04

102

~~109/~~PETE/84/06/07/0

JUN 2 1 1984

stribution:
WM sf
WMGT rf
NMSS rf
RBrowning
MBell
HMiller
JBunting
JGreeves
LHigginbotham
MKnapp
POrnstein & RF
JPohle
PDR

MEMORANDUM TO: Seth Coplan
Repository Projects Branch
Division of Waste Management

THRU: Malcolm Knapp, Chief
Geotechnical Branch
Division of Waste Management

FROM: Peter Ornstein
Hydrology Section
Geotechnical Branch
Division of Waste Management

SUBJECT: ANALYSIS OF NON-ISOTHERMAL UNSATURATED FLOW CONDITIONS

Attached is the report I prepared entitled "Analysis of Non-Isothermal Hydrologic Conditions in the Unsaturated Zone." This report is a write-up of the presentation I gave to the NRC NNWSI team last month and describes the possible hydrologic and thermal consequences resulting from canister size and repository size heat sources emplaced in unsaturated rock. A notable result of the analysis is that heat dissipation due to liquid evaporation will likely be the dominant thermal transport mechanism and significantly perturb the pre-emplacement hydrologic regime.

Peter Ornstein
Hydrology Section
Geotechnical Branch
Division of Waste Management

Enclosure:
As stated

8407160267 840621
PDR WASTE
WM-11 PDR

WM Record File
102

WM Project 11
Docket No.
PDR ✓
LPDR ✓

Distribution:

~~(Return to WM, 623-SS)~~

OFC	:WMGT	:WMGT	: WMGT	:	:	:
NAME	:POrnstein:dw	: JPohle	:MKnapp	:	:	:
DATE	:6/18/84	:6/18/84	: 6/14/84	:	: NM840469	: 00302

INTRODUCTION

Over the next several years, the Department of Energy will likely continue its appraisal of the Yucca Mountain area for disposal of high-level nuclear waste (HLW). The principal focus of their appraisal has been the unsaturated Topopah Spring Member underlying Yucca Mountain. A primary reason for considering disposal in the unsaturated zone is that the relatively low water content may not be amenable to hydrologic transport of leached waste.

Under the Nuclear Waste Policy Act of 1983, Congress has delegated to the NRC the responsibility to ensure that disposal of HLW meets appropiate NRC and EPA regulations (10 CFR Part 60 and 40 CFR Part 191). DOE must provide the NRC with reasonable assurance that performance objectives stated in NRC and EPA regulations will be met. These performance objectives prescribe minimum groundwater travel times, waste canister integrity, and maximum allowable radionuclide releases from the repository. For the NRC to be able to assess DOE's reasonable assurance that the performance objectives will be met, the NRC must be in a position to evaluate competently and carefully all technical assertions made by DOE. The NRC must have a full understanding of the physical processes that may affect waste isolation, and based on that understanding endorse or reject the DOE assertions.

This document describes a study designed to familiarize the NRC staff with the type and magnitude of physical interactions that may significantly affect waste isolation around a HLW repository located in unsaturated rock. The goal of this study is not to specifically define the likely hydrologic and thermal regime around a HLW repository located at Yucca Mountain, but to develop a conceptual framework from which a clearer definition of the site may evolve.

To attempt to define the potential thermal and hydrologic environment with the current paucity of available data would be premature.

CANISTER STUDY

A single canister with a thermal output of 3.4 kW was simulated using the TOUGH code to determine induced spatial and temporal thermal variations as well as changes in hydrologic characteristics. The canister was treated as a point heat source embedded in a cylindrical rock mass 4 M in diameter and 2 M high, which itself was embedded in a cylindrical rock mass 200 M in diameter and 1000 M high (Figure 1), with a pre-emplacement liquid saturation of 43 percent. The initial thermal load decayed exponentially with time (Figure 2). Although the initial canister loading is almost twice as high as what might be expected for either spent fuel or commercial high-level waste, the thermal loading is consistent to that used by Sandia in a recent study of thermal-hydrologic interactions for DOE (SAND83-0757).

The canister simulation was performed for a period of 2767 days. The average canister block temperature rose steadily for 508 days, peaked at 99.4°C, and then started to abate. At the close of simulation, the canister block temperature was still in excess of 92°C (Figure 3). As the canister block temperature rose, the net flux of fluid (primarily in the form of vapor) was away from the block, but was not sufficient to deplete the block of all liquid water. As the block dried out, the resulting capillary potential became much stronger than the surrounding blocks and tended to draw liquid water back into the block. A local hydrologic cycle was established whereby: 1) liquid water was heated and vaporized in the canister block; 2) vaporization of the water increased air phase pressure and forced vapor out of the canister block and into neighboring grid blocks; 3) the vapor condensed into liquid water in cooler neighboring blocks; and 4) uneven capillary potentials drew liquid water back into the canister block. This cycle, referred to as heat piping, is a highly effective way to dissipate thermal energy. The energy is consumed by fluid vaporization, transported with the vapor, and released some distance away as the vapor condenses (and thereby heats the rocks where condensation occurs).

At the close of this simulation the Δ10° isotherm (i.e., the contour indicating a 10° increase in temperature over ambient) had reached its maximum lateral extent of over 7.5 M from the center of the canister block and was starting to recede. The Δ5° isotherm was approximately 11.5 M from the canister and was still expanding outward. The Δ15° isotherm was approximately 6 M from the canister block and had started receding (Figure 4).

The numerical results of this particular canister simulation are not in and of themselves indicative of expected conditions within a HLW repository. However, similar simulations performed using site specific data (geologic, hydrogeologic, and thermal) will enable the NRC to assess canister emplacement schemes and resulting repository environments. These simulations need not be limited to the NNWSI project since similar thermal and hydrologic conditions will occur at other repositories during their respective operational stages, prior to resaturation.

REPOSITORY STUDY

A repository scale simulation was also performed to provide insight into processes and components of the hydrogeologic environment that will be affected by the disposal of high-level waste. The repository simulated was approximately 6.5 meters high and had a diameter of approximately 200 meters (Figure 5). An initially uniformly distributed thermal loading of 100 kW/acre was simulated and followed the same thermal decay function used in the canister scale simulation. With the exception of the rock-moisture characteristic curves and the surface recharge, the hydrogeologic and thermal parameters used were the same as those used in SAND83-0757. Characteristic curves were chosen on the basis of their shapes (i.e. similarity to those used by Sandia) (Figure 6) and their availibility in the TOUGH code's function library. Surface recharge was 1.0 cm/yr uniformly distributed in time and space.

The conceptualized porous medium within which the repository was emplaced was homogeneous, 320 meters thick and 650 meters in diameter; bounded on the side by a no-flow boundary, bounded on the top by a no-flow (air and thermal)/recharge (liquid water at 1cm/yr) boundary, and bounded on the bottom by an infinite volume reservoir with properties identical to the repository medium under pre-emplacement conditions. The purpose of the reservoir was to provide an infinite storage area for excess water and heat that would otherwise buildup in the lower portion of the study domain (i.e., below the repository).

