Characterization and Prediction of Subsurface Pneumatic Pressure Variations at Yucca Mountain, Nevada

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Yucca Mountain, Nevada is being investigated as the proposed site for geologic disposal of high level nuclear waste. A massive data collection effort for characterization of the unsaturated zone is being carried out at the site. The USGS is monitoring the subsurface pressure variations due to barometric pumping in several boreholes. Numerical models are used to simulate the observed subsurface pressure variations. Data inversion is used to characterize the unsaturated system and estimate the pneumatic diffusivity of important geologic features. Blind predictions of subsurface response and subsequent comparison to recorded data have built confidence in the models of Yucca Mountain.

Introduction

Barometric pumping of the subsurface was first described by Buckingham (1904), and he provided an analytical solution for gas pressure as a function of depth for the idealized conditions of a single homogeneous layer bounded above by a sinusoidally varying pressure boundary condition and bounded below by an impermeable boundary. Actual field measurements of subsurface response to barometric pumping have been used to estimate hydrologic properties by several researchers. Stallman (1967) and Stallman and Weeks (1969) describe estimation of permeability assuming a single layer bounded below by an impermeable boundary. Rozsa et al. (1975) describe estimation of diffusivity assuming a semi-infinite model. Weeks (1978) describes a numerical technique for estimation of permeability of a multilayered system and results from several field tests. Shan (1995) describes an analytical solution to the multilayered problem and its application to field data from one site.

This paper will present the results of subsurface pneumatic pressure data inversion using ITOUGH2 (Finsterle, 1997a), an automated inversion program based on the TOUGH2 (Pruess, 1991) multiphase numerical simulator. *In situ* measurements of surface and subsurface pneumatic pressure, gathered by the USGS, are used together with geologic based numerical models of Yucca Mountain to estimate the pneumatic diffusivity of several layers.

Site Description

Yucca Mountain, Nevada, located approximately 120 km northwest of Las Vegas, is the proposed location for a geologic repository designed to permanently store high level radioactive waste. Many surface based boreholes have been drilled in the Yucca Mountain area and several of these have been instrumented to monitor *in situ* air pressure. A 9 km long tunnel, the Exploratory Studies Facility, ESF, has been excavated to nearly 300 m below the surface in the unsaturated zone.

The unsaturated zone at Yucca Mountain is up to 700 m thick. The volcanic rocks that make up the unsaturated zone are alternating layers of welded and nonwelded ash flow and air fall tuffs. Figure 1 shows a cross section with the hydrogeologic units of Montazer and Wilson (1984) labeled. These units are based mainly on degree of welding. From the surface down, these units are the Tiva Canyon welded (TCw), the Paintbrush nonwelded (PTn), and the Topopah Spring welded (TSw). The TCw and TSw are highly fractured and very permeable to air. The PTn is less fractured and much more porous than the overlying or underlying units making it an impediment to gas flow and thus an important layer to characterize. Sublayering of the PTn using the nomenclature of Buesch et al. (1995) is also shown on Figure 1. The Yucca Mountain and the Pah Canyon Tuffs, Tpy and Tpp, respectively, are partially welded while the other PTn sublayers are nonwelded, bedded tuffs. Very little pneumatic pressure data is available to characterize rocks below the TSw.

Data

Subsurface gas (pneumatic) pressure data have been collected at twelve boreholes on the Yucca Mountain site by several principal investigators and organizations. For this paper, data from two boreholes, NRG-6 and NRG-7a, are analyzed. Data from NRG-7a, shown in Figure 2, are characteristic of a typical data set. The pressure at the land surface shows the largest variation (and the lowest pressure because it is at the highest elevation). With increasing depth below the surface, the pressure signal shows increasing amplitude

