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Post-Test Comparison of Thermal-Hydrologic Measurements and Numerical Predictions for the In Situ Single Heater Test, Yucca Mountain, Nevada

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ABSTRACT

The Single Heater Test (SHT) is a sixteen-month-long heating and cooling experiment begun in August, 1996, located underground within the unsaturated zone near the potential geologic repository at Yucca Mountain, Nevada. During the 9 month heating phase of the test, roughly 15 m^3 of rock were raised to temperatures exceeding 100 °C. In this paper, temperatures measured in sealed boreholes surrounding the heater are compared to temperatures predicted by 3D thermal-hydrologic calculations performed with a finite difference code. Three separate model runs using different values of bulk rock permeability (4 microdarcy to 5.2 darcy) yielded significantly different predicted temperatures and temperature distributions. All the models differ from the data, suggesting that to accurately model the thermal-hydrologic behavior of the SHT, the Equivalent Continuum Model (ECM), the conceptual basis for dealing with the fractured porous medium in the numerical predictions, should be discarded in favor of more sophisticated approaches.

KEYWORDS

Thermal, hydrology, hydraulic permeability, heating, Yucca Mountain, nuclear waste, numerical analysis.

INTRODUCTION

This paper presents the results of comparing thermal-hydrologic numerical models with experimental results of an in situ heater test conducted in the tuffaceous rock at Yucca Mountain, Nevada. The Yucca Mountain site is currently under investigation by the United States Department of Energy as the nation's first geologic repository for high-level radioactive wastes. Potential repository wastes will include spent nuclear fuel from commercial reactors with some defense high level waste.

The potential repository horizon is located deep within the unsaturated zone at Yucca Mountain, approximately 300-350 m below the ground surface and 250-300 m above the water table. The placement of heat generating wastes into a partially saturated, densely welded geologic medium will initiate thermally driven processes such as gas and water vapor movement, liquid flow, phase-change, heat transfer processes, and mechanical and chemical alteration to the ambient rock hydrologic properties. Quantification of these heat-driven processes will be essential for input into future performance assessment modeling studies of the

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mountain and repository. Site characterization efforts include performing heater experiments at the potential repository location in order to gain an understanding as to the extent and nature of the disturbance to the natural system as a consequence of a thermal perturbation.

Two heater tests have been planned at the Exploratory Studies Facility (ESF) at Yucca Mountain. The first was an in situ Single Heater Test (SHT) in which a single, 5 meter long line heater was emplaced directly into the potential repository host rock, the Topopah Spring Welded tuff (TSw2). The SHT was a 16 month-long heating and cooling experiment which commenced in late August, 1996 and ended in December, 1997. During the experiment, the host rock was heated for 9 months in order to determine how heat from stored high-level radioactive waste might affect coupled thermal-hydrologic-mechanical-chemical (T-H-M-C) processes. Following deactivation of the heater, the block was monitored for an additional 7 month cooling period so that the effects of re-wetting can be evaluated. The second test, which is referred to as the Drift Scale Test, is an in situ large-scale room and guard heater experiment in which heat driven processes on a drift scale will be studied. In this paper, we will compare the results from numerical models to the experimental data obtained from the heating phase of the SHT only.

Experimental Processes

The SHT set-up consists of a single heater element, 5 m in length, placed in an in situ block of TSw2 welded tuff approximately 13 m wide, 10 m long, and 5 m high (Fig. 1). The front face and two vertical sides of the block are defined by subsurface mined drifts 5 m high, while the top, bottom and back of the block are continuous with the host rock. The heater operated at approximately 3.8 kW of continuous power output for 9 months. A monitored cooling phase continued for 7 months after the heater was turned off. Temperature measurements were made on the heater surface, in the host rock and on the surfaces of the block, using approximately 300 thermocouple and resistance temperature device (RTD) sensors. (Fig. 1).

THERMAL-HYDROLOGIC (T-H) MODEL

Three-dimensional thermal-hydrologic (T-H) calculations were performed using the finite difference code TOUGH2 (Transport of Unsaturated Groundwater and Heat; Pruess, 1991). This computer code determines the coupled, simultaneous transport of heat (conduction and convection), liquid water, water vapor, and air in a partially saturated, fractured porous medium. The thermal and hydrologic material property data such as permeability, porosity, fracture frequency, grain density, heat capacity, and thermal conductivity required for the calculations are all based on site-specific data. The 3-D T-H model was used to quantify the vaporization and mobilization of in situ water in response to a heat source.

