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Calibration of a 3-D groundwater model of the post-Permian sedimentary cover at the Morsleben radioactive waste repository site

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Abstract A geometrically complex three-dimensional (3-D) finite element model is used for the simulation of groundwater flow in the sedimentary soft and hard rock at the Morsleben site. The model is calibrated by an automatic technique based on hydraulic head information, and by including prior information on hydraulic conductivity. Analysing the modelling results leads to a successive refinement of the conceptual model in terms of the applied boundary conditions. The hydraulic conductivity distribution obtained is believed to be of improved reliability, and overall the model uncertainty appears to be reduced.

INTRODUCTION

The waste repository at Morsleben in the German district of Saxony-Anhalt is presently used for the storage of short-lived low-level radioactive waste. The repository has been in operation since 1981. Comprehensive safety-related assessments are underway, contributing to the licensing procedure aiming at the final closure of the disposal facility.

The repository is located in an old salt mine in an uplift salt structure underlying the southeast–northwest trending Allertal zone. The Allertal zone is 1.5–2 km wide and separates the Lappwald block in the southwest from the Triassic Weferlingen block in the northeast. The folded and faulted Zechstein salt sequence of the Allertal zone is covered by a residual caprock of variable thickness and predominantly flat lying sediments of Mesozoic and Quaternary age (Fig. 1).

A geological/hydrogeological model of the caprock and the sedimentary layers was developed to enable assessment of the relevance of the geosphere with regard to the long-term safety of the repository. The corresponding three-dimensional (3-D) finite element (FE) mesh is used for the numerical simulation of groundwater flow, initially under freshwater conditions, neglecting the influence of the variable groundwater density resulting from dissolved salt.

As a result of comprehensive *in situ* investigations (hydraulic testing and piezometric survey) the hydraulic parameters and the associated uncertainties of the various hydrogeological units are relatively well known.

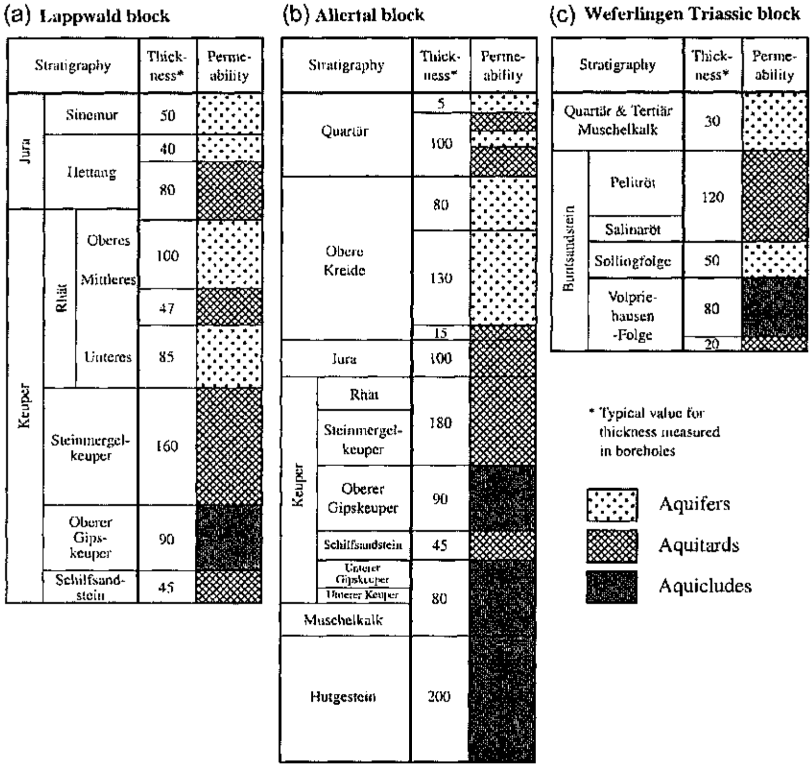

Fig. 1 Stratigraphic columns with major hydrostratigraphy of the post-Permian sedimentary cover at the Morsleben site: (a) Lappwald block, (b) Allertal zone, (c) Weferlingen Triassic block.

