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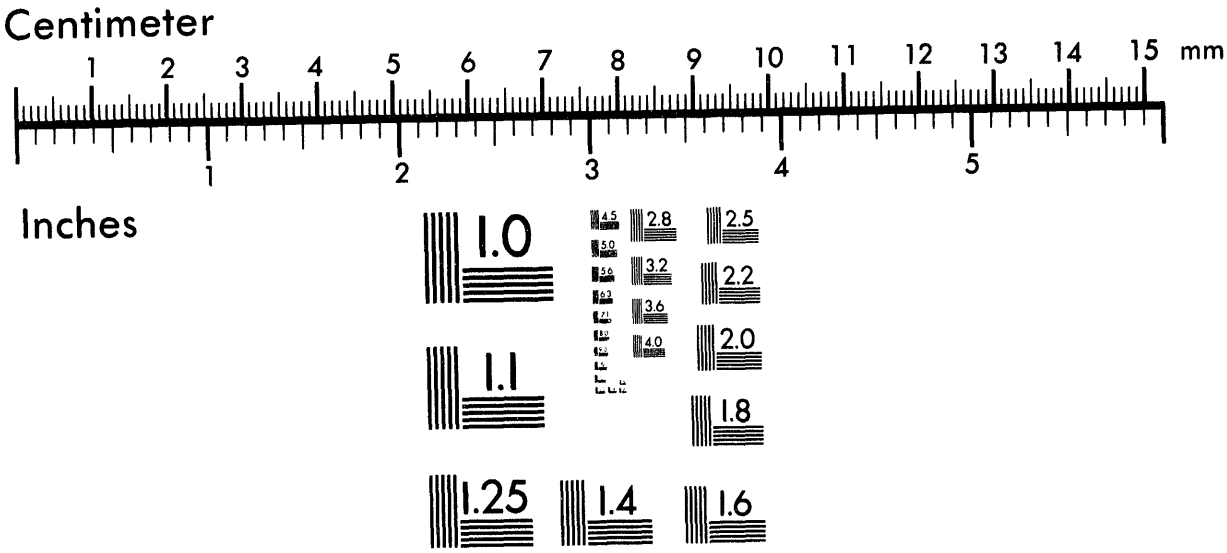

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Estimating Two-Phase Hydraulic Properties by Inverse Modeling

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ESTIMATING TWO-PHASE HYDRAULIC PROPERTIES BY INVERSE MODELING

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ABSTRACT

Disposal of high-level nuclear waste in geologic formations requires characterizing the hydrogeologic conditions at the potential site. This involves extensive data interpretation from laboratory and field experiments which are being performed on different scales. Two-phase flow processes are relevant if the potential site is located in the unsaturated zone, but they are also studied for repositories beneath the water table if the waste packages generate significant amounts of free gas. Numerical models are used for predicting the system behavior under different hydrologic and thermal loads. Parameters appearing in the governing equations are usually difficult to measure and subject to systematic errors. The strategy chosen to obtain model-related formation parameters is to calibrate the numerical model using observations of the system response. The practical relevance of parameter estimation for site characterization and design of field and laboratory experiments motivated the development. The purpose of this paper is to present the concept of parameter estimation, and to demonstrate the use of the proposed method for the interpretation of hydraulic tests conducted under two-phase flow conditions.

I. INTRODUCTION

Site characterization for nuclear waste repositories is based on the interpretation of data from laboratory and field experiments. The results of these studies provide a conceptual picture of the hydrogeological situation at the site, and numerical models are subsequently used to predict the system behavior for different hydrologic and thermal loads. The U.S. civilian radioactive waste management program focuses on a site in the unsaturated zone at Yucca Mountain, Nevada. Two-phase flow phenomena are also important for repositories situated beneath the water table, because gas is generated by the waste packages due to corrosion, hydrolysis, and microbial degradation.