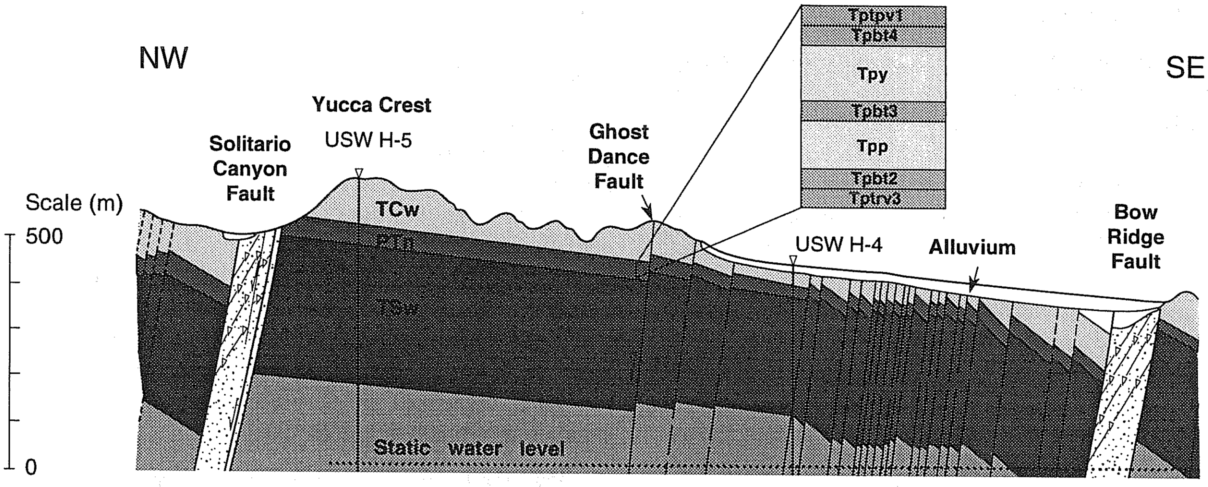

Figure 1. Cross-section of Yucca Mountain, Nevada, showing stratigraphic location of major hydrogeologic units (modified from Scott and Bonk, 1984). PTn is expanded to show sublayering. Vertical exaggeration is approximately 2:1.

attenuation and time lag with respect to the surface signal.

Both boreholes have one instrument station at the surface and one in the TCw. In NRG-6, there is one instrument station in PTn sublayer Tpp and five in the TSw. In NRG-7a, there is one instrument station in PTn sublayer Tpy and three in the TSw.

Physical Processes

Barometric pressure variation at the land surface is due to a variety of causes, each having a different characteristic period. Short period variations, which occur daily (diurnal) and every half day (semi-diurnal), are due to heating and cooling of the atmosphere and tidal effects. Longer period variations, on the order of days to weeks, are due to weather and frontal systems as they move across the earth's surface. The longest period variation occurs yearly and is due to seasonal heating and cooling of the atmosphere. This variation is more pronounced away from the equator where there are larger annual temperature variations.

The pneumatic diffusivity of the system is the property that describes how much attenuation and lag the barometric signal will undergo as it propagates into the subsurface. Pneumatic diffusivity is defined here as

$$D_g = \frac{k\overline{P}}{n_g \mu}$$

where D_g is pneumatic diffusivity, k is the intrinsic (saturated) permeability times the relative gas permeability at the prevailing saturation, n_g is the drained porosity (total porosity times gas saturation), μ is the dynamic viscosity of the gas, and $\overline{P}$ is the average gas pressure. Similar expressions are given by Weeks (1978) and Shan (1995).

The conceptual model of gas flow at Yucca Mountain is that gas flow occurs on a mountain scale mainly in the fractures. The gas filled matrix porosity in the welded units is not thought to contribute significant storage for transient gas flow because the high prevailing liquid saturation significantly reduces the already low matrix permeability for gas flow. In the nonwelded PTn, higher intrinsic matrix permeability coupled with lower matrix liquid saturation mean that matrix storage does affect transient gas flow in this unit.

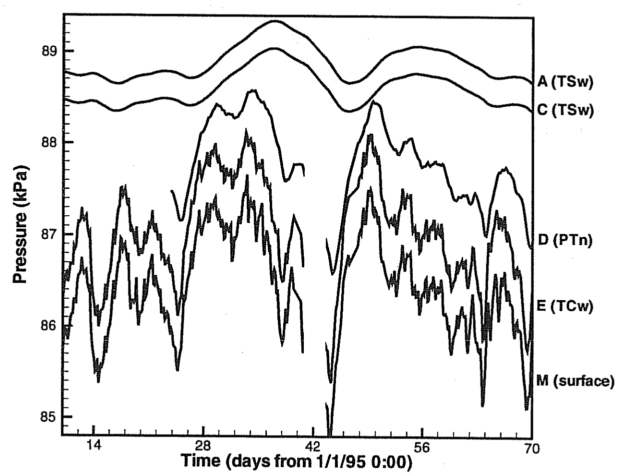

Figure 2. *In situ* pneumatic pressure data from borehole NRG-7a representing data sets typical of Yucca Mountain. Instrument stations are located in the middle TSw, upper TSw, PTn, and TCw geologic layers, and the surface. Sixty (60) days of data are shown from January 11th until March 12th, 1995.

