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### Title

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EFFECT OF SOURCE BOUNDARY CONDITIONS IN PREDICTING  
THE MIGRATION OF RADIONUCLIDES THROUGH GEOLOGIC MEDIA

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Both of the repository assessment programs have been ongoing for three years. This paper will present the progress that the assessment programs have made in the following areas:

1. mechanisms for radionuclide release (source term)
2. hydrology modeling
3. nuclide migration
4. environmental dispersion of nuclides
5. dosimetry
6. probabilistic approach
7. statistical approach

The paper will also provide a summary of the planned work for alternative media (i.e., other than bedded salt) and a summary of the research project.

#### 4. On Assessing the Long-Term Integrity of Nuclear Waste Repositories, Charles R. Hadlock, Peter D. Mattison (Arthur D. Little, invited)

In support of the U.S. Environmental Protection Agency in its development of environmental standards for high level radioactive waste disposal, Arthur D. Little, Inc., has developed a methodology for analyzing mechanisms that could lead to the release of radionuclides from deep geologic repositories and their possible transport to the accessible biosphere. Generic repository parameters were considered for five geologic host media: bedded salt, granite, basalt, shale, and salt domes. In all cases the repository was overlain by an aquifer; in the cases of bedded salt, basalt, and shale there was also an aquifer layer below the repository. Breach of containment mechanisms was identified for each repository type. These mechanisms were classified by cause (repository induced, human intrusion, natural events, engineering failures) and by release modes (direct release to air or land surface, release to overlying aquifer alone, release via aquifer interconnection, release to underlying aquifer alone, release to surface water). Depending on its expected likelihood of occurrence, mechanisms were modeled either probabilistically (usually in terms of an annual occurrence probability) or deterministically (in terms of an expected level or rate). Sufficient parameters to allow the calculation of the consequences of each breach mechanism were also estimated. In all cases, two sets of numerical estimates were generated. So-called "first estimates" were intended to apply to sites chosen so as to be favorable with respect to the mechanism in question. "Second estimates" were intended to apply to less than favorably chosen sites with respect to the mechanism in question, although they might be highly favorable with respect to other mechanisms. In the case of mechanisms that were not site dependent, second estimates were also used to cover other unfavorable circumstances. For the cases of both first and second estimates, the parameter values used were intended to be conservative; i.e., tending to bound the reasonably expected probabilities or consequences of the events.

#### 5. Effect of Source Boundary Conditions in Predicting the Migration of Radionuclides Through Geologic Media, M. Harada, F. Iwamoto, T. H. Pigford (UC-Berkeley)

Elsewhere we have presented the solution for the space-time-dependent concentration of radionuclides in one-dimensional (1-D) hydrogeologic transport through a sorbing

medium, using a boundary condition expressed as a time-dependent concentration of dissolved nuclides at the waste repository. Although this is the boundary condition commonly used in migration calculations, it is not consistent with a migration model which includes diffusional transport. It can introduce significant error in the prediction of concentration profiles near the source when diffusion and dispersion are appreciable and for low water velocities. Here we develop the solution in terms of a generalized time-dependent source, and we present the analytical solution resulting from using this boundary condition in a simple model of constant leach rate.

The 1-D transport is governed by the equation for the space-time-dependent concentration  $N_i$  of nuclide  $i$  in water flowing at velocity  $v$  through a sorbing medium

$$K_i \partial N_i / \partial t - D \partial^2 N_i / \partial z^2 + v \partial N_i / \partial z + \lambda_i K_i N_i = \lambda_{i-1} K_{i-1} N_{i-1} + F_i(t) \delta(z) \quad (-\infty < z < \infty, -\infty < t < \infty) \quad (1)$$

where  $F_i(t)$  represents the plane source (atoms/cm<sup>2</sup> s) of radionuclides dissolving in water at  $z = 0$ .