SELECTING THE INITIAL CONCEPTUAL MODEL

The 3-D groundwater model of the Morsleben site extends over an area of ~60 km^2 and covers the groundwater catchment area of the site (Fig. 2). It comprises all relevant stratigraphic layers (aquifers and aquitards) of the Lappwald block, Allertal zone, and Triassic Weferlingen block (Ehrminger *et al.*, 1998a). The numerical model as depicted in Fig. 4 consists of some 200 000 finite elements and 480 000 nodes, representing a total of 43 hydrogeological units. Steady state simulations of groundwater flow are performed with the numerical code CGM (Colenco Groundwater Model) (Genter & Schindler, 1996).

In a first preliminary conceptual model the elevation of the upper model boundary is defined by the groundwater table—represented by a manually constructed isoheadmap—derived from a large number of well observations. The prescribed hydraulic boundary condition along this surface is therefore of fixed head type. The lower impervious boundary is given by the base of the caprock (Allertal zone) and the transitions to the much less permeable hydrostratigraphic layers within the Lappwald and Weferlingen Triassic blocks, respectively. Vertical impervious model boundaries are defined to follow surficial groundwater water divides.

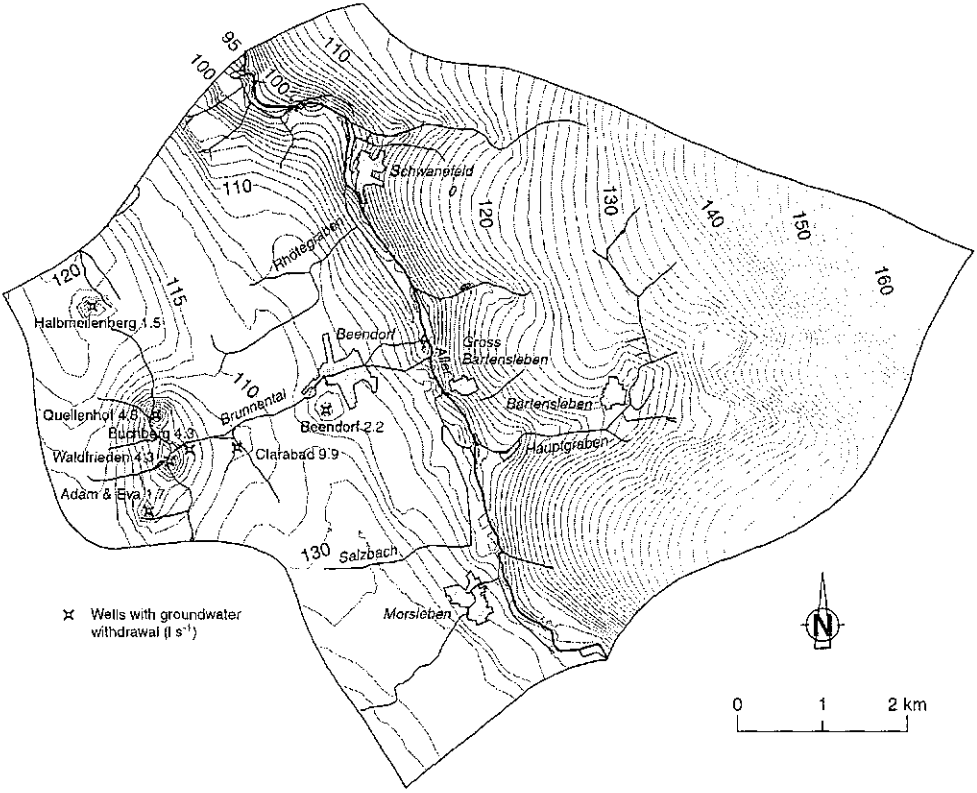

Fig. 2 Three-dimensional view of the groundwater model at the Morsleben site.

Model calculations based on the preliminary conceptual model described result in unrealistically high calculated areal discharge and recharge rates at the upper model boundary. This feature is prominent in areas where highly conductive hydrogeological units pinch out at the model surface, and controls the groundwater flow in a dominant aquifer (Rhaethian sandstone; in German: Rhät) of the Lappwald block. Therefore we conclude that the conceptual model chosen for defining prescribed hydraulic heads at the model surface does not result in a realistic model behaviour (Ehrminger *et al.*, 1998b).

