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Uncertainty reduction of hydrologic models using data from surface-based investigation

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SUMMARY

Geohydrologic model uncertainties include permeability, boundary, and initial conditions as well as the conceptual model it is based on. We present some examples of using information other than pressure data to constrain a geohydrologic model of the Horonobe area in Hokkaido, Japan. The initial model was constructed using information from surface geology and a few boreholes. Inversion analysis of pressure data implied the existence of a low-permeability cap rock. We then used river flow data and temperature data from a hot spring as a basis for estimating the recharge flux, which suggested that the overall permeability of the modeled area could be one order of magnitude larger than that of the base model. Next, we simulated a saltwater washout process and compared the simulated salinity distribution with the salinity data from a borehole. We found that a better match to the salinity data is obtained if the increase in permeability is taken up by a localized fault zone rather than uniformly by the entire model. A smaller-scale match to the temperature, pressure, and density profiles from two boreholes indicated that there was a low-permeability fault in between the two boreholes. The present study demonstrates that pressure data alone are insufficient to calibrate a model, and that additional observations are needed to accurately represent a site.

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1. Introduction

It is very difficult to characterize a large body of heterogeneous rock sufficiently, and to build a reliable groundwater flow model, particularly when the rock is fractured, which is most often the case. Available hydrological data are often limited and insufficient, both spatially and temporally. It is extremely challenging to scale-up detailed small-scale (tens of meters) measurements and to predict and verify large-scale (over several km) behavior. Unless there is an underlying known property that extends over scales, measurements conducted at a certain scale can only be used to describe the processes at the same scale. Some geostatistical tools may be used to predict the range of the model outcome. However, the more heterogeneous the rock is, the larger the uncertainty becomes.

Building a geohydrologic model of a large area involves many uncertainties from various sources, from the conceptual model to the input parameters. Model uncertainties include material parameters such as permeability and porosity. Often overlooked are boundary conditions and initial conditions. The most important element of a reliable model is the correct conceptual understanding of the geohydrologic processes within the area, which comes only after a long progression of model building, with much trial and error. Although model uncertainties originating from different modeling approaches have been addressed (e.g., Ijiri et al., 2009), uncertainty studies applied to actual field sites are limited. Most numerical models have implicit limitations that may lead to uncertainties that are inconspicuous and are seldom discussed. Many numerical models do not consider all the physical processes involved, which may or may not be necessary. A complete thermal, hydrological, mechanical, and chemical (THMC) simulation is very challenging and a subject of intense research at present. There are multiple reasons for this, including the difficulty in estimating the initial conditions and specifying the constitutive equations (such as the porosity–permeability relationship) that are applicable at a practical scale, in addition to the scarcity of relevant data such as the material properties and other *in situ* parameters.

The conditions at the outer boundaries of numerical models need to be specified all around, although they are usually impossible or impractical to measure. Therefore, they are often cho-

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sen for the convenience of modeling. The surface boundary conditions are often set to be a constant flux condition. Observations that can be made in the field are often severely limited in type, space, and time. One quantity that can be relatively easily observed is pressure, which can involve uncertainties of its own, such as gauge drift and borehole short-circuiting due to packer leak. To measure pressure at depth, we need to drill deep boreholes, which is very expensive. As a consequence, only a limited number of boreholes are drilled. Furthermore, the locations where boreholes can be drilled are often limited for reasons such as physical accessibility.

Ideally, tests should be designed to directly stress the system at the scale of interest, so that the observed response is the result of the averaging of the inherent properties up to that scale. However, this is difficult if the scale is over a kilometer or more. Moreover, in a very active tectonic environment like that of Japan, faults exist ubiquitously, which greatly affect the hydrology around their vicinity. Correct characterization of large faults is crucial in building a reliable geohydrologic model. Illman et al. (2009) successfully applied transient hydraulic tomography to large-scale ($\sim$1 km scale) cross-hole pumping tests to estimate the properties of fractured granite.

Large-scale groundwater flow models are typically calibrated to the steady-state pressure head data. An inversion scheme can be used to search for optimum parameters. However, we rarely have enough head data, and furthermore, head data alone are not sufficient for building a reliable model. Therefore, it is very important to utilize all available relevant data to constrain model uncertainties. In this paper, we show a progressive model improvement, in which information other than pressure data, such as temperature and salinity data, are used to constrain a hydrologic model to help reduce uncertainties in the conceptualization of a large heterogeneous rock formation, using the data from the Horonobe Underground Research Laboratory in Japan during the ground-surface-based initial investigation phase.

2. Horonobe site

The Japan Atomic Energy Agency (JAEA) is constructing an underground research laboratory (URL) in Horonobe Cho, Hokkaido (Fig. 1), to study physical and chemical processes deep underground and to develop technologies that may be applied to future geologic disposal of high-level radioactive waste elsewhere in Japan (Yamasaki et al., 2004; Ota et al., 2007). The formations of main interest, Koetoi and Wakkanai Formation are Neogene siliceous sedimentary rocks. Transecting the URL area is the Omagari Fault, an eastern dipping reverse fault with a left-lateral strike-slip component. Another fault of perhaps similar origin, the Nukanan Fault exists to the east of the Omagari Fault. A brief description of the lithology can be found in Table 1. At the Horonobe URL, 11 deep boreholes (HDB-1 to HDB-11) have been drilled, with depths ranging from 470 m to 1020 m (Fig. 2). After various investigations, loggings, and pressure tests were conducted, each borehole was isolated by packers into several intervals, and the pressure was monitored.

