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WASTE PIPE CALCULUS

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ABSTRACT

WASTE PIPE CALCULUS

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We present a rapid method of calculating transport in a network of one dimensional flow paths or "pipes". The method defines a Green's function for each flow path and prescribes a method of combining these Green's functions to produce an overall Green's function for the flow path network. A unique feature of the method is the use of the Laplace transform of these Green's functions to carry out most of the calculations.

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Waste Pipe Calculus

I. Introduction:

In studies of waste migration for the LLL Waste Management Project, a scheme for transporting waste along one dimensional flow-paths or "pipes" was implemented^[1]. A hydrology precalculation is used to define the flow-paths or "characteristics" for the one-dimensional convective diffusion equation. The solutions to this equation which satisfy appropriate boundary conditions are used to estimate the transport of waste.

The application of the solutions to this equation for successive flow-paths requires the evaluation of a convolution integral and several paths begins to increase the time spent for such a procedure by significant amounts. The main ingredient of this note is the representation of the solution to the convective diffusion equation as a Laplace transform. Such a representation lends itself to the problem of combining successive "pipes" on flow-paths by replacing a convolution in the time domain to a simple product in the transform space. The application of this technique to discrete and continuous flow-path models is the topic of this technical note.

II. Discrete Flow-Path Model

A. Definition

A discrete flow-path model (DFPM) is a set of nodes $\{N\}$ and a set of simple paths $\{P\}$. Any two nodes i and j in the DFPM are connected by some sequence of simple paths (or path). i and j are connected by a simple path if $P_{ij} \in \{P_k\}$.

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Each path has associated with it a set of parameters:

1) length	---- l
2) fluid velocity	---- v
3) dispersivity	---- α
4) retardation for nuclide group r	---- B_r

B. Single Nuclide Group Model

Let $C_r(z,t)$ be the density (K_g/m^3) of nuclide group r at position z and time t and $J_r(z,t)$ be its flux. Then C_r and J_r satisfy:

$$\begin{cases} \frac{\partial}{\partial z} J_r(z,t) + \frac{\partial}{\partial t} C_r(z,t) = 0 \\ J_r(z,t) - \frac{v}{B_r} C_r(z,t) + \alpha \frac{v}{B_r} \frac{\partial}{\partial z} C_r(z,t) = 0 \end{cases}$$

from which we can show that:

$$\frac{v}{B_r} \left(1 - \alpha \frac{\partial}{\partial z} \right) \frac{\partial}{\partial z} J_r + \frac{\partial}{\partial t} J_r = 0$$

Let us assume the following boundary conditions:

$$J_r = \delta(t) \text{ at } z = 0 \text{ (unit impulse)}$$

and $J_r \rightarrow 0$ as $z \rightarrow \infty$.

Then $J_r(z,t)$ is a Green's function and has the form:

$$J_r(z,t) = G_r(z,t) = \frac{z}{\sqrt{\frac{4\pi v \alpha t^3}{B_r}}} \exp \left[-\frac{\left(z - \frac{v}{B_r} t \right)^2}{4\alpha \frac{v}{B_r} t} \right]$$

and for the pipe with length L :

$$G_r(t) = \frac{L}{\sqrt{4\pi \frac{v}{B_r} \alpha t^3}} \exp - \left[\frac{\left(L - \frac{v}{B_r} t^2 \right)^2}{4 \frac{\alpha}{B_r} v t} \right]$$

The Laplace transform of this Green's function

$$G_r(s) = \int_0^\infty dt e^{-st} G_r(t) = \exp \left[\frac{L}{2\alpha} \left[1 - \sqrt{1 + \frac{4\alpha B_r s}{v}} \right] \right]$$

Let pipe p have input $J_{r,p-1}(t)$ and output $J_{r,p}(t)$. Then by the convolution theorem:

$$J_{r,p}(t) = \int_0^t dt' J_{r,p-1}(t') G_{r,p}(t-t')$$

But in transform space:

$$\overline{J_{r,p}}(s) = \overline{J_{r,p-1}}(s) \overline{G_{r,p}}(s)$$

And for a series sequence of pipes:

$$\overline{J_r}(s) = \prod_p \overline{G_{r,p}}(s) \overline{J_{r,0}}(s)$$

for each nuclide group r .

