ANALYSIS OF BOILING EXPERIMENTS USING INVERSE MODELING

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ABSTRACT

Numerical predictions of geothermal reservoir behavior strongly depend on the assumed steam-water relative permeabilities, which are difficult and time-consuming to measure in the laboratory. This paper describes the estimation of the parameters of the relative permeability and capillary pressure functions by automatically matching simulation results to data from a transient boiling experiment performed on a Berea sandstone. A sensitivity analysis reveals the strong dependence of the observed system behavior on effects such as heat transfer from the heater to the core, as well as heat losses through the insulation. Parameters of three conceptual models were estimated by inverse modeling. Each calibration yields consistent effective steam permeabilities, but the shape of the liquid relative permeability remains ambiguous.

INTRODUCTION

The experimental determination of relative permeability and capillary pressure functions for nonisothermal, single-component, two-phase flow problems as encountered in geothermal reservoir engineering is very challenging, mainly because of the need to measure saturation, matric potentials, and flow rates under high temperatures and pressures. Moreover, the standard concept of characteristic curves as saturation-dependent material properties may be inappropriate in such systems, because interfacial tension, wetting characteristics, and pore-level condensation-evaporation mechanisms are affected by temperature changes. The need for steam-water relative permeability and capillary pressure functions in numerical simulations of geothermal reservoirs prompted several investigators to analyze enthalpy data from production wells [e.g., *Grant*, 1977; *Horne and Ramey*, 1978] or to conduct steam-injection and boiling experiments in the laboratory [e.g., *Ambusso et al.*, 1996; *Satik*, 1997]. In this paper, we describe the estimation of the parameters entering the relative permeability and capillary pressure functions, by automatically matching simulation results to data from a transient boiling experiment performed on a Berea sandstone. If we use inverse modeling for parameter estimation, the functional form of the characteristic curves is part of the conceptual model, i.e., it cannot be directly inferred from the data. However, by subjecting competing conceptual models to the estimation process, we can find the function that best matches the observed data. If the match was achieved without overparameterization, the most likely model is identified.

We first discuss the inverse modeling approach implemented in ITOUGH2 [*Finsterle,* 1997a,b] and describe the boiling experiment. Next, we analyze the temperature, saturation, pressure, and heat flow data using inverse modeling with ITOUGH2.

INVERSE MODELING

Inverse modeling is a technique to derive model-related parameters from a variety of observations made on a hydrogeologic system, from small-scale laboratory experiments to field tests to long-term geothermal reservoir responses. 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]).

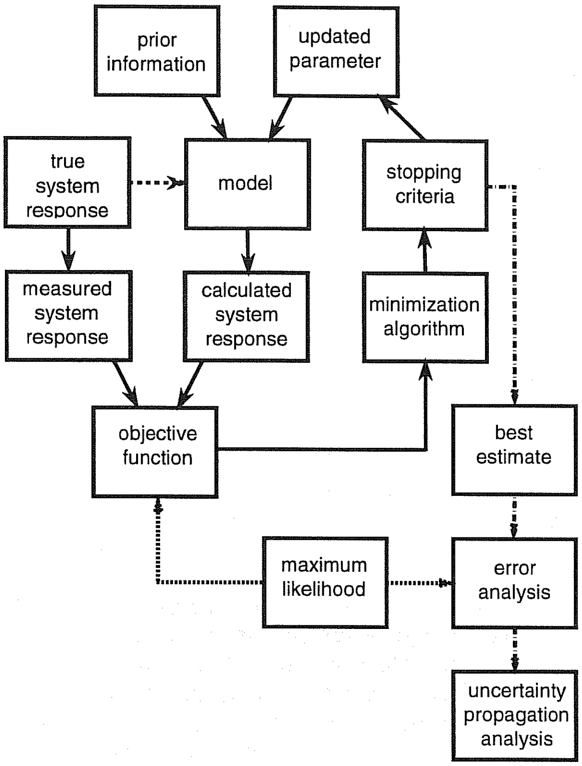

Figure 1. Inverse modeling flow chart showing main elements of automatic model calibration procedure.