3. Geohydrologic model

Groundwater in the Horobobe area in general is expected to flow from the higher hills in the east to the Japan Sea in the west. Based on the information obtained from early boreholes, geologic, and geophysical surveys, Imai et al. (2002) constructed a hydrogeologic model of the Horonobe area with updated fault geometry. They concluded that there are large uncertainties with the permeability and the recharge rate and showed that the salinity data may be useful to constrain a model. The original mesh of Imai et al.'s model was in a finite element model (FEM) format, which was converted to that of integrated finite difference (IFDM) for simulations using TOUGH2 (Pruess et al., 1999). Fig. 3 shows the geohydrological model used for the simulations. The total number of elements is 7,8000 with varying sizes from 50 m to 500 m that are classified into 11 material types. Based on borehole tests and core analyses the groundwater flow is thought to be mainly through fractures. We assume that an equivalent continuum can be used to represent the large-scale groundwater flow in the area. Heads observed in the boreholes show an increase with depth (Kurikami et al., 2008a,b), which can be caused by several sources, including the topography, geostatic load or gas generation. As shown in Fig. 2, most boreholes are in the proximity of the Omagari Fault. The initial version of the Imai et al. model shown in Fig. 3 failed to reproduce the observed head data: particularly the high heads observed in the Koetoi formation as shown in Fig. 4.

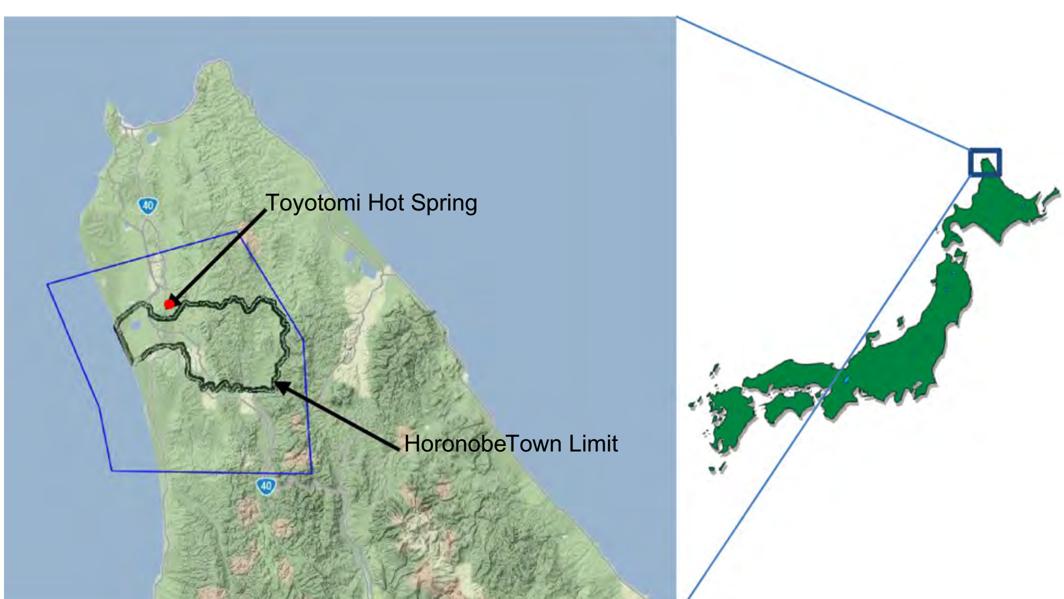

Fig. 1. Location of Horonobe Town in Hokkaido, Japan. Also shown is Toyotomi Hot Spring. The blue polygon denotes the model footprint shown in Fig. 3. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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Table 1
Permeability values of the base case.

Geological period	Epoch	Model units	Lithology	Hydraulic conductivity (m/s)
		Surface		2.0E−06
Quaternery		Quaternery sediments		1.0E−06
Neogene	Pliocene	Yuuchi F.	Fine to medium grained sandstone	1.0E−07
	Miocene	Low permeability zone		6.3E−11
		Koetoi F.	Diatomaceous mudstone	1.0E−09
		Wakkanai F.	Hard shale	1.0E−10
		Masuhoro F.	Alternating beds of conglomerate, sandstone, and mudstone	5.0E−10
Cretaceous		Cretaceous rock		1.0E−11
Faults		Oomagari fault core		1.0E−10
		Nukanan fault core		1.0E−10

