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FINITE MEDIUM GREEN'S FUNCTION
SOLUTIONS TO NUCLIDE TRANSPORT
IN POROUS MEDIA

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ABSTRACT

Current analytical techniques for predicting the transport of nuclides in porous materials center on the Green's function approach -- i.e., determining the response characteristics of a geologic pathway to an impulse function input. To date, the analyses all have set the boundary conditions needed to solve the 1-D transport equation as though each pathway were infinite in length. The purpose of this work is to critically examine the effect that this infinite pathway assumption has on Green's function models of nuclide transport in porous media. The work described herein has directly attacked the more difficult problem of obtaining suitable Green's functions for finite pathways whose dimensions, in fact, may not be much greater than the diffusion length.

Two different finite media Green's functions describing the nuclide mass flux have been determined, depending on whether the pathway is terminated by a high or a low flow resistance at the outlet end. Pulse shapes and peak amplitudes have been computed for each Green's function over a wide range of geohydrologic parameters. These results have been compared to both infinite and semi-infinite medium solutions.

It was found that predicted pulse shapes are quite sensitive to selection of a Green's function model for short pathways only. For long pathways all models tend toward a symmetric Gaussian flux-time history at the outlet. Thus, the results of our previous waste transport studies using the infinite pathway assumption are still generally valid because they always included at least one long pathway.

It was also found that finite medium models offer some unique computational advantages for evaluating nuclide transport in a series of connecting pathways.

TABLE OF CONTENTS

	<u>Page No.</u>
ABSTRACT	ii
1. OBJECTIVE	1-1
2. DESCRIPTION OF PROBLEM AND BACKGROUND	2-1
3. DERIVATION OF THE GREEN'S FUNCTIONS	3-1
3.1 The Transport Equation	3-1
3.2 Initial and Boundary Conditions for Finite Media	3-3
3.3 Laplace Transform Solutions	3-5
3.4 Solutions in the Time Domain	3-8
3.5 The Semi-Infinite Medium Problem	3-10
3.6 The WASTE Program Green's Function	3-11
4. NUMERICAL RESULTS FOR A SINGLE PIPE	4-1
5. INTERPRETATION OF GREEN'S FUNCTION SOLUTIONS	5-1
6. MULTIPLE PATHS	6-1
6.1 Current WASTE Model	6-1
6.2 Steepest Descent Method	6-2
6.3 Finite Medium Method	6-4
7. SUMMARY AND CONCLUSIONS	7-1
8. RECOMMENDATIONS	8-1
APPENDIX A THE TWO-MEDIUM PROBLEM	A-1
APPENDIX B SOLUTION OF THE TRANSPORT EQUATION FOR MULTIPLE PATHS WITH FINITE MEDIUM GREEN'S FUNCTIONS	B-1
REFERENCES	R-1

LIST OF FIGURES

<u>Figure No.</u>		<u>Page No.</u>
3.2-1	A One-Dimensional Pipe	3-3
4-1	Nuclide Flux Versus Time Histories for $\ell/\alpha = 2$	4-2
4-2	Nuclide Flux Versus Time Histories for $\ell/\alpha = 4$	4-3
4-3	Nuclide Flux Versus Time Histories for $\ell/\alpha = 8.8$	4-4
4-4	Nuclide Flux Versus Time Histories for $\ell/\alpha = 24$	4-5
4-5	Nuclide Flux Peak Height Versus Pipe Length (in units of α) for Four Green's Functions	4-8
4-6	Variation in Peak Amplitude with Diffusion Length for Fixed ℓ	4-9
5-1	Flow Pathways for Unflawed Repository (Ref. 1)	5-3

LIST OF TABLES

<u>Table No.</u>		<u>Page No.</u>
5-1	Baseline Parameters for Unflawed Salt Repository (Ref. 1)	5-4

1.

OBJECTIVE

The objective of the work described in this memorandum is to ascertain the sensitivity of one-dimensional nuclide transport in a porous medium to the selection of a Green's function transport model. The emphasis is on comparing proposed finite medium solutions to the convection-diffusion equation with the infinite medium solutions in current use.

2. DESCRIPTION OF PROBLEM AND BACKGROUND

It is important to develop mathematical models to estimate the release of buried radioactive waste to the biosphere and its potential impact on man. A necessary link in simulating this process is a model that accurately represents the subsurface transport of radionuclides in ground water. At the present time a particular model is embodied in the WASTE computer program, documented in Ref. 1. The model incorporates the effects of advective transport, hydrodynamic dispersion, and chemical interactions between waste components and rock.

To retain the greatest flexibility in handling a wide range of hydrogeologic parameters, the WASTE model approximates the three-dimensional groundwater flow pattern by a network of one-dimensional flowpaths or "pipes" that follow the stream flow lines. For each flow path segment the radionuclide transport equation is solved analytically in the form of a Green's function or impulse response. An assumption in the derivation of the impulse response is the following: all path segments are considered infinite or semi-infinite in extent for the purpose of setting boundary conditions. This assumption greatly simplifies the mathematics. Derivation of the Green's function is not difficult, and the solution for a single pipe is in closed form.

The above assumption is examined critically in this memo. More specifically, the work discussed here derives Green's function solution for finite length pipes and compares these results to the infinite or semi-infinite medium Green's

functions. The solutions obtained are not in closed form. Furthermore, there is ambiguity as to which of the finite medium solutions apply to the scenarios of interest. However, the finite medium boundary condition solutions are shown to possess considerable advantages, not the least of which is a more realistic physical model for highly dispersive flows. The remainder of the memorandum consists of derivations of finite medium Green's function, numerical results in the form of predicted pulse shapes for single pipes, discussion of their applicability to multi-segment networks, and an assessment of errors in the use of current models.

