vertical integrated model for the distribution of the parameters described above was created. This was done based on the thickness of the different stratigraphic units. A simplified acid–base balance was carried out in order to identify problem zones. This is a balancing of the predicted $H^+$-production by the sulphide weathering rate with the calcite content of the mixed sediment. The prediction of dump water quality was performed including all results using the hydrogeochemical equilibrium model PHREEQC (Parkhurst, 1995).

### 2.1. Data

To characterise the overburden sediments chemically, the results of about 40 forefield drilling points were used. For the material of each stratigraphic unit the following parameters were analysed (Frobenius, 1977–1986): total sulphur content ($S_t$), total carbon content ($C_t$), CEC, $CaCO_3$ content and a soil extraction by 10% hydrochloric acid. To characterise the effective weathering kinetics of pyrite, data from the field investigations of Rolland et al. (1998) was used. The distribution and thickness of the stratigraphic units is based on a large number (more than 500) of drilling points.

### 2.2. Results

The data interpretation confirms pyrite formation according to processes by Berner (1984) and show a strong dependence of the disulphide content from the genetical conditions of the sediments (Hoth et al.,1998). Fig. 2 shows the distribution of the acid–base balance. Positive values indicate a surplus of calcite with respect to the predicted amount of pyrite weathering. It is shown that the future dump body is well buffered in most parts. This is especially valid for the northern area due to the increasing part of quaternary overburden. The prediction of the dump water quality was carried out using PHREEQC-modelling as follows: The predicted amounts of weathering products ($H^+$, $Fe^{2+}$, $SO_4^{2-}$) were mixed,within the model, to a representative ground water analysis of the forefield. The precipitation of siderite, gypsum, melanterite, $Fe(OH)_{3(a)}$ and Kaolinite was allowed for the resulting solution. These secondary minerals are considered as model minerals. Only calcite and K-mica was allowed to dissolve. There was no kinetic approach for the feldspar weathering, which is approximated. Furthermore, equilibrium with the gas phase of the dump was considered.

A content of 10 vol% $CO_2$ was taken into account. These high $CO_2$ contents result mostly from reactions of tertiary organic matter within the dump body. This was shown by $\delta^{13}C$ isotope measurements at several locations (Nitzsche et al., 1999; Hoth, 2000).

The solution was put into equilibrium with the predicted CEC (derived from the forefield data). The exchanger composition was predicted based on the standard exchange coefficients of the PHREEQC 1.5 database.

## 3. Modelling of the migration process

The migration process is characterised by homogeneous (redox processes) and heterogeneous (mineral dissolution and precipitation, cation exchange) interactions. Transport models using isotherms were not able to cover the complexity of these processes. Eq. (1) shows that these models are single component approaches and chemical interactions will only be included by fitted parameters (retardation [$R$], rate constant of degradation [$\lambda$]). The other abbreviations are explained in the nomenclature.

$$\operatorname{div}\left(D \operatorname{grad} c - \frac{w}{n}c\right) - \lambda c R = R\frac{\partial c}{\partial t} - q \qquad (1)$$

A multicomponent reactive transport model must be used to reflect the interactive system.

### 3.1. Reactive transport model

The coupling of the 3D flow and transport code PCGEOFIM® (Sames and Boy, 1997) with the geochemical equilibrium model PHREEQC (Parkhurst, 1995) is based on a local equilibrium assumption (LEA) and was performed in cooperation