Simulation models recently developed for subsurface flow in the unsaturated zone can deal with many physical processes of increasing complexity. However, the question of how to choose appropriate parameter values for a specific flow system is difficult to answer. While some of the parameters affecting two-phase flow can be determined in the laboratory or directly measured in the field, such measured parameters may differ from their model counterparts both conceptually and numerically because of heterogeneity effects and the scale of observation. The strategy chosen to obtain model-related formation parameters is to calibrate the numerical model using observations of the system response at discrete points in space and time. The difficulty of parameter estimation in these systems has two aspects: the first is model conceptualization which aims at capturing the relevant physical processes and defining discrete units over which parameter values can be considered constant. The second deals with the actual procedure of how to derive model parameters from data observed in the field.

To address this point, a tool for automatic model calibration has been developed. In this paper we will discuss the methodology emplyed for inverse modeling of highly non-linear flow problems and demonstrate the applicability of the code by interpreting data from tests conducted under two-phase flow conditions.

II. INVERSE MODELING APPROACH

Inverse modeling requires developing a simulation tool capable of reproducing the overall behavior of the system under the given test conditions. In this work, Lawrence Berkeley Laboratory's general-purpose multiphase fluid and heat flow simulator TOUGH2 is used to solve the so-called direct problem.[1] The coupled transport of multiple components in multiple phases is calculated by means of integral finite differences. Fluid flow occurs under pressure, viscous, and gravity forces according to Darcy's law. Interferences between the phases are represented by parameterized relative permeability functions. Capillary forces are given as nonlinear functions of liquid saturation. Thermophysical properties of the fluids are calculated from a set of primary variables. The gaseous phase is considered ideal, and additivity of partial pressures is assumed for gas/vapor mixtures. Dissolution in the liquid phase is represented by Henry's law. Heat transport occurs through conduction and convection.

Solving the direct problem in an efficient and stable manner is one essential step for parameter estimation. Additionally, a procedure is needed to iteratively update the parameter set used for the direct problem, leading to an improvement of the fit between observations and the model output. In ITOUGH2 ("Inverse TOUGH2"), the inverse problem is formulated in the context of maximum likelihood estimation theory.[2] The performance criterion to be minimized, ζ, is a weighted norm of the differences between observed and model-predicted state variables which reflects the error structure of the residuals. If the errors are assumed to be Gaussian with covariance matrix **C**, the corresponding estimator is the sum of squared residuals, weighted by the inverse of the covariance matrix:

$$\zeta(\mathbf{p}) = \mathbf{r}^T \mathbf{C}^{-1} \mathbf{r} \tag{1}$$

Each element of vector **r** represents a residual calculated at a point in space and time at which data is available. The data may be of variable type, such as flow rate, capillary pressure, gas saturation, or temperature. In fact, any measurement for which a corresponding TOUGH2 result can be obtained is suitable for use in parameter estimation by inverse modeling. Furthermore, prior information about the model parameters can be treated as additional observations. Any TOUGH2 input parameter can be estimated if the observed data is sufficiently sensitive to it. The performance measure (1) to be minimized is a function of the unknown parameters which are summarized in vector **p** of length n.

The strong nonlinearity pertaining to multiphase flow is a complicating factor for both the optimization procedure and the subsequent error analysis. While several minimization algorithms have been implemented in the ITOUGH2 code, the Levenberg-Marquardt modification of the Gauss-Newton method has been found to be most robust. The basic idea of the Levenberg-Marquardt algorithm is to move along the steepest descent direction of the objective function (1) far from the minimum, switching continuously to the Gauss-Newton algorithm as the minimum is approached. This is achieved by decreasing the scalar μ, known as the Levenberg parameter, after a successful iteration, but increasing it if an uphill step is taken (Marquardt's method). The following nonlinear system of equations is solved for $\Delta\mathbf{p}$ at an iteration labeled by index k:

$$(\mathbf{J}_k^T \mathbf{C}^{-1} \mathbf{J}_k + \mu \mathbf{D}_k)\, \Delta\mathbf{p}_k^T = -\mathbf{J}_k^T \mathbf{C}^{-1} \mathbf{r}_k \tag{2}$$

