Electronic Supplementary Material – Hydrogeology Journal

Mapping fracture flow paths with a nanoscale zero-valent iron tracer test and a flowmeter test

Po-Yu Chuang¹, Yeeping Chia¹*, Yung-Chia Chiu², Mao-Hua Teng¹ and Sofia Ya Hsuan Liou¹

¹ Department of Geosciences, National Taiwan University, No. 1, Sec. 4, Roosevelt Rd., Taipei 106, Taiwan
² Institute of Applied Geosciences, National Taiwan Ocean University, No. 2, Beining Rd., Keelung 202, Taiwan
* Corresponding author: Yeeping Chia

Phone: + 886 (2) 33665873, e-mail: ypc@ntu.edu.tw

This document provides detailed information of preliminary field tests, including hydraulic tests and heat-pulse flowmeter tests, the spatial discretization and boundary conditions of the groundwater flow and solute transport model, and uncertainty and sensitivity analysis.

1. Preliminary Field Tests

1.1 Hydraulic Tests

Hydraulic tests are commonly implemented to estimate the transmissivity of an aquifer (Tiedeman and Hsieh 2001) and can be further applied to investigate the cross-hole hydraulic connectivity in fractured rock (Chuang et al. 2016). In this study, three hydraulic tests were conducted at two experimental wells, W4 and W6. First, W4 was pumped at a constant rate of 101 ml/s for about 45.4 minutes, and then stopped. The maximum drawdown of W4 was 5.15 m (Fig. S1a). In response, the water level of W6 dropped to 3.56 m at approximately 46 minutes and then recovered quickly after the
pumping ceased. The maximum drawdown at both wells occurred within 1 minute of each other, implying hydraulic connectivity between the two. To confirm the cross-hole hydraulic connectivity, a second hydraulic test was carried out. Pumping was conducted at a constant rate of 109 ml/s in W6 for about 49 minutes. The maximum drawdown at W6 was 4.41 m (Fig. S1b). The water level at well W4 declined up to 3.7 m in 50 minutes. This test further demonstrated the hydraulic connectivity between wells W4 and W6.

In addition, hydraulic test data were used to estimate the transmissivity of rock formation in the open hole or screen section of the well. As the well pipe storage might affect the drawdown during hydraulic tests, the drawdown data were analyzed by the Cooper-Jacob approximation that includes pumping well pipe storage effects (Cooper and Jacob 1946; Chapuis 1992). The estimated transmissivity of the rock formation in the 23.5-m screened section in W4 and open hole of W6 are $5.33 \times 10^{-6}$ and $6.08 \times 10^{-6}$ m$^2$/s, respectively.

Before the tracer tests, a 2.8-cm diameter tube screened at the depth between 31 and 32.5 m was inserted. After sealing with bentonite, a third hydraulic test was performed to re-examine the hydraulic connectivity between wells W4 and W6. W4 was used as the pumping well. Pumping was conducted at a constant rate of 27 ml/s for about 104 minutes and then stopped. The water level dropped 0.73 m in W6 after pumping for approximately 104 minutes (Fig. S1c). The water level recovery curve of W6 overlapped that from pumping well W4 after 105 minutes, indicating a hydraulic connection between W4 and W6 through the 1.5-m screened section in W6.
Fig. S1 Results of three cross-hole hydraulic tests. a Drawdown of groundwater level at W6 in response to pumping at W4. b Drawdown of groundwater level at W4 in response to pumping at W6. c Drawdown of groundwater level at screened W6 in response to pumping at W4.

1.2 Heat-Pulse Flowmeter Measurements

A heat-pulse flowmeter can be used to measure the flow velocity in the borehole. By integrating the velocities measured at various depths by the flowmeter and the transmissivity estimated by the hydraulic test, one can establish the vertical profile of horizontal transmissivity in the borehole (Molz et al. 1989; Day-Lewis et al. 2011; Lee et al. 2012). The heat-pulse flowmeter adopted in this study is manufactured by the Robertson Geologging Ltd. Flowmeter tests were firstly conducted at various positions without pumping for the measurement of ambient flow in the well. A repeated stationary measurement approach was applied at an interval of 100 cm along the two wells respectively. Because the ambient flow could not be detected in wells W4 and
W6, the vertical hydraulic gradients in the well were very small and could be ignored. Subsequently, W4 was pumped at a constant rate of 37 ml/s at the depth of 20 m to induce an upward flow in the testing well. After drawdown reached a steady-state, flowmeter measurements were undertaken between depths of 21.5 and 44.5 m in W4. The measurement interval ranged from 25 to 100 cm, depending on the change in measured flow velocity. Because errors can arise due to free convection and the shape factor associated with the irregular flow-through cell of the heat-pulse flowmeter, an empirical formula was used to correct the measurements (Lee et al. 2012). The corrected flowmeter data were subsequently analyzed using the FLASH program (Day-Lewis et al. 2011). The transmissivity obtained from the hydraulic tests and the corrected flow velocities in the borehole were used to calculate the transmissivity in each 25-cm section of the borehole. The vertical profile of section transmissivity varied with depth (Fig. S2). Two permeable zones were delineated in well W4. One was located between depths of 23.5 and 24 m, where 48.4 % of borehole flow issued; the other was between depths of 28 and 29 m, where 33.6 % of flow occurred.