3. DERIVATION OF THE GREEN'S FUNCTIONS

3.1 THE TRANSPORT EQUATION

In Appendix F of Ref. 1 the equations governing the transport and dispersion of ions in one-dimensional flow through porous media were presented. The equations described the concentrations of the various radionuclides in a decay chain dissolved in interstitial water and sorbed on the solid as a function of time and position. A number of assumptions were invoked in order to simplify the transport equations. Of particular importance were the assumptions of instantaneous ion exchange equilibrium between liquid and solid phases and of a retardation factor identical for all radionuclides in the same decay chain. The final equation (Eq. F.2-4 of Ref. 1) obtained was:

$$\frac{\partial c}{\partial t} + \frac{V}{B} \frac{\partial c}{\partial x} = \frac{\alpha V}{B} \frac{\partial^2 c}{\partial x^2} \quad (3.1-1)$$

where

- c = concentration of radionuclides in the pore water. Radioactive decay is ignored in Eq. 3.1-1, but may easily be accounted for by a renormalization
- V = interstitial water flow velocity
- B = retardation factor, which depends upon the ion exchange distribution coefficient, K_d .
- α = longitudinal dispersion length. Note that this model assumes that the dispersion coefficient is a linear function of velocity V.

Two further modifications of Eq. 3.1-1 are made here. First, define

$$U = V/B \quad (3.1-2)$$

as the effective radionuclide flow velocity. Second, the mass flux may be written in terms of concentration

$$q = Q(c - \alpha \frac{\partial c}{\partial x})^* \quad (3.1-3)$$

where

q = mass flux, and
 Q = water volumetric flow rate

By differentiating Eq. 3.1-3 and substituting into Eq. 3.1-1 it is readily demonstrated that an identical partial differential equation can be written with q as the dependent variable. Using Eq. 3.1-2 then gives

$$\frac{\partial q}{\partial t} + U \frac{\partial q}{\partial x} = \alpha U \frac{\partial^2 q}{\partial x^2} \quad (3.1-4)$$

It is often convenient to express the transport equation in terms of q instead of c because boundary conditions are often more easily expressed in q ; furthermore, mass flux is generally of more interest in studies of radionuclide transport through the geologic media than is concentration.

* Note that Appendix F of Ref. 1 erroneously sets $q = Qc$.

3.2 INITIAL AND BOUNDARY CONDITIONS FOR FINITE MEDIA

Solution of Eq. 3.1-4 requires two boundary conditions and an initial condition. Consider the case where no radionuclides are present in a pipe until time $t = 0$ when a unit amount of material is instantaneously injected at the upstream end of the pipe ($x = -\ell$), as depicted in Fig. 3.2-1. This situation implies an initial condition

$$q(x,0) = 0 \quad (3.2-1)$$

and one boundary condition

$$q(-\ell, t) = \delta(t) \quad (3.2-2)$$

where $\delta(t)$ is a delta function in time.

At the downstream end of the pipe ($x = 0$) it is necessary to match both mass flux, q , and concentration, c , with those of the succeeding pipe. Continuity of flux at a boundary is a consequence of conservation of mass, if no other sources are present in the vicinity of the boundary. Continuity of concentration is also necessary; otherwise, the derivative in Eq. 3.1-3 (and q as well) would become infinite at the boundary.

Figure 3.2-1 A One-Dimensional Pipe

The exact matching of boundary conditions at the interface between continuous pipes can involve tedious mathematics. In a sequence of many pipes, arbitrary constants in the solutions of Eq. 3.1-4 for each region may be found from a set of simultaneous equations. To illustrate this, a derivation of the two-medium problem is presented in Appendix A.

A much more tractable problem is one in which the various pipes are mathematically isolated from one another. That is, by suitably choosing limiting forms of the boundary conditions, the solutions to Eq. 3.1-4 for each region are effectively decoupled. This method is satisfactory if the limiting forms of the boundary conditions are justified on physical grounds.

For the present, two different situations at $x = 0$ will be considered. The arguments for the resultant boundary conditions will be qualitative here; further amplification is provided in Appendix A based on the exact solution for two consecutive pipes.

In the first case the pipe in question empties into a much larger body of water, or into an aquifer where there is considerable dilution of the waste. From Eqs. 3.1-3 and 3.1-4 the following relationship between mass flux and concentration at any point is derived:

$$U \frac{\partial q}{\partial x} + Q \frac{\partial c}{\partial t} = 0 \quad (3.2-3)$$

When the radionuclide concentration is very small in the medium that follows -- e.g., an aquifer -- then both c and $\frac{\partial c}{\partial t}$ are small at the boundary. Thus, for this limiting case, a suitable boundary condition at $x = 0$ is:

$$\frac{\partial q}{\partial x} (0, t) = 0 \quad (3.2-4)$$

Qualitatively, the zero gradient boundary condition is tantamount to ignoring advection in the vicinity of the $x = 0$ boundary and allowing nuclide flow across the boundary via hydrodynamic dispersion only. This argument follows from neglecting the second term in Eq. 3.1-4.

The second boundary condition deals with an opposite case, that of the pipe in question emptying into a very much smaller pipe. Obviously, the velocity increases rapidly at the boundary owing to the constriction. The appropriate boundary condition in this limiting case of infinite velocity at the boundary is obtained by assuming "slug flow". Slug flow depicts the flow as moving without axial mixing, that is, hydrodynamic dispersion is neglected. The mathematical description of slug flow at $x = 0$ is:

$$\frac{\partial q}{\partial t}(0,t) + U \frac{\partial q}{\partial x}(0,t) = 0 \quad (3.2-5)$$

This equation can be obtained from Eq. 3.1-4 by assuming its right-hand side is negligible.

3.3 LAPLACE TRANSFORM SOLUTIONS

A method of solving the 1-D transport equation is by the Laplace transform technique. The transformed equation, making use of initial condition Eq. 3.2-1, is

$$s\bar{q} + U\bar{q}_x = \alpha U\bar{q}_{xx} \quad (3.3-1)$$

In this notation, $\bar{q}$ is the transform of q . Each subscript x denotes a differentiation with respect to x ; s is the Laplace transform variable such that

$$\bar{q}(s) = \int_0^{\infty} e^{-st} q(t) dt \quad (3.3-2)$$

Independent solutions of the transformed equation can be shown to be of the form $A(s)e^{x/2\alpha} \sinh K(s)x$ and $B(s)e^{x/2\alpha} \cosh K(s)x$, where

$$K(s) = \frac{1}{2\alpha} \sqrt{1 + \frac{4\alpha s}{U}} \quad (3.3-3)$$

The constants $A(s)$ and $B(s)$ are specified by the boundary conditions.