The porous medium contains both fractures and rock matrix, each with its own set of characteristic properties. Typical conceptual models used to characterize such a system include an equivalent continuum model (i.e., an equivalent porous medium with averaged fracture and matrix properties), a dual permeability model (i.e., a porous medium containing separate fracture and matrix continua), and a random, discrete fracture model. This analysis makes use of the equivalent continuum model (ECM) for computational efficiency. The ECM assumes that capillary pressure and thermal equilibrium exist between the fractures and matrix. The fracture and matrix properties are pore volume averaged to produce parameters that represent a single effective porous material. The effective porous material can behave as matrix or fracture depending on the phase of the fluid and the bulk liquid saturation of the material.

Models were run with three different values of bulk rock permeability. The Low and High Permeability Models reflect the range of permeabilities measured at the site using air permeability testing (5.0×10^{-15} m^2 to 5.2×10^{-12} m^2). The Matrix Permeability case represents an unrealistic end-member situation in which the fractures do not exist at all and the bulk permeability of the rock is equivalent to the permeability of the matrix (4.0×10^{-18} m^2). It is assumed in this analysis that the rock fracture and matrix properties are homogeneous and isotropic. A more detailed description of the models, including descriptions of the mesh, the boundary conditions and the initial conditions, can be found in Francis et al. (1997).

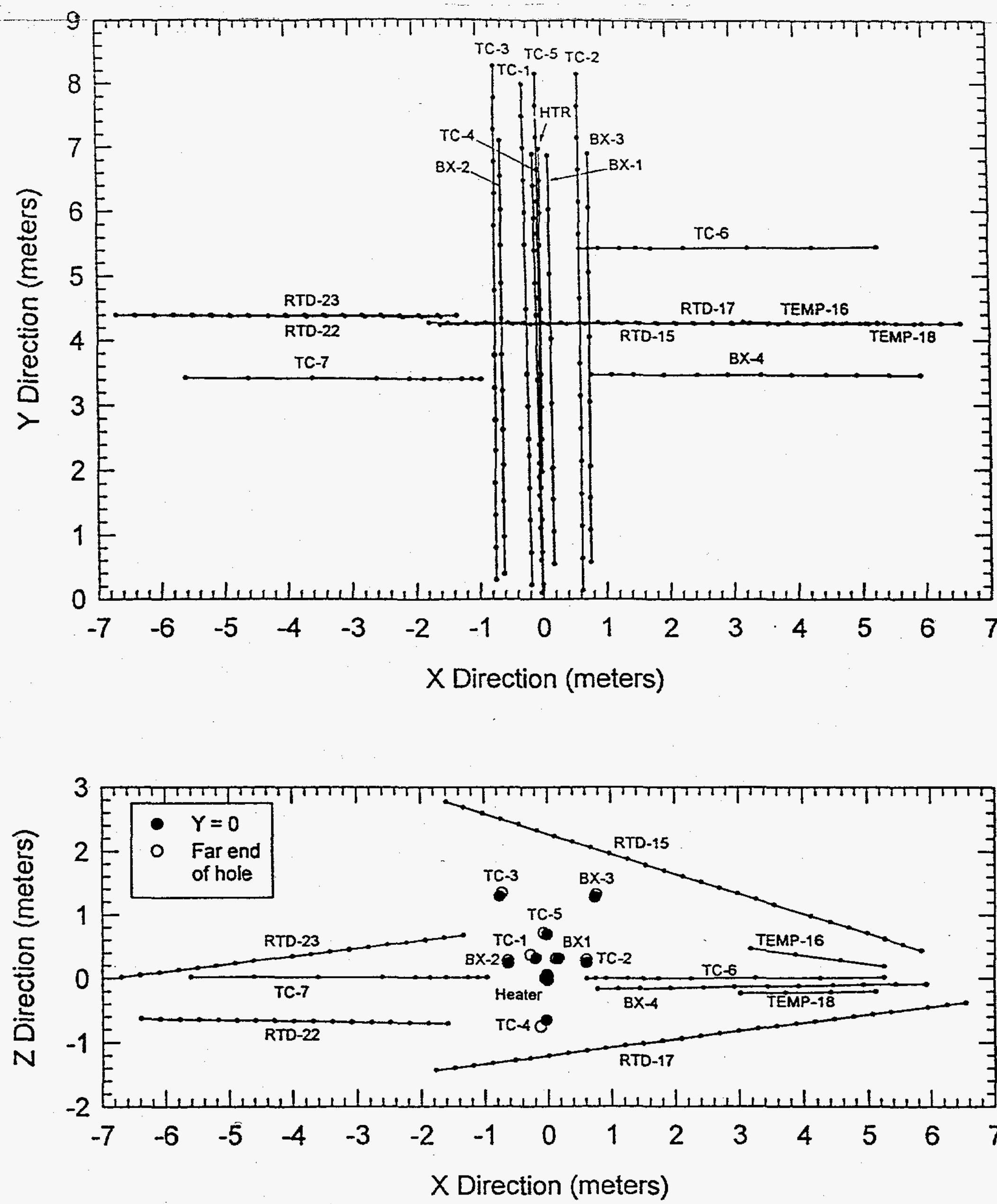

Figure 1 - Plan and cross section through the SHT block, showing locations of the heater and temperature gages.