Here, **J** is the Jacobian matrix with elements $J_{ij} = \partial r_i / \partial p_j$, and matrix **D** denotes a diagonal matrix of order n with elements equivalent to the diagonal elements of matrix $\mathbf{J}_k^T \mathbf{C}^{-1} \mathbf{J}_k$. The improved parameter set is finally calculated:

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \Delta\mathbf{p}_k \tag{3}$$

ITOUGH2 also provides an extensive residual analysis. A correction procedure for the a posteriori covariance matrix of the estimated parameter set has been developed in order to account for the effects of nonlinearity.[3] The uncertainty of modeling results in prediction runs can be calculated either by applying first-order second-moment error analysis or by Monte Carlo simulations. The performance of the code has been illustrated using synthetic data sets.[4] Here we present applications to laboratory and field data which exhibit strong two-phase flow effects.

Experiment	Scale	Main process	Data type	Parameter
Salt infiltration into granite disk	mm	capillarity diffusion	electrical conductivity	permeability characteristic curve
Ventilation experiment in granite	dm	evaporation capillarity	water potential evaporation rate	permeability characteristic curve
Pulse test in fracture zone	dm	liquid flow	pressure	permeability
Hydraulic tests in liquid-saturated fracture zone	m	liquid flow	pressure liquid flow rate	permeability storativity
Gas injection into liquid saturated fracture zone	m	gas-water displacement	pressure	characteristic curve
Water injection into fracture zone containing gas	m	water-gas-water displacement	pressure liquid flow rate	permeability
Hydraulic test in low permeability host rock, possibly containing free gas	m	water-gas displacement	pressure liquid flow rate	permeability storativity initial saturation
Gas injection into low permeability host rock, possibly containing free gas	10 m	gas-water displacement	pressure	permeability characteristic curve
Pump test in low permeability host rock, possibly containing free gas	10 m	two-phase flow degassing	pressure gas production	permeability characteristic curve initial saturation

Table 1: Summary of ITOUGH2 applications

III. OVERVIEW OF APPLICATIONS

Although computationally intensive, the indirect approach to calibration provides great flexibility in the experimental design and the nature of input data. In this paper, we present various ITOUGH2 applications for estimating gas-related formation parameters and for quantifying prediction uncertainties. Table 1 provides an overview. The tests have been conducted for the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra). Data interpretation using ITOUGH2 has been performed at the Swiss Federal Institute of Technology in Zürich (ETHZ) in collaboration with Nagra. We will briefly describe the main objectives and findings of each experiment. In Section IV, we discuss one of the examples in greater detail. The experiment chosen for this illustration is a series of water and gas injection tests into an initially fully liquid-saturated fracture zone at the Grimsel Rock Laboratory, Switzerland, a research facility operated by Nagra.

A. Salt Infiltration Into Granite Sample

In preparation for a combined ventilation and brine injection experiment at the Grimsel Rock Laboratory[5], the bottom of an air dry disk-shaped sample of granite, 20 mm thick and 110 mm in diameter, was brought in contact first with deionized water and then with a 0.1 M KCl salt solution. In order to detect the advancing wetting front which is driven by capillary forces, an electrical conductivity sensor was installed at the top of the sample (Figure 1). Electrical conductivity was calculated in ITOUGH2 as a function of liquid saturation and brine concentration, assuming that the electrical conductivity of water, salt solution, and the rock matrix are constant. An estimate of absolute permeability and capillary strength of the granite was obtained by fitting the model output to the measured electrical conductivity. The experiment confirmed that measurements of electrical conductivity can be used to detect changes of water and salt content in granite. The liquid infiltration velocity driven by capillary suction was calculated. Salt diffusion was found to be negligible compared to the convective flux of brine. This is a consequence of the relatively strong capillary forces which were determined by inverse modeling.