For a pure diffusion boundary condition where Eq. 3.2-4 is applicable, the transformed boundary conditions at $x = -\ell$ and $x = 0$, respectively, are

$$\bar{q}(-\ell) = 1 \quad (3.3-4)$$

and

$$\bar{q}_x(0) = 0 \quad (3.3-5)$$

These boundary conditions, when substituted into the general solution to Eq. 3.3-1, lead to the following equations in A and B (the argument s for A , B , and K will henceforth be dropped for convenience):

$$-Ae^{-\ell/2\alpha} \sinh K\ell + Be^{-\ell/2\alpha} \cosh K\ell = 1 \quad (3.3-6)$$

and

$$AK + \frac{B}{2\alpha} = 0 \quad (3.3-7)$$

We are interested in finding the mass flux at $x = 0$, the end of the pipe, given a delta function input at the pipe inlet. The transform of that response function (in the pure diffusion boundary case) is

$$\bar{q}(0) = \frac{Ke^{\ell/2\alpha}}{K \cosh K\ell + \frac{1}{2\alpha} \sinh K\ell} \quad (3.3-8)$$

For the slug flow boundary condition, the Laplace transform of Eq. 3.2-5, evaluated at $x = 0$, is

$$s\bar{q}(0) + U\bar{q}_x(0) = 0 \quad (3.3-9)$$

A substitution of Eq. 3.3-9 into the general solution yields

$$sB + U(AK + \frac{B}{2\alpha}) = 0 \quad (3.3-10)$$

which when combined with Eq. 3.3-6 gives the slug flow boundary result:

$$\bar{q}(0) = \frac{UKe^{l/2\alpha}}{UK \cosh Kl + (s + \frac{U}{2\alpha}) \sinh Kl} \quad (3.3-11)$$

It should be noted that the pure diffusion and slug flow transformed solutions are similar; deleting the s in the denominator of Eq. 3.3-11 gives Eq. 3.3-8 exactly. For convenience we can rewrite both solutions into a more general expression involving a parameter λ :

$$\bar{q}(0) = \frac{UKe^{l/2\alpha}}{UK \cosh Kl + (\lambda s + \frac{U}{2\alpha}) \sinh Kl} \quad (3.3-12)$$

with K given by Eq. 3.3-3. The parameter λ takes on the values

$$\lambda = 0 \quad \text{for pure diffusion at } x = 0$$

$$\lambda = 1 \quad \text{for slug flow at } x = 0$$

3.4 SOLUTIONS IN THE TIME DOMAIN

The important features of the inversion of transformed flux equations are discussed below.

It might appear that Eq. 3.3-12 has a branch point at $K = 0$, i.e., when $s = -\frac{4\alpha}{U}$. A Taylor series expansion of the denominator of $\bar{q}(0)$ about $K = 0$ would demonstrate that the only singularities are simple poles. The inversion is thus greatly expedited. Let s_n be the poles of $\bar{q}(0)$ so that the following equation is satisfied:

$$UK(s_n) \cosh K(s_n)\ell + (\lambda s_n + \frac{U}{2\alpha}) \sinh K(s_n)\ell = 0 \quad (3.4-1)$$

The inversion of $\bar{q}(0)$ is then given by the method of residues (Ref. 2) as

$$q(0,t) = \sum_n \frac{UK e^{s_n t}}{\frac{d}{ds} [UK \cosh K\ell + (\lambda s + \frac{U}{2\alpha}) \sinh K\ell]_{s=s_n}}$$

The results of the inversion process are more compact if the substitution

$$s_n = -\frac{U}{4\alpha} (1 + \xi_n^2) \quad (3.4-2)$$

or

$$K(s_n) = \frac{i\xi_n}{2\alpha} \quad (3.4-3)$$

are made, where the ξ_n are taken to be positive.

The quantities ξ_n are obtained from the transcendental equation

$$\tan \frac{\xi_n \ell}{2\alpha} + \frac{\xi_n}{1 - \frac{\lambda}{2} (1 + \xi_n^2)} = 0 \quad (3.4-4)$$

which derives from Eq. 3.4-1.

The mass flux at $x = 0$ is next found from:

$$q(0, t) = \frac{U}{2\alpha} e^{\ell/2\alpha} e^{-U\ell/4\alpha} \quad (3.4-5)$$

$$x \sum_n \frac{\xi_n^2 \cos \frac{\xi_n \ell}{2\alpha} e^{-U\xi_n^2 t/4\alpha}}{\left[\frac{\lambda}{2} (1 + \xi_n^2) - 1 \right] \left[\frac{\ell}{2\alpha} + \lambda \sin^2 \left(\frac{\xi_n \ell}{2\alpha} \right) \right] - \cos^2 \left(\frac{\xi_n \ell}{2\alpha} \right)}$$

Some observations about Eqs. 3.4-4 and 3.4-5 can be made:

- The ξ_n can be determined from Eq. 3.4-4 by iterative techniques. The identity $\tan (x - n\pi) = \tan x$ is useful to obtain higher order roots, which increase as n increases; here $n = 1, 2, \dots$
- The expression for $q(0, t)$ will, in general, converge rapidly. That is, only a few terms in the summation over n are required for a reasonable accuracy
- If Eq. 3.4-5 is integrated with respect to time it has been shown by computation that

$$\int_0^\infty q(0, t) dt = 1 \quad (3.4-6)$$

This follows from the initial assumption and serves as a check on the accuracy of the calculations.

3.5 THE SEMI-INFINITE MEDIUM PROBLEM

Eq. 3.4-5 with $\lambda = 0$ or 1 is the Green's function for a finite, one-dimensional medium. Currently, infinite or semi-infinite (Ref. 3) medium Green's functions are employed to estimate nuclide transport. For sake of comparison, the semi-infinite medium Green's function will be derived.

