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EVALUATION OF A 6-WIRE THERMOCOUPLE PSYCHROMETER FOR DETERMINATION OF IN-SITU WATER POTENTIALS

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ABSTRACT

A 6-wire, Peltier-type thermocouple psychrometer was designed and evaluated by the U.S. Geological Survey for monitoring *in-situ* water potentials in dry-drilled boreholes in the unsaturated zone at Yucca Mountain, Nye County, Nevada. The psychrometer consists of a wet-bulb, chromel-constantan, sensing junction and a separate dry-bulb, copper-constantan, reference junction. Two additional reference junctions are formed where the chromel and constantan wires of the wet-bulb sensing junction are soldered to separate, paired, copper, lead wires. In contrast, in the standard 3-wire thermocouple psychrometer, both the wet bulb and dry bulb share a common wire. The new design has resulted in a psychrometer that has an expanded range and greater reliability, sensitivity, and accuracy compared to the standard model.

For water-potential measurements at Yucca Mountain, thermocouple psychrometers are calibrated at five temperatures from 10 to 40 °C, in 5 °C increments over a 20 °C span, using six saline solutions ranging from 0.02 *m* (molal) (-90 kilopascals or, -0.9 bars) to 1.5 *m* (-7500 kilopascals or, -75 bars). A non-linear regression equation model was developed to characterize the relation between output voltage, temperature, and water potential. This model was developed using combined data from ten thermocouple psychrometers consisting of 900 data points. The best fit regression model is given by:

$$\psi = A + B(\mu V) + C(\mu V)(\mu V) + D(\mu V)(T) + E(T)(T) + F(\mu V)(T)(T)$$

where: ψ is water potential in bars, A, B, C, D, E, F are the regression coefficients, μV is the delta intercept in

microvolts, and T is temperature in °C. The resulting equation generated an $r^2 = 0.999$, and a standard error of the estimate = 1.01 bars, and when applied to data generated from 28 individual psychrometers, averaged an $r^2 = 0.999$, and a standard error of the estimate = 0.72.

Field trials and laboratory testing have shown that the 6-wire, modified thermocouple psychrometer supports an operational range in a stable temperature environment of -90 kilopascals (kPa) with 10% error to -7,500 kPa with 1% error. Measurement repeatability is on the order of 5 kPa (0.05 bars). A change of approximately 2% in the resistance of the wet bulb (nominally 8 ohms) of these sensors has been noted after two years of continuous field operations (4000 duty cycles).

I. INTRODUCTION

The U. S. Geological Survey has been conducting investigations at Yucca Mountain, Nevada, to provide information about the hydrologic and geologic suitability of this site for storing high-level nuclear wastes in an underground mined repository. Test drilling and instrumentation are a principal method of investigation. The main objectives of the deep unsaturated-zone test-hole program are: 1) to determine the flux of water moving through the unsaturated welded and nonwelded tuff units, 2) to determine the vertical and lateral distribution of moisture content, water potential, and other important geohydrologic characteristics in the rock units penetrated, and 3) to monitor stability and changes in *in-situ* fluid potentials with time. Thermocouple psychrometers will be used to monitor *in-situ* water potentials.

A thermocouple psychrometer is a temperature-sensing device that measures the difference between the ambient temperature of an atmosphere and the temperature of a freely-evaporating moist surface in the same atmosphere. The vapor pressure is inferred from these two quantities. Water potential is related to vapor pressure through the Kelvin equation:

$$\psi = \frac{RT}{V_w^0} \ln\left(\frac{e}{e_0}\right) \quad (1)$$

where:

- ψ = water potential, in bars
- R = ideal gas constant, $8.314 \times 10^7 \text{ erg}^\circ\text{K-mole}$
- T = absolute temperature, in $^\circ\text{K}$
- V_w^0 = molar volume of pure water, $18.015 \text{ cm}^3/\text{mole}$
- $\frac{e}{e_0}$ = relative humidity.

