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6 JACOB WAY READING, MASSACHUSETTS 01867 (617) 944-6850

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**ASPECTS OF NUCLEAR WASTE MANAGEMENT
VOLUME 2: POST-EMPLACEMENT HAZARDS**

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Lawrence Livermore Laboratory
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Prepared by:

Benjamin I. Ross
Lawrence E. Berman
Michael E. Hough
Gregory D. Pollak

Approved by:

John W. Bartlett
Thomas J. Kabele

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THE ANALYTIC SCIENCES CORPORATION
Six Jacob Way
Reading, Massachusetts 01867

ABSTRACT

This report describes studies of technical issues relating to nuclear waste management. It supplements previous TASC reports on this topic. Volume 1 addresses events occurring before emplacement of the waste in a repository. The subjects addressed are thermal analysis of interim storage accidents and doses to the worst-situated individual in all types of pre-emplacement accidents. Volume 2 deals with the possible release of waste from a geologic repository. Aspects of long-term repository performance which are discussed include water flow around shafts and boreholes and use of water from contaminated wells. New methods and results pertaining to the analysis of uncertainties in long-term risk predictions are also presented.

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1. INTRODUCTION

1.1 BACKGROUND

This report describes work done between February 1978 and June 1978 as part of a continuing program of systematic analysis of nuclear waste management issues. The purpose of this report is to record the results of analyses of some specific issues relating to the estimation of hazards to the public which might arise from the geologic disposal of high-level nuclear wastes.

These analyses are aimed at verifying the accuracy of the models presented in Ref. 1 and at broadening their scope. In the first volume of this report, studies of events which could occur before disposal of the waste were described. This volume presents the results of studies of long-term hazards from waste emplaced in a deep geologic repository.

1.2 ORGANIZATION OF THIS VOLUME

The study of long-term hazards of radioactive waste may be divided into three areas:

- Calculation of the probability of events which could lead to release of waste from a repository
- Analysis of the consequences of such releases
- Estimation of the uncertainties in predictions of probabilities and consequences.

The hazard analysis presented in Ref. 1 included all three of these aspects. The work reported here extends that study in the areas of consequence analysis and uncertainty estimation.

Chapter 2 of this volume describes studies involving consequence analysis. In Section 2.1, a detailed analysis of flow near a repository shaft is conducted in order to verify the previous assumption of independent parallel pathways. It is found that this assumption does not cause a significant error in the model results.

Section 2.2 describes an analysis of doses which might be received by individuals who used contaminated water from wells drilled near a repository. It is found that large doses are possible, but only a small number of people could be effected.

In Section 2.3, a method of summarizing repository performance by means of contour plots is presented.

Chapter 3 describes three aspects of the effect of parameter uncertainty on risk predictions:

- Description of probability density functions of repository performance measures by non-parametric statistics
- Application of the monte carlo method of uncertainty analysis to a salt repository
- An alternative to the monte carlo method for deriving estimates of performance uncertainty from input parameter probability distributions.

Finally, Chapter 4 summarizes the principal findings of the study and makes recommendations for further research.

2.

CONSEQUENCE ANALYSIS

2.1 FLOW IN AND AROUND A SHAFT

2.1.1 Introduction

The models used in Ref. 1 to analyze waste transport from a depository assume that the ground water flow is strictly one-dimensional -- i.e., that the flow is through a network of interconnected horizontal and vertical pathways which mix only at specified nodes and which do not allow flow into or out of these stream tube pathways or "pipes". Thus for a typical repository, the one-dimensional pathways might consist of the tunnel, shaft, and their associated fracture zones, faults, breccia pipes, etc.

The one-dimensional nature of the modeling precludes analyzing the extent to which flow across the stream tube boundaries may affect the waste concentration. Such effects as dilution, pressure equalization, migration to horizontal pathways, etc. could conceivably be quite important in the determination of the output concentrations. Three-dimensional modeling of the hydrology would be very useful in determining the range of validity of the stream tube models as well as providing guidelines for correcting for any significant departures from the one-dimensional approximation.

Unfortunately, three-dimensional hydrology computer codes are time-consuming to interface, debug, and run. They often encounter numerical difficulties when the modeling involves large, abrupt variations in flow velocities. They give

little information concerning the qualitative forms for the hydrology in various limiting cases. For these reasons, analytic solutions to some of the relevant hydrology problems are useful.

In this section, some solutions of this type are derived. The basic problem considered was a cylindrical shaft extending vertically through material with some specified vertical pressure gradient far from the shaft. The shaft and layer both admit water flow but with two different isotropic permeabilities. This analysis was extended to take into account the following phenomena:

- Anisotropy between horizontal and vertical flow
- A cylindrically symmetric fracture zone surrounding the shaft
- Multiple layers with identical sizes for the shaft and fracture zones. (A shaft extending down to a circular repository of some height is a special case of this.)
- Horizontal gradients, as well as vertical gradients, far from the shaft.

In Section 2.1.2 the differential equation for anisotropic flow is derived, general boundary conditions are discussed, and the general solutions to the differential equation are analyzed. In Section 2.1.3, the solution to the basic problem is presented, the details of the derivation being left to Appendix A. The appendix also contains the extension to both multi-layer and multi-radial zone problems, and the incorporation of horizontal gradients. Section 2.1.4 presents a derivation of "streamline functions" for cylindrically symmetric flow and the calculation of the quantity of water flowing

across a boundary surface in terms of the streamline function. Section 2.1.5 provides a summary of the numerical considerations which affect computer calculations using the solutions derived in the earlier sections, while Section 2.1.6 gives the results of calculations for some specific cases.

2.1.2 The Differential Equation, Boundary Conditions, and General Solutions

The differential equation for fluid flow through an anisotropic porous medium is the result of combining the law for mass conservation with the experimentally determined differential equation for specific discharge (Darcy's Law):

$$\vec{g} = k\nabla\phi \quad (2.1-1)$$

where $\vec{g}$ is the specific discharge vector, a component of which is the amount of water per unit time per unit area which passes through a surface perpendicular to the component axis; k is the permeability of the medium at the point in question; and ϕ is the piezometric head, defined as the sum of the pressure and potential energy per unit weight:

$$\phi = z + p/\rho g \quad (2.1-2)$$

(where ρ is the density, g is gravitational acceleration, p is the pressure, and z is the vertical distance from some arbitrary point).

The law of mass conservation, sometimes known as the law of current conservation, is

$$\nabla \cdot (\rho \vec{g}) + \frac{\partial(\rho \epsilon)}{\partial t} = 0 \quad (2.1-3)$$

where ϵ is the porosity.

For an incompressible fluid, ρ is independent of space and time, while for a non-deformable medium ϵ is a constant. Then Eq. 2.1-3 reduces to

$$\nabla \cdot \vec{g} = 0 \quad (2.1-4)$$

Combining Eqs. 2.1-1 and 2.1-4 gives

$$\nabla \cdot (k \nabla \phi) = 0 \quad (2.1-5)$$

If the medium is homogeneous in a given region, then k is a constant and Eq. 2.1-5 reduces to

$$\nabla^2 \phi = 0 \quad (2.1-6)$$

This equation is valid for an isotropic medium. For an anisotropic medium Eq. 2.1-1 is replaced by

$$\begin{aligned} g_x &= k_x (\nabla \phi)_x \\ g_y &= k_y (\nabla \phi)_y \\ g_z &= k_z (\nabla \phi)_z \end{aligned} \quad (2.1-7)$$

Combining this with Eq. 2.1-3 gives, in place of Eq. 2.1-6,

$$k_x \frac{\partial^2 \phi}{\partial x^2} + k_y \frac{\partial^2 \phi}{\partial y^2} + k_z \frac{\partial^2 \phi}{\partial z^2} = 0 \quad (2.1-8)$$

By defining new variables x' , y' , and z' related to the true coordinate variables x , y , and z by

$$x = \sqrt{k_x} x', \quad y = \sqrt{k_y} y', \quad z = \sqrt{k_z} z', \quad (2.1-9)$$

Equation 2.1-8 can be written as:

$$\frac{\partial^2 \phi}{\partial x'^2} + \frac{\partial^2 \phi}{\partial y'^2} + \frac{\partial^2 \phi}{\partial z'^2} = 0 \quad (2.1-10)$$

This equation is formally identical to Eq. 2.1-6, but it is solved as a function of the scaled variables x' , y' , and z' .

The boundary conditions for porous medium hydrology fall into two types. The first type are those boundary conditions which are imposed at the interface between media of two different permeabilities. Two requirements are imposed:

- The pressure must be continuous across such an interface (and thus the head as well, since z is continuous)
- The specific discharge (quantity of water per unit time per unit area) must be continuous. This is just the requirement that mass be conserved.

In mathematical terms, if the head function is described by the two forms $\phi_1(x)$ and $\phi_2(x)$ on either side of an interface, then, for a point s which lies on the interface, the required boundary conditions are, from Eq. 2.1-1

$$\phi_1(\vec{s}) = \phi_2(\vec{s}) \quad (2.1-11)$$

$$k_1 \left. \frac{\partial \phi_1}{\partial \hat{n}} \right|_{\vec{x}=\vec{s}} = k_2 \left. \frac{\partial \phi_2}{\partial \hat{n}} \right|_{\vec{x}=\vec{s}} \quad (2.1-12)$$

where $\hat{n}$ is the normal to the interface at the point $\vec{s}$.

The second type of boundary condition consists of those specific to the physical situation being considered.

For instance, the requirement that the head gradient far from the shaft be vertical and of some specified magnitude would be of this type. These boundary conditions will be enumerated for each problem as the need arises.

Equation 2.1-4 is known as Laplace's equation. Since the boundary conditions encountered throughout this section can best be described using cylindrical coordinates (ρ, θ, z) , general solutions to this equation are needed in this coordinate system. The separation of variables technique is the most manageable approach to solving Laplace's equation. It assumes that the solution can be written in the following form:

$$\phi(\rho, \theta, z) = R(\rho)Q(\theta)Z(z) \quad (2.1-13)$$

and inserts this into the differential Eq. 2.1-6 written in terms of cylindrical coordinates:

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \phi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} = 0 \quad (2.1-14)$$

The solution in the form of Eq. 2.1-13 will then be acceptable provided the functions R , Q , and Z satisfy the following ordinary differential equations:

$$\frac{d^2 Z}{dz^2} - \kappa^2 Z = 0 \quad (2.1-15)$$

$$\frac{d^2 Q}{d\theta^2} + r^2 Q = 0 \quad (2.1-16)$$

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial R}{\partial \rho} \right) + \left(\kappa^2 - \frac{r^2}{\rho^2} \right) R = 0 \quad (2.1-17)$$

Here κ^2 and r^2 are real (although not necessarily non-negative) constants. The solutions to the set of simultaneous differential equations 2.1-15 through 2.1-17 can then be classified into four different types, depending on the values κ^2 and r^2 . Explicitly, these solution sets are:

I) If $\kappa^2 > 0$, then

$$\begin{aligned} Z(z) &= A \sinh \kappa z + B \cosh \kappa z \\ Q(\theta) &= C \sin r\theta + D \cos r\theta \\ R(\rho) &= EJ_r(\kappa\rho) + FY_r(\kappa\rho) \end{aligned} \quad (2.1-18)$$

II) If $\kappa^2 < 0$, then

$$\begin{aligned} Z(z) &= A \sin |\kappa|z + B \cos |\kappa|z \\ Q(\theta) &= C \sin r\theta + D \cos r\theta \\ R(\rho) &= EI_r'(|\kappa|\rho) + FK_r'(|\kappa|\rho) \end{aligned} \quad (2.1-19)$$

III) If $\kappa^2 = 0$, $r^2 \neq 0$, then

$$\begin{aligned} Z(z) &= Az + B \\ Q(\theta) &= C \sin r\theta + D \cos r\theta \\ R(\rho) &= E\rho^r + F\rho^{-r} \end{aligned} \quad (2.1-20)$$

IV) If $\kappa^2 = 0$, $r^2 = 0$, then

$$\begin{aligned} Z(z) &= Az + B \\ Q(\theta) &= C\theta + D \\ R(\rho) &= E \ln \rho + F \end{aligned} \quad (2.1-21)$$

Here $J_r(x)$ and $Y_r(x)$ are the regular Bessel functions of order r , while $I_r(x)$ and $K_r(x)$ are the modified Bessel functions. The reader is referred to Ref. 2 for the derivation of these solutions, as well as various properties which they exhibit.

In any physical system the result should be the same after a rotation of 2π around the axis of symmetry. This implies not only that r^2 is non-negative, but also that r is an integer n . It also implies, in the fourth set of solutions above, that the constant C is equal to zero. In the case where no horizontal gradient component is present far from the shaft, then there is no preferred horizontal direction and the solution will not depend on θ . In that case, $n=0$ and $\phi(\rho, \theta, z) = R(\rho)Z(z)$. In the case where a horizontal gradient component does exist, values of n other than 0 will be necessary to describe the solution. It will be shown later that the only other value needed is $n=1$.

If a solution is sought for a problem where the allowed range of z is infinite and the solution is not constrained to be periodic, then a continuum of values for κ , either all real values or all pure imaginary values, will in general be needed to describe the solution. Either set of solutions, corresponding to pure real or pure imaginary κ , is complete and may be used in constructing the solution. The choice is usually dictated by the type of boundary conditions imposed. In all the problems considered in this section the range of z will be finite. In that case the Fundamental Theorem of Fourier Series states that, if one chooses κ to be pure imaginary, then only those values of $|\kappa|$ which are either 0 or integer multiples of some fundamental value need to be used in forming the solution. Explicitly:

$$|\kappa| = \frac{2m\pi}{L} = \frac{m}{z_0} \quad \text{or} \quad \kappa = 0 \quad (2.1-22)$$

where m is an integer and L is some constant. The solutions for $\kappa \neq 0$ so constructed will be periodic in z with period L . If one is only interested in some finite region for z , then

any function of z can be written as a sum of solutions indexed by m where the only restriction on L is that it be larger than the extent of the region of z being considered. Since the solution is only needed in this region, it is irrelevant that it is periodic outside it. How much larger L is than the region of z will generally be dictated by numerical considerations (Section A.1 of Appendix A). It is usually (although not always) chosen to be an integer multiple of the length of the region of interest.

The solutions for κ pure imaginary are given in Eqs. 2.1-19, 2.1-20, and 2.1-21 above. Even though the solutions for the z dependence when $\kappa=0$ are linear, rather than periodic, in z , these linear solutions can be expanded in a Fourier series of period L . Then the orthogonality of the sines and cosines over this interval will be very useful. It is for this reason that the solutions considered here will all correspond to κ pure imaginary rather than real.

The general form for a cylindrically symmetric solution (no horizontal gradient) will be:

$$\begin{aligned} \Phi(\rho, z) = & (Az + B)(E \ln \rho + F) + \sum_{m=1}^{\infty} \left[A_m \sin \frac{2m\pi z}{L} + B_m \cos \frac{2m\pi z}{L} \right] K_0 \left(\frac{2m\pi \rho}{L} \right) \\ & + \left[C_m \cos \frac{2m\pi z}{L} + D_m \sin \frac{2m\pi z}{L} \right] I_0 \left(\frac{2m\pi \rho}{L} \right) \end{aligned} \quad (2.1-23)$$

The constants A , B , E , F , A_m , B_m , C_m , and D_m must be determined from the boundary conditions. When the solution is no longer cylindrically symmetric, it has the more general form:

$$\begin{aligned} \Phi(\rho, \theta, z) = & Az + B + (A'z + B') \ln \rho + \sum_{n=1}^{\infty} \left\{ [C_n \cos n\theta + D_n \sin n\theta] \rho^n \right. \\ & + \left. [C'_n \cos n\theta + D'_n \sin n\theta] \rho^{-n} \right\} + \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \left\{ [A_{mn} \cos n\theta \cos \frac{2\pi mz}{L} \right. \\ & + B_{mn} \cos n\theta \sin \frac{2\pi mz}{L} + C_{mn} \sin n\theta \cos \frac{2\pi mz}{L} + D_{mn} \sin n\theta \sin \frac{2\pi mz}{L}] \\ & \times K_n \left(\frac{2\pi \rho}{L} \right) + [A'_{mn} \cos n\theta \cos \frac{2\pi mz}{L} + \dots \text{etc (with primes)}] I_n \left(\frac{2\pi \rho}{L} \right) \Big\} \end{aligned} \quad (2.1-24)$$

2.1.3 Solutions to the Single-Layer Shaft Problem

In this section the solution to the single-layer problem of a shaft and a surrounding fracture zone in a single rock layer is presented. Besides the requirement that only a vertical head be present far from the shaft, additional specific boundary conditions must be imposed. These are derived from the form of the geologic structure (permeability values and layer thicknesses) above and below the layer in question. As an example, far from the shaft the flow will be strictly vertical and the values of the head drops for the i^{th} layer, a_{3i} , are related from one layer to the next by Darcy's Law:

$$k_{3(i+1)} \frac{a_{3(i+1)}}{L_{i+1} - L_i} = \frac{k_{3i} a_{3i}}{L_i - L_{i-1}} \quad (2.1-25)$$

where k_{3i} is the permeability of the i^{th} layer in the undisturbed rock and $L_i - L_{i-1}$ is the thickness of the i^{th} layer. The head itself is continuous at the layer interfaces. Therefore, if one were to plot the head far from the shaft as a

function of z , a continuous, piecewise linear function would be the result (illustrated in Fig. A.3-1 in Appendix A). As mentioned in the previous section, to obtain an answer which is a sum (and thus subject to evaluation by computer), rather than an infinite integral, it is necessary to assume that the domain of z (the depth) is finite. The z dependence of the head will then be periodic of some period L . This imposition of periodicity is, in general, an approximation. The accuracy of the approximation depends on how large L is chosen compared to the thickness of the layer in question (L_1). The larger L is, the more layers are taken into account in modeling the behavior far from the shaft, and thus the more accurate the modeling of the flow in the vicinity of the shaft (which depends on the rock structure above and below the shaft layer) will be. However, the larger the value of L , the more terms must be computed to achieve a given accuracy.

Other boundary conditions must be specified besides the behavior of the head at infinity. To illustrate the nature of these boundary conditions, the general solution to the potential problem which is finite in each region must be written down. This is given by (see Appendix A):

$$\phi_1(\rho, z) = \frac{a_1 z}{L_1} + b_1 + \sum_{m=1}^{\infty} \left[C_m^1 \cos \frac{mz}{z_0} + D_m^1 \sin \frac{mz}{z_0} \right] I_0 \left(\frac{m\rho}{z_0} \right)$$

$$\rho \leq r$$

$$0 \leq z \leq L_1 \quad (2.1-26a)$$

$$\phi_2(\rho, z) = \frac{a_2 z}{L_1} + b_2 + \sum_{m=1}^{\infty} \left[A_m^2 \cos \frac{mz}{z_0} + B_m^2 \sin \frac{mz}{z_0} \right] K_0 \left(\frac{m\rho}{z_0} \right)$$

$$\rho \geq r$$

$$0 \leq z \leq L_1 \quad (2.1-26b)$$

where r is the radius of the shaft, and $z_0 = L/2\pi$. As $\rho \rightarrow \infty$, $\phi_2 \rightarrow a_2 z/L_1 + b_2$. a_2 is thus the vertical gradient far from the shaft, which is assumed known, and b_2 is the value of the head at the top of the layer far from the shaft, which can be taken to be zero. Note that these solutions are only defined for $0 \leq z \leq L_1$ whereas the period of expansion is $-L/2 \leq z \leq L/2$ (where $L \geq L_1$). In the appendix it is shown that to compute A_m^2 , B_m^2 , C_m^1 and D_m^1 it is necessary to know the fourier expansion for the two functions $f_1(z)$ and $f_2(z)$ defined over the entire expansion domain and whose forms on the subinterval $[0, L_1]$ are $a_1 z/L_1$ and $a_2 z/L_1$ respectively. This is where the known information concerning the hydrology far from the shaft is incorporated into the solution; it serves to completely determine $f_2(z)$ over the full domain. But $f_1(z)$ is unknown -- not only its form inside the subinterval (which is determined by a_1), but also its form outside this subinterval. It is at this point that new boundary conditions must be introduced. To determine a_1 , it will be assumed that the shaft dead-ends at the top of the layer in question. Thus the layer above has no discontinuities as ρ is varied and, in particular, at $\rho=r$. This translates into the mathematical requirements:

$$k_1 \left. \frac{\partial \phi_1}{\partial z} \right|_{z=0, \rho=r} = k_2 \left. \frac{\partial \phi_2}{\partial z} \right|_{z=0, \rho=r} \quad (2.1-27)$$

This determines a_1 in terms of A_m^2 , B_m^2 , C_m^1 , D_m^1 , and a_2 . The general boundary conditions Eqs. 2.1-11 and 2.1-12 determine A_m^2 , B_m^2 , C_m^1 , and D_m^1 in terms of the fourier components of $f_1(z)$ and $f_2(z)$. To determine the form of $f_1(z)$ outside this subinterval (and thus to determine its fourier coefficients) it is instructive to use the form dictated by the solution to the full multi-layer problem. In that case the function is piecewise linear as is $f_2(z)$, and the slopes of adjacent linear segments are related by a generalization of Eq. 2.1-25:

$$k_{2(i+1)-1} \frac{a_{2(i+1)-1}}{L_{i+1}-L_i} = k_{2i-1} \frac{a_{2i-1}}{L_i-L_{i-1}} \quad (2.1-28)$$

This incorporates the geologic structure below the layer in question, in the region $p < r$. The physical approximation corresponding to this mathematical assumption is discussed more fully in Section 2.1.5. This completely determines the problem since $f_1(z)$ is now determined in terms of a_1 .

2.1.4 Streamlines and Flux Calculations

This section deals with determination of a formula from which streamlines can be plotted and water flows calculated. The formulas given in Eq. 2.1-23 or Eqs. 2.1-25 and 2.1-26 determine the value of the head as a function of ρ and z . These formulas can be used to generate contours in the (ρ, z) plane along which the head is a constant (called "equipotential contours"). The velocity of the water flow will be in a direction perpendicular to these equipotential contours. It is generally more useful pictorially to have a set of curves which have the property that the velocity of the water at the point in question is tangent, rather than perpendicular, to the curve at that point. These curves are known as streamlines and are everywhere perpendicular to the equipotential lines.

In two-dimensional problems, or three-dimensional problems with cylindrical symmetry, there is only one condition between ρ and z which must be imposed to determine these streamlines. This condition may always be written in the form of a constraint that a function, $\chi(\rho, z)$, be a particular constant along a particular streamline. In general three-dimensional problems, two constraint equations must be specified to determine a streamline.

For cylindrically symmetric problems, the requirement that the streamlines (specified by $\chi(\rho, z) = \text{constant}$) must be tangent to the velocity can be used to derive a set of partial differential equations for $\chi(\rho, z)$. The gradient of $\chi(\rho, z)$ will be perpendicular to the $\chi = \text{constant}$ curves (the streamlines). Since the latter are parallel to the velocity, $\chi(\rho, z)$ must satisfy

$$\vec{g} \cdot \nabla \chi = 0 \quad (2.1-29)$$

where $\vec{g}$ is the velocity. In cylindrical coordinates with cylindrical symmetry ($g_\theta = 0$), Eq. 2.1-29 becomes

$$g_\rho \frac{\partial \chi}{\partial \rho} = -g_z \frac{\partial \chi}{\partial z} \quad (2.1-30)$$

Here, $g_\rho = k\partial\phi(\rho, z)/\partial\rho$ and $g_z = k\partial\phi(\rho, z)/\partial z$. Equation 2.1-30 will be satisfied if

$$\frac{\partial \chi}{\partial \rho} = -a(\rho, z)g_z, \quad (2.1-31)$$

$$\frac{\partial \chi}{\partial z} = a(\rho, z)g_\rho \quad (2.1-32)$$

where $a(\rho, z)$ is any arbitrary function. If the choice $a(\rho, z) = \rho$ is made, then the function χ so obtained will have a highly useful physical interpretation (derived in the next section). If the head $\phi(\rho, z)$ has the following general form:

$$\begin{aligned} \phi(\rho, z) = az + b + \sum_{m=1}^{\infty} \left\{ \left[A_m \cos \frac{mz}{z_0} + B_m \sin \frac{mz}{z_0} \right] K_0 \left(\frac{m\rho}{z_0} \right) \right. \\ \left. + \left[C_m \cos \frac{mz}{z_0} + D_m \sin \frac{mz}{z_0} \right] I_0 \left(\frac{m\rho}{z_0} \right) \right\} \end{aligned} \quad (2.1-33)$$

then the function $\chi(\rho, z)$ is given by:

$$\chi(\rho, z) = k \frac{a^2}{2} + k \sum_{m=1}^{\infty} \left\{ \left[-A_m \sin \frac{mz}{z_0} + B_m \cos \frac{mz}{z_0} \right] (-\rho) K_1 \frac{m\rho}{z_0} \right. \\ \left. + \left[-C_m \sin \frac{mz}{z_0} + D_m \cos \frac{mz}{z_0} \right] \rho I_1 \left(\frac{m\rho}{z_0} \right) \right\} \quad (2.1-34)$$

The quantity of water flowing across a surface can be calculated in terms of $\chi(\rho, z)$. For a cylindrically symmetric boundary value problem, the flow rate at a given point will have components:

$$k \frac{\partial \phi}{\partial z} \hat{z} \text{ and } k \frac{\partial \phi}{\partial \rho} \hat{\rho} \quad (2.1-34)$$

The amount of water per unit time flowing across a $\rho=\text{constant}$ surface will then be given by

$$k \int_{z_1}^{z_2} \frac{\partial \phi}{\partial \rho} \Big|_{\rho=a} 2\pi a dz = 2\pi [\chi(a, z_2) - \chi(a, z_1)] \quad (2.1-35)$$

where z_1 and z_2 delineate the endpoints of the portion of the cylinder being considered. Similarly the amount of water per unit time flowing across $z=\text{constant}$ surface will be given by:

$$k \int_{\rho_1}^{\rho_2} \frac{\partial \phi}{\partial z} \Big|_{z=L} 2\pi \rho d\rho = 2\pi [\chi_1(\rho_2, L) - \chi(\rho_1, L)] \quad (2.1-36)$$

Thus the streamline function, multiplied by 2π , gives the quantity of water flowing across a boundary surface. Knowing the values of χ which specify two streamlines, it is then possible to quickly determine the flow bounded by these streamlines. As a special case, the ratio of amount of flow through the

sides of the cylindrical surface of length L_1 to flow through the top end cap is:

$$\frac{\text{flow through sides}}{\text{flow through top}} = \frac{\chi(r, L_1)}{\chi(r, 0)} - 1 \quad (2.1-37)$$

2.1.5 Computational Methods

To implement the mathematics described in the previous sections and derived in Appendix A, a computer program was written. This program modeled a single layer with three radial zones, corresponding to a shaft, a fracture zone, and undisturbed rock. The program did not incorporate anisotropy or horizontal gradients as this would have been beyond the scope of the work. This single-layer program has exact expressions for the various unknown coefficients. A multi-layer program must solve a set of $8N$ simultaneous linear equations for the unknown parameters, where N is the number of terms kept in the sum over m in the equations for $\phi(\rho, z)$ and $\chi(\rho, z)$.