The transport equation, Eq. 3.1-4, is to be solved for an infinitely long pipe with an inlet at $x = 0$. A unit impulse of material is injected at $t = 0$; thus,

$$q(0,t) = \delta(t) \quad (3.5-1)$$

The second boundary condition invoked is that the mass flux must be finite at $x = \infty$; equivalently,

$$q(\infty,t) = 0 \quad (3.5-2)$$

As an initial condition Eq. 3.2-1 is applicable. Again using the Laplace transformation approach, the mass flux at a distance l from the source is readily obtained as

$$\bar{q}(l) = e^{l/2\alpha} e^{-K(s)l} \quad (3.5-3)$$

with $K(s)$ defined by Eq. 3.3-3. The inverse of Eq. 3.5-3 may be found in many standard tables of Laplace transforms; it is

$$q(l,t) = \frac{l}{[4\alpha U t^3]^{1/2}} \exp [-(l - Ut)^2/4\alpha Ut] \quad (3.5-4)$$

3.6 THE WASTE PROGRAM GREEN'S FUNCTION

The Green's function employed by the WASTE computer program is described in Ref. 1, Appendix F, although the derivation presented here will differ somewhat from the original. Since the intent of WASTE is to predict radionuclide transport in long pipes, the Green's function it uses is an infinite medium solution to the transport equation. The boundary conditions utilized are:

$$q(+\infty, t) = 0 \quad (3.6-1)$$

$$q(-\infty, t) = 0 \quad (3.6-2)$$

The initial condition corresponds to an instantaneous injection of a unit mass at $x = 0$; that is

$$q(x, 0) = U\delta(x) \quad (3.6-3)$$

where $\delta(x)$ is the delta function.

The Laplace transform method, when applied to Eq. 3.1-4 and Eqs. 3.6-1 to 3.6-3, yields the transformed solution at $x = \ell$

$$\bar{q}(\ell) = \frac{e^{\ell/2\alpha} e^{-K(s)\ell}}{K(s)} \quad (3.6-4)$$

The inverse of Eq. 3.6-4 is found from standard tables as

$$q(\ell, t) = \sqrt{\frac{U}{4\pi\alpha t}} \exp [-(\ell - Ut)^2/4\alpha Ut] \quad (3.6-5)$$

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This solution is somewhat similar in form to the results of the previous section for the semi-infinite medium Green's function. However, as will be demonstrated in Section 4, the two solutions may be very different; they are constrained to be identical only at time $t = l/U$.

4.

NUMERICAL RESULTS FOR A SINGLE PIPE

For identification purposes designate:

- q_D = finite medium Green's function with a pure diffusion boundary condition and given by Eq. 3.4-5 with $\lambda = 0$.
- q_{SF} = finite medium Green's function with a slug flow boundary condition and given by Eq. 3.4-5 with $\lambda = 1$.
- q_{SI} = semi-infinite medium Green's function given by Eq. 3.5-4.
- q_I = infinite medium Green's function given by Eq. 3.6-5.

The Green's functions q_D , q_{SF} , q_{SI} , and q_I have been numerically evaluated to compare their important features as a function of problem parameters. Figures 4-1 through 4-4 are plots of mass flux versus time at a fixed position a distance l from the pipe inlet at which a unit impulse of material is injected at $t = 0$. All four of the above Green's functions are presented in each figure. The coordinates are normalized. The abscissas have units of Ut/l , where l/U is the mean transit time of the material in the pipe. The ordinates are in units of ql/U so that all pulses shown have a unit area. Each of the first four figures represents a different value of l/α for the pipe; the range of l/α is from 2 to 24. Taking α to be 50 m gives pipe lengths of 100 m, 200 m, 440 m, and 1200 m.

Figure 1 compares the four Green's functions for a 100 m pipe ($l/\alpha = 2$) that is indicative of the depository

Figure 4-1 Nuclide Flux Versus Time Histories for $l/a = 2$

Figure 4-2 Nuclide Flux Versus Time Histories for $l/a = 4$

Figure 4.3 Nuclide Flux Versus Time Histories for $l/a = 8.8$

Figure 4-4 Nuclide Flux Versus Time Histories for $l/a = 24$

layer according to the model given in Section 5. The q_D curve has a considerably higher peak (by 81%) than the q_{SF} peak, a faster rise time, and an earlier arrival time. The q_{SF} curve is characterized by a longer tail. The q_D model represents a pipe joining a larger body of water with a much lower nuclide concentration. The large body of water will tend to draw the waste by diffusion rapidly out of the pipe. In contrast, the q_{SF} model represents a pipe joining a small area pipe. At the interface the flow resistance is high. Hence, nuclide transport across the first pipe is slower.

The semi-infinite pipe (q_{SI}) occupies an intermediary position. The transit time of the peak approximates that of the q_D model, although the overall shape is somewhat closer to the q_{SF} model.

The q_I result for the infinite pipe has by far the lowest peak and is the most delayed in time of the four Green's functions. This model allows backward diffusion from the injection point -- i.e., in a direction opposite from that of the bulk flow -- and therefore the pulse has more spread than for the other three models.

Figure 4-2 gives flux versus time histories similar to Fig. 4-1, but for a pipe with $l/\alpha = 4$. The peak of the q_D pulse is now considerably closer to that of the q_{SF} pulse; the difference is 37%. The q_{SF} and q_{SI} models are quite alike. As in Fig. 4-1, all pulses are noticeably asymmetric, but peak transit times are closer to the mean transit time, l/U , than Fig. 4-1.

Figure 4-3, which shows pulses for an $l/\alpha = 8.8$ pipe, indicates continuing trends toward increasing peak transit times, more symmetric pulses, and a smaller variation among the models in shape and height of the peak.

Finally, for the $l/\alpha = 24$ pipe, Fig. 4-4, the flux time histories for the four models are virtually identical and approach Gaussian distributions centered about $t = l/U$. In the limit of long pipes (or short diffusion lengths) there is little sensitivity of pulse shape to selection of model.

In Fig. 4-5 are plotted peak heights for all four Green's functions versus the quantity l/α . Note that these relative peak heights are not normalized as in the previous four figures. As expected, peak height decreases monotonically as l/α increases, the behavior expected from a model involving the diffusion process. Sensitivity to peak height on l/α is very high for pipes where l and α are comparable; the curves are nearly vertical in this region.

Figure 4-6, a plot of lq/U vs. α/l , illustrates the relationship between peak height and α , the diffusion length, for a fixed pipe length l . A result of interest is the behavior of the q_D and q_{SI} models. These curves first decrease with increasing α , reach a minimum, and then increase for large α . Such a result appears at first to be counter-intuitive. In contrast, the q_I and q_{SF} models predict a monotonically decreasing q vs. α curve.