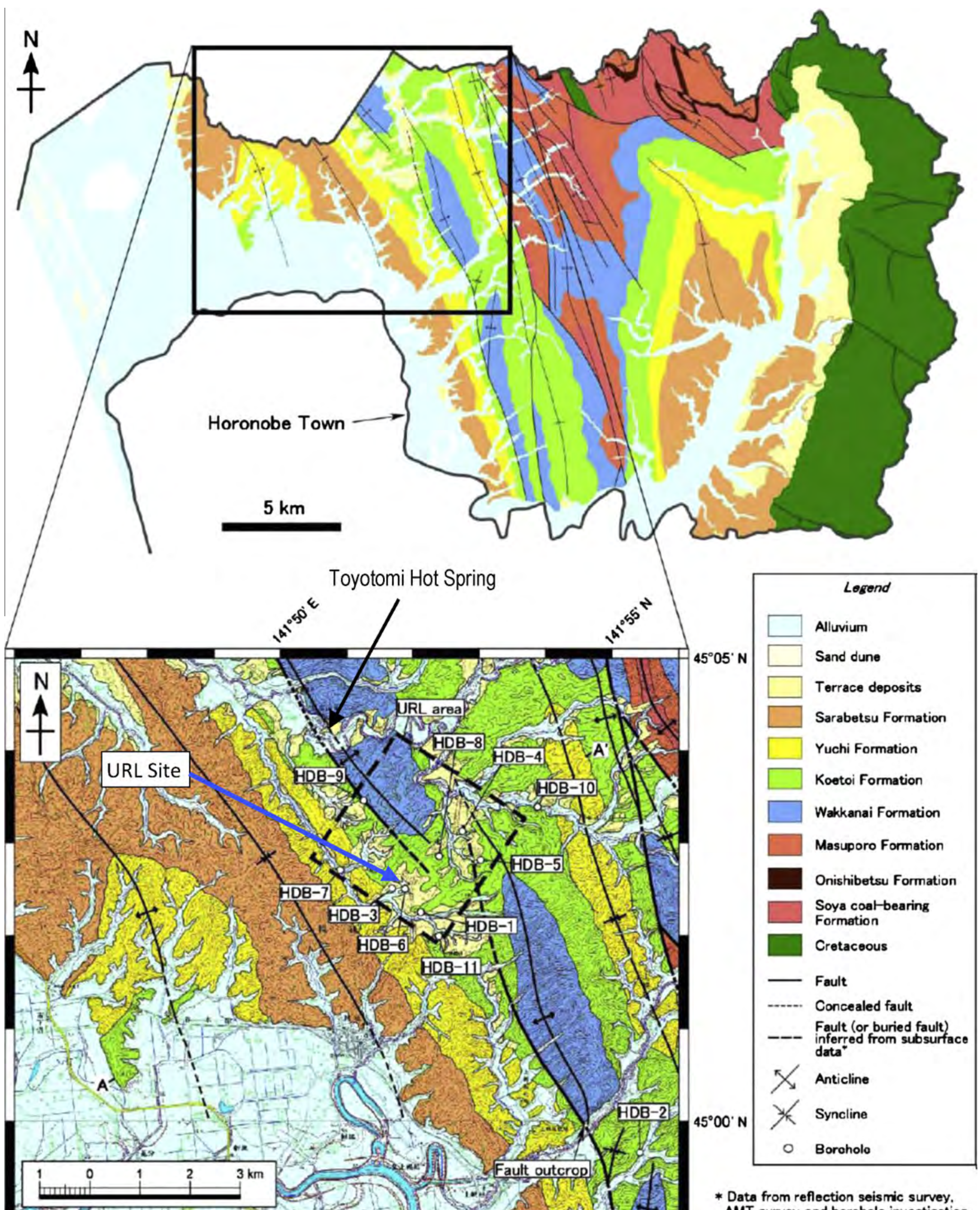

Fig. 2. Horonobe Town (top) and the URL study area (below, broken square) showing the borehole locations and the geology. Also shown are the location of Toyotomi Hot Spring and the URL site (modified from Ota et al., 2007).

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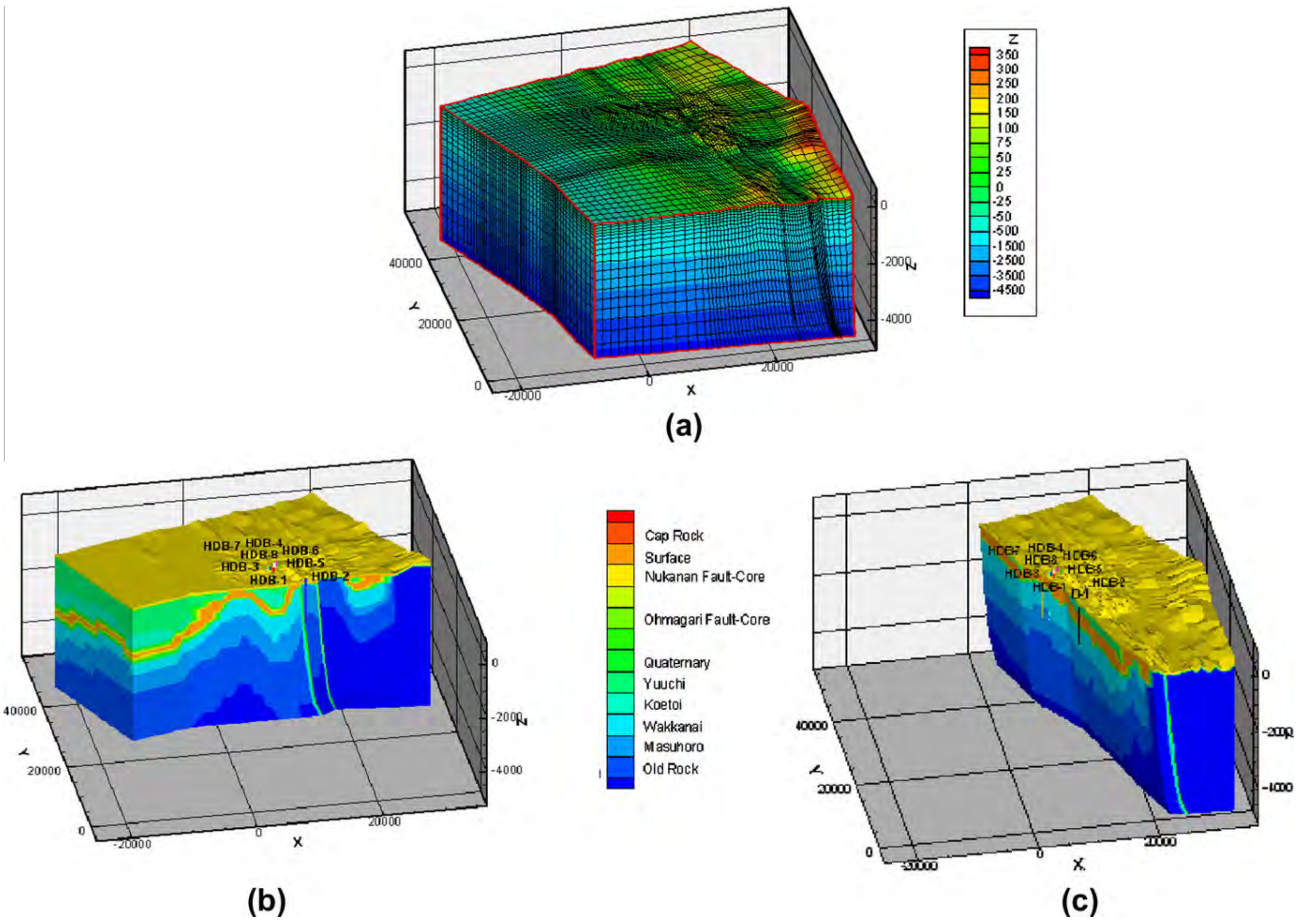

Fig. 3. (a) The numerical grid, (b) E–W and (c) N–S cross section of the geohydrological model of the Horonobe area showing the borehole locations, surface elevation (a), and geological formations (b and c). The model is 40 km × 40 km × 5 km centered on the Horonobe URL area shown in Fig. 2.

