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Calibration of spatial aquitard distribution using hydraulic head changes and regularisation

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SUMMARY

Irregularly expressed aquitards have a significant impact on hydraulics and redox conditions. The method expands the scope and applicability of characterising spatial structures close to well fields. The test site is an aquifer system with two aquifers divided by an aquitard (glacial till), located at a well field for drinking water abstraction. During operation, the wells are frequently switched and hydraulic head data are recorded at 10 wells in both aquifers. The data contain information about the impact of each abstraction well on each observation well. We develop an inverse modelling procedure to calibrate spatial aquifer parameters from this data. Instead of heads we calibrate to selected head differences to keep the model concise to short term fluctuations and to reduce data. The calibrated model parameters are storativity of the upper aquifer, hydraulic conductivity of both aquifers and leakage of the aquitard. The calibration is carried out spatially by pilot points with the software PEST using regularisation. Different cross validations show that the leakage can be calibrated in a physically meaningful way, but not the hydraulic conductivities and not the storativity. Geostatistic assumptions are not required. The calibrated spatial aquitard distribution coincides with bore profiles and explains anomalies of redox conditions.

1. Introduction

Drinking water often is abstracted from aquifer systems consisting of more than one groundwater story with the aquitards between the stories usually having a strong impact on flow conditions. Though they may be spatially very close together, from conceptual geologic models the flow areas above and below the aquitard are often assumed to be hydrologically well divided. But the dividing layer may have windows where water can penetrate from one aquifer to another. Due to their limited area, streamlines concentrate in these windows, resulting in complex flow fields, which seriously affect the groundwater quality in the managed aquifer system due to the mixing of water from different layers. The detection and location of such aquitard windows however is not trivial. Boreholes only provide information valid for a few square centimeters. Even tiny layers can affect the flow field but the probability of finding it decreases with the drilling diameter, e.g. for production wells. Tracer tests are expensive, may take a long time and often are not allowed if drinking water is abstracted. Geophysical methods may be an alternative, however they also are expensive, and have restricted applicability.

In an earlier study Krabbenhoft and Anderson (1986) demonstrated that ambiguous field data indicate the presence of unexpected factors that may have a marked effect on a subsurface hydrologic system. They prefer the use of groundwater models to isolate the factors that account for an anomalous flow field distribution and related hydraulic gradients in the case of a groundwater/lake system. The importance of the geologic structure for understanding a complex aquifer system is demonstrated in the paper of Martin and Frind (1998), postulating that flow is not so much controlled by the hydraulic conductivity of the different geological units but by their continuity and interconnectivity, particularly in the vertical direction. Their results illustrate the importance of aquitard windows having a controlling influence on flow field distribution. The development of detailed three-dimensional capture zone models for the local well fields with calibration/validation against environmental tracer data was proposed as key techniques to improve the knowledge of the aquifer system. Timms (2001) investigated groundwater quality changes in an aquifer–aquitard system, where near-surface saline water is percolating into a deeper aquifer due to aquitard windows. Inverse mass balance models and an axisymmetric radial groundwater flow model are determined using FEFLOW (Diersch, 1998), furthermore hydrochemical changes were accounted for with PHREEQC (Parkhurst and Appelo, 1999). Machado et al. (2007) studied an aquifer–aquitard system in order to understand whether rainfall

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waters could percolate an upper limestone aquitard and contribute to groundwater storage in the underlying aquifer. In this study they used the groundwater model MODFLOW (Harbaugh et al., 2000) for regional flow modelling and PHREEQC for hydrogeochemical inversion for identifying the contribution of groundwater flow through the Santana aquitard (of unknown hydraulic conductivity) to Cariri Valley aquifers. In a study of Gedeon et al. (2007) regional groundwater flow in NE Belgium was simulated considering two principal types of groundwater circulation. The shallow groundwater circulation is controlled by surface hydrology features. These features influence the groundwater flow in the second aquifer down to a clayey aquitard. In the south of the area, the recharge from the overlying upper aquifer is facilitated by the absence of clay in a limited area, where it has been eroded after sedimentation.

In the present study we investigate groundwater flow in a bank filtration site at the eastern bank of Lake Tegel, Berlin, Germany (Fig. 1). Surface water infiltrates into the groundwater and is abstracted by a well field about 100 m from the lake. The site forms part of Berlin's largest waterworks, affecting an area of 50 km^2. The two existing aquifers are divided by an irregularly formed aquitard consisting of low permeable glacial till. Water infiltrates from the lake into the near surface aquifer. Abstraction wells in the second aquifer cause a downward gradient of hydraulic heads, leading to a downward water flow where the till is nonexistent. A transect of observation wells aligned parallel to the general flow direction provides data about the hydraulic and geochemical situation. But only a few boreholes exist which show whether the till is existent or not. The picture which they provide about the shape of the till is rough and strongly non-unique and does not fit to hydraulic and geochemical observations. However, a lot of hydraulic information is available. Short term hydraulics at the transect are affected by 7 abstraction wells and recorded by 10 observation wells. A method is developed which allows a spatial aquitard characterisation using operational data and hydraulic heads.