One plausible explanation for the minimum in q is the following. In the limit of very small α , the transport process is pure advection, and the initial delta function shape is maintained. Hence, the peak is very large. In the limit of very large α , the transport process is pure diffusion. A diffusion model allows material near the source to move very rapidly; again the peak in the flux-time history is very large. It would, therefore, be necessary that for intermediate values of α a minimum would exist. For the q_{SI} model it can be shown that the minimum occurs exactly at $\alpha = 0.25l$. That there is no minimum for the q_{SF} model is possibly a

Figure 4-5 Nuclide Flux Peak Height Versus Pipe Length (in units of α) for Four Green's Functions

MODELS

- FINITE MEDIUM, DIFFUSION BOUNDARY (q_D)
- .- FINITE MEDIUM, SLUG FLOW BOUNDARY (q_{SF})
- SEMI-INFINITE MEDIUM (q_{SI})
- INFINITE MEDIUM (q_I)

Figure 4-6 Variation in Peak Amplitude with Diffusion Length for Fixed l

consequence of the fact that diffusion is not a dominant mechanism for material transport. For the q_1 model backward diffusion prevents material from leaving the source region rapidly even at large values of α and, thus, no minimum exists.

The point should be raised that regions of the curves in Fig. 4-6 to the right of the minimum (say $\alpha/l > 0.3$) may be physically unrealistic. According to the treatment of hydrodynamic dispersion in Ref. 4 the diffusion length is of the same order of magnitude as typical channel lengths in porous materials. It is difficult to imagine that these lengths could approach the actual pipe length and still have the one-dimensional transport equation considered here apply. This is strictly an intuitive comment; additional research into the validity of the constant α model is probably warranted.

5. INTERPRETATION OF GREEN'S FUNCTION SOLUTIONS

Given a one-dimensional pipe with nuclide transport, four response functions have been presented that allow the flux at the pipe outlet to be computed from a delta-function input at the pipe inlet. The choice of the appropriate Green's function is now addressed. As will be demonstrated in Appendix A there exist inequalities involving ratios of physical parameters of two consecutive pipes that determine the appropriate Green's function selection for the first pipe.

For the q_D model to be valid it is necessary that either

$$Q_2 \gg Q_1 \text{ and } U_1 \cong U_2 \quad (5-1)$$

or

$$U_1 \gg U_2 \text{ and } Q_1 \cong Q_2 \quad (5-2)$$

where the subscript 1 indicates the pipe of interest, and the subscript 2 indicates the following pipe.

For the q_{SF} model to be valid it is necessary that

$$U_2 \gg U_1 \quad (5-3)$$

and

$$Q_1 = Q_2 \quad (5-4)$$

The semi-infinite medium Green's function, of course, is never strictly applicable to finite length pipes, but may be the best choice when

$$Q_1 \cong Q_2 \quad (5-5)$$

and

$$U_1 \cong U_2 \quad (5-6)$$

or for pipes long compared to the diffusion length α when injection is at an endpoint.

The infinite medium Green's function q_1 is seemingly the most advisable choice to describe the aquifer or any long pipe when material is injected somewhere within the pipe boundaries, but not at an endpoint.

The above conditions lack definitiveness; additional analyses need be performed to quantify the regimes of validity of appropriate Green's functions. In certain circumstances, however, it would appear that these conditions are met. For instance, for the unflawed salt repository (Ref. 1) a current transport model considers one flow pathway through two tunnel fracture zones and then through two shaft fracture zones. This is one of the routes illustrated in Fig. 5-1. The geologic parameters for each of the four consecutive pathways are presented in Table 5-1. The total volumetric flow rate, Q , is the same in all four pathways up to the upper aquifer. Similarly, each pathway has the same porosity and retardation factor. Thus, the nuclide velocities, U , are inversely proportional to the cross-sectional area of each pathway. The velocity ratios between consecutive pathways, as can be computed from Table 5-1, are: 1:16.7, 1:3.3, and 1:12.0. Equations 5-3 and 5-4

are satisfied in this case of tunnel/shaft flow. It would be appropriate, then, to model the first three pathways in Table 5-1 with the q_{SF} Green's function.

In contrast, the flow rate in the aquifer is orders of magnitude larger than that in the tunnel/shaft pathway. Since Eq. 5-1 is obeyed, it is recommended that the q_D model be applied to pathway representing the fracture zone around the shaft in the shale barrier layer.

Similar considerations would lead to a recommendation that the q_D model Green's function be applied to both the depository layer and the barrier layer pathways (undisturbed rock) shown in Fig. 5-1, the parameters of which are described in Table 5-1.

Figure 5-1 Flow Pathways for Unflawed Repository (Ref. 1)

TABLE 5-1
 BASELINE PARAMETERS FOR UNFLAWED SALT REPOSITORY
 (Ref. 1)

T-1551

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	1	50
2 nd Segment of Tunnel Fracture Zone	440	198	10 ⁻³	10 ⁻⁶	1	50
Fracture Zone Around Shaft in Depository Layer	100	60	10 ⁻³	10 ⁻⁶	1	50
Fracture Zone Around Shaft in Shale Barrier Layer	200	5	10 ⁻³	10 ⁻⁴	1	50
Depository Layer	100	5 × 10 ⁶	10 ⁻²	10 ⁻⁹	1	50
Barrier Layer	200	5 × 10 ⁶	0.05	10 ⁻⁷	1	50
aquifer	1.6 × 10 ⁴	4 × 10 ⁵	0.1	10 ⁻⁴	¹²⁹ I, ⁹⁹ Tc: 1 Other Fission Products: 10 ² Actinides: 10 ⁴	50

6.

MULTIPLE PATHS

Computation of the transport of nuclides through a series of paths can be performed in a variety of methods. At present one method is employed in the TASC WASTE computer program; a second, more rapid method is also currently under consideration. Both of the above approaches utilize Green's functions that apply to semi-infinite or fully infinite media. A third technique, based upon finite media Green's functions, will be compared to the first two in a very general way with the purpose of showing some advantages to the latter method. Details of the computational techniques that extend the finite media Green's functions to multiple pipes are discussed in Appendix B.