REFINING THE CONCEPTUAL MODEL

A more realistic model behaviour, especially in shallow aquifers, has been achieved by modifying and refining the initial conceptual model along the upper model surface. The adopted modification is the transition from a pure Dirichlet boundary condition to a free surface boundary reflecting an unconfined aquifer system. Here, the transmissivity of shallow hydrostratigraphic units depends on computed groundwater heads. The resulting nonlinear system is solved iteratively.

Since the unsaturated zone is not considered in this concept, the surface elevation of the 3-D FE-mesh is modified according to the computed heads in each iteration.

With this approach the areal recharge by precipitation has to be specified as an additional flux boundary condition. This model parameter is derived independently by applying a separate soil water mass balance model to various soil types in the modelling domain.

Using the digital terrain model, groundwater discharge flux can be computed in those areas where the free groundwater surface equals the topography.

The numerical groundwater simulator CGM was modified in order to handle a deforming 3-D FE-mesh and to solve the numerical free surface problem iteratively.

DATABASE

The following hydrogeological data that may be used for calibration purposes are available in the project area:

- numerous water table observations from piezometers and head determinations from hydrotests,
- some measurements of the flow velocity and the flow direction carried out in piezometers,
- values of the hydraulic conductivity from hydrotests, probable *K* values and an uncertainty range for each hydrogeological unit,
- infiltration rates as evaluated with various methods and differentiated according to the range of physical conditions in the modelling area (vegetation, soil type, topography). Infiltration rates provided by the soil scientist have been evaluated by means of direct simulations. This led to the finding that in areas where aquitards pinch out, unrealistically high groundwater heads are computed, and in areas of groundwater withdrawal some wells become dry. Locally, infiltration rates were modified within their uncertainty to overcome these difficulties.

CALIBRATION CONCEPT

The objective of the calibration was to ascertain the validity of the permeability distribution in the complex model as provided by the hydrogeological testing and the derivation of mean values and uncertainty ranges for all hydrogeological units.

Because numerous measurements of head are available in the area of main interest (Allertal zone and Lappwald block), these values will be used for calibration. The other variables, which could affect head distribution, i.e. infiltration rate and lateral boundary conditions, will be kept constant during the calibration.

CALIBRATING THE NUMERICAL MODEL

The calibration procedure for the freshwater model is based on an inverse modelling approach and comprises the following steps: (a) sensitivity analysis for the calculated heads with respect to the hydraulic conductivities of all hydrogeological units within the model, (b) selection of the hydraulic conductivities to be optimized based on the sensitivity analysis, (c) definition of the objective function, and (d) iterative minimization of the objective function with respect to the selected parameters using the Simplex algorithm (Press *et al.*, 1992).

Within the optimization process a weighted least squares function is used to compare the calculated freshwater heads with the corresponding values of measured head. Because the numerical model neglects the variable groundwater density, a density weighting function is introduced in the objective function in order to weight the measured hydraulic head values according to the associated water density measurements. Moreover, the components constituting the objective function take into account the uncertainty intervals of individual head measurements and of hydraulic conductivity values to be estimated. The latter ensures that estimated parameters lie within their bounds. The objective function O is given by:

$$O = \sum_{i=1}^{n_H} w(d_i) F(H_i^s, H_i^m)$$

where n_H is the number of selected measured head values, d the fluid density corresponding to the measured head value, w the weighting function, F the weighted least squares component, H^s simulated head values and H^m measured head values. A total of 167 measured head values contribute to the objective function.

Based on sensitivity analyses, 39 hydraulic conductivity parameters have been chosen from a total of 43 to be considered for the model calibration. Starting from an initial value of 1.2×10^4 the objective function could be minimized to a value of 3.4×10^3 by performing a sequence of approximately 500 parameter estimation iterations before the inverse simulation was halted.

MODEL ERROR ANALYSIS AND FURTHER MODIFICATION OF THE CONCEPTUAL MODEL

A detailed analysis of the individual contributions to the objective function revealed the following pattern of spatial distribution of model errors. At the majority of the measurement locations in the modelling domain the model errors are rather small. The most substantial contribution to the objective function stems from a few measurement points which are clustered in the two Rhaethian sandstone aquifers in the southern part of the Lappwald block. Consistently, all of the simulated heads are lower than the measured counterparts.

