Modelling of mine flooding and consequences in the mine hydrogeological environment: flooding of the Koenigstein mine, Germany

A.T. Jakubick · U. Jenk · R. Kahnt

Abstract The approach to modelling of flooding of the underground mines and hydrogeological consequences in the downstream aquifers of the mine followed in the WISMUT Decommissioning and Reclamation Programme is illustrated for the case of the uranium underground leach mine in Koenigstein, near Dresden, Germany. The modelling of the present and future quantity and quality of the water in the mine workings (source of the potential groundwater contamination) and of the contaminant transport in the hydrogeological environment of the mine is central to finding the optimal courses of action for a safe (i.e. controlled) flooding of the mine and for decision-making regarding water-treatment strategy. The results gained in two large scale in-situ flooding experiment lasting over several years and the models developed, calibrated and validated on this basis for the mine flooding is presented. The modelling of the migration of reactive multi-component contaminants in the hydrogeological environment of the mine proved to be useful for the identification of the significance of the geochemical processes. Because of the problems of up-scaling the commonly inadequate database and limited accuracy of the data available, and because of the inherent uncertainty of approximations used in the reactive transport model, the assessment of the environmental impact caused by long-term migration of contaminants downstream of the mine had to be done using a simplified conventional, non-reactive, single component transport model that provided conservative results. For simulation of the mine flooding, it is recommended to use a concurrent monitoring and modelling approach and stepwise forward calculations that do not exceed the length of each preceeding observation period.

Received: 10 June 2001 / Accepted: 10 September 2001

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Keywords Decommission · Mine flooding · Modelling · Reclamation · Uranium

Introduction: decommissioning and reclamation of the Koenigstein mine

The post-war uranium production of the Soviet–East-German SDAG Wismut on the territory of the present federal states of Saxony and Thuringia amounted to approximately 220,000 t U_3O_8. After German reunification in 1990, the economic appraisal of the company showed that further mining was economically not feasible, and production was terminated. The duration of the decommissioning and reclamation of all Wismut liabilities was estimated to be approximately 15 years and cost DM 13 billion.

The remediation of the underground mines presents a substantial portion of the Wismut Remediation Program. The most important step in remediation of the underground mines is the flooding of the underground works. By flooding the mines, a stable regional water table is established and, in case of uranium mines, the radon exhalation into the atmospheric air is prevented. Because the mine water entering the groundwater or reaching the surface is contaminated, an evaluation of the environmental impact is required prior to flooding of the mine. In addition, knowledge of the flooding rate, mine-water quantity and quality are needed to decide about the mine-water treatment requirements and develop specifications for planning and building of the water-treatment plant and to calculate the costs associated with the water treatment. The description of the mine-flooding projects at the Wismut mine sites may be found in (Gatzweiler and Jakubick 1998).

Mining at Koenigstein, east of Dresden, started 1967 and ceased 1990 (Fig. 1). From the overall production (which amounted to 19,258 t U_3O_8) 6,122 t U_3O_8 were gained by underground block leaching.

Leach mining started in 1969. From 1971 to 1984, the production proceeded by both conventional mining and underground leaching. By 1984, leaching had entirely replaced conventional mining. The reasons for the

DOI 10.1007/s00254-001-0492-9

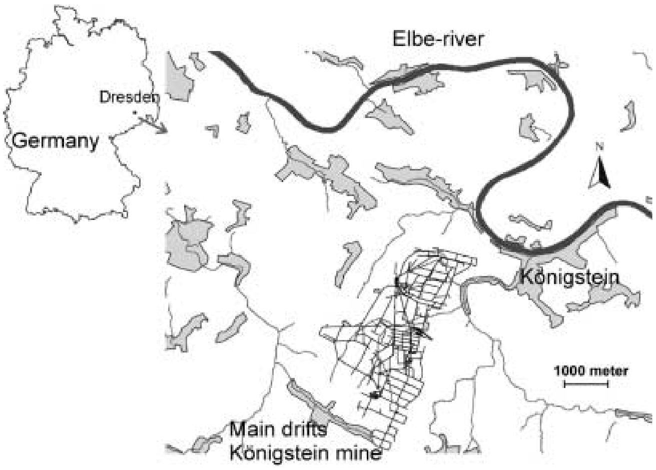

Fig. 1
Location of the Koenigstein mine

introduction of leaching technologies were the rising costs of conventional mining and milling procedures, the lower grade of ore, as well as the increasing complexity of geological and mining conditions.

Characteristics of the site and mine

The Koenigstein mine

The Königstein mine is located in the Elbsandsteingebirge Mountains, between the Erzgebirge (Ore Mountains) in the south and the River Elbe in the north. The uranium mineralisation (U content of 200–1,000 ppm) occurs in Cenomanian sandstones and siltstones overlying the granitic basement of the Cretaceous basin of Pirna. The thickness of the ore bearing layer varies from 2 to 10 m. In association with the uranium (present as pitchblende), approximately 2 to 3% sulphates (of Fe, Zn, Pb, Cu and others), 5% clay minerals and iron hydroxides are present in the ore. The U/Ra ratio is highly irregular because of secondary redepositions of uranium by groundwater.

The deposit extends over 26 km^2 at a depth of 150–250 m. The general dip of the ore body is approximately 3°N. The south field of the mine is developed down to 150 m, the north field of the mine is 300 m deep. The area of the mine is 5 km^2 . The maximum extension of the mine is 4.5 km from north to south. The maximum width (from east to west) is 2 km. There are 58.5 km of open mine drifts underground and five service and six ventilation shaft connections to the surface.

Because the exploitation started as a conventional underground mine and the underground works already existed, it was decided to apply the leaching agent directly underground rather than use solution mining from the surface. Typically, 10-m thick, 50–100-m-long and 100–200-m-deep sandstone blocks (with volumes reaching from 10^5 to 10^6 m^3) were leached. The leaching practice differentiated between:

1. Leaching of blocks (highly permeable sandstone);
2. Leaching of magazines (low-permeability rocks previously loosened by blasting).

By the time of closure, the number of leached blocks reached 104. The average concentration of the leaching agent (sulphuric acid) was 2–3 g H_2SO_4/l, pH=1.5–1.8, salinity 10–14 g/l. The liquid/solid ratio was 3–8 m^3/t at a feed rate of 0.003 to 0.1 m^3/t/day. The sulphuric acid was usually injected with a pressure of 0.6 MPa. The injection pressure was individually controlled and depended on the rock conditions and U content. The saturated leachate was collected at the bottom of the block. The recoveries were in the order of 65–75%.

The concentration of the dissolved uranium in the saturated leachate was 10 to 150 mg/l. Approximately 130,000 t of sulphuric acid was introduced into the mine and, in addition, a considerable amount of sulphuric acid got generated by the oxidation of pyrite.