The single-layer program still incorporates the influence of the layers above and below the particular one modeled. This is done by taking the Fourier expansion of $a_j z / L_1$ ($j=1,2,3$) using an expansion period which is larger than L_1 . Outside the interval $[0, L_1]$, the function is assumed continuous and piecewise linear, with the value of the slope in a given layer related to the slope of a neighboring layer by Eq. A.3-9:

$$k_{3(i-1)+j} \frac{a_{3(i-1)+j}}{L_i - L_{i-1}} = k_{3i+j} \frac{a_{3i+j}}{L_{i+1} - L_i} \quad (2.1-38)$$

It is possible to give a more specific, physical, analysis of this approximate incorporation of the effects of

other layers. The use of Eq. 2.1-38 to relate the various a 's has two significant features. The first is that this equation relates a given a_k to the neighboring layer's a_{k+1} , but only within the same radial zone. Second, the relationship between the a 's is what Darcy's Law would dictate if the shaft, fracture zone, and rock layer did not interact with one another so that the potentials were strictly linear in z . These two features are thus manifestations of two assumptions concerning the actual flow behavior in the various regions: the flow in the layer being modeled is principally vertical, and this behavior is essentially the same in all other layers as well. These assumptions are equivalent to modeling the lower layers by a pipe model. This is necessarily an approximation.

The single-layer program recognizes these approximations and compensates appropriately in the vicinity of the layer interfaces. For example, some streamline figures indicate that the streamlines near the lower boundary bend towards the lower layer. This is in accordance with the qualitative physics of the approximation since the flow in these examples is out of the shaft. Thus, neglecting the interaction between the shaft and rock in the lower layers means the head values in the undisturbed rock at the lower interface are lower than they would be if all layers were being modeled. In response to this the streamlines bend toward the lower face even though there is an overall upward gradient. As the distance from the lower layer increases, the streamlines reflect this effect less and less until finally they exhibit the expected upward bend. The point at which this reversal occurs depends on the specific problem and is somewhat sensitive to the expansion period chosen. The longer the period chosen, the less the distortion of the streamlines near the lower interface, and the less the influence of the periodic approximation itself.

The abnormal influence of the lower layer in the pipe approximation has its counterpart at the upper interface. As stated before, it was assumed that the shaft is in contact with a uniform overlying layer. Furthermore, for all the analyses to date, this upper layer was assumed to have no vertical head gradient and to have a large thickness (half the period of expansion). It thus serves as a sink for the upflowing water. (A similar source is present as the bottom-most layer with a thickness of one-fourth of the period.) When the water flowing up the shaft nears the upper interface it detects that the layer above is actually continuous in the radial direction and virtually all of the water then flows out the sides of the shaft. To compensate for this boundary effect the horizontal outflow from the shaft was computed ignoring this small region.

Multi-layer calculations provide a more explicit evaluation of the errors due to the effect of neglecting interactions between pathways. They avoid the ambiguities inherent in interpreting single-layer calculations, but there are much stricter computational constraints on a multi-layer program than there are on the single-layer program. This is because the amount of work necessary to compute a given number of the coefficients is much larger for the multi-layer program. To solve a set of N simultaneous equations requires an amount of time which varies approximately as N^3 , and memory space which varies approximately as N^2 . The single-layer program requires about 1.5 minutes and 1/10 of a megabyte for a 100-term sum on an IBM 370-158, and the execution time increases only linearly with N while the core requirements remain approximately constant. Thus there are essentially no computational constraints on the number of terms retained in the sums in the single-layer program. This is not the case for a multi-layer calculation, and in multi-layer computations it can be important to take care to retain only as many terms as are needed.

The question of what sets the minimum number of terms necessary to correctly model a given problem can be qualitatively investigated by looking at the finite difference approximations to the three differential equations, Eqs. 2.1-15 through 2.1-17. The results of this analysis are reviewed in Appendix A, but there is a more direct approach to the same answer. This is provided by the solutions given in Eq. 2.1-26. The series for the outer radial region will necessarily start to converge when $m \geq z_0/\rho_{\min}$ since $K_0(m\rho/z_0)$ exponentially damps out for large arguments. ("Large", to a good approximation, can be taken to be greater than 1.) The coefficients for the expansions are derived using the values $\rho=r_1$ and $\rho=r_2$. For the baseline repository shaft, $r_1=4\text{m}$ and $r_2=5\text{m}$. The minimum value for z_0 is $2L_5/\pi$ (including aquifers), where L_5 is the total thickness of all five layers. L_5 is 600 m for the baseline case and thus

$$\frac{\rho_{\min}}{z_0} = \frac{4\pi}{1200} \approx \frac{1}{100} \Rightarrow m_{\min} \approx 100. \quad (2.1-39)$$

This is the minimum number of terms required to correctly model the typical repository-shaft configuration.

A comparison of this analytic solution to finite element or finite difference approaches is useful. The considerations which govern the amount of computation required are similar for all techniques; however, the number of elements required for a finite-difference or finite-element solution is usually the square (or cube in three dimensions) of the number of terms needed in the analytic approach. Furthermore, the finite-difference and finite-element methods have great difficulty modeling large jumps in permeability. This is not a problem in the analytic solution.

2.1.6 Results for Specific Cases

A variety of single layer cases have been studied: two cases with a fracture zone only and four cases with failed backfill. In each case the layer modeled was the barrier layer overlying the layer in which the depository was located. Values for the permeabilities and layer thicknesses for the two baseline cases (one for fracture zone flow and one for shaft flow) are given in Table 2.1-1. The values for χ (the flow rate divided by 2π) for the shaft or fracture zone surfaces are given in Table 2.1-2, as well as the values of any parameters changed from baseline. All of these calculations are based on the structure shown in Fig. 2.1-1. They assume the presence of a relatively impermeable underlying depository layer ($k = 10^{-7}$ to 10^{-9} cm/sec) of thickness 100 m through which a shaft and fracture zone pass. Underlying this layer is a uniform layer of the same permeability as the fracture zone ($k = 10^{-4}$ cm/sec) and thickness 300 m which serves to model the presence of an actual repository and acts as a source for the flow. Finally, underlying this is the layer referred to above with zero vertical gradient.

The two fracture zone cases are a baseline case and a sensitivity study with the permeability of the underlying layer changed from 10^{-9} to 10^{-7} cm/sec. The effect of this change is dramatic. This is illustrated by the substantial differences in streamlines exhibited in Figs. 2.1-2 and 2.1-3 as well as by the calculated values of χ . Substantially more water is entering the fracture zone from below in the baseline case. Since more water is entering from below, more water exits through the side and the zone of influence is correspondingly larger. The case where the permeability of the underlying layer is 10^{-7} cm/sec exhibits very little distortion near the lower interface, since the lower layer is identical to the modeled layer.

TABLE 2.1-1
BASELINE PARAMETER VALUES

LAYER	THICKNESS (m)	UNDISTURBED PERMEABILITY (cm/sec)	FRACTURE ZONE PERMEABILITY (cm/sec)	SHAFT PERMEABILITY	
				UNFAILED	FAILED
Model Layer	200	10^{-7}	10^{-4}	10^{-9}	10^{-4}
Depository Layer	100	10^{-9}	10^{-4}	10^{-9}	10^{-4}
Source Layer	300	10^{-4}	10^{-4}	10^{-4}	10^{-4}

Head drop in model layer = 0.6 m
Baseline expansion period = $4L_5$

Figure 2.1-1 Structure of the Modeled Shaft Region (not to scale)

TABLE 2.1-2
CALCULATED FLOWS IN SHAFT REGION

CASE STUDIED	x (VERTICAL) $10^{-2} \text{ m}^3/\text{sec}$	x (LOWER END) $10^{-2} \text{ m}^3/\text{sec}$	PORION OF FLOW ENTERING BOTTOM OF SHAFT WHICH DOES NOT EXIT TOP OF SHAFT
Fracture Zone Only - Baseline	3.63×10^{-5}	5.04×10^{-5}	0.72
Fracture Zone Only - $k_6 = 10^{-7}$	0.73×10^{-6}	1.89×10^{-6}	0.39
Permeable Shaft - Baseline	0.57×10^{-4}	1.01×10^{-4}	0.56
Permeable Shaft - Period = $6L_5$	0.58×10^{-4}	1.05×10^{-4}	0.55
Permeable Shaft - $k_6 = 10^{-7}$	1.03×10^{-6}	3.38×10^{-6}	0.30
Permeable Shaft - $k_3 = 10^{-6}$	1.49×10^{-3}	1.62×10^{-3}	0.92

k_3 = modeled layer undisturbed permeability (cm/sec)
 k_6 = depository layer undisturbed permeability (cm/sec)

The four failed backfill cases are: a baseline case, a variation of the expansion period, a variation of the permeability of the underlying layer, and a variation of the permeability of the modeled layer. Figure 2.1-4 reproduces the streamlines for the baseline failed shaft case.

The key result of this analysis is the amount of water which enters the bottom of the shaft, but moves through the sides of the shaft and continues upward through undisturbed rock. The proportion of water entering the shaft which does this is given in the final column of Table 2.1-2. It can be

Figure 2.1-2 Streamlines Around the Baseline Shaft
With Fracture Zone Only

Figure 2.1-3 Streamlines Around a Shaft and Fracture Zone
With More Permeable Underlying Layer

seen that the amount of water which goes all the way through the shaft is comparable to the amount of water which leaves through the sides of the shaft. As long as this is so, the amount of water which is found to go all the way through the shaft will take comparable values whether calculated by the detailed method described in this section or using the simpler assumption that the shaft, fracture zone, and undisturbed rock are parallel independent pathways. The assumption of parallel independent pathways employed by the NUTRAN program in Ref. 1 therefore does not introduce any significant error.

Figure 2.1-4 Streamlines Around the Baseline Shaft With Permeable Backfill

2.2 WELL WATER DOSES

Water wells may be drilled into an aquifer overlying a formation containing a high-level nuclear waste depository if the water in the aquifer is potable and knowledge of the

location of the repository is lost at some future date. No attempt has been made here to assess the probability of this occurrence. Given that this may be a possibility, both individual and population doses from the contaminated well water withdrawn by such wells must be evaluated. Since it is impossible to predict where these wells might be drilled, calculations were made for wells placed at numerous downstream points in the aquifer, both on and off the flow axis.

The wells examined were categorized by the magnitude of their water withdrawal rates. Two limiting cases were considered:

- "Sampling wells", with small withdrawal rates. For sufficiently low withdrawal rates, no dilution occurs and the dose to a worst-situated individual takes a maximum value which is independent of the withdrawal rate. The withdrawal rate assumed in this case was the largest value consistent with no dilution. It thus yields a maximum value of individual dose and the greatest population dose which is consistent with the individual dose taking its maximum value.
- "Sink flow wells", with large withdrawal rates. The withdrawal rate chosen was that which would withdraw all water passing over the repository, but not any other uncontaminated water

Concentrations of radionuclides in the well water (and hence doses) are sensitive to the total mass of radionuclides withdrawn from the aquifer and their concomitant dilution, both of which depend upon the well withdrawal rate.

2.2.1 The Scope of the Analysis

Population doses and doses to a worst-situated individual with an average diet and life-style are calculated assuming the consumption of contaminated well water at any time during the entire history of the repository. For both types of dose, ingestion occurs over a 50-yr period. Two measures of dose were calculated: the whole-body dose, and a "whole-body-equivalent" dose in which the doses to the organs are weighted by their contribution to cancer risk (Ref. 3, Section 2.3).

The flow rate of water from the repository to the aquifer was determined for both categories of wells using the pipe network approach (Ref. 1) and the following four baseline repository designs:

- An unflawed shale repository with interstitial flow in the shale barrier layer
- An unflawed shale repository with fracture flow in the shale barrier layer
- An unflawed salt repository with interstitial flow in the shale barrier layer
- An unflawed salt repository with fracture flow in the shale barrier layer.

The parameter values characterizing the four baseline repositories are presented in Tables 2.2-1 through 2.2-4. The values for the unflawed salt repository (Tables 2.2-3 and 2.2-4) reflect a better understanding of the properties of bedded salt than those presented in Ref. 1, as described in Ref. 4.

In each case, the radionuclide inventory was that of high-level nuclear waste from the plutonium-stowaway fuel cycle (Ref. 3, Section 3.2.1).

TABLE 2.2-1
BASELINE PARAMETERS FOR UNFLAWED SHALE REPOSITORY
WITH INTERSTITIAL FLOW

PATHWAY	LENGTH (m)	CROSS SECTION (m ²)	EFFECTIVE POROSITY	PERMEABILITY (cm/sec)	RETARDATION FACTOR	DISPERSION (m)
1 st Segment of Tunnel Fracture Zone	1200	316	0.1	0.1	129, 99Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50
2 nd Segment of Tunnel Fracture Zone	440	18.96	0.1	0.1	129, 99Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50
Fracture Zone Around Shaft in Depository Layer	100	10	10 ⁻³	10 ⁻⁴	129, 99Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50
Fracture Zone Around Shaft in Shale Bar- rier Layer	200	5	10 ⁻³	10 ⁻⁴	129, 99Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50
Depository Layer	100	5x10 ⁶	0.05	10 ⁻⁹	129, 99Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50
Barrier Layer	200	5x10 ⁶	0.05	10 ⁻⁷	129, 99Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50
Aquifer	1.6x10 ⁴	4x10 ⁵	0.1	10 ⁻⁴	129, 99Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50

TABLE 2.2-2
BASELINE PARAMETERS FOR SHALE WITH FRACTURE FLOW

PATHWAY	LENGTH (m)	CROSS SECTION (m ²)	EFFECTIVE POROSITY	PERMEABILITY (cm/sec)	RETARDATION FACTOR	DISPERSION (m)
Depository Layer	100	5x10 ⁶	10 ⁻⁵	10 ⁻⁸	SAME	50
Barrier Layer	200	5x10 ⁶	10 ⁻⁴	10 ⁻⁶	SAME	50

TABLE 2.2-3
BASELINE PARAMETERS FOR UNFLAWED SALT REPOSITORY
WITH INTERSTITIAL FLOW IN SHALE BARRIER LAYERS

PATHWAY	LENGTH (m)	CROSS SECTION (m ²)	EFFECTIVE POROSITY	PERMEABILITY (cm/sec)	RETARDATION FACTOR	DISPERSION (m)
1 st Segment of Tunnel Fracture Zone	1200	3300	10 ⁻³	10 ⁻⁶	129I, ⁹⁹ Tc: 1 Other Fission Products: 1 Actinides: 1	50
2 nd Segment of Tunnel Fracture Zone	440	198	10 ⁻³	10 ⁻⁶	129I, ⁹⁹ Tc: 1 Other Fission Products: 1 Actinides: 1	50
Fracture Zone Around Shaft in Depository Layer	100	60	10 ⁻³	10 ⁻⁶	129I, ⁹⁹ Tc: 1 Other Fission Products: 1 Actinides: 1	50
Fracture Zone Around Shaft in Shale Bar- rier Layer	200	5	10 ⁻³	10 ⁻⁴	129I, ⁹⁹ Tc: 1 Other Fission Products: 10 Actinides: 10	50
Depository Layer	100	5×10 ⁶	10 ⁻²	10 ⁻⁹	129I, ⁹⁹ Tc: 1 Other Fission Products: 1 Actinides: 1	50
Barrier Layer	200	5×10 ⁶	0.05	10 ⁻⁷	129I, ⁹⁹ Tc: 1 Other Fission Products: 10 Actinides: 10	50
Aquifer	1.6×10 ⁴	4×10 ⁵	0.1	10 ⁻⁴	129I, ⁹⁹ Tc: 1 Other Fission Products: 10 ² ₃ Actinides: 10 ³	50

TABLE 2.2-4
BASELINE PARAMETERS FOR SALT WITH FRACTURE FLOW
IN SHALE BARRIER LAYERS

PATHWAY	LENGTH (m)	CROSS SECTION (m ²)	EFFECTIVE POROSITY	PERMEABILITY (cm/sec)	RETARDATION FACTOR	DISPERSION (m)
Depository Layer	100	5×10 ⁶	10 ⁻²	10 ⁻⁹	SAME	50
Barrier Layer	200	5×10 ⁶	0.05	10 ⁻⁶	SAME	50

Sampling Wells - A "sampling well" is one whose withdrawal rate is small enough that the velocity in the aquifer may be assumed to be unaffected by the presence of the well.

For such wells, the aquifer waste transport equation was solved assuming:

- A constant, unidirectional flow velocity independent of the pumping rate of the well
- A point source release of waste into the aquifer
- A Green's function (or aquifer impulse response) averaged over the height of the aquifer (Section F.8.1 of Ref. 1)
- Presence of both longitudinal and lateral dispersion.

Modeling a point source release regardless of whether the waste enters the aquifer through the undisturbed rock or through the shaft and tunnel introduces a degree of conservatism in the doses which were calculated for "close" wells (wells whose coordinates are less than the depository dimensions). Modeling the release from the shaft and tunnel by a point source is realistic. On the other hand, flow through the undisturbed rock is more akin to an area source than a point source. Concentrations (and hence doses) from close wells withdrawing the waste emanating from a plane source should be smaller than those from a point source. Farther downstream, well doses are not as sensitive to the point source assumption.

Concentrations at any time were calculated by convolving the impulse response with the flow rate of waste into the aquifer. Numerical difficulties were encountered in im-

plementing the discrete convolution integral (Section F.8.2 of Ref. 1). A modified numerical integration algorithm was developed to overcome these problems. Concentrations were then calculated as functions of the coordinates x (parallel to the flow) and y (perpendicular to the flow). These coordinates are measured from the point at which waste enters the aquifer.

Since dispersion is a factor, various sampling well locations were analyzed. The coordinates of each well are shown in Fig. 2.2-1. Six colinear wells (lying directly down-gradient from the repository) were chosen having x -coordinates of 300, 1200, 2700, 4800, 7500, and 10,800 meters. Since the center of the pulse of nuclear waste travels along the x -axis, the concentrations (and hence doses) calculated at each of these wells were larger than at off-axis locations at the same downstream distance. The lateral dispersivity was assigned an arbitrary value of one-third the longitudinal dispersivity, or 16.7 m.

The loci of x and y off-axis well coordinates are the parabolae in Fig. 2.2-1. For Gaussian distribution functions, 99% of a pulse is found between the parabola labeled $y=3\sigma$ and its reflection about the x -axis. At any time, 99% of the waste will lie within this parabola. The parabolic shape reflects the spreading of the waste pulse as it moves downstream. All concentrations (and hence doses) at points inside this parabola are within two orders of magnitude of the values on the x -axis. Since there is a single release point at $x=y=0$, concentrations are symmetric about the x -axis.

Since sampling wells do not dilute the waste, the worst-case doses to individuals are those calculated for such wells. The population doses were based on a well yield of $2 \times 10^4 \text{ m}^3/\text{yr}$ (Appendix B). This is the largest withdrawal rate

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Figure 2.2-1 Loci of Well Coordinates in the Aquifer Plane

possible over 50 years without dilution at a downstream distance of 300 m from the point source (the closest point studied) for the aquifer considered. This calculation placed an upper limit on how many people could be affected by the worst-case individual doses. Integrated population dose was not calculated because if withdrawal were to continue at the assumed rate for more than 50 years, the interaction of the well with the flow field would cause dilution.

Sink Flow Wells - The hydrology of sink flow wells is modeled by a sink (the well) embedded in a uniform flow (hence the nomenclature sink flow well).

Although of course the volumetric pumping rate of a well can take any value, the value chosen characterizes the smallest well which withdraws all of the water flowing over the depository. This ensures that all the radionuclides mix-

ing with this water are withdrawn by the well. The pumping rate decreases with increasing downstream well distance so as to maintain this flow configuration (Appendix B).

In order to simplify calculations, the aquifer waste transport equation was solved by the pipe network method described in Section F.9 of Ref. 1, which assumes:

- A constant, unidirectional flow velocity whose magnitude depends upon the pumping rate of the well
- A line source release of waste into the aquifer extending the full width of the depository
- Simple advection, with negligible dispersion.

A linear array of sink flow wells colinear with the flow axis ($y=0$) were located at downstream distances of 2, 4, 6, 8 and 10 km. Wells off the flow axis were not considered because wells at such locations cannot give greater doses than on-axis wells.

The closest well ($x=2$ km) is sufficiently far downstream of the depository that the flow over the depository is nearly parallel to the average flow direction. For closer wells, the flow across the face of the depository would not really be one-dimensional since radially-inward flow toward the well would be more noticeable. In such a situation, the one-dimensional flow approximation would not be valid.

In order to withdraw all the radionuclides in the aquifer, sink well water withdrawal rates are larger than those for sampling wells (Appendix B), thereby diluting the waste with a larger volume of water. Smaller individual doses re-

sult because of lower concentrations of radionuclides in the well water. Population doses, however, are larger because more contaminated water is available for distribution, affecting a larger number of people. The integrated population dose over three million years (if the well were operated continuously for that entire period) was also calculated.

2.2.2 Sampling Well Doses

Shale Repositories - For an unflawed shale repository with interstitial flow, peak individual and peak population doses for colinear sampling wells are shown in Fig. 2.2-2 as a function of their distance from the point source. The repository parameter values are listed in Table 2.1-1.

Long travel times between the depository and aquifer and the slowness with which the other fission products and actinides move relative to ^{129}I and ^{99}Tc make the latter two nuclides the primary contributors to the dose. In all cases, dose decreases by at least a factor of six between 300 m and 10,800 m from the repository because dispersion in the aquifer decreases the peak aquifer concentrations by a factor of $\sqrt{10,800/300}$, or 7.35.

The off-axis ($y \neq 0$) behavior of the peak average individual doses for this repository is shown in Fig. 2.2-3. Peak dose ratio, defined as the ratio of the peak dose at $y \neq 0$ to the peak dose at $y=0$ (Fig. 2.2-2) at a fixed x-coordinate, is plotted as a function of the dimensionless distance y/σ . Actual y-distances can be determined from Fig. 2.2-1. By using an ordinate which is a ratio, one set of curves is applicable to any of the four cases shown in Fig. 2.2-2. The peak dose ratios for the other repositories are very similar to those shown in Fig. 2.2-3 and are not displayed.

Figure 2.2-2 Peak Doses for Colinear Sampling Wells Near an Unflawed Shale Repository With Interstitial Flow in the Shale Barrier Layer

Figure 2.2-3 Peak Dose Ratio for Off-Axis Sampling Wells Near an Unflawed Shale Repository With Interstitial Flow in the Shale Barrier Layer

The logarithm of the peak dose ratio is a linear function of y when y is greater than 3σ . Each x -coordinate corresponds to a different straight line. As x increases, the slopes of these lines become increasingly negative, indicating a more rapid decline of the dose ratio. The logarithm of the peak dose ratio is a parabola for y less than 3σ (not shown).

Doses from sampling wells near an unflawed shale repository with fracture flow (Table 2.2-2) were also studied. For colinear wells, peak individual and peak population doses are shown in Fig. 2.2-4 as a function of well distance. The peak doses in Fig. 2.2-4 are one to two orders of magnitude larger than corresponding values in Fig. 2.2-2 because larger flow velocities through the fractured barrier and depository layers shorten the travel time between the depository and aquifer.

For individuals consuming water from wells drilled close to the depository, the whole-body and whole-body-equivalent doses are comparable to each other because fission products and actinides are escaping into the aquifer sooner. The contribution of iodine, which primarily affects the thyroid gland, is less important. The peak whole-body dose falls off rapidly at distances for which the fission product and actinide dose peaks occur at times greater than three million years (beyond the time period under consideration).