The simulation, described in detail below, lasted for 9867 days at which point an anomaly of the TOUGH code was discovered. The anomaly, which precluded resaturation via matric potential of a completely desaturated grid element, would have provided erroneous results had the simulation been allowed to continue. During the time frame for which the simulation had run, the results were not adversely significantly affected. At this writing, the author of TOUGH has been consulted and a remedy for the anomaly is being implemented.

The ambient conditions assumed a 1.0 cm/yr infiltration rate, a uniform temperature of 25°C, and an atmospheric pressure of 1 bar. Upon coupling the infiltration rate and rock-moisture characteristic functions, the resulting ambient liquid saturation was 43%, capillary pressure was -1.8 bars, and downward liquid velocity was approximately .24 m/yr. The ambient vapor content of the air was 2%.

The thermal load of the repository was instantaneously "turned on" at time zero and then proceeded to decay with time. Since the thermal load of the repository was the only stress placed on the thermal-hydrologic system throughout the simulation period, all hydrologic perturbations that occurred during the simulation resulted directly from repository heat generation. For convenience, the simulation history is broken up into four time periods; each of which will be discussed in turn.

2593 DAYS

During this period, repository temperature had risen to 103 °C and was still rising. Vapor pressure in the repository had increased and was equal to the air pressure (which had increased to 1.1 bars) indicating that boiling was occurring. Liquid saturation of the rock in the repository had dropped to 29% and vapor content of the air had risen to 99%. As expected, vapor flow was away from the repository in all directions. Conversely, liquid water was being drawn back into the repository from all directions as the capillary pressure within the repository dropped to -4.3 bars. Vapor leaving the repository in all directions was cooled and condensed in neighboring grid blocks.

5111 DAYS

At 5111 days, temperature within the repository blocks had risen to 109°C while temperatures within the grid blocks immediately above and below the repository had risen to 104°C and the water therein was in the process of boiling. The vapor content (i.e. the percent liquid saturation of air) within all blocks with temperatures in excess of 100°C had become approximately 100%. Liquid saturation within the repository had dropped to 18%; which is below the irreducible saturation set at 25% (The irreducible saturation is that saturation at which the capillary potential reaches a maximum negative value and hydraulic conductivity becomes zero.), and capillary pressure had dropped to -54.86 bars. The saturation in grid blocks above and below the repository in Layers E, F, L, M, N, and O was several several percent higher than ambient (due to condensation of vapor) with a slightly greater saturation in the layers above the repository than below. The Δ20° isotherm extended approximately 30 meters away from the repository in all directions, with the extension being somewhat further in the vertical directions than in the horizontal due in part to the flat geometric configuration of the repository. As at 2593 days, vapor flow was upward above the repository and downward below the repository. Fluid flow was downward through the entire domain except just beneath the repository where it was upward toward the repository (Figure 7).

7644 DAYS

At 7644 days, the repository temperature had reached 130.6°C and its liquid saturation had decreased to zero. A large temperature increase occurred between 5800 and 7000 days (Figure 8) due to total desaturation of the repository. Upon desaturation, thermal energy previously consumed by evaporation was made available to elevate repository temperatures. Temperatures in grid blocks just above and below the repository had reached 127°C. Saturation of grid blocks just above the repository was significantly higher than those just below (37% to 18%, respectively) since the higher grid blocks, unlike the lower ones, received direct recharge from above. Saturation in grid blocks above and below the repository was several percent higher than ambient in Layers E, F, M, N, and O. The Δ20° isotherm extended 45 meters above, 55 meters below, and 30 meters horizontally from the repository. The 100°C isotherm extended approximately 12 meters away from the repository in all directions and defined the extent of the 100% vapor environment. Again, the flow of vapor was upward above the repository and downward beneath it. Also, liquid flow was downward everywhere except: 1) just below the repository where it was upward; and 2) into or out of the repository where it was zero. The zero flow into or out of the repository was due to a TOUGH error which caused a zero hydraulic conductivity to be assigned to the repository blocks when their liquid saturations dropped to zero. The impact of this error would become significant during repository block cooling or an extended simulation period because it acts to proclude resaturation.

9867 DAYS

During the period from 7644 days to 8755 days, repository block temperatures decreased (due to the decay of the thermal source) slightly to 130°C and then started to increase again. The unanticipated increase was due to the total dehydration of the immediately underlying grid blocks (layer J) which effectively reduced the heat dissipation capabilities of the rock medium near the repository. In the field, however, the rock medium is a continuum and therefore would not display the temperature reversals which were caused by grid block discretization of the medium for purposes of the TOUGH simulation. The discrepency could be resolved with a much finer model griding.

At 9867 days, the close of simulation, repository block temperatures were approximately 132°C, and continued to have zero liquid saturation. The grid blocks immediately below the repository had temperatures in excess of 118°C and contained no liquid water. However, grid blocks immediately above the repository had temperatures in excess of 106°C and were 35% liquid water saturated. Only one layer above the repository showed liquid saturation levels greater than ambient while several layers below had higher than ambient saturation levels (Layer F and Layers M, N, O, and P, respectively) (Figure 9). The increased saturation of those grid blocks was predominantly due to condensation of vapor derived from the repository block, and was gradually moving downward toward the model's bottom boundary.

The Δ20°C isotherm extended approximately 45 meters above, 55 meters below, and 25 meters horizontally outward from the the repository. Vapor flow was away from the repository in all grid blocks. Fluid flow was downward everywhere except just beneath the repository where flow was upward (see Figure 7). The vertical temperature profile through the center of the repository (left edge of model grid) is shown in Figure 10.

The temperature history for the entire 9867 days taken at the center of the repository (Grid Block I-1) is shown in Figure 8. The inflections of the curve that show changes from steady temperatures to increasing temperatures are due to the complete drying out of either the repository grid blocks, or neighboring grid blocks. Due to the heat dissipation properties of heat piping, dehydrated grid blocks insulate much more effectively than non-dehydrated ones.

CONCLUSION

From this modeling study, several generic conclusions may be drawn: 1) As temperatures increase, vaporization increases, and the rate of heat dissipation also increases. This process is the predominant heat transfer process; 2) Increased vaporization near the heated zone will decrease liquid water saturation and will result in stronger capillary potentials closer to the heated zone. The end result will be a drawing of water into the heated zone and it's subsequent evaporation. Any disolved solids (e.g. salts) would likely precipitate out and concentrate in and adjacent to the heated zone; 3) A "dry" zone may be created if sufficient thermal loading is used and if the moisture characteric poperties of the rock medium are such that return liquid flow would be less than the amount of liquid evaporated by the thermal load; and 4) Since the thermal loading decays exponetially, a "dry" zone will likely have a short longevity.