At the time of termination of production (1990), approximately 9,500 t of uranium reserves were left underground and approximately 2 million m^3 of acidic solution (along with soluble secondary minerals) remained in the pores space of the mined formation.

Hydrogeology of the site

The ore body is located in the fourth and deepest aquifer of the Saxon Cretaceous basin carrying a major drinking water reservoir in the third aquifer. The two aquifers are separated by a 10- to 30-cm-thick clay layer (referred to as the Plenus clay or Planer) having an average hydraulic conductivity of k=10^{-9} m/s and an effective porosity of 1%. Leakages across the Plenus clay occur through the North-Fault intersecting the mine, disturbances caused by mining works and numerous old prospecting boreholes. Although the respective underground works were backfilled and the connections between the aquifers sealed, it is technically not feasible to completely isolate the artesian groundwater of the fourth aquifer (and mine) from the third aquifer. The groundwater of all aquifers discharge into the Elbe River, which, at the closest point, is approximately 600 m from the mine.

During mining, the fourth aquifer was completely drained around the mine. During leaching it was paramount to keep the circulation of the leaching fluid within the drained part of the formation, separate from the mining related draw down of the (artesian) groundwater in the fourth aquifer. The general direction of the ground-water flow toward the mine is in both the third and fourth aquifer from south to north–north-east, i.e. toward the Elbe River, which has a general flow direction from south-east to north-west. After flooding of the mine, the direction of the ground-water flow will remain the same.

To safely recover the leachate from the mine (thus removing the most mobile source of contamination), it remains imperative for the remediation phase to only gradually give up the control of the ground-water draw-down and maintain the separation of the two mine-water management systems.

Although the hydrogeological regime of the aquifers surrounding the mine is well understood to describe the regional flow field, the lithology and mineral content of the aquifer downstream of the mine is only known from early exploratory borings.

Remediation framework

The phasing out of leach mining without causing an inadmissible environmental impact is considerably more complex than closing down a conventional mine.

The amount of potential ground-water contaminants in the mine was assessed to be up to 75,000 t of sulphate, 19,000 t of iron, 2,300 t of aluminium, 1,600 t of tin, 1,200 t of uranium, 110 t of arsenic, 10 t of cadmium and 84 t of nitro-aromats.

The approach to flooding followed consists of a controlled increase of the mine water level with simultaneous monitoring of the hydrochemical, hydraulic and geo-mechanical conditions in the mine and the surrounding environment. Before giving up control, a number of measures (stipulated by the permitting authority) have to be impemented to prevent the contamination of the adjacent aquifers and nearby surface streams.

It was considered essential to

- preserve intact (and seal as far as possible) the groundwater barrier between the fourth and third aquifer;
- neutralise the leachate acid in the mine;
- remove or immobilise the dissolved or easily soluble uranium still present in the mine;
- equilibrate or neutralise the acid pore waters (approx. 2 million m^3);
- treat the contaminated water raised from the mine.

A cost–benefit analysis was used to select the optimal flooding strategy within the boundary conditions set by the stipulated measures. The selected option can be summarised as phasing out the leachate circulation by increasing gradually the groundwater inflow into the mine to displace the leachate in the pores of the mined formation, and pumping the mine water to the surface for treatment and discharge. During flooding, the hydraulic separation of the contaminated mine water from the aquifer is maintained by a specially constructed underground drift (the control drift) at the downstream end of the mine. The control drift is designed to drain the mine water through a series of boreholes drilled into the mine pillar of the control drift while simultaneously draining the groundwater from the aquifer on the downstream side of the drift through an other set of boreholes. Both water streams are managed separately. The separation of the mine and aquifer by the control drift is illustrated in Fig. 2.

An underground monitoring system was designed and implemented in the mine to control the rate of pumping from the mine. In case it becomes necessary, the flooding can be stopped and, if required, reactive materials introduce underground to control the geochemistry in the mine.

The water treatment technology was laid out to tolerate/adjust to changes of water quality during flooding.

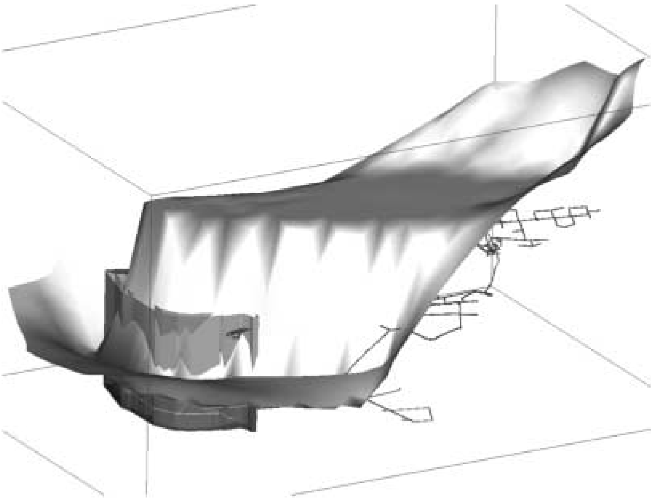

Fig. 2
The separation of the mine from the downstream aquifer by means of the mine-control drift. The equipotential surface of the mine water level after flooding (on the *right side*) and of the downstream groundwater level (on the *left side*) defines the interaction of the mine with the regional flow field

The described controlled mine flooding requires a dependable model for simulation of mine-water quality development, evaluation of the impact on the surrounding groundwater and the effective control of the flooding processes. However, to achieve the modelling objective there were insufficient data and knowledge of details to describe the individual contaminant sources (leaching blocks and magazines) in the mine. Particularly, the available data were insufficient for the description of the spatial variability of the pore volume, including acid liquid and contaminant content in the pores in statistically significant terms, and there were no measurements of flow and mass transport in the mine openings.

Data base development: the mine-flooding experiments

The main objective of the flooding experiment was to create a data base to handle the above-mentioned uncertainities, to specify the contaminants, which could be mobilised during flooding and subsequently calibrate and validate the mine-flooding model.

The first in-situ flooding experiment was started January 25, 1993 and was conducted in the deepest northern part of the mine, which included several leaching blocks, but had no direct contact with the fourth aquifer. The experimental area of the mine was flooded between 25 and 33.4 m a.s.l. by introducing first seepage water 26 m^3/h and later at 45 m^3/h of from the area of the North-Fault. Till November 1997, the water level was maintained constant at 33.4 m a.s.l. by means of an overflow. The maximum saturated thickness of the sandstone formation affected was approximately 8 m in the northern part of the experimental area, and decreasing towards the south because of the dipping of the sandstone layer. The volume of the rock mass and open mine space and pore space involved in the experiment was approximately 1.7 million m^3 and 160,000 m^3, resp. representing approximately 1% of the volume of the mine to be flooded. For purposes of comparison, the planned final flooding level is 140 m a.s.l. (below the leaky North-Fault), which corresponds to a water volume of 6,500,000–9,330,000 m^3.