Salt Repositories - Doses from sampling wells in an unflawed salt repository with interstitial flow in the shale barrier layer (Table 2.2-3) were also analyzed. Peak individual and peak population doses are shown in Fig. 2.2-5. Since sorption retardation of fission products and actinides is lessened by the salinity of the ground water, these radio-nuclides dominate the dose for wells close to the depository.

R-35890

R-35881

Figure 2.2-4 Peak Doses for Colinear Sampling Wells Near an Unflawed Shale Repository With Fracture Flow in the Shale Barrier Layer

Figure 2.2-5 Peak Doses for Colinear Sampling Wells Near an Unflawed Salt Repository With Interstitial Flow in the Shale Barrier Layer

Emphasis shifts to ^{129}I and ^{99}Tc as the wells move further away.

Doses from an unflawed salt repository with fracture flow in a shale barrier layer (Table 2.2-4) were also evaluated. Peak individual and peak population doses for colinear wells are shown in Fig. 2.2-6.

2.2.3 Sink Flow Well Doses

Doses from sink flow wells were calculated for the same four repositories as for sampling wells.

Shale Repositories - Peak individual, peak population and integrated population doses are shown in Fig. 2.2-7 for the case of an unflawed shale repository with interstitial flow.

As was observed for the sampling well near this repository, long travel times between the repository and aquifer and the slowness with which the other fission products and actinides move relative to ^{129}I and ^{99}Tc make the latter two nuclides the primary contributors to the dose. Since sink wells are far away from the waste release into the aquifer, only minor variations in the dose with downstream distance were observed.

Peak individual doses from sink flow wells are smaller than those from sampling wells. Although the sink flow wells withdraw a greater total mass of radionuclides, they also withdraw a larger volume of water which dilutes this waste. Since individual doses are sensitive to concentration and since concentration is smaller, individual doses are smaller.

Figure 2.2-6 Peak Doses for Colinear Sampling Wells Near an Unflawed Salt Repository With Fracture Flow in the Shale Barrier Layer

Figure 2.2-7 Doses for Colinear Sink Wells Near an Unflawed Shale Repository With Interstitial Flow in the Shale Barrier Layer

Since sink flow wells withdraw all radionuclides in the aquifer, the population doses computed are larger than those from sampling wells. The well withdrawal rate affects population doses only to the extent that aquifer flow velocities are increased, thereby reducing the time available for radioactive decay. For this repository scenario, radioactive decay was not a factor and withdrawal rate did not play a significant role in determining population dose.

Figure 2.2-8 shows sink well doses for the unflawed shale repository with fracture flow. The peak doses for this case are one to two orders of magnitude larger than corresponding values for the interstitial flow case because waste can reach the aquifer faster when flowing through fractures.

Salt Repositories - Figure 2.2-9 shows sink well doses from an unflawed salt repository with interstitial flow in the shale barrier layer. The fission products and actinides again dominate the dose for the closer wells, with emphasis shifting to ^{129}I and ^{99}Tc further downstream.

Doses from sink wells near an unflawed salt repository with fracture flow in the shale barrier are shown in Fig. 2.2-10.

2.2.4 Conclusions

In this section, the calculated doses are summarized. In order to simplify the discussion, the following worst-case conditions are considered:

Figure 2.2-8 Doses for Colinear Sink Wells Near an Unflawed Shale Repository With Fracture Flow in the Shale Barrier Layer

Figure 2.2-9

Doses for Colinear Sink Wells Near an Unflawed Salt Repository With Interstitial Flow in the Shale Barrier Layer

Figure 2.2-10

Doses for Colinear Sink Wells Near an Un-flawed Salt Repository With Fracture Flow in the Shale Barrier Layer

- The wells closest to the waste entry into the aquifer are considered
- The repository is assumed to contain 6×10^6 MWe-yr of nuclear waste, a projected upper bound for waste generation in the United States up to the year 2000.

Sampling Well Doses - Peak individual doses and peak population doses from sampling wells are presented in Table 2.2-5 for the four baseline repositories with wells situated 300 m downstream of the point source.

TABLE 2.2-5
SAMPLING WELL WATER DOSES 300 m DOWNSTREAM
FROM WASTE ENTRY INTO THE AQUIFER

REPOSITORY	PEAK INDIVIDUAL DOSE		PEAK POPULATION DOSE	
	WHOLE-BODY-EQUIVALENT (rem)	WHOLE-BODY (rem)	WHOLE-BODY-EQUIVALENT (man-rem)	WHOLE-BODY (man-rem)
Unflawed Shale	8.3×10^1	1.2×10^1	2.8×10^3	1.4×10^2
Shale With Fracture Flow	5.6×10^3	5.2×10^3	9.4×10^4	2.6×10^4
Unflawed Salt	9.3×10^2	1.4×10^3	3.3×10^5	5.0×10^5
Salt With Fracture Flow	1.8×10^4	3.2×10^4	6.5×10^5	1.1×10^6

The peak individual doses shown in Table 2.2-5 are considerably larger than the 5 rem dose to an individual from background radiation over a 50-year period. These individual doses should be construed as an upper bound because of the modeling assumptions of a point source repository, existence of potable ground water above the depository, and the loss of knowledge of the repository's location.

The population doses of Table 2.2-5 are the largest possible population doses which are consistent with the calculated individual doses. Although consumption of contaminated water from the sampling well results in very severe doses to individuals, the magnitude of the population dose indicates that only a small number of people can be exposed to these severe doses.

TABLE 2.2-6
SINK WELL DOSES 2 km DOWNSTREAM FROM
WASTE ENTRY INTO THE AQUIFER

REPOSITORY	PEAK INDIVIDUAL DOSE		PEAK POPULATION DOSE		INTEGRATED POPULATION DOSE	
	WHOLE-BODY-EQUIVALENT (rem)	WHOLE-BODY (rem)	WHOLE-BODY-EQUIVALENT (man-rem)	WHOLE-BODY (man-rem)	WHOLE-BODY-EQUIVALENT (man-rem)	WHOLE-BODY (man-rem)
Unflawed Shale	8.1×10^0	6.4×10^{-1}	1.2×10^3	5.8×10^1	3.9×10^6	2.5×10^5
Shale With Fracture Flow	2.6×10^2	1.5×10^2	3.8×10^4	1.9×10^3	1.2×10^7	2.7×10^6
Unflawed Salt	4.5×10^1	6.2×10^1	6.5×10^3	8.9×10^3	1.9×10^8	2.5×10^8
Salt With Fracture Flow	2.5×10^2	3.8×10^2	3.8×10^4	5.6×10^4	4.5×10^8	6.5×10^8

Sink Well Doses - Peak individual, peak population and integrated population doses from sink flow wells are presented in Table 2.2-6 for the four baseline repositories studied. In these cases the closest wells are situated 2 km downstream of the line source.

Individual doses from these sink flow wells are calculated to be much less than those from the sampling wells located at 300 m. Both greater dilution of the waste and the location of the well further downstream reduce the dose.

The peak population doses in Table 2.2-6 are the largest population doses possible for these repository scenarios if wells are constructed, primarily because all the radionuclides are being withdrawn. The magnitude of these doses indicates that a somewhat larger population (on the order of 100 people) is exposed to the accompanying individual doses.

2.3 CONTOURS OF EQUAL PERFORMANCE

The effect of various repository parameters on the performance of a repository may often be visualized more easily by use of contour plots. This section presents charts showing contour lines of various performance measures as functions of lumped parameters. The figures show doses to an average individual and aquifer concentrations of ^{129}I and ^{226}Ra as functions of flow times and pulse widths. The plutonium stow-away fuel cycle is assumed.

The contours have not been drawn in the region where pulse width exceeds flow time, as this would violate assumptions made in calculating the contours. Background levels or MPC_w have been divided by 6×10^6 MWe-yr, an estimate of the greatest amount of waste likely to be generated by the year 2000, and indicated on the plot.

Figure 2.3-1 shows the 50-yr whole-body-equivalent dose to an "average individual" as a function of the total flow time and total pulse width (dispersion time) defined in Ref. 12, Section 3.1.1. The curves are calculated by the method developed in that section, assuming all radionuclides move at the same velocity. If sorption retardation were to cause different groups of nuclides to have different velocities, each group of nuclides would have its own flow time and

Figure 2.3-1 Contours of Equal Peak 50-yr Whole-Body-Equivalent Dose to Average Individual, Assuming All Waste Travels at Same Speed. (Pu-stowaway fuel cycle)

pulse width. A set of curves similar to Fig. 2.3-1 could easily be prepared for each nuclide group.

As the pulse width does not enter into the approximate formula for integrated population dose (Eq. 3.1-5 of Ref. 12), such doses can be read directly off a plot of potential hazard without need for contour plots. Figure 2.3-2 shows whole-body-equivalent population dose as a function of time and can be used for that purpose, in the manner described in Ref. 3.

Figure 2.3-2 Whole-Body-Equivalent Population Dose As a Function of Time From Removal to Peak Release. (Pu-stowaway fuel cycle)

Peak aquifer concentrations can be calculated in a similar approximate manner from Eq. J-5 of Ref. 1. Concentration depends on the amount of water available to dissolve the contaminant; the aquifer characteristics given in Table 2.2-1 have been assumed. Figures 2.3-3 and 2.3-4 show contours of equal peak concentration of ^{129}I and ^{226}Ra . These two nuclides were selected to show the diversity of contours that can be obtained. Concentrations were calculated with the assumption that the entire inventory of the nuclides arrives in a single pulse. These contours are for concentration at any specified point in the aquifer; the pulse width and arrival time are the width and arrival time at that point.

Figure 2.3-3 Contours of Equal Peak ^{129}I Concentration

The ^{129}I concentration contours of Fig. 2.3-3 reflect the long half-life of this nuclide. Until the iodine starts to decay appreciably (after several million years), the peak concentration depends only on the pulse width and not on its time of arrival.

The ^{226}Ra concentration contours of Fig. 2.3-4 are more complex. Because the inventory of this nuclide grows over time as heavier parent nuclides decay, the highest con-

Figure 2.3-4 Contours of Equal Peak ^{226}Ra Concentration

centrations correspond to arrival times of the order of 10^5 yr. It should be noted that these contours are for concentration at a single point; peak concentration will differ from point to point as the ^{226}Ra inventory builds up and decays.

3. UNCERTAINTY ANALYSIS

The difficulty of accurately measuring many geologic parameters could affect confidence in risk assessments of nuclear waste disposal. For that reason, it is important to calculate the effect of measurement uncertainties on predictions of risk. This chapter discusses two different approaches to such calculations. First, a monte carlo technique is applied to a salt repository. The monte carlo technique does not require that any particular functional form be assumed for the probability distribution of risk which is being calculated. This represents a distinct advantage because these distributions seem not to be simple functions. Second, an analytic technique is developed for calculating probability distributions of model outputs. The costly computer runs and inherent statistical errors of the monte carlo approach can thus be avoided. However, since this method yields an expansion of the output probability distribution in terms of moments, it implicitly assumes a functional form. The further development and implementation of the analytic approach would require a substantial amount of additional work. The cost savings anticipated from its use would only justify this effort if an extremely large number of additional uncertainty analyses were anticipated.

3.1 UNCERTAINTY ANALYSIS OF A BEDDED SALT REPOSITORY

3.1.1 Introduction

Bedded salt is currently being considered for use as an emplacement medium for high-level nuclear wastes. The geom-

etry of a generic salt repository model and the associated baseline geologic and hydrologic parameters are defined in Table 2.2-3. This section describes a monte carlo study performed to evaluate the effect of parameter uncertainty on the statistics of repository performance measures, such as population dose.

The basic technique for the monte carlo analysis was developed in Ref. 1, which reports the results of a similar study for a shale repository. This method has been revised for use in the current study. The techniques developed here may be used in future uncertainty studies for salt repositories, or for analysis of other host rock formations.

3.1.2 Methods for Statistical Analysis of Data-Induced Uncertainty

A major objective of the monte carlo analysis is to identify the probability distribution functions (PDF's) of the repository performance measures. Such an identification should be useful in establishing confidence levels for the risks predicted for a generic repository. This section discusses the rationale for the methods used to analyze the outcomes of the monte carlo trials. In later sections these methods are applied to the uncertainty analysis of a salt repository.

Non-Parametric Statistical Analysis - The computer simulation system NUTRAN (NUclide TRANsport) is used to assess the risk from radioactive waste repositories (Ref. 1). Each run of the NUTRAN program package may be regarded as a simulated experiment, in which a repository with a given set of geologic and hydrologic parameters is constructed, and the time histories of the risks to man are followed over a three million year period. The outcome of a single monte carlo trial

may be regarded as a sample drawn from a parent population distribution. The monte carlo analysis enables one to infer the characteristics of this parent distribution.

There are two commonly used representations for characterizing probability distributions. They are:

- Specification by moments (parametric)
- Specification by quantiles (non-parametric).

From an analytic standpoint, moment specification is the most convenient way to describe a variety of PDF's. For instance, many random phenomena have Gaussian distributions, and consequently their statistical behavior may be completely specified by their first and second central moments -- their mean and variance. One approach to the analysis of the monte carlo outcomes would involve estimation of the moments of the output PDF from the sample output data. Unfortunately, there can be considerable difficulty interpreting the results of this type of analysis. The sample standard deviation, for instance, does provide a measure of the spread or dispersion of the output PDF. However, unless the parametric form of the output PDF (e.g., Gaussian) is known, the confidence levels associated with such a statistic may not be readily available. In addition, it was shown in Ref. 1 that the dose PDF's tend to be non-Gaussian.

As a consequence of the above-mentioned considerations, parametric statistical analysis is avoided in this study. Medians, rather than means, are estimated for the output PDF's. As a measure of statistical dispersion, the interquartile range is reported rather than the standard deviation. A number of results are available from statistical theory to assess confidence levels and test hypotheses for the sample distributions

(Refs. 5 and 6). These techniques have been applied to the results of this monte carlo study.

Multivariate Sensitivity Analysis - The monte carlo analysis may be regarded as a multivariate sensitivity study. The results of this study can be used to augment the deterministic sensitivity studies of the type presented in Ref. 1. Deterministic sensitivity analysis can be used to establish which model parameters are dominant in affecting repository performance. In a similar manner, monte carlo analysis can be used to establish which parameter uncertainties are dominant.

The assessment of dominant parameter uncertainties is facilitated by means of correlation analysis. With this type of analysis the relationships between the outputs of the NUTRAN program and the random inputs are evaluated by means of an appropriate correlation coefficient. For the analysis presented here, the Spearman rank correlation coefficient (Ref. 5) was used. The Spearman coefficient is a distribution-free measure of correlation and is therefore preferred to the standard Gaussian regression (or Pearson) correlation coefficient.

The Spearman coefficient for two data sets is computed simply by ordering or ranking the data sets from smallest to largest and computing the Pearson coefficient for the ranks. Its advantage over the standard Pearson correlation coefficient is illustrated by its property of indicating unity correlation between any two sets of data which are deterministically related by any monotonic (or order-preserving) function (e.g., if one is the logarithm of the other). The standard Pearson coefficient will indicate unity correlation only for data sets which are linearly related. Hence the Spearman coefficient is less restricted to a particular distribution and more sensitive to order relationships.

The magnitude of the Spearman coefficient, when interpreted correctly, can indicate the degree of dependence or correlation between an output and an input. This provides a means of comparing or ranking the impact of the various parameter uncertainties on the model performance predictions.

Figure 3.1-1 illustrates the procedure for generation and statistical analysis of the monte carlo outcomes. Using the assumed probability distributions for the input data the monte carlo program (WSRAND, see Ref. 1) generates random input data. These data are then input to the NUTRAN simulation system, which models the associated waste migration and computes nuclide concentrations and the dose to humans. These outputs are then subjected to various types of statistical analysis for specification of quantiles of the output PDF's and assessment of dominant uncertainties. In addition, hypothesis tests are available to assess confidence levels for the various statistics. In the next section the results of monte carlo analysis for a bedded salt repository are presented.

Figure 3.1-1 Structure of the Monte Carlo Analysis

3.1.3 Results of Monte Carlo Analysis

Model Parameters and Constraints - The baseline repository analyzed in this study is a bedded salt repository with flow paths to an overlying aquifer through a fracture zone surrounding the tunnel and shaft and through overlying layers of salt and shale. Flow through the shale layer is assumed to be interstitial flow. The nominal parameter values for this repository are described in Table 2.2-3; the baseline values of retardation factors have been modified as described in Ref. 4.

For the purposes of the monte carlo analysis the uncertain model parameters are considered random variables specified by probability distributions. The PDF's used in this study are defined in Appendix C. They are based on the assumption of moderate pre-mine phase exploration (fifty exploratory boreholes) and on a variety of physically determined constraints -- e.g., generic limits on the permeability of salt. In this study it is assumed that the baseline (or median) parameter values represent the best estimates of the site descriptors for a hypothetical salt repository. The PDF's used in the monte carlo analysis represent the estimation uncertainty of these parameters. This estimation uncertainty is due to a number of factors, including:

- Inaccurate and imprecise measurement
- Spatial variability of the model parameters.

The monte carlo analysis does not assess the impact of modeling errors. For instance, in running the NUTRAN simulation it is assumed that a single value of permeability will provide valid flow predictions for the aquifer. The PDF used to represent the uncertainty in permeability represents the

estimation error for that single value. The monte carlo analysis does not estimate the error due to using a single permeability value for this flow path.

Population Dose - Figure 3.1-2 displays a histogram and sample statistics of whole-body-equivalent integrated population dose for fifty monte carlo trials. The results are displayed on a logarithmic scale. The repository is assumed to contain 6×10^6 MWe-yr of solidified high-level waste.

Figure 3.1-2 Sample Histogram and Statistics of Whole-Body-Equivalent Integrated Population Dose for 50 Monte Carlo Trials

In Ref. 1 it was observed that for the case of a shale repository, the output PDF of population dose was multi-modal. This is also the case for the salt repository analysis presented here, although the scale chosen for the histogram in Fig. 3.1-2 is too coarse to show the multimodal nature of the fre-

quency distribution. Two dominant modes were observed: a major mode due to the fission products at approximately 2.0×10^{-2} man-rem/MWe-yr, and a minor mode at approximately 3.2 man-rem/MWe-yr. The latter is due strictly to a small number of cases in which significant amounts of actinides entered the biosphere during the three-million-year period which was considered.

An analysis of 500 random input data sets for a salt repository revealed that in approximately 19% of the cases, the mean passage time of the actinides across the aquifer was less than three million years, the maximum time period under consideration. A similar analysis of 1000 random input data sets for a shale repository (Ref. 1) showed approximately 3% of the cases had similar "short" passage times for the actinides, indicating a high level of population dose in many of those cases. These results indicate that given the input data statistics for the salt and shale repositories assumed here

Figure 3.1-3 CDF of Whole-Body-Equivalent Integrated Population Dose From 50 Monte Carlo Trials

and in Ref. 1 the probability of the actinides reaching the biosphere within three million years is significantly higher in salt than in shale. It should be noted, however, that these calculations may be highly sensitive to assumptions concerning the baseline permeability of the salt layer, which may be over-estimated here by several orders of magnitude (Ref. 6).

Distribution-Free Statistical Analysis of Population

Dose - Figure 3.1-3 shows the sample cumulative distribution function (CDF) for whole-body-equivalent integrated population dose. Also shown are the Kolmogorov 95% confidence limits for the CDF. The Kolmogorov bounds are an indication of the estimation accuracy that may be obtained from the number of samples. They are not necessarily an indication of uncertainty in the distribution of the actual physical outcomes. The uncertainty in predicting the physical outcome also depends on uncertainty in the input data PDF's and modeling errors in the waste transport and dose models, which are difficult to quantify.

Table 3.1-1 displays the key results of an analysis conducted to evaluate the correlations between the random input data and whole-body-equivalent integrated population dose (IPD) for fifty monte carlo trials. The input variates are listed according to the correlation with the output values of whole-body-equivalent IPD as reflected in the Spearman correlation coefficient. Also displayed is the probability of independence between the variate and IPD. The variates listed in the table are those which exhibited significant correlation with the output. The criterion of 5% probability of the null hypothesis was chosen arbitrarily as the significance level for this study.

TABLE 3.1-1
CORRELATION OF INPUT VARIATES WITH OUTPUT WHOLE-BODY-
EQUIVALENT INTEGRATED POPULATION DOSE

VARIATE	SPEARMAN CORRELATION COEFFICIENT	PROBABILITY OF INDEPENDENCE
Permeability of Salt Layer	0.56	0.0001
Porosity of Salt Layer	0.47	0.0006
Head Gradient in Upper Aquifer	0.37	0.0008
Actinide Retardation Factor in Aquifer	-0.36	0.01
Porosity of Shaft Fracture Zone in Barrier Layer	0.35	0.01
Porosity of Aquifer	0.34	0.017
Permeability of Aquifer	0.34	0.017

The entries in Table 3.1-1 indicate that the predominant uncertainties affecting population dose predictions may be those associated with the aquifer and depository layers. The strong positive correlation between salt permeability and population dose indicates that further evaluation of the properties of bedded salt may be desirable to reduce this uncertainty. It should be noted that the positive correlation of porosity in the various layers with dose is due to the assumed positive statistical correlation of porosity with permeability (Appendix C). Hence porosity is not regarded here as a dominant source of uncertainty.

Individual Dose - Figures 3.1-4 and 3.1-5 are, respectively, a histogram and cumulative distribution function for peak individual whole-body-equivalent dose. The 95% Kolomo-

Figure 3.1-4 Histogram and Statistics of Whole-Body-Equivalent Peak Individual Dose From Fifty Monte Carlo Trials

Figure 3.1-5 CDF of Whole-Body-Equivalent Peak Individual Dose From 50 Monte Carlo Trials

gorov confidence bounds for the sample CDF based on fifty monte carlo trials are shown in Fig. 3.1-5.

In general it should be noted that the predicted values of peak individual dose from the salt repository tend to be one to two orders of magnitude higher than those predicted for shale in Ref. 1. This is due to the low values of nuclide retardation factors assumed here and the conservative baseline value for the permeability of salt.

Table 3.1-2 lists the random input variates which exhibited significant correlation (<5% probability of independence) with peak individual dose.

TABLE 3.1-2
CORRELATION OF RANDOM INPUT VARIATES WITH
WHOLE-BODY-EQUIVALENT PEAK DOSE

	SPEARMAN COEFFICIENT	PROBABILITY OF INDEPENDENCE
Head Gradient in Upper Aquifer	0.43	0.002
Porosity of Shaft Fracture Zone in Barrier Layer	0.42	0.003
Dispersion in First Part of Tunnel Fracture Zone	-0.39	0.006
Actinide Retardation Factor in Aquifer	-0.37	0.008
Permeability of Aquifer	0.37	0.008
Porosity of Aquifer	0.37	0.008
Permeability of Salt Bed	0.35	0.014
Fission Product Retarda- tion Factor in Aquifer	-0.30	0.034
Porosity of Salt Bed	0.29	0.038
Permeability of First Part of Tunnel Fracture Zone	0.28	0.047

Table 3.1-2 indicates that the peak dose predictions are sensitive to the same uncertainties as integrated population dose (Table 3.1-1) and in addition may be more sensitive to other uncertainties, particularly those associated with the shaft and tunnel fracture zones. This is a reasonable observation in view of the fact that high predicted peak doses are frequently a result of the early escape of nuclides through the shaft and tunnel fracture zones due to the high assumed permeabilities of these areas.

Nuclide Concentrations - Table 3.1-3 lists the statistics for maximum concentrations of various nuclides in the aquifer for 50 monte carlo trials. The repository is assumed to contain 6×10^6 MWe-yr of waste.

TABLE 3.1-3
PEAK AQUIFER CONCENTRATIONS
FROM 50 MONTE CARLO TRIALS (Ci/m^3)

NUCLIDE	MPC _w	BASELINE	FIRST QUARTILE	SAMPLE MEDIAN	THIRD QUARTILE
^{99}Tc	3×10^{-4}	1.3×10^{-4}	1.4×10^{-5}	7.7×10^{-5}	9.7×10^{-4}
^{126}Sn	2×10^{-5}	5.9×10^{-7}	4.8×10^{-8}	6.4×10^{-7}	6.7×10^{-6}
^{90}Sr	3×10^{-7}	3.2×10^{-13}	*	8.1×10^{-30}	1.4×10^{-17}
$^{239}\text{Pu}^\dagger$	5×10^{-6}	3.3×10^{-6}	1.9×10^{-9}	3.8×10^{-7}	5.7×10^{-6}
$^{226}\text{Ra}^\dagger$	3×10^{-8}	1.8×10^{-8}	1.2×10^{-9}	9.5×10^{-9}	9.4×10^{-8}

*Concentration less than 10^{-50} Ci/m^3 .

†For ^{239}Pu and ^{226}Ra the true peaks often occur after three million years and were not calculated. The statistics computed here are for maximum concentrations within three million years.

Table 3.1-3 indicates that for ^{99}Tc , ^{239}Pu , and ^{226}Ra at least 25% of the nuclide concentrations exceeded their MPC_w values within three million years.

3.1.4 Summary

This section has presented the results of a monte carlo uncertainty analysis of a bedded salt repository. The techniques used for the analysis have been expanded from those used in Refs. 1 and 3 to include correlation analysis of inputs and outputs and distribution-free statistical analysis of the outputs. The results of the correlation analysis indicate that further evaluation of the properties of bedded salt may be particularly important to reduce uncertainties in predictions of integrated population dose from salt repositories.

