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# Sensitivity analysis of transport modeling in a fractured gneiss aquifer

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ABSTRACT

Modeling solute transport in fractured aquifers is still challenging for scientists and engineers. Tracer tests are a powerful tool to investigate fractured aquifers with complex geometry and variable heterogeneity. This research focuses on obtaining hydraulic and transport parameters from an experimental site with several wells. At the site, a tracer test with NaCl was performed under natural gradient conditions. Observed concentrations of tracer test were used to calibrate a conservative solute transport model by inverse modeling based on UCODE2013, MODFLOW, and MT3DMS. In addition, several statistics are employed for sensitivity analysis. Sensitivity analysis results indicate that hydraulic conductivity and immobile porosity play important role in the late arrive for breakthrough curve. The results proved that the calibrated model fits well with the observed data set.

## 1. Introduction

In the past decade, fluid flow and solute transport in a fractured aquifer attracted many geo-engineers and geoscientists. Hydraulic and transport properties controlling fluid flow are of high heterogeneity in fractured aquifers. Fractured aquifer may have main three different characteristics: (i) fluid flow mainly occurring in the fractured zones, (ii) discrete flow paths, and (iii) channelized fluid flow.

Fluid flow and solute transport in a fractured gneiss aquifer are known to be highly heterogeneous over the range of scale. Moreover, understanding the transport process in fractured gneiss aquifers is of great importance to groundwater protection and improves the ability to predict the contaminant behavior in fractured aquifer. Rasmuson and Neretnieks (1986a, 1986b) show that only a very small portion of the fracture plane allows groundwater flow. However, modeling of solute transport in fractured aquifers has been addressed by many scientists (e.g. Bear et al., 1993; Feehley et al., 2000; Jørgensen et al., 2004; Simmons et al., 2001; Neuman, 2005; Reimus et al., 2003; Dagan and Neuman, 2005). Fractured zones are mostly dominant in igneous and metamorphic rock rocks. Identifying fracture zones by means of remote sensing is rather straight forward, but to define fracture properties and apertures precisely is still a challenge. Snow (1970) investigated the frequency of joints and the mean and variance of fractured apertures for gneiss using a packer injection test. Bear (1979, 2012) pointed out that mass flux for contaminant transport is a mix of two mechanisms: (i) contaminants travelling with the average velocity of groundwater flow, and (ii) dispersivity controlled flux.

Tracer tests have been widely used by many scientists and researchers around the world to acquire fluid flow and solute transport parameters. Tracer tests can be carried out under a natural gradient (Ptak and Teutsch, 1994; Schreiber and Bahr, 2002; Liou et al., 2011), under divergent flow (Welty and Gelhar, 1994; Ghergut et al., 2009; Chen et al., 2007), or under convergent flow tracer tests (Moench, 1995; Karasaki et al., 2000; McKenna et al., 2001; Riva et al., 2008). In fact, the goal of the tracer test varies from case to case. Gutiérrez et al. (1997) conducted a tracer test to determine the absorption and diffusion in fractured rock, while Sánchez-Vila and Carrera (1997) carried out tests to calculate the porosity and anisotropy of the flow system, however, the goal of Welty and Gelhar (1994) was to calculate dispersivity.

Dual-porosity approaches were developed by Barenblatt et al. (1960), Warren and Root (1963), and Coats and Smith (1964)). Bourdet and Gringarten (1980) proposed a new type curve to analyze well test data in dual-domain aquifers. Gringarten (1984) presented an intensive review of double porosity behavior in fissured and multilayer reservoirs. A further step forward was made by Streltsova (1983) who developed an analytical solution, which depends on the inter porosity flow regime. Moench (1984) developed a fracture skin model based on linear or diffusive flow. Sudicky (1990) solved Laplace transform Galerkin finite element equations to solve the solute transport through double porosity

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media. Dykhuizen (1990) suggested an improvement for the quasi-static condition in a dual-domain aquifer because the common approach assumed that the flow exchange transfer term is linear (first-order term). In the improved approach, the first order term is associated to the geometry of block matrix (size and shape) and hydraulic conductivity of the matrix at the interface between fracture and block matrix. Then, a coupling term that could be applied in early and later times was proposed (Dykhuizen, 1990; Zheng and Samper, 2005). Zimmerman et al. (1993) applied the coupling term into one nonlinear ordinary differential equation. Because the second-order term failed to determine the water transfer in the early stage for a non-equilibrium pressure head, Zimmerman et al. (1996) suggested a new term called second order term for water transfer. This term is determined by weighted arithmetic averages of conductivities using functions in the dual domain. Mckenna et al. (2001) applied single and multiple rates to interpret the results obtained from multi-well tracer test and depicted evidence that matrix diffusion is important in fractured systems. Later Köhne et al. (2004) implemented two modifications in the second-order transfer term. However, Feehley et al. (2000) compared the results from single-domain and double-domain models and observed that the single domain model is insufficient to simulate diffusive spreading at a low concentration.

The idea behind this latter approach is that there are two distinct zones. The first zone is the mobile phase, which contains the fractured area. The second zone is an immobile phase that contains the block matrix (un-fractured area). In the mobile area, the advection is the dominant phenomena for solute transport while in the immobile area; diffusion is the most dominant domain phenomena. The porosity in the mobile zone is generally higher than in the immobile zone. Such dual-domain model was implemented in the chemical reactions package MT3DMSv5.3. The dual-porosity approach is a powerful tool, which is more appropriate than the classical single-porosity approach for modeling the solute transport in particular for fractured aquifers because of the complexity and heterogeneity in the fractured system. In this study, the model was run with a dual domain mass transfer without sorption.