While attempting to explain this feature, the initial conceptual model was re-evaluated. A hypothesis for refinement was formulated with respect to the influx along a lateral boundary in the Lappwald block. The hydrostratigraphic units within this tectonic block, including two Rhaethian sandstone aquifers, form a gentle north–south oriented synclinal structure with a northward plunging axis. As mentioned previously, the vertical model boundaries were designed to follow the surficial groundwater water divides, thereby cutting through the Rhaethian sandstone aquifers and allowing them to outcrop outside of the model domain. In retrospect we concluded that the adopted impervious vertical boundaries neglect and prevent a sizeable lateral groundwater inflow into the model.

Based on this hypothesis, the potential amount of lateral inflow via the Rhaethian sandstone was estimated independently in a few direct model simulations by changing the external boundary condition of the Rhaethian sandstone from impervious to a prescribed flux type boundary. A reasonable total inflow rate of 7.5 l s^{-1} was determined iteratively by comparing measured and simulated heads in the area of concern and by independently evaluating the total recharge flux on the outcrop of the Rhaethian sandstone.

After modifying the conceptual model as described above, a new inverse simulation was started. Optimized hydraulic conductivities obtained in the previous inverse run were re-used as initial parameters. The technique currently employed by us for inverse modelling is not capable of optimizing the values of a prescribed flux boundary condition. Therefore the groundwater inflow in the Rhaethian was kept constant and again only hydraulic conductivities were optimized. Because of the modified boundary condition, the inverse simulation was started with an objective function's value of 4.4×10^3. After more than 300 iterations the objective function had decreased even further to a value less than 3.1×10^3. The optimization was then halted due to ceasing parameter changes. This improvement of the objective function supports the plausibility of our hypothesis and justifies our conclusion of having generated a superior conceptual model.

RESULTS AND CONCLUSIONS

The permeability distribution which is the result of the automatic model calibration performed is shown in Fig. 3. The experiences and insights gained during the project

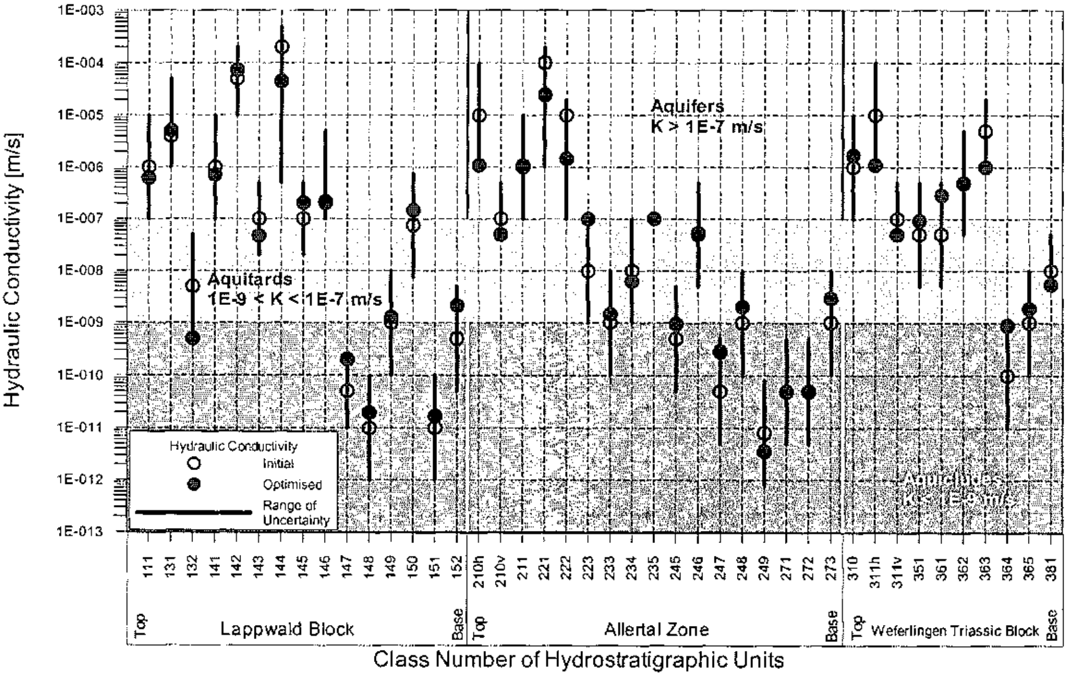

Fig. 3 Initial and optimized values of hydraulic conductivities and their associated range of uncertainty.