3.2 PREDICTOR APPROACH TO UNCERTAINTY ANALYSIS

One of the greatest disadvantages of the monte carlo method of uncertainty analysis is its high cost. In this section an analytic technique is developed which has the potential to calculate the same quantities as the monte carlo method, but at lower cost per case analyzed.

3.2.1 Introduction

The current monte carlo approach to uncertainty analysis in the nuclear waste management project consists of two distinct parts. First, probability distributions for the physical parameters of the model are constructed. Constraints are imposed on and among various parameters and a large number of parameter value sets are generated by random sampling of these constrained distributions. Second, the hydrology and transport

program is run for each of these parameter sets, and probability distributions of doses or concentrations are computed. In this way both the average (over the physical parameters) and higher moments of the time evolution of the concentration are computed.

The monte carlo approach has the virtue of generating distributions, not just selected moments, of doses. However, it uses a lot of computer time; consequently it is expensive. Moreover, if it is desired to change the input distributions not only must a new set of random samples be generated, but a new series of deterministic runs performed for each set. The second aspect is highly expensive and thus substantially reduces the flexibility of the uncertainty analysis. A more efficient and versatile approach is usually taken in uncertainty analysis whenever possible. This is to multiply the predictor equation by probability distributions for the physical parameters and integrate over the parameter space. If the probability distributions are not time dependent (and sometimes even when they are), it is usually possible to derive a predictor equation for the expected value, and perhaps higher moments, of the output quantities. The predictor equation approach has the following virtues:

- It is quick to run on a digital computer
- It offers versatility in choosing the parameters of the input distributions and thus facilitates sensitivity studies of the uncertainty analysis
- It exhibits analytic forms for the moments in terms of these distribution parameters so that limiting behavior can be seen explicitly.

In the stream tube models used for the nuclear waste transport predictions, two drawbacks exist to implementing this approach. The first is that the hydrogeologic parameters, which are usually (although not always) considered independent from one pipe to the next, enter in the calculation of concentrations in a form which couples the velocities of the various pipes. This is entirely due to the fact that the overall head difference between upper and lower aquifers is not a function of the immediate repository geology, but rather of the regional geology (except in cases of extremely high flow and consequent depressurization). This means that it is not possible to integrate the distributions for the transport and hydrology parameters independently of one another, even excluding possible correlations between permeabilities and porosities within a pipe or among retardation factors for different pipes. Note, though, that the correlations between velocities are deterministic -- i.e., given the values of permeabilities, porosities, cross sections, and lengths of all the pipes and a specified value of overall head difference, the velocities are completely determined (unlike the correlations between permeabilities and porosities). Therefore these quantities and their associated distributions contain all the information required for the expected value of a concentration.

The second difficulty in using this approach with the stream tube transport model is the mathematical complexity of any moment calculations when attempting to find analytically tractable, yet physically reasonable, probability distributions for the physical parameters. The following two sections deal with the mathematical aspects of this problem, and detail how, under a certain approximation, such distributions can be found and the first few moments calculated.

3.2.2 Mathematical Structure of the Predictor Equation

In the model discussed here the concentrations of the nuclides in the aquifer as a function of time are completely specified by the leaching behavior of the canisters and the Green's functions for each of the pipes and nuclides. This excludes time-dependent phenomena associated with geologic and deterioration events. These are easily incorporated --about which more will be said below. Since doses are linearly related to concentrations, only the latter quantities need to be studied.

The output concentration at the end of a pipe is related to the input concentration by the equation:

$$c^{\text{out}}(z,t) = \frac{1}{Q} \int_0^t R(t') G(z, t-t') dt' \quad (3.2-1)$$

where $R(t)$ is the rate at which waste enters the pipe, Q is the volumetric water flow rate (and, therefore, $c^{\text{in}}(t) = R(t)/Q$), z is the length of the pipe, and $G(z,t)$ is given by

$$G(z,t) = \frac{1}{\sqrt{\pi} \sqrt{\alpha \frac{B}{V} t}} \exp - \frac{(z - \frac{V}{B} t)^2}{4\alpha \frac{V}{B} t} \quad (3.2-2)$$

Here α , V , and B are, respectively, the dispersion constant, water velocity, and retardation factor for the nuclide and pipe being considered.

Note that with this normalization G has the dimensions of $(\text{time})^{-1}$, as is evident from Eq. 3.2-1. If the argument of the exponential is multiplied and divided by α^2 then Eq. 3.2-2 can be written as

$$G(z,t) = \frac{1}{\sqrt{\pi} \sqrt{Tt}} \exp - \frac{(\bar{z}-t/T)^2}{4t/T} \quad (3.2-3)$$

where

$$T = \frac{\alpha B}{V} \text{ and } \bar{z} = \frac{z}{\alpha} \quad (3.2-4)$$

Thus each pipe is characterized by a set of T's (one for each nuclide) and a normalized length $\bar{z}$. The T's for different pipes are not in general independent of each other because of the coupling between velocities. Note that T has units of time. The lumped parameter T is the only variable considered throughout the remainder of this discussion, and its definition should be kept in mind.

For computer implementation the amount of waste, $F(l)$, leaving the pipe during a time period $(t(l), t(l+1))$ indexed by some integer l must be known. This is given approximately by:

$$\begin{aligned} F(l) &= \int_{t(l)}^{t(l+1)} Q c(z,t) dt \\ &= \frac{1}{2} \int_0^{t(l)} dt' R(t') [g(z, t(l+1) - t') - g(z, t(l) - t')] \\ &\quad + \frac{1}{2} \int_{t(l)}^{t(l+1)} dt' R(t') g(z, t(l+1) - t') \end{aligned} \quad (3.2-5)$$

where

$$g(z,t) = \operatorname{erfc} \frac{\bar{z}-t/T}{4t/T} - e^{-\bar{z}} \operatorname{erfc} \frac{\bar{z}+t/T}{4t/T} \quad (3.2-6)$$

In performing the uncertainty analysis, the relationships between the T's for various pipes and the hydrogeologic parameters must be known. Appendix D presents the fundamental

equations for velocities (and consequently, T's) as a function of the resistances for each pipe in a simple repository pipe configuration (interstitial flow through repository and barrier rock layers and flow through a fracture zone around the shaft and tunnel). Here the resistance of a pipe is defined by

$$R = \frac{z}{kW} \quad (3.2-7)$$

where z is length, k is permeability and W is cross-sectional area. From the equations in Appendix G, it can be seen that there is no simple relationship between the physical parameters and the velocities.

In the monte carlo simulation used to date, the physical parameters have been assumed to follow log-normal distributions, sometimes truncated for values outside of some generic range. There is no particular reason why the parameters should follow such a law; rather, the log-normal distribution is chosen because it exhibits qualitative characteristics (a single maximum, vanishing probability at the origin, and rapid fall-off for large argument values) which are considered intuitively appropriate for the real distributions. However, any other distribution satisfying these characteristics would be just as valid.

The log-normal distributions do have certain features which make them analytically attractive. If two independent variables are log-normally distributed, then the product and quotient of these variables are also log-normally distributed. However, the sum (or difference) of two log-normally distributed variables does not have an analytically tractable form. From these facts it is evident that the resistances will be log-normally distributed when the pipe lengths, permeabilities,

and areas are. But the head differences, and consequently the velocities, will not have a simple distribution. (Actually they can only be written as a multidimensional integral representation.) In fact, no distributions for the physical parameters with the correct qualitative features will produce an analytically simple distribution for the variable T .

The unfortunate interdependence of the T 's for different pipes does not necessarily preclude an analytic approach to uncertainty analysis. This is due to two features of the model. The first is the fact that the random sampling of the input distributions, subject to all the correlations and constraints, generates a probability surface for values in the full parameter space. Thus the output of the random sampling gives the probability that the N -parameter vector $(K_1, \dots, K_n, W_1, \dots, W_n, \epsilon_1, \dots, \epsilon_n, \dots, H_0)$, (where ϵ is the porosity, H_0 is overall head drop, and n is the number of pipes times the number of nuclides) will have some specified vector value. If the values of T_i ($i=1, \dots, n$) associated with each value of the parameter vector are then computed, it is possible to calculate a probability surface for the n T_i 's, along with $N-n$ of the other parameters (i.e., a simple change of variables). This surface incorporates the correlations between the T_i 's. This distribution is then usually multiplied by a loss function (the concentration) and integrated. However, as an approximation, it is possible to take the values of a given pipe's T_i , computed for each of the N -component vectors generated by the random sampling, and compile a histogram distribution for this T_i . This can be done for each value of i separately. This would give a set of n single variable (univariate) distributions -- one for each pipe and nuclide. These distributions, since they were produced by a random sampling of the full N -dimensional probability surface with the sampling frequency per unit surface "area" weighted by the value of the probability density at that point on the surface, are the same as

those n univariate distributions obtained by averaging the multivariate probability density over all the variables except for the T_i in question. Mathematically, if the joint probability density function is denoted by $g(\vec{T}, \vec{x}_{N-n})$ where $\vec{T} = (T_1, \dots, T_n)$ and $\vec{x}_{N-n}$ is a vector whose $N-n$ components are the residual $N-n$ physical variables, then the exact expected value for the output concentration (as a function of time) is given by:

$$\int_C^{\text{out}} (t; \vec{T}) g(\vec{T}, \vec{x}_{N-n}) (d^{N-n}x) (d^n T) \quad (3.2-8)$$

On the other hand, denoting by $f_i(T_i)$ the univariate distributions defined by

$$f_i(T_i) = \int g(\vec{T}, \vec{x}_{N-n}) (d^{N-n}x) (d^{n-1}T)$$

then the approximation explained above is equivalent to:

$$\int_C^{\text{out}} (t; \vec{T}) \prod_i f_i(T_i) dT_i \quad (3.2-9)$$

Equations 3.2-8 and 3.2-9 are equal only when the T_i are independent variables. This "projection" approximation will take into account most of the correlations between T_i 's when their effective distributions are generated. The accuracy of the approximation will depend somewhat on the degree of uncertainty in H_0 -- the overall head drop -- since if it was completely unknown then the T 's would be independent. It should be pointed out that some repository models assume constant recharge rate for the aquifers as opposed to a constant head difference. In this case the approximation is more accurate.

The second feature of the modeling involves assigning an analytic form to these distributions which will allow the integrations involved in the expectation values to be analytically performed. The primary result of the next section is that such distributions have been found.

3.2.3 Probability Distributions

The simplest distribution considered was the Gamma distribution. This is a two-parameter distribution denoted $\gamma(x|\alpha, \beta)$ and given by:

$$\gamma(x|\alpha, \beta) = \begin{cases} \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x} & , \quad x \geq 0 \\ 0 & , \quad x < 0 \end{cases} \quad (3.2-10)$$

This has the qualitative form which the projected distributions for the T's are likely to have (based on the qualitative form for the physical parameter distributions). Furthermore, the origin for these distributions can be shifted without destroying integrability, so that they can be thought of as 3-parameter distributions. If a richer structure is needed, a generalization of Eq. 3.2-10 is given by

$$\gamma(x|\alpha, \beta, \delta, m) = \begin{cases} N(\alpha, \beta, \delta, m) \frac{x^{\alpha-1} e^{-\beta x}}{(1+\delta x)^m} & , \quad x \geq 0 \\ 0 & , \quad x < 0 \end{cases} \quad (3.2-11)$$

where N is a normalization factor. This is a 4-parameter distribution with the same behavior near the origin as the usual Gamma distribution, but with a different asymptotic behavior. (Again, this can be considered a 5-parameter distribution by shifting the origin.) Virtually any single-peak distribution

can be effectively fit by Eq. 3.2-11. Appendix E gives the relevant properties of these two distributions.

With these distributions it is possible to compute the expectation value of Eq. 3.2-1 directly. For computer implementation, it is still necessary to integrate the concentration (either actual or its expectation value) over some time interval. The order in which the time integration and the parameter averaging are done is immaterial as long as the distributions for the parameters are constant over the time interval $(t(\ell), t(\ell+1))$. For purposes of convenience the time averaging will be done first in this derivation. Later, when looking at the higher moments, it will be necessary to do the parameter averaging first.

To compute the expectation value of the quantity of waste leaving the pipe between $t(\ell)$ and $t(\ell+1)$, multiply Eq. 3.2-5 by these distributions and integrate. It is assumed that the parameters have been appropriately fit to the projected distributions. First consider the 2-parameter distribution. This gives

$$\bar{F}(\ell) = \int_0^{\infty} dT F(\ell, T) \gamma(T|\alpha, \beta) \quad (3.2-12)$$

Consider only integer values for α for the present and note the identity

$$x^m e^{-\beta x} = (-1)^m \frac{\partial^m}{\partial \beta^m} e^{-\beta x} \quad (3.2-13)$$

Using this, the following integral is needed:

$$\int_0^{\infty} e^{-\beta T} \operatorname{erfc} \frac{\bar{z} \pm t/T}{2\sqrt{t/T}} dT = \frac{\exp\left\{\pm 2\sqrt{t/T} \left[\frac{\bar{z}}{\sqrt{4t}} + \sqrt{\frac{\bar{z}^2}{4t} + \beta}\right]\right\}}{\sqrt{\frac{\bar{z}^2}{4t} + \beta} \left(\frac{\bar{z}}{\sqrt{4t}} + \sqrt{\frac{\bar{z}^2}{4t} + \beta}\right)} \quad (3.2-14)$$

A formula for an arbitrary number of derivatives of Eq. 3.2-14 is the next step in the analysis:

$$\begin{aligned} \frac{\partial^m}{\partial b^m} \frac{e^{\pm 2c(\sqrt{a} + \sqrt{b})}}{\sqrt{b}(\sqrt{a} + \sqrt{b})} &= \frac{\partial^m}{\partial b^m} \left[-\frac{2}{\sqrt{b}} \int_{\infty}^{\sqrt{c}} e^{-2y(\sqrt{a} + \sqrt{b})} dy \right] \\ &= -2 \sum_{i=0}^m \binom{m}{i} \left[\frac{\partial^{m-i}}{\partial b^{m-i}} \frac{1}{b^{1/2}} \right] \frac{\partial^i}{\partial b^i} \int_{\infty}^{\sqrt{c}} e^{-2y(\sqrt{a} + \sqrt{b})} dy \end{aligned} \quad (3.2-15)$$

A formula is thus needed for $\frac{\partial}{\partial b^{\ell}} f(\sqrt{b})$. By dimensional analysis this can be written as

$$\frac{d^{\ell}}{db^{\ell}} f(\sqrt{b}) = \sum_{k=0}^{\ell-1} \frac{a_k^{\ell}}{(\sqrt{b})^{\ell+k}} \frac{d^{\ell-k}}{d(\sqrt{b})^{\ell-k}} f(\sqrt{b}) \quad (3.2-16)$$

In Appendix F, an explicit formula for the a_k^{ℓ} is derived. For convenience, the result is simply quoted here:

$$a_k^{\ell} = \frac{(\ell+k-1)!(-1)^k}{k!(\ell-k-1)!2^{\ell+k}} \quad (3.2-17)$$

Note that this is not related to the binomial coefficient. Combining Eqs. 3.2-17 and 3.2-16 with Eq. 3.2-15 gives:

$$-2 \sum_{i=0}^m \binom{m}{i} \frac{(-1)^{m-i} (2m-2i-1)!}{2^{2m-2i-1} (m-i-1)! (\sqrt{b})^{2m-2i+1}} \sum_{k=0}^{i-1} \frac{a_k^i}{(\sqrt{b})^{i+k}} \\ \times \int_0^{\sqrt{c}} (-2y)^{i-k} e^{-2y(\sqrt{a} + \sqrt{b})} dy \quad (3.2-18)$$

Now using the identity

$$\int_0^1 x^m e^{-ax} dx = \frac{m!}{a^{m+1}} \left[-e^{-a} \sum_{r=0}^m \frac{a^r}{r!} \right]$$

gives for Eq. 3.2-18:

$$\sum_{i=0}^m \sum_{k=0}^{i-1} \binom{m}{i} \frac{(i+k-1)! (-1)^m (2m-2i-1)! (i-k)}{k! 2^{i+k} 2^{2m-2i-1} (m-i-1)! (\sqrt{b})^{i+k+2m-2i+1}} \\ \times \frac{e^{\pm 2\sqrt{c}(\sqrt{a} + \sqrt{b})} (i-k-1)! (\pm 2\sqrt{c}(\sqrt{a} + \sqrt{b}))^r}{(\sqrt{a} + \sqrt{b})^{i-k+1} r!} \quad (3.2-19)$$

Multiplying this by $\frac{(-1)^m (\beta)^{m+1}}{m!}$ and identifying $c = t/4$,

$b = (\bar{z}^2/4t) + \beta$, $a = \bar{z}^2/4t$, gives the expectation value of the components of the g function in Eq. 3.2-6 (and consequently for components of the g function in Eq. 3.2-5 for $F(\ell)$ with $\gamma(T|m-1, \beta)$). Since this expression is a finite sum, it can be calculated by a digital computer.

Turning to a preliminary discussion of the 4-parameter distribution, first note the identities

$$\frac{x^n e^{-\beta x}}{(1 + \gamma x)^m} = \frac{\partial^n}{\partial (-\beta)^n} \frac{\partial^{m-1}}{\partial \gamma^{m-1}} \frac{(-1)^{m-1}}{(m-1)!} \frac{e^{-\beta x}}{1 + \gamma x} \quad (3.2-21)$$

and

$$\frac{e^{-\beta x}}{1 + \gamma x} = -e^{\beta/\gamma} \int_{\infty}^{\beta/\gamma} e^{-y(1 + \gamma x)} dy \quad (3.2-22)$$

Concentrating on Eq. 3.2-21, multiplying it by the erfc function and integrating gives:

$$\begin{aligned} & \int_0^{\infty} \frac{e^{-\beta T}}{1 + \gamma T} \operatorname{erfc} \left(\sqrt{aT} \pm \sqrt{\frac{c}{T}} \right) dT \\ &= -e^{\beta/\gamma} \int_{\infty}^{\beta/\gamma} dy \int_0^{\infty} dT e^{-y(1 + \gamma T)} \operatorname{erfc} \left(\sqrt{aT} \pm \sqrt{\frac{c}{T}} \right) \\ &= -e^{\beta/\gamma} \int_{\infty}^{\beta/\gamma} dy \frac{e^{\mp 2\sqrt{c}(\sqrt{a} + \sqrt{a+\gamma y})}}{\sqrt{a+\gamma y}(\sqrt{a} + \sqrt{a+\gamma y})} e^{-y} \\ &= -e^{\beta/\gamma} \int_{\infty}^{\beta/\gamma} e^{a/\gamma} e^{-\sigma^2/\gamma} \frac{e^{\mp 2\sqrt{c}(\sqrt{a+\sigma})}}{\sigma(\sqrt{a+\sigma})} \frac{2\sigma d\sigma}{\gamma} \\ &= (-2)^2 \frac{e^{-\beta/\gamma} e^{a/\gamma}}{\gamma} \int_{\infty}^{\sqrt{c}} dy' \int_{\infty}^{\beta/\gamma} d\sigma e^{-\sigma^2/(\gamma + 2y'\sigma)} e^{\mp 2y'\sqrt{a}} \end{aligned}$$

where $\sigma^2 = a + \gamma y$. This last integral reduces to the form

$$e^{ax} \operatorname{erfc} bx \, dx$$

which can be integrated by parts.

Recurrence relations for derivatives with respect to β and γ can be developed in exact analogy to the previous discussion. However, these relations are complex and only useful

for actual computer implementation. They pose no special problems, since the derivation of the basic integral is the critical component in the analysis.

The procedure outlined in Eqs. 3.2-12 through 3.2-19 computes the expectation value of the concentration. It is then possible to extract the maximum value of the expectation value. This is in general different from the expectation value of the maximum value of the concentration. The latter can in principle be calculated but requires solving an integral equation for the maximum value.

An equivalent preliminary investigation of the higher moments of the concentrations can now be done. As previously mentioned, it will be necessary to use Eq. 3.2-1 and integrate over the parameter space first. This is because integrals of powers of error functions with exponentials are not a priori computable.

The following quantity must be computed for the second moment (using the basic Gamma distribution):

$$\begin{aligned} & \int_0^{\infty} T^m \frac{e^{-\beta T}}{\sqrt{4\pi t_1 T} \sqrt{4\pi t_2 T}} \exp \left\{ -\frac{(\bar{z} - t_1/T)^2}{4t_1/T} \right\} \exp \left\{ -\frac{(\bar{z} - t_2/T)^2}{4t_2/T} \right\} dT \\ &= C \int_0^{\infty} T^{m-1} e^{-\beta T} \exp \left[-a'T - \frac{b}{T} \right] dT \stackrel{a=a'+\beta}{=} C \int_0^{\infty} T^{m-1} e^{-(aT + b/T)} dT \\ &= 2C \left(\frac{b}{a} \right)^{m/2} K_m(2\sqrt{ab}) \end{aligned}$$

where $C = e^{-\bar{z}^2/4\pi\sqrt{t_1 t_2}}$ and $K_m(x)$ is the m^{th} -order modified Bessel function. This expression is valid for noninteger values of m as well. Identifying $a = \beta + \bar{z}^2/4t_1 + \bar{z}^2/4t_2$ and $b = (t_1 + t_2)/4$,

this Bessel function must now be integrated over intervals for t_1 and t_2 . This can be done numerically or, by changing variables from (t_1, t_2) to $(t_1 + t_2, 1/t_1 + 1/t_2)$, can be done analytically. Higher moments can be generalized from the first two moments.

To implement this program and make possible analytic calculations of uncertainty distributions, the following additional tasks must be performed:

- The computer programs generating the sample sets must be augmented by code to compute the T's and to project their distributions
- A curve fitting program must be written to fit the gamma distributions
- The WASTE program must be changed to compute $\bar{F}(\ell)$ rather than $F(\ell)$. This includes the numerical analysis aspects
- Codes to compute higher moments must be written and debugged
- The output must be checked against previously generated monte carlo data.

A substantial additional effort would be required and this effort must be balanced against the expected gains in efficiency of the uncertainty analysis.

3.2.4 Summary

The procedure for uncertainty analysis outlined in this section consists of three parts:

- A set of probability distributions for the physical parameters are chosen. A random sample is taken from these distributions and the values of the key param-

eter T associated with each parameter vector are computed, taking into account all correlations and constraints

- Probability distributions (histograms) are compiled for each pipe and nuclide's T. These histograms are fit to one of the distributions indicated in Section 3.2.3.
- The waste transport code is run with the formula for the expectation value of the quantity of waste leaving each pipe, $\bar{F}(\ell)$, substituted for $F(\ell)$ everywhere. Additional changes are made to the code to compute higher moments as well.

This approach provides efficiency and versatility in the uncertainty analysis since the following features are implicit in its formulation:

- Changes in dose moments induced by changes in the parameters characterizing the distributions of the physical variables can be easily calculated. A new random sample is taken, the generic distributions fit to the new histograms, and the modified waste transport program run again. Thus sensitivity analysis of the uncertainty analysis can be performed efficiently.
- Changes in the form of the physical parameter distribution can be investigated in exactly the same manner. It is no longer necessary to rely on log-normal input distributions.
- Time-dependent changes are easily incorporated as long as the change takes place at the dividing point between two time periods. The time periods can be arbitrarily chosen. Thus borehole failure, faulting, breccia pipe formation, etc. are easily accommodated.
- Conditional expectations are easily analyzed. These fall into two types. The first would be associated with time-dependent events

(e.g., "what is the expected dose given that a borehole failed within the first 200 yr") while the second conditional expectation would be concerned with whether or not the actinides reach the aquifer or the river within 3 million years. This can be investigated by putting a lower limit on the transit time for a given pipe (equivalent to moving the origin for a T distribution over by some specified amount).

- This procedure is efficient in the sense that no monte carlo simulation is used and that the less one knows about the value of T, the less work must be done, since there are fewer terms in the sums, to extract the moments.

Much additional work would be required to bring the analytic uncertainty analysis technique to the point where it is usable. The required effort must, of course, be weighed against the anticipated improvements in the efficiency of the analysis. It would appear that the necessary effort would only be justified if a very large number of uncertainty analyses were planned.

4.

CONCLUSIONS AND RECOMMENDATIONS

4.1 CONCLUSIONS

The analyses described in this report have considerably extended the previous work reported in Refs. 1 and 3. Among the principal conclusions are:

- Individuals consuming well water from aquifers contaminated by radioactivity escaping from a nuclear waste repository could receive, at a maximum, doses of many rems over 50 years; however, only a very small number of people would receive such doses.
- If radioactivity were to escape from a depository through a shaft, borehole, or other small flaw, a considerable fraction of the waste flowing through the flaw would escape into the surrounding rock if the flaw passed through a layer of substantially greater permeability than the depository layer. However the magnitude of this effect is not sufficient to significantly affect risk predictions.
- Uncertainties in risks calculated for a bedded salt repository due to uncertainties in parameter values are similar to those calculated for a shale repository.
- The hydrologic properties of bedded salt make the largest contribution to uncertainties in predictions of integrated population dose from a salt repository; further research on these properties is advisable.

