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### Publication Date

1995-05-01



# Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

## EARTH SCIENCES DIVISION

Presented at the International High Level Radioactive Waste Management Conference, Las Vegas, NV, May 1, 1995, and to be published in the Proceedings

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LBL-36527  
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**Inverse Modeling as a Step in the Calibration of the  
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This work was supported by the Director, Office of Civilian Radioactive Waste Management, Yucca Mountain Site Characterization Project Office, Suitability and Licensing Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

# INVERSE MODELING AS A STEP IN THE CALIBRATION OF THE LBL-USGS SITE-SCALE MODEL OF YUCCA MOUNTAIN

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## ABSTRACT

Calibration of the LBL-USGS site-scale model of Yucca Mountain is initiated. Inverse modeling techniques are used to match the results of simplified submodels to the observed pressure, saturation, and temperature data. Hydrologic and thermal parameters are determined and compared to the values obtained from laboratory measurements and conventional field test analysis.

## I. INTRODUCTION

The three-dimensional site-scale model of the unsaturated zone at Yucca Mountain developed by Lawrence Berkeley Laboratory (LBL) and United States Geological Survey (USGS) has been continuously updated, taking into account new data as they become available. Adjustments of thermal and hydrologic parameters as well as boundary fluxes are performed in order to calibrate the model so it reproduces the saturation, capillary pressure, and temperature distributions measured in boreholes. The calibrated site-scale model is being used to predict conditions in new boreholes and in the Exploratory Study Facility (ESF).

## II. CALIBRATION PROCESS

Calibration of the Yucca Mountain site-scale model is an inherently iterative procedure involving several cycles of data and model analysis. First, the data intended to be used for calibration are reviewed to assess their uncertainty, and to identify potential systematic deviations from their model counterparts. Next, the relative weighting between data of different types (e.g. saturation, moisture tension, temperature, etc.) as well as the prior estimates of the thermal and hydrologic parameters is determined. Numerical models of increasing complexity (higher

dimensionality, incorporation of additional physical processes, etc.) are developed and calibrated against the available data using non-linear optimization algorithms. The residuals are interpreted, pointing towards aspects of the model that need to be modified. Simulation of moisture and gas flow as well as heat transport is performed using the TOUGH2<sup>1</sup> code, and ITOUGH2<sup>2</sup> ("Inverse TOUGH2") is used for automatic model calibration.

The site-scale model of Yucca Mountain is being calibrated against moisture tension and saturation data from various wells at Yucca Mountain. The approach used is to apply ITOUGH2 along with simple one- and two-dimensional models to match the observed data and then incorporate the resulting parameters into the three-dimensional model. This procedure has started with wells UZ-16 and UZ-14 and data from more wells will be added.

## III. RESULTS

Figure 1 shows the fit between the observed and calculated saturation profile at borehole UZ#16. Steady-state infiltration of 0.1 mm/year is calculated in a one-dimensional model, taking into account phase interferences, gravity and capillary forces. Formation properties are taken from the three-dimensional site-scale model<sup>3</sup>, and reasonable variances are assigned to both the saturation data and the initial parameter values. Absolute permeabilities and the air entry pressures  $1/\alpha$  of the van Genuchten model are updated in order to fit the saturation profiles without deviating significantly from the prior parameter values which are based on laboratory measurements and conventional analysis of field tests. The differences between the prior information values and the parameter estimates after model calibration are shown in Figure 2. This preliminary calibration indicates that a more sophisticated model structure is required to integrate field

observations of state variables and laboratory measurements of rock properties into a consistent numerical site-scale model. For example, two- and three-dimensional effects would have to be considered to properly account allow for lateral movement of moisture, water vapor removal from the upper part of Yucca Mountain, and density effects due to the geothermal gradient. Incorporation of moisture tension, temperature and gas flow data into the inverse problem formulation will reduce non-uniqueness of the inverse problem and thus improve the identifiability of model parameters.

#### IV. CONCLUSIONS

We have initiated the calibration process for the LBL-USGS three-dimensional site-scale model. Thermal and hydrologic parameters are determined by calibrating numerical models against available saturation, temperature, and capillary pressure data. Inverse modeling techniques have been applied to simplified submodels in order to identify sensitive parameters, and to investigate the importance of specific hypotheses and processes. Calibration of two-dimensional cross-sections through Yucca Mountain are being performed as an intermediate step toward the calibration of the three-dimensional site-scale model.

