ITOUGH2: Solving TOUGH Inverse Problems

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paper presented at the TOUGH workshop '95

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Abstract

ITOUGH2 is a program that provides inverse modeling capabilities for the TOUGH2 code. While the main purpose of ITOUGH2 is to estimate two-phase hydraulic properties by calibrating a TOUGH2 model to laboratory or field data, the information obtained by evaluating parameter sensitivities can also be used to optimize the design of an experiment, and to analyze the uncertainty of model predictions. ITOUGH2 has been applied to a number of laboratory and field experiments on different scales. Three examples are discussed in this paper, demonstrating the code's capability to support test design, data analysis, and model predictions for a variety of TOUGH problems.

Introduction

Simulating multiphase fluid flow in porous or fractured media using TOUGH2 requires specifying a number of parameters that are difficult to determine. Parameters measured in the laboratory may significantly differ from their model counterparts both conceptually and numerically mainly because of scale effects. Calibration of a TOUGH2 model against a test response that is relevant to the ultimate application, is a strategy to obtain model-related formation parameters. These parameter estimates represent effective properties at the scale of interest, thus greatly improving the reliability of the subsequent model predictions.

ITOUGH2 is a program that provides inverse modeling capabilities for the TOUGH2 simulator. The core of the program contains an algorithm that examines the impact of model parameters on the simulation results by repeatedly solving the flow problem using TOUGH2. The information about parameter sensitivities, combined with an efficient and robust optimization technique and a detailed error analysis, makes ITOUGH2 a powerful tool not only for parameter estimation, but also for the optimization of test designs and the analysis of prediction uncertainties.

ITOUGH2 solves the inverse problem by automatic model calibration based on the maximum likelihood approach. All TOUGH2 input parameters including initial and boundary conditions as well as geometrical features such as fracture spacing can be considered unknown or uncertain. The parameters can be estimated based on any type of observations for which a corresponding TOUGH2 output is available. Furthermore, user-specified parameters and observations can be introduced. The user can select from a number of different objective functions and minimization algorithms. One of the key features of ITOUGH2 is its extensive error analysis which provides statistical information about final residuals, estimation uncertainties, and the ability to discriminate among model alternatives. The theoretical background as well as the usage of the hierarchically structured command language are documented in *Finsterle* [1993]. Three examples are discussed in this paper, demonstrating the capability of ITOUGH2 to support test design, data analysis, and model predictions.

Test Design

Design of a laboratory or field test can be optimized, so that the uncertainty of the estimated parameters is as small as possible. The basic idea supported by ITOUGH2 is the following:

- Conceive a test design, i.e. sequence of test events, type of data to be collected, location of sensors, number and type of parameters to be identified, etc.
- Generate synthetic data using TOUGH2. A random noise can be added to represent measurement errors.
- Solve the inverse problem for all unknown or uncertain parameters using ITOUGH2.
- Analyze sensitivity matrix. Revise test design to improve sensitivity of data .
- Analyze covariance matrix. Optimize test design to reduce parameter correlation and estimation uncertainty.
- Examine impact of conceptual model on parameter estimates. Check whether the data are selective with respect to competing model alternatives.

As an example, we simulated the response to a series of standard borehole tests, including pulse withdrawal (PW) and pulse injection (PI) tests, a constant rate pumping (RW) - recovery (RWS) test, as well as injection of water (RI) and gas (GRI) at a constant rate, followed by shut-in recovery periods (RIS, GRIS). A synthetic inverse problem is first solved under the assumption that only data from test sequence 1 are available (Figure 1). The covariance matrix of 10 unknown parameters is calculated, and the standard deviations and correlation coefficients are analyzed. Table 1 demonstrates that performing test sequence 1 alone is insufficient to identify a number of two-phase flow parameters. Adding test sequences 2 and 3 considerably improves the ability to determine parameter values by reducing both the estimation error and the correlations between the parameters. Details can be found in *Finsterle* [1995].