4.2 RECOMMENDATIONS

A number of methods of calculation or presentation of results which may be applicable to future waste management studies are described in this report. The following recommendations are made for their use:

- Series-expansion calculation of flow near small flaws: This method of calculation should be used before the construction of flow path networks to check the validity of the assumption of pathway independence in cases where the results presented in this report are not applicable.
- Calculation of doses from well water: Such doses should be calculated in assessing sites which have potable aquifers. However, as the calculated doses are contingent on loss of knowledge of the repository's location, the results are not directly comparable to calculations of doses from release to surface waters. The likelihood and potential for future water well construction in the vicinity of a repository site should be investigated.
- Contour plots of performance: Such plots present potential hazard information in an easily assimilable form and should be prepared when appropriate.
- Use of non-parametric statistics to describe repository performance probabilities: Results of future monte carlo analyses should be presented in this form.
- Predictor equation method of uncertainty analysis: A substantial amount of additional work would be required to complete the development of this approach; this might be justified if uncertainty analysis of a very large number of individual scenarios were anticipated.

APPENDIX A

SOLUTION OF LAPLACE'S EQUATION FOR THE SHAFT

In this appendix the boundary value problems discussed in Section 2.1 will be solved. The analysis will be divided into three parts. The problem of a shaft, with no associated fracture zone, in a single layer, with only a vertical gradient far away, will be solved in Sections A.1 and A.2. Section A.3 will extend the analysis to multiple radial zones and multiple layers. Section A.4 will incorporate the presence of horizontal gradients into the basic problem, and generalize the solutions. Finally, the equation for the streamline function of Section 2.1.4 will be solved in Section A.5.

A.1 SINGLE-LAYER HYDROLOGY PROBLEMS

The simple case of a shaft in a single layer is illustrated in Fig. A.1-1. Since the problem has cylindrical symmetry, the expansion given in Eq. 2.1-23 is sufficient. The region exterior to the shaft will be designated Region II; the inside of the shaft will be designated Region I. The head in the two regions will be described by a different form in each region. The first requirement imposed on the head in the two regions is that it be finite everywhere. As $\rho \rightarrow \infty$, $I_0(k\rho) \rightarrow \infty$, $K_0(k\rho) \rightarrow 0$ and $\ln \rho \rightarrow \infty$. Therefore, the coefficients of $I_0(k\rho)$ and $\ln \rho$ must be zero in this region. Thus, in the exterior region the head must have the form:

$$\phi_2(\rho, z) = \bar{a}_2 z + b_2 + \sum_{m=1}^{\infty} \left[A_m^2 \cos \frac{mz}{z_0} + B_m^2 \sin \frac{mz}{z_0} \right] K_0\left(\frac{m\rho}{z_0}\right)$$

for $\rho \geq r_1$

(A.1-1)

Figure A.1-1 Shaft in a Single Layer

The subscripts on a and b , as well as the superscripts on A_m and B_m , refer to the region of validity.

As $\rho \rightarrow 0$, $I_0(k\rho) \rightarrow 1$, $K_0(k\rho) \rightarrow \infty$ and $\ln \rho \rightarrow \infty$. Therefore, the head inside the shaft must have the form

$$\phi_1(\rho, z) = \bar{a}_1 z + b_1 + \sum_{m=1}^{\infty} \left[C_m^1 \cos \frac{mz}{z_0} + D_m^1 \sin \frac{mz}{z_0} \right] I_0\left(\frac{mr_1}{z_0}\right)$$

for $\rho \leq r_1$ (A.1-2)

The general boundary conditions 2.1-11 and 2.1-12 must now be applied at the interface of the two regions. Equation 2.1-11 gives:

$$\bar{a}_1 z + b_1 + \sum_{m=1}^{\infty} \left[C_m^1 \cos \frac{mz}{z_0} + D_m^1 \sin \frac{mz}{z_0} \right] I_0\left(\frac{mr_1}{z_0}\right) =$$

$$\bar{a}_2 z + b_2 + \sum_{m=1}^{\infty} \left[A_m^2 \cos \frac{mz}{z_0} + B_m^2 \sin \frac{mz}{z_0} \right] K_0\left(\frac{mr_1}{z_0}\right) \quad (\text{A.1-3})$$

This is required to hold for all z , such that $0 \leq z \leq L_1$. Similarly Eq. 2.1-12 gives:

$$k_1 \left. \frac{\partial \phi_1}{\partial \rho} \right|_{\rho=r_1} = k_2 \left. \frac{\partial \phi_2}{\partial \rho} \right|_{\rho=r_1} \quad (\text{A.1-4})$$

Using the formulas:

$$\frac{dK_o(x)}{dx} = -K_1(x) \text{ and } \frac{dI_o(x)}{dx} = I_1(x) \quad (\text{A.1-5})$$

Eq. A.1-4 becomes

$$\begin{aligned} -k_2 \sum_{m=1}^{\infty} \frac{m}{z_o} \left[A_m^2 \cos \frac{mz}{z_o} + B_m^2 \sin \frac{mz}{z_o} \right] K_1\left(\frac{mr_1}{z_o}\right) = \\ k_1 \sum_{m=1}^{\infty} \frac{m}{z_o} \left[C_m^1 \cos \frac{mz}{z_o} + D_m^1 \sin \frac{mz}{z_o} \right] I_1\left(\frac{mr_1}{z_o}\right) \end{aligned} \quad (\text{A.1-6})$$

In this last equation, if the interval L over which the fourier expansion is based (by Eq. 2.1-22, $L = 2\pi z_o$) were the same as the layer thickness L_1 , then the orthogonality of the sines and cosines over the interval L could be used to justify equating the coefficients of the cosines:

$$-k_2 K_1\left(\frac{mr_1}{z_o}\right) A_m^2 = k_1 I_1\left(\frac{mr_1}{z_o}\right) C_m^1 \quad (\text{A.1-7})$$

and the sines:

$$-k_2 K_1\left(\frac{mr_1}{z_o}\right) B_m^2 = k_1 I_1\left(\frac{mr_1}{z_o}\right) D_m^1 \quad (\text{A.1-8})$$

Since the only requirement on L is that it be at least as large as L_1 , in principle they could be chosen the same. However, it will be made clear in the next paragraphs that, for a variety of reasons, expansions where L is considerably larger than L_1 are often the most desirable. It is possible to use Eqs. A.1-7 and A.1-8 when L is larger than L_1 provided that only a single layer is being analyzed. The validity of equating coefficients when L is greater than L_1 follows from the uniqueness theorem for Laplace's equation, which states that if a solution is found which satisfies all the boundary conditions of a problem, then it is the solution.

The analysis of Eq. A.1-3 presents more formidable problems, since the z dependence is not fully contained in the sines and cosines. To use the uniqueness argument, it is necessary to know what $\bar{a}_1$, $\bar{a}_2$, b_1 and b_2 are and to have a Fourier expansion over the interval L_0 which converges to $\bar{a}_i z + b_i$ ($i=1,2$) over the subinterval L_1 . In this subinterval, term-by-term coefficient matching could then be performed.

Bypassing for the moment the derivation of this expansion, the dependence of A_m^2 , B_m^2 , C_m^1 , D_m^1 on the expansion coefficients can be derived from Eqs. A.1-3, A.1-7, and A.1-8. Specifically, suppose the series

$$\begin{aligned} f_1(z) &= \frac{c_0^1}{2} + \sum_{m=1}^{\infty} \left[s_m^1 \sin \frac{mz}{z_0} + c_m^1 \cos \frac{mz}{z_0} \right] \\ f_2(z) &= \frac{c_0^2}{2} + \sum_{m=1}^{\infty} \left[s_m^2 \sin \frac{mz}{z_0} + c_m^2 \cos \frac{mz}{z_0} \right] \end{aligned} \quad (\text{A.1-9})$$

converge to $\bar{a}_1 z + b_1$ and $\bar{a}_2 z + b_2$, respectively, over the interval $[0, L_1]$ (if L is larger than L_1 , there will be many such expansions). Eq. A.1-3 is then given by

$$\frac{c_o^2}{2} + \sum_{m=1}^{\infty} \left[c_m^2 + A_m^2 K_o \left(\frac{mr_1}{z_o} \right) \right] \cos \frac{mz}{z_o} + \left[s_m^2 + B_m^2 K_o \left(\frac{mr_1}{z_o} \right) \right] \sin \frac{mz}{z_o} =$$

$$\frac{c_o^1}{2} + \sum_{m=1}^{\infty} \left[c_m^1 + C_m^1 I_o \left(\frac{mr_1}{z_o} \right) \right] \cos \frac{mz}{z_o} + \left[s_m^1 + D_m^1 I_o \left(\frac{mr_1}{z_o} \right) \right] \sin \frac{mz}{z_o}$$

(A.1-10)

Equating coefficients term by term now gives:

$$c_o^1 = c_o^2 \quad (A.1-11)$$

$$c_m^2 - c_m^1 = C_m^1 I_o \left(\frac{mr_1}{z_o} \right) - A_m^2 K_o \left(\frac{mr_1}{z_o} \right) \quad (A.1-12)$$

$$s_m^2 - s_m^1 = D_m^1 I_o \left(\frac{mr_1}{z_o} \right) - B_m^2 K_o \left(\frac{mr_1}{z_o} \right) \quad (A.1-13)$$

Equations A.1-7 and A.1-12 constitute two equations in the two unknowns A_m^2 and C_m^1 . Similarly for Eqs. A.1-8 and A.1-13.

Their solutions are

$$A_m^2 = (c_m^2 - c_m^1) / K_o \left(\frac{mr_1}{z_o} \right) (1 + 1/x_m)$$

$$C_m^1 = -(c_m^2 - c_m^1) / I_o \left(\frac{mr_1}{z_o} \right) (1 + x_m)$$

(A.1-14)

$$B_m^2 = (s_m^2 - s_m^1) / K_o \left(\frac{mr_1}{z_o} \right) (1 + 1/x_m)$$

$$D_m^1 = -(s_m^2 - s_m^1) / I_o \left(\frac{mr_1}{z_o} \right) (1 + x_m)$$

where

$$x_m = \frac{k_1}{k_2} \frac{I_1 \left(\frac{mr_1}{z_o} \right) K_o \left(\frac{mr_1}{z_o} \right)}{I_o \left(\frac{mr_1}{z_o} \right) K_1 \left(\frac{mr_1}{z_o} \right)} \quad (A.1-15)$$

Thus, the general boundary conditions generate the solution for A_m^2 , B_m^2 , C_m^1 and D_m^1 in terms of the coefficients s_m^1 , s_m^2 , c_m^1 and c_m^2 . These latter quantities are determined by the specific boundary conditions of the problem in question as will now be shown.

Up to this point, nothing has been said about incorporating boundary conditions at infinity. From Eq. A.1-1 and the fact that $K_0(x)$ is exponentially decreasing as $x \rightarrow \infty$, it can be seen that:

$$\lim_{\rho \rightarrow \infty} \phi_2(\rho, z) = \bar{a}_2 z + b_2 \quad (\text{A.1-16})$$

Thus the coefficient b_2 corresponds to the value of the head at the top of the layer ($z=0$), far from the shaft. It is usually chosen to be zero, since only derivatives of the head influence the velocity. Furthermore $\bar{a}_2$ is seen to be the vertical head gradient far from the shaft. It is presumably known. However, knowing $\bar{a}_2$ and b_2 does not fully specify the structure of the solution at infinity.

Although only a single layer is being modeled here, layers above and below the one considered do have a substantial effect on the flow. This is physically intuitive and can be seen explicitly from Figs. A.1-2a through A.1-2f. These curves all have the property that over the interval $(0, L_1)$, their functional form is $\bar{a}_2 z$. They differ drastically in their forms outside this interval, and thus in the values of their respective expansion coefficients. The form they take in these other intervals corresponds to the behavior which the head is assumed to take far from the shaft in the layers above and below the layer in question. Besides their identical behavior in the primary layer, they all share the property that they are periodic. This is intrinsically an approximation, since the head will never be strictly periodic in nature.

Figure A.1-2 Functions Whose Behavior on $(0, L_1)$ is $\bar{a}_2 z$

In Fig. A.1-2a, for example, the period of expansion is the same as the layer thickness L_1 . Physically, this would correspond to a situation where the head changed very quickly from a value of zero at the top of the primary layer ($z=0$) to a non-zero value at the bottom of the next overlying layer. A similar discontinuity occurs at the bottom of the primary layer ($z=L_1$). Such discontinuities do not occur in nature. In Fig. A.1-2b, where the period of expansion is twice the layer thickness, the discontinuity at the top of the layer has been removed but the one at the bottom remains. In Fig. A.1-2c, where the period is the same as in Fig. A.1-2b, both discontinuities are no longer present, but the derivatives have discontinuities. These discontinuities are actually required by Eq. 2.1-12, but they are of an unphysical nature: the derivatives (and thus the directions of water flow) change sign.

In Figs. A.1-2d and A.1-2e, which have periods of $4L_1$ and $8L_1$ respectively, the derivatives are continuous at $z=0$ and $z=L_1$. Thus these surfaces do not represent layer interfaces. Figure A.1-2f, however, illustrates a head function which takes into account a significant amount of geologic information. The curve consists of a series of straight line segments of differing slopes and lengths. The lengths L_1 , L_2-L_1 , L_3-L_2 and L_4-L_3 are the thicknesses of successive layers. The slopes ($\bar{a}_2$, $\bar{a}_4$, $\bar{a}_6$) of the line segments represent the head gradients in each of these layers. As illustrated here the layer between $z=L_3$ and $z=L_4$, as well as the region of negative z , have zero slope. This would correspond physically to ideal confined aquifers -- regions not allowing vertical flow. (To be complete, it would be necessary to include a horizontal gradient in the model. This will be done in the following sections.) The function is still periodic and thus still represents an approximation.

Physically, the more layers taken into account, the better the approximation. It would thus seem appropriate to choose a value of L quite large so the effects of the periodicity are reduced. However, the farther removed a layer is from the primary layer, the less impact that layer's hydrology will have on the flow in the primary layer. Moreover, the larger the value of L chosen, the more terms that must be kept in the sum (over m) to achieve reasonable accuracy. This is because the higher the order the term is in the Fourier series, the finer the structure (in the coordinate z) that term is probing.

Mathematically, if the maximum number of terms kept in the Fourier series is N , then the minimum distance (Δz) over which the series will be capable of representing an appreciable change in a function of z (e.g., the head), will be:

$$\Delta z \cong \frac{L}{N} \quad (\text{A.1-17})$$

Thus, the larger the value of L , the larger the value of N needed to maintain the same accuracy. Therefore there is a trade-off in taking a large value of L , and maintaining an acceptable degree of accuracy for a given computation time. The next section (A.2) gives a derivation of the Fourier coefficients for the function reproduced in Fig. A.1-2f. The derivation is straightforward and may be generalized to an arbitrary number of layers.

This completes the discussion of the boundary conditions far from the shaft. It is now necessary to consider the constants $\bar{a}_1$ and b_1 which characterize the linear (in z) portion of the solution inside the shaft. The constant b_1 is determined by the general boundary condition that the head be continuous

at the interface $\rho=r_1$. First, though, the value of $\bar{a}_1$ and then the Fourier expansion for the function whose form over the interval $(0, L_1)$ is $\bar{a}_1 z$, must be determined.

If no specific boundary conditions other than the head gradients at infinity are known, then these constants are undetermined. However, the addition of more boundary conditions of certain types can serve to fix $\bar{a}_1$. For instance, the knowledge of the value of the pressure at $z=0$ (or $z=L_1$) for all $\rho \geq r_1$ would serve to fix c_m^1 . Similarly, the knowledge of the vertical component of the water velocity (or flux) at $z=0$ for all $\rho \leq r_1$, would serve to fix s_m^1 . Generally such precise information is lacking in realistic problems and then approximations based on physical intuition can be useful. As an example, consider the situation where the shaft deadends at $z=0$ (i.e., the overlying layer is continuous in ρ for all ρ). The amount of water per unit area per unit time which flows out of the end of the shaft into the layer above, as a function of ρ , is given by Darcy's law as

$$-k_1 \left. \frac{\partial \phi_1}{\partial z} \right|_{z=0} \quad (\text{A.1-18})$$

Similarly, the flux of water flowing out of the region exterior to the shaft into the overlying layer, as a function of ρ , is

$$-k_2 \left. \frac{\partial \phi_2}{\partial z} \right|_{z=0} \quad (\text{A.1-19})$$

Since above the shaft the flux is assumed to be continuous at $\rho=r_1$, the two fluxes in Eqs. A.1-18 and A.1-19 should be equal for this value of ρ :

$$k_2 \frac{\partial \phi_2}{\partial z} \bigg|_{z=0, \rho=r_1} = k_1 \frac{\partial \phi_1}{\partial z} \bigg|_{z=0, \rho=r_1}$$

This is equivalent to:

$$k_2 \bar{a}_2 + \sum_{m=1}^{\infty} \frac{m}{z_0} B_m^2 K_0\left(\frac{mr_1}{z_0}\right) = k_1 \bar{a}_1 + \sum_{m=1}^{\infty} \frac{m}{z_0} D_m^1 I_0\left(\frac{mr_1}{z_0}\right) \quad (\text{A.1-20})$$

Substituting the expressions of Eq. A.1-14 for B_m^2 and D_m^1 gives

$$\sum_{m=1}^{\infty} \frac{m}{z_0} \left[(s_m^2 - s_m^1) \frac{k_2 x_m + k_1}{1+x_m} \right] = \bar{a}_1 k_1 - \bar{a}_2 k_2 \quad (\text{A.1-21})$$

s_m^2 and s_m^1 are the sine coefficients for the Fourier series which converge to $\bar{a}_2 z$ and $\bar{a}_1 z$, respectively, on the interval $[0, L_1]$. If a new set of coefficients R_m^2 , T_m^2 , R_m^1 and T_m^1 are defined by:

$$\begin{aligned} s_m^j &= a_j R_m^j \\ c_m^j &= a_j T_m^j \end{aligned} \quad \text{for } j = 1, 2 \quad (\text{A.1-22})$$

then these new expansion coefficients represent two series which converge to the same function, z , over the interval $[0, L_1]$. However, this does not imply the coefficients are equal -- this would only be true if the series converged to the same function over the entire interval $[0, L]$. It is at this point that some assumption must be made concerning the structure of the solution outside the primary layer. It is most physically realistic to assume that:

$$k_{2(i-1)+1} \bar{a}_{2(i-1)+1} = k_{2i+1} \bar{a}_{2i+1} \quad (i=1, \dots, n) \quad (\text{A.1-23})$$

This expression relates the $\bar{a}$ for a given layer inside the shaft to the $\bar{a}$ for the overlying layer inside the shaft. As explained in Section 2.1-5, this formula is equivalent to assuming that the pipe model is a reasonably good approximation to the modeled layer and all underlying layers. Using this expression, $\bar{a}_3, \bar{a}_5 \dots \bar{a}_{2n+1}$ are then seen to be proportional to $\bar{a}_1$, and using Eqs. A.2-11, A.2-12, and A.1-22 then gives the explicit formula:

$$\begin{Bmatrix} R_m^j \\ T_m^j \end{Bmatrix} = \frac{1}{L} \sum_{i=1}^n \frac{k_j}{L_1} \frac{L_i - L_{i-1}}{k_2(i-1) + j} \begin{Bmatrix} P_m(i) + U_m(i) \\ Q_m(i) + V_m(i) \end{Bmatrix} \quad (j=1,2) \quad (\text{A.1-24})$$

where $P_m(i)$, $U_m(i)$, $Q_m(i)$, and $V_m(i)$ are all defined in the next section.

Once the assumption represented by Eq. A.1-23 is made, then Eqs. A.1-21 and A.1-22 give:

$$\bar{a}_1 = \frac{\frac{k_2}{k_1} + \frac{1}{k_1} \sum_{m=1}^{\infty} \frac{m}{z_o} R_m^2 \left(\frac{k_2 x_m + k_1}{1 + x_m} \right)}{1 + \frac{1}{k_1} \sum_{m=1}^{\infty} \frac{m}{z_o} R_m^1 \left(\frac{k_2 x_m + k_1}{1 + x_m} \right)} \bar{a}_2 \quad (\text{A.1-25})$$

It is then possible to solve for b_1 by using Eqs. A.1-11 and A.1-9. This completes the solution to this example.

It should be clear from the above that the form the solution takes for a single layer is dependent on the behavior in neighboring layers. For this reason, a full analysis of a multi-layer problem is necessary. This will be undertaken in Section A.3. Satisfying the general boundary conditions will not be as easy as it was for a single layer. But there will

be a corresponding increase in the definiteness of the specific boundary conditions.

A.2 FOURIER EXPANSION OF A PIECEWISE LINEAR FUNCTION

In this section, the Fourier expansion for a continuous, piecewise linear function, periodic with some period L is derived. A single period of a typical example is plotted in Fig. A.2-1.

Figure A.2-1 Graph of Piecewise-Linear Periodic Function

Specifically, the function has the form:

$$f(z) = \begin{cases} \frac{-\bar{a}_n(z - \bar{L}_{n-1})}{\bar{L}_n - \bar{L}_{n-1}} - (\bar{a}_1 + \bar{a}_2 + \dots \bar{a}_{n-1}), & z \in [\bar{L}_n, \bar{L}_{n-1}] \\ \frac{-\bar{a}_{n-1}(z - \bar{L}_{n-2})}{\bar{L}_{n-1} - \bar{L}_{n-2}} - (\bar{a}_1 + \dots \bar{a}_{n-2}), & z \in [\bar{L}_{n-1}, \bar{L}_{n-2}] \\ \vdots \\ \frac{-\bar{a}_1 z}{\bar{L}_1} & , z \in [\bar{L}_1, 0] \\ \frac{a_1 z}{L_1} & , z \in [0, L_1] \\ \vdots \\ \frac{a_n(z - L_{n-1})}{L_n - L_{n-1}} + (a_1 + a_2 + \dots a_{n-1}), & z \in [L_{n-1}, L_n] \end{cases} \quad (A.2-1)$$

The bars over the various symbols indicate that they refer to the region $z < 0$. For the particular application of this research, the coefficients a_i and $\bar{a}_i$ are related to one another by Darcy's Law (Eq. A.1-23).

The Fourier expansion over the period $L = L_n + |\bar{L}_n|$ is:

$$f(z) = \frac{c_0}{2} + \sum_{m=1}^{\infty} \left[s_m \sin \frac{2m\pi z}{L} + c_m \cos \frac{2m\pi z}{L} \right] \quad (A.2-2)$$

where

$$s_m = \frac{2}{L} \int_{\bar{L}_n}^{L_n} f(z) \sin \frac{2m\pi z}{L} dz \quad (A.2-3)$$

$$c_m = \frac{2}{L} \int_{\bar{L}_n}^{L_n} f(z) \cos \frac{2m\pi z}{L} dz \quad (A.2-4)$$

$$c_0 = \frac{2}{L} \int_{\bar{L}_n}^{L_n} f(z) dz \quad (A.2-5)$$

Using C.2-1:

$$\begin{aligned} \begin{pmatrix} s_m \\ c_m \end{pmatrix} &= \frac{2}{L} \left[\sum_{i=1}^{\bar{n}} \int_{\bar{L}_i}^{\bar{L}_{i-1}} \left(\frac{-\bar{a}_i(z - \bar{L}_{i-1})}{\bar{L}_i - \bar{L}_{i-1}} - \sum_{k=1}^{i-1} \bar{a}_k \right) \begin{pmatrix} \sin \frac{2m\pi z}{L} \\ \cos \frac{2m\pi z}{L} \end{pmatrix} dz \right. \\ &\quad \left. + \sum_{i=1}^n \int_{L_i}^{L_{i-1}} \left(\frac{a_i(z - L_{i-1})}{L_i - L_{i-1}} + \sum_{k=1}^{i-1} a_k \right) \begin{pmatrix} \sin \frac{2m\pi z}{L} \\ \cos \frac{2m\pi z}{L} \end{pmatrix} dz \right] \end{aligned} \quad (A.2-6)$$

Now

$$\begin{aligned} \int_{L_{i-1}}^{L_i} z \sin bz \, dz &= - \frac{\partial}{\partial b} \int_{L_{i-1}}^{L_i} \cos bz \, dz = - \frac{\partial}{\partial b} \left(\frac{1}{b} \sin bz \right) \Big|_{L_{i-1}}^{L_i} \\ &= \left(\frac{1}{b^2} \sin bz - \frac{z}{b} \cos bz \right) \Big|_{L_{i-1}}^{L_i} = \frac{1}{b^2} (\sin bL_i - \sin bL_{i-1}) \\ &\quad - \frac{1}{b} (L_i \cos bL_i - L_{i-1} \cos bL_{i-1}) \end{aligned} \quad (A.2-7)$$

Similarly

$$\int_{L_{i-1}}^{L_i} z \cos bz \, dz = \frac{\cos bL_i - \cos bL_{i-1}}{b^2} + \frac{L_i \sin bL_i - L_{i-1} \sin bL_{i-1}}{b} \quad (\text{A.2-8})$$

Defining

$$P_m(i) = \frac{1}{L_i - L_{i-1}} \int_{L_{i-1}}^{L_i} (z - L_{i-1}) \sin \frac{2m\pi z}{L} \, dz$$

$$Q_m(i) = \frac{1}{L_i - L_{i-1}} \int_{L_{i-1}}^{L_i} (z - L_{i-1}) \cos \frac{2m\pi z}{L} \, dz$$

$$U_m(i) = - \int_{L_n}^{L_i} \sin \frac{2m\pi z}{L} \, dz, \quad \bar{U}_m(i) = - \int_{\bar{L}_n}^{\bar{L}_i} \sin \frac{2m\pi z}{L} \, dz$$

$$V_m(i) = - \int_{L_n}^{L_i} \cos \frac{2m\pi z}{L} \, dz, \quad \bar{V}_m(i) = - \int_{\bar{L}_n}^{\bar{L}_i} \cos \frac{2m\pi z}{L} \, dz \quad (\text{A.2-9})$$

then using Eqs. A.2-7 and A.2-8 gives:

$$\begin{aligned} P_m(i) &= \frac{1}{L_i - L_{i-1}} \left(\frac{L}{2m\pi} \right)^2 \left[\sin \frac{2m\pi L_i}{L} - \sin \frac{2m\pi L_{i-1}}{L} \right. \\ &\quad \left. - \frac{2m\pi}{L} (L_i - L_{i-1}) \cos \frac{2m\pi L_i}{L} \right] \\ Q_m(i) &= \frac{1}{L_i - L_{i-1}} \left(\frac{L}{2m\pi} \right)^2 \left[\cos \left(\frac{2m\pi L_i}{L} \right) - \cos \left(\frac{2m\pi L_{i-1}}{L} \right) \right. \\ &\quad \left. + \frac{2m\pi}{L} (L_i - L_{i-1}) \sin \frac{2m\pi L_i}{L} \right] \end{aligned}$$

$$\begin{aligned}
 U_m(i) &= \left(\frac{L}{2m\pi} \right) \left[\cos \left(\frac{2m\pi L_i}{L} \right) - \cos \left(\frac{2m\pi L_n}{L} \right) \right] \\
 V_m(i) &= - \left(\frac{L}{2m\pi} \right) \left[\sin \left(\frac{2m\pi L_i}{L} \right) - \sin \left(\frac{2m\pi L_n}{L} \right) \right]
 \end{aligned}
 \tag{A.2-10}$$

Using Eqs. A.2-9 in Eq. A.2-6 then gives:

$$\begin{aligned}
 \begin{Bmatrix} s_m \\ c_m \end{Bmatrix} &= \frac{2}{L} \left[\sum_{i=1}^{\bar{n}} (-\bar{a}_i) \begin{Bmatrix} P_m(i) + U_m(i) \\ Q_m(i) + V_m(i) \end{Bmatrix} \right. \\
 &\quad \left. + \sum_{i=1}^n a_i \begin{Bmatrix} P_m(i) + U_m(i) \\ Q_m(i) + V_m(i) \end{Bmatrix} \right]
 \end{aligned}
 \tag{A.2-11}$$

Finally:

$$\begin{aligned}
 c_o &= \frac{2}{L} \int_{L_n}^{L_n} f(z) dz = \frac{2}{L} \left[\sum_{i=1}^{\bar{n}} \bar{a}_i \frac{(L_i - L_{i-1})}{2} + (L_n - L_i) \right. \\
 &\quad \left. + \sum_{i=1}^n a_i \frac{(L_i - L_{i-1})}{2} + (L_n - L_i) \right]
 \end{aligned}
 \tag{A.2-12}$$

This completes the derivation of the Fourier transform of $f(z)$.

