**Assessment of Effectiveness of Geologic
Isolation Systems**

Systems Approximate Simulator: Fiscal Year 1982 Progress

May 1982

**Prepared for the U.S. Department of Energy
Office of Nuclear Waste Isolation
under Contract DE-AC06-76RLO 1830**

**Pacific Northwest Laboratory
Operated for the U.S. Department of Energy
by Battelle Memorial Institute**

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PACIFIC NORTHWEST LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC06-76RLO 1830

Printed in the United States of America
Available from
National Technical Information Service
United States Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

NTIS Price Codes
Microfiche A01

Printed Copy

Pages	Price Codes
001-025	A02
026-050	A03
051-075	A04
076-100	A05
101-125	A06
126-150	A07
151-175	A08
176-200	A09
201-225	A010
226-250	A011
251-275	A012
276-300	A013

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SYSTEMS APPROXIMATE SIMULATOR:
FISCAL YEAR 1982 PROGRESS

J. L. Devary
G. M. Petrie

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Pacific Northwest Laboratory
Richland, Washington 99352

ACKNOWLEDGMENTS

This research supported by the Assessment of Effectiveness of Geologic Isolation Systems (AEGIS) Program, was conducted by Pacific Northwest Laboratory, managed by Battelle Memorial Institute for the U.S. Department of Energy under Contract DE-AC06-76RLO 1830. The AEGIS Program is sponsored by the Office of Nuclear Waste Isolation (ONWI). The authors wish to thank R. G. Baca of Rockwell-Hanford, Richland, Washington, for supplying flow-path information of the Hanford basalt.

SUMMARY

The 'Systems' task of the Assessment of Effectiveness of Geologic Isolation Systems (AEGIS) Program is developing a Systems Approximate Simulator (SAS); a computer code of low-level technical complexity that incorporates the most significant waste-package, repository, and site processes affecting geologic nuclear waste isolation. This report discusses the AEGIS 1982 fiscal year progress toward building a SAS.

A computer code, SAS(82), has been developed as the site module of the SAS development effort. The SAS(82) is an efficient and accurate simulator of one-dimensional radionuclide transport. Features of the SAS(82) are direct (Monte Carlo) simulation, linear decay and sorption models, spatially and temporally varying hydrologic and geochemical variables, general travel-time distributions (possibly non-Fickian), and multinuclide release.

The SAS(82) was used to simulate radionuclide transport from a nuclear waste repository located within the Hanford basalts. A ^{99}Tc analysis along a thermally influenced path through the Grande Ronde Formation demonstrated the complexity of modeling near-field transport. Perturbed hydrologic conditions corresponding to "Hanford Basalt Geologic Simulation Model" results (Petrie et al. 1981) were evaluated, using the SAS(82).

Future work will include the development of SAS waste-package and repository modules as simplified process models become available. The SAS may eventually be used as the basis for parametric sensitivity and uncertainty studies for the entire geologic nuclear waste isolation system.

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1.0 INTRODUCTION

For the 1982 fiscal year (FY82), the Assessment and Evaluation of Geologic Isolation Systems (AEGIS) Program has adopted the basic work breakdown structure of the Office of Nuclear Waste Isolation (ONWI) and the Department of Energy National Waste Terminal Storage (DOE NWTs) by separating research into four areas: 1) waste-package research, 2) repository research, 3) site research, and 4) system research. Four computer models of low-level technical complexity are being developed by ONWI:

- PACSYM---waste package
- REPSYM---repository
- SITSYM---site
- SYSSIM---system.

The AEGIS 'Systems' task is developing a Systems Approximate Simulator (SAS), a computer model of low-level technical complexity that would qualify as a SYSSIM. The SAS is a modularized computer code that incorporates the most important aspects of waste-package, repository, and site processes of nuclear waste isolation. Figure 1 indicates the development status of the SAS for FY82. The SAS consists of three modules:

- Waste Package---This 'PACSYM'-type module is being developed by other ONWI contractors and will be included in the SAS when completed. The three characteristics of the waste package to be modeled are corrosion of the canister and overpack materials, leaching of the waste form, and transport of the radionuclides out of the emplacement niche. The output of this module would be 1) the radionuclide inventory at the repository at any time, and 2) the release time, duration, and leach rates for each radionuclide.
- Repository---This 'REPSYM'-type module also is being developed by other ONWI contractors and will be included within the SAS when available. Detailed modeling of repository effects on waste migration is an immense task due to the physical complexity of the problem. The output of this module would be 1) repository-induced,

FIGURE 1. Systems Approximate Simulator Development for Fiscal Year 1982

flow-field perturbations (i.e., the perturbations to the ground-water pore velocities and travel paths due to physical and thermal buoyancy effects), and 2) source locations or embarkation points in the flow field for radionuclide transport.