Use of this equation is based on the thermodynamic principle that when vapor is in equilibrium with liquid, the vapor pressure of water in the air will reflect the potential of the liquid water in the system^{1,2}. The vapor pressure, or relative humidity, is determined by cooling the thermocouple psychrometer to condense water vapor onto the wet bulb and then observing the evaporation of the liquid water.

A modified, 6-wire, Peltier-type thermocouple psychrometer was designed for monitoring *in-situ* water potentials in dry drilled boreholes in the unsaturated zone at Yucca Mountain, Nye County, Nevada. Hydraulic gradients calculated from these data are necessary to determine the direction and magnitude of water flux in the unsaturated zone of Yucca Mountain. *In-situ* measurements offer several distinct advantages over laboratory measurements of water potentials using core samples. *In-situ* measurements record the dynamics of the equilibration process and provide more accurate water-potential determinations. Core may be dried slightly during the coring process and hence, measurements made from these cores tend to underestimate true water potentials. The degree of underestimation is primarily a function of the porosity and volumetric water content of the core. The moisture retention curve determines the sensitivity to drying. Depending on the original water content and its position on the moisture retention curve, small changes in saturation may result in large changes in water potential or large changes in saturation may result in small changes in water potential.

For water potential measurements at Yucca

Mountain, thermocouple psychrometers are calibrated at five temperatures ranging from 10 to 40 $^\circ\text{C}$, in 5 $^\circ\text{C}$ increments over a 20 $^\circ\text{C}$ span, using six molal calibration solutions of sodium chloride (NaCl), ranging from 0.02 m (-90 kPa) to 1.5 m (-7500 kPa). The molal calibration solutions provide a standard vapor pressure when temperature is held constant^{1,2}. Calibration data is then fitted to a regression equation. Once a calibration curve has been established for a sensor, the sensor can be used for *in-situ* measurements of water potentials in rock.

Evaluation of the modified 6-wire thermocouple psychrometers involved a 3-phase testing program. Phase 1 consisted of extensive laboratory-based testing and calibrations in order to determine the sensitivity, range of operation, repeatability, and accuracy of the sensor. Phase 2 involved long-term field trials of these thermocouple psychrometers in three 12.2 m deep boreholes located adjacent to the Hydrologic Research Facility (HRF) in Area 25, Nevada Test Site. Phase 3 of this program, which began in December, 1993, consists of laboratory recalibration of thermocouple psychrometers removed from HRF borehole # 2 after over two years of continuous operation.

II. TECHNICAL DEVELOPMENT

A 6-wire, Peltier-type thermocouple psychrometer was designed to replace the standard 3-wire thermocouple psychrometer previously used for *in-situ* measurements of water potentials. The 6-wire, Peltier-type thermocouple psychrometer consists of a wet-bulb chromel-constantan sensing junction and a separate dry-bulb copper-constantan sensing junction. Two reference junctions are formed where the chromel and constantan wires of the wet-bulb sensing junction are soldered to separate, paired, copper, lead wires. This is in contrast to the 3-wire thermocouple psychrometer where both sensing junctions share a common copper wire lead. A schematic diagram and the instrumentation of a 6-wire thermocouple psychrometer is shown in Figure 1.

The 6-wire configuration offers some distinct advantages over the 3-wire configuration: 1) voltage output can be measured immediately following excitation, thus providing accurate determinations of water potential in the very dry or low water potential range (-7500 kPa); 2) the wet bulb can be read during current excitation as a 4-wire resistor to track any change in the resistance of the wet bulb over time; and 3) the circuit is balanced to reduce noise, thus improving the signal-to-noise ratio of the sensor. The result is that