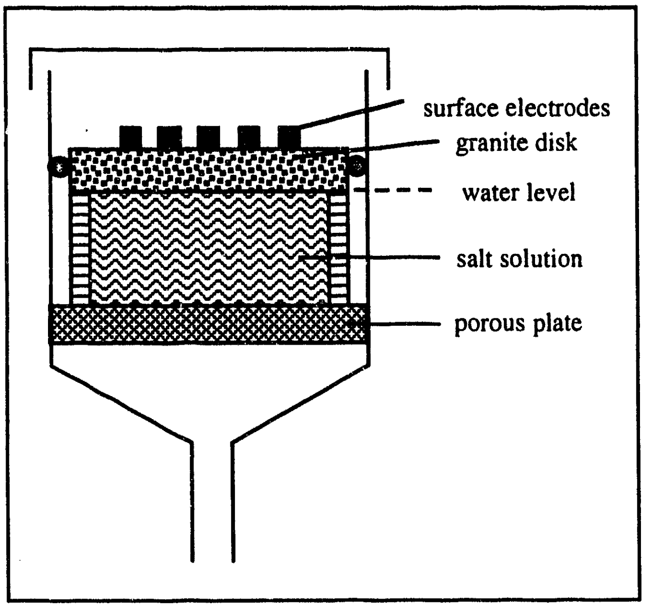

Fig. 1: Experimental setup

B. Ventilation Experiments

Ventilation tests were originally conceived to determine the macro-permeability of crystalline rocks by measuring the inflow of moisture into drift sections with controlled ventilation. It was found, however, that the estimated matrix permeability may be affected by partial drying of the drift wall, leading to substantial regions with two-phase flow conditions. In order to quantify the extent of the two-phase region and study its hydraulic properties, in-situ measurements of water potential, water content, temperature, and ambient air humidity were performed. We developed an ITOUGH2 model which takes into account evaporation at the drift surface as a function of relative humidity in the circulated air, vapor pressure lowering due to strong capillary pressures, and diffusive flux of air and vapor in the unsaturated zone which slowly propagates into the formation as a result of the drying process. Precise water potential measurements (Figure 2), as well as estimates of the evaporation rate at the drift wall, were used to determine absolute permeability and three parameters of van Genuchten's characteristic curves. [3,5] The results show that subtle two-phase flow processes can be successfully modeled to match field observations of various types.