The flow chart shown in Figure 1 illustrates the process and main elements of inverse modeling. The core of an inverse modeling code is an accurate, efficient, and robust simulation program such as TOUGH2 [*Pruess*, 1991] to solve the so-called forward problem. A problem- and site-specific conceptual model has to be developed, capable of simulating the flow and transport processes that govern the observed system behavior. 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:

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

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 to reduce the impact of outliers in the data or systematic modeling errors [*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. Of special interest is the covariance matrix of the estimated parameter set, which is given by

$$\mathbf{C}_{pp} = s_0^2 (\mathbf{J}^T \mathbf{C}_{yy}^{-1} \mathbf{J})^{-1} \tag{2}$$

where $\mathbf{J}$ is the Jacobian matrix, updated at the solution. Its elements are the sensitivity coefficients of the calculated system response with respect to the parameters:

$$J_{ij} = -\frac{\partial r_i}{\partial p_j} = \frac{\partial y_i}{\partial p_j} \tag{3}$$

In Equation (2), s_0^2 is the estimated error variance, a goodness-of-fit measure given by

$$s_0^2 = \frac{\mathbf{r}^T \mathbf{C}_{yy}^{-1} \mathbf{r}}{M - N} \tag{4}$$

where M is the number of observations and N is the number of parameters.

More than its efficiency, the formalized sensitivity, residual, and error analyses make inverse modeling superior to conventional trial-and-error model calibration.

BOILING EXPERIMENT

A vertical boiling experiment was performed at Stanford, taking advantage of the high-resolution X-ray computer tomography (CT) scanner, which measures porosity and steam saturation during the course of the experiment. A schematic of the experimental setup is shown in Figure 2. A 43-cm-long Berea sandstone core of radius 2.54 cm was sealed with epoxy and insulated with a ceramic fiber blanket. The core was saturated with water before being heated from the bottom. At the top, the core is open to atmospheric conditions. During the 7-day experiment, the heater power was increased stepwise, eventually reaching 10.4 Watts; boiling conditions were reached after about 5 days. Temperature, water pressure, and heat flux were measured at 41 points along the core, using thermocouples, pressure transducers and heat flux sensors, respectively; four CT scans were run at $t = 4$, 5, 6, and 7 days to measure steam saturation. The CT numbers depend on fluid density and thus temperature, which was evident during the first 5 days of heating. A simple linear correction was employed to avoid unreasonable steam saturation values in the first part of the experiment, when temperatures were below the boiling point. The differences between a CT scan of the fully liquid-saturated core and the dry core yielded a porosity estimate of 0.22. A detailed description of the experiment is given in *Satik* [1997]. Table 1 summarizes the assumed properties of the materials used in the experiment.

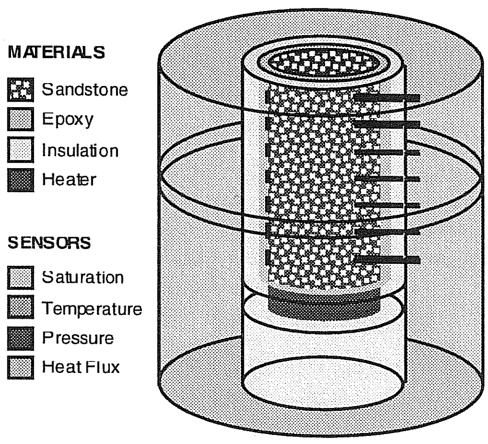

Figure 2. Schematic of experimental setup for boiling experiment.

Table 1. Thermal Properties of Materials Used in the Boiling Experiment

Material	Density [kg m^{-3}]	Heat cond. [W m^{-1} K^{-1}]	Spec. heat [J kg^{-1} K^{-1}]
Sandstone	2160	4.33 (4.93$^{\#}$)	858
Heater	2200	2.89	245
Heater insulator	530	0.13 (0.15$^{\#}$)	1047
Epoxy	1200	0.58	1047
Core insulator	192	0.09 (0.12$^{\#}$)	105

$^{\#}$ Determined by inverse modeling, see below

MODEL DEVELOPMENT

A two-dimensional, radial TOUGH2 model was developed for simulating the boiling experiment. It consists of 51 layers along the core axis, to discretize—from the bottom to the top—the heater insulation, the heater, the core, and the atmospheric boundary. In the radial direction, the model consists of 4 rings, the innermost representing the sandstone core, followed by two rings for the epoxy and the insulation material, and finally the outer boundary blocks. Material properties, nodal distances, and initial conditions for the heater and insulation materials were selected such that they were impermeable to fluid flow, but pervious to conductive heat transfer. The capillary pressure functions of *Brooks and Corey* [1964] and *van Genuchten* [1980] were modified (see *Finsterle* [1997a] for details) so that a finite value is obtained when saturation is at or below residual liquid saturation, conditions achieved as a result of boiling.