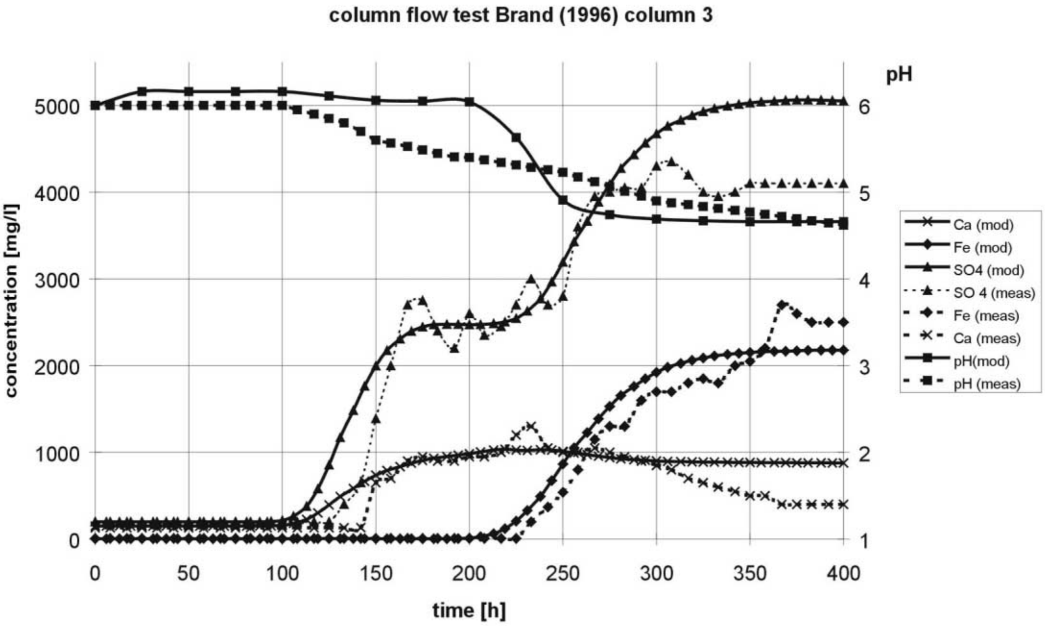

Fig. 3. Simulation results (mod) in comparison to measured values (meas) for a column flow test from Brand (1996).

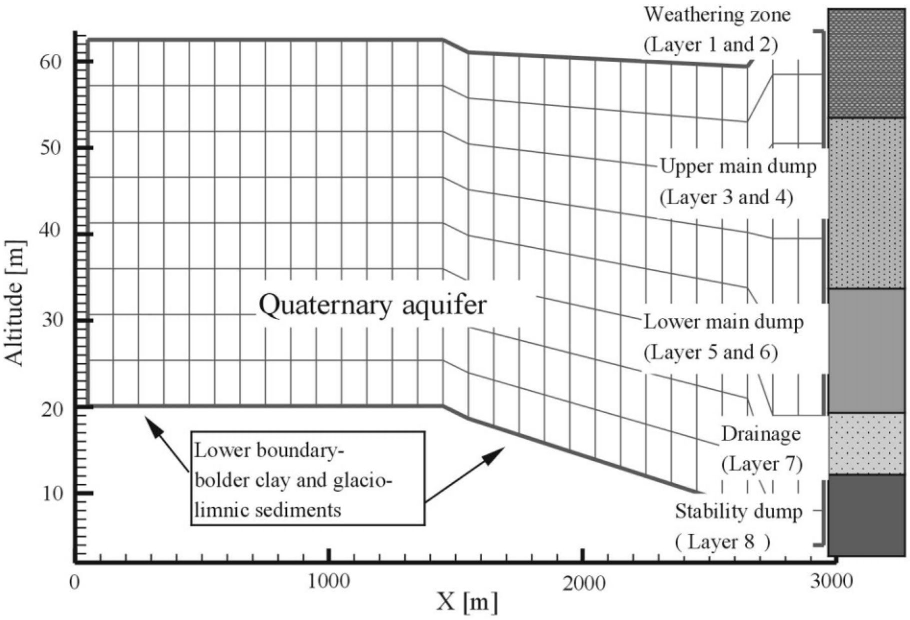

Fig. 4. Basic structure of the 2D cross section model.