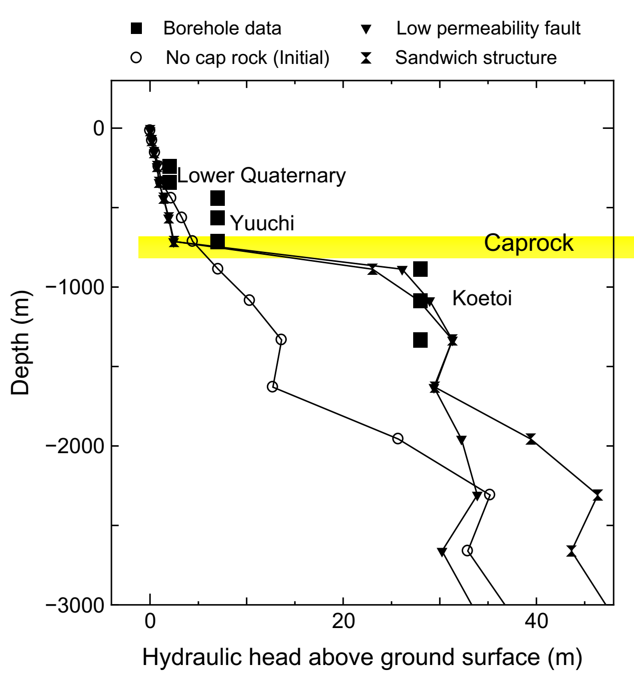

Fig. 4. Head inversion results for two different structures of fault.

3.1. Static head inversion

Ito et al. (2004) attempted to assess whether the topography and permeability structure shown in Fig. 3 alone can explain the high heads at depth, by changing the input permeabilities. To match model predictions to observed data, modelers often employ a trial and error approach, in which forward model runs are repeated numerous times by adjusting input parameters. This approach is often useful, because it gives the modeler insights into which parameters are more important relative to one another. However, it is often very tedious and difficult to conduct in a systematic manner. Ito et al. (2004) used iTOUGH2 (Finsterle and Najita, 1998; Finsterle, 2008), which solves the inverse problem by automatically calibrating a TOUGH2 model against observed data. They inverted for the log-permeabilities of the main layers including Yuchi and Wakkanai Formations as wells those of the faults. They did not invert for the boundary conditions nor the initial conditions, although these are admittedly huge and important unknowns.

Ito et al. (2004) showed that the high heads at depth can be explained by assigning a low-permeability to the model material denoted caprock in Fig. 3. They also examined the influence of fault zone properties on the observed data. In one model, the faults are assumed to have a sandwich structure, with a low-permeability core and high-permeability damaged zones on both sides. In another model, the fault was assumed to be a simple low-permeability structure (base case). The head at depth greater than

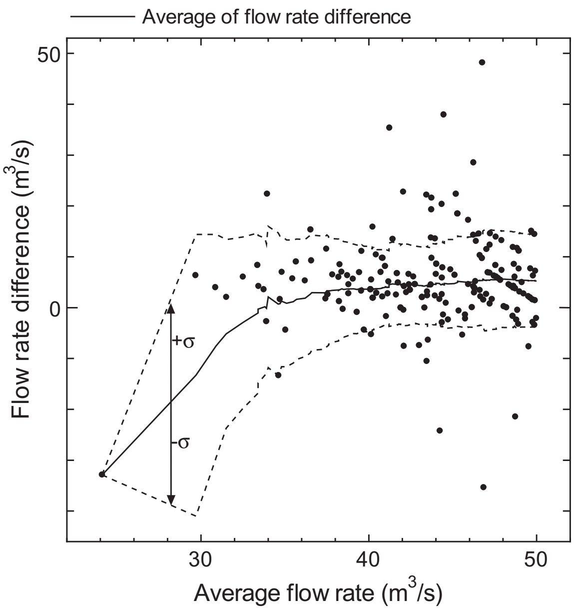

Fig. 5. Flow-rate difference between two points of the Teshio River. Broken lines indicate one standard deviation.

1700 m diverged between the two fault models (Fig. 4). Because there were no data available from these depths, the results were inconclusive regarding the structure of the fault. Table 1 shows the calibrated values of permeabilities, which we call the base case.

3.2. Use of river flow data

One of the important but very difficult parameters to estimate for a geohydrologic model is the surface boundary condition. This is especially true when the model area is very large, i.e., several tens of square kilometers. One approach is to use river flow data, if there is a river that runs across the area of interest, preferably forming a well-defined basin that covers the study area. Ito et al. (2004) used the data from the Teshio River, which flows from east to west within the modeled area, to estimate the recharge rate, by taking the difference of the average monthly flow rate between two measurement locations that are approximately at the east and west end of the area. Fig. 5 shows the calculated difference between the two locations for flow rates less than 50 m^3/s, which is assumed to be the maximum base flow rate. Based on the figure, the flow-rate difference is approximately 5 m^3/s, considered to be closely related to the recharge rate in the area. However, note that the variance is very large; thus, it should only be considered as approximate. The 5 m^3/s recharge rate for the area translates to roughly 80 mm/year of recharge for the entire area. Using data from much smaller sub-basins in the area, Kurikami et al. (2008a,b) found the estimated recharge rate to vary from 64 mm/year to 283 mm/year from sub-basin to sub-basin, or approximately from 5% to 20% of the annual average rainfall of 1400 mm/year.