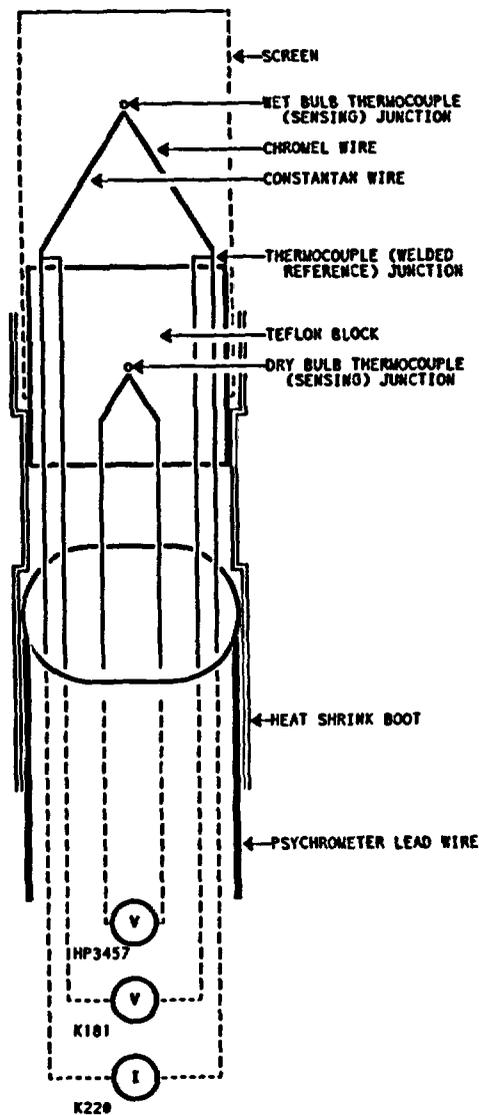


Figure 1. Schematic and instrumentation of a 6-wire thermocouple psychrometer.

the 6-wire thermocouple psychrometer is characterized by an expanded range, greater reliability, sensitivity, and accuracy compared to that of the standard 3-wire thermocouple psychrometer.

A. Instrumentation

Instrumentation for the calibration of 6-wire thermocouple psychrometers consists of an automated data acquisition system designed to accommodate 16 psychrometers at a time.

The electronic system includes a Hewlett-Packard^{*} HP3497A signal multiplexer, HP3457A digital multimeter, Keithley^{*} K220 programmable current source which supplies a 5 mA current for thermocouple excitation during Peltier cooling, and a K181 nanovoltmeter which is used to read voltages from the thermocouple psychrometer wet bulb. A Hart Scientific^{*} programmable temperature water bath is used to ensure temperature stability to 0.0005°C.

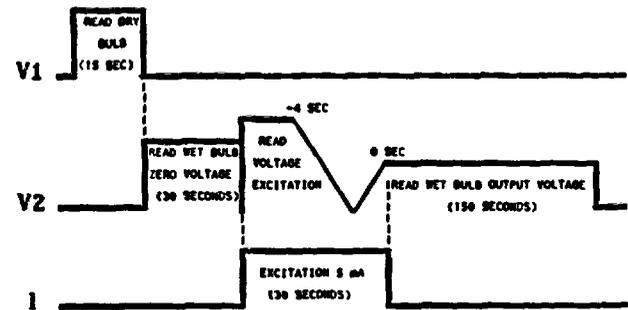


Figure 2. Psychrometer Scanning Sequence.

B. Scanning Sequence

Figure 2 shows the thermocouple psychrometer calibration scanning sequence. The dry bulb temperature is measured for 15 seconds using the HP3457A digital multimeter. Immediately following this, the voltmeter zero offset is measured for 30 seconds using the K181 nanovoltmeter. A 5 mA excitation current, supplied by the K220 current generator, runs for 30 seconds. During excitation the voltage of the wet bulb is read by the K181 nanovoltmeter until four seconds before the end of the excitation period, at which point the K181 is switched to a more sensitive range. This four second interval allows time for the nanovoltmeter to come into range so that the wet bulb output voltage readings may begin immediately at the end of current excitation. The wet bulb output voltage is measured for 150 seconds; data are collected at approximately 0.5 second intervals during this period. Except for very wet conditions, 150 seconds is sufficient to measure the entire re-equilibration curve.

^{*} Use of trade or firm names in this report is for identification purposes only and does not constitute endorsement by the U. S. Geological Survey.