Table 1
Initial and boundary concentrations and hydraulic quantities

| | Layers 1–2 | Layers 3–6 | Layer 7 | Layer 8 | Quaternary aquifer |
|---|---|---|---|---|---|
| Ca (mg/l) | 519 | 680 | 542 | 542 | 94.7 |
| Fe (2) (mg/l) | 463 | 4.6 | 160 | 160 | 0.4 |
| Fe (3) (mg/l) | $8 \times 10^{-3}$ | $l \times 10^{-3}$ | $l \times 10^{-2}$ | $l \times 10^{-2}$ | 0.04 |
| TIC (mg/l) as $HCO_3$ | 378 | 794 | 592 | 592 | 152.5 |
| S (6) (mg/l) as $SO_4$ | 2003 | 1280 | 2463 | 2463 | 123 |
| Calcite (mol/l) | 0 | $7.7 \times 10^{-2}$ | 0 | 0 | $5.9 \times 10^{-3}$ |
| Gypsum (mol/l) | $1.8 \times 10^{-1}$ | $2.8 \times 10^{-2}$ | $3.0 \times 10^{-3}$ | $3.0 \times 10^{-3}$ | 0 |
| $Fe(OH)_{3(a)}$ (mol/l) | $5.6 \times 10^{-1}$ | $6.9 \times 10^{-1}$ | 0 | 0 | $7.13 \times 10^{-1}$ |
| Siderite (mol/l) | $2.08 \times 10^{-2}$ | $1.97 \times 10^{-2}$ | 0 | 0 | 0 |
| CaX2 (mol/l) | $2.39 \times 10^{-2}$ | $3.09 \times 10^{-1}$ | $2.7 \times 10^{-1}$ | $2.7 \times 10^{-1}$ | $4.37 \times 10^{-2}$ |
| FeX2 (mol/l) | $7.13 \times 10^{-2}$ | $5.58 \times 10^{-4}$ | $2.72 \times 10^{-2}$ | $2.72 \times 10^{-2}$ | $4.93 \times 10^{-3}$ |
| pH | 5.49 | 6.51 | 5.3 | 5.3 | 7.59 |
| pE | 4.36 | 3.34 | 3.53 | 3.53 | 2.67 |
| $k_f$ (m/s) | $2 \times 10^{-3}$ | $2 \times 10^{-3}$ | $8 \times 10^{-4}$ | $5.8 \times 10^{-1}$ | $2.3 \times 10^{-4}$ |
| Recharge (mm/a) | 60 | | | | 150 |

with Mr Sames. Within PHREEQC, the set of geochemical equations (representing the interactions) is solved based on a thermodynamic database.

The geochemical reactions are related to the transport equation by the source/sinkterm $q_k$ in Eq. (2).

$$\mathrm{div}\left(D\ \mathrm{grad}\ c_k - \frac{w}{n}c_k\right) + q_k = \frac{\partial c_k}{\partial t} \tag{2}$$

For time step $t$ the transport Eq. (2) is solved for $n$ cells and $k$ master components $k$ times. A simulation of chemical interactions at each cell within PHREEQC follows. The resulting changes of the $n \times k$ concentrations will be considered in the next time step $t + 1$ within the transport equation as the source/sinkterm $q_k$. The solution of the transport equation is carried out by the 'Front Limitation' algorithm (Haefner et.al., 1997). This algorithm overcomes the limitations of the 'Grid Peclet number', in contrast to conventional algorithms. Therefore, it is possible to use coarse grids, which are adjusted for the data. This results in a drastic saving in CPU time.

### 3.2. Verification of the reactive transport model

Among other examples a column flow test from Brand (1996) was simulated. This test is related to the problem of dump water migration in a calcium siderite buffered aquifer. Fig. 3 shows the comparison of measured and simulated concentrations at the column outflow. The basic processes (calcium–iron exchange, siderite dissolution and gypsum precipitation) are covered well by the model in their effects of the column outflow.