An extensive underground monitoring system was established for the experiment consisting of observation points at the periphery of the flooded mine space and boreholes in the flooded space. The contaminants concentrations and flux, as well as the outflow from the flooded area, were continuously monitored. The first experiment lasted till 2 November 1997, i.e. for more than 57 months.

In the second flooding experiment the mine water level was raised to 40.0 m.a.s.l. by introducing additional drainage water; thus, increasing the involved volume of rock mass to 7.7 million m^3 and of mine space to 800 thousand m^3, i.e. 5% of the estimated final flooding volume. The water in the second experiment was introduced at a rate of approximately 52–56 m^3/h over a period of 2 years. At 40.0 m a.s.l. a constant flooding level was maintained. During the experiment, approximately 1,876,000 m^3 of mine water flowed through the experimental mine section (515,000 m^3 were stored) and approximately 2,630 t of sulphate, 620 t of iron and 34 t of uranium were released.

The quality of the flooding water reflected the conditions created by the previous leaching: pH=2–3, TDS=10 g/l, 3 g/l sulphates, 500 mg/l iron and 10 mg/l uranium.

The second experiment lasted for 24 months (from 3 November 1997 to 1 January 2001).

Since 16 October 2000, the flooding level has been decreased to test the hysteresis between mine flooding and mine dewatering.

Testing of the high density sludge (HDS) treatment process for handling the mine water was part of the experiment. In addition, the feasibility of in-situ geochemical mine-water treatment measures was tested underground.

The flooding model concept

Modelling framework

The overall goal of the model development was to have a performance assessment tool to select the optimal mine flooding strategies, source control and management of the flooding process. A specific modelling task was to evaluate the concentration of the contaminants (U, Cd, Zn, As and others) downstream of the mine, during and after flooding. A multistage modelling approach was applied to simulate the following sequence of processes:

1. Release of the contaminated pore waters from leaching blocks and magazines;
2. Movement of water and contaminants in the mine drifts;
3. Leakage through the North Fault and other discontinuities into the third aquifer;
4. Transport of the contaminants and their geochemical interaction downstream of the mine.

The modelling of the processes involved a wide range of spatial dimensions. For the downstream flow and contaminant transport in the aquifer a range of 30 to 40 km had to be considered; the flow in the mine openings (drifts) involves distances from 100 to 4 km; the density-dependent flow from the leaching blocks acts over 1–200 m and the diffusional flux occurs over distances less than 1 m.

To simulate the processes acting at different scales, the conceptual model had to comprise several independent models: (1) a regional hydraulic model (the FEFLOW code was used for this purpose) that provided the in- and outflow boundaries for the mine as a function of hydraulic head and time; (2) the mine flooding geochemical balance model, FLOODING (including the commercial code PHREEQC), which provided the source term as a function of time; (3) detailed flow and mass release models (FEFLOW) that describe the prevailing processes and parameters within the mine; (4) the mass transport model for the downstream aquifers, which included a conventional (non-reactive) mass transport model (FEFLOW) and a reactive mass transport model (MINTRAN).

For purposes of evaluation models for risk analysis, analysis of uncertainty, time integration and cost–benefit analysis codes such as GOLDSIM or @risk were employed. The decision making regarding the optimal flooding option was based on sensitivity analysis with the above models. The clarification of the conceptual issues required decoupled model calculations and calibration of the detailed flow and mass release models. The model-specific parameters and relevant data base were attached to each model individually.

The interaction of the individual models is illustrated in Fig. 3. The detailed description of the conceptual model is presented in Heinzelmann and others (1998) and Kahnt and others (2000).

Geochemical concepts

Within the open mine space and pore space the species were assumed to be in thermodynamic equilibrium. The state of equilibrium was calculated for each time step with PHREEQC (Parkhurst 1995; Parkhurst and others 1999). For calculations, the geochemical data base of CHEMVAL2 was used (Pearson and others 1992; Falck and others 1996).

Table 1 presents the 'mean' pore water composition estimated on the basis of pore-water analysis. A neutral charge balance was achieved by adding SO_4^{2-}.

Beside the pore water, the most immediate source of contamination is from the secondary minerals present as sulphate salts. Adsorption of U and As on secondary minerals was of considerable importance. Valent metals, such as Cd, were of negligible importance.

Table 2 shows the composition of the secondary minerals. Secondary minerals present in the mine are given as solids (mol/kg SO_4) and are related to 1 kg of total sulphate.

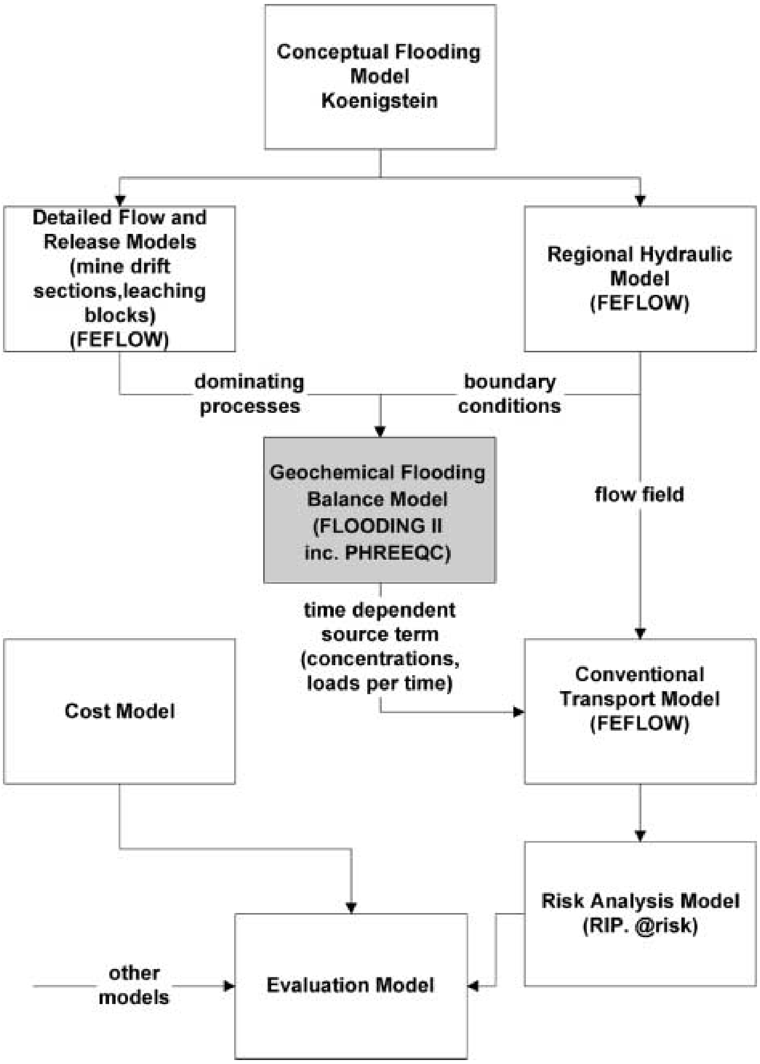

Fig. 3
The conceptual modelling approach and interaction of the individual models (the reactive transport model not included)