In well W6, flowmeter measurements were implemented at a pumping rate of 30.5 ml/s in the open-hole section from 21.75 to 34 m in depth. Three identified permeable zones were located at depths of 24–25, 29.5–29.75 and 33–33.5 m in W6 (Fig. S3). The most permeable fracture, as indicated by the highest section transmissivity, is expected to locate at the permeable zone between depths of 33–33.5 m.
**Fig. S2** Vertical distribution of well screen positions, borehole flow rate and section transmissivity from flowmeter measurements at W4. Each section is 25-cm thick.
Fig. S3 Vertical distribution of well screen positions, borehole flow rate, section transmissivity from flowmeter measurements and rock core images at W6. Each section is 25-cm thick. The black dashed rectangle represents the design position of the well screen, while the red dashed rectangle represents the actual position of the well screen. The flowmeter test was conducted in the open hole before W6 was sealed with bentonite.

2. Groundwater Flow and Solute Transport Model

Although the entire well field is a three-dimensional setting, simplified flow and transport processes through two thin permeable fracture zones were identified (Fig. 7). Therefore, a two-dimensional groundwater flow and solute transport model was developed using MODFLOW-2005 (Harbaugh 2005) and MT3DMS (Zheng and Wang 1999). The flow field during the tracer test was simulated by the groundwater flow model. Assuming the fluid density is constant, the governing equation for groundwater flow is
\[
S \frac{\partial h}{\partial t} = \frac{\partial}{\partial x_i} \left( K_{ii} \frac{\partial h}{\partial x_i} \right) \tag{S1}
\]

where \( h \) is hydraulic head, \( K_{ii} \) are the principal components of hydraulic conductivity aligned with the coordinate axes, \( t \) is time and \( S \) is specific storage. After the flow field was determined, the solute transport was simulated using a version of the MT3DMS code (Zheng and Wang 1999). The advection-dispersion equation is

\[
\frac{\partial (\theta c)}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left( \theta v_i c \right) \tag{S2}
\]

where \( C \) is the solute concentration, \( \theta \) is the porosity and \( D_{ij} \) is the dispersion coefficient tensor, which is a product of dispersivity and flow velocity. The flow velocity is determined from the groundwater flow model. The model assumed the same flow field for both saline and nZVI tracer tests.

The model grid consists of 50 rows and 100 layers with a grid spacing of 0.1 m \( \times \) 0.1 m (Fig. S4). The vertical direction of the model domain spans depths from 25 to 35 m. The total simulation time is 50 minutes. The temporal discretization consists of 50 one-minute stress periods with 10-second time steps. All boundaries are assumed to be no-flow.

Two adjacent permeable zones in W6 are assumed to connect with W4 (Figs. 7 and S4). Based on the flowmeter measurements and the nZVI tracer test results (Figs. 6 and S3), the dominant permeable zone is assumed to extend from 33–33.5 m in W6 to 28–29 m in W4. Considering the depth resolution of the flowmeter measurements, the thickness of the subordinate permeable zone is assumed to be 50 cm. Based on the acoustic televiewer log and the core log, eight fractures were found at the screen section in W6 with a dominant dip angle of 50°. Accordingly, the subordinate permeable zone with a dip of 50° between 31.5 and 32 m in W6 is assumed to connect to the dominant
permeable zone (Fig. 7).

Aside from the permeable zones, the horizontal hydraulic conductivity is set to $1.7 \times 10^{-10}$ m/s and the ratio of vertical hydraulic conductivity to horizontal hydraulic conductivity ($K_z/K_x$) is assumed to be 0.1. According to the flowmeter measurements in injection well W6, the transmissivity ratio of dominant permeable zone to the subordinate permeable zone is 6.89 (Fig. S3). The $K_x$ of the permeable zone can be calculated by the transmissivity divided by the thickness. As the thicknesses of both the permeable zones is 50 cm in W6, the ratio of $K_x$ of dominant permeable zone to the subordinate permeable zone is 6.89. The $K_z/K_x$ in the two permeable zones is set equal to 1. The lateral distance between the injection well W6 and the observation well W4 is 2.5 m (Fig. S4).

