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Multiphase Inverse Modeling: An Overview

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ABSTRACT

Inverse modeling is a technique to derive model-related parameters from a variety of observations made on hydrogeologic systems, from small-scale laboratory experiments to field tests to long-term geothermal reservoir responses. If properly chosen, these observations contain information about the system behavior that is relevant to the performance of a geothermal field. Estimating model-related parameters and reducing their uncertainty is an important step in model development, because errors in the parameters constitute a major source of prediction errors. This paper contains an overview of inverse modeling applications using the ITOUGH2 code, demonstrating the possibilities and limitations of a formalized approach to the parameter estimation problem.

INTRODUCTION

Numerical modeling of nonisothermal multiphase flow in fractured-porous media has reached a level of sophistication that allows one to accurately simulate coupled flow, transport, and heat exchange processes in a geothermal reservoir under a variety of natural and production-induced conditions (Pruess et al., 1997). However, uncertainties in the parameters describing the hydrogeologic properties of the geothermal reservoir often obliterate the theoretically high precision of numerical simulations. An even greater impact on the predicted system behavior is generated by errors in the conceptual model, making the identification of the relevant features and parameters the most important step in model development.

Data describing the geothermal reservoir characteristics are usually obtained using a variety of methods, each of which producing information pertinent to a specific scale and a particular process. In previous publications (Finsterle and Pruess, 1995; Finsterle et al., 1997) we have argued that hydrogeologic parameters should be determined based on production data (flow rates, enthalpies, and temperatures) and using a model with a structure similar to that employed for the subsequent predictions. Automatic history matching of relevant test and production data assures that *model-related* parameters are estimated, thus increasing the reliability of the predictions.

The project described in this paper aims at enhancing automatic history matching and optimization techniques for analyzing problems in geothermal reservoir engineering. Developing inverse modeling capabilities for a nonisothermal multiphase reservoir simulator provides the means to reduce errors and uncertainties in the input parameters. The fact that parameter uncertainties constitute a major source of prediction uncertainty emphasizes the importance of the parameter estimation process in general, and the assessment of parameter sensitivities and estimation errors in particular.

We have developed inverse modeling capabilities for the TOUGH2 simulator (Pruess, 1991) for applications in nuclear waste isolation, environmental sciences, and geothermal engineering. The ITOUGH2 code ("Inverse TOUGH2") permits the estimation of TOUGH2 input parameters based on any type of observation for which a corresponding TOUGH2 output can be calculated (Finsterle, 1997a). Furthermore, a detailed residual and error analysis can be performed, and the uncertainty of model predictions can be evaluated using either a linear analysis or Monte Carlo simulations.

The purpose of this paper is to provide an overview of ITOUGH2 applications to a variety of multiphase flow problems on a wide range of scales and involving different processes. The ability of inverse modeling to extract information from measured data will be demonstrated, along with its limitations, which are usually a consequence of systematic errors in either the model or the data.

ELEMENTS OF INVERSE MODELING

In this section, we briefly summarize the various steps involved in the iterative procedure of automatic model calibration. A detailed discussion of inverse modeling theory can be found elsewhere (e.g., Carrera and Neuman, 1986).

The flow chart shown in Figure 1 illustrates the process and main elements of inverse modeling.