The delta intercept, shown in Figure 3, is calculated by extrapolating a line through the plateau region back to the initial time (the end of excitation). The voltmeter zero is then subtracted from the calculated intercept to give a final delta intercept value.

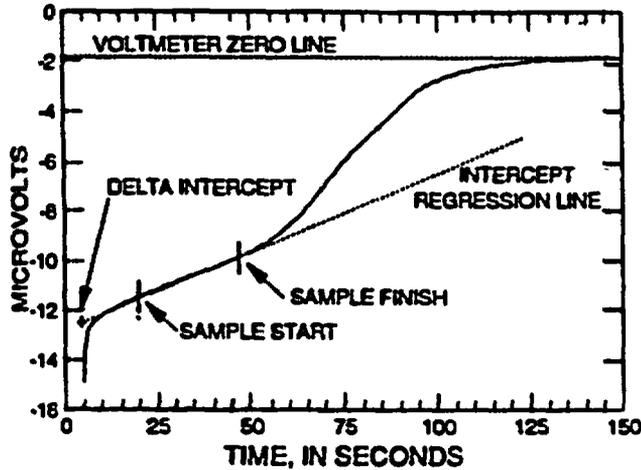


Figure 3. Calculation of the delta intercept. The area bounded by sample start and sample finish is the section of the curve used for the calculation of the regression line and the delta intercept.

C. Calibration

The relationship between thermocouple psychrometer output and water potential is not linear, and the wet bulb outputs of several different salt solutions must be measured at each of several temperatures³. The saline solutions and temperatures used in calibration span the estimated range of temperatures and water potentials likely to be encountered in boreholes at Yucca Mountain. Calibrations are performed in a water bath to provide isothermal conditions. Thermocouple psychrometer voltage outputs are collected from each calibration run and the delta intercept calculated⁴. The delta intercepts are then plotted against all water-potential values (in bars or kilopascals) at the various temperatures to yield a family of curves. Three delta intercepts are collected at each temperature and molality; six calibration solutions and five temperatures yield 90 delta intercepts as shown in Figure 4.

D. Field Testing

Sixteen calibrated thermocouple psychrometers were installed in two 12.2 meter boreholes (HRF borehole #1