The model calibrated to the measured heads described in the previous section calculates only 8 mm/year of recharge. Calibration to head values alone is only sensitive to the relative contrast (ratio) of the permeability of each layer and not to the absolute values of permeability. Therefore, permeability values can be multiplied by a constant value for all layers and still maintain the same goodness of fit for the steady-state head analysis. Because the model calibrated only to the measured heads severely underpredicts recharge in the area, it is possible that the absolute permeabilities of the layers are too low, although their ratios may be approximately correct. To improve the base case, we would be justified increasing the permeability by a factor of 10.

3.3. Hot spring data

Adjacent to the north of Horonobe Town is Toyotomi Onsen, a hot spring (see Fig. 2). Hot spring water has been produced since the 1920s from a depth of ~800 to 900 m. The water temperature is reportedly around 42 °C (Toyotomi Onsen, 2009). We use TOUGH2 with the EOS3 module to simulate coupled heat and fluid flow using the 3D grid shown in Fig. 3. The bottom boundary condition is set at a constant heat flux of 20 mW/m^2 with no fluid flow. The heat flux value is based on Tanaka et al. (2004). The top boundary condition is set at atmospheric pressure with 10 °C, the annual average temperature of the area.

Fig. 6 shows a comparison of the steady-state temperature profiles when the permeability of each layer in the model is multiplied by a constant value. Also shown in the figure is the approximate depth and temperature of the hot-water production zone for the hot spring (double-headed arrow). As can be seen from the figure, the case with ten to twenty times the permeability of the base-case model matches the temperature of the production zone best. The 3D temperature distribution in the model is generally monotonic (not shown) except near the surface with small scale irregularities reflecting the effects of the topography controlled recharge and the sea. It might be added that the hot spring was discovered during a natural gas exploration, not due to hydrothermal expressions near the surface.

3.4. Use of salinity data

The salinity distribution in groundwater may yield some clues as to how the groundwater has evolved. High-salinity water is encountered at depths in HDB boreholes, whereas near-surface water is fresh. It is believed that the study area was once under

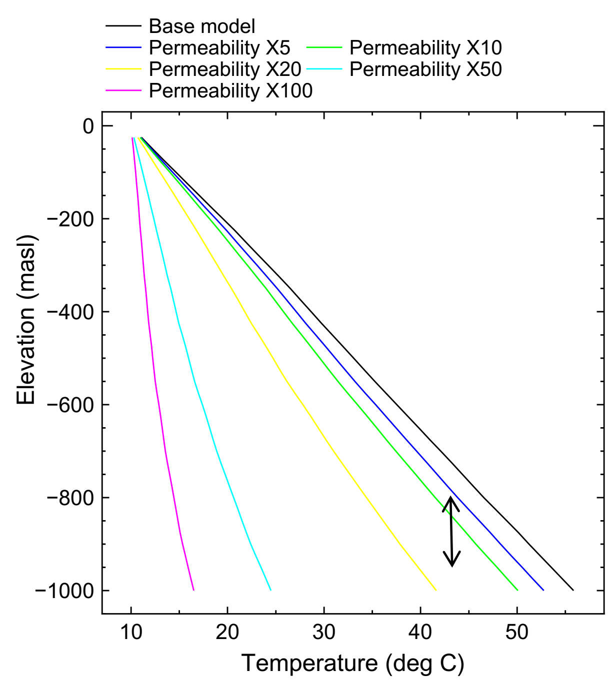

Fig. 6. Modeled temperature profile at Toyotomi Hot Spring for various permeability multipliers. The arrow indicates approximate temperature and depth of the source of Toyotomi Hot Spring.

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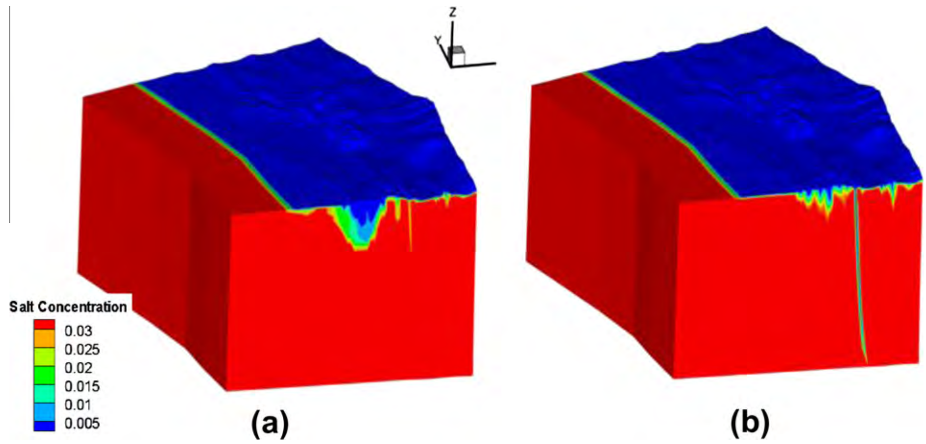

Fig. 7. Salt concentration distribution after 2.5 Ma for the cases: (a) 10 times the base case permeability, and (b) high-permeability fault. Fresh water intrudes deeply along the faults.