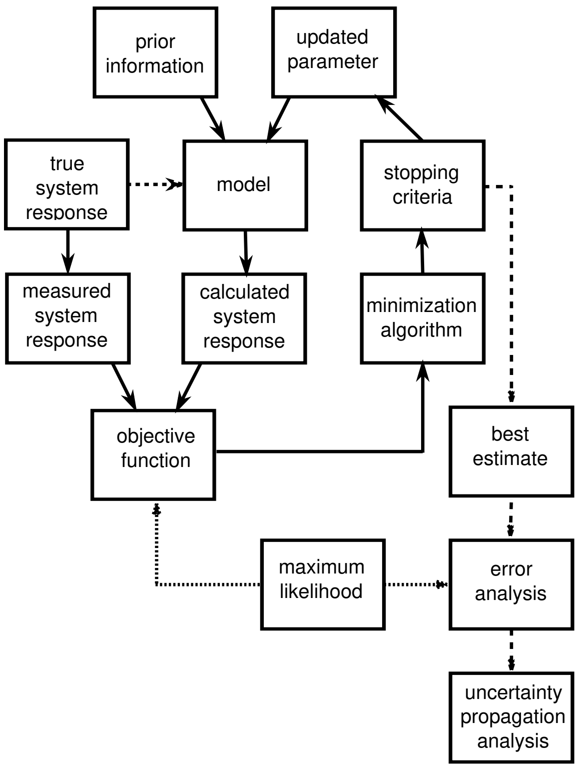

Figure 1. *Inverse modeling flow chart showing main elements of automatic model calibration procedure.*

The core of an inverse modeling code is an accurate, efficient, and robust simulation program that solves the so-called forward problem. It must be capable of simulating the flow and transport processes that govern the observed system response. As mentioned above, we use TOUGH2 (Pruess, 1991) to model multiphase fluid and heat flow in fractured-porous media. In addition to selecting the simulator, a problem- and site-specific conceptual model has to be developed. Note that any error in the conceptual model leads to a bias in the parameter estimates, which is usually much larger than the uncertainty introduced by random measurement errors.

Next, an objective function has to be selected to obtain an aggregate measure of deviation between the observed and calculated system response. The choice of the objective function can be based on maximum likelihood considerations, which for normally distributed measurement errors leads to the standard weighted least squares criterion (Carrera and Neuman, 1986):

$$S = \mathbf{r}^T \mathbf{C}_{zz}^{-1} \mathbf{r} \tag{1}$$

Here, $\mathbf{r}$ is the residual vector with elements $r_i = z_i^* - z_i(\mathbf{p})$, where z_i^* is an observation (e.g., pressure, temperature, flow rate, etc.) at a given point in space and time, and z_i is the corresponding simulator prediction, which depends on the vector $\mathbf{p}$ of the unknown parameters to be estimated. The i-th diagonal element of the covariance matrix $\mathbf{C}_{zz}$ is the variance representing the measurement error of observation z_i^*. Note that alternative objective functions are available, which may have significant advantages over the traditional least-squares formulation (Finsterle and Najita, 1997).

The objective function S has to be minimized in order to maximize the probability of reproducing the observed system state. Due to strong nonlinearities in the functions $z_i(\mathbf{p})$, an iterative procedure is required to minimize the objective function S. A number of minimization algorithms are available in ITOUGH2. They reduce the objective function by iteratively updating the parameter vector $\mathbf{p}$ based on the sensitivity of z_i with respect to p_j. Details about the minimization algorithms implemented in ITOUGH2 can be found in Finsterle (1997a).

Finally, under the assumption of normality and linearity, a detailed error analysis of the final residuals and the estimated parameters is conducted. As demonstrated in Finsterle and Pruess (1995a,b), these analyses provide valuable information about the estimation uncertainty, the adequacy of the model structure, the quality of the data, and the relative importance of individual data points and parameters. In addition to its efficiency, it is mainly the formalized sensitivity, residual, and error analyses that make inverse modeling preferable over the conventional trial-and-error model calibration.

APPLICATIONS

ITOUGH2 has been applied to a number of synthetic and actual multiphase inverse problems on different scales and with different objectives. Applications to geothermal engineering problems have been described in Finsterle and Pruess (1995b), White (1995), Finsterle and Pruess (1997), Finsterle et al. (1997), and Guerrero et al. (1998). An additional set of sample problems with a detailed description of the ITOUGH2 program options can be found in Finsterle (1997b). Table 1 shows the four selected applications of increasing scale that will be discussed in the remainder of this paper.