6.1 CURRENT WASTE MODEL

The current WASTE transport model, described in Ref. 1, employs a numerical approach in which the input to a path is divided into discrete time intervals, and the input is approximated by impulses entering at the midpoint of each time interval. The Green's function for the pipe gives an output corresponding to each impulse (or delta-function) input. Finally, the net output is obtained by integrating (summing) the impulse responses over a time interval; the net output yields the input to the next path segment. The Green's function for the WASTE model (Eq. 3.6-5) is the solution for an infinite medium in the region $x > 0$ when a unit mass of material is injected at the point $x = 0$ (flow is directed toward positive x). These conditions quite reasonably approximate an aquifer.

The same Green's function, however, is also used to describe flow in finite length pathways, such as the fracture zones depicted in Figure 5-1.

Readily identifiable deficiencies in the current WASTE treatment are:

- an inappropriate Green's function for finite length pathways when the dispersion length is comparable to the length of the pathway. Moreover this Green's function allows dispersion in both directions at the source, which is not strictly correct for consecutive pipes in a network.
- a somewhat cumbersome numerical solution to problems involving a series of consecutive pipes.

6.2 STEEPEST DESCENT METHOD

The second method now under scrutiny at TASC and elsewhere (Ref. 3) involves the semi-infinite Green's function, q_{SI} , given by Eq. 3.5-4. This approach assumes that the output from a series of pipes is given by convolution of expressions of the form of Eq. 3.5-4, one from each of the individual pathways. A straightforward means of handling this problem is to use Laplace transform techniques. The transform of the output of a series of pipes is merely the product of the transforms of the individual pipes. For the case of the q_{SI} model, Eq. 3.5-3 can be used for each pipe; the transform of the output from a set of N pipes is given by

$$\tilde{q}_N(\ell, s) = \exp \sum_{i=1}^N \frac{\ell_i}{2\alpha_i} \left[1 - \sqrt{1 + \frac{4\alpha_i s}{U_i}} \right] \quad (6.2-1)$$

where α_i , l_i , and U_i are respectively, the diffusion lengths, actual physical lengths, and effective flow velocities for each of the path segments, and

$$l = \sum_{i=1}^N l_i \quad (6.2-2)$$

The inversion of Eq. 6.2-1 is accomplished by means of the method of steepest descent (see Ref. 5). In outline, this solution method involves the following steps:

- Evaluate the contour integral

$$q(l, t) = \frac{1}{2\pi i} \oint_c \exp \left[st + \sum_{i=1}^N \frac{l_i}{2\alpha_i} \left[1 - \sqrt{1 + \frac{4\alpha_i s}{U_i}} \right] \right] \quad (6.2-3)$$

- Differentiate the argument of the exponential, $f(s)$, and set the resulting expression equal to zero to obtain the maximum value of the argument and the value of $s = s_0(t)$ at which the derivative is zero, i.e.,

$$f'(s_0) = 0 \quad (6.2-4)$$

- Expand the argument $f(s)$ in a Taylor series about $s = s_0(t)$
- Find the inverse transform from the expression (see Ref. 5)

$$q(l, t) = \frac{e^{f(s_0)}}{\sqrt{2\pi f''(s_0)}} \quad (6.2-5)$$

The steepest descent inversion method may be exact for certain forms of $f(s)$; for other forms Eq. 6.2-5 is just the first term in an asymptotic expansion for large time t with errors that are difficult to estimate.

The semi-infinite medium Green's function/steepest descent solution method is computationally much more rapid than is the WASTE procedure because a larger proportion of the solution procedure is performed analytically in the former approach. Moreover, there is the advantage that for a series of cases the semi-infinite medium Green's function, q_{SI} , better represents the physics of nuclide transport than does the infinite medium Green's function (although WASTE could be modified to accept other Green's function forms). However, the drawbacks to the steepest descent method are similar to the WASTE model. First the Green's function employed may not be a good representation of the response of short pipes when the coefficient of dispersion is large. Second, the inversion formula, Eq. 6.2-5, is an approximation appropriate for large t whose accuracy has not been determined.

6.3 FINITE MEDIUM METHOD

The finite medium Green's function approach appears to be superior to the previous two in certain respects. It would be expected that either the q_{SF} or q_D models would better describe the behavior of a finite pipe than either the q_I or q_{SI} models. Hence, the Green's functions are finite media should be an improvement over the semi-infinite or the infinite medium Green's function where results are sensitive to the ratio l/α .

There is another advantage. The Laplace transforms of the finite medium Green's functions are analytic and can be written in terms of simple poles. This property, as shown in Appendix B, allows the following statement to be made: if the solutions for individual pathways are known exactly, then the overall solution for the series of pathways is also known exactly. The poles corresponding to the transform of the solution for the series of pipes are simply the accumulation of these for all the individual pipes. The solution for the nuclide flux in each pipe can be obtained to any degree of accuracy by retaining sufficient terms in Eq. 3.4-5; the same statement can be made with regard to an entire series network of consecutive pipes. Thus, a rapidly converging series analogous to Eq. 3.4-5 can be obtained for a series of pipes using the values of ξ_n derived from equations identical to Eq. 3.4-4 for each single pipe.

7.

SUMMARY AND CONCLUSIONS

The WASTE computer code and comparable nuclear waste transport models approximate 3-D groundwater flow in porous media by 1-D flowpaths. Along each flowpath segment of a flow network the transport equation is solved by means of Green's functions. To simplify the mathematics and to allow a closed form solution, flowpath segments are assumed to be infinite or semi-infinite when setting boundary conditions. The infinite pathway assumption has been examined in this memorandum.

The work described here has obtained, analytically, Green's functions for representative flow pathways of finite length. Two boundary conditions at the outlet of 1-D pipes were investigated: one depicted outlet flow as a pure diffusion process; the second assumed that outlet flow was a non-diffusion (advection) process. The two boundary conditions are extremes and bound actual flow pathway outlet conditions. Boundary conditions of this sort allow a decoupling of flow pathways so that the solution for one pipe does not depend upon the properties of subsequent pipes. It is necessary, however, to select which of the two models for finite medium Green's functions is appropriate based upon the general characteristics of the next pipe, although the details of the next pipe are not needed.