Inverse modeling is an automatic approach for searching the parameter values, which minimize the residual between computed and observed values (LaVenue and Pickens, 1992). Parameter estimation (inverse modeling) is challenging task for groundwater modelers due to the many uncertainties associated with the conceptual model, observations and model parameters (Liu and Gupta, 2007), which usually leads to an ill-posed problem (Mishra and Kuhlman, 2013). The inverse problem has become widely used for solving the groundwater flow (LaVenue and Pickens, 1992; RamaRao et al., 1995; LaVenue et al., 1995; LaVenue and Marsily, 2001). Gómez-Hernánez et al. (1997) developed stochastic approach for using pilot points in conjunction with stochastic fields to obtain multiple hydraulic property distributions. Doherty (2003) and Kowalsky et al. (2004) included regularization in the context of pilot points. Alcolea et al. (2006) combined prior information with Pilot point method. Doherty (2008) suggested using the regularized inversion techniques with practical tools like PEST (Doherty, 2008, 2013) and UCODE (Poeter et al., 2008). More information regarding UCODE can be found in Poeter et al. (1988, 2008).

Simply, sensitivity analysis is a technique for changing a set of parameters and see how the output will be altered. Sensitivity analysis is commonly used in many diverse areas of sciences for different purposes. It is a vital step for contaminant transport modeling. Saltelli et al. (2008) classified the sensitivity methods into the local sensitivity method, and the global sensitivity method. The local sensitivity method (first-order sensitivity) relates to the impact of change of one parameter value on the results in the model while the global sensitivity method deals with the sensitivity of whole sets of parameter distribution (van Griensven et al., 2006). Tilden et al. (1981) addressed the distinction between the local and global sensitivity method in more details. Saltelli et al. (2000, 2004, 2008) gave an intensive overview of global sensitivity analysis methods. Nonlinear regression is widely used in the field of water resource management and water protection (Knopman and Voss, 1988; Anderman and Hill, 1999; Foglia et al., 2009; Shi et al., 2012). Poeter and Hill (1998) made the first version of UCODE public. So far only UCODE 2005 is available at the USGS website as a public domain code but UCODE2013 will be released soon.

Sensitivity analysis, residual analysis, and inverse modeling were performed in this study using UCODE2013. UCODE is applied widely as the inverse modeling module in groundwater flow simulators. Recently, UCODE coupled with PHREEQC was used for reactive transport modeling (Skold et al., 2007). In addition, UCODE2013 offers a set of new statistical tests e.g. a parameter correlation coefficient (PCC). The PCC in UCODE 2013 can be determined for any pairs of estimated parameters. It is calculated by the covariance between two parameters using means of their standard deviations.

Coupling MOFLOW2005 and MT3DMS with UCODE to simulate conservative tracer transport in a fractured gneiss rock was to our knowledge not performed until now. Thus, in this work UCODE was used, for the first time, for inverse modeling of contaminant transport in a gneiss aquifer to appropriately explore the interaction between model parameters. The main advantages for UCODE2013 over other codes are: (1) the ability to couple it with any model that provides ASCII output files, (2) the freedom to specify the desirable weight of the observation depending on quality of the observations, (3) it provides a very useful information statistics (Poeter et al., 2008), (4) the parameter estimation by UCODE2013 is straightforward (Scott et al., 2003), (5) MCMC capability (using DREAM algorithm), and (6) parallel computing capability. Thus, UCODE 2013 is commonly used for auto-calibration, sensitivity analysis, and quantifying the parametric and predictive uncertainty analysis. More information about UCODE2013 and new features included e.g. evaluation uncertainty will be described elsewhere. Local sensitivity analysis was calculated using the Gauss–Newton nonlinear regression method (Hill and Tiedeman, 2007).

## 2. Method

Andrews (1861) was the first one to establish the principle of dual-porosity in the field of petroleum production (Ngien et al., 2012). In the double porosity model (Feehley et al., 2000), the transport equation for conservative tracer can be written as given below (Eq. (1)):

$$\theta_m \frac{\partial C_m}{\partial t} + \theta_{im} \frac{\partial C_{im}}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta_m D_{ij} \frac{\partial C_m}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\theta_m v_i C_m) + q_s C_s \tag{1}$$

where $C_m$ is the concentration in the mobile zone, $C_{im}$ is the concentration in the immobile zone, $\theta_{im}$ is the porosity in the immobile zone, $\theta_m$ is the porosity in the mobile zone, $\lambda_{1,im}$, $\lambda_{1,m}$ are the first-order rates for mobile-sorbed and immobile-sorbed phases respectively, whereas Eq. (2) represents the mass conservation in the immobile zone. The total porosity is the sum of the porosities in the area (Eq. (3)). A detailed explanation of these equations can be found in Zheng (2010) and Zheng et al. (2010)).

$$\theta_{im} \frac{\partial C_{im}}{\partial t} = \zeta(C_{im} - C_{im}) - \lambda_{1,im}\theta_{im}C_{im} \tag{2}$$

$$\theta = \theta_m + \theta_{im} \tag{3}$$

where $\zeta$ is the mass transfer rate between the mobile and immobile zones. However, double porosity is employed in this research to accomplish the task of simulating a single-phase flow in fractured