Table 1. *Summary Description of Selected ITOUGH2 Applications*

#	Application	Parameters	Observations
1	Gas-pressure-pulse-decay experiment	Permeability Porosity Klinkenberg factor	Pressure in upstream and downstream gas reservoir
2	Ventilation experiment	Permeability van Genuchten parameters	Water potentials Pressures Evaporation rate
3	Atmospheric pressure fluctuation	Gas diffusivity	Pneumatic pressure
4	Calibration of geothermal reservoir model	Permeability Porosity Steam saturation van Genuchten parameters	Pressure Enthalpy

In Application 1, permeability and porosity of a very tight fine-grained graywacke core plug from the Geysers Coring Project are determined using the gas-pressure-pulse-decay (GPPD) method, in which a reservoir attached to the dry sample is rapidly pressurized using nitrogen gas (see Figure 2). Gas starts flowing through the sample, and the pressure change over time is observed in both the upstream and downstream reservoirs. Using nitrogen gas as opposed to water has the advantage of shorter test duration due to the increased mobility of the fluid. Furthermore, the high compressibility allows the determination of a relatively independent porosity estimate from the steady-state pressure data. Knudsen diffusion effects, however, lead to increased gas fluxes and thus require estimating a third parameter, the Klinkenberg gas slip factor *b*, along with absolute permeability and porosity. Details can be found in Finsterle and Persoff (1997).

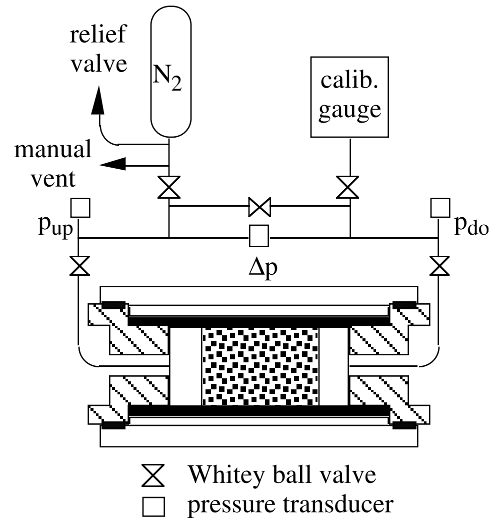

Figure 2. *Gas-pressure-pulse-decay apparatus.*

Figure 3 shows the data (symbols), the simulated pressures with an initial set of parameters (dash-dotted lines), and the match obtained after 5 ITOUGH2 iterations (solid lines).

The almost perfect match shown in Figure 3 may lead to the conclusion that the parameters were estimated with a high degree of precision. However, the covariance matrix of the estimated parameters (Table 2) reveals that the very strong negative correlation between the permeability *k* and the Klinkenberg factor *b* yields an estimation uncertainty of more than an order of magnitude.

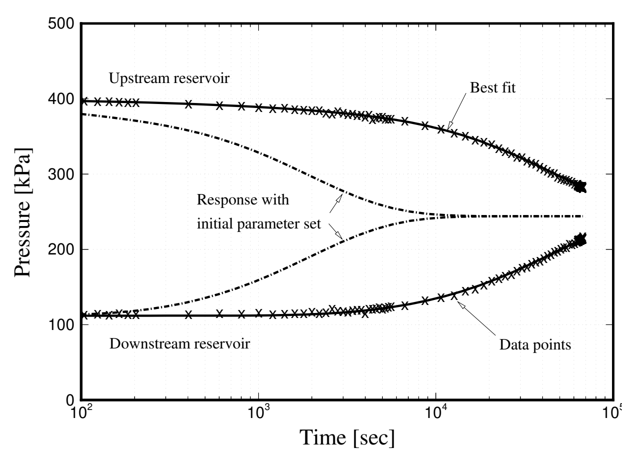

Figure 3. *Inversion of data from a GPPD experiment. Comparison between measured and calculated pressure transient curves in the upstream and downstream gas reservoirs.*

Table 2. Estimation Covariance Matrix, Inversion of One GPPD Experiment

	log(k)	log(b)	porosity
log(k)	1.67	-0.99	-0.87
log(b)	-1.90	2.16	0.87
porosity	-5.79E-4	6.59E-4	2.64E-7

Diagonal contains variances, lower triangle is covariance matrix, upper triangle is correlation matrix.

Table 3. Estimation Covariance Matrix, Simultaneous Inversion of Three GPPD Experiments.

	log(k)	log(b)	porosity
log(k)	1.05E-4	-0.52	-0.12
log(b)	-1.07E-4	4.10E-4	-0.02
porosity	-1.30E-6	-3.62E-7	1.06E-6

Diagonal contains variances, lower triangle is covariance matrix, upper triangle is correlation matrix.

