

200
6/20/95 WB. (2)

BNL-52468
FORMAL

RELEASE OF RADON CONTAMINANTS

FROM YUCCA MOUNTAIN:

The Role of Buoyancy Driven Flow

T. M. Sullivan

C. Pescatore

February, 1994

Brookhaven National Laboratory

Environmental and Waste Technology Center

Upton, NY 11973

The submitted manuscript has been authored under Contract No. DE-AC02-76CH00016 with the U.S. Department of Energy.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER *go*

DISCLAIMER

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ABSTRACT

The potential for the repository heat source to promote buoyancy driven flow and thereby cause release of radon gas out of Yucca Mountain has been examined through a critical review of the theoretical and experimental studies of this process. The review indicates that steady-state buoyancy enhanced release of natural radon and other contaminant gases should not be a major concern at Yucca Mountain. Barometric pumping and wind pumping are identified as two processes that will have a potentially greater effect on surface releases of gases.

TABLE OF CONTENTS

1.) Introduction	1
2.) Predicted Gas Flow Based on the General Literature on Coupled Mass and Heat Transport in Porous and Fractured Media	3
2.1) The Critical Condition for Buoyancy Driven Flow in Porous Media: Theoretical Studies	3
2.2) The Critical Condition for Buoyancy Driven Flow in Porous Media: Experimental Studies	7
2.3) Application to Yucca Mountain	9
2.4) Conclusions	12
3.) Predicted Gas Flow Based on the Specific Literature of Yucca Mountain	13
3.1) Modeling Approaches and Results for Post-Emplacement Conditions	13
3.1.1) Levels of Sophistication	13
Level 1: Solution of the Coupled Set of Equations for Energy Momentum, and Mass	13
Level 2: Decouple the Energy Equation from the Momentum and Mass Balance Equations	14
Level 3: Assume a hydrostatic pressure distribution	15
3.1.2) Common Assumptions	15

3.2) Conclusions	18
4.) Coupling Between Buoyancy Flow and Surface Driven Flow	19
4.1) Natural Flow Systems at Yucca Mountain	19
4.2) Barometric Pumping at NTS	20
4.3) Conclusions	22
5.) Conclusions	23
6.) References	26

**Appendix A: Fundamental Equations for Heat and Mass Transport of a Compressible
Fluid in a Porous Media**

1. INTRODUCTION

The issue of gas flow and contaminant transport out of the proposed repository site at Yucca Mountain has recently received much attention [Knapp, 1987; Ross, 1988; Amter, 1991; Ross, 1992; Codell, 1992; Pescatore, 1992; White, 1992; Ross, 1993]. Particular concern is given to the potential for enhanced release due to buoyancy caused by heating of the rock mass.

This program is charged with examining the potential for releases of natural radon from Yucca Mountain. In order to do so, we have reviewed the literature on predicting gas flow and contaminant transport in non-isothermal media and have performed ancillary calculations (Appendix A).

Chapter 2 of this report reviews the literature on coupled experimental and theoretical work on buoyancy driven flow in porous media. It also presents an application of these findings to conditions representative of Yucca Mountain.

Chapter 3 presents a qualitative overview of direct attempts to model the release of contaminant gases from Yucca Mountain. The predicted results are discussed in terms of the findings reported in Chapter 2. Based on these comparisons, limitations in current post-emplacment modeling are discussed.

Chapter 4 presents information on the natural gas flow system at Yucca Mountain. Results are presented from experimentally measured and predicted flows at Yucca Mountain under present unheated conditions. The role of barometric pumping in contaminant transport in fractured systems is also presented. These naturally occurring flows are compared to the predicted flows after emplacement. The potential for coupling between flow and transport by buoyancy and barometric pumping are discussed.

Chapter 5 summarizes the findings of this study. The role of buoyancy is compared to

other flow inducing processes. Recommendations for methods to improve current analyses are provided.

2. PREDICTED GAS FLOW BASED ON THE GENERAL LITERATURE ON COUPLED MASS AND HEAT TRANSPORT IN POROUS AND FRACTURED MEDIA

Gas contaminants at Yucca Mountain will travel as impurities in air/vapor. Thus, the first important issue to address is whether macroscopic movement of air out of the mountain due to buoyancy can take place. The literature on flow out of Yucca mountain has generically addressed this very issue from a strict modelling and simplified point of view. Their assumptions and results are examined in Chapter 3. It is important to recognize that substantial efforts in understanding coupled mass and heat transport from both the experimental and theoretical view points have been performed and are available in the literature. This chapter reviews some of this work and applies these findings to relevant conditions at Yucca Mountain.

2.1) The Critical Condition for Buoyancy Driven Flow in Porous Media: Theoretical Studies

Beginning with an isothermal porous system in which a fluid is at rest, if a heat source is applied at the bottom, the fluid will begin to move due to buoyancy. As it moves, it encounters resistance due to friction between the fluid and solid as well as internal friction within the fluid. Depending on the fluid properties (viscosity and coefficient of thermal expansion) and porous medium properties (permeability) the flow can be damped out due to frictional losses or energy exchange from the heated fluid to the stationary porous medium. Or, if the conditions are favorable, the flow will develop and lead to convective currents. *Thus, a threshold set of conditions must exist for the macroscopic steady-state movement of air due to buoyancy at Yucca Mountain.*

A review of the early studies on buoyancy driven flow in a porous media heated from below is presented in [Bear, 1972]. Recent studies on buoyancy driven flow in porous media have expanded on the earlier work to include the effects temperature dependent properties [Straus, 1977; Nield, 1982], different boundary conditions [Rajan, 1987; Phillips, 1991],

non-homogeneous media [Phillips, 1991] and of evaporation/condensation [Ross, 1993]. All of the studies, with the exception of [Ross, 1993], apply to a homogeneous single phase fluid.

The conditions for the establishment of steady-state convective currents were studied first theoretically for an infinite uniform, isotropic, horizontal porous media heated from below. The boundary conditions were constructed to have fixed temperature at the surfaces with no net flow out of either boundary. It was also assumed that density and viscosity variations are important only in the buoyancy term, i.e., the Boussinesq approximation. Perturbation analysis on the resulting coupled set of conservation equations for energy, momentum (Darcy's law), and mass was used to study the formation of convection currents. The host media was saturated with water and thermal equilibrium was assumed between the solid and liquid phases. The results of this study indicate that non-zero steady-state flow would be established if the Rayleigh number, a dimensionless parameter that relates buoyancy forces to viscous forces, is greater than $4\pi^2$ [Lapwood, 1948]. For a homogenous, isotropic porous medium and using the Boussinesq approximation, the Rayleigh number, Ra , is defined as [Elder, 1967];

$$Ra = \frac{k \gamma g \Delta T H}{\kappa_m \nu}$$

where g is the acceleration due to gravity, γ is the coefficient of thermal compressibility, ΔT is the temperature change over the height, H of the system, κ_m is the effective thermal diffusivity of the medium (see section 2.3), ν is the kinematic viscosity of the gas, and k is the permeability.

The theory of convective flow in porous media was generalized [Straus, 1977] to incorporate temperature and pressure dependent properties for density, viscosity, thermal expansion coefficient and specific heat. Removing the Boussinesq approximations leads to a decrease in the value for the critical Rayleigh number for water while it increases the value for (ideal) gases [Nield, 1982]. The major reason for the destabilizing effect of temperature

and pressure dependent properties of water on convective flow is that the thermal expansion coefficient increases with temperature and the viscosity decreases. The opposite is true for gases.

As reported in Phillips [Phillips, 1991] the critical Rayleigh number for a Boussinesq fluid in an isotropic porous medium is specific to the choice of boundary conditions. For example, if the heat flux is specified at both impermeable boundaries, the critical Rayleigh number is 12. When the upper surface is at constant pressure (i.e. flow can occur through the boundary) while the lower boundary is impermeable; if the upper and lower boundary temperatures are fixed, the critical value is 27.1; if the upper temperature and the lower heat flux is fixed, it is $\pi^2 = 9.87$. These last two situations are more representative of the Yucca Mountain site than having an impermeable upper boundary.

Phillips reports an expression for the critical Rayleigh number, Ra , for a porous medium with impermeable boundaries and directionally dependent permeabilities as [Phillips, 1991]:

$$Ra = \frac{g\gamma\Delta T H}{\kappa_m \nu} \frac{k_h k_v}{[k_h^{1/2} + k_v^{1/2}]^2} \leq \pi^2$$

where k_h and k_v are the vertical and horizontal permeabilities, respectively. If the permeabilities are equal in each direction, the preceding expression reduces to the classical expression for the Rayleigh number. If the permeabilities differ by a factor of two, the critical Rayleigh number increases to $5.83 \pi^2$ (using the homogeneous medium expression with the permeability selected as the larger of the two values). If an order of magnitude difference in permeabilities occurs, the critical value becomes $17.3 \pi^2$.

At Yucca Mountain studies indicate that over 75% of the fractures are within 10 degrees of being vertical [MacDougall, 1987]. This would indicate that the permeability

should be much smaller in the horizontal than in the vertical direction.¹

Non-homogeneous fluids

[Ross, 1993] has recently extended the Lapwood infinite porous media analysis to air constrained to be at 100% humidity. Thus, the effects of evaporation and condensation of water vapor are included in the analysis. The studies of Ross indicate that for a homogenous infinite layer with fixed temperatures at the repository horizon and the surface, incorporation of evaporation/condensation effects would lower significantly the critical Rayleigh number. In Ross's studies, the critical Rayleigh number is a function of the temperature change as well as the surface temperatures. For the conditions at Yucca Mountain the critical Rayleigh number is approximately two orders of magnitude lower than that found by Lapwood. Ross's studies also indicate that for typical Yucca Mountain conditions the time constant for establishing convective flow is on the order of 1000 years.

A potentially important limitation of the [Ross, 1993] analysis is the use of Darcy's law for a non-homogeneous fluid (air plus water vapor). This neglects the momentum transfer between water in the gas phase (vapor) and liquid in the pores of the rock upon condensation. In the most general approach to solving multi-phase flow problems, there is a momentum balance equation for each phase (liquid, air, and water vapor). The influence of this assumption on the value of the critical Rayleigh number is not known, but the more complex numerical simulations of buoyancy-driven flow [Buschek, 1992; White, 1992] would indicate that it should increase significantly [see Section 3.1.1]. Other reasons why the critical Rayleigh number should be greater than Ross predicts are discussed in Section 2.2.

In any event, the long time required to reach steady-state convection, (on the order of

¹However, the several orders of magnitude difference between matrix and in-situ permeability indicate that the fractures are interconnected [Wang, 1984]. Estimated values of the equivalent porous media permeability for these two directions typically are within a factor of two [Wang, 1986].