## 4. Migration modelling for the site Jänschwalde

Reactive transport simulation was done for a 2D vertical cross section (compare Fig. 2). The chemical components $Ca^{2+}$, $Fe^{2+}$, $Fe^{3+}$, DIC, $SO_4^2$ were included in the simulation. Redox reactions, mineral dissolution and precipitation as well as cation exchange were considered. Fig. 4 shows the basic model structure. The area of $x = 2700$ up to 3000 m represents the dump body, which is vertically divided into different parts. It was assumed that the dump water quality is equal over the whole simulation time (first order boundary condition). Therefore, only 300 m of the dump were included in the model area.

From $x = 0$ up to 2700 m the model represents the undisturbed quaternary aquifer. A grid size of 100 m and a longitudinal dispersivity of $\delta_l = 10$ m was chosen for the model. An anisotropic factor of 10 between the horizontal and vertical hydraulic conductivities was used. The hydraulic gradient was $I = 1 \times 10^{-3}$. Table 1 shows initial and boundary conditions as well as parameters for the different parts of the model. Chemical concentrations result from the prediction procedure described above. The water

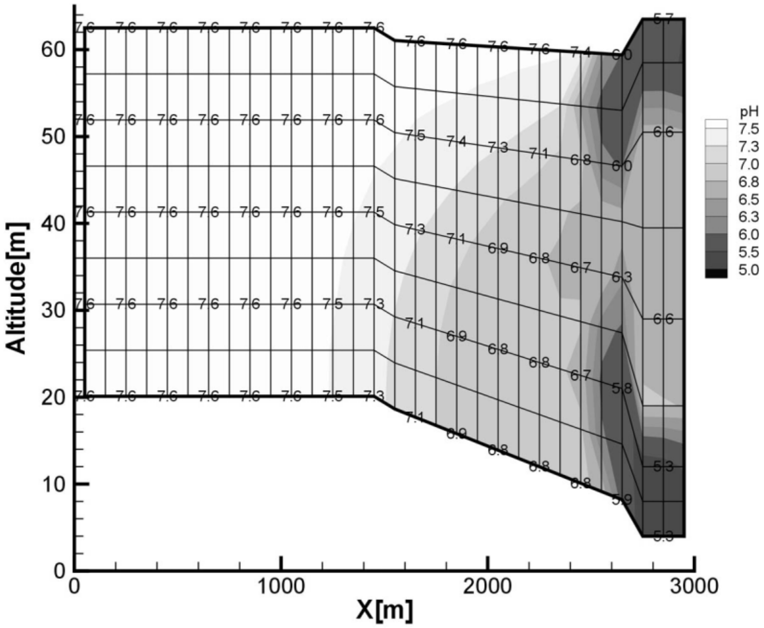

Fig. 5. Predicted pH values after 100 years steady state flow.