Numerical evaluation of the finite medium Green's functions have been made and compared to the semi-infinite and infinite medium Green's functions currently in use for 1-D waste transport calculations. The following principal conclusions have been drawn:

- The finite medium Green's function models developed here represent an important improvement over current waste transport models. While not invalidating the results of current transport models, the finite medium models do extend the range of applicability of the Green's function approach to solving radionuclide transport problems
- The q_p model, which represents flow into an aquifer or larger area body, gives an earlier and higher peak than does either the infinite medium q_i model or the semi-infinite q_{si} model for short pipes. Hence, currently considered infinite or semiinfinite Green's functions may not be conservative. In this domain (where l/a is not large) the sensitivity of results for a single pipe to model selection is high
- All models examined for pipe outlet mass fluxes tend toward Gaussian shaped Green's functions centered at the mean transit time as pipe length becomes large compared to the diffusion length. Therefore, in this regime (large l/a), model selection is not critical
- The response of a flow path to an impulse function input is sensitive to α as the ratio α/l approaches unity. The validity of the transport equations with a constant diffusion length in this range of l/a values is in doubt
- The q_{si} and q_{sp} models give fairly similar results. Both models implicitly assume a high flow resistance beyond the length of pipe being considered so that the similarity in Green's function is qualitatively reasonable
- Characteristics of actual flow pathways in an unflawed salt repository do closely correspond to the end boundary conditions necessary to apply the finite medium Green's functions. This conclusion, however,

is based on the limited extent to which important geologic parameters such as the dispersion length are known

- The use of finite medium Green's functions has computational advantages. The Laplace transform of the Green's functions are analytic, with all singularities being simple poles. The inversion of a single pipe is not difficult, and the result is a rapidly converging series of exponentials. The application to stacked pipes offers no apparent additional problems. Given the solutions for individual paths, the solution for a series of connected pathways can be formed exactly (a property of the analytic nature of the transformed Green's function). In contrast, the use of non-analytic semi-infinite or infinite medium Green's functions requires inversion techniques that are approximations only for stacked pipes.

8.

RECOMMENDATIONS

The finite medium Green's functions appear to have certain advantages over techniques currently considered for the determination of nuclide transport in porous media. To exploit these advantages fully the following work is recommended:

- Investigate other plausible boundary conditions at the pipe outlet in addition to the slug flow and pure diffusion boundary conditions. One example is the finite pipe with a source injection within the boundaries, not at an endpoint
- Obtain more definitive limits on the regimes of validity of the various outlet boundary conditions
- Extend comparison of the various models proposed to date -- the q_D , q_{SI} , q_I , and q_{SF} models -- to two or more connected pipes in series with varying ratios of flow parameters such as pipe length, diffusion length, nuclide velocity, and volumetric flow rate
- Examine the potential implementation of the finite medium Green's function approach into the NUTRAN nuclide transport code network.

APPENDIX A

THE TWO-MEDIUM PROBLEM

The purpose of this appendix is to derive boundary conditions for the outlet of a finite length pipe that serve to isolate that pipe from successive pipes. That is, outlet boundary conditions are sought that will enable a solution for the flux-time history at the outlet of a single pipe to be obtained independently of the exact flow parameters of successive pipes. To this end, the exact solution of the two-medium problem will be found first, and then useful limiting cases of this solution will be investigated.

Medium 1, the pipe of interest, is taken to extend from $x = -l$ to $x = 0$. Medium 2, for simplicity, is semi-infinite and extends from $x = 0$ to $x = \infty$. Equation 3.3-1, the Laplace transform of the transport equation (Eq. 3.1-4), must be satisfied in both media.

In medium 1, a general solution of Eq. 3.3-1 is:

$$\bar{q}_1(x,s) = e^{x/2\alpha_1} [A(s) \sinh K_1 x + B(s) \cosh K_1 x] \quad (A-1)$$

where

$$K_1 = \frac{1}{2\alpha_1} \sqrt{1 + \frac{4\alpha_1 s}{U_1}} \quad (A-2)$$

In medium 2, a solution of Eq. 3.3-1 that is finite at $x = \infty$ is

$$\bar{q}_2(x,s) = C(s) e^{x/2\alpha_2} e^{-K_2 x} \quad (A-3)$$

where

$$K_2 = \frac{1}{2\alpha_2} \sqrt{1 + \frac{4\alpha_2 s}{U_2}} \quad (A-4)$$

The quantities $A(s)$, $B(s)$, and $C(s)$ are arbitrary constants to be determined by the boundary conditions. Both Eqs. A-1 and A-3 are valid when the initial condition is

$$q(x,0) = 0 \quad (A-5)$$

At $x = -l$ we adopt the previously discussed delta function input, Eq. 3.2-2. Therefore,

$$\bar{q}(-l) = 1 \quad (A-6)$$

and

$$B \cosh K_1 l - A \sinh K_1 l = e^{l/2\alpha_1} \quad (A-7)$$

By virtue of continuity of mass flux across the boundary at $x = 0$ we have

$$\bar{q}_1(0,s) = \bar{q}_2(0,s) \quad (A-8)$$

Therefore

$$B(s) = C(s) \quad (A-9)$$

The nuclide concentration must also be continuous across the boundary at $x = 0$. The concentration and mass flux are related through Eq. 3.2-3, i.e.,

$$U \frac{\partial q}{\partial x} + Q \frac{\partial c}{\partial t} = 0 \quad (\text{A-10})$$

If the concentration c is continuous (for all time) than $\frac{\partial c}{\partial t}$ must also be continuous; hence, the continuity condition at $x = 0$ is

$$\frac{U_1}{Q_1} \frac{\partial q_1}{\partial x} (0, t) = \frac{U_2}{Q_2} \frac{\partial q_2}{\partial x} (0, t) \quad (\text{A-11})$$

or

$$\frac{U_1}{Q_1} \frac{d\bar{q}_1}{dx} (0) = \frac{U_2}{Q_2} \frac{d\bar{q}_2}{dx} (0) \quad (\text{A-12})$$

Therefore

$$\frac{U_1}{Q_1} \left(AK_1 + \frac{B}{2\alpha_1} \right) = \frac{U_2 C}{Q_2} \left(\frac{1}{2\alpha_2} - K_2 \right) \quad (\text{A-13})$$

Solving Eqs. A-7, A-9, and A-13 for A , B , and C gives the following result:

$$B(s) = \bar{q}_1(0, s) = \bar{q}_2(0, s) \quad (\text{A-14})$$

$$= \frac{K_1 e^{\ell/2\alpha_1}}{K_1 \cosh K_1 \ell + \frac{1}{2\alpha_1} \sinh K_1 \ell - \frac{Q_1 U_2}{Q_2 U_1} \left(\frac{1}{2\alpha_2} - K_2 \right) \sinh K_1 \ell}$$

the transform of the mass flux at the boundary $x=0$.