1000 years [Ross, 1993]) makes the applicability of his critical Rayleigh number questionable. The repository temperature will not remain constant for this length of time. The influence on the critical Rayleigh number of having a constant repository temperature as compared to a decreasing temperature is not known. However, intuitively as the heat source decreases one would expect the driving force for buoyancy to decrease. In addition, if the time constant for establishing convective flow is thousands of years, this indicates that a transient flow field will be in effect for this duration. This implies that the Rayleigh stability analysis, which determines whether steady-state flow will occur, is not appropriate on this time scale.

2.2) The Critical Condition for Buoyancy Driven Flow in Porous Media: Experimental Studies

Elder conducted experimental and numerical studies of finite sized heat sources at the bottom of the heated region [Elder, 1967]. His studies specified a fixed temperature in the heated region and covered a range of the ratio of the heated width to the total width between 1/2 and 4/5. Elder found that the critical Rayleigh number was insensitive to the heated length fraction and remained near the Lapwood value of $4\pi^2$. The aspect ratio in these experiments, (ratio of the height above the heat source to the length at the bottom of the experimental apparatus) ranged from 1/5 to 1/2. Elder's studies indicate the following:

- below the critical Rayleigh number heat transfer is by conduction and no mass flow occurs, whereas above this point convection plays an important role;
- "... as the critical Rayleigh number is approached (from above) the time for the establishment of the steady motion is considerably larger than the time to heat the slab solely by conduction." Elder goes on to say, "For this reason attempts to study the instability of a layer of fluid suddenly heated from below by the assumption that the temperature field is quasi-steady, are bound to fail."

- mass discharge occurs only above the critical Rayleigh number. The discharge will be centered on the heated region and mass will be recirculated (i.e. a convection cell forms). As the Rayleigh number increases, less mass is recirculated until eventually the flow is dominated by a boundary layer near the heated surface and a plume rising above it.

More recent studies [Rajen, 1987] for a uniform heat flux at the bottom of the porous medium filled with water, experimentally demonstrated convective flow at a Rayleigh number of 30. This is above the critical value for a uniform heat flux source. Data or computations at Rayleigh numbers less than 30 are not provided and therefore the precise value for the onset of convection can not be determined from this report. These experiments considered aspect ratios of 1/16 and 1/4.8 and heated length fractions of 1, 1/2, and 1/12. The values specifying the geometry are more consistent with values expected at Yucca Mountain than those of Elder.

Another important conclusion of the work of Rajen is that the use of an equivalent medium permeability may be questionable at Rayleigh numbers slightly above the critical value. In these cases, recirculation effects were localized to a small region above the edge of the heated region. [Rajen, 1987] concludes "The equivalence of a fissure system with a porous medium for a partially heated layer will not be dependent solely on the geometry of the fissure system, and a Rayleigh number dependence will probably exist." This implies that the volume of the region over which buoyancy driven flow will occur is a function of the Rayleigh number. At Rayleigh numbers slightly in excess of the critical value, the buoyancy driven flow will be localized to directly above the edge of the heated region. In this case, the presence of fissures above the edge of the repository would play an important role in buoyancy driven flow. If the distribution of fissures in this region is not representative of the average in the system, it may be difficult to define an equivalent porous medium permeability.

2.3 Application to Yucca Mountain

For a homogenous, isotropic porous medium and using the Boussinesq approximation, the Rayleigh number, Ra , is defined as [Lapwood, 1948, Elder, 1967];

$$Ra = \frac{k \gamma g \Delta T H}{\kappa_m \nu}$$

To allow calculation of the Rayleigh number, typical values of the parameters at Yucca Mountain along with their definition with dry air as the reference fluid are supplied in the following table. Namely:

where k = permeability of the porous medium (m^2)	$10^{-11} m^2$;
γ = coefficient of thermal compressibility (K^{-1});	$3 \cdot 10^{-3} K^{-1}$;
g = acceleration due to gravity (m/s^2);	$9.8 m/s^2$
ΔT = temperature difference across the porous medium (K);	80 K
H = height of the porous medium;	350 m
$\kappa_m = K_m/\rho c$ = thermal diffusivity (m^2/s)	$1.8 \cdot 10^{-3} m^2/s$
K_m = thermal conductivity of the porous medium ($W/(m K)$);	$1.8 W/(m K)$
ρc = thermal capacity of the fluid ($W/(m^3 \cdot s K)$)	1000 ($W/(m^3 \cdot s K)$)
ν = kinematic viscosity of the fluid (m^2/s);	$2 \cdot 10^{-5} m^2/s$

The values of all parameters are typical of those found in the temperature range of 300 - 350 K. Following [Elder, 1967], the thermal diffusivity is obtained through a weighted-average conductivity term of the whole system (solid plus fluid). The typical weighting is by the volume fraction of each phase. However, the thermal capacity is that of the fluid.

Using the values provided we see that the Rayleigh number is 0.23. This is two orders of magnitude below the critical value determined experimentally [Elder, 1967; Rajan, 1987]. If the behavior of the air/vapor mixture is more like that of an ideal gas, it is

expected that the critical Rayleigh number would be slightly higher when accounting for non-Boussinesq effects. The calculated Rayleigh number is of the same order of magnitude as that found by Ross when including the effects of evaporation/condensation.

The parameter with the largest uncertainty in the Rayleigh number is the permeability. While the value selected is on the high end, higher values have been estimated in the literature [Klavetter, 1986; Kipp, 1987]. Using the properties of air saturated with water vapor would not cause large changes in the thermal expansion coefficient, thermal capacity of the fluid or viscosity. Therefore, it would not cause large changes in the Rayleigh number.

A recent study [Buschek, 1992] which considered coupled heat transfer with water, air, and host rock at the Yucca Mountain site is in qualitative agreement with the above analysis as they found that far-field convection significantly contributes to heat flow at bulk permeabilities greater than 10^{-10} m², while for permeabilities below 10^{-11} m² convective heat transfer is insignificant.

A similar Rayleigh number analysis [Rasmussen, 1987] which factors in inhomogeneity and anisotropy of the geologic setting has also concluded that buoyancy driven flow is unlikely at Yucca Mountain. [Rasmussen, 1987] reports of a study [Donaldson, 1970] of gas flow through a series of vertically oriented high permeability fracture zones separated by zones of low gas permeability. The critical Rayleigh number was found to exceed that of the homogeneous porous medium case. The key parameter in determining the increase in the critical Rayleigh number is the aspect ratio defined as the area of all fractures divided by the column height. Based on this, Rasmussen claims that "*... to have convective flow, the presence of flow channels and low gas permeability zones require the system to exist under conditions of higher Rayleigh numbers than would be necessary for a system with uniformly distributed flow paths (i.e. an equivalent porous medium). The occurrence of narrow zones of high gas permeability rather than large zones of uniform moderate permeability can be impediments to the formation of convection cells at a HLW repository.*"

We concur with Rasmussen that, if the vertical permeability (directed up and out of the mountain) is much larger than the horizontal permeability, the horizontal flow may be insufficient to replenish the fracture flow and a steady-state convection system will not arise. In any directionally fractured system, (i.e. non-isotropic permeability), the possibility of buoyancy induced convection is reduced over that of a uniform porous media. This is supported theoretically by the work reported in [Phillips, 1991].

Another impediment to setting up convection cells is the layered, non-homogeneous distribution of permeabilities at Yucca Mountain. Different stratigraphic layers have substantially different permeabilities. If the permeability in any of these layers is much less than the value assumed in estimating the Rayleigh number, the likelihood for buoyancy driven flow is decreased. In general, the least permeable layer controls the flow through the system. The effects of lowering the permeability for a 50 m region above the repository horizon by a factor of 10 and 100 is presented in appendix A. The examples with the reduced permeability zone showed a substantial reduction in predicted flow out of the mountain.

The issue of the regions of applicability of the equivalent porous medium approach has been addressed recently [Buschek, 1992]. In [Buschek, 1992] it is stated that for far field convection to occur, the fractures would have to be connected on a scale of the order of hundreds of meters and they would have to be distributed so that they behaved as an isotropic continuum.²

²This may not be the case at Yucca Mountain, however, almost all state-of-the-art codes and models (e.g. TOUGH, TOUGH-2, MST5, PORFLOW, etc.) rely on the equivalent porous medium approach.

2.4 Conclusions

A threshold set of conditions, taken into account by the Rayleigh parameter, must exist at Yucca Mountain before macroscopic steady-state movement of air and vapor can take place due to buoyancy. The critical value of this parameter is not known exactly at Yucca Mountain. The experimental studies of buoyancy-driven flow in finite porous media with a finite heat source at the bottom suggest for a homogeneous fluid a critical Rayleigh number of approximately 30. This value would be greater at Yucca Mountain due to the directionally fractured and layered geology. For the quantities appearing in the Rayleigh parameter based on a) a homogeneous porous media, b) typical reference values applicable to Yucca Mountain, and c) a permeability on the high end of the measured values, the Rayleigh parameter is calculated to be approximately 0.2. Thus, buoyancy-driven flow should not take place at Yucca Mountain. This implies that the release of naturally occurring radon should not be enhanced over existing conditions.

In only one theoretical study, [Ross, 1993], the critical Rayleigh number was determined to be as low as 0.2. However, at this time, the underlying assumptions of this study have not been verified. In any event, even with this approach, the inclusion of non-Boussinesq effects in the analysis and the presence of different stratigraphic layers and anisotropies will certainly yield a larger value for the critical Rayleigh number indicating the onset of convection.

3. PREDICTED GAS FLOW BASED ON THE SPECIFIC LITERATURE OF YUCCA MOUNTAIN

Concern over potential releases of ^{14}C and ^{222}Rn and other contaminated gases at Yucca Mountain has caused a number of studies predicting gas flow and contaminant transport after heating by the waste to be performed. These studies are reviewed in this chapter.

3.1 Modeling Approaches and Results for Post-Emplacement Conditions

The movement of contaminated gas in a porous media heated from below involves solution of the continuity equations for mass, momentum, and energy for each phase (air, water, host rock). Temperature differences may exist between the different phases. Further, the boundary conditions are a function of time due to atmospheric variations. This coupled set of equations is complicated and many assumptions are made to simplify the equations to permit a solution. Currently, there have been three levels of sophistication used in solving the system of equations. These three approaches are discussed below. Common assumptions of the models are presented after the models are discussed.

3.1.1 Levels of Sophistication

Level 1: Solution of the Coupled Set of Equations for Energy, Momentum, and Mass

The most detailed analyses of flow at Yucca Mountain solve the multi-phase coupled system of conservation equations under the assumption of thermal equilibrium between phases. They include the effects of boiling and evaporation/condensation and capture the effects of convection on heat transport. The momentum equation is assumed to be adequately represented by Darcy's law. This reduces the system of coupled partial differential equations from three to two. That is, the Darcy's law expression for volumetric flow is used in the continuity and energy equations which are solved simultaneously.