A number of forward simulations were performed to better understand the system behavior before inverse runs were initiated. During the first five days of the experiment, the temperature condition in the core depends exclusively on the heat source, the heat transfer from the heater to the core, and the thermal properties of the sandstone as well as the insulation materials, which determine heat losses. No hydrologic parameters affect the system behavior as long as single-phase liquid conditions prevail. A sensitivity analysis indicates that the heat loss from the heater as well as from the core to the environment have a significant impact on the initial steam development. Once the boiling point has been reached, the upward propagation of steam is influenced by the two-phase flow properties. Both steam and water relative permeabilities determine the pressure and temperature conditions, the steam front propagation, and saturation distribution within the core. Counterflow of liquid and steam by buoyancy and capillarity is an important mechanism transporting water to the heater, affecting the instance when single-phase steam conditions are reached and temperatures start to rise beyond the boiling temperature.

INVERSIONS

While the objective of the inversions is to estimate parameters of the steam-water relative permeability and capillary pressure functions, the discussion above reveals that the system behavior is strongly affected by a number of additional, uncertain or variable parameters, such as the absolute permeability, the thermal properties, and the source terms. Since these parameters are correlated to the parameters of interest, any errors in the fixed values will lead to errors in the estimated parameters. This problem can only be solved (1) by obtaining accurate and independent measurements of these parameters, or (2) by considering them to be unknown, and including them into the estimation process. We follow the latter approach because it helps reduce estimation bias, allows examination of parameter correlations, and provides increased, more reasonable uncertainty estimates. Furthermore, if we select the first approach, very accurate measurements of the thermal properties would be required, in order for them to be sufficiently known so they can be fixed in the model. The requirement for high measurement accuracy of the thermal parameters is a consequence of heat losses—and thus the insulation material properties—strongly affecting the experiment.

In order to reduce the correlation between the thermal properties and the two-phase flow parameters of interest, we perform the inversion in two steps. First, we estimate the thermal properties from the data obtained during the first 5 days of heating, when the temperatures were below the boiling point. In the second inversion, we fix the thermal properties and estimate hydrogeologic parameters from the remainder of the data that exhibit two-phase flow effects.

The matches to the temperature and heat flow data during the single-phase period are visualized in Figures 3 and 4, respectively. The vertical distance of the symbol to the diagonal line represents the residual. The numbers indicate the sensor locations, where Sensor 1 is closest to the heater, Sensor 2 is 3 cm higher, etc. The random scattering of the points around the diagonal line indicates that the average behavior is identified as intended by minimizing the least-squares objective function (1). Note, however, that the matches to the individual sensors are not optimal in the least-squares sense. Specifically, the heat flow rates show a systematic under- or overprediction of the heat losses at different points along the core. Since this pattern is not reflected in the temperature data, we suspect that the heat flux sensors exhibit systematic trends. Nevertheless, we believe that by estimating the heat conductivity of the insulation material from all available heat flow data, the average heat loss is well captured. The estimates are shown in Table 1.

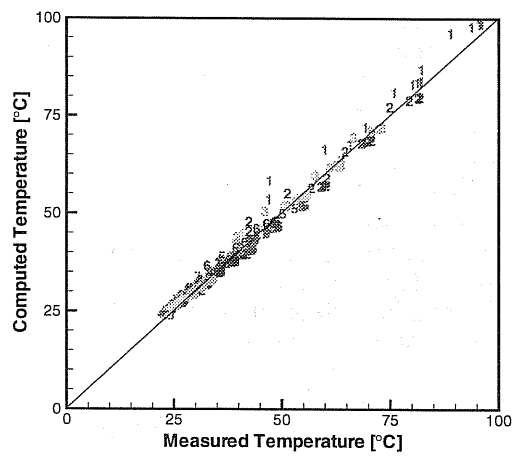

Figure 3. Measured versus calculated temperatures after calibration of single-phase period.