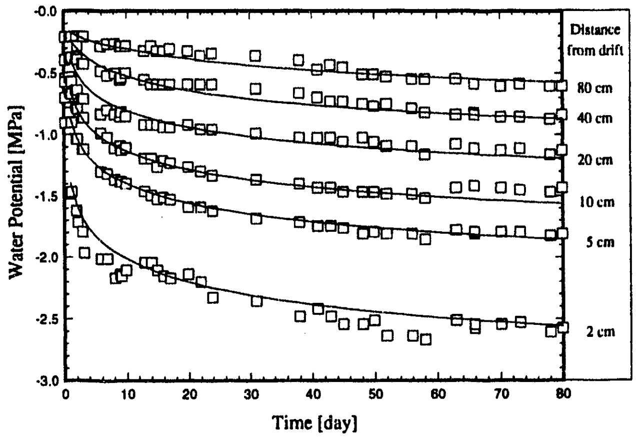

Fig. 2: Fit between computed (lines) and measured (symbols) water potentials

C. Interpretation of Hydraulic Tests

Standard hydraulic tests such as pulse tests, constant head injection tests, constant rate withdrawal tests, shut-in pressure recoveries, etc. may be interpreted using ITOUGH2. The multiphase formulation of the TOUGH2 code allows interpretation of these data even if the test is conducted in a two-phase environment. The initial gas saturation of the formation can be considered an unknown parameter to be determined by inverse modeling. Preliminary experiences with data from a potentially gas-bearing, low-permeability formation show, however, that due to water injection during drilling operations and injection periods it is difficult to obtain reliable information about the two-phase flow properties of the rock. While the permeability of the inner, liquid-saturated region can easily be determined, long pumping or pressure recovery periods are required to estimate initial gas saturation of the gas-bearing zone at greater distances from the well. This is visualized in Figure 3, which shows contours of the objective function in the two-dimensional parameter space. The shape of the objective function, as well as the eigenanalysis of the a posteriori error covariance matrix, indicate that absolute permeability can be estimated within relatively narrow bounds independent of the initial gas saturation. The latter cannot be identified only on the basis of the injection rates, which are measured during a constant pressure water injection test. However, by adding pressure data from the shut-in recovery period, it is possible to estimate the gas content of the formation (see Figure 4).

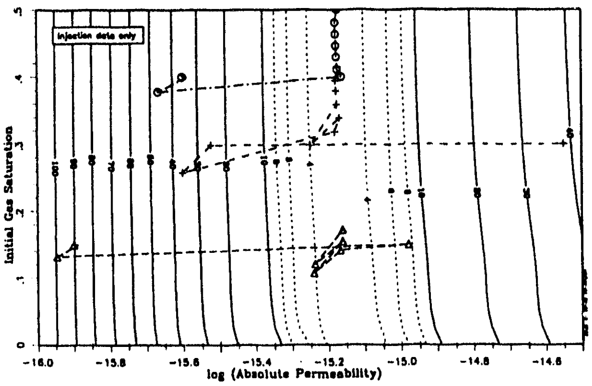

Fig. 3: Objective function and solution paths using injection data only

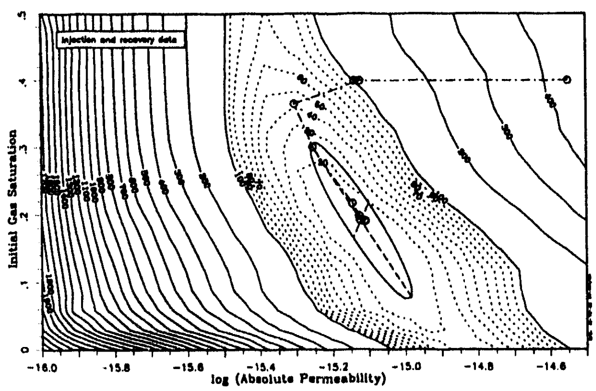

Fig. 4: Objective function, solution path, and confidence region using injection and recovery data

Data from pump tests may exhibit an unusual reponse if a free gas evolves in the borehole, as shown in Figure 5. The gas produced at a well head may be dissolved in the liquid phase under ambient conditions, coming out of solution when the pressure is decreased. It may also originate from a gas-bearing zone in the formation. This is not only a incertitude of one of the parameters to be estimated, but may also be considered an uncertainty of the conceptual model. In this case, ITOUGH2 can by used to examine and compare different model structures on an objective basis. Note that the pressure response shown in Figure 5 cannot be analyzed using standard wellbore simulators because degassing and expansion of the gas phase in the borehole are important mechanisms to be taken into account.