THERMAL-HYDROLOGIC MODEL COMPARISON TO MEASURED DATA

Figure 2 illustrates the measured and predicted temperatures as a function of time at the location of temperature gage TMA-TC-1A-7, located about 41 cm away from the heater. Note the behavior of the model temperatures as the rock warms through the boiling point of water (96°C at the SHT elevation). In the high permeability model, the rock near this gage location remains at the boiling point for several weeks. As the water in the rock pores boils, all the thermal energy entering the rock near this gage location is devoted to boiling water rather than raising the rock temperature. After all the water has boiled off, the rock temperature begins to rise once again.

The low permeability model exhibits an inflection in the temperature profile near the boiling point, but not an isothermal period as did the high permeability model. When the rock near the location of gage TMA-TC-1A-7 reaches 96°C in the low permeability model, the water in the pores begins to boil, but the water vapor is somewhat inhibited from escaping from the pores of the rock, so the pore pressure begins to build. This increase in pressure causes the boiling point of water to rise. The result is that not all of the thermal energy entering the rock is consumed by the process of boiling water; a portion is devoted to raising the temperature of the rock.

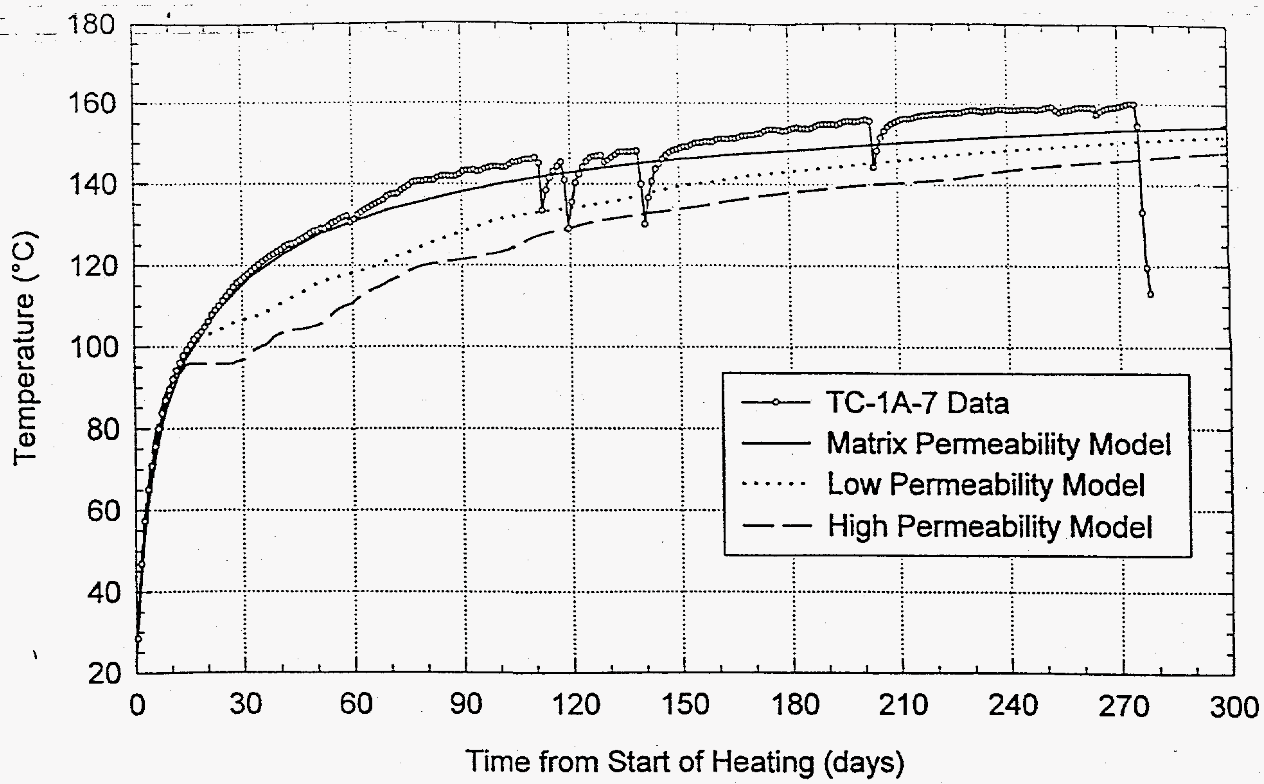

Figure 2 - Temperature-time history for gage TMA-TC-1A-7, located 41 cm from the heater in the vertical plane which is perpendicular to the heater and intersects the heater at its midpoint.