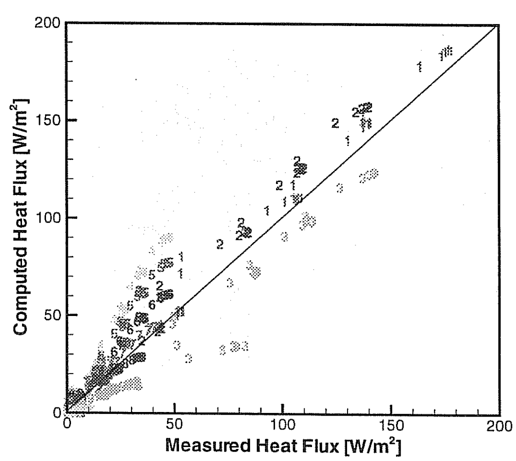

Figure 4. Measured versus calculated heat flow rates after calibration of single-phase period.

Three different relative-permeability and capillary-pressure models were calibrated against the available temperature, saturation, pressure, and heat-flow data from the boiling period. The first model consists of linear (LI) functions, the second is the Brooks-Corey (BC), and the third is the van Genuchten (VG) model as modified by *Finsterle* [1997a].

The distribution of the residuals obtained with the BC model is visualized in Figures 5 and 6; the *a priori* assumed measurement error and the *a posteriori* standard deviations of the final residuals are given in Table 2, along with the contribution of each observation type to the final value of the objective function. The assumed accuracy of the attainable match was overestimated, especially for the saturation data, which may include a systematic measurement error. The estimated error variance $s_0^2 = 5.5$, which is significantly greater than one, reflects the fact that the match is not as good as expected. Nevertheless, the contributions of each observation type to the objective function are relatively well balanced.

Using the estimated error variance as a goodness-of-fit criterion, none of the three models performs significantly better than the competing alternatives, indicating that the data do not contain sufficient information for us to distinguish among different conceptual models. This result is unfortunate, because the three models are believed to be sufficiently different from one another, such that key questions regarding the nature of steam-water relative permeabilities could have been answered by a clear preference of a specific model. For example, while the BC and VG model exhibit strong phase interference, the linear relative permeability functions suggest that steam flow is not greatly affected by the presence of liquid water. The BC and VG models also differ in regard to the presence or absence of a finite gas entry pressure, leading to a sharper or more diffuse saturation front.

Table 2. Assumed Measurement Error, Standard Error of Final Residuals, and Contribution to Objective Function (COF)

Observation type	Measurement error	Std. dev. of residuals	COF [%]
Temperature [°C]	1.0	1.9	17.2
Pressure [kPa]	1.0	1.4	12.7
Saturation [%]	1.0	0.9	33.7
Heat flux [W/m²]	10.0	27.7	36.4

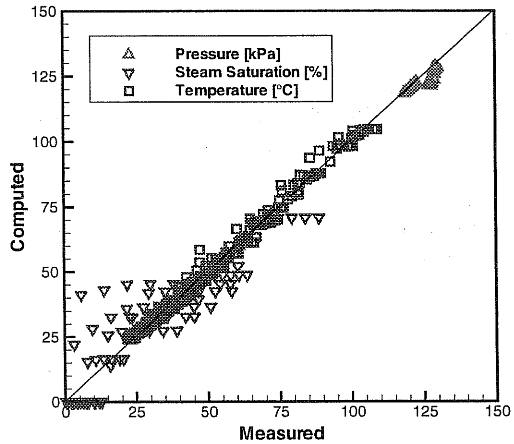

Figure 5. Measured versus calculated temperatures, pressures and steam saturations.