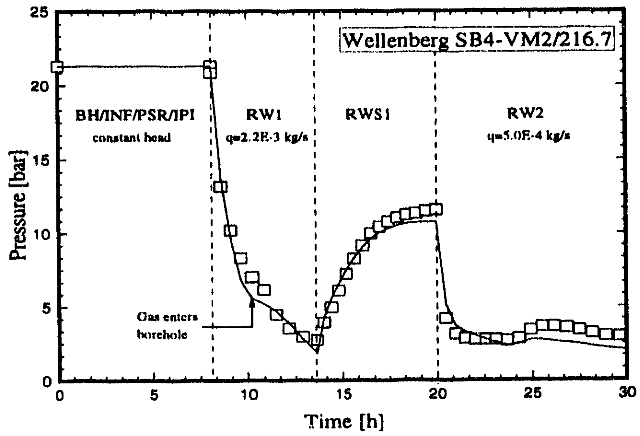

Fig. 5: Well test analysis

IV. GAS TESTS AT GRIMSEL ROCK LABORATORY

The remainder of this paper discusses the interpretation of a series of water and gas injection tests into a fracture zone. The purpose of the experiment was to assess the appropriateness of standard evaluation techniques applied to data from tests conducted under two-phase flow conditions. A discrete fracture zone was selected at the Grimsel Rock Laboratory. A number of boreholes were drilled, intersecting the fracture zone. Inflatable packers were installed to isolate injection and observation intervals. The test layout is shown in Figure 6. Interval I1.2 of borehole BoFR 87.001 was used to inject liquid and gas. The pressure response was observed in interval I0.2 of borehole BoGA 89.001.

The basic idea behind the test sequence is to perform a series of standard hydraulic tests (pulse tests, constant-head injection tests, etc.) into the fully liquid-saturated fracture zone (Phase 1). Subsequently, gas is injected in order to artificially create an unsaturated zone around the borehole (Phase 2). The same tests as the ones conducted during Phase 1 are then repeated (Phase 3). The results of Phase 1 and Phase 3 are compared to study possible impacts of the gas phase on test performance and interpretation.

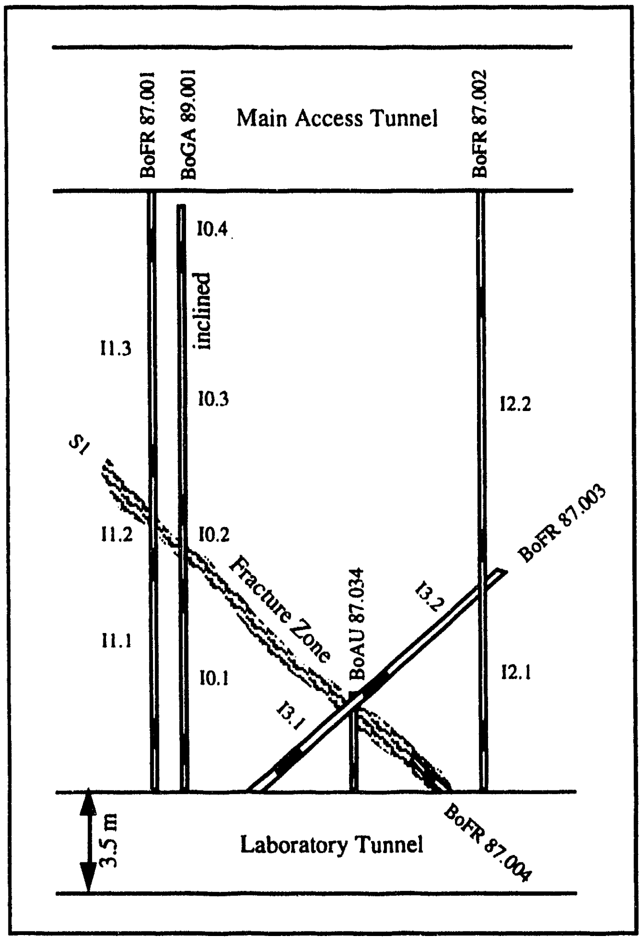

Fig. 6: Plan view of test layout

Figure 7 shows a schematic of the conceptual model. The injection borehole intersects the fracture zone which is depicted as a horizontal disk. Both the borehole and the fracture are connected to a region representing the granodiorite matrix. A skin zone and two zones with different hydraulic properties are introduced. The test response is observed in a borehole intersecting the fracture plane at a distance of approximately 2 m.

An initial guess of the absolute permeabilities was obtained from two pulse tests. The second pulse test was conducted using a 0.2 m^3 tank attached to the injection line, increasing the volume of water being injected and therefore increasing the radius of influence of the pulse test. ITOUGH2 allows us to model both tests simultaneously, yielding a consistent parameter set of higher accuracy. The fits are shown in Figure 8 with symbols representing the measured data; the solid lines are the pressures calculated by ITOUGH2.