Calculated flow velocities are extremely sensitive to fracture permeability and the hydrologic properties of the fractures. Predicted velocities are as large as 3 meters per day (1000 m/yr) along the repository centerline in the boiling region 100 years after emplacement [Pruess, 1988]. However, these dropped to 0.03 m/day (10 m/day) or less 100 m or more above the repository level.

Recent studies on the thermal response to the repository heat load [Buschek, 1992] indicate that convection is an important heat transfer mechanism only in the boiling region above the repository. Above this region, conduction is the only effective heat transfer mechanism. Accordingly, diffusion is the dominant mass transfer mechanism.

A study of ^{14}C release using the multi-phase continuity equations [White, 1992] arrives at the conclusion that diffusion in the gas phase was the dominant transport mechanism as the advection velocities were so low.

These analyses do not predict large scale buoyancy generated convection currents. They do, however, predict buoyancy driven flow in the boiling region. This region is limited to within approximately 100 m of the repository and is subject to substantial recirculation. Thus, the net flow out of this region is negligible.

Level 2: Decouple the Energy Equation from the Momentum and Mass Balance Equations

In the next level of sophistication, evaporation and condensation are still considered, however, convective heat transport is not. In these models, the energy equation is solved independently of the continuity equation. This requires the model to neglect convective heat flow and permits a temperature distribution to be calculated prior to obtaining the fluid flow field.

The temperature field obtained based on conduction is used to calculate temperature dependent properties such as density and viscosity. The flow field is obtained using Darcy's

law is to represent the momentum equation. Darcy's law is placed in the continuity equation and the pressure is determined from the resulting partial differential equation.

Ignoring heat convection is equivalent to ignoring mass convection. Thus, there should be no buoyancy-induced mass flow. Nevertheless, these models calculate buoyancy driven flow. Ross calculates gas transport times to the surface of approximately 100 years, implying an average velocity of about 0.3 m/yr [Ross, 1992]. ^{14}C transport times were considerably longer due to retardation. It is interesting to recall, it has been experimentally shown [Elder, 1967] that when convective heat transport is not important, it implied that the Rayleigh number is less than the critical value and at steady-state there is zero flow.

Level 3: Assume a hydrostatic pressure distribution

In the simplest approach, Darcy's law is used for the momentum equation with the approximation that the hydrostatic pressure distribution adequately describes the pressure field. As in the Level 2 models, convective heat transport is ignored. This completely decouples all three conservation equations. The velocity is calculated directly from the density difference due to thermal heating [Pescatore, 1992]. This gives the largest flow rates with values on the order of meters per day. However, this prediction, as those in level 2, is inconsistent with the assumption of negligible heat convection.

3.1.2 Common Assumptions

As indicated earlier, although there have been three distinct levels of computational sophistication implemented to predict gas and contaminant flow out of Yucca Mountain, all approaches rely on a number of important and common assumptions and simplifications. For instance, we have already noted that the full momentum equation is not solved in any of the above approaches rather Darcy's law is used instead. These assumptions are reported hereafter and their impact is reviewed.

1. Isotropic Permeability

The fractured nature of Yucca Mountain leads to the possibility of anisotropies in permeability. If these occur, the flow fields will adjust accordingly. In particular, if the horizontal permeability is less than the vertical permeability this will tend to further mitigate the possibility of buoyancy driven flow. At this time, all simulations of flow through Yucca Mountain are based on isotropic permeability. An example of the changes in flow that could arise from anisotropic permeability is found in Appendix A. For a factor of ten difference in the vertical and horizontal permeabilities predicted flow rates were substantially reduced from the isotropic case.

In addition, some models assume a homogeneous porous media. The permeabilities of the different stratigraphic units at Yucca Mountain are different and this will further reduce the likelihood of buoyancy.

2. Preferential Flow Paths

The fractured nature of Yucca Mountain also leads to the possibility of preferential flow paths. The presence of preferential flow paths would have similar effects to having anisotropic permeability, i.e., reduced potential for buoyancy driven flow.

Preferential flow paths were found in the Stripa-3D saturated fracture flow experiments [Tsang, 1991] and it was concluded that "tracer transport in such a medium cannot usually be interpreted by theories which assume flow in a homogeneous porous medium." Preferential flow paths were also found in the barometric pumping experiments at the NTS [Nilson, 1992] and in the gas injection tests in the U.K. [Lineham, 1993]. The presence of preferential flow paths would make the use of an equivalent porous medium model more difficult to justify and the likelihood of buoyancy driven flow to decrease. The Stripa-3D experiments were successfully modeled using a discrete fracture model [Tsang, 1991].

3. Thermal Equilibrium

Given a fractured porous media heated from the bottom. If convective flow occurs, gas from the hotter region will travel up the fracture much faster than conduction will carry heat up the host media. Therefore, there is a potential for temperature disequilibrium between phases exist. If the flow velocities at the repository level are on the order of 1000 m/yr as predicted [Pruess, 1988] it is likely that temperature disequilibrium will occur. If the gas is hotter than the host rock, it is likely that energy will be removed from the gas, therefore, further reducing the probability of buoyancy.

4. Time - Invariant Boundary Conditions and Barometric Pumping

All of the simulations use time - invariant boundary conditions. In contrast, experimental studies and simulations of seasonal and even daily variations of the flow out of wells in Yucca Mountain clearly indicate the response of gas flow to changes at the surface [Kipp, 1987]. These experiments will be presented in more detail in Chapter 4.

Barometric pumping will also exist at Yucca Mountain as it has been experimentally shown to occur under similar situations at the Nevada Test Site (NTS). These experiments and the modeling of barometric pumping will be discussed in Chapter 4.

Both barometric pumping and time-dependent changes in the boundary conditions at Yucca Mountain are important for realistic estimates of the actual flow of air and contaminants out of the mountain. However, from the point of view of assessing purely buoyancy effects, pumping can be neglected as a first approximation. Similarly, estimating the surface temperature as constant will be an adequate approximation in determining buoyancy effects. This is what has been done in all Yucca Mountain gas contaminant release studies. However, these approximations do not permit investigation of the potential for coupling of buoyancy with surface driven flow.

5.) Darcy's Law for non-homogeneous fluids

Use of a single expression for the momentum balance (Darcy's law) for a non-homogeneous fluid (air plus water vapor) has not been demonstrated for a condensible gas. This approach ignores the momentum transfer between the liquid in the pores and the water vapor in the gas. In principle, a momentum balance should be written for each phase with terms to represent the transfer between phases during evaporation/condensation. Often when considering evaporation/condensation effects, this is simplified to a Darcy's law type expression for the air and the water vapor.

3.3 Conclusions

All Yucca mountain gaseous contaminant release studies address buoyancy only (i.e. they neglect surface driven flows and barometric pumping effects) and work at three levels of sophistication. The most sophisticated approaches do not predict significant macroscopic movement of air/water out of the mountain due to buoyancy effects. Their results are in agreement with those based on the Rayleigh parameter analysis in Chapter 2, i.e., buoyancy driven flow should not occur under the conditions found at Yucca Mountain. The less sophisticated approaches do predict buoyancy driven flow and mass releases; however they are internally inconsistent as they fail to recognize that if heat transfer by convection does not take place, as they assume, buoyancy-driven flow should not take place. Furthermore, there are theoretical difficulties common to all Yucca Mountain studies, i.e., the use of thermal equilibrium. The extent that these assumptions influence the predicted flow is not known. However, the consistency between the sophisticated analysis and the Rayleigh parameter analysis, which at least has an experimental foundation, gives heuristic support to the modeling predictions and conclusions.

4.0 COUPLING BETWEEN BUOYANCY FLOW AND SURFACE DRIVEN FLOW

Measurement and prediction of gas flow at Yucca Mountain under existing conditions has been performed. These studies stress the influence of surface processes on flow through the mountain. In addition, the role of barometric pumping in removing man-made contaminants from fractured-volcanic rock has been studied at the Nevada Test site, which is adjacent to the Yucca Mountain site. These studies are reviewed in this chapter.

4.1 Natural Flow System at Yucca Mountain

Near the surface of Yucca Mountain gas flow is strongly influenced by atmospheric pressure, temperature, wind velocity, and topography. This has been recognized by researchers from the United States Geological Survey (USGS). The USGS has studied [Weeks, 1987] the flow into and out of two wells at Yucca mountain. Their data indicate an almost continual exhaust from the wells during the winter months. This was expected based on the topography and temperature within the mountain exceeding that in the atmosphere. The air being released from the wells was saturated with water vapor. In the summer months, the flow direction was quite sensitive to changes in atmospheric temperature. The well would intake air when the atmospheric temperature exceeded the well temperature and reverse itself when the conditions reversed. This reversal typically happened several times per day.

Based on these findings the flow in and out of Yucca Mountain due to seasonal temperature variations was modeled numerically by the USGS [Kipp, 1987]. Their predictions indicate that in summer, air enters the mountain near the crest and exits along the lower half of the valley wall. In winter, the flow is reversed. Maximum pore velocities are near five m/day [Kipp, 1987]. Flow during spring and autumn is about an order of magnitude lower. Within the mountain, responses to changes in the surface conditions

influenced flow to a depth of 50 - 100 meters.

More recent work [Weeks, 1991] indicates that wind flow is an important mechanism for moving air into the mountain. Theoretically, as wind blows against the canyon wall of the mountain, the pressure increases due to frictional drag and decreases at the crest due to an airfoil effect. Their data showed a direct correlation of anomalously high discharge from the wells during high westerly flows. Weeks estimates that wind pumping is responsible for approximately 30% of the flow through the mountain. With 70% being due to thermal effects. The correlation with high winds indicates that flows will be relatively high for short periods of time.

The pressure differential caused by these effects is generally less than 100 Pa, i.e., one mbar or 0.1% of atmospheric pressure. This highlights the sensitivity of flow in and out of Yucca Mountain due to boundary effects.

4.2 Barometric Pumping at NTS

Flow into and out of the mountain due to barometric pressure effects are believed to contribute little to net flow. However, they can be important in removing man-made contaminants. Extensive studies of the role of barometric pumping on releases at the NTS have been performed [Nilson, 1991; 1991a; 1992]. Nilson reports of experiments where gas tracers are injected into the loosely compacted postshot rubble zone. The injection site is overlain by 320 m of fractured rock. They found that the tracers reached the surface within two months of injection. This indicates an average velocity of a few meters per day. Surface tracer concentrations were near zero during periods of high barometric pressure and would rapidly increase as the pressure decreased. Although there was one clearly defined fracture at the surface, it was not the dominant release pathway. Sampling at many sites indicated a wide distribution of concentrations, some larger than collected from the visible crack. Thereby, indicating a highly fractured system.