In the matrix permeability model, the temperature at the location of gage TMA-TC-1A-7 rises smoothly through 96°C without the flat spots or inflections observed in the other two models. As the temperature in the model rises, minute amounts of liquid water vaporize but cannot escape from the pore space, so the pore pressure rises dramatically. This pressure increase very effectively inhibits further evaporation of the pore water, and the liquid saturation remains near ambient levels, even up to temperatures of 160°C. Very little thermal energy is devoted to boiling water, and most of the heat being input to the rock contributes to raising its temperature. Because there is very little liquid or vapor flow in the system, heat is transferred in the rock almost entirely by conduction; convection is an insignificant process.

Note that the temperatures measured by TMA-TC-1A-7 exhibited a very smooth temperature profile as they warmed through the boiling point. Note that the temperatures measured by gage TMA-TC-1A-7 near the end of the test are underpredicted by the models by 5 to 12 °C. Of the three numerical simulations, the matrix permeability model most closely matches the data recorded from this temperature gage.

The measured and modeled temperatures after 266 days of heating, as a function of radial distance from the heater, are compared in Figure 3. At radial distances greater than about 1.2 m, where the measured temperatures are less than 96°C, all three models yield essentially the same results, indicating that conduction is the primary mechanism for heat transfer predicted in this region. Also in this region the models overpredict the measured temperature by as much as about 5°C. This overprediction could be easily corrected by increasing the wet thermal conductivity of the rock in the simulations from 2.1 W/m/K to perhaps 2.2 W/m/K, which would cool the predicted rock temperatures. At radial distances from the heater less than 1 m, the three models exhibit very different thermal behaviors. The high permeability model has a "flat spot" where the temperature is at about 96°C over a radial distance range from about 1 m out to 1.2 m. The low permeability model exhibits a significant inflection in this region while the matrix permeability model rises smoothly through 96°C. These isothermal regions and temperature inflections are due to the same phenomena which caused the isothermal time periods and temperature inflections in the temperature vs time plot for gage TMA-TC-1A-7.

The data exhibit a very smooth temperature profile as a function of radial distance. Even though data are scarce in the annular region 1 m from the heater, where inflections in the temperature profile would be anticipated, the available data do not indicate that any such inflections exist.