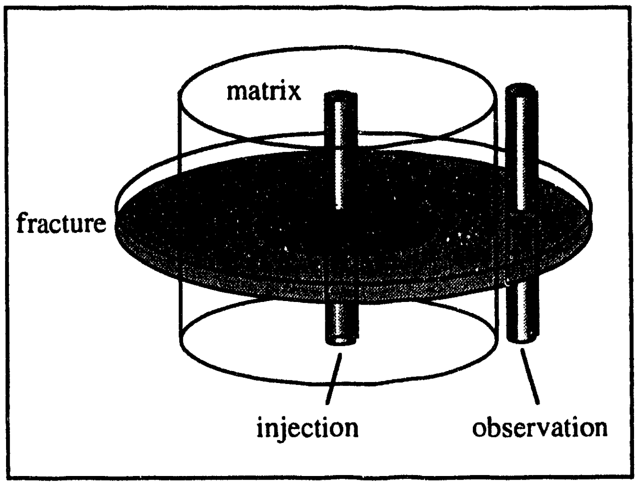

Fig. 7: Schematic of the conceptual model

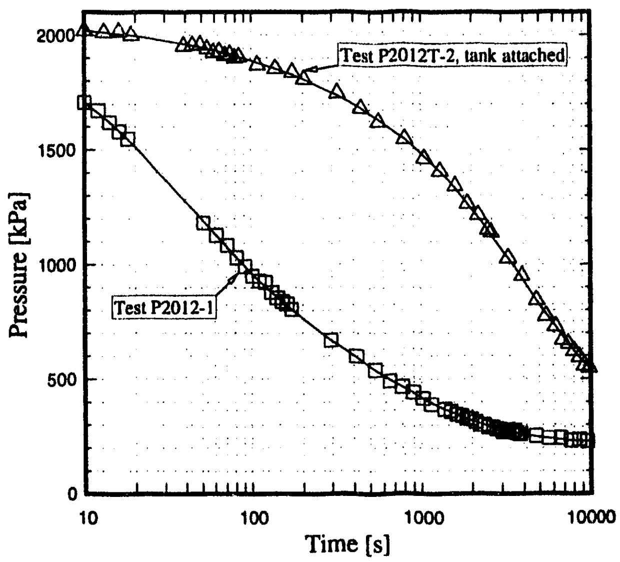

Fig. 8: Simultaneous pulse test interpretation

A constant-head water injection test, followed by a shut-in pressure recovery period, was then performed. Injection rate, as well as pressure measurements in both the injection and observation borehole, are used to estimate the permeabilities of the fully liquid saturated system. The results of this test sequence are discussed elsewhere.[6] Next, nitrogen gas is injected at a constant pressure of 20 bars for about 8 hours (QCHG-1), creating an unsaturated region around the well. The test response is used to estimate two-phase hydraulic properties of the fracture zone. Figure 9 shows the comparison of the measured and predicted pressures in the two intervals I1.2 and I0.2. Note that only the pressure data observed in interval I0.2 during the test period QCHG-1 are used for parameter estimation, whereas the remaining data (pressure recovery PRG-1 and extraction period EXTR-1) are utilized to test the predictive capability of the calibrated model. The system behavior is very well predicted in both intervals during the test period PRG-1. The fit shows significant deviations, however, for the final extraction test. This makes clear that the predictability of a model is restricted to cases governed by similar flow processes under similar conditions. Switching from gas injection to withdrawal of a mixture of gas and liquid reverses the flow direction, triggering new processes and phenomena such as hysteresis which are not accounted for in the numerical model.