The effects of barometric pumping have been modeled [Nilson, 1991] using a dual porosity model for flow and transport of contaminants in an isothermal system which undergoes small deviations in pressure. The model is able to successfully predict the general trends found in this process, but it has not been calibrated to predict actual releases.

Although, the geologic setting at Yucca Mountain imposes conditions that restrict buoyancy effects, i.e., non-homogenous and fractured rock, these same conditions are favorable for air movement at considerable depths due to barometric pumping. Currently, there has been no investigation of release of contaminants from Yucca Mountain due to barometric pumping. The results from such a study under pre-emplacment conditions would prove to be extremely useful. If it could be demonstrated experimentally that this was an important transport mechanism, then future release models would have to incorporate this phenomena. The existing barometric pumping transport models are based on isothermal systems and may require modification to account for the thermal effects of the repository.

If barometric pumping is the dominant transport mechanism, it is likely that excess releases of natural radon due to heating of the mountain will be non-existent or small. However, ingrowth of radon from U-238, Pu-238, and U-234 will introduce a substantial source at the repository level. Assuming no removal of uranium and plutonium at the repository level, after 20,000 years, the radon inventory from the spent fuel will be approximately 0.3 Ci /MTHM. This will increase to 1.26 Ci/MTHM at 200,000 years and will eventually attain secular equilibrium with U-238 and have an inventory of 0.32 Ci/MTHM for millions of years. Assuming a repository area of $5.58 \cdot 10^6 \text{ m}^2$ [SCP, 1988] and a height of 5 m for the containers gives a radon density at the repository horizon of $3 \cdot 10^{-3} \text{ Ci/m}^3$. These levels of radon are orders of magnitude greater than expected background levels. Radon levels in air samples at the Ranier Mesa have been found to range from 25 - 200 pCi/l [Fauver, 1987]. If a substantial fraction of the radon in the spent fuel is available for release, radon may be a long term issue as radon anomolies over depths as great as 600 m are known [Cameron, 1987].

4.3 Conclusions

Surface driven flows due to wind pumping and thermal effects cause substantial flows within 100 m of the surface. Further, the experimental data on barometric pumping at the NTS clearly indicate that pumping to depths of the repository horizon can occur in fractured media. In addition, modeling predictions of buoyancy driven flow at Yucca Mountain indicate large flows within 100 m of the repository at 100 years. It remains to be seen how the natural (pre-emplacment) flows will interact with the heat driven flows. This is a problem of both natural and forced convection. The problem is non-linear and simple addition of these two individual cases can not be performed.

To accurately simulate this phenomena will require solution of the coupled energy, momentum, and mass equations subject to time-dependent boundary conditions which simulate the atmospheric pressure and temperature variations. The potential for barometric pumping will require the use of a double porosity model for flow and transport. Simulated flows due to changes in boundary conditions are contained within 50 - 100 meters of the mountain. The predicted values of these flows exceeds that of buoyancy driven flow. Therefore, to properly estimate the release from the surface of the mountain it is clear that the boundary conditions must be accurately represented. This will most likely require time-varying boundary conditions.

At this time, there is no obvious method of obtaining a time-invariant boundary condition that conservatively predicts release. Originally, it was assumed that using the lowest surface temperature would lead to the largest buoyancy effects and therefore, highest release rate. With this assumption, gas exited through the crest of the mountain. Simulations of gas flow through Yucca Mountain under pre-emplacment conditions [Kipp, 1987] indicate that in summer, gas flows downwards from the crest and exits the side of the mountain. This may act to shorten the travel distance and thereby increase release.

5. CONCLUSIONS

Steady-state buoyancy-enhanced releases of natural radon and other contaminant gases should not be of concern at Yucca Mountain. This indication is derived from both the theoretical and experimental literature on coupled-heat and mass transport in porous media and it is reinforced at Yucca Mountain due to the layered and directionally-fractured nature of the geologic setting. The more complex simulations of gaseous transport at Yucca Mountain also suggest the same conclusions. The less sophisticated approaches predicting buoyancy-driven mass flow have been found to be internally inconsistent.

Even though some analyses indicate that for permeabilities on the high end of the expected values at Yucca Mountain buoyancy may play a role in movement of the gas. The validity of these analyses has been questioned. In any event, in these simulations, the predicted velocities are much less than those predicted near the surface due to boundary effects, and they are much less than transport velocities from barometric pumping. Thus, even if buoyancy were to take place, it is not likely to be the dominant process. Nevertheless, some attention should be devoted to the experimental determination of the critical Rayleigh number under conditions representative of those expected at Yucca Mountain.

While buoyancy may not be of major concern, flow induced by barometric pumping requires further attention. Even if pumping does not add a net flow into the mountain, the actual flow of man-made contaminant gases may still be positive outwards. Transport of gaseous contaminants from the repository depth may take place within months. In the case of radon, the potential problem of barometric pumping will pose itself later in time (after 100,000 years) when the containers will be perforated, the UO_2 will be oxidized to UO_{2+x} , and the radon will be produced in significant amounts from the ^{238}U decay chain.

Experimental and theoretical investigations indicate that the flow through Yucca

Mountain will be a complex function of surface pressure and temperature, the fracture network and its flow properties, and the thermal effects caused by repository heating. Currently, none of the simulations predicting long term contaminant transport provide this level of detail. In addition, the complexity of the flow system suggests that in-situ permeability and tracer testing will be required to adequately characterize the system.

RECOMMENDATIONS:

Barometric and wind pumping at Yucca Mountain may cause long-term ^{222}Rn removal from the oxidized spent fuel waste. The problem of enhanced ^{222}Rn release to the accessible environment would pose itself later in time (after 20,000 years and peaking at roughly 200,000 year, say), and would last for as long as unsaturated conditions would prevail at Yucca Mountain.

From a waste management point of view three items appear to need further assessment: 1. the extent and location (i.e. existence of preferential flow channels) of the potential releases; 2. the relevance of the induced radon anomaly for uranium prospecting with the attending significance for human intrusion scenarios and siting considerations; and 3. the extra dose that this radon source may deliver to affected individuals over a practically indefinite period of time.

In order to address the above questions one needs to examine both the potential for barometric- and wind-pumping induced flow at Yucca Mountain and the extent to which oxidized spent fuel or the presence of backfill in the borehole may provide a reasonable barrier to radon release. The study has not touched upon the latter aspects. Regarding the former, we observe that computation of flow and transport subject to barometric pumping and time-dependent boundary conditions will be a computationally intensive exercise and the costs may be prohibitive.

Prior to using this brute force approach, efforts should be made to simplify the

system. Following are the areas that should be examined:

- a) As a minimum, the role of barometric pumping on the movement of air through Yucca Mountain should be studied under pre-emplacment conditions.

- b) Methods to simplify the boundary conditions used in attempting to model wind pumping and other short duration high flow events should be performed. Ideally, a time-independent boundary condition would be found that bounded flow out of the mountain. Due to the complexity of the geologic units, mountain surface, and variation in weather patterns it may not be possible to define a single boundary condition that will bound flow.

6. REFERENCES

[Amter, 1990]

Amter, S., and B. Ross, "Simulation of Gas Flow Beneath Yucca Mountain, Nevada, with a Model Based on Freshwater Head," Waste-Management '90, R.G. Post ed., Vol 2., pp. 915-925, 1990.

[Bear, 1972]

J. Bear, Dynamics of Fluids in Porous Media, Dover Publications, New York, 1972.

[Buschek, 1992]

Buschek, T.A., and J.J. Nitao, "The Impact of Thermal Loading on Repository Performance at Yucca Mountain," Proceedings of the Third International Conference on High Level Radioactive Waste Management, pp. 1003 - 1017, Las Vegas, NV, 1992.

[Cameron, 1987]

Cameron, C.P., "A Review of Radon Emanation and Mobilization in Minerals and Rocks," WES-MP-GL-87-27, US Army Engineer Waterways Experiment Station, Vicksburg, MS, September, 1987.

[Codell, 1992]

Codell, R. B., and W.M. Murphy, "Geochemical Model for ^{14}C Transport in Unsaturated Rock," Proceedings of the Third International Conference on High Level Radioactive Waste Management, V. 2, pp. 1959-1965, Las Vegas, NV, 1992.

[Donaldson, 1970]

Donaldson, L.G., "The Simulation of Geothermal Systems with a Simple Convection Model," Geothermics, Special Issue 2, 1970.

[Elder, 1967]

Elder, J.W., "Steady Free Convection in a Porous Media Heated From Below," J. Fluid Mech., V. 27, pp. 29-48, 1967.

[Fauver, 1987]

Fauver, D.N., "Survey of Radon and Radon Daughter concentrations in selected Ranier Mesa tunnels," DOE/NV/10327-31, prepared for the U.S. Department of Energy, Nevada Operations Office, Las Vegas, Nevada, 1987.

[Klavetter, 1986]

Klavetter, E.A., and R.R. Peters, "Estimation of Hydrologic Properties of an Unsaturated Fractured Rock Mass," SAND84-2642, Sandia National Laboratories, Albuquerque, NM, 1986.

[Kipp, 1987]

Kipp, K.L., Jr., "Effect of Topography on Gas Flow in Unsaturated Fractured Rock: Numerical Simulation," in Flow and Transport Through Unsaturated Fractured Rock, D.D. Evans and T.J. Nicholson, eds., pp. 171 - 176, American Geophysical Union, Washington, 1987.

[Knapp, 1987]

Knapp, R.B., "An Approximate Calculation of Advective Gas Phase Transport of ^{14}C at Yucca Mountain, Nevada," UCRL-97805, Lawrence Livermore National Laboratory, Livermore, CA, 1987.

[Lapwood, 1948]

Lapwood, E.R., "Convection of a Fluid in a Porous Media," Proc. Cambridge Phil. Soc., V. 44, pp. 508-521, 1948.

[Lineham, 1993]

Lineham, T.R. et. al., "Gas Migration in Fractured Rock: Results and Modeling of a Helium Gas Injection Experiment at the Reskajeage Farm Test Site, S.W. England, United Kingdom," Migration '93, Ed. S.B. Clark, Charleston, SC, December, 1993.

[MacDougall, 1987]

H.R. MacDougall, L.W. Scully, and J.R. Tillerson, "Site Characterization Plan Conceptual Design Report, Volume 1, Chapters 1-3," SAND84-2641, Sandia National Laboratory, Albuquerque, NM, 1987.

[Nield, 1982]

Nield, D.A., "Onset of Convection in a Porous Layer Saturated by an Ideal Gas," Int J. Heat Mass transfer, Vol. 25, No. 10 pp. 1605-1607, 1982.