A.3 MULTI-LAYER, MULTI-RADIAL ZONE HYDROLOGY

In this section, two generalizations in the boundary structure will be incorporated. The first will be a generalization to more than one layer. Each layer will have its own thickness and permeability associated with the undisturbed portion. The second generalization will be to include radial zones concentric with the shaft. Physically these would cor-

respond to fracture zones (of varying radial thicknesses) or a circular depository of some height. The head functions will be superscripted by the numeral $j_{\max}(i-1)+j$ where i indexes the layers (with $i=1$ the top layer) and j indexes the radial zones (with $j=1$ the shaft). In this section, $i_{\max}$ will be set to 5 and $j_{\max}$ to 3, although the derivation will be entirely general and readily extendable to more layers and radial zones. Figure A.3-1 illustrates the zones and superscript notation. The form for the head inside the shaft ($j=1$) will still only contain $I_0(x)$ since $K_0(x)$ is not finite at the origin:

$$\phi^{3i-2}(\rho, z) = f_1(z) + \sum_{m=1}^{\infty} \left[C_m^{3i-2} \cos \frac{mz}{z_0} + D_m^{3i-2} \sin \frac{mz}{z_0} \right] I_0\left(\frac{m\rho}{z_0}\right) \quad (\text{A.3-1})$$

Here $f_1(z)$ is of the general form illustrated in Fig. C.1-2f. Specifically:

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	j=1	j=2	j=3	
	ϕ_1	ϕ_2	ϕ_3	i = 1
	ϕ_4	ϕ_5	ϕ_6	i = 2
	ϕ_7	ϕ_8	ϕ_9	i = 3
	ϕ_{10}	ϕ_{11}	ϕ_{12}	i = 4

Figure A.3-1 Indexing System Used to Label Shaft, Fracture Zone, and Surrounding Rock Regions

$$f_j(z) = \frac{a_{3(i-1)+j} (z-L_{i-1})}{L_i-L_{i-1}} + \sum_{\ell=1}^{i-1} a_{3(\ell-1)+j} + b_j$$

$$\text{when } z \in [L_{i-1}, L_i] \quad (\text{A.3-2})$$

The a 's used here differ from the a 's of Section A.1 in that they have the layer thickness factored out. The unbarred a 's thus have the same units as the head (length).

Outside the shaft and fracture zones the form of the head is:

$$\phi^{3i}(\rho, z) = f_3(z) + \sum_{m=1}^{\infty} \left[A_m^{3i} \cos \frac{mz}{z_0} + B_m^{3i} \sin \frac{mz}{z_0} \right] K_0\left(\frac{m\rho}{z_0}\right) \quad (\text{A.3-3})$$

As before, $f_3(z)$ is the head structure far from the shaft. The constants appearing in its definition are all presumably known.

Inside the fracture zone or depository, both I_0 's and K_0 's are allowed:

$$\begin{aligned} \phi^{3i-1}(\rho, z) = f_2(z) + \sum_{m=1}^{\infty} \left\{ \left[A_m^{3i-1} \cos \frac{mz}{z_0} + B_m^{3i-1} \sin \frac{mz}{z_0} \right] K_0\left(\frac{m\rho}{z_0}\right) \right. \\ \left. + \left[C_m^{3i-1} \cos \frac{mz}{z_0} + D_m^{3i-1} \sin \frac{mz}{z_0} \right] I_0\left(\frac{m\rho}{z_0}\right) \right\} \quad (\text{A.3-4}) \end{aligned}$$

In principle a $\log \rho$ term would also be allowed in the intermediate radial zones, but it is straightforward to show that its coefficient is necessarily zero if this type of term is

excluded in the inner and outer regions, as it is by the finiteness requirement at $\rho=0$ and $\rho \rightarrow \infty$.

There are ten general boundary conditions for each layer:

$$a) \quad \phi_{3i} \Big|_{\rho=r_2} = \phi_{3i-1} \Big|_{\rho=r_2}$$

$$b) \quad k_{3i} \frac{\partial \phi_{3i}}{\partial \rho} \Big|_{\rho=r_2} = k_{3i-1} \frac{\partial \phi_{3i-1}}{\partial \rho} \Big|_{\rho=r_2}$$

$$c) \quad \phi_{3i-1} \Big|_{\rho=r_1} = \phi_{3i-2} \Big|_{\rho=r_1}$$

$$d) \quad k_{3i-1} \frac{\partial \phi_{3i-1}}{\partial \rho} \Big|_{\rho=r_1} = k_{3i-2} \frac{\partial \phi_{3i-2}}{\partial \rho} \Big|_{\rho=r_1}$$

$$e) \quad \phi_{3i+3} \Big|_{z=L_i} = \phi_{3i} \Big|_{z=L_i}$$

$$f) \quad k_{3i+3} \frac{\partial \phi_{3i+3}}{\partial z} \Big|_{z=L_i} = k_{3i} \frac{\partial \phi_{3i}}{\partial z} \Big|_{z=L_i}$$

$$g) \quad \phi_{3i+2} \Big|_{z=L_i} = \phi_{3i-1} \Big|_{z=L_i}$$

$$h) \quad k_{3i+2} \frac{\partial \phi_{3i+2}}{\partial z} \Big|_{z=L_i} = k_{3i-1} \frac{\partial \phi_{3i-1}}{\partial z} \Big|_{z=L_i}$$

$$i) \quad \phi_{3i+1} \Big|_{z=L_1} = \phi_{3i-2} \Big|_{z=L_2}$$

$$j) \quad k_{3i+1} \frac{\partial \phi_{3i+1}}{\partial z} \Big|_{z=L_i} = k_{3i-2} \frac{\partial \phi_{3i-2}}{\partial z} \Big|_{z=L_i} \quad (A.3-5)$$

Boundary conditions (hereafter abbreviated B.C.) A.3-5a and A.3-5b refer to the fracture zone - rock layer interfaces; B.C.'s A.3-5c and A.3-5d refer to the shaft - fracture zone interfaces; B.C.'s A.3-5e and A.3-5f refer to the layer interfaces exterior to the shaft and fracture zone; B.C.'s A.3-5g and A.3-5h refer to the layer interfaces in the fracture zone; B.C.'s A.3-5i and A.3-5j refer to the layer interfaces inside the shaft. Full generality is allowed in that each region has its own permeability. In any case likely to be studied, some of the regions (such as the shaft in each layer) will have the same permeability.

It will not turn out to be possible to satisfy all these boundary conditions simultaneously by matching coefficients term-by-term as was done in the single layer case. There are fundamental reasons why problems which have overlapping boundaries, such as constant ρ and constant z boundaries, cannot be solved this way. However, it is possible to match coefficients for either the constant ρ boundaries or the constant z boundaries. For various reasons, it will turn out to be necessary to match the coefficients for the latter type of boundary. The full sums must then be matched for the constant ρ boundaries. After careful analysis, it will then be possible to obtain the various coefficients to arbitrary accuracy.

Thus B.C.'s A.3-5e, A.3-5g and A.3-5i yield:

$$e) \Rightarrow f_3(z=L_i) - f_3(z=L_i) = 0 = \sum_{m=1}^{\infty} \left[(A_m^{3i+3} - A_m^{3i}) \cos \frac{mL_i}{z_0} + (B_m^{3i+3} - B_m^{3i}) \sin \frac{mL_i}{z_0} \right] K_0\left(\frac{m\rho}{z_0}\right) \quad \text{for } \rho \geq r_2$$

$$\Rightarrow A_m^{3i+3} \cos \frac{mL_i}{z_0} + B_m^{3i+3} \sin \frac{mL_i}{z_0} = A_m^{3i} \cos \frac{mL_i}{z_0} + B_m^{3i} \sin \frac{mL_i}{z_0} \quad (C.3-6)$$

$$g) \Rightarrow A_m^{3i+2} \cos \frac{mL_i}{z_0} + B_m^{3i+2} \sin \frac{mL_i}{z_0} = A_m^{3i-1} \cos \frac{mL_i}{z_0} + B_m^{3i-1} \sin \frac{mL_i}{z_0}$$

$$\begin{aligned} & C_m^{3i+2} \cos \frac{mL_i}{z_0} + D_m^{3i+2} \sin \frac{mL_i}{z_0} \\ & = C_m^{3i-1} \cos \frac{mL_i}{z_0} + D_m^{3i-1} \sin \frac{mL_i}{z_0} \end{aligned} \quad (A.3-7)$$

$$\begin{aligned} i) \Rightarrow & C_m^{3i+1} \cos \frac{mL_i}{z_0} + D_m^{3i+1} \sin \frac{mL_i}{z_0} = C_m^{3i-2} \cos \frac{mL_i}{z_0} \\ & + D_m^{3i-2} \sin \frac{mL_i}{z_0} \end{aligned} \quad (A.3-8)$$

Similarly B.C.'s A.3-5f, h, and j give: ($i=1, \dots, 4$; j as specified)

$$\frac{k_{3(i-1)+j} a_{3(i-1)+j}}{L_i - L_{i-1}} = \frac{k_{3i+j} a_{3i+j}}{L_{i+1} - L_i} \quad j=1,2,3 \quad (A.3-9)$$

$$k_{3(i-1)+j} (A_m^{3(i-1)+j} \sin \frac{mL_i}{z_0} - B_m^{3(i-1)+j} \cos \frac{mL_i}{z_0}) =$$

$$k_{3i+j} (A_m^{3i+j} \sin \frac{mL_i}{z_0} - B_m^{3i+j} \cos \frac{mL_i}{z_0}) \quad (j=2,3) \quad (A.3-10)$$

$$k_{3(i-1)+j} (C_m^{3(i-1)+j} \sin \frac{mL_i}{z_o} - D_m^{3(i-1)+j} \cos \frac{mL_i}{z_o}) =$$

$$k_{3i+j} (C_m^{3i+j} \sin \frac{mL_i}{z_o} - D_m^{3i+j} \cos \frac{mL_i}{z_o}) \quad (j=1,2) \quad (A.3-11)$$

Equations A.3-10, A.3-6 and A.3-7 can be used to solve for A_m^{3i+j} and B_m^{3i+j} in terms of $A_m^{3(i-1)+j}$ and $B_m^{3(i-1)+j}$ (i.e., the coefficients in one layer in terms of the coefficient of the overlying layer):

$$A_m^{3i+j} = \bar{f}_m^{3i+j} A_m^{3(i-1)+j} + e_m^{3i+j} B_m^{3(i-1)+j} \quad (A.3-12)$$

$$B_m^{3i+j} = e_m^{3i+j} A_m^{3(i-1)+j} + \bar{f}_m^{3i+j} B_m^{3(i-1)+j} \quad (A.3-13)$$

where

$$e^{3i+j} = \frac{1}{k_{3i+j}} (k_{3i+j} - k_{3(i-1)+j}) \sin \frac{mL_i}{z_o} \cos \frac{mL_i}{z_o} \quad (A.3-14)$$

$$f^{3i+j} = \frac{1}{k_{3i+j}} \left[k_{3i+j} \sin^2 \frac{mL_i}{z_o} + k_{3(i-1)+j} \cos^2 \frac{mL_i}{z_o} \right] \quad (A.3-15)$$

$$\bar{f}^{3i+j} = \frac{1}{k_{3i+j}} \left[k_{3i+j} \cos^2 \frac{mL_i}{z_o} + k_{3(i-1)+j} \sin^2 \frac{mL_i}{z_o} \right] \quad (A.3-16)$$

Similarly:

$$C_m^{3i+j} = \bar{f}_m^{3i+j} C_m^{3(i-1)+j} + e_m^{3i+j} D_m^{3(i-1)+j} \quad (A.3-17)$$

$$D_m^{3i+j} = e_m^{3i+j} C_m^{3(i-1)+j} + \bar{f}_m^{3i+j} D_m^{3(i-1)+j}$$

Since each layer's coefficients are linearly related to the overlying layer's, they can all be linearly related to the uppermost layer. The coefficients g_m^{3i+j} , h_m^{3i+j} , $\bar{g}_m^{3i+j}$ and $\bar{h}_m^{3i+j}$ may be defined by the following equations:

$$\begin{pmatrix} A_m^{3i+j} \\ C_m^{3i+j} \end{pmatrix} = \bar{g}_m^{3i+j} \begin{pmatrix} A_m^j \\ C_m^j \end{pmatrix} + \bar{h}_m^{3i+j} \begin{pmatrix} B_m^j \\ D_m^j \end{pmatrix} \quad (\text{A.3-18})$$

$$\begin{pmatrix} B_m^{3i+j} \\ D_m^{3i+j} \end{pmatrix} = h_m^{3i+j} \begin{pmatrix} A_m^j \\ C_m^j \end{pmatrix} + g_m^{3i+j} \begin{pmatrix} B_m^j \\ D_m^j \end{pmatrix}$$

Then a set of recursion relations can be generated from Eq. A.3-17 for g_m^{3i+j} , h_m^{3i+j} , $\bar{g}_m^{3i+j}$, and $\bar{h}_m^{3i+j}$.

$$\begin{aligned} \bar{g}_m^{3i+j} &= \bar{f}_m^{3i+j} \bar{g}_m^{3(i-1)+j} + e_m^{3i+j} h_m^{3(i-1)+j} \\ \bar{h}_m^{3i+j} &= \bar{f}_m^{3i+j} \bar{h}_m^{3(i-1)+j} + e_m^{3i+j} g_m^{3(i-1)+j} \\ h_m^{3i+j} &= e_m^{3i+j} \bar{g}_m^{3(i-1)+j} + f_m^{3i+j} h_m^{3(i-1)+j} \\ g_m^{3i+j} &= e_m^{3i+j} \bar{h}_m^{3(i-1)+j} + f_m^{3i+j} g_m^{3(i-1)+j} \end{aligned} \quad (\text{A.3-19})$$

Although the solutions can be written out, they become quite complicated for more than three layers. They are, however, easily calculated by computer.

The boundary conditions for the constant z surfaces thus relate the lower layer coefficients to those of the uppermost layer. The radial boundary conditions must now be

used to solve for these unknowns in terms of the specific boundary conditions.

B.C. A.3-5a gives:

$$\begin{aligned} f_3(z) + \sum_{m=1}^{\infty} \left[A_m^{3i} \cos \frac{mz}{z_0} + B_m^{3i} \sin \frac{mz}{z_0} \right] K_0 \left(\frac{mr_2}{z_0} \right) = \\ f_2(z) + \sum_{m=1}^{\infty} \left\{ \left[A_m^{3i-1} \cos \frac{mz}{z_0} + B_m^{3i-1} \sin \frac{mz}{z_0} \right] K_0 \left(\frac{mr_2}{z_0} \right) \right. \\ \left. + \left[C_m^{3i-1} \cos \frac{mz}{z_0} + D_m^{3i-1} \sin \frac{mz}{z_0} \right] I_0 \left(\frac{mr_2}{z_0} \right) \right\} \end{aligned} \quad (A.3-20)$$

Similarly B.C. A.3-5b gives:

$$\begin{aligned} k_{3i} \sum_{m=1}^{\infty} \left[A_m^{3i} \cos \frac{mz}{z_0} + B_m^{3i} \sin \frac{mz}{z_0} \right] K_1 \left(\frac{mr_2}{z_0} \right) = \\ k_{3i-1} \sum_{m=1}^{\infty} \left\{ \left[A_m^{3i-1} \cos \frac{mz}{z_0} + B_m^{3i-1} \sin \frac{mz}{z_0} \right] K_1 \left(\frac{mr_2}{z_0} \right) \right. \\ \left. - \left[C_m^{3i-1} \cos \frac{mz}{z_0} + D_m^{3i-1} \sin \frac{mz}{z_0} \right] I_1 \left(\frac{mr_2}{z_0} \right) \right\} \end{aligned} \quad (A.3-21)$$

Analogous expressions can be written down corresponding to B.C.'s A.3-5c and A.3-5d and the resulting expressions solved for the first layer coefficients by the same steps used in the solution of the single layer problem (the answer will be more complicated since there are now three radial regions instead of just two). If, then, the lower layer's coefficients in the various radial zones are solved in terms of the first layer's coefficient by Eq. A.3-18, the resulting coefficients will not satisfy A.3-20 or A.3-21 for layers other than the first. Thus these equations cannot be solved by equating the coefficients within the individual layers. How then are they

to be satisfied? The z dependence must be eliminated and this is done by multiplying both sides of Eqs. A.3-20 and A.3-21 (as well as the corresponding equations for B.C.'s A.3-5c and A.3-5d) by $\sin \frac{m'z}{z_0}$ and $\cos \frac{m'z}{z_0}$ and integrating over the full period. This gives eight equations for each value of m' :

$$\begin{aligned} a) \quad s_{m'}^3 - s_{m'}^2 = & - \sum_{m=1}^{\infty} \sum_{i=1}^5 \left[((A_m^{3i} - A_m^{3i-1})K_0(\frac{mr_2}{z_0}) - C_m^{3i-1}I_0(\frac{mr_2}{z_0})) \right. \\ & \times (SC_{m'm}(i) - SC_{m'm}(i-1)) + ((B_m^{3i} - B_m^{3i-1})K_0(\frac{mr_2}{z_0}) - D_m^{3i-1}I_0(\frac{mr_2}{z_0})) \\ & \left. \times (SS_{mm}(i) - SS_{mm}(i-1)) \right] \end{aligned}$$

a') $c_{m'}^3 - c_{m'}^2$ = as above but with the replacements: $SC_{mm} \rightarrow CC_{mm}$,
and $SS_{mm} \rightarrow SC_{mm}$.

$$\begin{aligned} b) \quad s_{m'}^2 - s_{m'}^1 = & - \sum_{m=1}^{\infty} \sum_{i=1}^5 \left[(B_m^{3i-1}K_0(\frac{mr_1}{z_0}) + (D_m^{3i-1} - D_m^{3i-2}) \right. \\ & \times I_0(\frac{mr_1}{z_0})) (SS_{mm}(i) - SS_{mm}(i-1)) + (A_m^{3i-1}K_0(\frac{mr_1}{z_0}) + (C_m^{3i-1} - C_m^{3i-2}) \\ & \left. \times I_0(\frac{mr_1}{z_0})) (SC_{m'm}(i) - SC_{m'm}(i-1)) \right] \end{aligned}$$

b') $c_{m'}^2 - c_{m'}^1$, as in b) but with same replacements as in a')

$$c) \quad 0 = \sum_{m=1}^{\infty} \sum_{i=1}^5 \left[m ((k_{3i}B_m^{3i} - k_{3i-1}B_m^{3i-1})K_1(\frac{mr_2}{z_0}) + k_{3i-1}D_m^{3i-1} \right.$$

$$\begin{aligned} & \times I_1\left(\frac{mr_2}{z_0}\right) (SS_{mm}(i) - SS_{mm}(i-1)) + ((k_{3i}A_m^{3i} - k_{3i-1}A_m^{3i-1})K_1\left(\frac{mr_2}{z_0}\right) \\ & + k_{3i-1}C_m^{3i-1}I_1\left(\frac{mr_2}{z_0}\right) (SC_{m,m}(i) - SC_{m,m}(i-1))) \end{aligned}$$

c') as in c) but with the same replacements as in a').

$$\begin{aligned} d) \quad 0 = & \sum_{m=1}^{\infty} \sum_{i=1}^5 m \left[(k_{3i-1}B_m^{3i-1}K_1\left(\frac{mr_1}{z_0}\right) - (k_{3i-1}D_m^{3i-1} - k_{3i-2}D_m^{3i-2}) \right. \\ & \times I_1\left(\frac{mr_1}{z_0}\right) (SS_{mm}(i) - SS_{mm}(i-1)) + (k_{3i}A_m^{3i-1}K_1\left(\frac{mr_1}{z_0}\right) \\ & \left. - (k_{3i-1}C_m^{3i-1} - k_{3i-2}C_m^{3i-2})I_1\left(\frac{mr_1}{z_0}\right) (SC_{m,m}(i) - SC_{m,m}(i-1))) \right] \end{aligned}$$

d') as in d) but with the same replacements as in a')

Here

$$s_{m'}^j = \frac{1}{L_5} \int_{-L_5}^{L_5} f_j(z) \sin \frac{m'z}{z_0} dz \quad (A.3-22)$$

$$c_{m'}^j = \frac{1}{L_5} \int_{-L_5}^{L_5} f_j(z) \cos \frac{m'z}{z_0} dz \quad (A.3-23)$$

(explicitly given in Section A.2) and

$$SS_{mm}(i) - SS_{mm}(i-1) = \int_{L_{i-1}}^{L_i} \sin \frac{mz}{z_0} \sin \frac{m'z}{z_0} dz$$

$$SC_{mm'}(i) - SC_{mm'}(i-1) = \int_{L_{i-1}}^{L_i} \sin \frac{mz}{z_0} \cos \frac{m'z}{z_0} dz$$

$$CC_{mm'}(i) - CC_{mm'}(i-1) = \int_{L_{i-1}}^{L_i} \cos \frac{mz}{z_0} \cos \frac{m'z}{z_0} dz$$

(A.3-24)

The sum over i in the above equations comes from integrating the different forms of Eq. A.3-20 and A.3-21 (etc.) over the full period.