Table 1: Reduction of estimation error and parameter correlation as a result of adding test sequences 2 and 3, van Genuchten model

	van Genuchten					
Parameter	Sequence 1 only		Sequence 1 and 2		Sequence 1, 2 and 3	
	σ	χ	σ	χ	σ	χ
log (k [m^2])	0.32	0.04	0.03	0.26	0.03	0.27
p_i [bar]	N/D	0.01	0.64	0.19	0.21	0.50
S_{gi} [-]	N/D	0.03	0.03	0.12	0.02	0.14
AEP $1/\alpha$ [bar]	N/D	0.02	0.52	0.14	0.26	0.27
PSDI n [-]	N/D	0.01	0.87	0.05	0.43	0.09
S_{lr} [-]	N/D	0.02	0.16	0.06	0.10	0.10
S_{gr} [-]	N/D	0.02	0.01	0.06	0.01	0.07
ϕ [-]	N/D	0.01	0.01	0.07	0.01	0.11
log (c_{tz} [Pa^{-1}])	N/D	0.29	0.19	0.09	0.19	0.09
p_{bh} [bar]	0.62	0.19	0.25	0.45	0.22	0.51

σ : standard deviation from joint probability density function
χ : ratio of conditional and joint standard deviation; low value indicates high correlation
N/D : not determinable, i.e. standard deviation much larger than parameter value

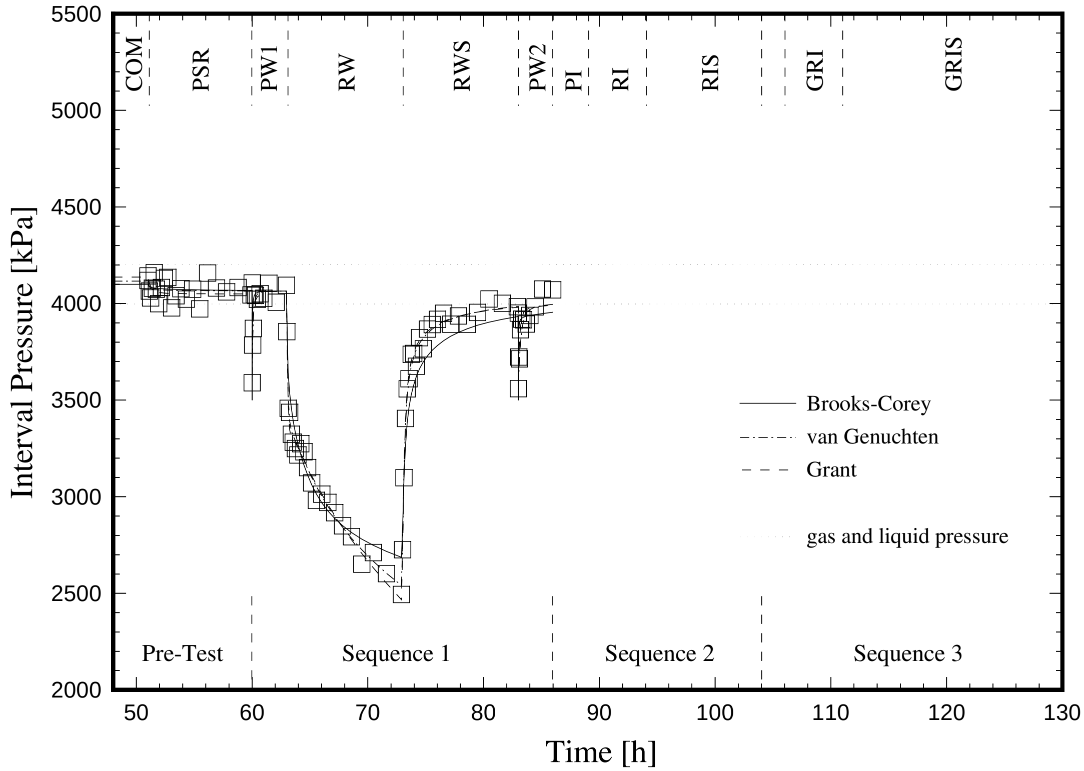

Figure 1: Fitting alternative models to data synthetically generated for test sequence 1