[Nilson, 1991]

Nilson, R., E. Peterson, K. Lie, N. Burkhard, and J. Hearst, "Barometric Pumping of Contaminated Gases Through Fractured Porous Media," Proceedings of the Second International Conference on High Level Radioactive Waste Management, V. 1, pp. 86- - 868, 1991.

[Nilson, 1992]

Nilson, R.H., et. al., "Field Measurements of Tracer Gas Transport Induced by Barometric Pumping," Proceedings of the Third International Conference on High Level Radioactive Waste Management, V. 1, pp. 710-716 Las Vegas, NV, 1992.

[Phillips, 1991]

Phillips, O.M., Flow and Reactions in Permeable Rocks, Cambridge Universtiy Press, 1991.

[Rajan, 1987]

Rajen, G. and F.A. Kulacki, "Natural convection in a Porous Layer Locally Heated from Below - A Regional Laboratory Model for a Nuclear Waste Repository," ASME/AiChE National Heat Transfer Conference, Pittsburgh, 1987.

[Rasmussen, 1987]

Rasmussen, T.C., and D.D. Evans, "Unsaturated Flow and Transport Through Fractured Rock Related to High-Level Waste Repositories," NUREG/CR-4655, Department of Hydrology and Water Resources, University of Arizona prepared for the U.S. Nuclear Regulatory Commission, 1987.

[Ross, 1988]

Ross, B., "Gas-Phase Transport of Carbon-14 Released From Nuclear Waste into the Unsaturated Zone," Scientific Basis for Nuclear Waste Management XI, pp. 273 -284, M.J. Apted and R.E. Westerman, eds., Materials Research Society, Pittsburgh, 1988.

[Ross, 1992]

Ross, B., S. Amter, and N. Lu, "Numerical Studies of Rock-Gas Flow in Yucca Mountain," SAND91-7034 Sandia National Laboratories, 1992.

[Ross, 1993]

Ross, B., Y. Zhang, N. Lu, "Implications of Stability Analysis for Heat Transfer at Yucca Mountain," Proceedings of the Fourth International Conference on High Level Radioactive Waste Management, V. 1, pp. 584 - 589, Las Vegas, NV, 1993.

[Pescatore, 1992]

Pescatore, C., and T.M. Sullivan, "Potential Increases in Natural Radon Emission Due to Heating of the Yucca Mountain Rock Mass," Proceedings of the Third International Conference on High Level Radioactive Waste Management, V. 2, pp. 1599-1606, Las Vegas, NV, 1992.

[Pruess, 1988]

Pruess, K., J.S.Y. Wang, and Y.W. Tsang, "Effective Continuum Approximation for Modeling Fluid and Heat Flow in Fractured Porous Tuff," SAND86-7000, Sandia National Laboratories, Albuquerque, NM, 1988.

[SCP, 1988]

USDOE, Site Characterization Plan-Overview, DOE/RW-0198, Department of Energy, December, 1988.

[Strauss, 1977]

Strauss, J. M. and G. Schubert, "Thermal convection of Water in a Porous Medium: Effects of Temperature- and Pressure-Dependent Thermodynamic and Transport Properties," Journal of Geophysical Research, Vol. 82, No. 2, pp. 325 - 333, 1977.

[Tsang, 1991]

Tsang, Y.W., "Tracer Transport in Fractures," in Proceedings of Workshop V: Flow and Transport in Unsaturated Fractured Rock - Related to High-Level Radioactive Waste Disposal, ed., D. D. Evans, and T.J. Nicholson, NUREG/CR-0040, pp. 23 - 26, 1991.

[Wang, 1984]

Wang, J.S.Y. and T.N. Narasimhan, "Hydrologic Mechanisms Governing Fluid Flow in Partially Saturated, Fractured, Porous Tuff at Yucca Mountain," LBL-18473, Lawrence Berkeley Laboratory, Livermore, CA, 1984.

[Wang, 1986]

Wang, J.S.Y. and T.N. Narasimhan, "Hydrologic Mechanisms Governing Partially Saturated Fluid Flow in Fractured Welded Units and Porous Non-welded Units at Yucca Mountain," SAND85-7114, Sandia National Laboratory, Albuquerque, NM, 1986.

[Weeks, 1987]

Weeks, E.P., "Effect of Topography on Gas Flow in Unsaturated Fractured Rock: Concepts and Observations," in Flow and Transport Through Unsaturated Fractured Rock, D.D. Evans and T.J. Nicholson, eds., pp. 165 - 170, American Geophysical Union, Washington, 1987.

[Weeks, 1991]

Weeks, E.P., "Does the Wind Blow Through Yucca Mountain?" in Proceedings of Workshop V: Flow and Transport in Unsaturated Fractured Rock - Related to High-Level Radioactive Waste Disposal, ed., D. D. Evans, and T.J. Nicholson, NUREG/CR-0040, pp. 43 - 53, 1991.

[White, 1992]

White, M.D. M.D. Freshley, and P.W. Eslinger, "Simulation of Two-Phase Carbon-14 Transport at Yucca Mountain, Nevada," PNL-SA-20324, Pacific Northwest Laboratory, 1992.

[Wooding, 1957]

Wooding, R.A., "Steady-State Free Thermal Convection of Liquid in a Saturated Porous Media," J. Fluid Mech., V. 2, pp. 273- 285, 1957.

[Wooding, 1962]

Wooding, R.A., "Free Convection of Fluid in a Vertical Tube Filled with Porous Material," J. Fluid Mech., V. 13, pp. 129-144, 1962.

APPENDIX A:

FUNDAMENTAL EQUATIONS FOR HEAT AND MASS TRANSPORT OF A COMPRESSIBLE FLUID IN A POROUS MEDIA

Originally, this program started to examine the effects that heterogeneities and anisotropies in permeability could have on flow out of Yucca Mountain. However, during the progress of the work, it was realized that surface conditions would have a major influence on flow. At that point, we began to review the literature to determine which conditions and events would influence flow and the findings in the body of this report were obtained. The review clearly indicated that any modeling that did not account for changes at the surface would inaccurately predict flow. However, simulating flow under constant boundary conditions can provide useful insight into the sensitivity of flow to changes in flow parameters. Therefore, we present our modeling work on predicted flow in this Appendix.

In general, the movement of the gas phase can be obtained by solving the coupled set of partial differential equations for conservation of mass, momentum, and energy. In our system there are four components: solid (the host rock); liquid (water in the pores); and two gasses (dry air and water vapor). Each component has its own set of conservation equations. For our system we assume that the solid does not deform. This removes the need for continuity and momentum equations for the solid. Further, we are not interested in the motion of the liquid. As compared to the motion of the gas, liquid flow rates will be quite small and we ignore them. Thus, we do not need momentum or continuity equations for the water. We also assume that the air moves only through the fractures and is always saturated with water vapor. This removes the need for equations describing the movement of water vapor. At this point, we are left with a system of four equations: conservation of mass, momentum, and energy for the gas (air plus water vapor) and conservation of energy for the solid and liquid.

For the gas phase the continuity equations is:

$$\frac{\partial \eta \rho}{\partial t} = \nabla \cdot \rho \vec{q}$$

where η = volume of air in the fractures per unit volume of porous media

ρ = density of air

q = volumetric flux of air per unit area (a vector quantity)

Here, we have assumed that the air is a single component and ignored the fact that it contains water vapor. Therefore, we have implicitly assumed that there is no evaporation or condensation that would provide a source/sink for the gas phase.

The momentum equation for the gas phase is:

$$\rho \frac{\partial q}{\partial t} + \rho q \nabla \cdot q = -\nabla P - \rho g \nabla z + \nabla \cdot \tau$$

where P is the gas pressure, and

τ = shear stress and this represents frictional losses in momentum

For steady, creeping flow the first two terms on the right hand side are approximately zero and the frictional loss term can be approximated as [Bear, 1972]:

$$\nabla \cdot \tau = -v \frac{q}{k}$$

where v is the kinematic viscosity and k is the permeability of the porous medium and it is a measure of the resistance to flow. With these assumptions the simplified momentum balance becomes the well-known Darcy's law:

$$q = -\frac{k}{v} \nabla [P - \rho g z]$$

The momentum balance gives an expression for the volumetric flux in each of the principal directions and in general the permeability is a tensorial quantity that is not necessarily isotropic.

The energy balance equation for the solid and liquid (which we treat as a single, stationary component) is:

$$\frac{\partial [(1-\eta)(\rho c_p)_{sw} T_s]}{\partial t} = \nabla \cdot (1-\eta) K_s \nabla T_s + \gamma_{ws} - \gamma_{sg}$$

where η is the air filled fracture porosity;

$(\rho c_p)_{sw}$ is the heat capacity of the soil/water component;

T_s is the temperature of the soil/water component;

K_s is the thermal conductivity of the soil/water component;

γ_{ws} is the source of thermal energy from the radioactive waste to the soil/water component.

γ_{sg} is the source of thermal energy transferred from the solid/water component to the gas component.

The gas phase energy balance is similar except for a convective heat transport term and is:

$$\frac{\partial[\eta(\rho c_p)_g T_g]}{\partial t} = \nabla \eta K_g \cdot \nabla T_g - \nabla \cdot (\eta(\rho c_p)_g q T_g) + \gamma_{sg} + \gamma_{wg}$$

where $(\rho c_p)_g$ is the heat capacity of the gas component;

T_g is the temperature of the gas;

K_g is the thermal conductivity of the gas;

γ_{wg} is the thermal energy source from the radioactive waste supplied directly to the gas.

Typically when modelling gas flow it is assumed that the heat transfer rate between the gas phase and the rock/water phase is sufficiently fast such that we have thermal equilibrium between components. In this case, the rate of energy transfer between the two components is zero and we can write a single energy balance equation as follows:

$$\frac{\partial[(\rho c_p)_{pm} T]}{\partial t} = \nabla K_{pm} \cdot \nabla T - \nabla \cdot [\eta(\rho c_p)_g q T] + \gamma_w$$

where T is the temperature in the system,

$K_{pm} = (1 - \eta) K_s + \eta K_g =$ equivalent porous media thermal conductivity;

$(\rho c_p)_{pm} = (1 - \eta) (\rho c_p)_{sw} + \eta (\rho c_p)_g =$ equivalent heat capacity of the porous media

γ_w is the total thermal energy source from the radioactive waste.

One final assumption is made: the amount of energy transferred by convection in the gas phase is small compared to that carried away by conduction. This allows the qT term in the energy balance to be dropped and allows solution of the energy equation without consideration of the flow field. However, the flow field still depends on the temperature because the pressure, density, and viscosity depend on temperature.

The time-dependent heat conduction equation is solved analytically assuming a

homogeneous infinite medium. The surface temperature is maintained at 20 C by including a negative source 350 m above the surface. Superposition of these two sources gives the temperature within the region of interest.