Using Eq. A.3-18 and defining:

$$SO_{mm'}^{3(i-1)+j} = \bar{g}_m^{3(i-1)+j} (SC_{m'm}(i) - SC_{m'm}(i-1)) + h_m^{3(i-1)+j} \\ \times (SS_{mm'}(i) - SS_{mm'}(i-1))$$

$$SN_{mm'}^{3(i-1)+j} = \bar{h}_m^{3(i-1)+j} (SC_{m'm}(i) - SC_{m'm}(i-1)) + g_m^{3(i-1)+j} \\ \times (SS_{mm'}(i) - SS_{mm'}(i-1))$$

$$CO_{mm'}^{3(i-1)+j} = \bar{g}_m^{3(i-1)+j} (CC_{m'm}(i) - CC_{m'm}(i-1)) + h_m^{3(i-1)+j} \\ \times (SC_{mm'}(i) - SC_{mm'}(i-1))$$

$$CN_{mm'}^{3(i-1)+j} = \bar{h}_m^{3(i-1)+j} (CC_{m'm}(i) - CC_{m'm}(i-1)) + g_m^{3(i-1)+j} \\ \times (SC_{mm'}(i) - SC_{mm'}(i-1))$$

(A.3-25)

(Note the interchange in the order of m and m' between SO and CO and between SN and CN). Then the Eqs. A.3-22 a-d' can be written as:

$$\begin{aligned}
 \text{a) } s_m^3 - s_m^2 &= \frac{-1}{L_5} \sum_{m=1}^{\infty} \sum_{i=1}^5 \left[(SO_{mm}^{3i}, A_m^3 - SO_{mm}^{3i-1}, A_m^2) K_0 \left(\frac{mr_2}{z_0} \right) + \right. \\
 &\quad \left. (SN_{mm}^{3i}, B_m^3 - SN_{mm}^{3i-1}, B_m^2) K_0 \left(\frac{mr_2}{z_0} \right) - (SO_{mm}^{3i-1}, C_m^2 + SN_{mm}^{3i-1}, D_m^2) I_0 \left(\frac{mr_2}{z_0} \right) \right] \\
 \text{b) } s_m^2 - s_m^1 &= \frac{-1}{L_5} \sum_{m=1}^{\infty} \sum_{i=1}^5 \left[(SO_{mm}^{3i-1}, A_m^2 + SN_{mm}^{3i-1}, B_m^2) K_0 \left(\frac{mr_1}{z_0} \right) + \right. \\
 &\quad \left. (SO_{mm}^{3i-1}, C_m^2 - SO_{mm}^{3i-2}, C_m^1) I_0 \left(\frac{mr_1}{z_0} \right) + (SN_{mm}^{3i-1}, D_m^2 - SN_{mm}^{3i-2}, D_m^1) I_0 \left(\frac{mr_1}{z_0} \right) \right] \\
 \text{c) } 0 &= \sum_{m=1}^{\infty} \sum_{i=1}^5 \left[m (k_{3i} SO_{mm}^{3i}, A_m^3 - k_{3i-1} SO_{mm}^{3i-1}, A_m^2) K_1 \left(\frac{mr_2}{z_0} \right) + \right. \\
 &\quad \left. (k_{3i} SN_{mm}^{3i}, B_m^3 - k_{3i-1} SN_{mm}^{3i-1}, B_m^2) K_1 \left(\frac{mr_2}{z_0} \right) + (k_{3i-1} SO_{mm}^{3i-1}, C_m^2 + \right. \\
 &\quad \left. k_{3i-1} SN_{mm}^{3i-1}, D_m^2) I_1 \left(\frac{mr_2}{z_0} \right) \right] \\
 \text{d) } 0 &= \sum_{m=1}^{\infty} \sum_{i=1}^5 \left[m - (k_{3i-1} SO_{mm}^{3i-1}, A_m^2 + k_{3i-1} SN_{mm}^{3i-1}, B_m^2) K_1 \left(\frac{mr_1}{z_0} \right) + \right. \\
 &\quad \left. (k_{3i-1} SO_{mm}^{3i-1}, C_m^2 - k_{3i-2} SO_{mm}^{3i-2}, C_m^1) I_1 \left(\frac{mr_1}{z_0} \right) + (k_{3i-1} SN_{mm}^{3i-1}, D_m^2 \right.
 \end{aligned}$$

$$- k_{3i-2} S_{mm'}^{3i-2} D_m^1 I_1 \left(\frac{mr_1}{z_0} \right)] \quad (A.3-26)$$

a'), b'), c'), and d') are similar to a), b), c), and d) but but with replacements $SO_{mm'} \rightarrow CO_{mm'}$, $SN_{mm'} \rightarrow CN_{mm'}$, and $s_m^j \rightarrow c_m^j$.

These equations are the desired equations for the coefficients in the top layer. However they involve, as previously mentioned, an infinite sum over these coefficients. There are a corresponding infinite number of equations - eight for each value of m' . Since the head functions, which are the ultimate goal of this research, are infinite sums, to produce equipotential and streamline plots it is necessary to truncate the sums in Eqs. A.3-1, A.3-2, and A.3-3 at some value N . To the same degree of accuracy, the sums in Eqs. A.3-25 may be truncated. The resulting equations constitute a finite set of linear equations for $A_m^3, B_m^3, A_m^2, B_m^2, C_m^2, D_m^2, C_m^1$, and D_m^1 for $m=1, \dots, N$. This set of equations can be formulated as a matrix equation, the matrix inverted and the coefficients obtained. Before this can be done, though, the various constants $a_{3(i-1)+j}$ for $j=1,2; i=1, \dots, 5$ must be solved for in terms of the first layer's coefficients.

Equation A.3-9 relates the a in a given region to the a for the same radial zone but one higher layer. Thus only a_1 and a_2 need be expressed in terms of A_m^j, B_m^j, C_m^j , and D_m^j . To determine this dependence it is necessary to specify additional boundary conditions. Since there are only 2 constants, there need be only two conditions. Furthermore, they must involve the derivative of ϕ at $z=0$ for some specified values of ρ , since the value of ϕ itself at $z=0$ does not involve a_1 or a_2 (they occur in ϕ multiplied by z). Without any further know-

ledge it is not possible to specify the necessary conditions. If, however, it is assumed that the shaft and fracture zones are not present above $z=0$, then continuity conditions may be imposed just as in the single layer problem previously discussed. Specifically, the z components of fluid flux must be continuous for all values of ρ along the surface $z=0$. Thus:

$$k_2 \left. \frac{\partial \phi_2}{\partial z} \right|_{\substack{z=0 \\ \rho=r_2}} = k_3 \left. \frac{\partial \phi_3}{\partial z} \right|_{\substack{z=0 \\ \rho=r_2}} \quad (\text{A.3-27})$$

$$k_2 \left. \frac{\partial \phi_2}{\partial z} \right|_{\substack{z=0 \\ \rho=r_1}} = k_1 \left. \frac{\partial \phi_1}{\partial z} \right|_{\substack{z=0 \\ \rho=r_1}} \quad (\text{A.3-28})$$

Using Eqs. A.3-1 through A.3-3 then gives:

$$k_2 \left[\frac{a_2}{L_1} + \sum_{m=1}^{\infty} \frac{m}{z_o} \left(B_m^2 K_o \left(\frac{mr_2}{z_o} \right) + D_m^2 I_o \left(\frac{mr_2}{z_o} \right) \right) \right] = k_3 \left[\frac{a_3}{L_1} + \sum_{m=1}^{\infty} \frac{m}{z_o} B_m^3 K_o \left(\frac{mr_2}{z_o} \right) \right] \quad (\text{A.3-29})$$

$$k_1 \left[\frac{a_1}{L_1} + \sum_{m=1}^{\infty} \frac{m}{z_o} D_m^1 I_o \left(\frac{mr_1}{z_o} \right) \right] = k_2 \left[\frac{a_2}{L_1} + \sum_{m=1}^{\infty} \frac{m}{z_o} \left(B_m^2 K_o \frac{mr_1}{z_o} + D_m^2 I_o \frac{mr_1}{z_o} \right) \right] \quad (\text{A.3-30})$$

The first of these equations may be solved for a_2 in terms of a_3 and the unknowns B_m^2 , B_m^3 , and D_m^2 . Then the second of these equations may be solved for a_1 in terms of a_3 and B_m^3 , B_m^2 , D_m^2 , and D_m^1 .

From Eq. A.2-11 (with $\bar{a}_i = 0$),

$$\begin{pmatrix} s_m^j \\ c_m^j \end{pmatrix} = \frac{1}{L_5} \sum_{i=1}^5 a_{3(i-1)+j} \begin{pmatrix} P_m(i) + U_m(i) \\ Q_m(i) + V_m(i) \end{pmatrix} \quad (\text{A.3-31})$$

together with Eq. A.3-9 gives:

$$\begin{pmatrix} s_m^j \\ c_m^j \end{pmatrix} = \frac{1}{L_5} \sum_{i=1}^5 \frac{k_j}{L_1} \frac{L_i - L_{i-1}}{k_{3(i-1)+j}} \begin{pmatrix} P_m(i) + U_m(i) \\ Q_m(i) + V_m(i) \end{pmatrix} a_j = \begin{pmatrix} R_m^j \\ T_m^j \end{pmatrix} a_j \quad (\text{A.3-32})$$

On the left hand side of Eqs. A.3-26a and A.3-26b the differences $s_m^3 - s_m^2$, and $s_m^2 - s_m^1$, occur. Using Eqs. A.3-32, A.3-29 and A.3-30, these differences may be written as the sum of a term proportional to a_3 plus terms proportional to sums over the unknowns B_m^2 , B_m^3 , D_m^2 , and D_m^1 . The latter terms may be moved to the right hand side of Eqs. A.3-26. These equations may then be written in matrix form:

$$V_k = \sum_{\ell=1}^{8N} M_{k\ell} x_\ell \quad (\text{A.3-33})$$

where

$$\begin{aligned} x_{1+8(m-1)} &= A_m^3 & V_{1+8(m-1)} &= (R_m^3 - \frac{k_3}{k_2} R_m^2) a_3 \\ x_{2+8(m-1)} &= A_m^2 & V_{2+8(m-1)} &= (T_m^3 - \frac{k_3}{k_2} T_m^2) a_3 \\ x_{3+8(m-1)} &= B_m^3 & V_{3+8(m-1)} &= (R_m^2 \frac{k_3}{k_2} - R_m^1 \frac{k_3}{k_1}) a_3 \\ x_{4+8(m-1)} &= B_m^2 & V_{4+8(m-1)} &= (T_m^2 \frac{k_3}{k_2} - T_m^1 \frac{k_3}{k_1}) a_3 \end{aligned}$$

$$x_{5+8(m-1)} = C_m^2 \quad v_{5+8(m-1)} = 0$$

$$x_{6+8(m-1)} = C_m^1 \quad v_{6+8(m-1)} = 0$$

$$x_{7+8(m-1)} = D_m^2 \quad v_{7+8(m-1)} = 0$$

$$x_{8+8(m-1)} = D_m^1 \quad v_{8+8(m-1)} = 0$$

and N is the numbers of terms in the m summation which are retained. The matrix elements (64 for each value of m and m') are tedious but straightforward to write out; therefore only one example will be given. $M_{1+8(m'-1), 3+8(m-1)}$ is given, from Eqs. A.3-32, A.3-29, and A.3-26a, by:

$$\left[-\frac{1}{L_5} \sum_{i=1}^5 SN_{mm'}^{3i} + R_m^2 \frac{m}{z_0} \frac{k_3}{k_2} K_0\left(\frac{mr_2}{z_0}\right) \right] \quad (\text{A.3-34})$$

The variables x_ℓ in Eq. A.3-33 can then be solved for by matrix inversion or least-squares methods. b_1 and b_2 may be computed from the identity:

$$b_j = f_j(0). \quad (\text{A.3-35})$$

Explicitly:

$$b_2 = \sum_{m=1}^{\infty} \left[(A_m^3 - A_m^2) K_0\left(\frac{mr_2}{z_0}\right) - C_m^2 I_0\left(\frac{mr_2}{z_0}\right) \right] \quad (\text{A.3-35a})$$

and

$$b_1 = b_2 + \sum_{m=1}^{\infty} \left[(C_m^2 - C_m^1) I_0\left(\frac{mr_1}{z_0}\right) + A_m^2 K_0\left(\frac{mr_1}{z_0}\right) \right] \quad (\text{A.3-35b})$$

After solving the matrix equation for A , B , C , and D , b_2 and then b_1 may be computed. This completes the solution of this boundary value problem.

A.4 HORIZONTAL GRADIENTS

The incorporation of horizontal gradients into the boundary conditions is, fortunately, straightforward. In any given layer the boundary condition far from the shaft is now given by:

$$b_{3i} + \bar{a}_{3i}z + d_{3i}x + c_{3i}xz \quad (A.4-1)$$

where the x axis has been chosen to lie along the direction of the horizontal gradient, and the magnitude of that gradient in the layer in question is $d_{3i} + c_{3i}z$. The presence of c_{3i} allows for the possibility of correlation between the horizontal and vertical gradients -- a necessity when dealing with confined flow. Converting x to cylindrical variables gives:

$$x = \rho \cos \theta. \quad (A.4-2)$$

In the general form for the head given by Eq. 2.1-24, there are terms whose θ dependence is $\cos \theta$, as well as $\sin \theta$ and higher order terms ($\cos n\theta$ and $\sin n\theta$). These latter terms may have their coefficients set to zero since the specific boundary conditions represented by Eq. A.4-1 only contain $\cos \theta$ terms, and the $\cos \theta$ term is orthogonal to the $\sin \theta$ and higher order terms. Thus the general form for the head in the undisturbed rock in the presence of both a vertical and a horizontal gradient far from the shaft is:

$$\begin{aligned} \phi_{3i}(\rho, \theta, z) = & \bar{a}_{3i}z + b_{3i} + \sum_{m=1}^{\infty} \left[A_m^{3i} \cos \frac{mz}{z_o} + B_m^{3i} \sin \frac{mz}{z_o} \right] K_o \left(\frac{m\rho}{z_o} \right) \\ & + \cos \theta \left\{ (c_{3i}z + d_{3i}) \left(\rho + \frac{e_{3i}}{\rho} \right) + \sum_{m=1}^{\infty} \left[E_m^{3i} \cos \frac{mz}{z_o} + F_m^{3i} \sin \frac{mz}{z_o} \right] K_1 \left(\frac{m\rho}{z_o} \right) \right\} \end{aligned} \quad (A.4-3)$$

Similarly, inside the shaft the general form is:

$$\begin{aligned} \phi_{3i-2}(\rho, \theta, z) = & \bar{a}_{3i-2} z + b_{3i-2} + \sum_{m=1}^{\infty} \left[C_m^{3i-2} \cos \frac{mz}{z_0} + D_m^{3i-2} \right] \sin \frac{mz}{z_0} \\ & \times I_0\left(\frac{m\rho}{z_0}\right) + \cos \theta \left[(c_{3i-2} z + d_{3i-2}) \rho + \sum_{m=1}^{\infty} \left[G_m^{3i-2} \cos \frac{mz}{z_0} \right. \right. \\ & \left. \left. + H_m^{3i-2} \sin \frac{mz}{z_0} \right] I_1\left(\frac{m\rho}{z_0}\right) \right] \end{aligned} \quad (A.4-4)$$

In the intermediate radial zone the solution is

$$\begin{aligned} \phi_{3i-1}(\rho, \theta, z) = & \bar{a}_{3i-1} z + b_{3i-1} + \sum_{m=1}^{\infty} \left\{ \left[A_m^{3i-1} \cos \frac{mz}{z_0} + B_m^{3i-1} \sin \frac{mz}{z_0} \right] \right. \\ & \times K_0\left(\frac{m\rho}{z_0}\right) + \left[C_m^{3i-1} \cos \frac{mz}{z_0} + D_m^{3i-1} \sin \frac{mz}{z_0} \right] I_0\left(\frac{m\rho}{z_0}\right) \left. \right\} + \\ & \cos \theta \left[(c_{3i-1} z + d_{3i-1}) \left(\rho + \frac{e_{3i-1}}{\rho} \right) + \sum_{m=1}^{\infty} \left\{ \left[E_m^{3i-1} \cos \frac{mz}{z_0} \right. \right. \right. \\ & \left. \left. + F_m^{3i-1} \sin \frac{mz}{z_0} \right] K_1\left(\frac{m\rho}{z_0}\right) + \left[G_m^{3i-1} \cos \frac{mz}{z_0} + H_m^{3i-1} \sin \frac{mz}{z_0} \right] I_1\left(\frac{m\rho}{z_0}\right) \right\} \right] \end{aligned} \quad (A.4-5)$$

The general boundary conditions are the same as those given in Eqs. A.3-5a through A.3-5j. Since the terms proportional to $\cos \theta$ are independent of the constant (in θ) terms, the A_m , B_m , C_m , D_m , a , and b coefficients appearing in Eqs. A.4-3 through A.4-5 may be solved for among themselves in the same manner as in the preceding section, while the E_m , F_m , G_m , H_m , c , and d coefficients may likewise be solved for in the same manner as before. The horizontal gradient can thus be dealt with as a separate problem from the vertical gradient problem, at least for the purpose of satisfying the general boundary conditions. If there are any correlations between

the vertical and horizontal flow far from the shaft, these boundary conditions may be imposed after the various coefficients have been solved for. (The coefficients e_{3i-1} and e_{3i} can be shown to vanish since the $\frac{1}{\rho}$ term is not allowed in the interior of the shaft.)

As an example of a case where the horizontal and vertical flow are correlated, consider the case of a series of layers confined by impervious rock above and below. Then water flowing up to the top layer will cause that layer's flow rate to increase as a function of the distance downstream, because of conservation of mass. Conversely, to generate the vertical flow, either the top or the bottom layer must have a higher horizontal gradient than its opposing member. The interdependence of a_{3i} , d_{3i} , and c_{3i} for this example can be calculated, although this will not be done here.

This concludes the discussion of the incorporation of horizontal gradients into the specific boundary conditions.

A.5 STREAMLINE FUNCTIONS

In this section the differential equations for the streamline function are solved. These equations are given in Eqs. 2.1-31 and 2.1-32:

$$\frac{\partial \chi}{\partial \rho} = -\rho k \frac{\partial \Phi}{\partial z} \quad (\text{A.5-1})$$

$$\frac{\partial \chi}{\partial z} = \rho k \frac{\partial \Phi}{\partial \rho} \quad (\text{A.5-2})$$

If $\Phi(\rho, z)$ is given by

$$\begin{aligned}\phi(\rho, z) = az + b + \sum_{m=1}^{\infty} \left[A_m \cos \frac{mz}{z_0} + B_m \sin \frac{mz}{z_0} \right] K_0 \left(\frac{m\rho}{z_0} \right) \\ + \left[C_m \cos \frac{mz}{z_0} + D_m \sin \frac{mz}{z_0} \right] I_0 \left(\frac{m\rho}{z_0} \right)\end{aligned}\quad (A.5-3)$$

then

$$\begin{aligned}\frac{1}{k} g_\rho = \frac{\partial \phi}{\partial \rho} = \sum_{m=1}^{\infty} \left\{ \left[A_m \cos \frac{mz}{z_0} + B_m \sin \frac{mz}{z_0} \right] \left(-\frac{m}{z_0} \right) K_1 \left(\frac{m\rho}{z_0} \right) \right. \\ \left. + \left[C_m \cos \frac{mz}{z_0} + D_m \sin \frac{mz}{z_0} \right] \frac{m}{z_0} I_1 \left(\frac{m\rho}{z_0} \right) \right\}\end{aligned}\quad (A.5-4)$$

and

$$\begin{aligned}\frac{1}{k} g_z = \frac{\partial \phi}{\partial z} = a + \sum_{m=1}^{\infty} \left\{ \frac{m}{z_0} \left[-A_m \sin \frac{mz}{z_0} + B_m \cos \frac{mz}{z_0} \right] K_0 \left(\frac{m\rho}{z_0} \right) \right. \\ \left. + \frac{m}{z_0} \left[-C_m \sin \frac{mz}{z_0} + D_m \cos \frac{mz}{z_0} \right] I_0 \left(\frac{m\rho}{z_0} \right) \right\}\end{aligned}\quad (A.5-5)$$

Using the identities

$$\int \rho I_0 \left(\frac{m\rho}{z_0} \right) \frac{m d\rho}{z_0} = \rho I_1 \left(\frac{m\rho}{z_0} \right) \quad (A.5-6)$$

and

$$\int \rho K_0 \left(\frac{m\rho}{z_0} \right) \frac{m d\rho}{z_0} = \frac{z_0}{m} - \rho K_1 \left(\frac{m\rho}{z_0} \right) \quad (A.5-7)$$

and integrating Eq. A.5-1 with respect to ρ then gives

$$\begin{aligned}\chi(\rho, z) = g(z) + k \sum_{m=1}^{\infty} \left\{ \left[-A_m \sin \frac{mz}{z_0} + B_m \cos \frac{mz}{z_0} \right] \left(\frac{z_0}{m} - \rho K_1 \left(\frac{m\rho}{z_0} \right) \right) \right. \\ \left. + \left[-C_m \sin \frac{mz}{z_0} + D_m \cos \frac{mz}{z_0} \right] \rho I_1 \left(\frac{m\rho}{z_0} \right) \right\} + \frac{k a \rho^2}{2}\end{aligned}\quad (A.5-8)$$

Here $g(z)$ is an undetermined function of z . Similarly, integrating Eq. A.5-2 with respect to z gives:

$$\chi(\rho, z) = h(\rho) + k \sum_{m=1}^{\infty} \left[-A_m \sin \frac{mz}{z_0} + B_m \cos \frac{mz}{z_0} \right] (-\rho) K_1 \left(\frac{m\rho}{z_0} \right) \\ + \left[-C_m \sin \frac{mz}{z_0} + D_m \cos \frac{mz}{z_0} \right] \rho I_1 \left(\frac{m\rho}{z_0} \right) \quad (\text{A.5-9})$$

Equations A.5-8 and A.5-9 will be equal provided:

$$g(z) = -k \sum_{m=1}^{\infty} \left[B_m \cos \frac{mz}{z_0} - A_m \sin \frac{mz}{z_0} \right] \frac{z_0}{m}$$

and

$$h(\rho) = \frac{k\rho^2}{2} \quad (\text{A.5-10})$$

This completes the calculation of the streamline function for cylindrically symmetric problems. When a horizontal gradient is present two functions are needed, in general, to describe the streamlines. The differential equations for this case are coupled and nonlinear and not transparently solvable.

APPENDIX B
WELL WITHDRAWAL RATES

The sampling well and sink flow well withdrawal rates used for the analysis presented in Section 2.2 are derived in this appendix.

B.1 SAMPLING WELL WITHDRAWAL RATE

A volumetric flow rate of $2 \times 10^4 \text{ m}^3/\text{yr}$ for a well 300 m from a point source of contamination is used to calculate population doses for all sampling wells.

A sampling well is one which extracts radioactive water from the contaminant plume without diluting it with cleaner water outside the plume. The greatest volume that can be withdrawn without significant dilution may be expressed as:

$$V^* = \pi r^2 b \epsilon \quad (\text{B-1})$$

This is the volume of the water in a right circular cylinder of height b equal to the vertical thickness of the aquifer (200 m), porosity ϵ , and radius r given by:

$$r = 1.5\sigma = 1.5 \sqrt{2\gamma x} \quad (\text{B-2})$$

where σ , γ , and x are as defined in Fig. 2.2-1.

Over the circle with radius given by Eq. B-2, centered on the flow axis downstream of the waste release point, concentrations do not change appreciably.

Since population doses are calculated over a 50 year period, the largest possible sampling well is presumed to extract a volume V^* over that period. Hence, the volumetric withdrawal rate Q cannot exceed:

$$Q = \frac{1}{50} V^* \quad (B-3)$$

For a sampling well located at $x = 300$ m, the closest well to the source of contaminants, the volumetric flow calculated using Eq. B-3 is $2 \times 10^4 \text{ m}^3/\text{yr}$.

B.2 SINK FLOW WELL WITHDRAWAL RATE

The volumetric pumping rate used for the sink flow well characterizes the smallest well which withdraws all of the water flowing over the depository. Unlike sampling wells which were all assigned the same withdrawal rate, the sink flow well withdrawal rates used in our study depended on the location of the well. These rates were used in Section 2.2.2 to calculate ground water concentrations of radionuclides at the well and individual doses.

The aquifer flow field with a sink flow well is drawn schematically in Fig. B-1. The velocity field is approximated by superposing a uniform stream parallel to the x -axis and a sink at the location of the well. Hence, the aquifer interstitial velocity vector is the resultant of the two constituent velocities:

$$\vec{v} = \frac{U_0}{\epsilon} \hat{x} - \frac{Q}{2\pi r b \epsilon} \hat{r} \quad (B-4)$$

where

Figure B-1 Aquifer Flow Field With a Sink Flow Well

- U_0 is the undisturbed stream velocity magnitude (0.15 m/yr)
- ϵ is the porosity (0.10)
- Q is the volumetric withdrawal rate (m^3/yr) of the well
- b is the thickness of the aquifer (200 m)
- r is the radial distance outward from the well along a unit radius vector $\hat{r}$
- $\hat{x}$ is the unit vector parallel to the x-axis (the flow direction)

The distance r_0 between the well and its downstream stagnation point (point of zero velocity) is determined by using Eq. B-4 and requiring that $\vec{v} \cdot \hat{x} = 0$ for $y = 0$:

$$r_0 = \frac{Q}{2\pi b U_0} \quad (\text{B-5})$$

For a fixed aquifer thickness b , observe that r_0 is large if Q is large, or U_0 is small, or both. The quantity r_0 is referred to as the radius of influence of the well. Far upstream of the well ($r \gg r_0$), the flow velocity is nearly parallel and equal in magnitude to the uniform stream.

The streamline shown in Fig. B-1 passing through the stagnation point is called the stagnation streamline or limit line (Ref. 1). We require that at the depository, the area enclosed by this streamline is as wide as the depository and is nearly parallel to the depository edges. As a result, all the waste entering the aquifer from a line source at the center of the depository mixes with the water passing above it and flows directly into the well, provided lateral dispersion is small. Uncontaminated water flowing to either side of the depository does not mix with the waste and flows past the well. Hence the waste in the well water is diluted to the least extent that is consistent with all the radionuclides being withdrawn by the well.

The flow regime shown in Fig. B-1 is established by adjusting the well withdrawal rate Q according to the location of the well. If the well is located sufficiently far downstream of the center of the depository, the stagnation streamline is nearly parallel to the x -axis. The withdrawal rate is then adjusted so the distance between the two branches of the stagnation streamline is equal to the width of the line source, which is as wide as the depository.