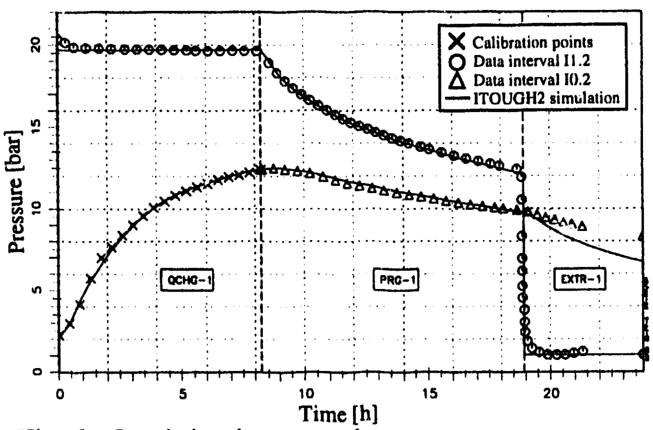

Fig. 9: Gas injection experiment

In Phase 3, a constant-pressure water injection test is conducted similar to the one in Phase 1. Both tests are analyzed using ITOUGH2 assuming single-phase liquid conditions. Recall that the fracture zone is liquid saturated in Phase 1, whereas it contains a significant amount of free gas in Phase 3. The measured and calculated flow rates are shown as a Jacob-Lohman plot in Figure 10.

Both data sets can be matched almost perfectly. The parameters estimated by inverse modeling reveal that identical values are obtained for the absolute permeability of the inner zone, regardless of whether the system is initially liquid saturated or whether it contains a free gas phase. This is mostly due to the fact that in the Phase 3 experiment a composite system is created by injecting water into an unsaturated environment. The zone around the borehole is almost fully liquid saturated with some gas at residual gas saturation. Consequently, the correct value for the absolute permeability is obtained. However, in the outer region where gas is present, the absolute permeability would be greatly underestimated using Phase 3 data, as indicated by the steeper slope of the data after about 1000 seconds (see Jacob-Lohman plot, Figure 10). The estimated storage coefficient of this zone is very large, suggesting that a free gas phase is present. Once there is clear evidence for the system being two-phase, the conceptual model can be modified accordingly to account for phase interferences.

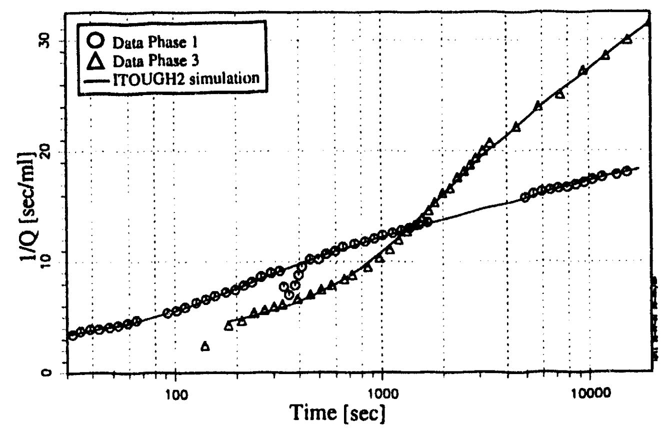

Fig. 10: Jacob-Lohman plot of constant pressure water injection test into saturated and unsaturated fracture zone

CONCLUDING REMARKS

The purpose of this paper was to present various applications of the ITOUGH2 code for the design and interpretation of experiments to characterize the host rocks of potential radioactive waste repositories.

Estimating hydrogeological parameters by inverse modeling has the advantage that the calibrated model is able to describe the field scale behavior in a manner which is optimal with respect to the given data and the actual model structure. Numerical simulation provides remarkable flexibility in adapting complex flow processes, geometries, initial and boundary conditions. Data of almost any type can be used simultaneously to estimate input parameters of a prediction model. Furthermore, the efficiency of the automatic model calibration allows the examination of alternative conceptual models to explain the data. From this perspective, inverse modeling can be used for process identification in a complex multiphase environment, and provide guidance for future model of performance assessment at Yucca Mountain.

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