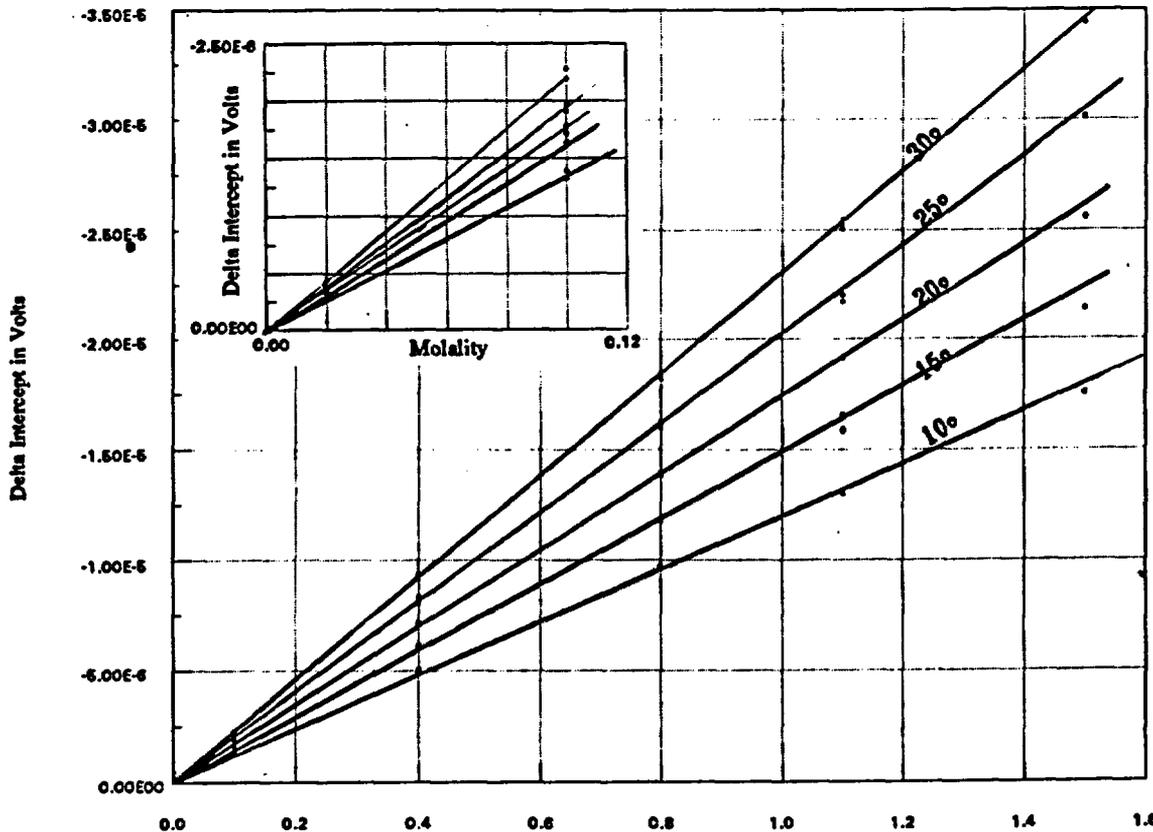


Figure 4. Plot of molality vs. delta intercept at 6 molalities, 5 temperatures, 3 replications at each molality and temperature.

and HRF borehole #2) located adjacent to the HRF in October, 1991. In each borehole, two sensors were located at each of four instrument stations at depths of approximately 3.0, 6.1, 9.1, and 12.2 meters. Primary sensors have been read every 3 to 5 hours with approximately 4000 duty cycles to date. The secondary sensors are activated periodically to confirm the reading of the primary sensor.

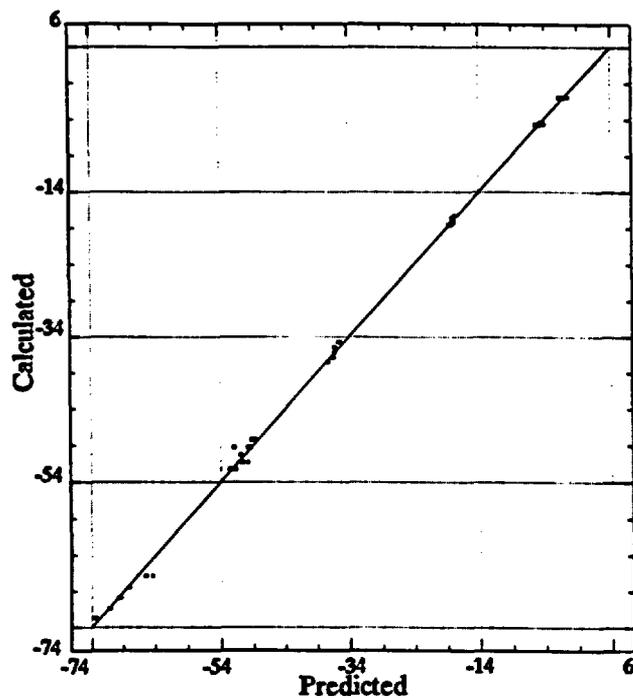


Figure 5. Regression plot (in bars) of calculated vs. predicted water potentials

III. RESULTS

A. Calibration Equation

The data from ten thermocouple psychrometers (over 900 data points) were pooled and several model equations were evaluated. The selected best-fit regression model is:

$$\psi = A + B(\mu V) + C(\mu V)(\mu V) + E(T)(T) + F(\mu V)(T)(T) \quad (2)$$

where:

A, B, C, D, E, F are regression coefficients
 μV is the delta intercept, in microvolts
T is temperature, in degrees Celsius
 ψ is water potential, in bars.