are summarized as follows:

- The calibrated values for the hydraulic conductivity of four units (out of 29) in the Lappwald block and the Allertal zone—the Weferlingen Triassic block is of less interest—reach the maxima or minima of the uncertainty ranges.
- The final conductivity values in the Lappwald block show two trends: those in the upper part of the block are generally somewhat reduced while those of the lower units are systematically increased, even if only to a small degree.
- The same tendency can be observed in the Allertal zone, where lower conductivities result in the layered Quaternary and in the Upper Cretaceous aquifers, whereas the conductivities of the lower (hard rock) aquifers are slightly increased.
- The values of the Weferlingen Triassic block are of less importance for the study; the few available observations of the water level do not warrant their representation and, therefore, their usefulness for calibration purposes.
- The final distribution of hydraulic conductivity is considered hydrogeologically plausible, i.e. the new values are compatible with the lithology.
- Substantial differences between measured and calculated head remain in particular in the area of the Lappwald block, but the final *K* distribution is considered to be more reliable than the initial one. Furthermore, the calibration process enhanced our knowledge and understanding of the hydrogeological system and in particular of the sensitivity of the boundary conditions in the Lappwald block.
- The resulting free groundwater surface (Fig. 4) is similar to the manually constructed map of the head isolines but contains significantly more detail than the latter; the geological structure of the underground and the influence of the topography (i.e. valleys) on shallow aquifers and aquitards is clearly visible.

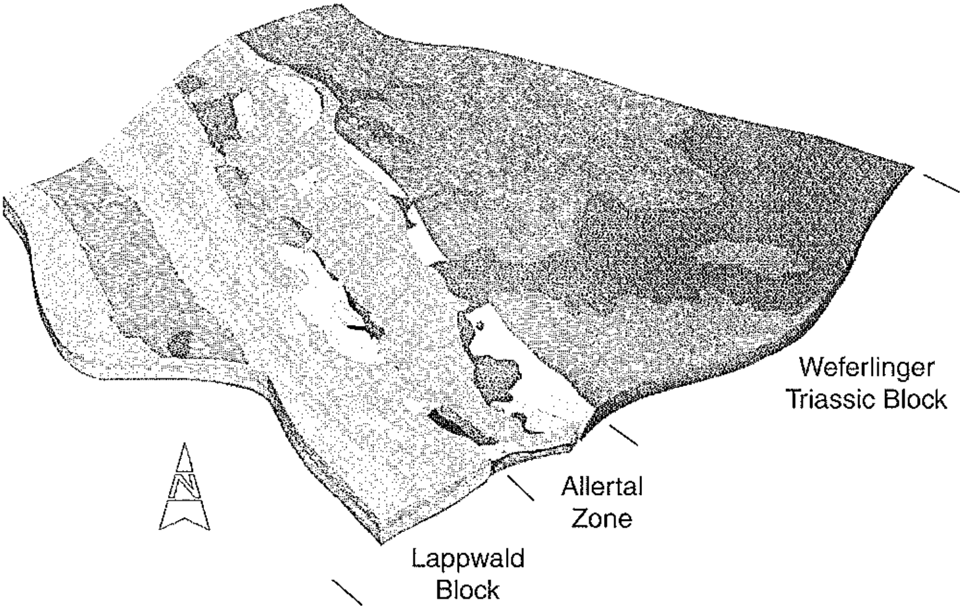

Fig. 4 Free groundwater surface, river network, pumping stations and location of modelled area.

- Due to a systematic trend in the potential distribution in the Lappwald block, water inflow over the lateral boundary of the Lappwald block has been incorporated in the second phase of the calibration process. As a result, a substantial further decrease of the objective function was achieved.

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