Simulations performed herein underscore the complexities associated with a repository in unsaturated rock. Coupled relationships between hydrology/thermomechanics and hydrology/geochemistry (both aqueous and hard-rock) pose additional complexities which must be sorted out and assessed in a site evaluation.

For the purposes of hydrology, the TOUGH code appeared amenable to simulating the complex hydrologic processes in a porous medium. Despite its degree of complexity, TOUGH relies upon many assumptions both in its mathematical formulation and in the data it receives as input. These assumptions include that a comprehensive characterization of the site has been performed thereby providing all the neccessary data, that a mathematical formulation based on porous media theory can be accurately applied to the site, and that the various constitutive relationships employed by TOUGH will be accurate over the entire range of pressures and temperatures encountered in a simulation. Therefore, use of TOUGH with the current paucity of data and the current state of theoretical knowledge with respect to flow through unsaturated fractured rocks should be limited to determining critical parameters (via sensitivity studies) and then provide general assessments of repository performance.

REFERENCES

SAND81-7210; Klasi, M.L., Russell, J.E., McClain, W.C., and Brandshaug, T.; Far-Field Thermal Analysis of a High Level Waste Repository in Tuff; 1982.

SAND83-0757; Monday, L.A., Wilson, R.K., and Bixler, N.E.;Comparison of Waste Emplacement Configurations for a Nuclear Waste Repository in Tuff. IV. Thermal-Hydrological Analysis; 1983.

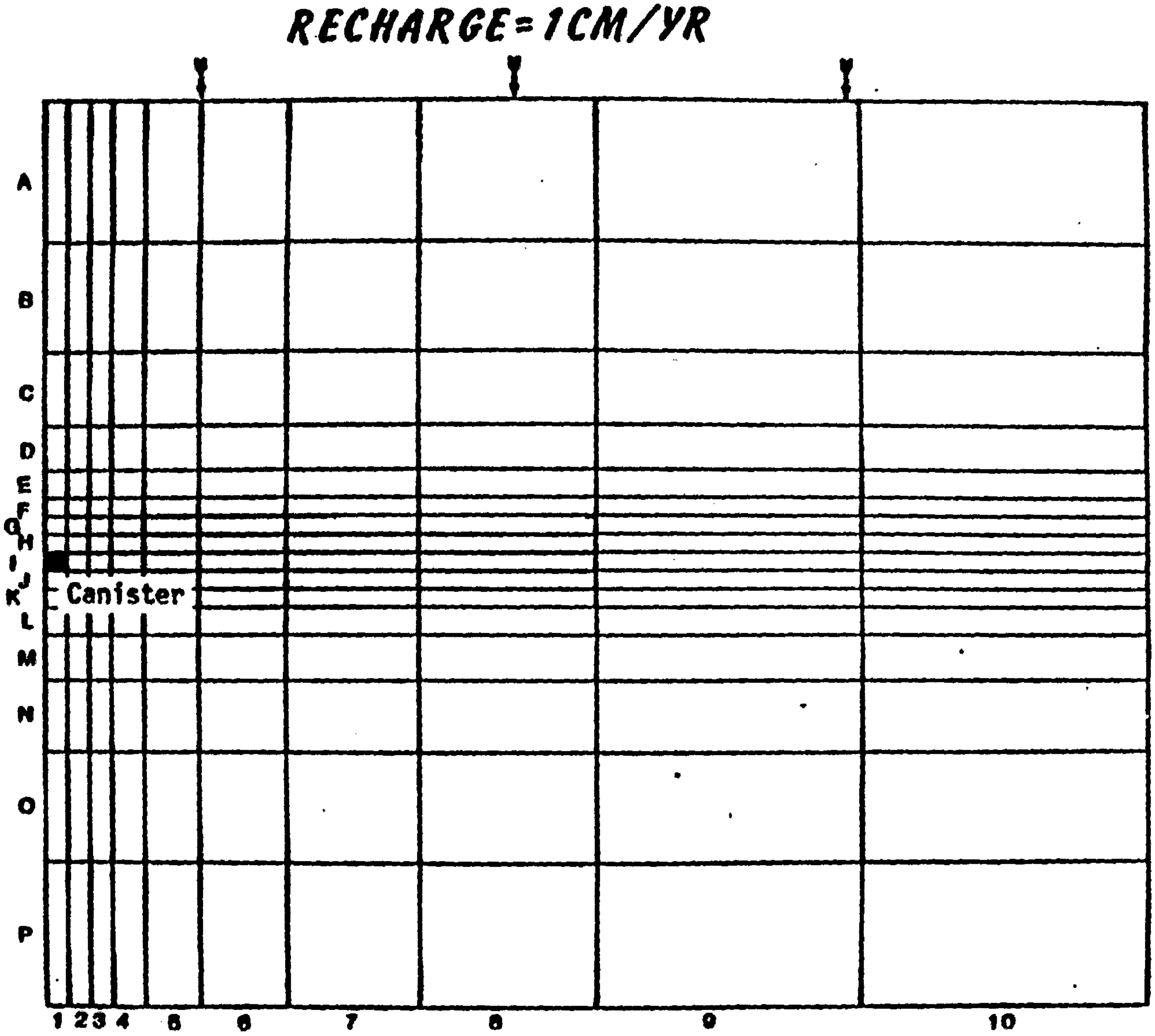

Figure 1. Cylindrical half-cross-section showing gridding of canister scale problem.