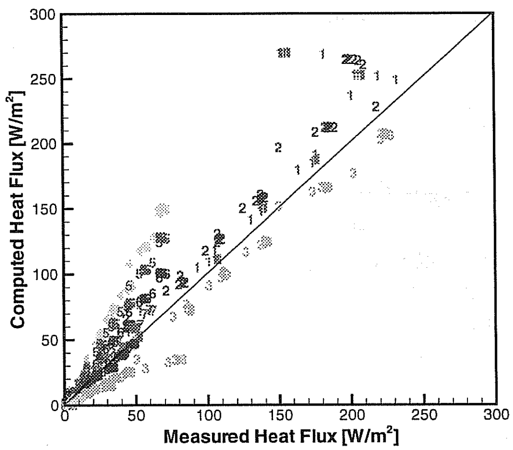

Figure 6. Measured versus calculated heat fluxes.

The relative permeability functions as obtained with the best estimate parameter sets are shown in Figure 7. The linear functions estimated by inverse modeling are in good agreement with the data obtained by *Ambusso et al.* [1996], who determined relative permeabilities by concurrently injecting steam and water into a Berea sandstone core. The VG steam relative permeability also coincides with the latter two functions. The BC function is somewhat lower, which is partly compensated for by a 50% higher absolute permeability estimate. In conclusion, the effective steam permeabilities as obtained with all three models are consistent and in agreement with the results of *Ambusso et al.* [1996]. The relative liquid permeability, however, is significantly lower in the BC and VG model as compared to LI and Ambusso et al. Since the observations made during the boiling experiment are more sensitive to steam than to liquid relative permeability, inverse modeling makes the former consistent, and allows the latter to deviate according to the restrictions imposed by the individual models. Note that unlike the BC and VG model, the linear steam and liquid relative permeability functions are independent from one another, allowing the water relative permeability to vary more easily, which eventually came to agree with the data of Ambusso et al.

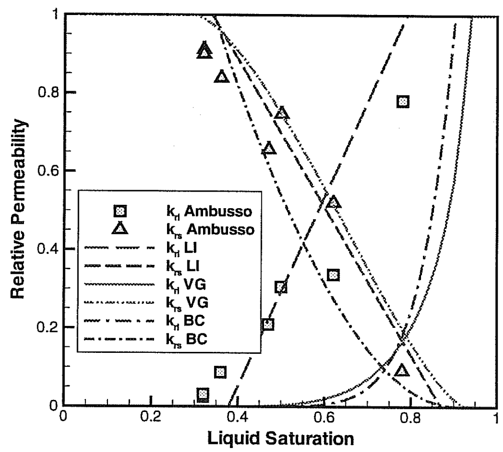

Figure 7. Relative permeability functions estimated by inverse modeling. Independent data obtained by *Ambusso et al.* [1996] are shown as symbols.

One might argue that the inverse problem as formulated here, with 6 parameters estimated for each model, is ill-posed due to over-parameterization. This is certainly true given the apparent nonuniqueness of the solution. The situation can be improved only if independent estimates for some of the key parameters can be obtained. The difficulties encountered here are also a result of the overall test design, in which two-phase flow conditions are initiated not by steam injection, but by boiling. This scheme makes the heat source the main driving force, which becomes dependent on the thermal properties of the core and the laboratory equipment, possibly introducing additional uncertainties. While the experiment provided interesting insights into the boiling process in porous media [*Satik*, 1997], a quantitative analysis of the data for the determination of steam-water relative permeability proved difficult and ambiguous.

CONCLUDING REMARKS

Temperature, steam saturation, pressure, and heat flux data from a vertical boiling experiment were used to estimate thermal and hydrogeologic properties of a Berea sandstone core. Since heating was the only driving force in this experiment, the development of a two-phase flow field was strongly coupled to the temperature conditions in the core. Consequently, the thermal properties, not only of the sandstone, but also of the insulation material, became a major factor in understanding the system behavior. From an inverse perspective, the high sensitivity of the insulation and heater properties, as well as the strong correlation of these properties to the parameters of interest, make it difficult to obtain accurate estimates.

All three conceptual models used for calibration yield similar matches to the data, i.e., no conclusive statement about the appropriate form of the relative permeability functions can be made. However, all three models produce consistent effective permeabilities for the steam phase, which is a major factor governing the propagation of the boiling front.

The comprehensive analysis of all available data from a nonisothermal multiphase flow experiment provided insight into the coupling of processes and the correlation of parameters. This information is useful for the design of future experiments.

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