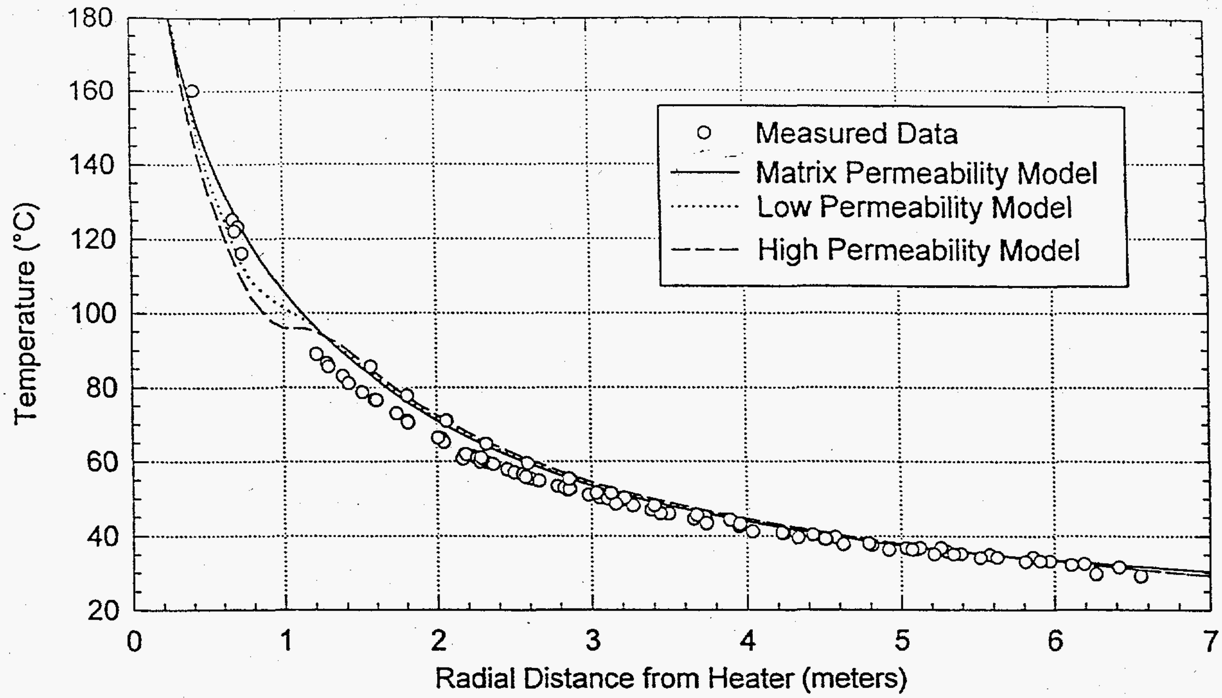

Figure 3 - Radial temperature distribution in the vertical plane that intersects the heater at its midpoint, after 266 days of heating.

To compare the models and data from a more global perspective, the amounts by which the models overpredict the measured temperatures at the conclusion of heating are plotted as a function the measured temperatures in Figure 4. The models and data agree very well at temperatures less than about 50°C, which is not surprising because the temperatures are not elevated very significantly above ambient. In the range from 50 to 85°C the models for the most part overpredict the measurements by up to 6 or 7°C. As noted earlier, these discrepancies could be easily corrected by increasing the wet thermal conductivities in the models slightly.

Above about 90°C the discrepancies between the models and the data are different for the three models. The high permeability model yields the poorest match between the measured and predicted temperature, with the model underpredicting the measurements by a substantial amount. Underprediction indicates that the model is allowing too much heat to escape from regions where the temperature exceeds 90°C. The low permeability model provides a better match, but the measured temperatures above 100°C are still systematically underpredicted by the model. These discrepancies between the models and the data may indicate that the value of dry thermal conductivity used in the models (1.67 W/m/K) is too high: a lower value would allow less heat to escape. Lower values of dry thermal conductivity are not supported by laboratory measurements, however. Alternatively, the discrepancies may indicate that the models overpredict the amount of convective heat transfer occurring in the rock. The matrix permeability model, in which convective heat transfer is insignificant, does not systematically violate the data at temperatures exceeding 100°C and therefore does the best job of matching the measured temperature data.

The comparisons between the measured data and the numerical predictions presented so far suggest that the matrix permeability model yields the best match between measured and modeled temperatures. For one observation, however, this is not true. In Figure 5 the amount by which the temperature of the gages in the interior of the SHT block increased between days 186 and 266 is plotted as a function of the temperature measured on day 186. The temperatures recorded by gages whose temperature on day 186 were less than 100°C increased by about 2.5 to 3.5°C, while the temperature of gages whose temperature on day 186 exceeded 100°C rose by 6 to 7°C. This can be taken as evidence for the formation of a dry-out zone around the heater. As the water in the rock evaporated, two thermal properties of the rock changed. Drying the rock reduced its heat capacity, with the result that after drying the same rate of heat input to the rock resulted in faster warming of the rock. Evaporation of the water in the rock also reduced its thermal conductivity. As the drying front propagated radially outward, the temperature of the relatively low thermal conductivity rocks in the dry-out zone increased more rapidly than the temperature of rocks outside the dry-out zone. The data in Figure 5 suggest that by the end of the SHT heating phase, the dry-out zone extended out to the 100°C isotherm, located about 1 m from the heater (Figure 3).