The gas density is determined from the ideal gas law:

$$\rho = \frac{P}{RT}$$

where R is the universal gas constant.

To model a two-dimensional axial slice of the Yucca Mountain system, the preceding system of equations has four equations for four unknowns: temperature, pressure, axial and horizontal volumetric flow rate. The temperature field can be obtained first and then used to define the density in terms of pressure. Then, the two expressions for volumetric flow rate can be placed into the continuity equation leaving the following equation to determine the pressure:

$$\frac{\partial}{\partial t} \frac{\theta P}{RT} = - \frac{\partial}{\partial z} \frac{Pq_z}{RT} - \frac{\partial}{\partial x} \frac{Pq_x}{RT}$$

where:

$$q_z = - \frac{k_z}{\mu} \frac{\partial [P + \rho_0 g z]}{\partial z} - \frac{k_z g}{\mu} \left[\frac{P}{RT} - \rho_0 \right]$$

and,

$$q_x = - \frac{k_x}{\mu} \frac{\partial P}{\partial x}$$

Here, we have assumed that the permeability tensor is aligned along the principal co-ordinate axis and therefore, we ignore cross terms. We have, however, explicitly acknowledged that the permeability may be different in the x and z directions.

These expressions for q_x and q_z are substituted into the continuity equation leaving a non-linear equation for the pressure P. usually, the steady-state solution for pressure is obtained by requiring the time derivative term to be zero.

A.1 Modeling Results

The simulation geometry assumes symmetry about the midplane of the repository. The lower boundary is the water table located 150 m beneath the repository. There is no gas flow into the system at the water table. The upper boundary is the surface of the mountain and it is 350 above the repository ($z = 500$ m). Symmetry is assumed about the center of the repository, therefore, there is no flow out of this boundary (left boundary). The heated region of the repository extends 1250 m from the centerline. The right boundary is at 5000 m. This is far enough to prevent the effects at the boundary from influencing flow into the repository.

Table A.1 Base Case Parameters

<u>Permeability:</u>	$k_z = k_x = 10^{-11} \text{ m}^2$
<u>Density of air:</u>	$\rho = 1.07 (T_0/T) \text{ kg/m}^3$; T degrees K
<u>Viscosity of air:</u>	Table look-up $(1.7 - 2.2) 10^{-5} \text{ kg/m/s}$ (T= 20 - 100 C)

Fracture porosity = 0.001

Heat source [Pescatore, 1992]: $\gamma_w(t) = 1.14 Q_0(10 + t)^{-0.64982}/(\rho c_p)$
where Q_0 = areal heat source in kW/acre
 t = time in years.

Initial and Boundary Conditions:

Temperature: Repository heat source at 100 years
Temperature obtained through an analytical solution.
Geothermal gradient : $T(z=500,t) = 20$ C
 $T(z = 150, t = 0) = 28.3$ C (repository level)

Pressure: $q_z = 0$ at $z = 0$ m (the water table)
 $q_x = 0$ at $x = 0$ (symmetry)
 $P = P_{atm}$ at $z = 500$ m (top boundary)
 $P(5000,z) = P_h(5000,z)$ (right boundary)
where P_h is the calculated hydrostatic pressure
with the geothermal gradient temperature profile.

Model results:

In the base case the velocity profile is provided in Figure A.1 where it is shown that the velocity profile is radially inward beneath the repository. A plume forms above the repository carrying gas upward. Figure A.2 presents the axial velocity contours. The highest flows in both directions occur near the repository edge where temperature gradient is largest. Horizontal flows are largest just above the water table. Flow out of the mountain occurs above the entire heated region. Pore velocities (not Darcy velocities) out of the mountain are about $6 \cdot 10^{-6}$ m/s (0.5 m/d).

Layered Medium

In this case, the permeability was decreased by an order of magnitude to $k = 10^{-12} \text{ m}^2$ in the region $z = 350 - 400 \text{ m}$. This reduced flow out of the surface by a small amount. The flow pattern has shown a major shift due to the layered region as seen in Figure A.3. Now, a circulation pattern above repository edge at interface between the two permeability regions can be seen. Peak exit velocities, Figure A.4, are a factor of three lower than the base case.

The effect of a low permeability layer was examined further by once again reducing the permeability another order of magnitude, $k = 10^{-13} \text{ m}^2$ for $z = 350 - 400 \text{ m}$. This further reduced the flow out of the surface. In Figure A.5 the flow patterns reveal two distinct flow systems. One system is contained within the region above the low permeability layer, while the other is contained below. There is a strong convection cell above the repository edge and bounded by the low permeability region. Peak exit velocities, Figure A.6, are a factor of six lower than the base case.

Anisotropic Media

The effects of anisotropy were examined by reducing the horizontal permeability by an order of magnitude, $k_x = 10^{-12} \text{ m}^2$; $k_z = 10^{-11} \text{ m}^2$. The flow pattern is fairly similar to the base case, Figure A.7, however, the average flow out of the surface has been reduced by an order of magnitude while the peak flow rates are a factor of three lower than the base case, Figure A.8.

To test the effects of anisotropy further, the horizontal permeability was decreased two orders of magnitude beneath the vertical permeability, $k_x = 10^{-13} \text{ m}^2$; $k_z = 10^{-11} \text{ m}^2$. The flow pattern changed dramatically in this case, Figures A.9 and A.10. Over most of the heated region, the velocity is negative (i.e. directed into the mountain) and small (essentially zero) for much of the top surface. Maximum exit velocities were a factor of 30 less than the base case.

A.2 Conclusions

A detailed derivation of the equations of flow and transport were presented using the assumptions of an equivalent porous medium, conduction dominated heat transport, an ideal gas, and Darcy's law. Effects of boiling and evaporation/condensation were not considered.

The resulting equations were applied to examine the effects of a low permeability layer and anisotropies on gas flow out of Yucca Mountain. Both have the potential for significantly reducing flow as compared to the homogeneous case. In both cases, large changes in the flow patterns were recognized for a two - order of magnitude change in permeability from the reference values.

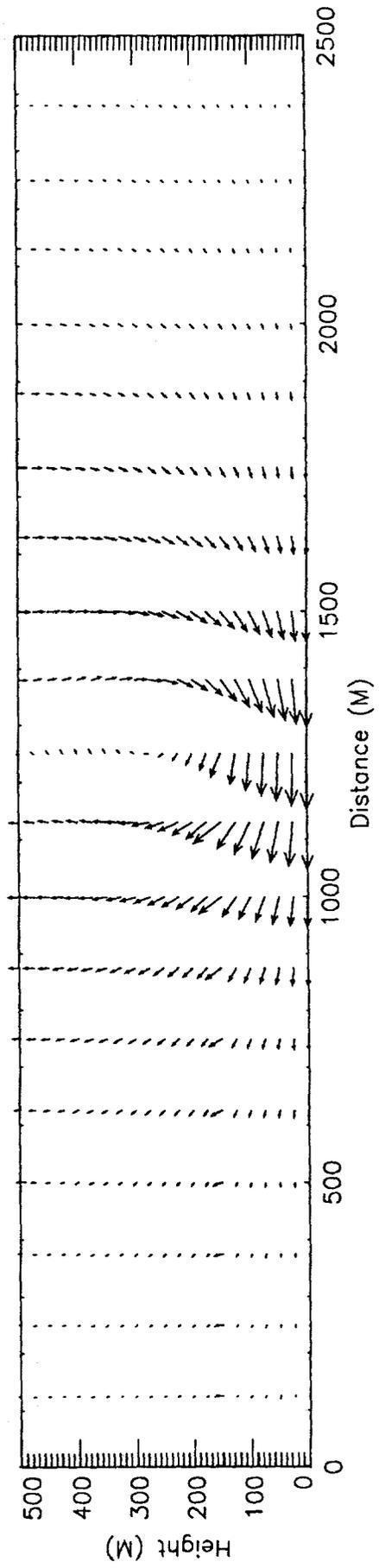


Figure A.1 Velocity Vectors at 100 years, base case.

Vertical Velocity Contours

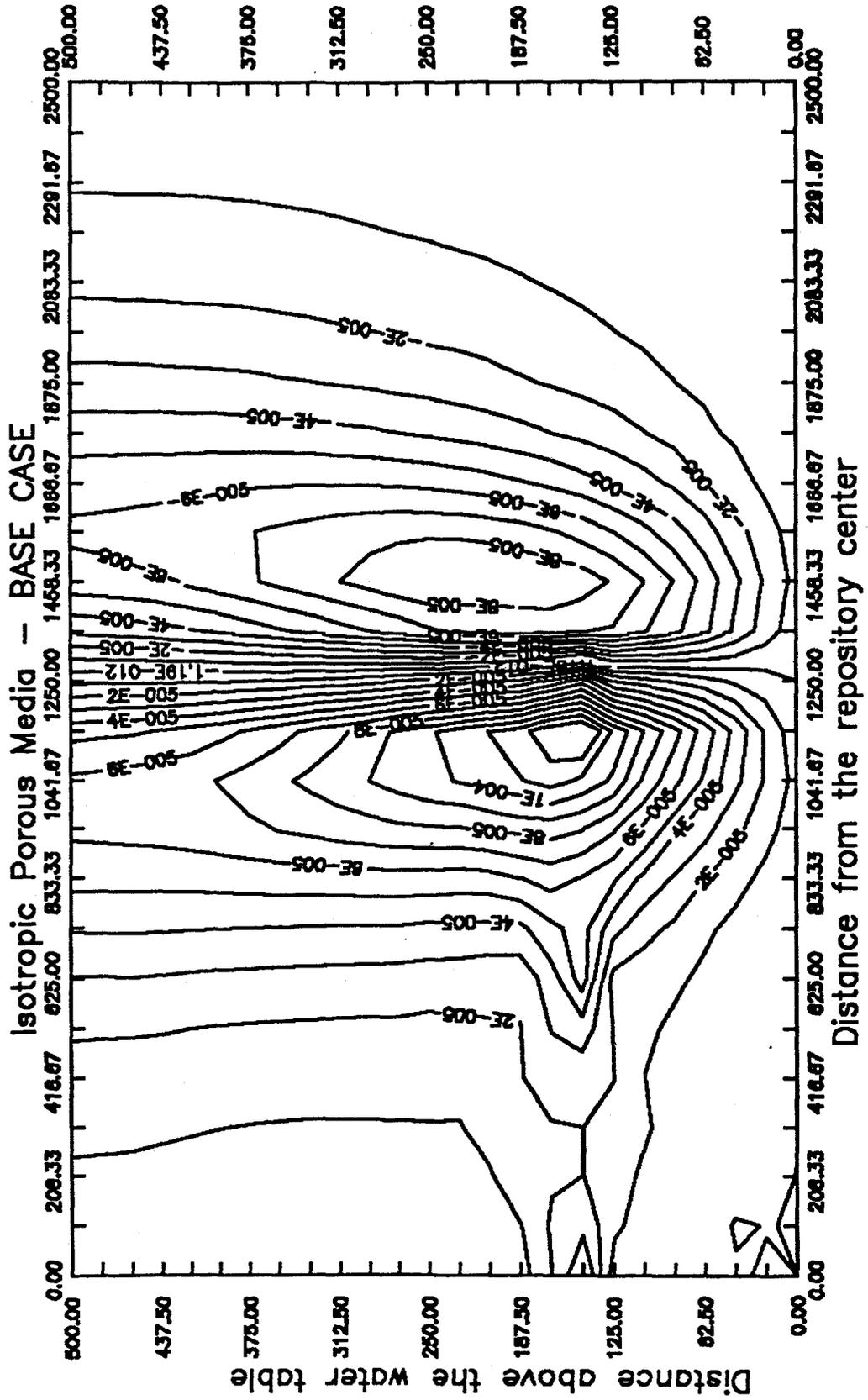


Figure A.2 Vertical Velocity Contours at 100 years, base case.