The iron hydrolysis is accounted for as an effective mineral phase (the 'Koenigstein mineral'), the composition of which was estimated by mixing mine and groundwaters.

$$3\mathrm{Fe} + \mathrm{SO}_4^{2-} + 7\mathrm{H}_2\mathrm{O} = \mathrm{Fe}_3\mathrm{SO}_4(\mathrm{OH})_7 + 7\mathrm{H}^+$$

$$k = \frac{[\mathrm{Fe}^{3+}]^3[\mathrm{SO}_4]}{[\mathrm{H}^+]^7} \qquad \log\ k = 1.6$$

Because of its importance, the iron hydroxide phase is specified in detail in Table 3. In the first approximation the assumption was made that the geochemical equilibrium during flooding is controlled by hydrolysis of iron.

The model codes

Regional flow model

The model describes the flow field in the hydrogeological environment of the mine and considers the hydrological conditions on the surface, such as streams, water removal for drinking, industrial and emergency purposes. The model specifies the position of the mine in the hydrogeological field and the volume of the mine in terms of the open mine space and rock mass porosity. The separation/communication of the mine and ground-water-flow field through the control drift is demonstrated in Fig. 2, showing the equipotential surface of the mine water and groundwater in the aquifer for flooded mine conditions. However, a dependable simulation of the mine-water drainage into the control drift requires a reliable quantification of the hydraulic conductivity of the sandstone pillar of the control drift, which is (for safety reasons) unattainable. The modelling is performed by the commercial code FEFLOW (MODFLOW can be used alternatively). The inflow and outflow rates of the regional flow model provide the boundary conditions for the FLOODING code and describe the contamination source for the aquifer.

Detailed flow and mass release models

Detailed models are used to derive the assumptions for conceptualisation by simulating the flow and contaminant release from the individual mine sections (model compartments). The compartments are non-dimensional

Table 1
Mean pore water composition (concentrations in mg/l)

pH	2.1	Mn	20.7
pE	12.0	S(6)	7211
Na	476	Cl	371
K	5.	U(6)	35
Ca	378	Zn	109
Mg	42.3	As	0.65
Al	198	Cd	1.08
Fe	1,569		

Table 2
Amount of salts expressed as secondary minerals of ideal composition in mol/kg SO_4

Na_2SO_4	7.65e-1
K_2SO_4	3.79e-2
$CaSO_4$	1.71e-1
$FeSO_4$	4.73e-0
$Fe_2(SO_4)_3$	8.36e-1
$Al_2(SO_4)_3$	6.05e-1
$NiSO_4$	1.65e-2
$ZnSO_4$	2.84e-1
UO_2SO_4	1.04e-1
$CdSO_4$	2.25e-3
H_3AsO_4	1.04e-2

elements that consist of a section of the open mine space and associated pore space (composed of a volume effectively accessible to flooding and a volume occupied by the pore water).

The pore space in the compartment represents either a leached mining block or a water-conducting mine pillar through which the mine water drains.

The open mine space in the compartment has one inflow and two outflows (open outflow in the mine drift and drainage through the pore space). The unrestricted water flow in the mine drifts and the water movement in the draining mine pillars are simulated as an advective flow. The flow Q_A^{FP} between the open mine space and the pore space is determined by the difference of average water levels in the mine drift and pore space, Δh and effective hydraulic conductivity, L:

$$Q_A^{FP} = L_A \cdot \Delta h$$

Considering the fact that there is a delay between the flooding level in the rock mass and flooding level in the mine drift, three combinations of flooding level states are possible:

1. The mine drift is partly flooded and the surrounding pore space is unsaturated; the hydraulic gradient is directed from the flooded part of the drift towards the pore space. The non-flooded part of the drift receives and conducts air along with an influx of radon that is pushed out by the increasing flood level from the unsaturated pore space.
2. The mine drift is completely flooded (except for small air pockets) and the pore space below the mine floor is saturated; the hydraulic gradient from the flooded drift is directed towards the unsaturated mine wall and roof.
3. Both mine drift and surrounding pore space are completely saturated.

Prior to flooding, the contaminants in the open mine space are present as secondary minerals. Their amount is assumed to be proportional to the open mine space. The contaminant transport in the communicating open mine space and in the pore space of the pillars includes hydrodynamic dispersion.

In the pore space of the blocks, the contaminants are present in the pore water secondary minerals and sorbed on the mineral surfaces. Because of the difference in the mean density of the pore water in the leaching blocks and the water in the mine space, $\Delta\rho$, the contaminant release with the water flux, Q_A^{wash} from the blocks is mainly by density-dependent flow. The quantity of the contaminant flux is controlled by an effective coupling parameter, Λ, which is quantified by calibration:

$$Q_A^{wash} = \Lambda_A \cdot \frac{\Delta\rho}{\rho_0}$$

In the first model, predictions of the parameters of the contaminant flux from the pore space, Λ, L, and initial contaminant mass were considered constant for all blocks in the mine. Later, a more differentiated approach was adopted. The time dependent load release functions distinguish between the contamination release from a combined source of secondary minerals and pore liquid producing an initial peak followed by a decline (described by an error or complementary error function) and release from a pore liquid source only following a steady load decrease curve (described by an exponential or power function).

The contaminant release from the stagnant mine sections is of significance for long-term predictions. The release curves are described by either an exponential or power function on one hand or by a linear decrease or constant load release on the other. Based on the flooding experiment both maximal and minimal load relase functions were estimated.

The detailed model required in support of the FLOODING code is switched on after the significance of the contribution of the particular mine section has been analytically established.

Mine flooding geochemical balance model

The code was developed for WISMUT by Kalka and others (1998) in two stages. The original FLOODING I code used a simple mixing cell approach. All drifts and shafts were assumed to be freely interconnected and were treated as a single compartment. The pore space was divided into 1-m-slices, each coupled with the mine openings, the contaminant release from the pore space was by density-dependent flow. The only chemical process taken into account was iron hydrolysis.

The presently used second version of the code, FLOODING II, includes the FREEQEC code and describes the hydraulic and hydrogeochemical processes in the underground mine space. FLOODING II is a flexible multi-compartment model that calculates the mass and contaminant balance in the mine works. The code presents the source term in the conceptual model of the mine.