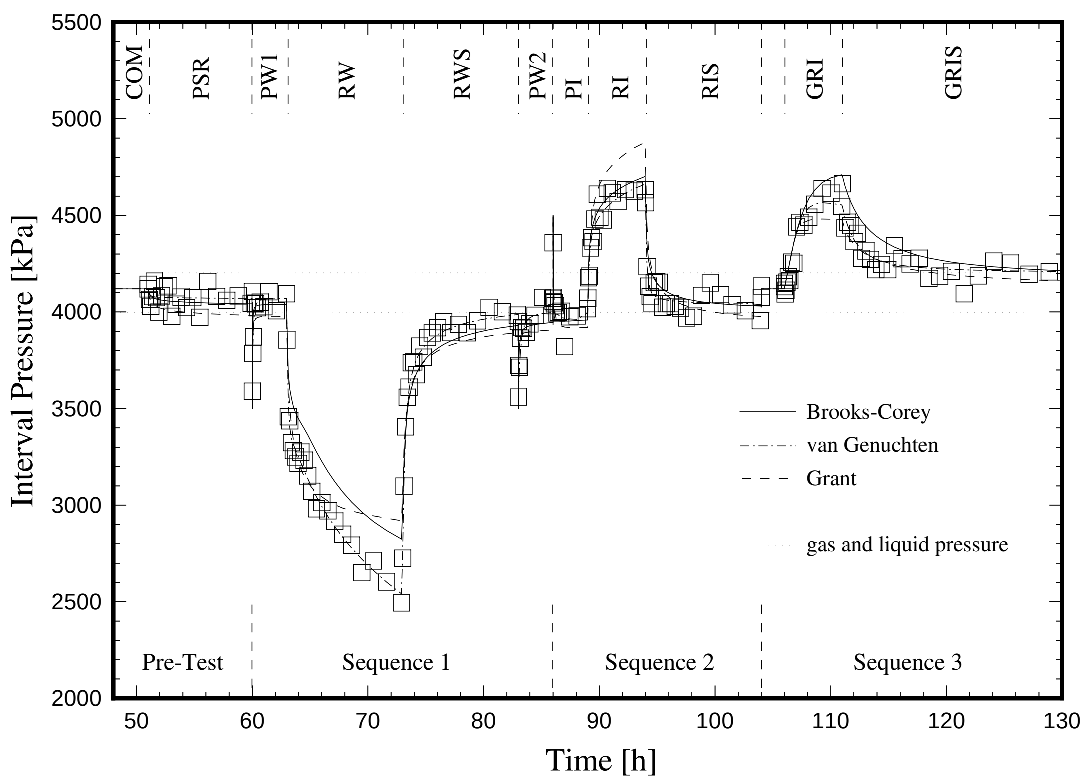

Figure 2: Fitting alternative models to data generated for test sequences 1, 2, and 3

Table 2: Estimated error variances using different characteristic curves; data are generated using the van Genuchten model, perturbed by a normally distributed noise with σ_0 = 50 kPa.

Estimated Error Variance s_0^2/σ_0^2			
Model	Sequence 1 only	Sequence 1 and 2	Sequence 1, 2 and 3
data (van Genuchten)	1.00	1.00	1.00
van Genuchten	0.92	0.99	1.06
Brooks-Corey	0.89	*2.81*	*4.39*
Grant	0.95	*5.77*	*4.78*
s_0^2 : estimated error variance = *a posteriori* error variance of residuals; if s_0^2/σ_0^2 is greater than $F_{0.95}$=1.35 (*italic*), the model is unlikely to explain the data			

The synthetic data for each test design are inverted using three different characteristic curves (Brooks-Corey, van Genuchten, and Grant). The goodness-of-fit can be used to examine the capability of the test design to discriminate among alternative conceptual models.

It can be seen (Table 2, Figure 1) that each model explains the flow system equally well if only data from test sequence 1 are available. If data from sequences 2 and 3 are added (Figure 2), however, one of the models performs significantly better, and provides a basis for rejecting the competing alternatives. In conclusion, the extended test design has the potential of identifying a model that is more likely to represent field conditions.

Model Calibration

The main purpose of the ITOUGH2 code is to estimate model-related parameters by automatically calibrating an appropriate TOUGH2 model to laboratory or field data. The indirect approach to calibration provides great flexibility in choosing scale and layout of an experiment that can be analyzed to determine two-phase hydraulic properties.