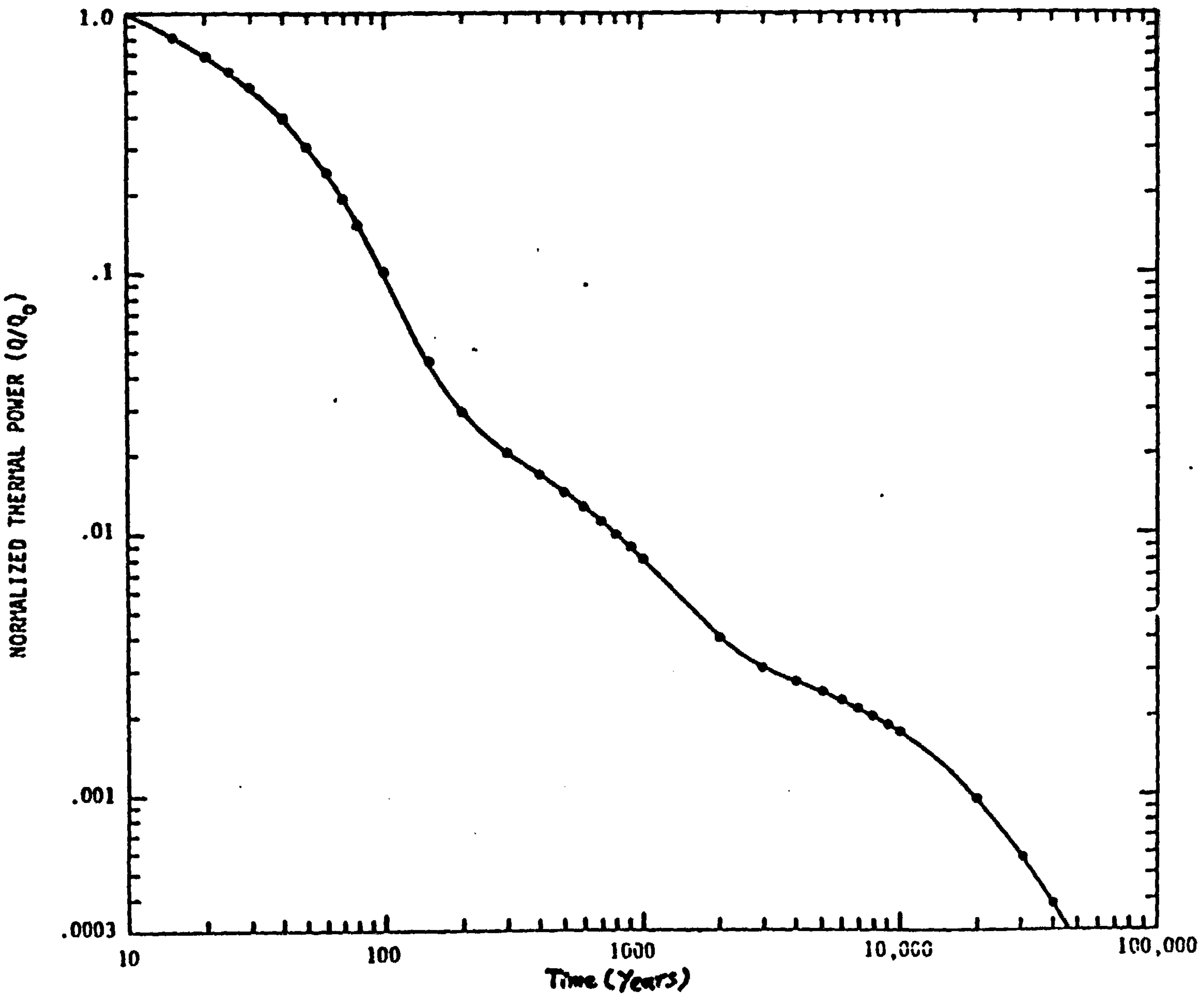

Figure 2. Normalized thermal loading as a function of time (from SAND81-7210).

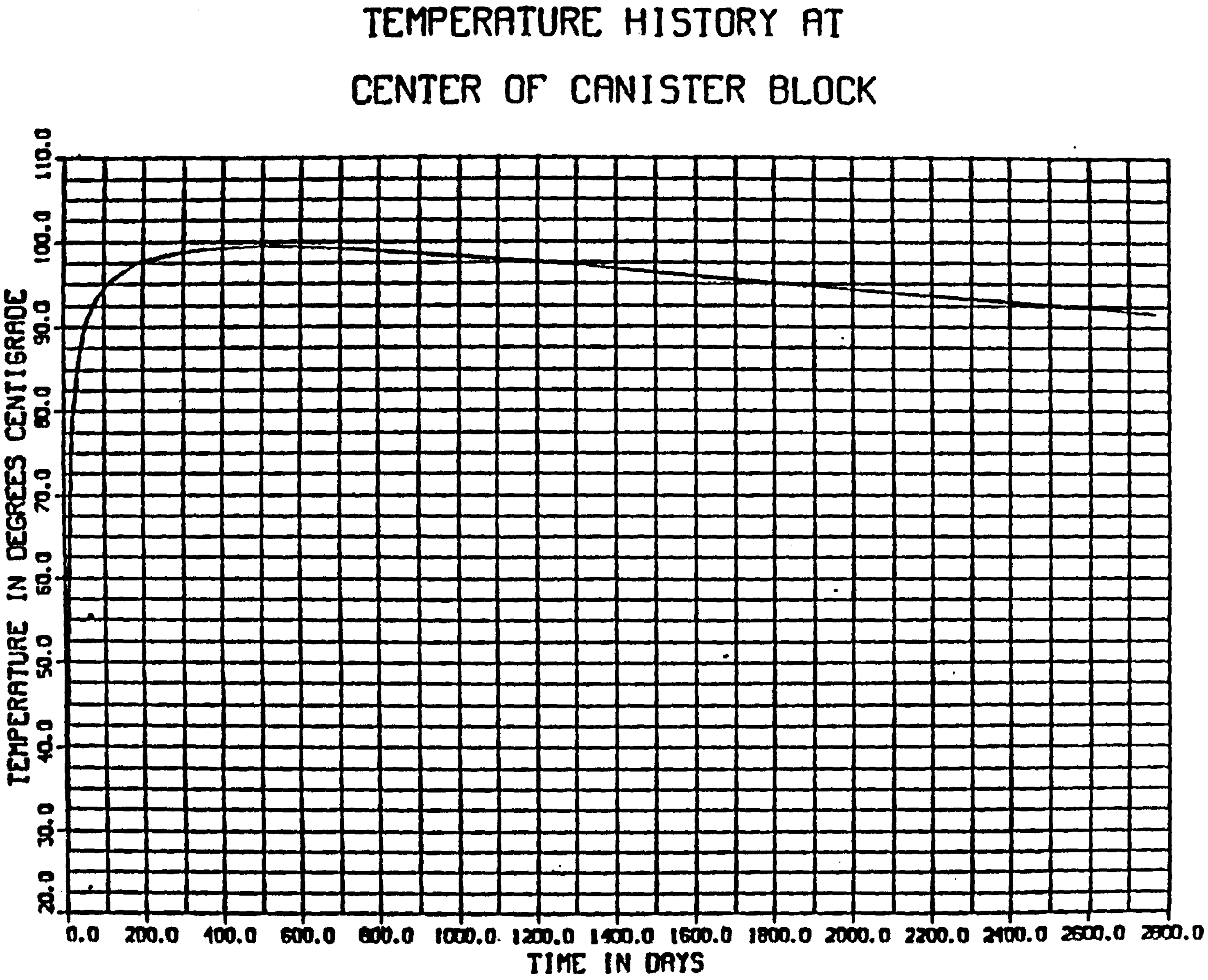

Figure 3. Temperature history at center of canister block.