- Site--This 'SITSYM'-type module has been developed by the AEGIS program in FY82 and is referred to as the SAS(82) for the remainder of this report. The SAS(82) is a one-dimensional radionuclide transport code that includes 1) spatial and temporal variation in pore velocity, dispersion, and sorption, 2) multinuclide leach rates and release times, 3) linear decay chains, and 4) linear sorption.

Two other detailed process models are required as input to the SAS. The first, a three-dimensional ground-water flow and transport model, must exist for the proposed repository site for the calculation of nuclide travel paths from the repository to the biosphere. In the near-field, such a model must

include repository-induced, thermal buoyancy effects. In the far-field, a three-dimensional, finite element ground-water flow code such as FE3DGW may be used to determine the flow paths.

The second required process model, a dynamic geohydrologic model for the repository site, predicts changes in the radionuclide travel pathways corresponding to ongoing geologic processes for the period of time that the repository is considered to be active (10,000 to 1,000,000 years). The AEGIS Program has developed a Geologic Simulation Model computer code that fulfills these requirements (Petrie et al. 1981).

The information flow between the various computer models (shown in Figure 1) is as follows:

1. Changes in repository geometry caused by ongoing geologic processes are input to the Repository Module from the Geologic Simulation Model.
2. Repository thermal effects are input to the Waste Package Module from the Repository Module.
3. Repository breaching conditions (e.g., ground-water flow, percentage of radionuclide inventory affected) are input to the Waste Package Module from the Geologic Simulation Model.
4. The type, time, and quantities of radionuclides to be released to the ground-water flow system are input to the Site Module [SAS(82)] from the Waste Package Module.
5. The present-day flow system including pore velocities and pathways are input to the Site Module [SAS(82)] from the three-dimensional Hydrologic Flow and Transport Model.
6. Geologic perturbations of the present-day flow system are input to the Site Module [SAS(82)] from the Geologic Simulation Model.
7. The radionuclide release point from the repository is input to the Site Module [SAS(82)] from the Repository Module to determine the proper travel path to the biosphere.
8. The radionuclide activity-level distribution (over time) at the biosphere discharge point is output from the Site Module [SAS(82)].

The SAS research effort has purposely followed the path of modular computer code development so that state-of-the-art process models may be incorporated as they become available.

This report describes FY82 activities with an emphasis on the development of the SAS(82). Section 2 discusses conclusions and suggestions to future work; Section 3 describes the individual process models incorporated into SAS(82); Section 4 describes the numerical implementation of these process models; Section 5 examines test cases for SAS(82); and Section 6 provides an application of SAS(82) to radionuclide transport in the Hanford basalt.

2.0 CONCLUSIONS

The 'Systems' task of the Assessment of Effectiveness of Geologic Isolation Systems (AEGIS) Program is developing a Systems Approximate Simulator (SAS), a computer code of low-level technical complexity that incorporates the most significant waste-package, repository, and site processes affecting geologic nuclear waste isolation.

A computer code, SAS(82), has been developed as the site module of the SAS development effort. The SAS(82) is an efficient and accurate simulator of one-dimensional radionuclide transport. Features of the SAS(82) are direct (Monte Carlo) simulation, linear decay and sorption models, spatially and temporally varying hydrologic and geochemical variables, general travel-time distributions (possibly non-Fickian), and multinuclide release.

A waste package module must be developed that uses the material properties of the waste, canister, and overpack, as well as repository ground-water and temperature conditions to calculate radionuclide release times, rates, and durations. The AEGIS Program expects to receive a simplified waste-package model the latter part of FY82. The model is planned to be incorporated into SAS in FY83.