Analysis of a ventilation test performed by *Gimmi et al.* [1992] at the Grimsel Rock Laboratory is shown here. A TOUGH2 model that simulates evaporation at a ventilated drift surface and propagation of a drying zone into the initially fully saturated rock matrix was calibrated against transient water potential measurements at six different depths. Pressure data in two boreholes as well as estimates of evaporation rates at the drift surface were also considered. Absolute permeability and the parameters of van Genuchten's characteristic curves were determined. Figure 3 shows the comparison between observed and calculated water potentials. Minimization was started from different initial parameter sets. All inverse runs resulted in parameter sets that are almost identical, suggesting that the solution is unique within the parameter space of interest.

The predicted water potentials, plotted as solid lines in Figure 3, are close to the measured values. The calculated flow rate of 0.31 mg m^{-2} s^{-1} compares very well to the observed value of 0.3 mg m^{-2} s^{-1}. The difference between measured and calculated gas pressures in the two boreholes is less than 0.01MPa. This example shows that inverse modeling of the ventilation experiment provides reliable estimates of model-related formation parameters affecting two-phase flow. It requires, however, a high model sophistication to simulate the physical processes relevant to desaturation of a granitic rock matrix. The error analysis indicates that if the absolute permeability can be determined independently, the parameters of van Genuchten's characteristic curves are estimated with less uncertainty because of a more favorable correlation structure. Details can be found in *Finsterle and Pruess* [1995].

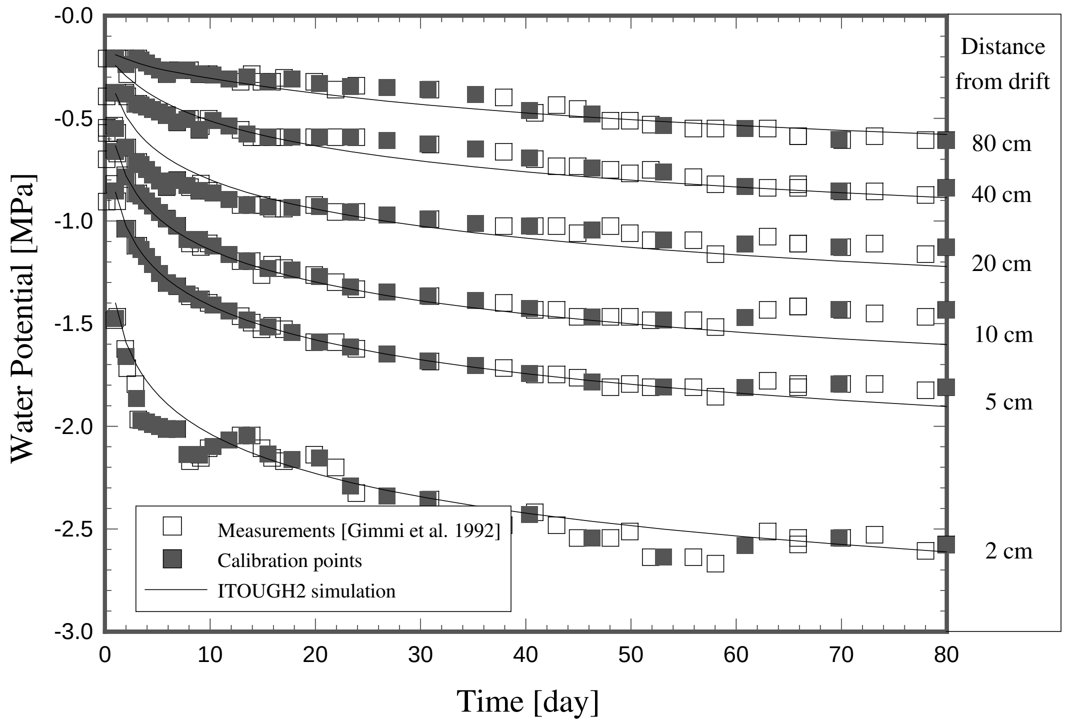

Figure 3: Comparison between calculated and measured water potentials during a ventilation period of 80 days. Data from six tensiometers at different depths are available. Calibration points are linearly interpolated between actual data points. Data from *Gimmi et al.* [1992].