The two highly correlated parameters can be effectively decoupled by simultaneously inverting data from three experiments performed at three different pressure levels. Weakening the correlation coefficient from -0.99 to -0.52 allows for a more independent determination of all parameters, thus significantly reducing the estimation uncertainty as shown in Table 3. The match to all three GPPD experiments is shown in Figure 4.

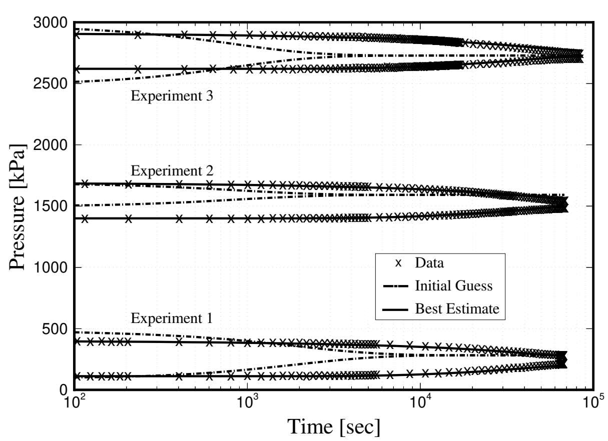

Figure 4. *Comparison between measured and calculated pressure transient curves from three simultaneously inverted GPPD experiments.*

This example shows the importance of a formalized error analysis for a comprehensive interpretation of inverse modeling results. More details about correlations, the impact of systematic errors and their removal by parameterization, and the use of robust estimators can be found in Finsterle and Persoff (1997) and Finsterle and Najita (1997).

Application 2 demonstrates the flexibility of inverse modeling. A variety of different data from an unconventional experiment are used for the determination of two-phase hydraulic properties.

Figure 5 shows a schematic of a ventilation experiment performed at the Grimsel Rock Laboratory, Switzerland. In order to determine the macropermeability of crystalline rocks, the total inflow of moisture into an isolated, ventilated drift section is measured in a cooling trap. Due to ventilation, the initially saturated granodiorite formation starts to dry out radially from the drift despite a strong water pressure gradient. By measuring the water potential using thermocouple psychrometers (TP), the gas pressure in two boreholes (see Figure 6), and the average evaporation rate, it was possible to determine the absolute permeability as well as the two-phase flow parameters of the van Genuchten model (Luckner et al., 1989). The example demonstrates that virtually any type of sensitive data can be used in a joint inversion to estimate parameters that affect the observed system behavior. This flexibility of inverse modeling can be exploited to conceive new experimental designs and to analyze a larger variety of observations obtained under natural and testing conditions. The ventilation experiment, the problem of nonuniqueness, and a nonlinear error analysis are discussed in detail in Finsterle and Pruess (1995).

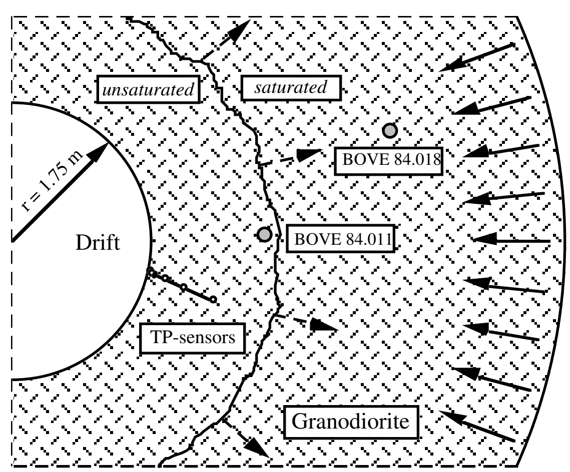

Figure 5. *Schematic of ventilation experiment, showing thermocouple psychrometer (TP) and borehole locations.*