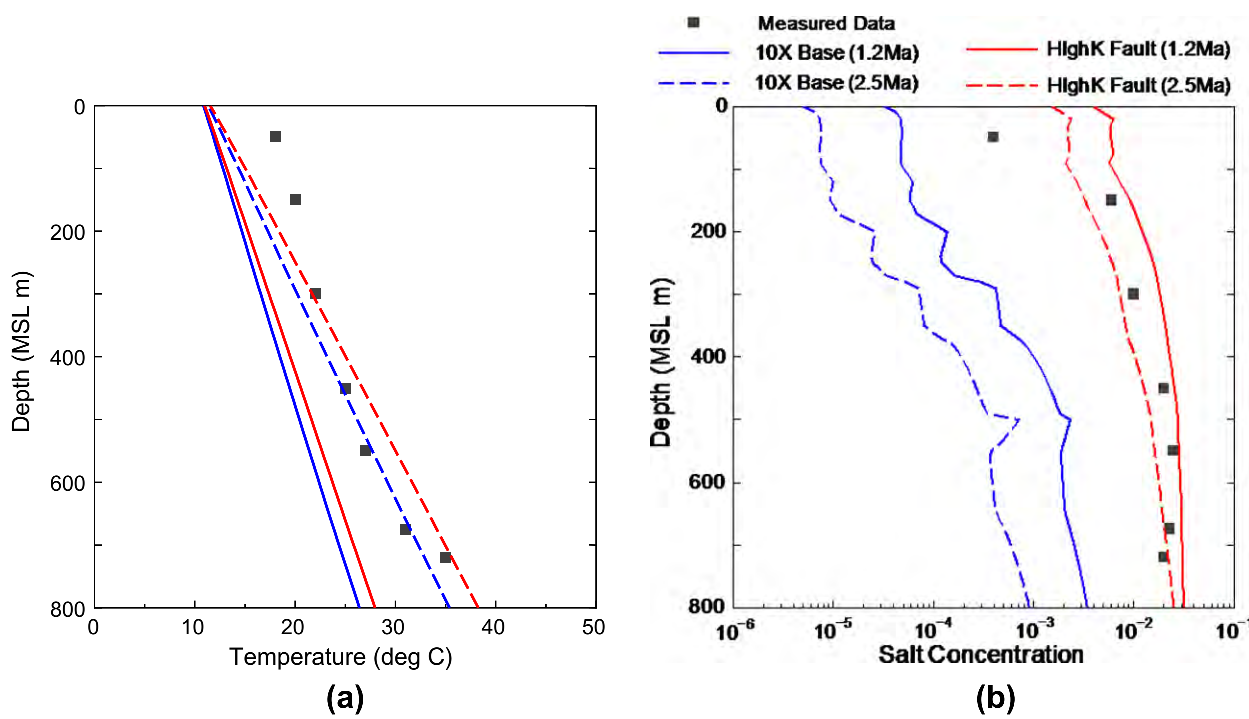

Fig. 8. Saltwater washout simulation results. Markers denote measured data along HDB-1. Blue colored lines are for the case with 10 times the base permeability. Red lines are for the high-permeability-fault case. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the sea before it rose to its present state. The land mass was initially saturated with saltwater, but as a result of rainfall, which recharges fresh water into the ground, the saltwater has been gradually washed out, particularly near the surface. We model the saltwater washout process by using TOUGH2 with the EOS7 module to simulate nonisothermal, density-driven, single-phase flow. As the initial condition for the salt concentration, we assume that the entire model is saturated with seawater (3.2% salt concentration). The boundary conditions are much the same as in the previous study for static head inversion. By setting the top boundary condition at atmospheric pressure, recharge of fresh water takes place from the surface, with the strength and pattern of recharge a function of permeability and topography.

Fig. 7 shows the simulation results after 2.5 Ma: (a) the case with 10 times larger permeability than the base case, and (b) the case in which the permeability of the fault zone is 100 times larger than the base case, while the rest of the permeabilities are kept the same as the base case. Note that the study area is thought to have been uplifted above sea level approximately 13–1 Ma. (Iwatsuki et al., 2009). The latter case still allows a similar amount of total recharge ($\sim$50 mm/year), but the flow is localized to the fault zone. The high-permeability fault model is consistent with the finding by Ishii et al. (2006), who suggested deep intrusions of fresh water along the Omagari Fault based on the AMT (audio-frequency magnetotelluric) surveys. Fig. 8 shows a comparison of the salt concentration and the temperature data from HDB-1 with the simulation results, whose initial condition for the temperature is set as uniform at the surface temperature and the uniform sea water salt concentration. It should be noted that the data were collected shortly after the drilling and may not reflect true *in situ* conditions. The model with 10 times larger permeability than the base case matches reasonably well with the temperature data after 2.5 Ma,

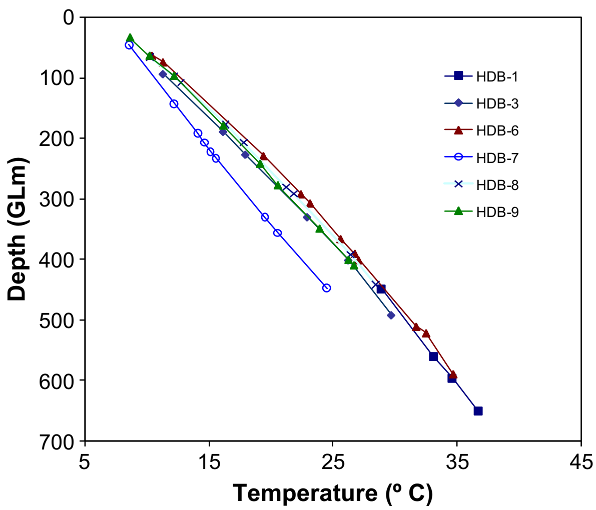

Fig. 9. Temperature profile along HDB boreholes. The blue line is the temperature profile along HDB-7. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

but does poorly against the salt concentration data. The permeability appears to be too large, and the freshwater washes out the salt too quickly. The high-permeability-fault case matches reasonably well with the temperature and salt concentration data. Now we have a model that can explain the pressure, temperature and the salt concentration distribution as well as the geophysical data. In addition, the high-permeability fault zone model heuristically explains the sustained operation of the hot spring. In the next section we will examine the fault zone properties at a smaller scale.