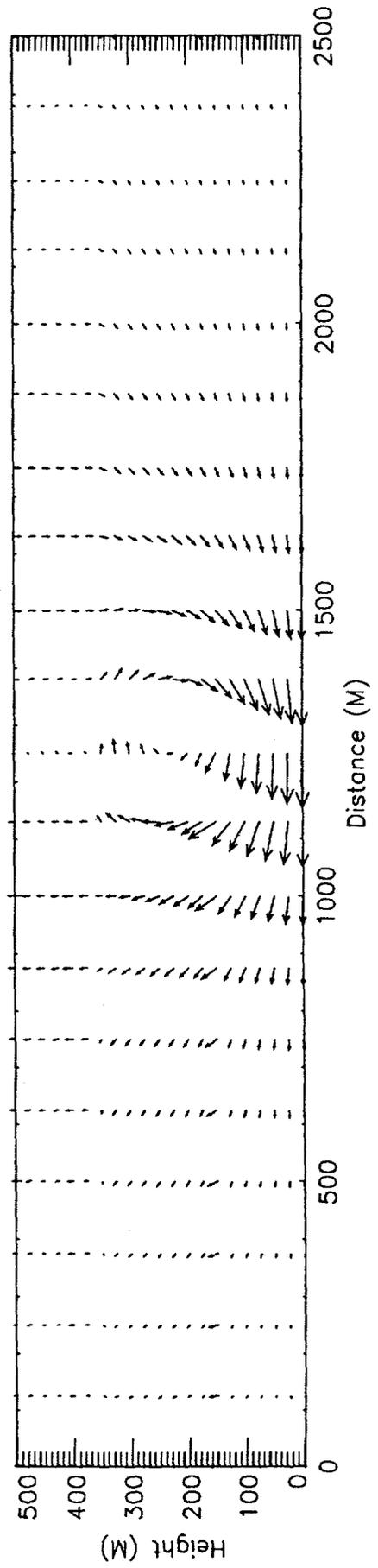


Figure A.3 Velocity Vectors at 100 years for a layered medium having a permeability of one-tenth of the base case value in the region $Z = 350-400$ m.

Vertical velocity contours

permeability = 0.1 k for z = 350 - 400

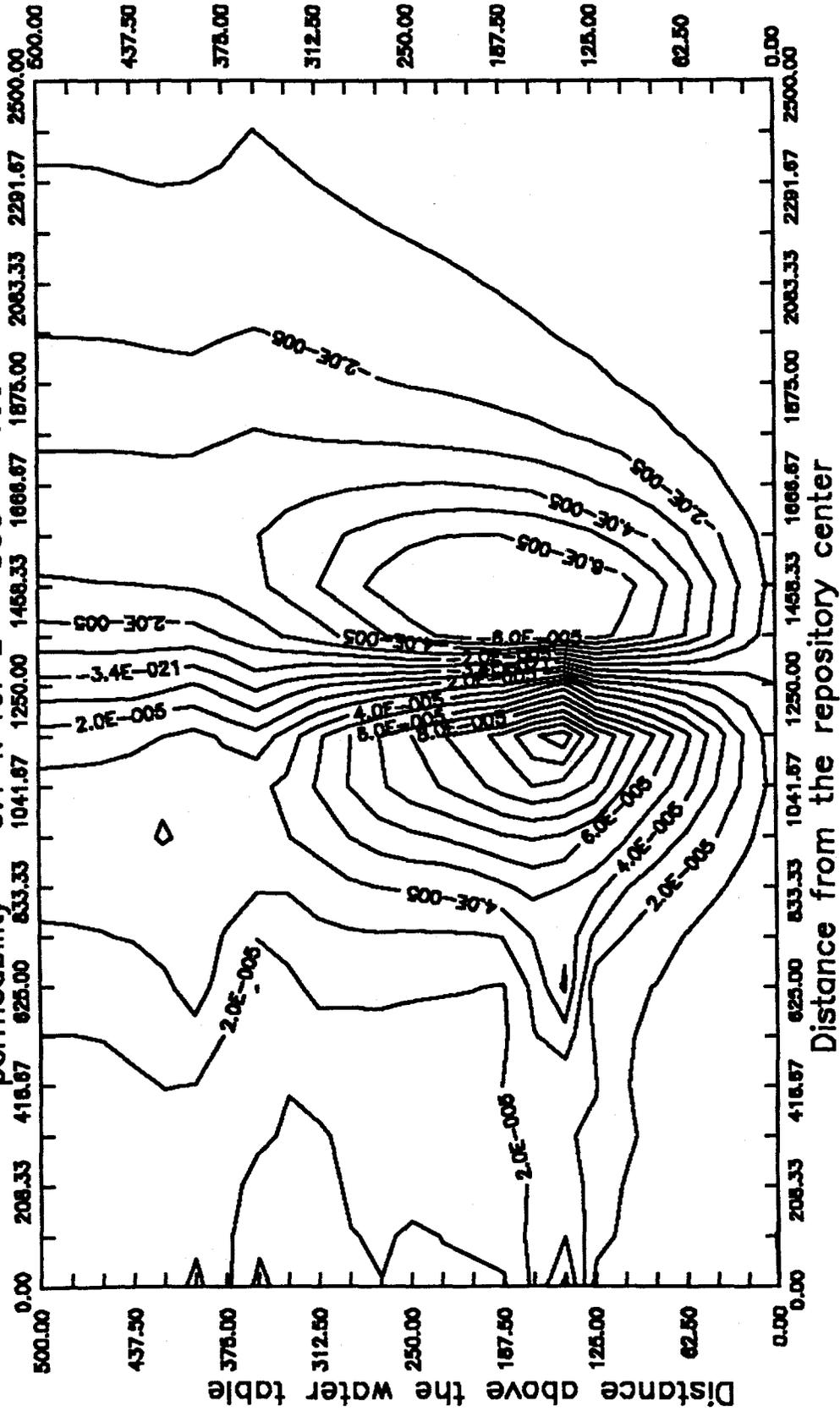


Figure A.4 Vertical Velocity Contours at 100 years for a layered medium having a permeability of one-tenth of the base case value in the region Z = 350-400 m.

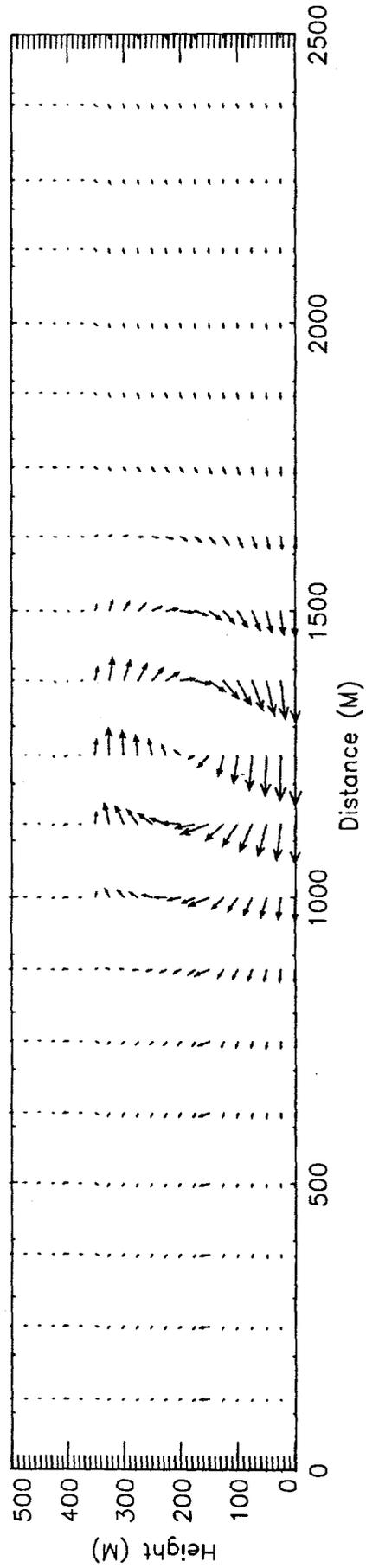


Figure A.5 Velocity Vectors at 100 years for a layered medium having a permeability of one-hundredth of the base case value in the region $Z = 350-400$ m.

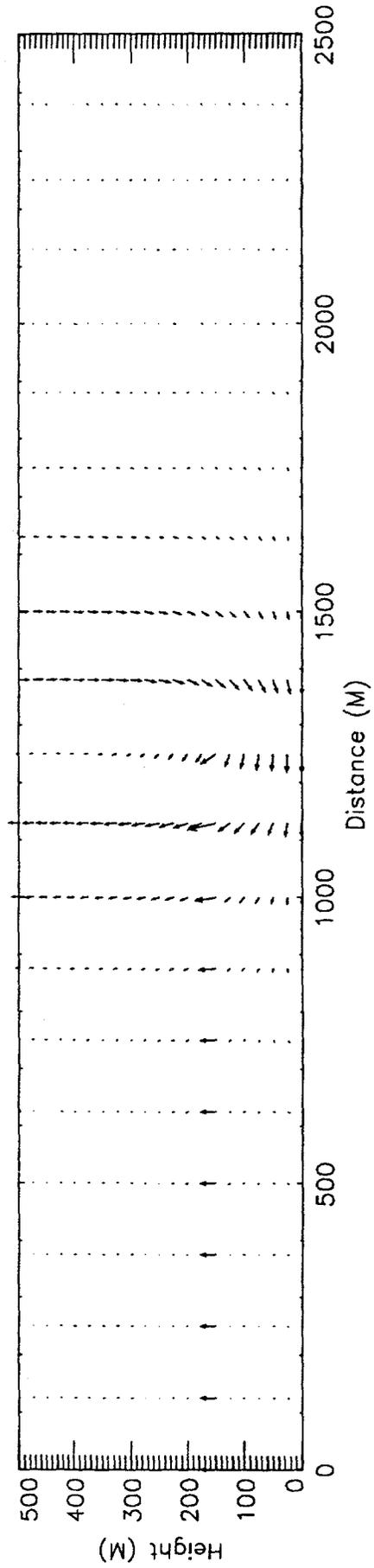


Figure A.7 Velocity Vectors at 100 years for an anisotropic medium having the horizontal permeability one-tenth of the vertical value.