Uncertainty Analysis for Model Predictions

Model predictions using TOUGH2 are uncertain due to the uncertainty associated with the input parameters. ITOUGH2 provides two options to analyze prediction errors. The variance of a model output can be calculated using standard First Order Second Moment error analysis which may take into account the correlations between the parameters. This method results in normally distributed prediction errors. It assumes, however, that the model is linear in the parameters, and that the probability density function of the input parameters is close to Gaussian. The strong nonlinearities inherent in multiphase flow modeling may require performing Monte Carlo simulations. The probability density function of the prediction error is then obtained by statistically analyzing a large number of TOUGH2 realizations.

The difference between the two methods is demonstrated for a synthetic laboratory experiment, in which the outflow of water at the bottom of a column is measured during injection of gas at a constant pressure from the top. The flow rate initially increases as a result of increasing total mobility. Once the gas has reached the outlet, the flow rate drops sharply due to the reduced relative permeability and water content. Values for absolute permeability and three parameters of the characteristic curves are sampled from a normal distribution, and 100 Monte Carlo simulations are performed. The results indicate (Figure 4) that the prediction errors are not symmetrical around the mean, i.e. that the linearity assumption is violated. Nevertheless, the simple First Order Second Moment error analysis provides a reasonable estimate of prediction uncertainties during the initial and final stages of the experiment.

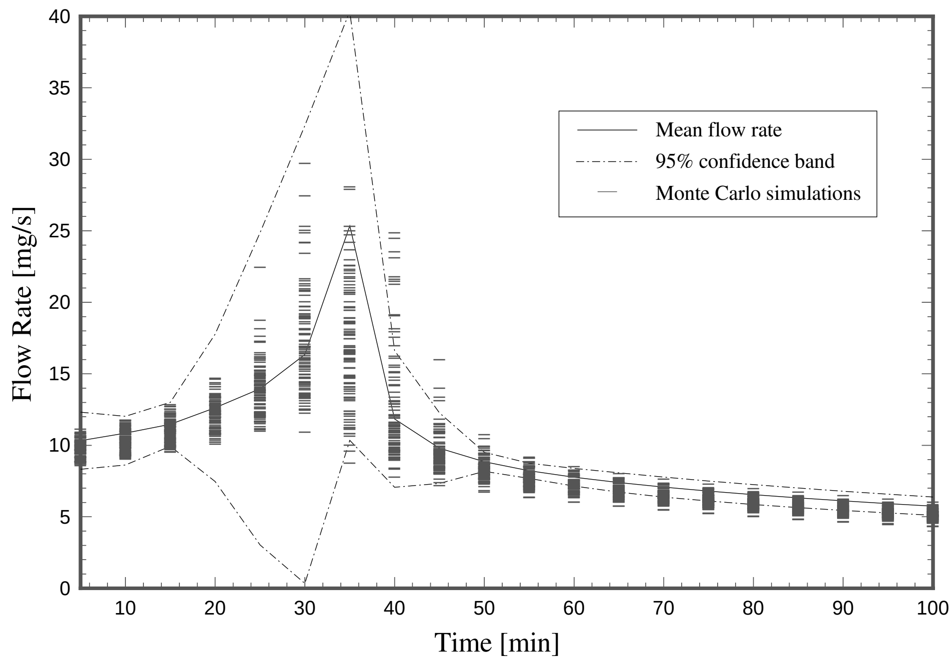

Figure 4: Uncertainty of model prediction for synthetic laboratory experiment. The results of 100 Monte Carlo simulations represent the probability density function of the model output. The uncertainty is fairly well reproduced by a First Order Second Moment error analysis.

Concluding Remarks

Inverse modeling provides an appealing technique to obtain model-related TOUGH2 parameters by calibrating the numerical model against sensitive observations of the system state. The combination of sophisticated process description (TOUGH2) and a flexible and robust inverse approach with detailed error analysis (ITOUGH2) yields a powerful tool for test analysis under two-phase flow conditions. The design of an experiment can be optimized prior to testing in order to improve the subsequent estimation of parameter values. Finally, the impact of parameter uncertainties on model predictions can be studied using ITOUGH2.

Acknowledgment This work was carried out under U.S. Department of Energy Contract No. DE-AC03-76SF00098 for the Director, Office of Civilian Radioactive Waste Management, Office of External Relations, and was administered by the Nevada Operations Office, U.S. Department of Energy, in cooperation with the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra).

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