The pooled data fit the model with an r^2 of 0.9983 and a standard error of the estimate of 1.0083 bars. When the data generated from 28 psychrometers including the original ten were fit individually to the model equation,

the average r^2 was 0.9992 and the average standard error of the estimate was 0.7165 bars. The accuracy of the regression equation is illustrated in Figure 5, which shows an example comparison between measured water potentials and those predicted from the regression equation. The 95% confidence residuals are less than 1.04 bars.

B. Water Potential Measurements

Figure 6 shows the water potential measurements made by the primary and secondary psychrometers at 12.2 meters in HRF borehole #1 over a 20,000 hour period (approximately 27 months) starting in October, 1991. Temperature variation at this depth has been less than 0.3°C over the entire time period. Measurements made when the hole was first instrumented were drier than -6500 kPa (-65 bars). Current measurements are around -400 kPa (-4 bars). The difference between these two sensors has never been greater than 150 kPa (1.5 bars) over the entire 27 month period. The spike in the water potential curve resulted from a period of gas sampling and subsequent aspiration of the thermocouple psychrometer.

C. Voltmeter Zero Measurement

The voltmeter zero represents the net combination of any residual voltages generated from the thermocouple junctions in the psychrometer, and any non-zero offsets in the nanovoltmeter or measuring electronics. Temperature gradients across the psychrometer will induce a voltage drop and cause current to flow and thereby increase the magnitude of the voltmeter zero. This is evident in Figure 7, where temperature and voltmeter zero changes at the 3.0 meter and 12.2 meter stations in HRF borehole #1 are compared. The 3.0 meter station shows an 8°C range of temperature in contrast to the 0.3°C temperature range measured at 12.2 meters. The voltmeter zero of the station at 12.2 meters shows some seasonal variation, but the predominant cause of the offset is noise from the nanovoltmeter itself. The net offset is less than 300 nanovolts. The station at 3.0 meters shows a pronounced seasonal effect that mirrors the temperature change suggesting the offset is caused by a temperature gradient induced current. The variation in the offset is close to 4000 nanovolts.

The cooling of the psychrometer bead through the Peltier effect represents a displacement of the vapor equilibrium state from the initial state measured by the voltmeter zero. The delta intercept calculation, in fact, represents the difference between the voltmeter zero