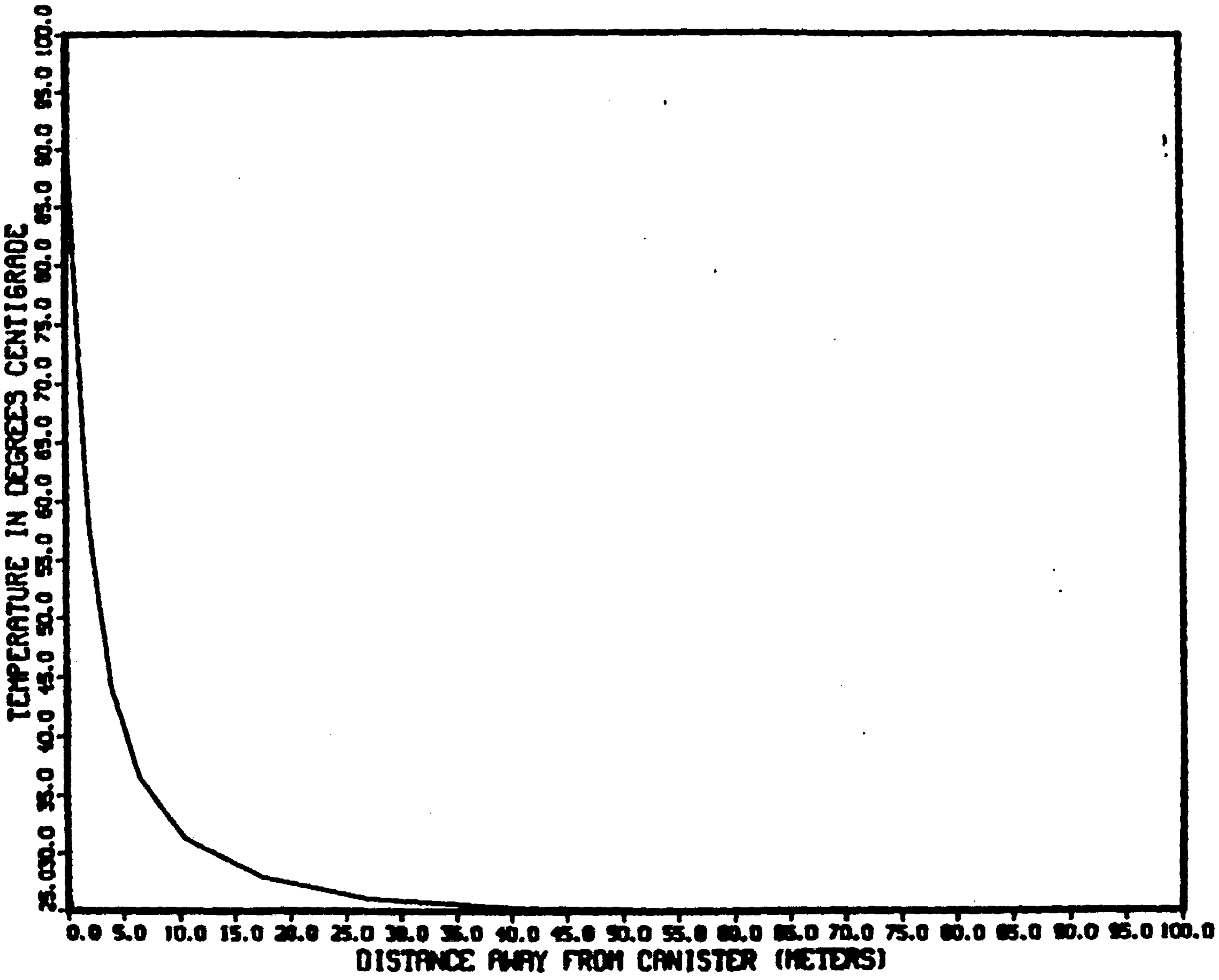

Figure 4. Horizontal temperature profile for canister at 2767 days.

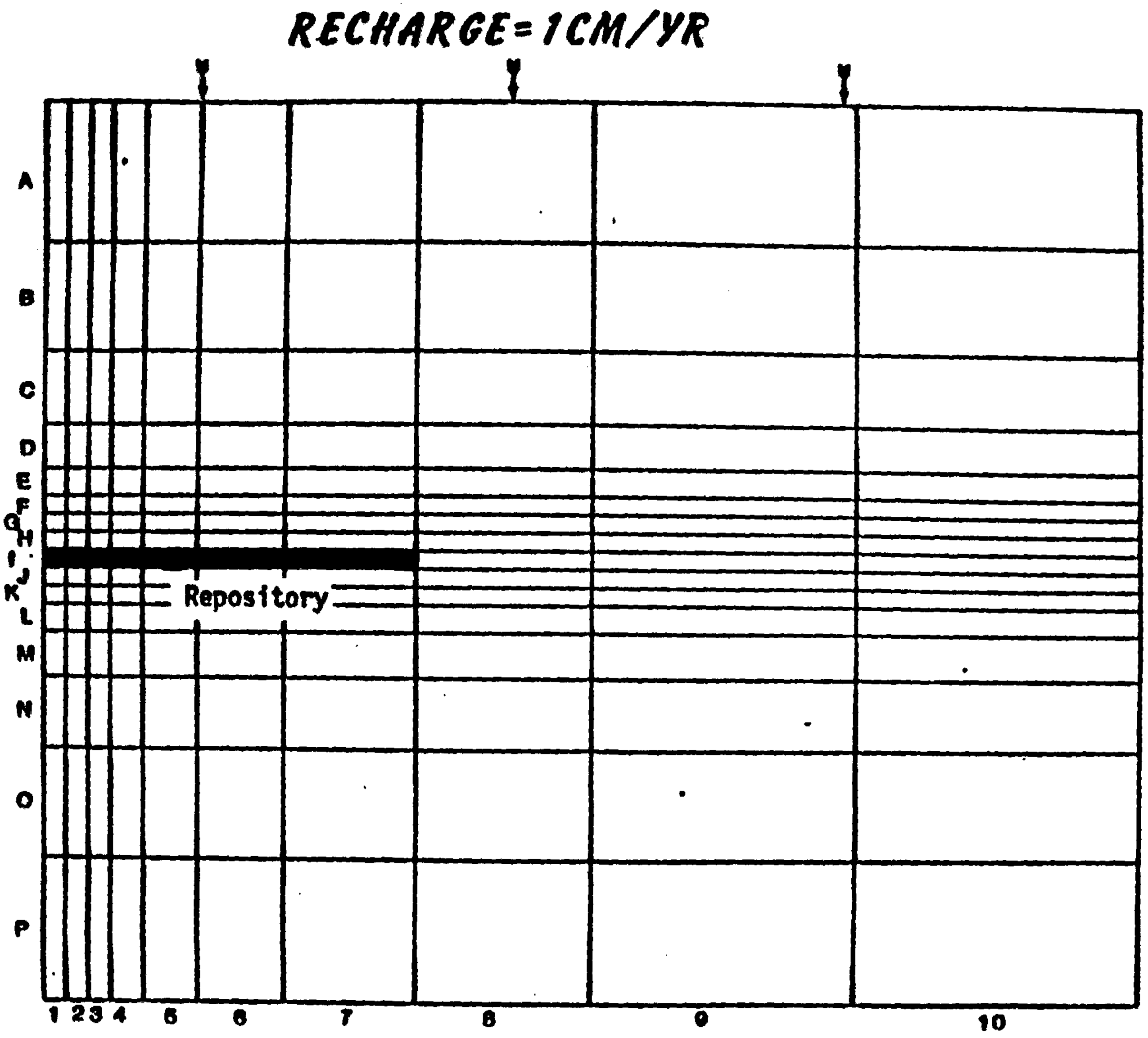

Figure 5. Cylindrical half-cross-section showing gridding of repository scale problem.