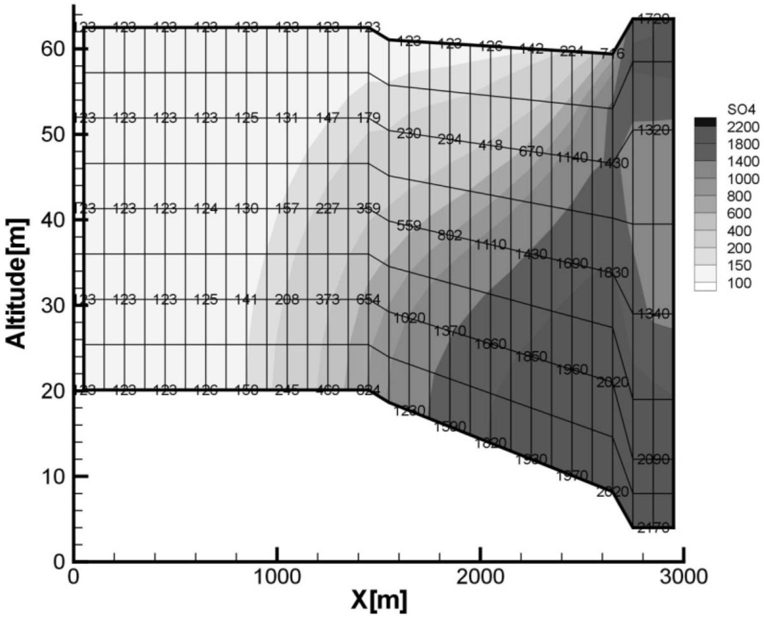

Fig. 6. Predicted $SO_4^{2-}$ concentrations (mg/l) after 100 years steady state flow.

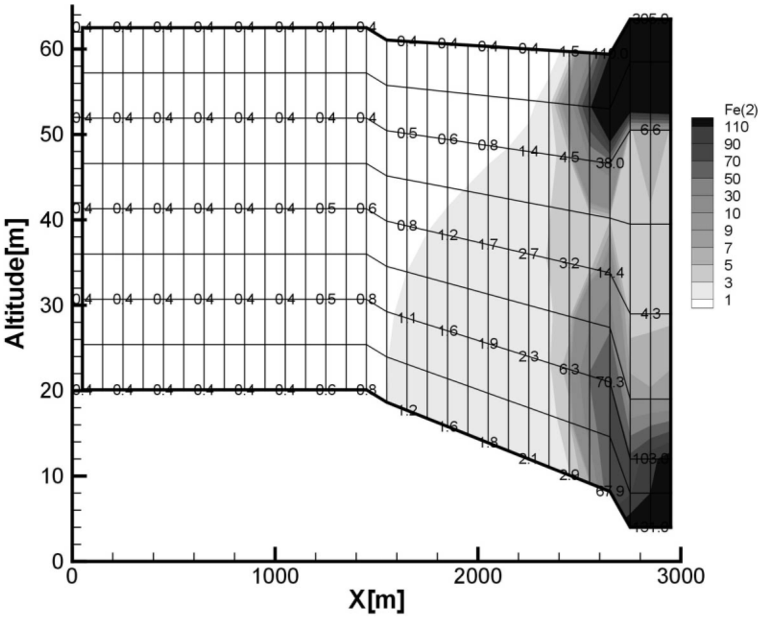

Fig. 7. Predicted $Fe^{2+}$ concentrations (mg/l) after 100 years steady state flow.

quality of the recharge was set to the initial values of the quaternary aquifer. The coefficients of hydraulic conductivity and the recharge rate result from parameter estimation calculations for the already existing part of the dump.

### 4.1. Results

Figs. 5–7 present the results for the pH-value, the sulphate and iron distribution after 100 years of steady state flow. The impact on the pH-values is concentrated on the immediate surroundings of the dump site. This is caused by the calcite buffering within the aquifer. The influence of the undisturbed aquifer by sulphate is much higher. Only, for higher concentration levels gypsum precipitation takes place. The process of cation exchange on the aquifer material limits the iron impact on the aquifer drastically.

The figures show the important role of the unaffected recharge due to the resulting flow system. The result is a dilution of the dump water plume. An approach to steady state was observed. How far from the dump site the equilibrium state will be reached depends strongly on the outflow rates of the dump.

## 5. Future work

The reactive transport calculations show, that the hydraulic conductivity of the dump body and the recharge rate are significant. Up to now the water levels of dump gauges represents only the lower part of the dump. Therefore, the parameter estimation of hydraulic parameters could only be performed for this part of the dump body. There will be a flooding of residual structure (‘Klinger See’) in the south of the dump site. This will allow an estimation of the hydraulic parameters for the whole dump body.

The buffering potentials of the aquifer are very important for the migration process. Column flow tests will be performed with aquifer material and dump waters as infiltrating fluid. These experiments are necessary to show that the buffering potentials of the aquifer material will be effective. The modelling of these experiments will be used as a verification case for the coupled reactive model.

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