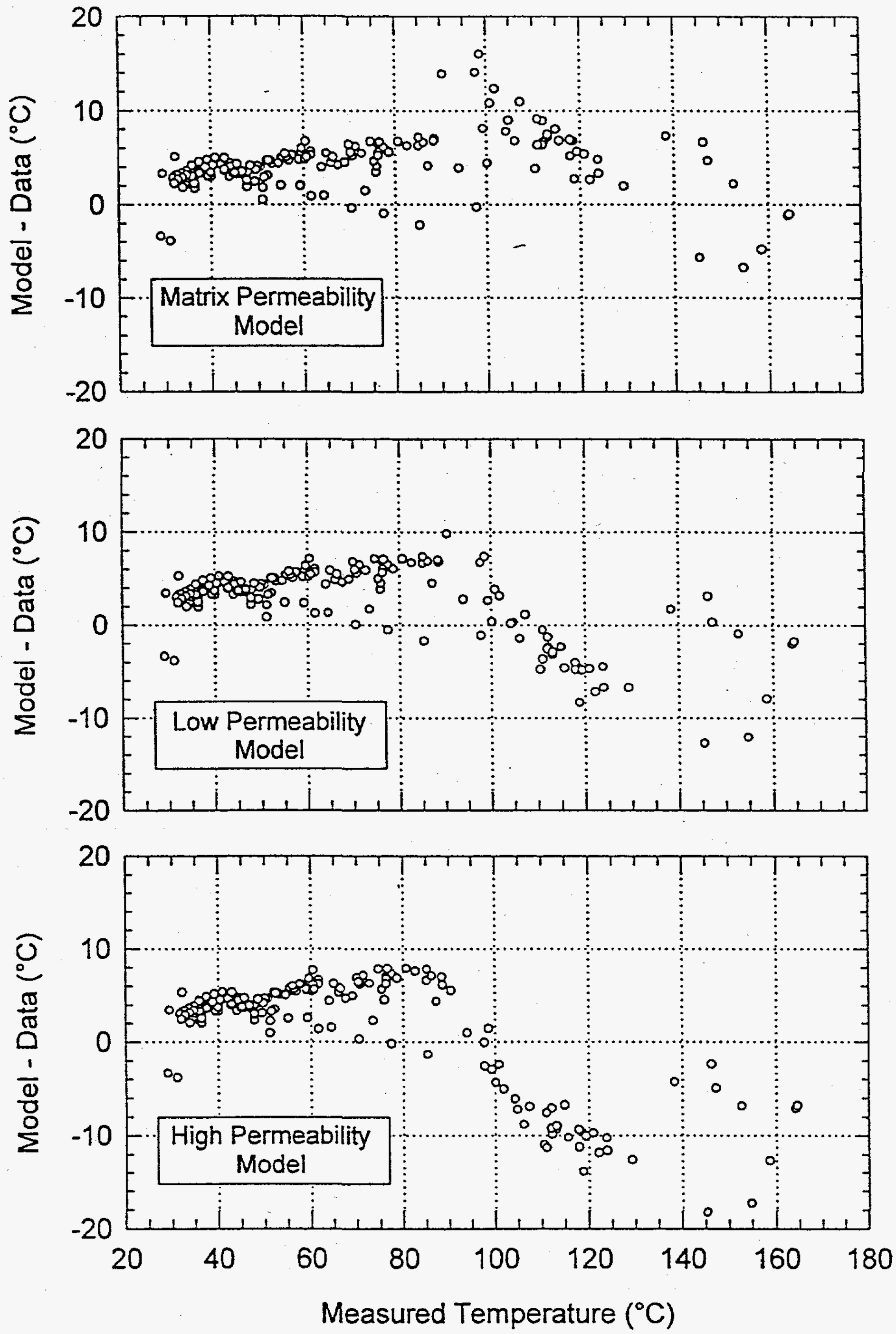

Figure 4 - Comparison of measured data and numerical models after 266 days of heating.

Dry-out zone formation can similarly be deduced from the temperature increases predicted by the models. The matrix permeability model exhibits enhanced temperature increases only at temperatures well in excess of temperatures actually observed during the SHT, suggesting only a very small dry-out zone within about 15 cm of the heater. The low permeability and high permeability models exhibit enhanced temperature increases extending to considerably lower temperatures (i.e., greater radial distances from the heater), and are therefore more consistent with the data. In addition to regions with enhanced temperature increases, the low and high permeability models also have regions right near the boiling point where the temperature increases are lower than those observed at cooler temperatures. These correspond to annular regions where liquid water and steam coexist in the pores of the rock and thermal energy is being devoted to evaporating water instead of raising the temperature of the rock. Although the measured data show a very slight decline in the temperature increases in this temperature range, the effect is much less pronounced than predicted by the low and high permeability models.