4. Fault zone characterization

Geothermal gradients or temperature profiles are very sensitive to, and thus useful in, estimating water percolation fluxes in the subsurface (e.g., Wu et al., 2004, 2007). In particular, temperature profiles near a fault are often used to assess fault properties (Fairley and Hinds, 2004a,b; Heffner and Fairley, 2006; Doan and Cornet, 2007). Wu and Karasaki (2009) used the measured temperature data to estimate both flow rate and flow directions in two HDB boreholes at Horonobe (Fig. 1). It is suspected that a fault or a set of faults exist at the Horonobe site, one of which is the Omagari Fault as shown in Fig. 3. The HDB boreholes at the site are packed off into several monitoring intervals using packers. Pressure and temperature are monitored in each interval. Fig. 9 shows the temperature profiles along the HDB boreholes. As the figure shows, the temperature profile along HDB-7 is different from that of other boreholes—slightly concave upward, generally indicating colder groundwater flowing downward. The other profiles are all concave downward, indicating that warm groundwater may be flowing upward. Wu and Karasaki (2009) used the TOUGH2 code with the modified EOS3 module to simulate nonisothermal flow of single-phase water with density dependence on mineral compositions, in addition to pressure and temperature in the two wells, HDB-7 and HDB-8. For each layer, the most recent permeability value based on borehole tests was used. The basic assumption was that the system is at vertically steady-state conditions for water flow, solute transport, and heat flow. Aqueous mineral concentration distribution was assumed at steady state as a function of depth only for each well. Therefore, the water density is correlated to mineral compositions by extrapolating and interpolating the measured mineral compositional data from the two wells, in addition to its dependence to pressure and temperature. Independent simulation was conducted for each well, which implies a horizontal variability. The water density is correlated to mineral compositions by extrapolating and interpolating the measured mineral compositional data from the two wells including Na^+, Ca^{2+}. Cl^-, SO_4^{2-} and others, and its dependence on pressure and temperature. Fig. 10 shows the simulated temperature profile. A downward flow of 3 mm/year matches the HDB-7 data, and an upward flow of 6 mm/year matches HDB-8 data. Note that the two wells, HDB-7 and HDB-8, are close to each other, with HDB-8 further inland. Head values in HDB-8 are ~10 m higher than those in HDB-7. Fig. 11 shows the simulated pressure profile. The 6 mm/year simulation matches the pressure profile in HDB-8 (Fig. 11a) very well while it over-predicts the data in HDB-7 at 3 mm/year (Fig. 11b). Comparing the simulation results with the data indicates different flow directions, i.e., flow at HDB-8 is upwards (discharge) and flow at HDB-7 is downwards (recharge). This finding indicates a fault is likely separating the two boreholes, with the fault behaving as a closed boundary or low-permeability barrier to flow across it. It is conceived that the water flowing upward passes over the fault through the weathered bedrock, and perhaps through the alluvium as well, eventually flow downward on the

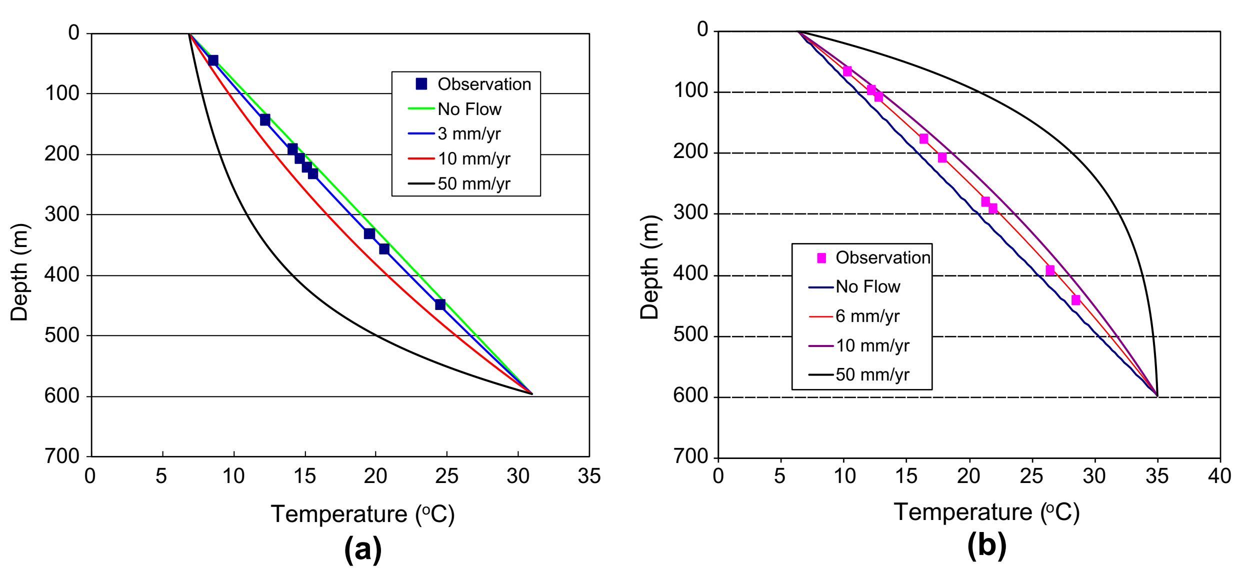

Fig. 10. Simulated and observed temperature profile along: (a) HDB-7 and (b) HDB-8 for various (a) downward and (b) upward flow rates.