Code Modifications

In order to apply a transient pressure boundary condition, it was necessary to slightly modify ITOUGH2 (Finsterle, 1997a). Moridis and Pruess (1992) recommend using large boundary elements and applying a similarly large source or sink to the boundary element in order to apply a transient pressure boundary condition to a model. For this problem, that technique did not work well, mainly because of the large number of barometric pressure data points necessary to adequately describe the surface pressure signal (no less than 8 per day for simulations that are 60 days long). We found that in order to use this technique it was necessary to use ITOUGH2 on the generation table to optimize the source and sink values to better match the observed surface pressure data. Even then, the match was not always satisfactory.

In order to directly use the surface pressure data, we have implemented a tabular input to ITOUGH2 that describes the transient pressures at the surface boundary element (Finsterle, 1997b). The input table includes a table of times at which the surface pressure is defined and tables of pressures at those times for each boundary element. Defining pressures for each element allows mean pressure differences due to elevation difference to be included. At each time step, the pressure for each element named in the table is calculated by linear interpolation, and that pressure is passed to the EOS module for calculation of other primary and secondary variables.

Pneumatic Data Inversion

One-dimensional, vertical models of the stratigraphy at boreholes NRG-6 and NRG-7a are used to simulate the effect of barometric pumping on the subsurface, which is assumed to be a one-dimensional, vertical process. Water is assumed to be immobile over the time scale of the simulations (60 days to several years). This assumption is based on the low estimates of infiltration to the unsaturated zone at Yucca Mountain, an average of approximately 5 mm/yr over the site, and the low matrix permeability of the rocks that make up Yucca Mountain, on the order of milli-darcys to micro-darcys. With the assumption of immobile water, a single continuum model is assumed to be adequate for simulation of the pneumatic system. These models extend from the mountain surface to the water table.

No flow boundary conditions are specified on the lateral boundaries and at the lower boundary, which is coincident with the water table. A time varying pressure boundary condition is applied to the upper boundary that simulates the observed barometric pressure signal, as explained above.

Initial conditions are gas static equilibrium (i.e., gravity equilibrium in the gas phase) with the initial boundary pressure. Because the barometric pressure is constantly changing, gas static conditions are never actually expected to exist. Therefore, the simulation is allowed to run for 30 days so that the subsurface pressures are in a dynamic state reflecting the constantly changing conditions in the mountain. Only after 30 days of simulation time are the observed pressures compared to the calculated pressures for estimation of pneumatic diffusivity.

Practically, because diffusivity is proportional to the ratio of permeability to porosity, ITOUGH2 estimates either permeability or porosity; a value for the other parameter is assumed. In this case, we assume a value for the porosity of each layer and estimate the permeability.

Time step size is limited to six hours so that the diurnal component of the barometric signal is appropriately simulated.

Because the welded layers are intensely fractured, they have a very high diffusivity. This can be seen in Figure 2. There is very little difference between the surface signal and the signal recorded in the TCw (i.e., there is little difference between the amplitude and phase of the two signals; mean pressure difference is caused by a difference in elevation between the instrument stations). There is no difference between the two signals recorded in the TSw. The largest change in the signal that is observed occurs across the PTn, from instrument station E to instrument station C. For the inverse problem, we have chosen to estimate five values of diffusivity corresponding to five sublayers in the PTn. These five sublayers are 1) Tpcpv1 and Tpbt4, 2) Tpy, 3) Tpbt3, 4) Tpp, and 5) Tpbt2 and Tptrv3 as shown in Figure 1.

Data from both NRG-6 and NRG-7a are jointly inverted. This means that models of both boreholes are run simultaneously. Data from both NRG-6 and NRG-7a are matched to the computed pressures. A single value of diffusivity is estimated for each geologic layer and applied to that layer in the models of both boreholes. This assumes that each geologic layer at Yucca Mountain is homogeneous. By making this assumption, we have better constrained the problem by increasing the amount of data that is inverted for the estimation of any one parameter.

The optimized match between the data and the simulation for borehole NRG-7a is shown in Figure 3 (a). Note that the amplitude attenuation at instrument station D appears to be slightly over-predicted by the simulation, and the lag at instrument station C is under-predicted.

As a comparison, the data from each borehole are individually inverted (i.e., the layers are not assumed to be homogeneous between the two borehole, thus separate estimates of diffusivity are made for the layers in each of the boreholes). Figure 3 (b) shows the comparison between the observed data and the calculated pressures for borehole NRG-7a. Note that the amplitude at instrument station D and the lag at instrument station C predicted by the simulation appear to match the observed data better than in the joint inversion.