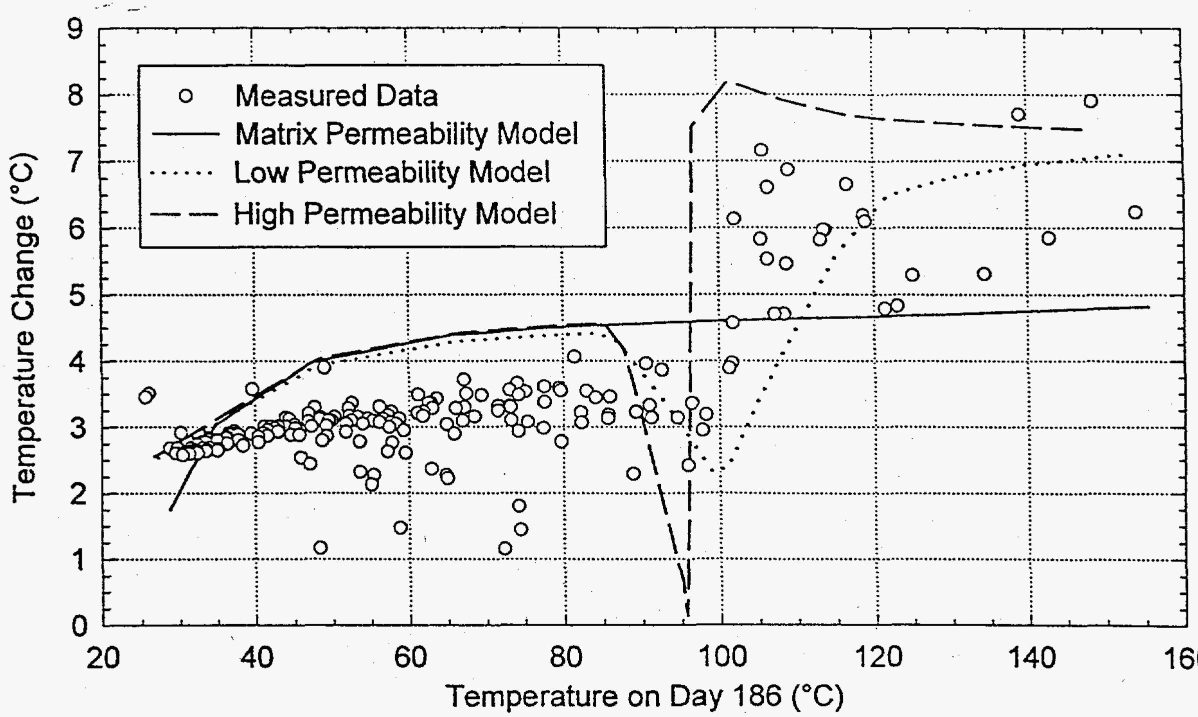

Figure 5 - Amount by which the temperature increased between day 186 and day 266 as a function of the temperature measured on day 186; data and model predictions.

DISCUSSION

In this section, our intuitive conceptual model of how the thermal and hydrologic processes are coupled will be described. Then the conceptual model that is the basis of the numerical simulations which have been run to date, and which have been compared to the measured data in this report, will be described. Finally, the two conceptual models will be compared and contrasted.

From a thermal perspective, there were two heat transport mechanisms at work in the SHT: conduction and convection. Although both contributed to the overall heat transfer, convection was likely inhibited by the limited permeability of the rock, and hence conduction was likely the predominant heat transfer mechanism. The other important thermal effect operative in the SHT was the change in thermal properties of the rock, which occurred as its liquid saturation decreased as a result of boiling. Drier rock will have lower thermal conductivity and heat capacity compared to rock with a higher liquid saturation. Because a substantial amount of heat was being transferred conductively through the rock, lowering the thermal conductivity of the rock likely increased the temperature gradient within it. A higher gradient resulted in higher temperatures in the dry-out zone. Lower heat capacity, and lower thermal conductivity coupled with a radially propagating drying front, caused temperatures within the dry-out zone to rise more rapidly than temperatures outside the dry-out zone.

From a hydrologic perspective, the rocks at the SHT site consist of a low permeability matrix intersected by numerous fractures that have a much higher permeability. There were two fluid phases of concern in the SHT: liquid water and water vapor. The permeability of the matrix was such that liquid water residing in the matrix could be considered essentially immobile at the time scale of the SHT. Water vapor, on the other hand, could flow at a significant rate through the matrix because of its much lower viscosity. Liquid water and water vapor could both move easily through the fractures and along the boreholes.

At ambient conditions, the matrix was partially saturated, with about 92% of the pore space occupied by liquid water (Engstrom and Rautman, 1996). The fractures were probably fairly dry because, if they contained significant water, that water would have drained due to gravity. The liquid water in the matrix was held in place by capillary suction.

During the SHT, as the rock was heated to temperatures exceeding the boiling point of water, liquid phase buoyant convection was probably of fairly minor significance due to the limited permeability of the matrix. Once the water began to boil, however, the resulting water vapor flowed readily. Because boiling occurred close to the heater first, a substantial pore pressure gradient developed, which caused the vapor to flow in a net direction that was radially away from the heater. Because the fractures had a much higher permeability than the matrix, the vapor tended to first flow from the matrix into the nearest fracture or borehole and then along the fracture or borehole in a direction away from the heater.