It is to be noted that Eq. A-14 contains the properties of both media. For certain limiting cases Eq. A-14 can be simplified to a form which contains the properties of medium 1 only. The first case occurs when

$$\frac{Q_1 U_2}{Q_2 U_1} \ll 1 \quad (\text{A-15})$$

In this situation Eq. A-14 reduces to Eq. 3.3-8, and Eq. A-12 reduces to Eq. 3.3-5. Hence, the zero flux-gradient boundary condition leads to the q_D model when Eq. A-15 (or, equivalently, Eqs. 5-1 and 5-2) is satisfied.

The second case occurs when the quantity α_2/U_2 represents a time that is short compared to typical pulse observation times. For this limit, $K_2(s)$, given by Eq. A-4, can be approximated by

$$K_2 = \frac{1}{2\alpha_2} \left(1 + \frac{2\alpha_2 s}{U_2} \right) \quad (\text{A-16})$$

If it is also assumed that $Q_1 = Q_2$, then substituting Eq. A-16 into Eq. A-14 gives Eq. 3.3-11, the q_{SF} model. Similarly, a substitution of Eq. A-16 into Eq. A-12 yields Eq. 3.3-9, the slug flow boundary condition. Since we are interested in observation times of the order of (or larger than) α_1/U_1 , and since

$$\alpha_1 \approx \alpha_2 \quad (\text{A-17})$$

the previous condition on α_2/U_2 is roughly equivalent to Eq. 5-3, that is

$$U_2 \gg U_1 \quad (\text{A-18})$$

Finally, when $Q_1 = Q_2$, $U_1 = U_2$, and $\alpha_1 = \alpha_2$, then $K_1 = K_2$, and Eq. A-14 reduces to

$$\bar{q}_1(0) = e^{\ell/2\alpha_1} e^{-K_1\ell} \quad (\text{A-19})$$

the q_{SI} model (see Eq. 3.5-4).

APPENDIX B

SOLUTION OF THE TRANSPORT EQUATION FOR
MULTIPLE PATHS WITH FINITE MEDIUM GREEN'S FUNCTIONS

Consider a single pipe with a Green's function whose Laplace transform has the form

$$\bar{q}_1(s) = \frac{u_1(s)}{v_1(s)} \quad (B-1)$$

If the singularities of $\bar{q}_1(s)$ are all simple poles the inverse transform of Eq. B-1 is found from (Ref. 2)

$$q_1(t) = \sum_i \frac{u_1(s_i)}{v_1'(s_i)} e^{s_i t} = \sum_i H_1(s_i, t) \quad (B-2)$$

where $v_1(s_i) = 0$ and the $H_1(s_i, t)$ are the residues at the poles s_i .

Next add a second pipe in series with the first pipe. Assume the Green's function for pipe 2 may be likewise expressed as

$$\bar{q}_2(s) = \frac{u_2(s)}{v_2(s)} \quad (B-3)$$

with

$$q_2(t) = \sum_j \frac{u_2(s_j)}{v_2'(s_j)} e^{s_j t} = \sum_j H_2(s_j, t) \quad (B-4)$$

and

$$v_2(s_j) = 0 \quad (B-5)$$

The required solution for the flux at the outlet of the second pipe is the convolution of Green's functions for the two pipes:

$$q_{\text{net}}(t) = \int_0^t q_1(\tau) q_2(t-\tau) d\tau \quad (B-6)$$

The Laplace transform of the net flux is

$$\bar{q}_{\text{net}}(s) = \bar{q}_1(s) \bar{q}_2(s) \quad (B-7)$$

$$= \frac{u_1(s)}{v_1'(s)} \frac{u_2(s)}{v_2'(s)}$$

Thus

$$q_{\text{net}}(t) = \sum_k \frac{u_1(s_k) u_2(s_k) e^{s_k t}}{v_1'(s_k) v_2'(s_k) + v_1(s_k) v_2'(s_k)} \quad (B-8)$$

where

$$v_1(s_k) v_2(s_k) = 0$$

It is easily seen the set of poles s_k is merely the sum of the set s_i plus the set s_j .^{*} Using Eqs. B-3 and B-5 in Eq. B-8 then gives

$$\begin{aligned} q_{\text{net}}(t) &= \sum_i \frac{u_1(s_i) u_2(s_i) e^{s_i t}}{v_1'(s_i) v_2(s_i)} + \sum_j \frac{u_1(s_j) u_2(s_j) e^{s_j t}}{v_1(s_j) v_2'(s_j)} \\ &= \sum_i \bar{q}_2(s_i) H_1(s_i, t) + \sum_j \bar{q}_1(s_j) H_2(s_j, t) \end{aligned} \quad (\text{B-9})$$

Notice that the solution for two pipes in series can be written in terms of the residues for each of the individual pipes. If Eqs. B-2 and B-4 may be considered exact solutions for each pipe (since any arbitrary degree of accuracy may be obtained), then Eq. B-9 is an exact solution as well.

The above method may be readily generalized to any number of pipes, say N , as

$$\bar{q}_{\text{net}}(s) = \sum_{n=1}^N \sum_m H_n(s_m^n, t) \prod_{\substack{\ell=1 \\ \ell \neq n}}^N \bar{q}_\ell(s_m^n, t) \quad (\text{B-10})$$

^{*} If any of the poles from the two sets coincide, then the procedure must handle second order poles in addition, requiring some modification of the above method.

where

$$\bar{q}_n(s) = \frac{u_n(s)}{v_n(s)} ; \quad n = 1 \dots N \quad (B-11)$$

$$v_n(s_m^n) = 0 ; \quad m = 1, 2, \dots \quad (B-12)$$

and

$$H_n(s_m^n, t) = \frac{u_n(s_m^n)}{v_n'(s_m^n)} e^{s_m^n t} \quad (B-13)$$

The quantity s_m^n is defined as the m^{th} pole for the n^{th} pipe.

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