Rötting et al. (2006) carried out inversion of cross hole pumping tests to determine simultaneously aquifer parameters and the hydraulic connection to an adjacent river. We propose an alternative approach of characterising the aquifer properties by using operational data from well fields instead of data from defined tests. By recording the signal of multiple wells in multiple observation wells a large amount of data may be easily collected but the uncertainty has to be estimated because the interval of the recoded data is in the same time scale as the simulated processes. Since the initial water level is not in equilibrium and the geometry usually is complex, traditional pumping test evaluations are not applicable. Numerical simulation is necessary but calibration parameters are strongly cross correlated and simulation results have to be compared and calibrated to a large amount of data. Under these circumstances a thorough calibration cannot be performed manually and inverse modelling becomes necessary. The detection of spatial structures which are not known in advance requires a spatial discretisation with numerous parameters. The solution is often not unique and a subset of parameters turns out to be sensitive. The inverse modelling tool PEST (Doherty, 2004) is suitable to solve this problem by constraining a large amount of parameters using regularisation and offering the possibility of performing the inversion within a reasonable time using coarse grain parallel computing.

The probably most important contribution of this study is that subsurface structures are directly deduced from hydraulic data, i.e. the calibrated structure has a pronounced deterministic part that is demonstrated not to be affected by uncertainty. Except for a smoothing constraint, that effectively provides the lower spatial resolution, no assumptions about the aquifer structure are required.

Applied inverse methods demonstrate well matching of observation data and prove predictive capability with respect to observation data. We provide a more rigorous approach and demonstrate that the principal model results are not compromised by model or data inherent uncertainty. The method shows that the conductivity of the glacial till is unique with regard to different subsamples and also to aquifer hydraulic conductivity.

While prediction uncertainty is frequently estimated by resampling in surface water hydrology (Dingman, 2008), we have not found this applied to groundwater. Feyen and Caers (2006) applied resampling to synthetic data. We only found that uncertainty analyses for field data have been carried out by using the complete data set (e.g. Datta et al., 2009; Alcolea et al., 2009). Furthermore, the calibration results are prerequisite for a consistent geochemical

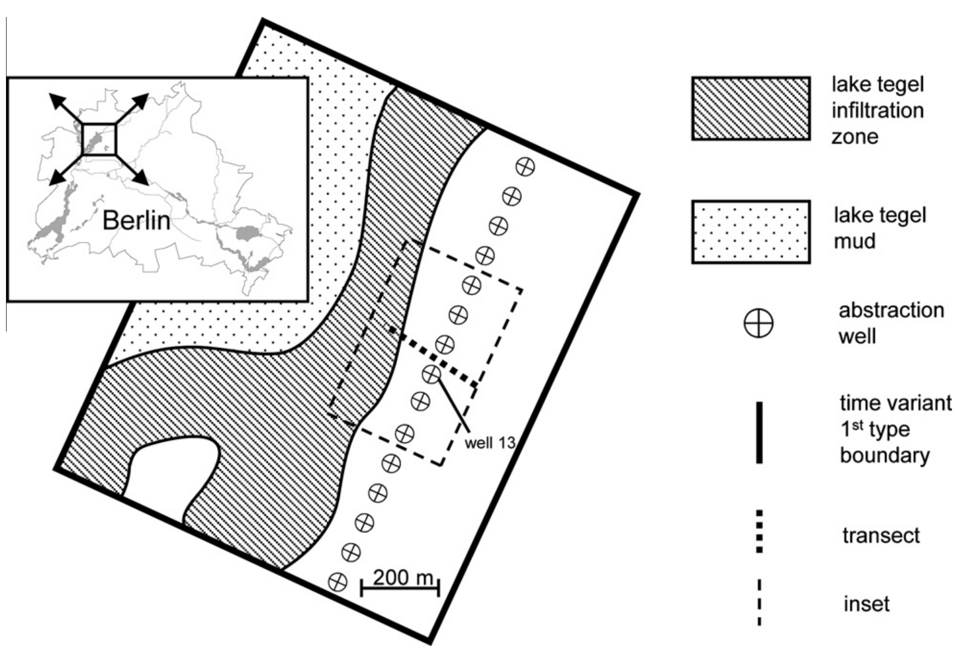

Fig. 1. Investigation area and model domain. Outer boundary conditions are extracted from a regional flow model (Wiese and Nützmann, 2009).