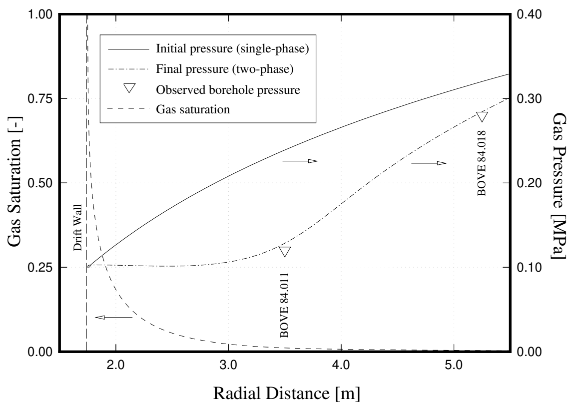

Figure 6. *Calculated gas saturation and pressure profiles after 80 days of ventilation. The measured borehole pressures are shown as triangles.*

Application No. 3 uses transient gas pressure data on a regional scale to estimate gas diffusivity of a thick, heterogeneous, unsaturated zone. Atmospheric pressure variations at the land surface are damped as they propagate through the formation. The pneumatic pressure signals observed at several levels in a deep borehole exhibit a specific time lag and reduction in amplitude depending upon gas diffusivity. Figure 7 shows the pressure fluctuations at the land surface, and the comparison between the measured and calculated pneumatic signals. Analyzing pneumatic pressures by inverse modeling provides a means to determine effective fracture network properties in the unsaturated zone on a large scale. More details can be found in Finsterle (1997b).

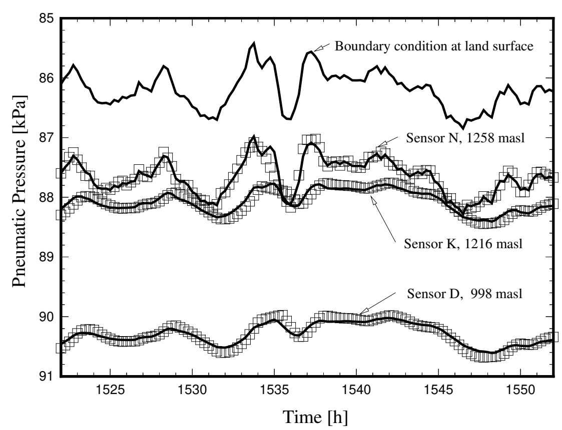

Figure 7. *Match of pneumatic pressures at three elevations in a deep borehole. The applied boundary pressure fluctuations at the land surface (1371 masl) are also shown.*

The final application presents preliminary results of an inversion of pressure and enthalpy data from a geothermal well, using a simple, one-dimensional, radial model with homogeneous rock properties. The thickness of the reservoir is assumed to be 200 m; the feed zone is at a depth of about 1600 m. Initial reservoir temperature was measured to be 336 ˚C.

Note that the pressure and enthalpy data were obtained at the wellhead, whereas the simulation results refer to downhole conditions. While heat loss and enthalpy changes along the wellbore are not expected to be large, the pressure drop, a function of flow rates and phase composition, is significant. Here, we assume that the pressure drop is independent of flow rate; it will be treated as an unknown parameter to be estimated simultaneously with the reservoir properties.

The parameters to be estimated are selected based on a sensitivity analysis. Only the most sensitive parameters of relative low overall correlation are subjected to the estimation process. They include the logarithm of the absolute permeability, porosity, initial vapor saturation, residual liquid saturation, the van Genuchten parameter n in the relative permeability function (Luckner et al., 1989), and a constant c_{well} representing the pressure drop along the wellbore.

Data from 85 days of production were used to calibrate the model. The production rate during this period varied around 4 kg/s. Data are again available after t=106 days, when production rate was increased to about 10 kg/s. This latter period was not used for calibration but for testing the model predictions. Figure 8 shows the prescribed production rate, the observed and calculated enthalpies and pressures for the initial parameter set as well as the best estimate, along with the 95% error band. The corresponding parameter sets are given in Table 4.

Comparison of the responses obtained with the initial and final parameter set demonstrates the sensitivity of the modeling results with respect to the relatively minor updates needed to improve the match. More important, it reveals the difficulties of the current model to simulate the relatively strong pressure drop between t=55 and t=70 days, without resulting in excessively low pressures once the production rate is increased. Recall that wellbore effects are not modeled. While the enthalpies are matched reasonably well (except at early times, when fracture flow may be dominant), the model fails to predict the enthalpy during the last period of high production, when most of the produced fluid in the model consists of vapor.