The initial condition and the infinite-medium boundary condition are

$$N_i(z, t) = 0, \quad t < 0; \quad N_i(\pm\infty, t) = 0 \quad (2)$$

The recursive solution, obtained by using Green's functions, is

$$N_i(z, t) = \int_0^t f_i(t - \theta) \exp(-\lambda_i \theta) \exp[-(z - v_i \theta)^2 / 4\kappa v_i \theta] / (4\pi\kappa v_i \theta)^{1/2} d\theta + \frac{\lambda_{i-1} v_i}{v_i - 1} \int_0^t \int_{-\infty}^{\infty} N_{i-1}(\xi, t - \theta) \times \exp(-\lambda_i \theta) \frac{\exp[-(z - \xi - v_i \theta)^2 / 4\kappa v_i \theta]}{(4\pi\kappa v_i \theta)^{1/2}} d\xi d\theta \quad ,$$

where

$$f_i(t) = F_i(t) / K_i \quad (3)$$

The recursive solution yields the concentration of nuclide  $i$  in explicit form

$$N_i(z, t) = \int_0^t f_i(t - \theta) \exp(-\lambda_i \theta) F(v_i \theta, z - v_i \theta) d\theta + \sum_{j=1}^{i-1} (\lambda_{i-1} \cdot \lambda_{i-2} \cdot \dots \cdot \lambda_j v_j / v_j) \times \int_0^t d\theta_i \int_0^{t-\theta_i} d\theta_{i-1} \dots \int_0^{t - \sum_{k=j+1}^i \theta_k} d\theta_j \times \exp\left(-\sum_{k=j}^i \lambda_k \theta_k\right) \times F\left(\sum_{k=j}^i v_k \theta_k, Z - \sum_{k=j}^i v_k \theta_k\right) \quad (4)$$

where

$$F(\alpha, \beta) = \exp(-\beta^2 / 4\kappa\alpha) / (4\pi\kappa\alpha)^{1/2} \quad .$$

The source term  $F_i(t)$  depends on the rate of solution of nuclide  $i$  from the waste material. To illustrate, assume an initial amount  $W^0$  of waste material per unit cross-sectional area for water flow, and assume that the waste matrix and its contained radionuclides dissolve at a constant total rate