C. Coupled Nuclide Groups

The previous formalism may be extended to a vector set of radioactive waste fluxes $J_r(z,t)$ which is not only retarded in their motion through the host rock but also coupled to each other by the process of radioactive decay. The equations governing such a process are:

$$\frac{\partial}{\partial z} J_r(z,t) + \frac{\partial}{\partial t} C_r(z,t) = \sum_{p \neq r} q_{pr} C_p(z,t) - \sum_{s \neq r} q_{rs} C_r(z,t)$$

$$J_r(z,t) = \frac{v}{B_r} \left(1 - \alpha \frac{\partial}{\partial z} \right) C_r(z,t)$$

where q_{rs} is the transition rate from species r to species s .

Then:

$$v \left(1 - \alpha \frac{\partial}{\partial z} \right) \frac{\partial}{\partial z} J_r(z,t) + \frac{\partial}{\partial t} J_r(z,t) = \sum_p Q_{pr} J_p(z,t)$$

$$\text{where } Q_{pr} = q_{pr} B_r \quad p \neq r$$

$$= - \sum_{p \neq r} B_r q_{rp} \quad p = r$$

We apply the Laplace transform to the equation and obtain:

$$v \left(1 - \alpha \frac{\partial}{\partial z} \right) \frac{\partial}{\partial z} \overline{J_r}(z,s) = - \sum_p \left[\delta_{pr} s - Q_{pr} \right] \overline{J_p}(z,s) = - \sum_{p \neq r} M_{pr}(s) \overline{J_p}(z,s)$$

and diagonalize the matrix $M_{pr}(s)$ using the orthogonal transformation:

$D_{pq}(s)$. That is

$$\sum_{q,r} D_{pq}(s) M_{qr}(s) D_{ru}^{-1}(s) = \delta_{pu} m_p(s)$$

where the $m_p(s)$ are the eigenvalues of $M_{qr}(s)$.

If we define $\overline{J_k}(z,s)$ to be an eigen function of $\{M_{qr}(s)\}$

then

$$\overline{J_k}(z,s) = \sum_r D_{kr}(s) \overline{J_r}(z,s)$$

and the differential equations in $J_k(z,s)$ decouple:

$$\frac{\partial^2}{\partial z^2} J_k(z,s) - \frac{1}{\alpha} \frac{\partial}{\partial z} \overline{J_k}(z,s) - \frac{m_k(s)}{\alpha v} J_k(z,s) = 0 \quad k = 1, \dots,$$

In particular, we look at those solutions $\overline{G}_{rp}(z,s)$ for which

$\overline{G}_{rp}(0,s) = \delta_{rp}$. That is, $\overline{G}_{rp}(z,s)$ is the flux of species r at z given an injection of species p at $t = 0$.

Then:

$$\overline{J}_{kp}(0,s) = D_{kp}(s)$$

The solution $\overline{J}_{kp}(z,s)$ which vanishes as $z \rightarrow \infty$ is then:

$$\overline{J}_{kp}(z,s) = D_{kp}(s) \exp \left[\frac{z}{2\alpha} \left(1 - \sqrt{1 + \frac{4\alpha m_k(s)}{v}} \right) \right]$$

$$\text{and } \overline{G}_{rp}(z,s) = \sum_k D_{rk}^{-1}(s) D_{kp}(s) \exp \left[\frac{z}{2\alpha} \left(1 - \sqrt{1 + \frac{4\alpha m_k(s)}{v}} \right) \right]$$

Application of successive flow paths q with ℓ_q , α_q , v_q , and retardation B_{rq} gives:

$$\overline{G}_{rp}(z,s) = \prod_q \overline{G}_{qr,p}(\ell_q, s)$$

where the index q denotes successive matrix multiplications.

D. Series - Parallel Connection of Flow-Paths

In the formulation of the transport calculation defined so far, the flux was allowed to pass through a set of flow-paths connected in series. The resultant propagation in its most general form is described by a product of matrix operators:

$$\overline{G}(z,s) = \prod_q \overline{G}_q(\ell_q, s)$$

The index q is taken in the order of the connection of each serial flow-path.

If there are flow-paths in parallel, the evaluation of the transport resulting from such paths becomes a sum of products over series path

segments. The coefficient of each product is the fraction of the flow that participates in each series flow segment. Thus, for a series parallel connection the form of the Green's function describing the transport would be:

$$\bar{G}(z,s) = \sum_k \phi_k \prod_{q \in p_k} \bar{G}_q(z_q,s)$$

where ϕ_k is the flow fraction participating in path k and $\{q \in p_k\}$ is the set of series segments of that participate path p_k . Thus, the formulation of flow-path calculus for series-parallel path segments is quite straight forward.

An example with a sample discrete series-parallel flow-path model is illustrative.