Table 4. *Initial Guess, Best Estimate, and Estimation Uncertainty*

Parameter	Initial Guess	Best Estimate	Standard Deviation
log (perm. [m^2])	-14.50	-14.48	0.01
porosity [-]	0.02	0.05	0.01
initial vapor sat. [-]	0.02	0.01	0.01
res. liq. sat. [-]	0.20	0.18	0.04
vG parameter n [-]	3.00	2.45	0.08
c_{well} [bar]	40.00	45.40	1.14

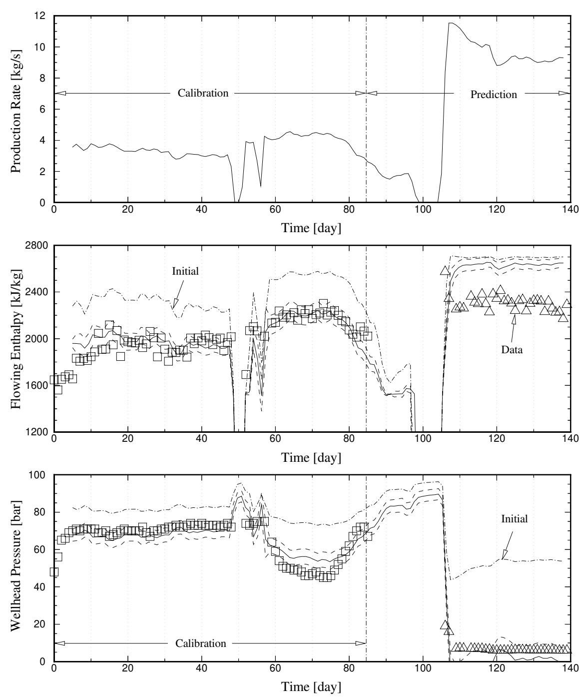

Figure 8. *Calibration and prediction of flowing enthalpy and wellhead pressure. The top panel shows the prescribed production rate. Squares are measured data used for calibration. Triangles are measured data used for validation. The dash-dotted lines are the model results with the initial parameter set (see Table 4). Simulation results based on the estimated parameter set are shown as solid lines. Error bands (dashed lines) are calculated using linear uncertainty propagation analysis.*

It should be realized that the conditions during the validation phase are quite different from the ones encountered while calibrating the model. Vapor saturation near the well is increased, i.e., the relative permeabilities are extrapolated beyond the calibrated range. It is obvious that the systematic errors in the simplified model must be eliminated before the parameter set can be further assessed.

CONCLUDING REMARKS

The purpose of this paper was to demonstrate the power and flexibility of an inverse modeling approach for automatic history matching. Four selected ITOUGH2 applications on different scales have been discussed. It was shown that model-related parameters can be estimated by performing a joint inversion of a variety of data collected under testing conditions or during production. The advantages of inverse modeling procedures are that they overcome the time and labor-intensive tedium of trial-and-error model calibration. More importantly, the formalized approach allows one to obtain objective measures of estimation uncertainty, parameter correlation, and overall goodness-of-fit.

Forward and inverse modeling improve our understanding of the basic multiphase flow processes and allow us to study the impact of parameters on model predictions. The reliability of model predictions in complicated nonisothermal multiphase flow systems strongly depends on the accuracy with which the input parameters can be determined. Inverse modeling aims at assessing and reducing the estimation uncertainties. The success of inverse modeling, however, depends on our ability to develop a model that is *in principle* capable of reproducing the observed system state. This crucial and difficult step of model conceptualization is the limiting factor in both forward and inverse modeling, because any error in the conceptual model leads to systematic prediction errors and biased parameter estimates.

The ITOUGH2 code used in these studies is continually revised and updated to account for newly incorporated physical processes, and to improve the robustness and effectiveness of the optimization algorithm.

ITOUGH2 is planned to be released through DOE's Energy Science and Technology Software Center in the summer of 1998. More

information can be obtained at the following web site:
http://www-esd.lbl.gov/ITOUGH2

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