As the vapor flowed away from the heater, it eventually encountered the boiling point isotherm, where it condensed back to a liquid. Because the vapor had been preferentially flowing along fractures and boreholes, the liquid saturation of the fractures on the cool side of the boiling point isotherm would increase substantially. As a result of capillary suction, some of the liquid water would be imbibed into the matrix and some drawn back into the dry-out zone and revaporized. Much of the water, however, may have flowed downward in the fractures and boreholes due to gravity, ultimately leaving the region of influence of the SHT. From a broad spatial perspective, then, the heating process can be viewed as a mechanism for moving liquid water from the matrix, where it was relatively immobile due to capillary suction and the relatively low permeability of the matrix, to the fractures, where it could flow more easily due to the higher permeability of the fractures.

The numerical simulations that have been compared to the measured data in this report are based on the Equivalent Continuum Model (ECM). To achieve computational efficiency, the ECM assumes that the matrix and the fractures are in thermodynamic equilibrium. With this assumption, the thermal and hydrologic properties of the matrix and the fractures can be combined into single, bulk values. The model then computes the temperature, pressure, and saturation that would exist in a single medium with those bulk properties. In the implementation used for the SHT, the bulk permeability and bulk capillary suction more closely resembled those of the matrix until such time as the liquid saturation approached unity. This means that it was very difficult for liquid water to flow in the model until near total saturation was achieved. In the SHT models, when the rock temperature exceeded the boiling point of water, vapor formed and flowed radially away from the heater in response to the pore pressure gradient. When the water vapor flowed past the boiling point isotherm it condensed, but then the resulting liquid water could not readily flow anymore because complete saturation was only rarely achieved in the SHT models. As the boiling point isotherm progressively moved radially outward away from the heater in response to the continued addition of heat, the liquid water boiled once again and moved radially outward where it recondensed. This process is called refluxing because the water was continually vaporized, transported radially away from the heater, condensed when it crosses the boiling point isotherm, and then was later revaporized, ad infinitum.

The key difference between our intuitive conceptual model and the ECM is that the ECM almost never allows liquid water to leave the system whereas, in reality, this probably occurred. This means that in the ECM there was more liquid water filling the pores of the rock near the boiling point isotherm than there likely was in reality. Consider a cylindrical surface 40 cm in radius whose axis coincided with the axis of the heater. In the ECM, when the temperature of this surface reached the boiling point, all the water that originally filled the pores of the cylindrical volume of dry rock enclosed by the cylindrical surface was filling the pores in close proximity to the surface of the cylinder. Throughout the time period required to vaporize all of this liquid water, virtually all the thermal energy entering the rock was consumed by the vaporization process, and very little was devoted to raising the temperature of the rock. This lead to the development of the substantial predicted isothermal time periods and isothermal annular regions described earlier in this report. If, once the vapor condensed, it had done so in a material with the permeability of the fractures, the resulting condensate could readily have drained out of the system under the influence of gravity, thereby reducing the amount of liquid water that would have had to be re-vaporized as the boiling point isotherm expanded. In this case, the isothermal time periods and annular regions would still have existed because the water that was originally in the pores still needed to be vaporized, but their magnitudes might have been greatly reduced due to the reduction in the amount of water that had to be refluxed.

The implication of this analysis is that the ECM may have significantly overpredicted the magnitude of the isothermal temporal and spatial regions observed in the numerically predicted temperature profiles by retaining condensate water in the system. Because these features were the primary evidence suggesting that the matrix permeability model fit the measured data better than the low and high permeability models, it is likely inappropriate to draw any conclusion from those comparisons. The observation of a dry-out zone extending out to the 100°C isotherm is compelling evidence that the bulk permeability of the rock was substantially higher than the permeability of the matrix. This conclusion is more robust than conclusions based on the shapes of the spatial and temporal temperature profiles because it is not as dependent on comparisons with the numerical model; it can be gleaned from the measured data alone. The apparent poor fit between the measured data and the low and high permeability models should not be interpreted as evidence that convective heat transfer is not important in the rock. More likely, the poor fit is due to shortcomings of the conceptual model on which the ECM is based. To achieve better predictions of the thermal-hydrologic response to thermal loading of the rock mass at Yucca Mountain, the ECM approach should be abandoned in favor of other conceptual models which allow more gravity drainage of water in the condensate zone surrounding the heater.

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