Figure 1 displays a sample flow-path network involving eight distinct flow-path segments but three distinct flow-paths. The Green's functions for each segment are designated by G_p $p = 1, 8$, while the branching flow fractions are given by f_1 and f_2 .

Figure 1. Sample flow-path model

Based on Figure 3 there are 3 paths:

- $k = 1 : p = 1, 2, 3, 4 \quad \phi_1 = f_1$
- $k = 2 : p = 5, 6, 3, 4 \quad \phi_2 = (1-f_1)f_2$
- $k = 3 : p = 5, 7, 8, 4 \quad \phi_3 = (1-f_1)(1-f_2)$

We note $\phi_1 + \phi_2 + \phi_3 = 1$ and:

$$G = \phi_1 G_4 G_3 G_2 G_1 + \phi_2 G_4 G_3 G_6 G_5 + \phi_3 G_4 G_8 G_7 G_5$$

E. Evaluation of Moments

One advantage of the Laplace transform representation of Green's function is the ease with which one may obtain moments of the components of the net flux $J_p(z,t)$.

For each component nuclide r , we wish to calculate its mean arrival time $\bar{t}_r$ and the dispersion about that arrival time σ_{tr}^2 . These quantities are given by:

$$\bar{t}_r = \frac{\int_0^\infty dt' t' J_r(t')}{\int_0^\infty dt' J_r(t')}$$

$$\sigma_{tr}^2 = \left[\frac{\int_0^\infty dt' t'^2 J_r(t')}{\int_0^\infty dt' J_r(t')} \right] - \bar{t}_r^2$$

An elementary result from Laplace transform theory states that:

$$t_r = - \left. \frac{\partial}{\partial s} \ln J_r(s) \right|_{s=0}$$

$$\sigma_{tr}^2 = \left. \frac{\partial^2}{\partial s^2} \ln J_r(s) \right|_{s=0}$$

Then for series flow-paths where

$$J_r(s) = \prod_p \overline{G}_{rp}(p,s) J_0(s)$$

we obtain:

$$\bar{t}_r = \sum_p \bar{t}_{rp} + \bar{t}_0$$

$$\sigma_{tr}^2 = \sum_p \sigma_{trp}^2 + \sigma_{tro}^2$$

by applying logarithmic derivatives. The quantities $\bar{t}_{sp}$ and σ_{tsp}^2 are given by:

$$\bar{t}_{rp} = - \frac{\partial}{\partial s} \ln \bar{G}_{rp} (s_p, s) \Big|_{s=0}$$

$$\sigma_{tr}^2 = \frac{\partial^2}{\partial s^2} \ln \bar{G}_{rp} (s_p, s) \Big|_{s=0}$$

For flow-paths which are connected in parallel, where

$$\bar{J}_r(s) = \sum_p \phi_p \bar{J}_{rp}(s), \quad \sum_p \phi_p = 1$$

we obtain:

$$\bar{t}_r = \sum_p \phi_p \bar{t}_{rp}$$

$$\sigma_{tr}^2 = \sum_p \phi_p (\sigma_{trp}^2 + \bar{t}_{rp}^2) - \bar{t}_r^2$$

F. Conversion to Time Domain

Conversion to the time domain is obtained by applying the inverse Laplace transform to each series segment.

$$J_r(t) = \frac{1}{2\pi i} \sum_p \phi_p \int_{-i\infty+c}^{i\infty+c} ds' \exp(s't) J_{rp}(s')$$

The evaluation of each series segment can be accomplished by the use of the method of steepest descents. Thus:

$$J_{rp}(t) = \frac{1}{2\pi i} \int_{-i\infty+c}^{i\infty+c} ds' \exp(s't + g_{rp}(s'))$$

where $g_{rp}(s) = \lambda \eta J_{rp}(s)$.

Then:

$$J_{rp}(t) = \frac{1}{\sqrt{2\pi g'_{rp}(s)}} \exp \left[st + g_{rp}(s) \right]$$

with $t = g'_{rp}(s)$.

The general form of $-g'_{rp}(s)$ is plotting in Figure 2.

Figure 2. Expected form of $-g'(s)$.

$g'_{rp}(s)$ tends to have a singularity at some finite negative value of s and then decrease to zero as $s \rightarrow \infty$. Therefore, contributions for small t will come from large values of s while those for large t will come from negative values of s near the singularity.

References:

1. Berman, L. E. et al., "Analysis of Some Nuclear Waste Management Options," TASC, Report No. TR-1103-1-1, 28 June 1978, Appendixes D and F.