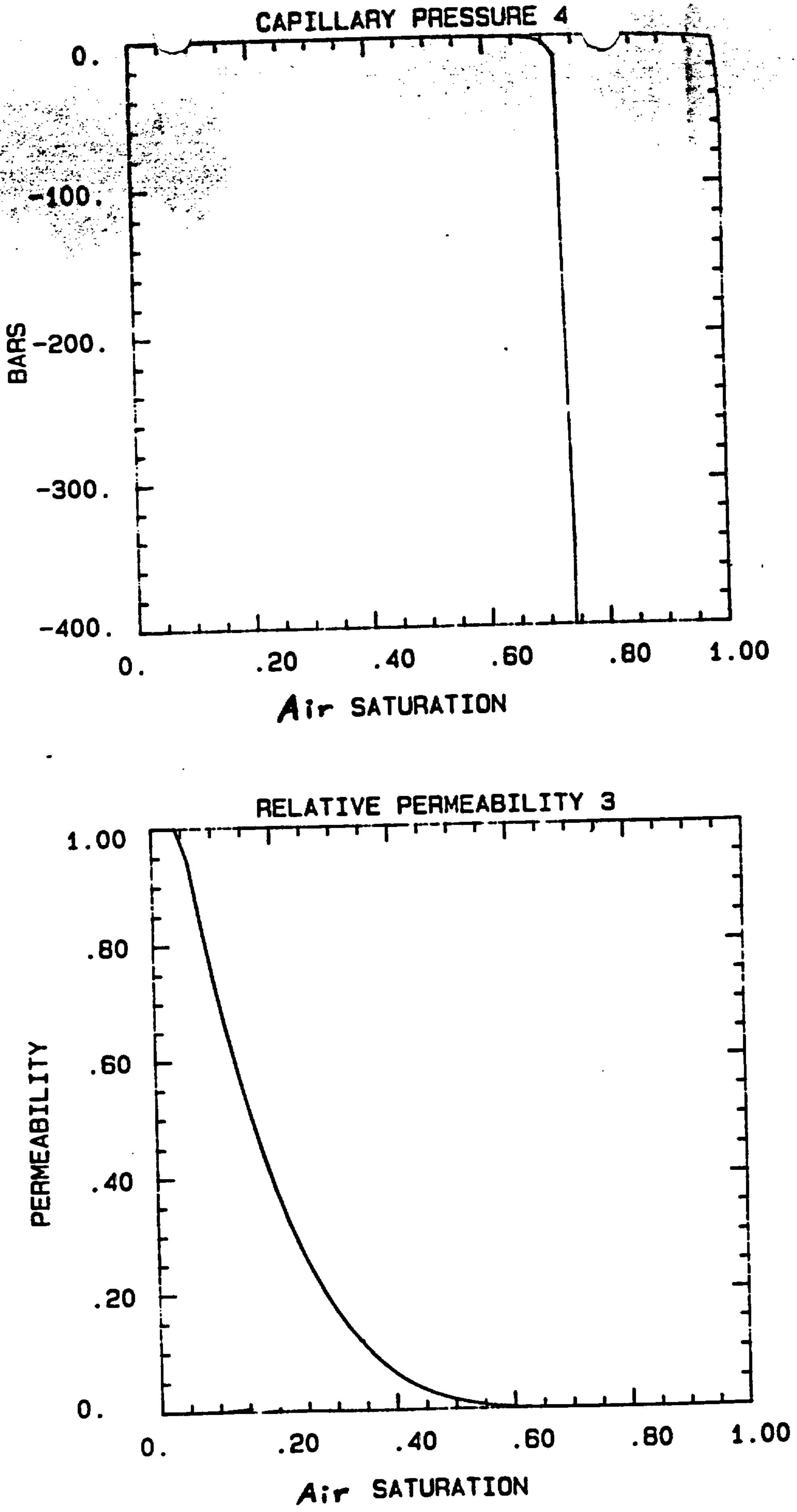

Figure 6. Moisture characteristic curves used in both repository and canister problems.