Vertical velocity contours

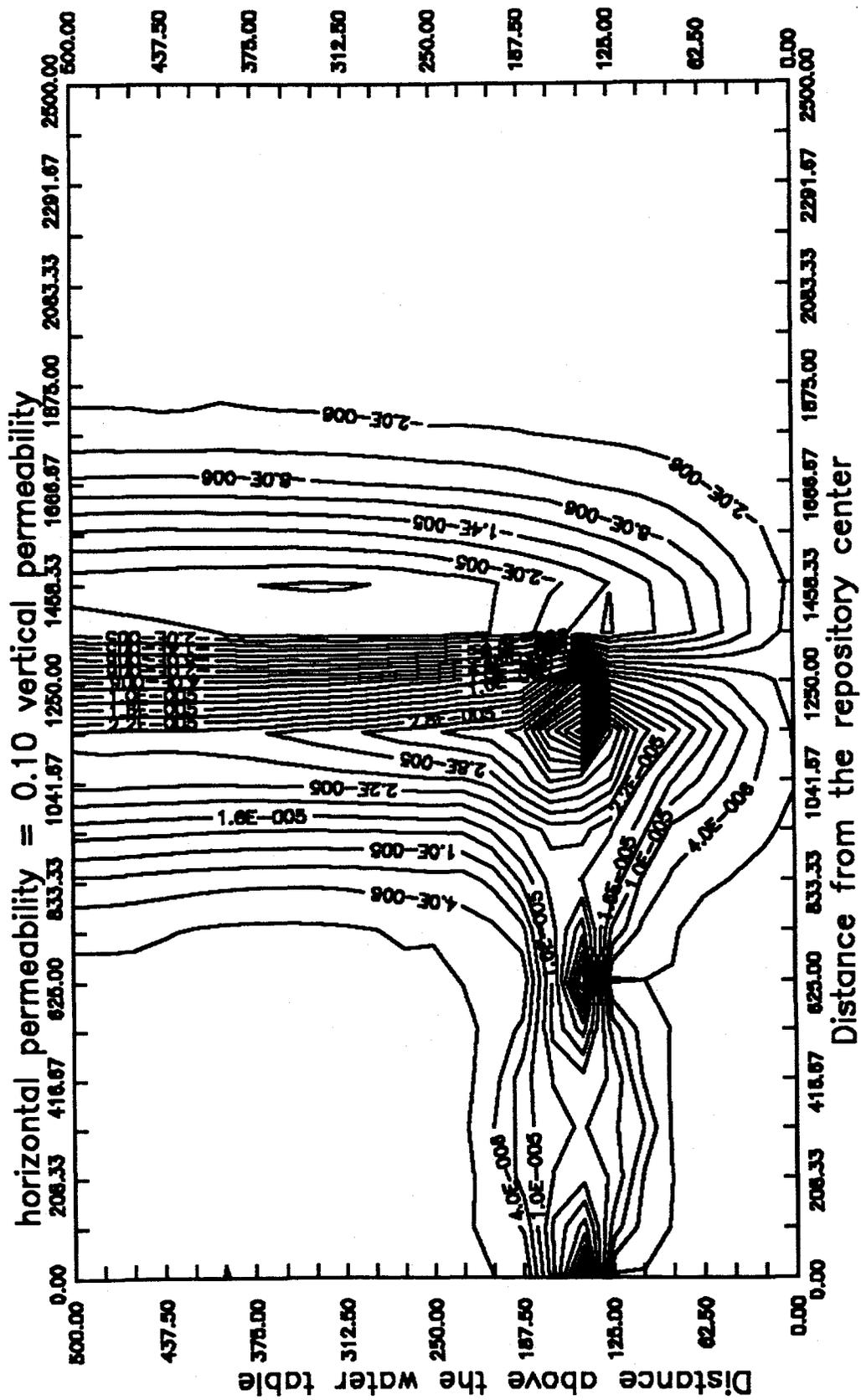


Figure A.8 Vertical Velocity contours at 100 years for an anisotropic medium having the horizontal permeability one-tenth of the vertical value.

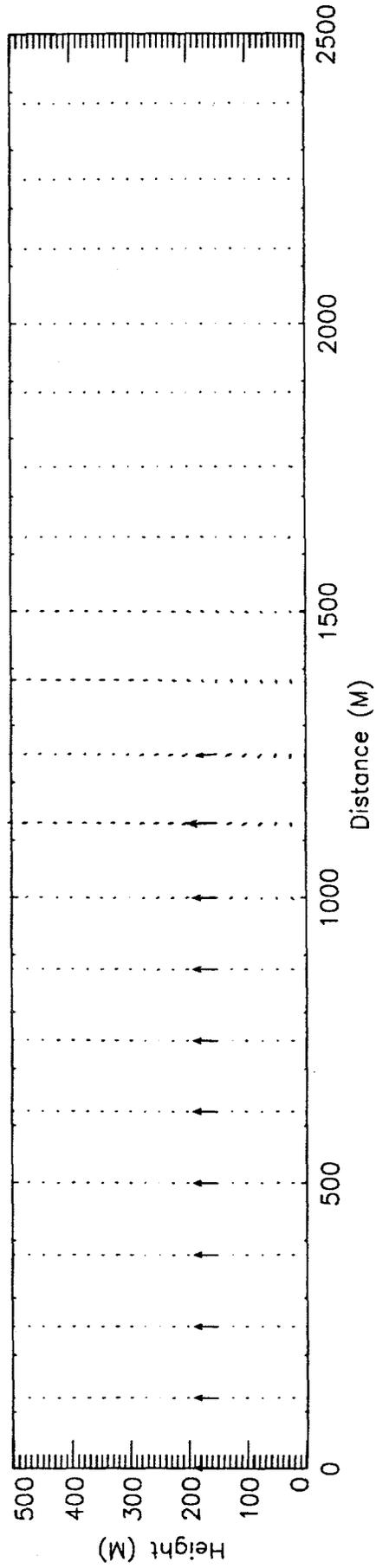


Figure A.9 Velocity Vectors at 100 years for an anisotropic medium having the horizontal permeability one-hundredth of the vertical value.

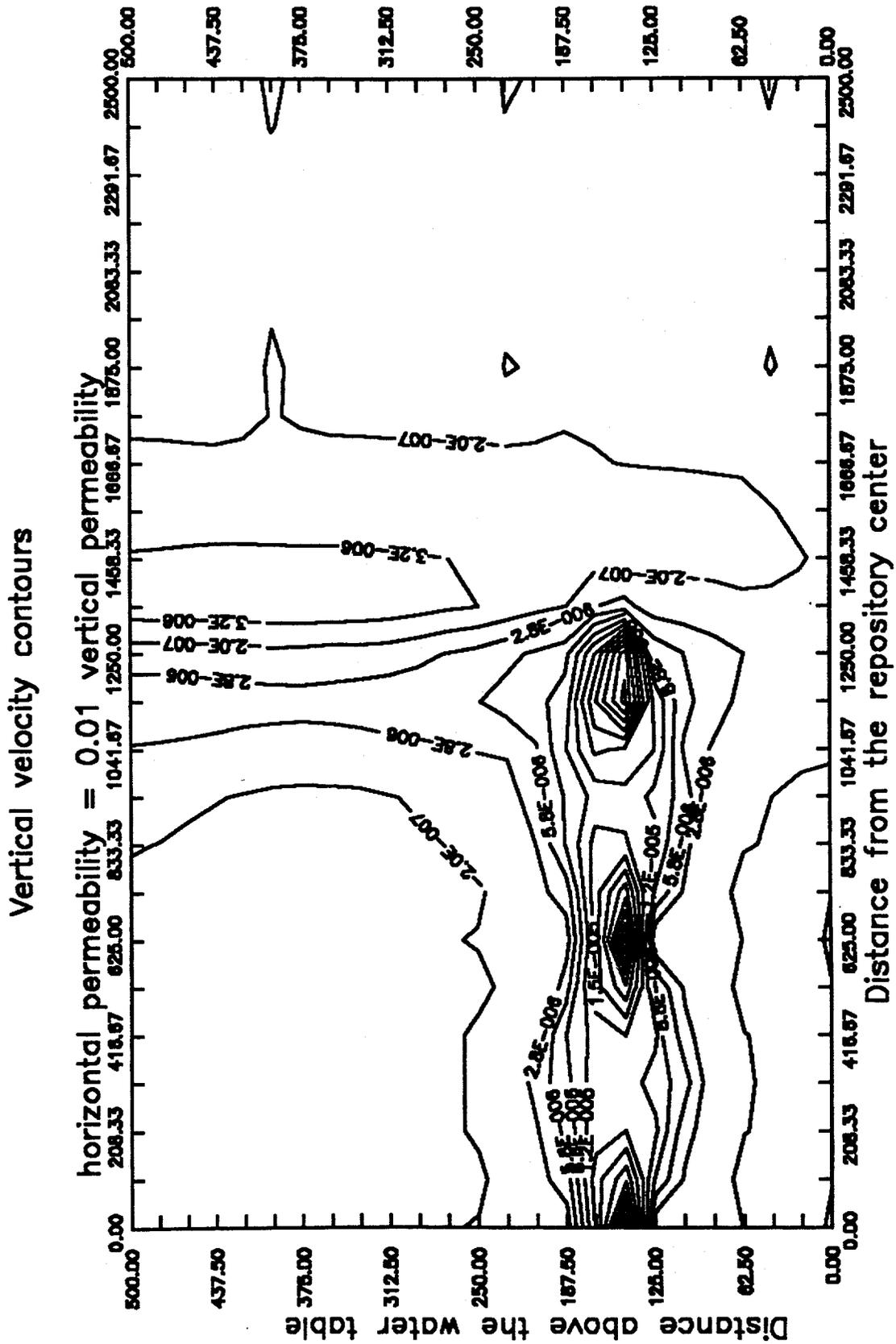


Figure A.10 Vertical Velocity contours at 100 years for an anisotropic medium having the horizontal permeability one-hundredth of the vertical value.