Table 3
Composition of the iron hydroxide phase

Dilution ratio $f=V(GW)/V(PW)$	Composition dependent on	Koenigstein mineral (charge balanced ?)
2.6	$Fe_{3,10}SO_4(OH)_7K_{0,125}$:x H_2O	$Fe_3SO_4(OH)_7$:x H_2O
5.0	$Fe_{2,60}SO_4K_{0,087}$:x H_2O	
7.3	$Fe_{3,06}SO_4(OH)_7K_{0,068}$:$x$ H_2O	
9.0	$Fe_{2,98}SO_4(OH)_7K_{0,102}$:$x$ H_2O	

The level of flooding in the mine is controlled by the boundary conditions provided by the regional flow model (time-dependent hydraulic heads, in- and outflows). The flooded volume of the mine is considered to be a function of the flooding level in the mine.

The neighbouring mine compartments are hydraulically connected. The overall connection of the mine compartments is determined according to their geodetic elevation in the mine, which determines when the compartments become active (accessible to flooding).

Apart from the compartments describing the mining blocks and sandstone pillar (P-boxes) there are separate compartments for:

- the experimental flooding (WS, WN, E1, E2);
- mine workings in the crystalline basement;
- mine workings in the productive strata.

The involvement of the mine compartments with a restricted connection to the mine workings depends on whether a long-term contribution to the source term has been established or not. The contribution is estimated in a separate calculation.

The schematic model structure of the Koenigstein mine is shown in Fig. 4.

The different compartment groups have different hydraulic and contaminant release characteristics, expressed by the dominant processes (hydraulic, pore water release and geochemistry) in the code.

The model calculates the time-dependent mass flow balance for each mine compartment and flooding situation. The contribution of the open mine space and of the effectively available pore space are considered separately. The output of the Flooding code is the prediction of the time-dependent mine water quality provided as a function of flooding level.

Transport models

The downstream contaminant transport in the third aquifer was simulated by using the commercial FEFLOW code and by modelling the conventional (non-reactive, single species) transport in a 3-D flow field, which ascertained a conservative assessment of the ground-water contamination in the evaluation models.

For investigation of the geochemical behaviour of the contaminants, a reactive (multi-component) contaminant transport code, MINTRAN, developed by K.U. Mayer, University of Waterloo, Canada, was used (Mayer 1998). The objective was to identify the effect of the possible geochemical reactions on the mobility of the contaminants, estimate the buffer capacity of the aquifer and to test the robustness of the geochemical assumptions and the parameter uncertainties.

The code uses a global-implicit approach to handle the transport of the contaminants as an advective–diffusive flux of dissolved multi-component substances. The diffusive transport of gases can be include in the code. The geochemical interactions considered involve complexation, oxidation/reduction, ion exchange, gas exchange between the gas and water phases, and solution/precipitation of mineral phases. For the calculation of the geochemical processes the MINTEQA2 and WATEQ4F databases were used (Dzombak and others 1990; Bruno and others 1995).

The investigated parameters and elements included the change of pH and the fate of the sulphate (originating from the leaching) as well as the fate of the dissolved metals Al, Cd, Cr, Fe, Ni, Pb, Ra, U and Zn following their release into the fourth aquifer.

The simulations were first done with a 2-D model. Following a detailed evaluation involving the use of the non-reactive transport model, a reduction to a 1-D evaluation was considered sufficient for the task. The average aquifer porosity was taken as 19% and the flow regime assumed in steady state. The mass transport simulation did not include macroscopic dispersion in order to make certain that the results would not be distorted by any potential numerical problems commonly associated with sharp concentration fronts. The extreme simplification of the aquifer hydraulics was considered to be justified for the particular task because the ratio of the minimum length of the flow path and the thickness of the aquifer was greater than 100.

The modelling was done in co-operation with University of Waterloo (Bain and others 2002) and involved two cross sections (Fig. 5) that had extreme values of length and velocity:

1. a long section (length 5 km, average particle velocity 30 m/year);
2. a short section (length 1 km, average particle velocity 180 m/year)

The hydrogeological cross section of the short profile B is shown in Fig. 6. Based on the available cores from the fourth aquifer, the following ranges (in % volume) of minerals contents were specified:

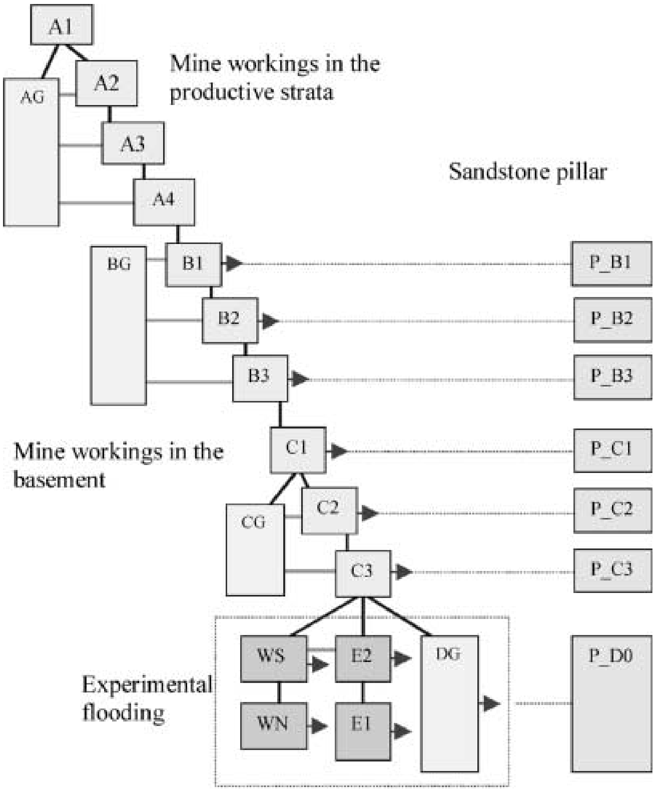

Fig. 4
Compartmentalisation of the Koenigstein mine for the Flooding II code

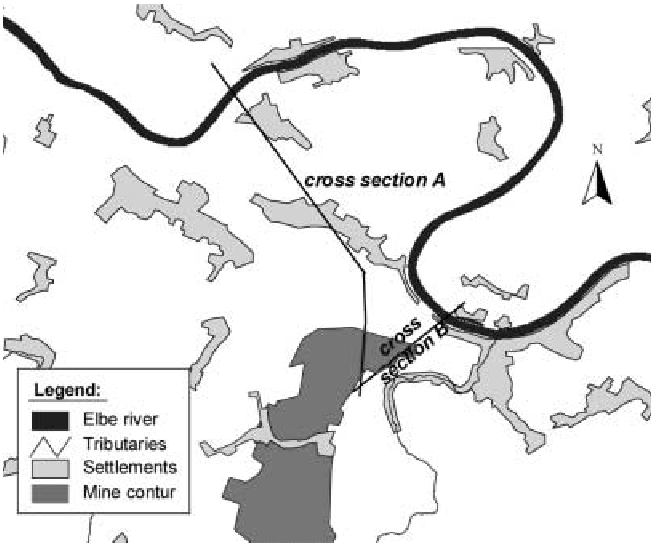

Fig. 5
The two cross sections used in the mass transport modelling

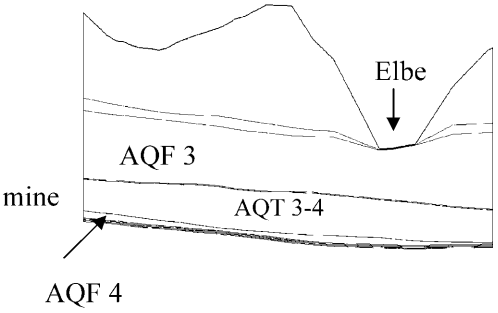

Fig. 6
Cross section B (the short section) through the aquifers downstream of the mine. The vertical exaggeration is 1 to 30