The grid for the mass transport model is the same as the flow model. The specified mass flux boundaries in the transport model coincide with the specified head boundaries in the flow model. As the fractures were partially filled with unconsolidated deposits based on the core samples, the porosities of two fracture zones are assumed to be 0.2. According to the deployment of electrical conductivity sensors in the field, the cell located at 29 m in W6 is assigned to release the tracer. The cell located at 28.5 m in W4 is designated the observation point (Fig. S4).
3. Uncertainty and Sensitivity Analysis

PEST (Doherty 2015) was used to calibrate the model and the weight for each observation is set equal to one. The optimal results showed that the root-mean-square error (RMSE) was equal to $4.434 \times 10^{-3}$. The uncertainty and sensitivity analysis is also important during the model calibration process and the uncertainty-related index, i.e., sensitivity coefficient (Jacobian matrix), covariance matrix, AIC (Akaike 1974), AICC (Hurvich and Tsai 1989), BIC (Schwarz 1978), and KIC (Kashyap 1982), can be calculated in PEST. These calculated indices are summarized in the Table S1. The covariance matrix for the saline tracer test is shown below:

---

**Fig. S4** Geometric configuration and finite-difference mesh for the groundwater flow and transport model.
Table S1 The model uncertainties of saline tracer test

| Index                  | Saline test                      |
|------------------------|----------------------------------|
| Sum of squared weighted residuals | 9.86×10⁻⁴ (RMSE = 4.434×10⁻³) |
| Composite sensitivities ² | $K^a = 2.488\times10^{-2}$  
$D^b = 2.203\times10^{-3}$ |
| AIC                    | -1077.696                       |
| AICc                   | -1077.446                       |
| BIC                    | -1069.881                       |
| KIC                    | -1068.011                       |

² $K$=Hydraulic conductivity  
³ $D$=Dispersivity  
² Hill et al. (1998)

References

Akaike H (1974) A new look at the statistical model identification, IEEE Transactions on Automatic Control 19:716-723, doi 10.1109/tac.1974.1100705

Chapuis RP (1992) Using Cooper-Jacob Approximation to Take Account of Pumping Well Pipe Storage Effects in Early Drawdown Data of a Confined Aquifer, Ground Water 30:331-337, doi 10.1111/j.1745-6584.1992.tb02000.x

Chuang PY, Chia Y, Liou YH, Teng MH, Liu CY, Lee TP (2016) Characterization of preferential flow paths between boreholes in fractured rock using a nanoscale zero-valent iron tracer test, Hydrogeol J 24:1651-1662, doi 10.1007/s10040-016-1426-7

Cooper HH, Jacob CE (1946) A generalized graphical method for evaluating formation constants and summarizing well-field history, Transactions, American Geophysical Union 27:526, doi 10.1029/TR027i004p00526
Day-Lewis FD, Johnson CD, Paillet FL, Halford KJ (2011) A computer program for flow-log analysis of single holes (FLASH). Ground Water 49:926-931, doi 10.1111/j.1745-6584.2011.00798.x

Doherty J. (2015) Calibration and Uncertainty Analysis for Complex Environmental Models, Watermark Numerical Computing, Brisbane, Australia. ISBN: 978-0-9943786-0-6.

Harbaugh AW (2005) MODFLOW-2005, the US Geological Survey modular ground-water model: the ground-water flow process US Department of the Interior, US Geological Survey Reston, VA, USA

Hill MC, Cooley RL, Pollock DW (1998) A controlled experiment in ground water flow model calibration, Ground Water 36:520-535, doi 10.1111/j.1745-6584.1998.tb02824.x

Hurvich CM, Tsai CL (1989) Regression and Time-Series Model Selection in Small Samples, Biometrika 76:297-307, doi 10.1093/biomet/76.2.297

Kashyap RL (1982) Optimal Choice of AR and MA Parts in Autoregressive Moving Average Models, IEEE Trans Pattern Anal Mach Intell 4:99-104, doi 10.1109/TPAMI.1982.4767213

Lee TP, Chia YP, Chen JS, Chen HE, Liu CW (2012) Effects of free convection and friction on heat-pulse flowmeter measurement, Journal of Hydrology 428:182-190, doi 10.1016/j.jhydrol.2012.02.001

Molz FJ, Morin RH, Hess AE, Melville JG, Guven O (1989) The Impeller Meter for Measuring Aquifer Permeability Variations - Evaluation and Comparison with Other Tests, Water Resources Research 25:1677-1683, doi 10.1029/WR025i007p01677

Schwarz G (1978) Estimating the Dimension of a Model, The Annals of Statistics
Tiedeman CR, Hsieh PA (2001) Assessing an open-well aquifer test in fractured crystalline rock, Ground Water 39:68-78, doi 10.1111/j.1745-6584.2001.tb00352.x

Zheng C, Wang PP (1999) MT3DMS: a modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems; documentation and user's guide DTIC Document.