ITOUGH2 also provides a quantitative assessment of the match between the data and the simulation. The mean and the standard deviation of the residuals (difference between observation and simulation at each data point) give a measure of the goodness of fit. Table 1 shows the mean and standard deviation of the residuals for each borehole for both the joint and individual inversions. With the exception of the mean for NRG-6, the numbers indicate an improved match for the individual inversions. The increase of the mean from the joint to the individual inversions for borehole NRG-6 reflects a small systematic error between the observed and predicted pressures.

Although the individual inversions provide a better match to the data, the uncertainty of the diffusivity estimates is expected to increase. This is because less data is being used for each estimate of diffusivity. In the joint inversion, there were estimates of diffusivity for five layers; in the individual inversion, the same amount of data was used for two estimates of diffusivity for each layer or nine estimates of diffusivity (the Tpy layer is not present in NRG-6). ITOUGH2 also provides a measure of the uncertainty of each parameter estimate. Figure 4 shows the diffusivity estimates and the uncertainty of the estimate for each layer from each of the three inversions. Note that the values of uncertainty are not meant to reflect all the uncertainty in the system, but are measures of relative uncertainty between the different inversions. For three of the sublayers, the uncertainty of the individual inversion estimates is increased with respect to the joint inversion estimate, as expected. The small uncertainty of the joint inversion estimate of Tpbt3 diffusivity (as compared to the individual inversion estimates) is because data from the overlying layer (from NRG-7a) and underlying layer (from NRG-6) are used in the inversion effectively bounding layer Tpbt3. Interestingly, the uncertainty of both individual inversion estimates for layer Tpbt2/Tptrv3 and one for layer Tpp are less than the uncertainty of the joint inversion estimate for those layers. Both boreholes have several instrument stations in the TSw, and all this data was used in the inversions. The improvement of the overall match between the simulation and the

Borehole	Joint		Individual	
	Mean [Pa]	Std. Dev. [Pa]	Mean [Pa]	Std. Dev. [Pa]
NRG-6	13.8	80.1	15.4	78.9
NRG-7a	26.2	70.0	24.4	62.2

Table 1. Comparison of mean and standard deviation of residuals for joint vs. individual inversion of *in situ* pneumatic pressure data.

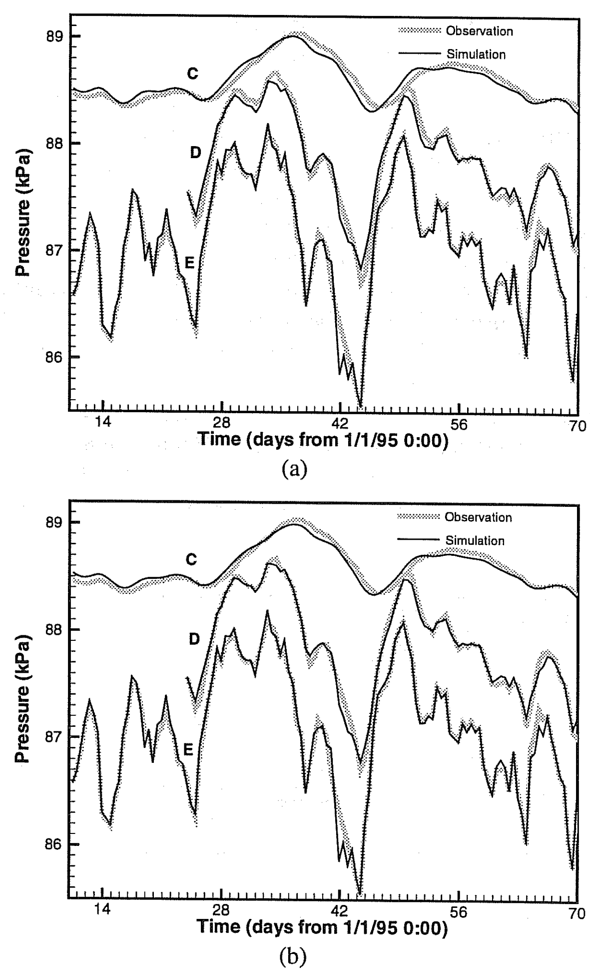

Figure 3. Simulated pressure response at stations C (upper TSw, D (PTn) and E (TCw) in borehole NRG-7a using diffusivity estimated by joint inversion of NRG-6 and NRG-7a data (a) and individual inversion of NRG-7a data (b).

observations for the individual data inversion is significant because the TSw data represents a large portion of the data being inverted. The improved match between simulation and observation means that the estimates of diffusivity between the lowest instrument station in the PTn and the highest in the TSw are more certain.