For distant downstream wells, the flow over the depository only has an x -component of velocity whose magnitude does not change appreciably along any streamline. Hence the volumetric flow rate Q may be derived by averaging the x -component of velocity across the streamlines passing over the depository

and multiplying the result by the thickness and porosity of the aquifer:

$$Q = \varepsilon b \int_{-\beta}^{+\beta} (\vec{v} \cdot \hat{x}) d\xi = U_0 b \int_{-\beta}^{+\beta} \left[1 + \frac{r_0^2 x}{1 + (\xi/x)^2} \right] d\xi \quad (\text{B-6})$$

where

x is the distance between the well and the waste release into the aquifer

2β is the width of the depository (2 km)

Performing the required integration results in:

$$Q = 2bU_0 \left[\beta + r_0 \tan^{-1}(\beta/x) \right] \quad (\text{B-7})$$

Since the radius of influence r_0 also depends on Q according to Eq. B-5, Eq. B-7 must be solved explicitly for Q :

$$Q = 2b\beta \left[\frac{U_0}{1 - \frac{1}{\pi} \tan^{-1}(\beta/x)} \right] \quad (\text{B-8})$$

This solution is equivalent to finding an analytic expression for the stagnation streamline and adjusting the width of the streamline at the depository to be equal to 2β . The volumetric flow rate Q given by Eq. B-8 is shown as a function of x in Fig. B-2. The closest sink well which satisfies these requirements corresponds to $x = 2$ km (Fig. B-2).

The bracketed expression in Eq. B-8 is the average flow velocity in the x -direction across the face of the depository. This velocity is faster than U_0 because of the pumping of the well. Since the well withdrawal rate Q decreases with distance (Fig. B-2), this average velocity ap-

Figure B-2 Sink Well Volumetric Flow Rate Q

Figure B-3 Average Flow Velocity to the Sink Flow Well

proaches U_0 in the limit that x gets very large (Fig. B-3). This average velocity was used in the one-dimensional pipe network for the pipe leading into the well.

Alternatively, the velocity of flow to the well could have been derived by computing the solute travel time to the well along a streamline coinciding with the x -axis ($y=0$) and dividing into the distance to the well. For distant wells, the results obtained from this procedure are nearly the same as using the average x -velocity across the streamlines appearing in Eq. B-8.

APPENDIX C
INPUT DATA PROBABILITY DISTRIBUTIONS

This Appendix contains the statistical parameters and model constraints which were used by the monte carlo routine (WSRAND) to generate random data for input into the NUTRAN simulation. These parameters and constraints determine the input data PDF's. The procedure for generating and analyzing random data from such information is discussed in Ref. 1.

The input data PDF's defined here reflect the assumed measurement uncertainties that exist after moderate preexcavation phase exploration of the repository has been performed. The values reported here were obtained from Golder Associates, Inc., Geotechnical Engineers, Inc., and Lawrence Livermore Laboratory as described in Ref. 1.

C.1 DISPERSION CONSTANTS

Table C.1-1 lists the median values and geometric standard deviations for the randomly generated dispersion constants. Also listed are the minimum and maximum generic limits for these data.

C.2 STREAM TUBE CROSS-SECTIONS

Table C.2-1 lists the assumed statistics for the crosssections of the shaft and tunnel fracture zones.

TABLE C.1-1
ASSUMED STATISTICS FOR DISPERSION CONSTANTS

PATHWAY	MINIMUM VALUE (m)	MEDIAN VALUE (m)	MAXIMUM VALUE (m)	GEOMETRIC STD. DEV.
Depository layer (salt)	10	50	100	2
First segment of tunnel fracture zone	10	50	100	2
Second segment of tunnel frac- ture zone	10	50	100	2
Shaft fracture zone in de- pository layer	10	50	100	2
Shaft fracture zone above de- pository	10	50	100	2
Shale barrier layer	10	50	100	2
Aquifer	10	50	100	2

TABLE C.2-1
ASSUMED STATISTICS FOR PIPE CROSS-SECTIONS

PATHWAY	MINIMUM (m ²)	MEDIAN (m ²)	MAXIMUM (m ²)	GEOMETRIC STD. DEV.
First segment of tunnel fracture zone	190	330	6400	2
Second segment of tunnel fracture zone	11.4	198	384	2
Shaft fracture zone in salt layer	4	60	110	2
Shaft fracture zone in barrier layer	0	5	100	10

C.3 NUCLIDE RETARDATION FACTORS

There are five regions of flow through the baseline salt repository. They are:

- Flow through the aquifer
- Flow through the undisturbed shale layer
- Flow through the undisturbed salt layer
- Flow through the fracture zone in shale
- Flow through the fracture zone in salt.

The three nuclide groups are numbered as follows:

1. ^{99}Tc , ^{129}I
2. Other fission products
3. Actinides and their daughters.

There are three nuclide groups flowing through five different regions, requiring the generation of fifteen distinct random retardation factors for each set of input data. The following notation is used for the random retardation factors:

- $B_A(j)$ = retardation factor for flow of nuclide group j through the aquifer; $j = 1, 2, 3$.
- $B_S(j)$ = retardation factor for flow of nuclide group j through the undisturbed shale; $j = 1, 2, 3$.
- $B_{SLT}(j)$ = retardation factor for flow of nuclide group j through undisturbed salt; $j = 1, 2, 3$.

- $B_F(j)$ = retardation factor for flow of nuclide group j through the shale fracture zone; $j = 1,2,3$.
- $B_{FSLT}(j)$ = retardation factor for flow of nuclide group j through the salt fracture zone; $j = 1,2,3$.

Retardation of radionuclides dissolved in groundwater is affected by the physical and chemical properties of the subsurface and by the chemistry of the groundwater and the dissolved species. These factors will often operate in more than one rock stratum, or on more than one class of nuclide. For this reason, the various retardation factors are not independent random variables. In an attempt to represent this non-independence, constraints and correlations were imposed on the retardation factors.

Constraints Within Flow Regions - The following constraints apply to the retardation factors (denoted here by $B(j)$; $j = 1,2,3$) in each of the five flow regions:

$$B(1) \geq 1.0 \quad (C.3-1)$$

$$B(2) \geq B(1) \quad (C.3-2)$$

$$B(3) \geq B(1) \quad (C.3-3)$$

Within each flow region $B(2)$ and $B(3)$ are assumed to have a jointly lognormal distribution with correlation coefficient $\rho = 0.5$.

The following special constraints for nuclide group 1 apply in the two salt regions and the aquifer:

$$B_A(1) = B_{SLT}(1) = B_{FSLT}(1) = 1.0 \quad (C.3-4)$$

The following constraints apply to relationships between retardation factors in different regions.

Undisturbed Salt and Aquifer

$$B_{SLT}(2) \leq B_A(2) \quad (C.3-5)$$

$$B_{SLT}(3) \leq B_A(3) \quad (C.3-6)$$

Fractured Shale and Undisturbed Shale

$$B_F(2) \leq B_S(2) \quad (C.3-7)$$

$$B_F(3) \leq B_S(3) \quad (C.3-8)$$

Fractured Salt and Undisturbed Salt

$$B_{FSLT}(2) \leq B_{SLT}(2) \quad (C.3-9)$$

$$B_{FSLT}(3) \leq B_{SLT}(3) \quad (C.3-10)$$

Generic Ranges and Uncertainties - Table C.3-1 lists the assumed retardation factor statistics used to generate the random input data along with the above-mentioned constraints (Ref. 4).

C.4 PERMEABILITIES AND EFFECTIVE POROSITIES

This section contains the statistics used for the generation of random permeabilities and porosities.

C.4.1 Fracture Zones

Tables C.4-1 and C.4-2 list the assumed statistics for the input permeabilities and effective porosities in the repository fracture zones. These values apply to fracture zones which have partially resealed as described in Ref. 1.

TABLE C.3-1
ASSUMED RETARDATION FACTOR STATISTICS

PATHWAY	NUCLIDE GROUP	MINIMUM	MEDIAN	MAXIMUM	GEOMETRIC STD. DEV.
Aquifer	1	1	1	1	1
	2	1	10^2	10^3	10
	3	10	10^3	10^4	10
Und. sturbed Shale	1	1	1	$2 \cdot 2$	10
	2	1	10	10^2	10
	3	1	10	10^3	10
Undisturbed Salt	1	1	1	1	1
	2	1	1	10^3	10
	3	1	10	10^3	10
Shale Fracture Zone (Shaft)	1	1	1	$2 \cdot 2$	10
	2	1	10	10^2	10
	3	1	10	10^3	10
Fractured Salt (Shaft and Tunnel)	1	1	1	1	1
	2	1	1	10	10
	3	1	1	10	10

TABLE C.4-1
ASSUMED PERMEABILITY STATISTICS FOR FRACTURE ZONES

PATHWAY	MEDIAN (cm/sec)	GEOMETRIC STD. DEV.
Tunnel	1.0×10^{-6}	10.0
Shaft in Depository Layer (Salt)	1.0×10^{-6}	10.0
Shaft in Shale Barrier Layer	1.0×10^{-4}	10.0

TABLE C.4-2

ASSUMED EFFECTIVE POROSITY STATISTICS FOR FRACTURE ZONES

PATHWAY	MEDIAN (cm/sec)	GEOMETRIC STD. DEV.
Tunnel	1.0×10^{-3}	10
Shaft in Depository Layer (Salt)	1.0×10^3	10
Shaft in Shale Barrier Layer	1.0×10^{-3}	10

Within each pathway it was assumed that the random variates $\log_{10}$ (permeability) and $\log_{10}$ (porosity) have a bivariate normal distribution with a correlation coefficient $\rho=0.8$.

C.4.2 Flow Through Undisturbed Rock

Table C.4-3 lists the statistics used to generate the random permeabilities for flow in the aquifer and the shale barrier layers.

TABLE C.4-3

ASSUMED STATISTICS FOR PERMEABILITY
IN THE UNDISTURBED ROCK

LAYER	MINIMUM	MEDIAN	MAXIMUM	GEOMETRIC STD. DEV.
Shale Barrier Layer Above Depository	1.0×10^{-9}	1.0×10^{-7}	1.0×10^{-5}	10
Shale Barrier Layer Below Depository	1.0×10^{-9}	1.0×10^{-7}	1.0×10^{-5}	10
Aquifer	1.0×10^{-6}	1.0×10^{-4}	1.0×10^{-2}	10

For flow through these layers the effective porosities, ϵ , were generated from the horizontal permeabilities, k_H , by the relationship (Ref. 8):

$$\epsilon = c \log_{10} \left(\frac{k_H}{A} \right) \quad (C.4-1)$$

The constants c and A are dependent on the geologic layer and are listed in Table C.4-4.

TABLE C.4-4
CONSTANTS USED TO GENERATE EFFECTIVE
POROSITY FROM PERMEABILITY

LAYER	c	A
Shale Barrier Layer Above Repository	2.3×10^{-2}	4.0×10^{-9}
Shale Barrier Layer Below Repository	2.3×10^{-2}	4.0×10^{-9}
Aquifer	4.5×10^{-2}	4.0×10^{-7}

C.4.3 Permeability and Porosity of Salt

The statistics used for generating the random permeabilities and porosities in the undisturbed salt were obtained from Geotechnical Engineers, Inc.* The generic limits for the permeability of salt, k_{salt} , are defined by

$$0 < k_{salt} < 10^{-5} \quad (C.4-2)$$

where k_{salt} is measured in cm/sec. The random salt permeabilities were generated with an assumed lognormal distribution with a median of 10^{-9} cm/sec and a geometric standard deviation of 100.

*Bart Paulding, Geotechnical Engineers, Inc., personal communication.

The corresponding salt porosities were assumed to be normally distributed and were generated jointly with $\log_{10}$ (permeability) using a correlation coefficient of 0.8. The generic limits used were 0.0 to 0.015 with an assumed mean of 0.01. The statistics for salt have since been revised (Ref. 9), but these revisions were not incorporated into this study.

C.5 ADDITIONAL VARIATES

Table C.5-1 lists the statistics used to generate the following random variates:

- Horizontal head gradient in the aquifer
- Vertical head of the underlying aquifer
- Dissolution rate of the waste (Λ)
- Time required to saturate the repository void space (T_{fill}).

TABLE C.5-1
STATISTICS OF RANDOM VARIATES

VARIATE	MINIMUM	MEDIAN	MAXIMUM	GEOMETRIC STD. DEV.
Horizontal Head Gradient in the Aquifer	0.0005	0.005	0.05	1.3
Vertical Head of Underlying Aquifer (m)	3.0	60.0	150.0	1.3
$\Lambda(\text{yr}^{-1})$	*	1.0×10^{-4}	*	10.0
$T_{fill}(\text{yr})$	20	100.0	1000.0	10.0

*No generic limits were used for the leach rate.

APPENDIX D
EQUATIONS FOR FLUID VELOCITIES

A pipe is defined by its two end nodes. For the baseline repository, the nodes are:

Node 0 = Node at interface between lower
aquifer and lower barrier layer

Node 1 = Node at center of depository

Node 2 = Node in tunnel at interface
between depository and repository layer

Node 3 = Node at interface between depository layer and upper barrier layer

Node 4 = Node at junction of shaft and tunnel

Node 5 = Node in shaft at interface between
depository and upper barrier layers

Node 6 = Node at interface between upper
barrier layer and the upper aquifer.

Pipes (0,1), (1,3), (3,6) are considered to correspond to flow (either interstitial or fracture) directly through the rock layers. Pipes (1,2), (2,4), (4,5), (5,6) are considered to correspond to flow through the fracture zone surrounding the shaft and tunnel.

If R is defined as in Eq. 3.2-7, then Darcy's law is equivalent to Ohm's law, with the current identified with the flow rate, and the voltage drop identified with the head difference. Kirchoff's laws can be used to solve the resistance network for the head differences. Specifically, the current conservation law gives:

$$\left(\frac{\Delta H}{R}\right)_{01} = \left(\frac{\Delta H}{R}\right)_{12} + \left(\frac{\Delta H}{R}\right)_{13}$$

$$\left(\frac{\Delta H}{R}\right)_{13} = \left(\frac{\Delta H}{R}\right)_{36}$$

$$\left(\frac{\Delta H}{R}\right)_{12} = \left(\frac{\Delta H}{R}\right)_{24} = \left(\frac{\Delta H}{R}\right)_{45} = \left(\frac{\Delta H}{R}\right)_{56}$$

For a closed circuit loop, the total net head drop must be zero by Kirchoff's second law. This gives:

$$(\Delta H)_{01} + (\Delta H)_{13} + (\Delta H)_{36} = H_0$$

$$(\Delta H)_{01} + (\Delta H)_{12} + (\Delta H)_{24} + (\Delta H)_{45} + (\Delta H)_{56} = H_0$$

Here H_0 is the total head difference between upper and lower aquifers.

These seven equations in seven unknowns can be solved to give:

$$\left(\frac{\Delta H}{R}\right)_{13} = \left(\frac{\Delta H}{R}\right)_{36} = \frac{H_0 R_{12456}}{D}$$

$$\left(\frac{\Delta H}{R}\right)_{12} = \left(\frac{\Delta H}{R}\right)_{24} = \left(\frac{\Delta H}{R}\right)_{45} = \left(\frac{\Delta H}{R}\right)_{56} = \frac{H_0 R_{136}}{D}$$

where $R_{136} = R_{13} + R_{36}$, $R_{12456} = R_{12} + R_{24} + R_{45} + R_{56}$, and

$$D = (R_{01} + R_{12456})R_{136} + R_{01}R_{12456} = (R_{01} + R_{136})R_{12456} + R_{01}R_{136}.$$

The velocity in a given pipe is then given by $\frac{1}{\epsilon W} \frac{\Delta H}{R}$.

APPENDIX E

PROBABILITY DISTRIBUTION CHARACTERISTICS

The following table lists the important properties which characterize the two types of distributions considered in Section 3.2.3. These properties would be the most useful in fitting empirical data to one of the two types.

Gamma Distribution: $n!e^{-\beta x}x^n\beta^{n+1}$

- Mode (Maximum Value): $\frac{df(x)}{dx} = \frac{d\left[\frac{n!x^n e^{-\beta x}}{\beta^{n+1}}\right]}{dx} = 0$
 $\Leftrightarrow x_{\max} = \frac{n}{\beta}$
- Value at Mode: $n!n^n e^{-n}\beta$
- Average Value: $\bar{x} = \int_0^{\infty} xf(x)dx = \frac{n+1}{\beta} = x_{\max} + \frac{1}{\beta}$
- Standard Deviation:
 $\overline{(x-\bar{x})^2} = \int_0^{\infty} (x-\bar{x})^2 f(x)dx = \frac{n+1}{\beta^2} = \frac{\bar{x}}{\beta}$
- Inflection Points: $\frac{d^2f(x)}{dx^2} = 0 \Leftrightarrow x_i = \frac{n \pm \sqrt{n}}{\beta}$
 $= \left[1 \pm \frac{1}{\sqrt{n}}\right] x_{\max}$

Generalized Gamma Distribution: $N^{\beta\gamma} \frac{x^n e^{-\beta x}}{(1+\gamma x)^m}$

- Mode: $\frac{df(x)}{dx} = 0 \Leftrightarrow x_{\max} = \left(\frac{n-m}{2\beta} - \frac{1}{2\gamma}\right) + \sqrt{\left(\frac{n-m}{2\beta} - \frac{1}{2\gamma}\right)^2 + \frac{n}{\beta\gamma}}$

$$\begin{aligned}
 \bullet \quad \text{Normalization: } N_{nm}^{\beta\gamma} &^{-1} = \int_0^{\infty} \frac{x^n e^{-\beta x}}{(1+\gamma x)^m} dx \\
 &= (-1)^n \frac{\partial^n}{\partial \beta^n} \int_0^{\infty} \frac{e^{-\beta x}}{(1+\gamma x)^m} dx \\
 &= (-1)^n \frac{\partial^n}{\partial \beta^n} \left(\frac{e^{-\frac{\beta}{\gamma}}}{\gamma} \int_1^{\infty} \frac{e^{-\frac{\beta}{\gamma} y}}{y^m} dy \right) \\
 &= \frac{(-1)^n}{\gamma^{n+1}} \frac{\partial^n}{\partial z^n} (e^z E_m(z)) \\
 &= \frac{(-1)^n}{\gamma^{n+1}} \sum_{i=0}^n \binom{n}{i} e^z E_{m-i}(z) (-1)^i
 \end{aligned}$$

where

$$\begin{aligned}
 z &\equiv \beta/\gamma, \quad E_m(z) \equiv \int_1^{\infty} \frac{e^{-zy}}{y^m} dy \\
 &= e^{-z} \sum_{\ell=0}^{m-2} \frac{(-z)^{\ell} (m-2-\ell)!}{(m-1)!} + \frac{(-z)^{m-1}}{(m-1)!} E_1(z)
 \end{aligned}$$

and the formula $\frac{dE_n(z)}{dz} = -E_{n-1}(z)$ has been used.

$$\bullet \quad \text{Average Value: } \bar{x} = \int_0^{\infty} x f(x) dx$$

$$\begin{aligned}
 &= N_{nm}^{\beta\gamma} \frac{(-1)^{n+1}}{\gamma^{n+2}} \frac{\partial^{n+1}}{\partial z^{n+1}} (e^z E_m(z)) \\
 &= -\frac{1}{\gamma} \frac{\frac{\partial^{n+1}}{\partial z^{n+1}} (e^z E_m(z))}{\frac{\partial^n}{\partial z^n} (e^z E_m(z))}
 \end{aligned}$$

- Standard Deviation: $\int_0^{\infty} x^2 f(x) dx - \bar{x}^2$

$$= - \frac{1}{y} \left[\frac{\frac{\partial^{n+1}}{\partial z^{n+1}} e^{z E_m(z)}}{\frac{\partial n}{\partial z^n} e^{z E_m(z)}} - \frac{\frac{\partial^{n+1}}{\partial z^{n+1}} e^{z E_m(z)}}{\frac{\partial n}{\partial z^n} e^{z E_m(z)}} \right]^2$$

- Inflection Points: These satisfy the following equation

$$\left(\frac{n}{x_i} - \beta - \frac{my}{1 + yx_i} \right)^2 = \frac{n}{x_i^2} - \frac{my^2}{(1 + yx_i)^2}$$

$$\Leftrightarrow (n(1 + yx_i) - \beta x_i(1 + yx_i) - myx_i)^2$$

$$= n(1 + yx_i)^2 - my^2 x_i^2$$

(which is a quartic equation).

APPENDIX F
DERIVATION OF EQUATION 3.2-17

Differentiating both sides of Eq. 3.2-16 yields:

$$\begin{aligned} \frac{d^{\ell+1}}{db^{\ell+1}} f(\sqrt{b}) &= \sum_{k=0}^{\ell+1} \frac{a_k^{\ell+1}}{(\sqrt{b})^{\ell+k+1}} \frac{d^{\ell-k+1} f(\sqrt{b})}{d(\sqrt{b})^{\ell-k+1}} \\ &= \sum_{k=0}^{\ell} \left[\frac{a_k^{\ell}}{(\sqrt{b})^{\ell+k}} - \frac{(\ell+k)}{2(\sqrt{b})^2} + \frac{1}{2} \frac{1}{\sqrt{b}} \frac{d}{d(\sqrt{b})} \frac{d^{\ell-k}}{d(\sqrt{b})^{\ell-k}} f(\sqrt{b}) \right] \end{aligned} \quad (F-1)$$

Equating coefficients of $\frac{1}{(\sqrt{b})^{\ell+k+1}} \frac{d^{\ell-k+1}}{d(\sqrt{b})^{\ell-k+1}}$ gives the recurrence relation,

$$\begin{aligned} a_k^{\ell+1} &= a_k^{\ell} - (\ell+k-1) a_{k-1}^{\ell} \\ &= a_k^{\ell-1} - (\ell+k-2) a_{k-1}^{\ell-1} - (\ell+k-1) a_{k-1}^{\ell} \\ &= a_k^{\ell-2} - (\ell+k-1) a_{k-1}^{\ell} + (\ell+k-2) a_{k-1}^{\ell-1} + (\ell+k-3) a_{k-1}^{\ell-2} \\ &\vdots \\ &= a_k^{\ell} - \sum_{j=0}^{\ell-k} a_{k-1}^{\ell-j} (\ell+k-j-1) \end{aligned} \quad (F-2)$$

a_k^{ℓ} is zero, as can be seen from Eq. 3.2-16; therefore, letting $j \rightarrow \ell-j$ in Eq. F-2 gives

$$a_k^{\ell+1} = - \sum_{j=k}^{\ell} a_{k-1}^j (j+k-1) \quad (F-3)$$

For $k=0$, Eq. 3.2-16 gives $a_0^{\ell} = 1$ and therefore

$$a_1^{\ell+1} = - \sum_{j=1}^{\ell} (j) = - \frac{\ell(\ell+1)}{2} \quad (F-4)$$

For $k=2$, Eq. 3.2-16 gives:

$$\begin{aligned} a_2^{\ell+1} &= - \sum_{j=2}^{\ell} a_1^j (j+1) = - \sum_{j=2}^{\ell} \frac{(j+1)j(j-1)}{2} \\ &= - \sum_{j=3}^{\ell+1} \frac{j(j-1)(j-2)}{2} \end{aligned} \quad (F-5)$$

This can be written as:

$$\begin{aligned} a_2^{\ell+1} &= \frac{1}{2} \frac{\partial^3}{\partial x^3} \sum_{j=0}^{\ell+1} x^j \bigg|_{x=1} = \frac{1}{2} \frac{\partial^3}{\partial x^3} \left[\frac{x^{\ell+2}-1}{x-1} \right]_{x=1} \\ y=x-1 &= \frac{1}{2} \frac{\partial^3}{\partial x^3} \left[\frac{(1+y)^{\ell+2}-1}{y} \right]_{y=0} \\ &= \frac{1}{2} \frac{\partial^3}{\partial y^3} \sum_{j=2}^{\ell+2} \binom{\ell+2}{j} y^{j-1} \bigg|_{y=0} \\ &= \frac{1}{2} \frac{\partial^3}{\partial y^3} \sum_{j=2}^{\ell+2} \binom{\ell+2}{j} y^{j-1} \bigg|_{y=0} \\ &= \frac{1}{2} \sum_{j=1}^{\ell+1} \binom{\ell+2}{j} (j-1)(j-2)(j-3) y^{j-4} \bigg|_{y=0} \\ &= \frac{1}{2} \binom{\ell+2}{4} 3 \cdot 2 \cdot 1 = \frac{1}{2} \frac{(\ell+2)! 3!}{4! (\ell-2)!} = \frac{1}{2^3} (\ell+2)(\ell+1)\ell(\ell-1) \end{aligned} \quad (F-6)$$

Comparing Eqs. F-5 and F-6, it can be seen that a generalization for $a_k^{\ell+1}$ for arbitrary k is given by

$$a_k^{\ell+1} = \frac{(\ell+k)!(-1)^k}{k!(\ell-k)! 2^{\ell+k+1}} = \frac{\Gamma(\ell+k+1)(-1)^k}{\Gamma(k+1)\Gamma(\ell-k+1) 2^{\ell+k+1}} \quad (F-7)$$

This can be checked by combining Eqs. 3.2-16 and F-7 and repeating the reasoning of Eq. F-1.

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