- Quartz at 90–96% (vol);
- Feldspar at <1;
- Clay minerals at 0–3;
- Metal-oxides and metal-sulphides at 1–2;
- Carbonates at <1;
- Organic substances at 0–0.1;
- Trace minerals at 1.

The uranium content was 0.03% and assumed to be in form of uraninite. A more detailed mineralogy was not available. The type of carbonates (dolomite, calcite) present in the aquifer was unknown. The required data on the ratio of metal-oxides and metal-sulphides were lacking. The presence of ferrihydrite could not be ascertained.

A typical water sample analyses was used as the initial water concentration for the fourth aquifer.

Table 4 summarises the constitution of the ground- and mine-water. In the observed range, the chemical composition of the aquifer water had no significant effect on the geochemical behaviour of the dissolved metals. The water composition observed during the flooding experiment was considered representative for the mine water constitution. The two waters were equilibrated at the mine/aquifer boundary. For most of the simulations, the concentration was assumed to be constant.

The solid phases listed in Table 5 were assumed to act as sources or sinks for the listed dissolved metals. Although clearly relevant to migration, ion-exchange and sorption processes could not be included in the evaluation because quantitative, site-specific data were missing and the pH and Eh buffer capacity of the aquifer was unknown.

To overcome the lack of mineralogical data, the effect of variation of the content of the relevant minerals (in the observed ranges) on the geochemical behaviour of the contaminants was evaluated in a sensitivity analysis. The sensitivity analysis involved the variation of the carbonate mineralogy, mineralogy of the metal-oxides, carbonate content, metal-oxide content, metal-sulphide content, ion exchange and use of steady state and transient boundary conditions.

Based on the observed dominance of particular parameters, more than 20 scenarios were developed and tested for both cross sections, thus covering the range of the possible geochemical behaviour of the investigated parameters. The most important scenarios were 1% (mass) ferrihydrite; 0.2% (mass) calcite; 0.2% (mass) calcite, 1% (mass) ferrihydrite = calcite + ferrihydrite; 0.2% (mass) calcite; and 1% (mass) pyrite.

A generalised overview of the characteristic concentrations of the dissolved metals for four scenarios in the short cross section is presented in Table 6. Only qualitative

Table 4 Constitution of the mine and groundwater

Element	Source term (mol/l)	Source term equiv. (mol/l)	Background groundwater (mg/l)
pH	2.3	2.3	6.6
Eh (mV)	13.5	13.3	197
Al	6.52e-3	6.57e-3	
Ba	1.09e-7	3.54e-8	
Ca	1.16e-2	1.17e-2	7.4
Cd	8.78e-6	8.85e-6	
Cl	1.3e-2	1.31e-2	32.8
Total CO_3	1.67e-7	1.01e-8	82.6
Cr	1.64e-5	1.64e-5	
Fe(II)	2.69e-4	1.36e-4	Fe_{tot}=0.17
Fe(III)	1.07e-2	1.06e-2	
H_4SiO_4	1.6e-3	9.33e-4	6.77
K	1.97e-4	5.79e-7	81.8
Mg	2.02e-3	2.03e-3	4.1
Na	2.38e-2	2.4e-2	41
Ni	1.12e-4	1.13e-4	
Pb	4.83e-7	4.86e-7	
PO_4	8.32e-5	8.38e-5	0.06
Ra	3.1e-4	3.12e-4	880 mBq/l
SO_4	5.28e-2	5.3e-2	26
UO_2^{2+}	1.78e-4	1.78e-4	0.0454
Zn	1.53e-3	1.54e-3	0.011

statements comparing the characteristic concentrations with the ‘conservative’ scenario (assuming no chemical reactions) appeared to be justified because the calculated concentration of the considered metals varied by more than four orders of magnitude for the specified observation points. The modelling results for a point 1,000 m downstream of the source and 100 years after completion of the mine flooding are given in Table 6.

Based on the detailed evaluation of the results, the following conclusions can be drawn:

1. The carbonate minerals controlled the
- pH level
- precipitation of secondary carbonate and hydroxide phases
- retardation of the Cd, Cr and Zn transport
- dissolution of secondary mineral phases affecting high metal concentrations
- the creation of Fe(III)-hydroxide, which led to an oxidative dissolution of uraninite.
2. Sulphide mineral phases controlled the
- redox potential
- U(VI) reduction and precipitation of uraninite
- caused the potential release of Ni, Pb and Zn.

None of the simulated scenarios resulted in a simultaneous decrease of all metals and radionuclides (e.g. either the uranium concentration was low while the zinc concentration was high or vice versa).

The comparison of the non-reactive and reactive mass transports and the effect of using transient (instead of constant) boundary conditions (that resulted in a slow, long-lasting decrease of contaminant concentration) is demonstrated for uranium migration in Fig. 7.

The mobility of the dissolved metals strongly depends on the mineralogy of the aquifer. Already, trace mineral contents (below 1%) significantly affected the mobility. The sensitivity to parameter variation (in the relatively narrow range of mineral content in the aquifer) indicates that the scale up presents the most significant problem in using the multi-component, reactive model for calculation of a large-scale, long-term migration.

Because it is not feasible to collect all the geochemical information needed for the code and to perform large-scale field tests for model calibration, it was concluded that the only possibility of improving the accuracy of migration calculations would mean to reduce the uncertainty of the relevant geochemical processes by very involved field investigations.

Based on the results of the sensitivity analyses it was decided to view the reactive transport model at this stage as an investigative tool rather than a functional part of the FLOODING code.

Evaluation models

For selection of the best flooding alternative, the performance-assessment model, which integrated the results of all model calculations, was extended by a cost–benefit analysis.

The results of the conventional (non-reactive) transport modelling were used to quantify the environmental impact and risks associated with a particular flooding option. The quantified environmental impact and estimated costs of the alternative options served to select the best option. The evaluated flooding options contain an inherent uncertainty, primarily due to the uncertainty of the data and incomplete knowledge of the processes involved.