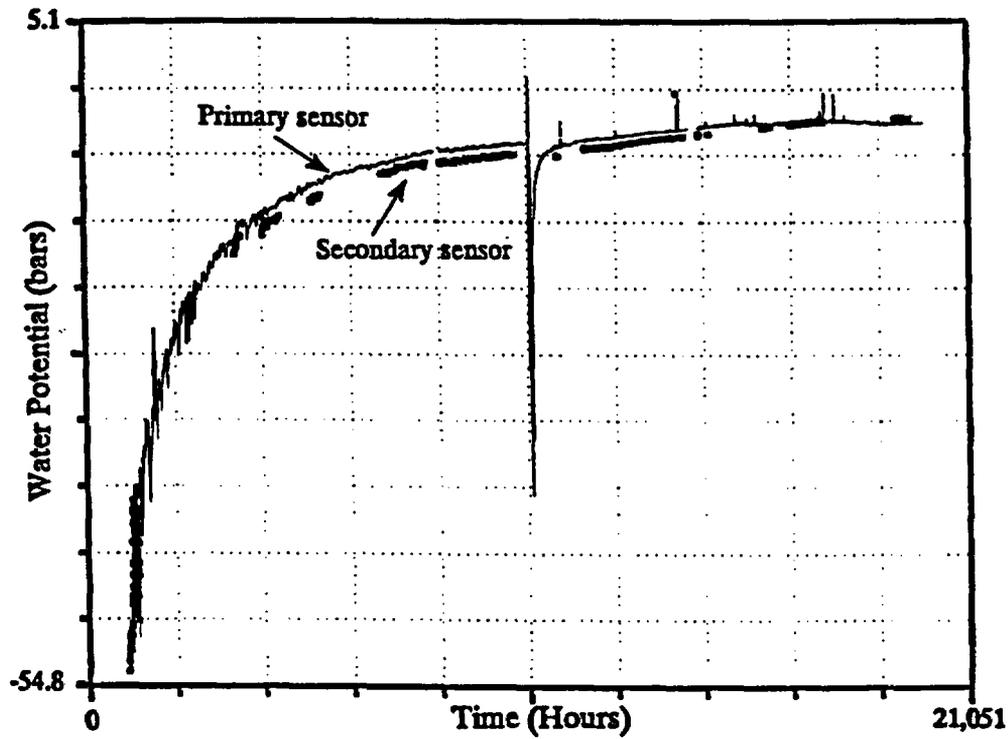


Figure 6. Water potential readings of two thermocouple psychrometers at depths of 12.2 meters, in HRF Borehole #1.

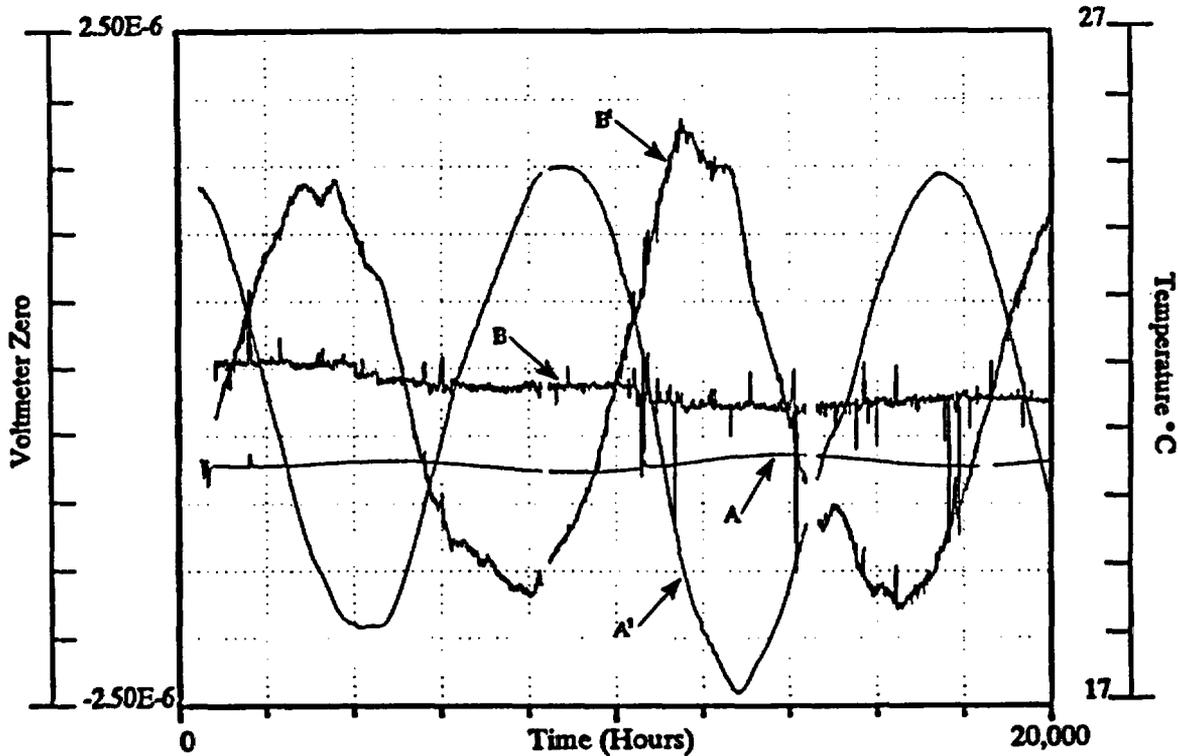


Figure 7. Observed temperature effects on voltmeter zero readings for four psychrometers in HRF Borehole #1 located at depths of 12.2 m (A = zero voltage, B = temperature °C), and at 3.0 m (A' = zero voltage, B' = temperature °C).

and the displaced equilibrium. Thermal gradients and large thermal changes, such as those seen in the station at 3.0 meters, can result in non-equilibrium conditions that are reflected in large changes in the voltmeter zero and corresponding error in the calculation of water potential. This has led to observed differences of 1000 to 2000 kPa (10 to 20 bars) between the two psychrometers at the shallow station.