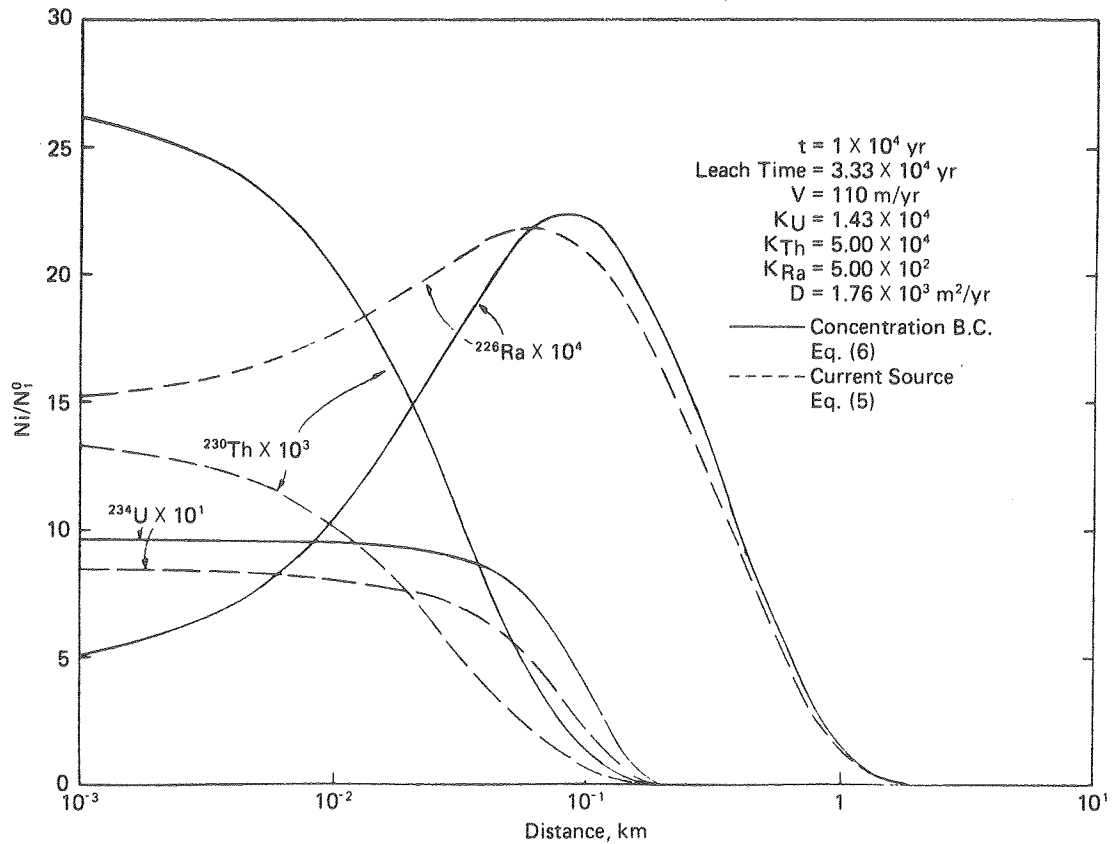


Fig. 1. Comparison of concentration profiles for different source boundary conditions (pure  $^{234}\text{U}$  source at  $t = 0$ ).

$W^0/F$ , where  $T$  is the leach time. The source term is then

$$F_i(t) = \frac{N_i(t)W^0}{T}, \quad (5)$$

where  $N_i(t)$  is the time-dependent amount of nuclide  $i$  per unit amount of waste material, given by the Bateman equation. In the special case of no diffusion or dispersion, the source term must equal the convection flow at  $z = 0$ , which yields the usual approximation of a concentration boundary condition

$$N_i(0, t) = \frac{F_i(t)}{V}. \quad (6)$$

The analytical solutions for the concentration boundary condition have been presented elsewhere.

The source boundary condition of Eq. (5) then results in the analytical solutions for a step release in Ref. 1, but with the function  $E(i, j; k)$  defined as

$$E(i, j; k) = \exp(z/2\kappa - \beta_{ij}t) \int_0^{(v_k t/4\kappa)^{1/2}} \frac{2}{\sqrt{\pi}} \times \exp\{-[\gamma y^2 + (z/4\kappa y)^2]\} dy \\ = \frac{\exp(-\beta_{ij}t + z/2\kappa)}{2\sqrt{\gamma}} \left\{ \exp(-Z\sqrt{\gamma}/2\kappa) \operatorname{erfc} \left[ \frac{Z - v_k t \sqrt{\gamma}}{(4\kappa v_k t)^{1/2}} \right] - \exp(Z\sqrt{\gamma}/2\kappa) \operatorname{erfc} \left[ \frac{Z + v_k t \sqrt{\gamma}}{(4\kappa v_k t)^{1/2}} \right] \right\} \\ (\gamma > 0). \quad (7)$$

The band-release solution is then obtained by applying the superposition method of Foglia et al.<sup>2</sup>

Figure 1 is an illustration showing the differences of the concentration profiles for the two different boundary conditions, calculated for the decay chain  $^{234}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra}$ , and with assumed parameters listed on the figure. The concentration profiles for the two boundary conditions are appreciably different in the regions near the repository. At greater penetrations into the geologic medium, the errors due to the use of the concentration boundary condition become less important. The two solutions become identical in the case of no dispersion.

1. M. FOGLIA, F. IWAMOTO, M. HARADA, P. L. CHAMBRÉ, and T. H. PIGFORD, "The Superposition Solution of the Transport of a Radionuclide Chain Through a Sorbing Medium," UCB-NE-3348 (June 1979).

2. M. FOGLIA, T. H. PIGFORD, and P. L. CHAMBRÉ, "The Superposition Equation for the Band Release of Decaying Radionuclides Through Sorbing Media," UCB-NE-3935 (Mar. 1979).

## 6. The Superposition Solution of the Transport of a Radionuclide Chain Through a Sorbing Medium, M. Foglia, F. Iwamoto, M. Harada, P. L. Chambré, T. H. Pigford (UC-Berkeley)

The prediction of the space-time-dependent concentrations of radionuclides undergoing hydrogeologic transport is of primary concern in the evaluation of geologic disposal of