Prediction

Once the models are calibrated through data inversion, predictions of the subsurface response to barometric pumping are made for portions of the observed data not used in the calibration. The predictions allow evaluation of the models under different conditions than those of calibration, providing insight into possible conceptual model deficiencies.

Figure 5 shows the predicted pressures at instrument station D in the upper TSw. From day 196 (July 16, 1995) through day 270 (September 28, 1995), the simulation matches the observation reasonably well, indicating that the conceptual model and the calibration from the previous time period are valid.

However, after day 270, the simulation systematically over-predicts the amplitude attenuation at station D. Since we know that the model has not changed, we can assume that the real system has changed. In the original conceptual model, it was assumed that NRG-6 was too far from the ESF tunnel to be affected by the barometric signal introduced into the subsurface through the tunnel. This was confirmed because when the tunnel excavation passed closest to NRG-6 no change in the signal was observed. However, around the same time as the change in the observed data, excavation of the ESF tunnel intersected a fault (beyond the point of closest approach to NRG-6) that also passes near NRG-6. It seems very likely that the barometric signal is transmitted from the ESF, through the fault, which is assumed to have a high diffusivity, to instrument station D in NRG-6. This would account for the added amplitude in the observed signal after September 28.

Conclusions

Measurements of the subsurface response to barometric pumping of the unsaturated zone can be used to determine pneumatic diffusivity. In this study, we have used independently determined geology to define layering in two boreholes. Diffusivity of these layers is then estimated through inversion of observed time-series pressures from the subsurface. Using the data from two boreholes, we have compared the match between observation and simulation for a joint inversion and individual inversions and compared the uncertainty of the estimated parameters for the joint and individual inversions. In both cases, the matches between observation and simulation were reasonable though slightly better for the individual inversions. At the same time, the uncertainty of the estimated parameters increased for six of the nine individual inversion estimates with respect to the uncertainty of the joint inversion estimates. Because the match for the individual inversions is not overwhelmingly better or the uncertainty of the diffusivity estimate much less for the joint inversion, one technique does not seem to be clearly better than the other for this case. If the assumption of layer homogeneity were absolutely true, then the joint inversion should have been the better approach. If, however, the layers were strongly heterogeneous, then the individual inversion should have been clearly better. This would seem to indicate that the system is strongly heterogeneous between layers and homogeneous or weakly heterogeneous within layers.

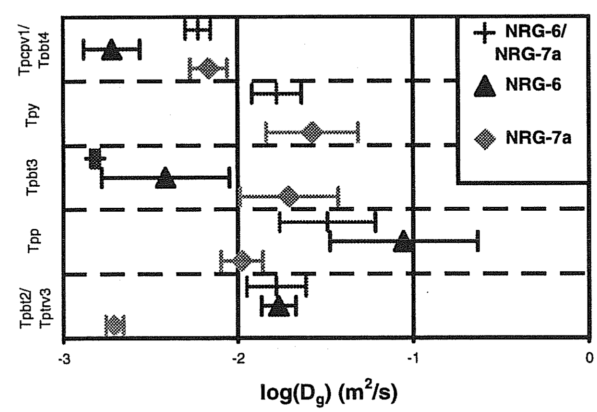

Figure 4. Estimated diffusivity and uncertainty of the estimates from joint and independent inversions of NRG-6 and NRG-7a data.

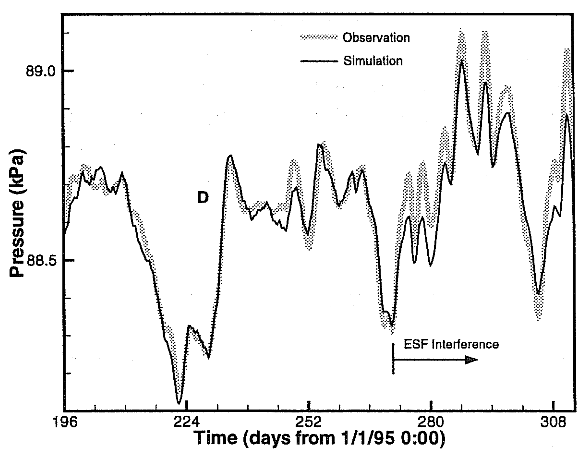

Figure 5. Prediction of pressures at instrument station D (upper TSw) in NRG-6.

Predictions of subsurface response, based on calibrated models, have helped to validate not only the estimated values but also the conceptual model of gas flow. The predictions have also pointed out where and when other factors, such as the introduction of the barometric signal into the subsurface by the ESF tunnel, are of importance to the models.

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