D. Voltage Output during Excitation

Changes in the voltage measured during excitation of the psychrometer with a 5 mA current represents a change in the resistance of the thermocouple probably due to corrosion on the surface of the bead. This may ultimately have an effect on the accuracy of the measurement. However, the changes in voltage shown in Figure 8 represent less than a 2% change in the resistance over a two year period, with the largest percentage change seen at the shallowest station. Variations in the initial resistance of the psychrometer are normal. With a 6-wire device it is possible to track these changes, and perhaps adjust water potential measurements accordingly. Tests are underway to determine the significance of these resistance changes.

IV. CONCLUSIONS

The 6-wire thermocouple psychrometer has been successfully used to measure water potential for over two years in shallow boreholes. The redesigned psychrometer, combined with improved electronics, has exhibited enhanced accuracy and precision, an expanded range of measurement, and improvements in long term stability and reliability.

ACKNOWLEDGMENTS

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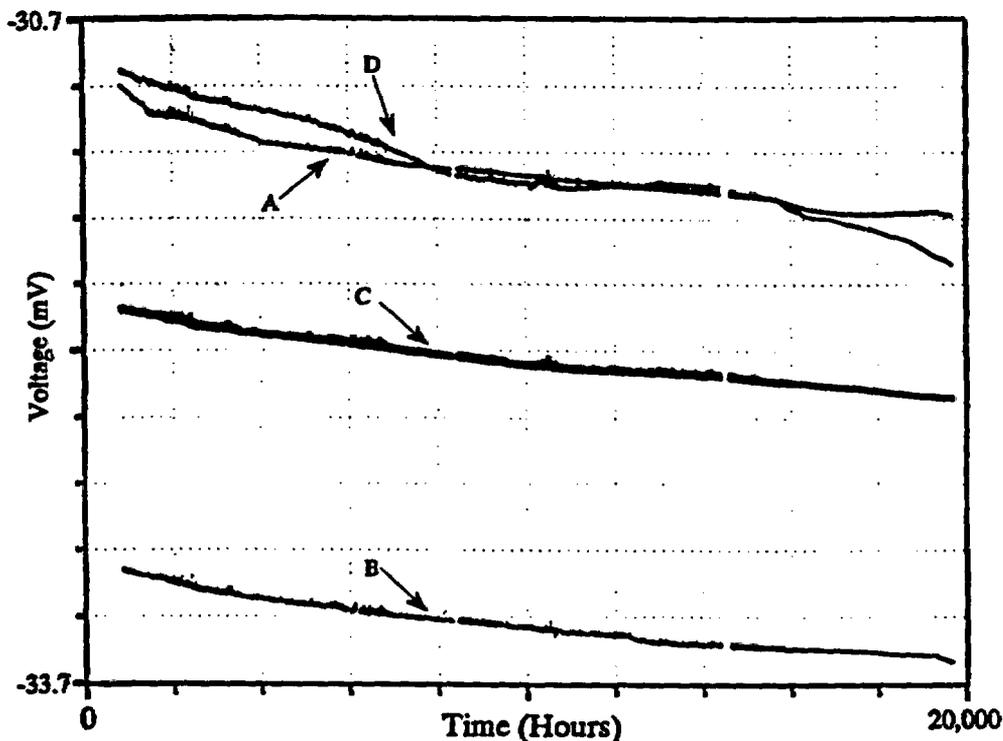


Figure 8. Voltage output values during current generation for four psychrometers in HRF Borehole #1 located at depths of 12.2 m (A), 9.1 m (B), 6.1 m (C), and 3.0 m (D).

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