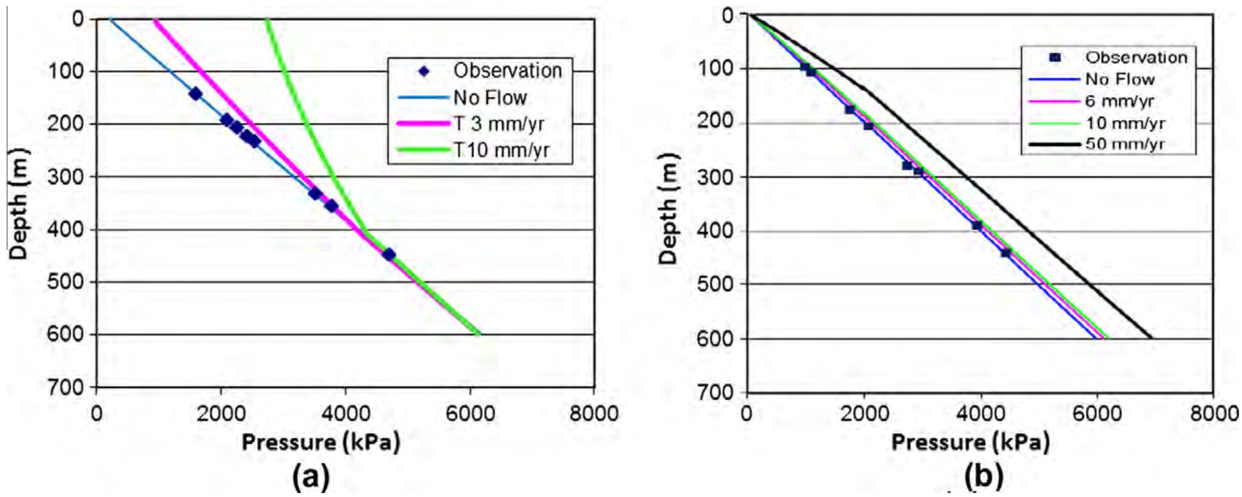

Fig. 11. Simulated and observed pressure profile along (a) HDB-7 and (b) HDB-8 for various (a) downward and (b) upward flow rates.

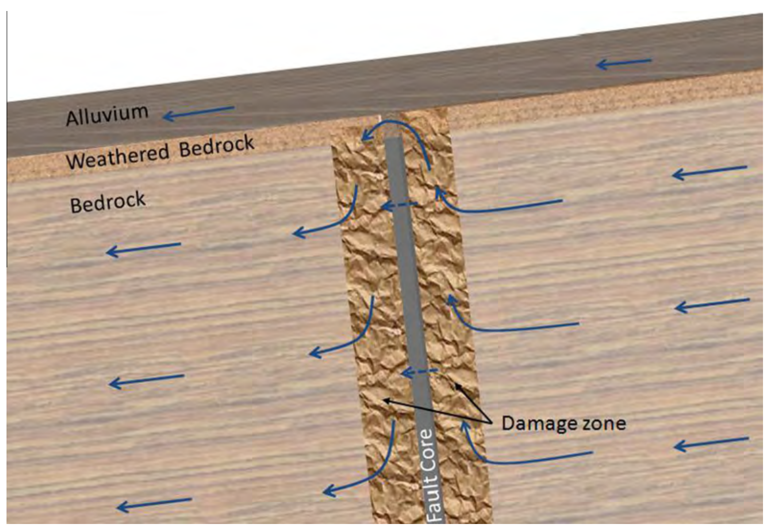

Fig. 12. Conceptual model of fault zone flow.

Table 2
Summary of geohydrologic model evolution.

Section no.	Data used (additional)	Processes modeled	Module used	Findings
3.1	Hydraulic head	Groundwater flow	EOS9, iTOUGH	Low permeability layer
3.2	River flow rate	Groundwater flow	EOS3	Larger recharge rate
3.3	Hot spring data	Groundwater and heat flow		10 × larger overall permeability
3.4	Fluid salinity, temperature profiles	Groundwater, brine, and heat flow	EOS7	Localized fault zone permeability
4	Pressure, temperature, salinity profiles	Groundwater flow, heat, mineral composition	Modified EOS3	Flow direction and flux in fault zone

other side of the fault, while a small amount of water may permeate directly through the fault. Fig. 12 shows a conceptual model of groundwater flow crossing a fault zone. A similar model was proposed by Bense and Kooi (2004) for Peel Boundary Fault in The Netherlands. The Fig. 12 model most likely applies to the Omagari Fault zone: upward flow along the damage zone east of the fault (HDB-8) and downward flow along the damage zone to the west (HDB-7)—and overall higher head in HDB-8 than in HDB-7.

5. Summary and discussion

In this paper, we presented (through some examples) the use of information other than pressure data to constrain a geohydrologic model. The initial model was constructed using information on surface geology and from a limited number of boreholes. The inversion analysis of pressure implied the existence of a low-permeability cap rock. We then used river flow data and temperature data from a hot spring for estimating the recharge rate. The estimated recharge rate was 10 times larger than the original model had calculated, which suggested that the overall permeability of the model may be one order of magnitude larger than that of the base model. Next, we simulated the saltwater washout process and compared it with salinity data from a borehole. We found that a better match to the salinity data is obtained if the increase in permeability were taken up by the fault zone rather than assigning larger permeability uniformly to the entire model. At a smaller scale, we conducted a 1D simulation and matched the temperature, pressure, and density profiles from two boreholes. We found that there may be a low-permeability fault in between the two boreholes. A conceptual flow model across a fault is proposed. Table 2 summarizes the model evolution.

Inclusion of additional processes in a geohydrologic model, such as heat and salt transport, requires additional parameters and may actually increase uncertainty. For example, heat-conductivity and heat-flux data are needed, in addition to the usual hydrologic parameters. Although the initial saltwater distribution is unknown, the model assumes that the rise and formation of the present-day Hokkaido Island happened instantaneously. However, when a model successfully matches temperature and salinity data in addition to pressure data, the model may be deemed more reliable than a model constructed by simply extrapolating or upscaling small-scale observations. This is because pressure, temperature, and salinity data reflect the results of the natural averaging process that takes place at a large-scale and over a long time duration. Thus, we believe that we now have more enhanced understanding of the large-scale geohydrologic processes at the Horonobe Site.

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