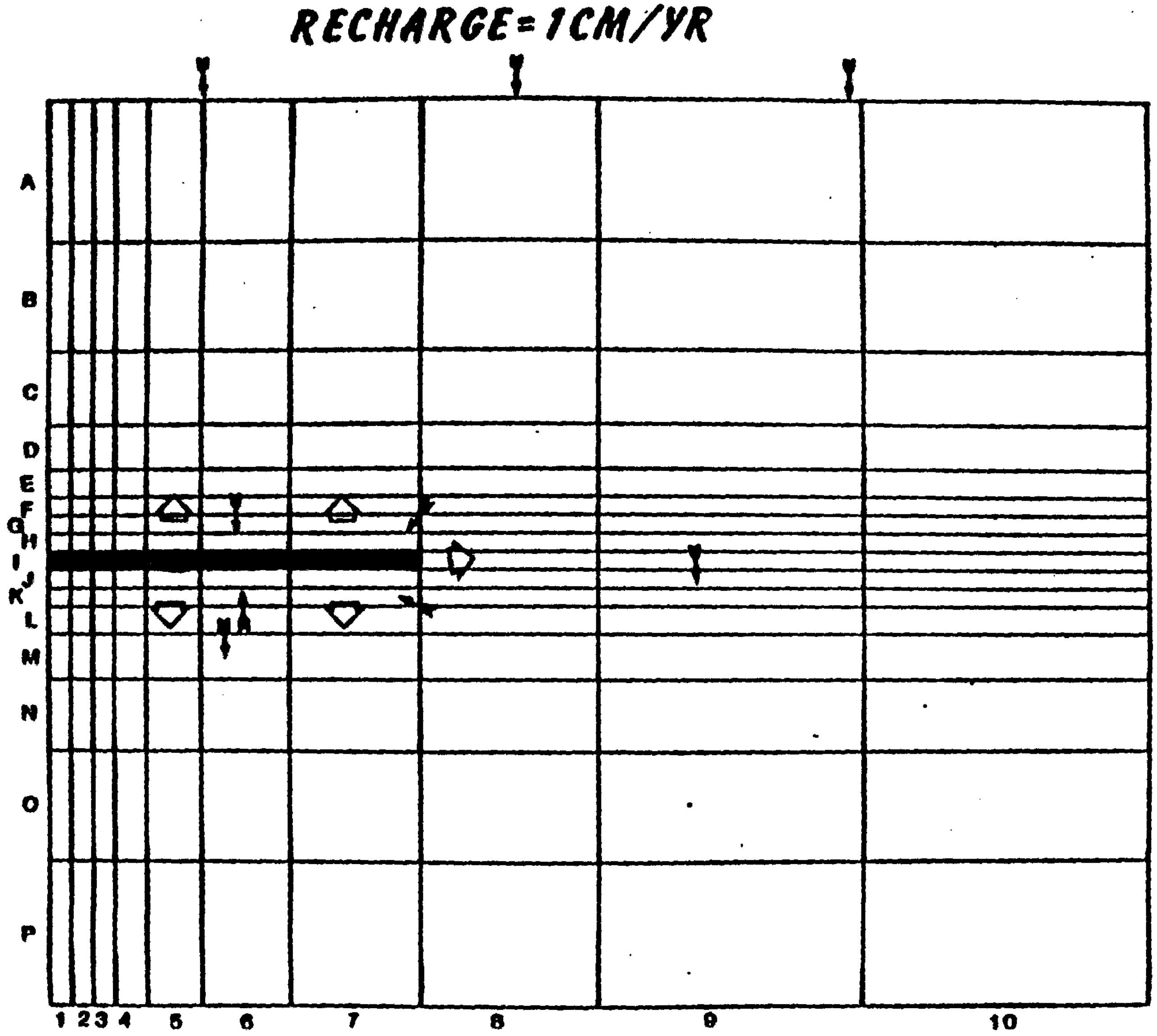

Figure 7. Schematic representation of water movement. Open arrows indicate vapor. Closed arrows indicate liquid.

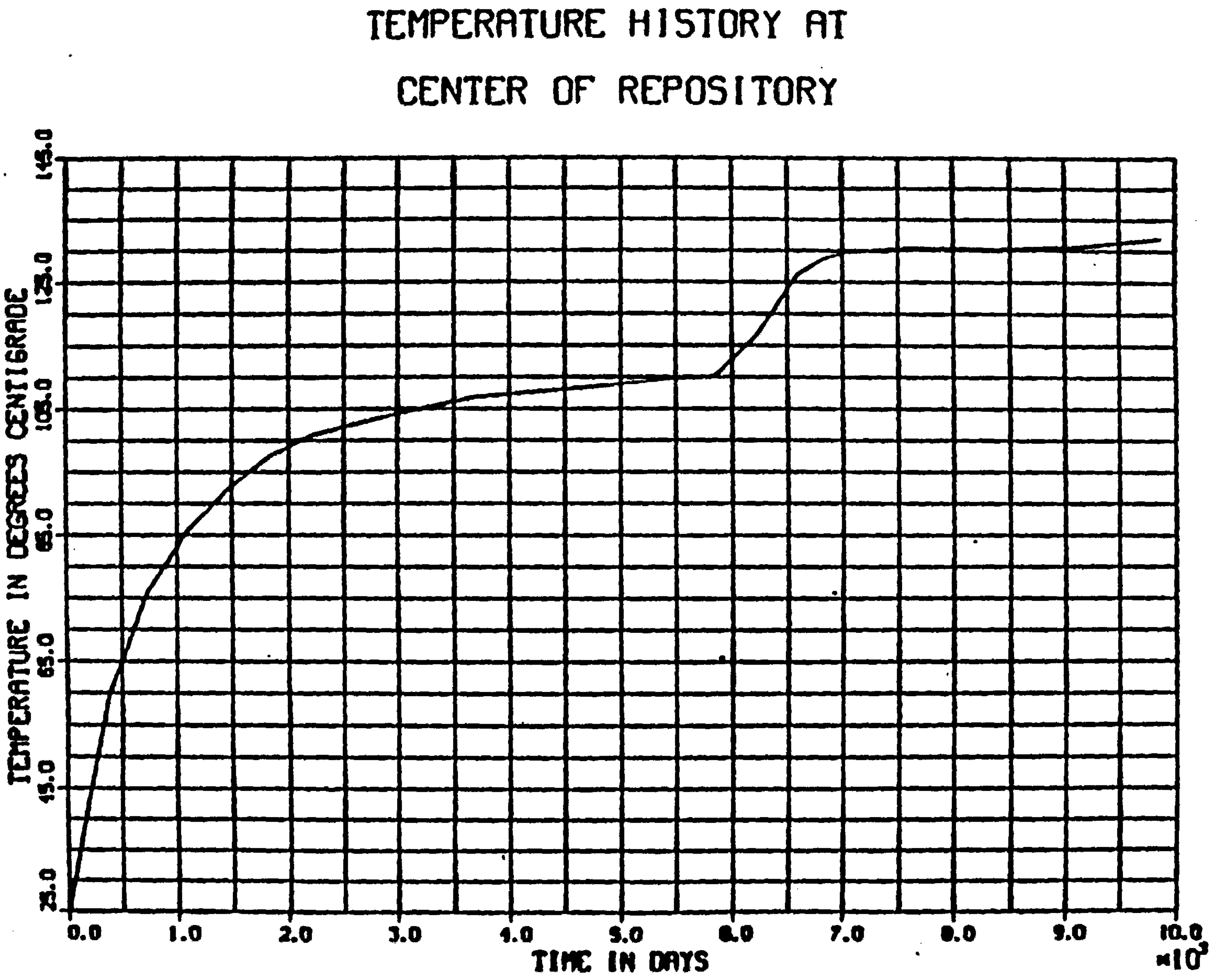

Figure 8. Temperature history at center of repository.