#### ACKNOWLEDGMENT

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Yucca Mountain Site Characterization Project Office, Suitability and Licensing Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

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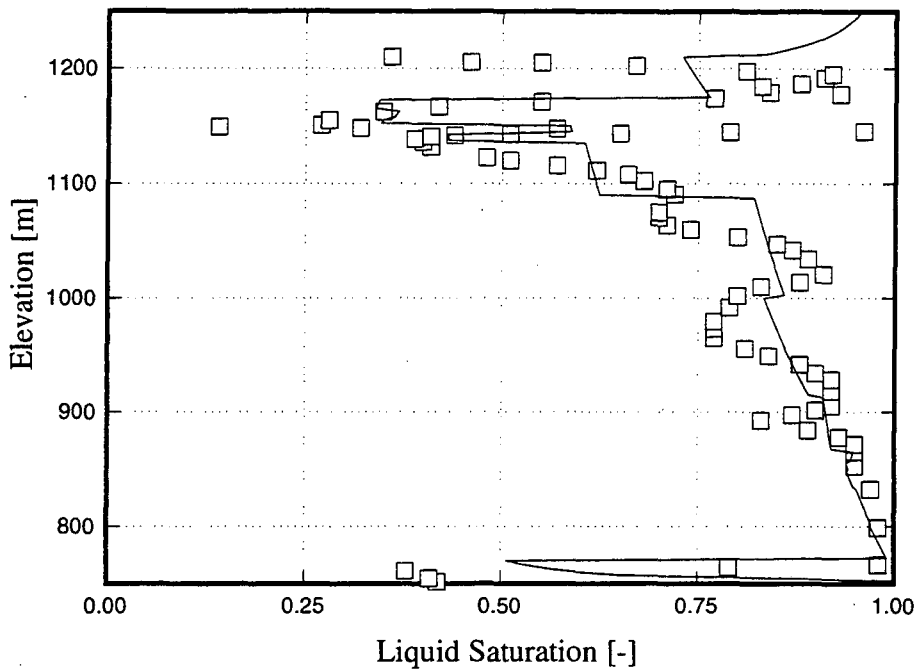


Figure 1: Fit between the observed (symbols) and calculated (solid lines) saturation profile at UZ#16, using a one-dimensional steady-state model.

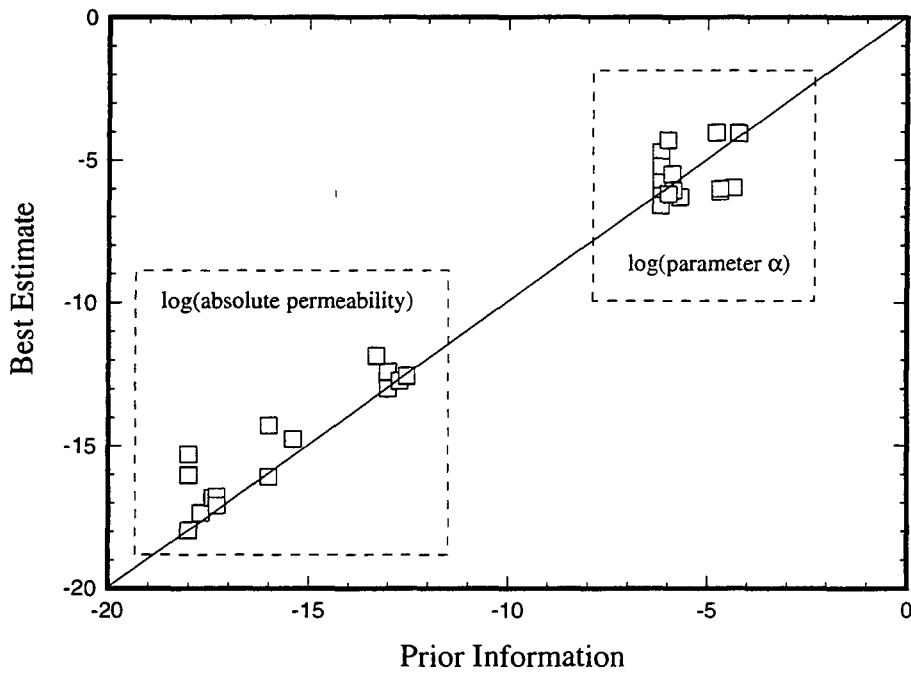


Figure 2: Difference between parameter estimates and their prior values. The optimum parameter set is determined by fitting the observed saturation profile at UZ#16.

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