Probabilistic methods to assess the likelihood of the possible outcomes were used to demonstrate rational decision making to the regulator. However, such highly formalised approaches are not necessary for the technical understanding of the sensitivity of the model to parameter variation.

Table 5
Assumptions concerning sources and sinks for the metals

Element	Possible source	Mass	Possible sink
Al	Gibbsite	1% as Al_2O_3	Gibbsite, jurbanite
Cd	Ottavite	0.5 ppm Cd	Ottavite
Cr	no	0	$Cr(OH)_3$
Fe	Pyrite, siderite	Bis 2 mass%	Pyrite, siderite, ferrihydrite
Ni	Millerite	4 ppm Ni	$Ni(OH)_2$
Pb	Galena	3 ppm Pb	Anglesite
U	Uraninite	4 bis 460 ppm	Uraninite
Zn	Sphalerite	20 ppm Zn	Smithonite, sphalerite

Table 6
Comparison of the migration of the metal contaminants calculated by reactive mass transport modelling for the B cross section (short profile) with the migration calculated by using a non-reactive (conservative) mass transport model for the main geochemical scenarios

	Ferrihydrite	Calcite	Calcite + ferrihydrite	Calcite + pyrite
Fe	High	Small	Small	High
SO_4	Equal	Small	Small	Small
U	High	High	High	Small
Cd	High	High	High	High
Cr	Equal	Equal	Equal	Equal
Ni	Equal	Equal	Equal	High
Pb	Equal	Equal	Equal	High
Zn	Equal	Equal	Equal	High

Calibration and discussion of modelling results

The evaluation of the flooding experiments aimed to identify the dominant hydraulic and geochemical processes and to derive the contaminant-release functions from the leaching blocks. The evaluation was based on the observed behaviour of the contaminants.

The overall conclusions from the flooding experiments were that (1) the contaminant mass behaviour was mainly determined by the hydraulics of the mine water, (2) the chemistry of the mine water corresponded to various degrees of dilution of the pore leachate and (3) the geochemical equilibria were controlled by $FeSO_4$ and the stabilisation of the geochemical processes was reached at pH $\leq =3$.

The model was adjusted to the data obtained from the first phase of the flooding experiment and a prognosis was made for the second phase of the experiment. The parameter identification and calibration were based on the measured contaminant flux. The calibration and the modelling phases are illustrated for uranium in Fig. 8. The figure demonstrates a good match between the measured and the calculated uranium load.

The good correspondence of calculated and measured results are believed to have been achieved because:

- The period of prediction is comparable to the duration of the experimental phase over which the data were collected;
- The volume of the second flooding experiment was only five times larger than the volume of the first experiment.

Based on the experience of the first experiment, the FLOODING I code was extended to:

- Include PHREEQC;
- Represent separately the remote (more isolated) parts of the open mine space;
- Adjust the type of boundary conditions of the model to the observed behaviour.

Figures 9 and 10 illustrate the effect of including PHREEQC in the FLOODING code using the example of sulphate release and the prediction of acidity.

Because the volume scale of the experiments can be considered sufficiently large to be representative for the overall mine volume, a realistic prediction for the mine flooding was considered feasible, if the time scale of forward calculation would not exceed the observational period of the experiment. The comparison of the modelling results and experiment (shifted in time) is given in Fig. 11 for different scenarios to illustrate the range of the remaining uncertainties over a time period comparable with the experiments. The uncertainties associated with long-term simulations are not included. The good match between measured sulphate load from the experimental

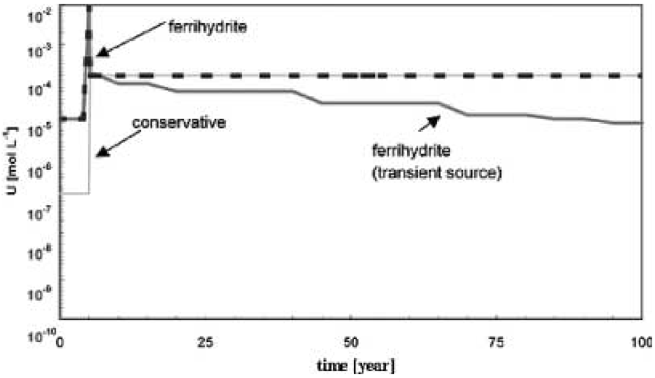

Fig. 7
Uranium breakthrough concentration in the B cross section calculated for non-reactive mass transport (conservative) and for reactive mass transport using transient (*lower line*) and stationary (*upper line*) boundary conditions

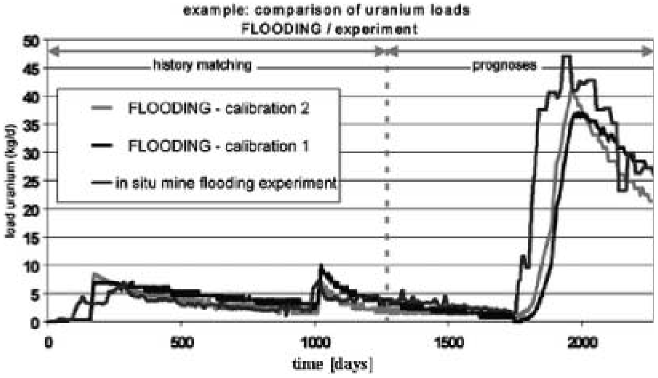

Fig. 8
Calibration of the FLOODING I and II codes by matching the observed development of the source during the in-situ flooding experiment followed by a subsequent prediction of the source development for the next phase of the flooding experiment

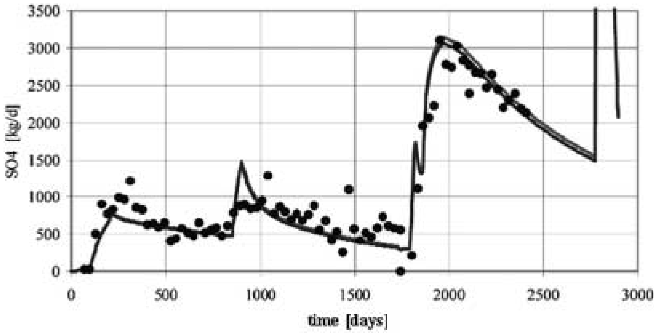

Fig. 9
Comparison of the sulphate release prediction with the mine flooding experiment with use of PHREEQC in the Flooding code (*lower line*) and without (*upper line*)

flooding (dots) and the calculations with the FLOODING code (line) are demonstrated in Fig. 11. The analysis of the results showed that:

- The reliability of predictions increased when data measured in in-situ experiments were applied to comparable scales.
- Within the tested scale and time limits it was possible to simulate the contaminant release by means of multi-compartment model.
- Based on the experimental data it appears that the contaminant release is dominated by flushing out the secondary minerals from the open mine space. The mobilisation of the secondary minerals is instantaneous, producing an initial contamination peak. The dilution of the contaminants that occurs in the early phases of the flooding depends on the volume of the water available for mixing and volume of the open mine space. The process of contaminant release from the leaching blocks proceeded simultaneously with the instant flushing out of the secondary contamination minerals at a slower pace.
- During the observation period of the flooding experiments, the geochemical reactions, such as sorption, were of secondary importance compared with the dissolution of the secondary minerals and the iron hydrolysis. It follows that the system is at least initially (i.e. over several years) dominated by the conditions created by the in-situ ore leaching. Other important controlling factors are the oxidation introduced by the continuous mine-water pumping and the physical limitations of the pore-water release into the open mine space.
- Although the modelling of the contaminant release during the mine flooding is reasonably reliable for a time span comparable with the observation time of the experimental flooding, considerable uncertainties remain concerning long-term modelling.

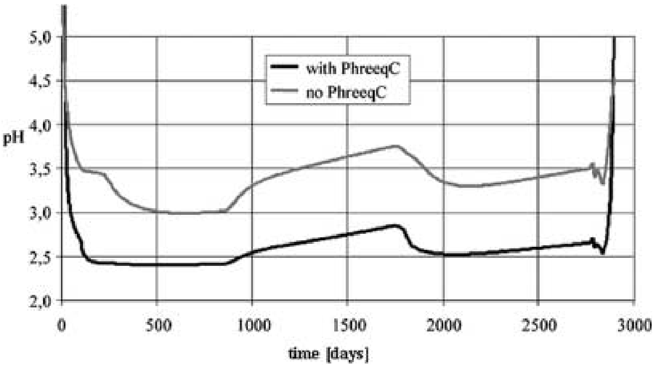

Fig. 10
Prediction of the pH development with use of PHREEQC in the Flooding code (*lower line*) and without (*upper line*)

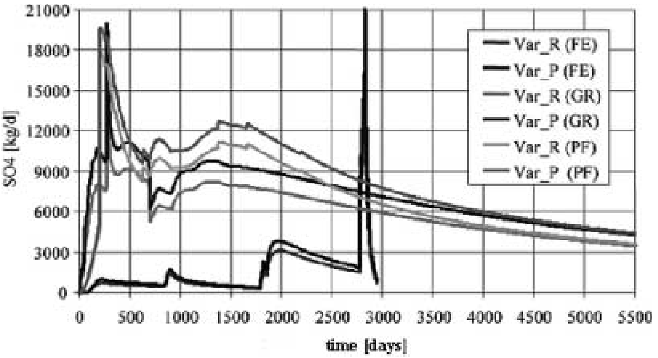

Fig. 11
Prediction and sensitivity analysis (*R* realistic; *P* pessimistic) of the sulphate concentration for the mine flooding compared with the flooding experiment (shifted in time)

Conclusions

The key elements of the conceptual model developed for the Koenigstein mine flooding are the (1) mine-flooding geochemical balance model (FLOODING II) that describe the source term (i.e. the interior of the mine) and (2) the downstream transport model that describes the spreading of the contaminants in the aquifers adjacent to the mine. Although the simulation capability of the mine-flooding geochemical balance model proved to be satisfactory, the modelling of the reactive transport of the contamination in the aquifer provided strikingly less conclusive results, in spite of using similar geochemical concepts.

We contribute the main reasons for the different reliability of the results to the key significance of data acquisition on a scale relevant to the size of the problem modelled. This was clearly confirmed by the good match of the model calculations with the source term development in the mine during the second phase of the experimental flooding. The calibration was done by matching the development of the first flooding experiment over a period of several years (57 months) to predict the second experimental flooding, which lasted 24 months. The prediction involved a spatial (volume-related) up-scaling of 1:5.

For prediction of the reactive transport in the aquifer over a period of hundreds of years and a distance of 1–5 km, the uncertainty of the calculated downstream contaminant concentrations ranged over four orders of magnitude. In this case, only laboratory data combined with site-specific field information could be employed, i.e. the data used were obtained on an inadequate scale. The uncertainty of the modelling results is likely to be caused by the spatial heterogeneity of the migrational field not reflected in the data base and the high sensitivity of the model to the content of trace minerals.

For the simulation of the overall mine flooding (development of the source term) it is recommended to keep modelling in pace with the observations made during flooding and progressively improve the simulation capability of the models. The time horizon of forward calculations should not exceed the duration of the preceeding observational phase. The limitation dictated by the duration of the previous observation period will keep the spatial scale-up (presently 1:14) within reasonable limits.

To follow this step-by-step approach to model predictions, it is unavoidable to monitor the flooding progress in the mine. With help of the data collected in the course of flooding, a continuous refinement of the modelling parameters and a periodic calibration of the model to the new scale is easily achievable. By forward feedback of progressively improving data base in the model it will become possible to flexibly respond to unexpected developments.

In this respect it is important to note that the observations during the flooding experiments showed that integral data collection provided more reliable indications of the flooding/release parameter changes than the differential measurements. This gives us the confidence that by using cumulative data collected in course of the flooding the reliability of long-term prediction assessments will further improve.

To base predictions on the monitoring of flooding rather than on the historical data from the mine de-watering is of significance because of the considerable hysteresis observed between flooding and de-watering during flooding experiments.

Because it is unattainable to collect all the data with the quality required for reactive multi-component transport modelling, it is preferable for the evaluation of the potential downstream contaminant migration to identify the geochemical interaction that dominates the modelled scale and to apply a conventional (non-reactive) mass transport model accompanied by a broadly based sensitivity analysis to test the limits of the simplification.

Finally, it must be reminded that the prediction of the flooding process and migration in the adjacent aquifer necessitates the compartmentalisation of the mine space, discretisation of the hydrogeological field and simplification of the time dependence of the acting processes, thus only approximating the modelled reality. For this reason, the simulation of future hydraulic and hydrochemical states will always bear an inherent risk of uncertain predictions caused already at the most elementary level of modelling. Nevertheless, the model predictions of the contaminant response to mine flooding are essential for a rational selection of the mine decommissioning measures to alleviate the risk of contamination of the hydrogeological environment in a densely populated area, such as exists at the Koenigstein site.

Acknowledgements The authors like to thank the contributions of D.W. Blows, E.O. Friend, K.U. Mayer, W.H. Molson and J.G. Bain, all from the University of Waterloo, for the reactive transport modelling. In conjunction with the Flooding code and the conceptual model we would like to acknowledge the work of Drs. Kalka and Muenze of UIT Dresden. Last, but not least, we like to acknowledge the work of our colleague Metschies of Wismut, who provided the hydrogeological input for the model predictions.

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