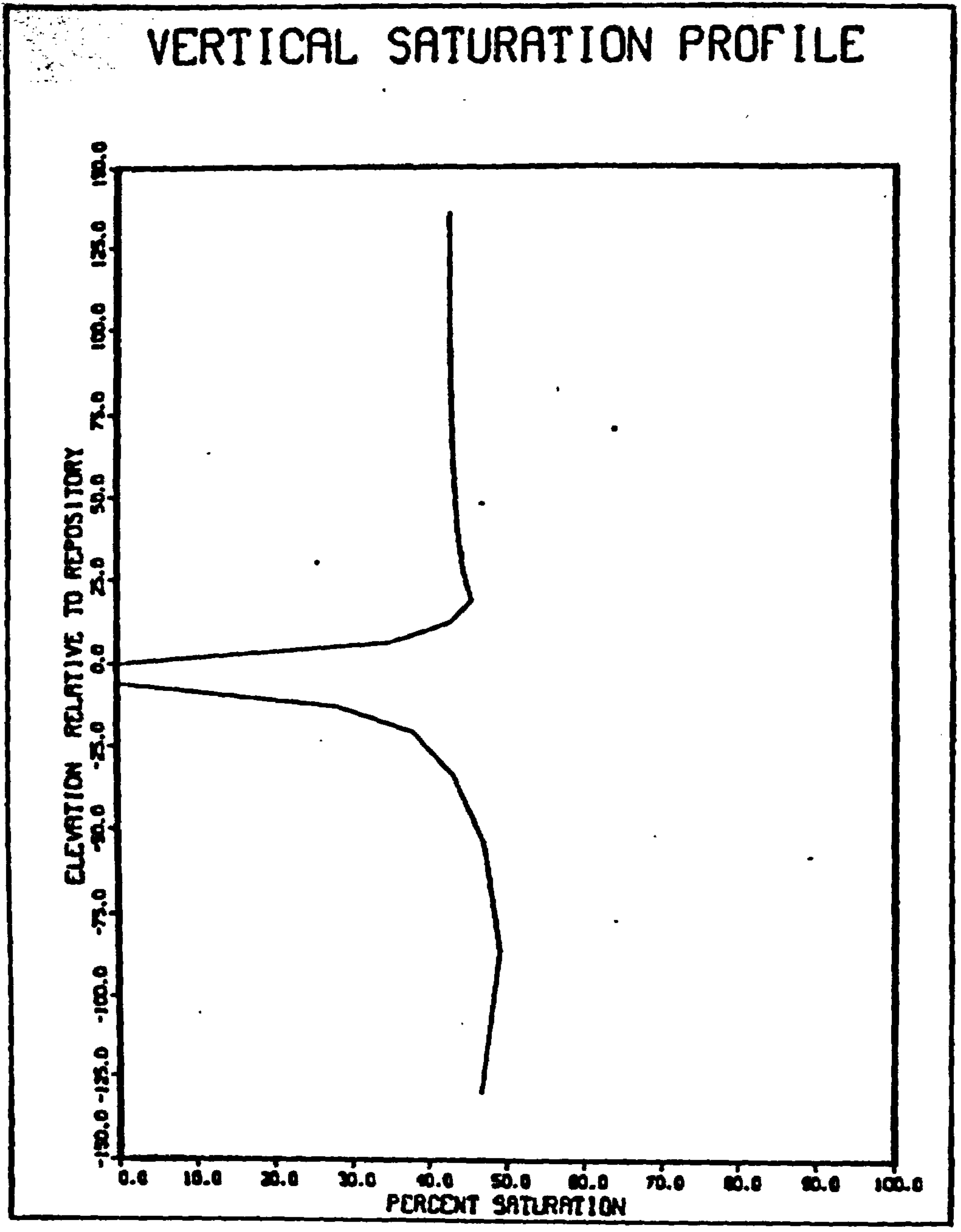

Figure 9. Vertical saturation profile through center of repository.

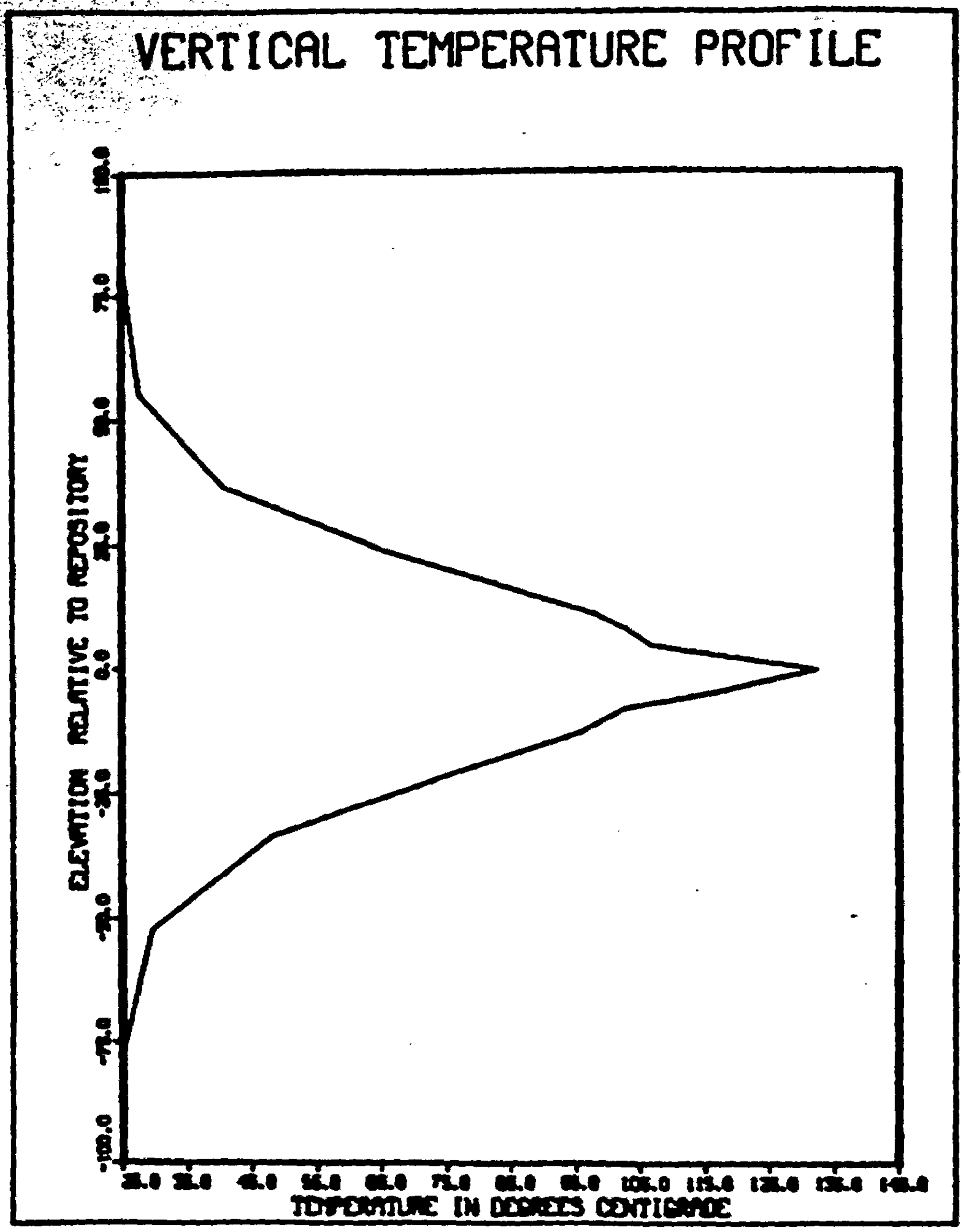

Figure 10. Vertical temperature profile through center of repository.