A repository module must also be developed that accepts as input the waste package leaching information, repository dimensions and thermal conditions, and ground-water flow to calculate the radionuclide distribution on the near-field/far-field boundary as a function of time. This involves a three-dimensional analysis with coupled flow, heat transfer, stress, and transport models for fractured media. Development of a computer code to cover this physical complexity is an enormous undertaking. A simplified version embodying these concepts probably will not be available in the near future. Thus, development of a SAS repository module to calculate near-field radionuclide transport does not now appear to be feasible in FY83.

3.0 SAS(82) PROCESS MODELS

The SAS(82) represents the development during FY82 toward a Systems Approximate Simulator (SAS), a computer code of low-level technical complexity that includes the most significant waste package, repository, and site processes that affect geologic nuclear waste isolation.

The SAS(82) is a one-dimensional transport code that calculates the arrival time distribution of radionuclides to a discharge point in the biosphere via a fixed travel path. To model random effects such as longitudinal dispersion and radioactive decay, the SAS(82) has been developed as a direct (Monte Carlo) simulation code. Radionuclide particles are released from the repository and are propagated along the travel path according to spatially and temporally varying pore velocities, sorption, and dispersion coefficients to the discharge point.

Radioactive decay is modeled into the SAS(82) as a linear chain

$$\alpha_1 \rightarrow \alpha_2 \rightarrow \dots \rightarrow \alpha_s \quad (3.1)$$

where α_1 is the parent element, $\alpha_2, \dots, \alpha_{s-1}$ are the daughter elements, and α_s represents the final nonradioactive stable element of the chain.

Geologic media sorption or retardation effects on radionuclide transport are modeled as follows:

$$V_\alpha = \frac{V}{R_\alpha} \quad , \quad D_\alpha = \frac{D}{R_\alpha} \quad (3.2)$$

where V_α and D_α are the pore velocity and dispersion coefficient of radionuclide- α , V and D are the pore velocity and dispersion coefficient corresponding to ground-water transport, and R_α is the retardation coefficient of radionuclide- α . Equation (3.2) assumes that sorption occurs rapidly relative to the ground-water pore velocity, allowing the chemistry of the ground water to be at or near equilibrium at all times.

The source module of the SAS(82) includes different release times, rates, and durations for each of the elements of the linear decay chain [Equation (3.1)] to reflect the exponentially decaying inventory of the repository, corrosion times of the cannister and overpack materials, and the different solubilities of individual radionuclides of a decay chain. A description of the transport, arrival time, decay, and sorption models implemented within SAS(82) are given below.

TRANSPORT EQUATIONS

The equations for mass transfer are extensions of the continuity equation for a specific chemical species. Stated in nonmathematical terms for a given control volume:

$$\begin{array}{lclcl} \text{Net rate of mass} & & \text{Net rate of accumu-} & & \text{Rate of chemical pro-} \\ \text{efflux of species A} & + & \text{lation of A within} & - & \text{duction of A within} \\ \text{from control volume} & & \text{control volume} & & \text{the control volume} \end{array} = 0$$

A general continuity equation in three-dimensions for multiphase transport of species α (Gray 1975) is written for porous media as:

$$\begin{aligned} \epsilon \frac{\partial \langle \rho_{\alpha} \rangle}{\partial t} + \langle \rho_{\alpha} \rangle \frac{\partial \epsilon}{\partial t} + \nabla \cdot (\langle V \rangle \langle \rho_{\alpha} \rangle) + \nabla \cdot \langle \hat{\rho}_{\alpha} \hat{V} \rangle \\ + \frac{1}{V} \int_{A_{fs}(t)} \rho_{\alpha} (V_{\alpha} - W_{\alpha}) \cdot n_{\alpha} dA = - \nabla \cdot \langle J_{\alpha} \rangle \\ - \frac{1}{V} \int_{A_{fs}(t)} J_{\alpha} \cdot n_{\alpha} dA + \epsilon \langle R_{\alpha} \rangle^f \end{aligned} \quad (3.3)$$

where

ρ_{α} = mass concentration of radionuclide- α in the fluid

V = fluid pore velocity

W = velocity of the interface

ϵ = porosity

J_{α} = diffusive flux of α with respect to the fluid pore velocity

R_α = rate of production of α in the fluid phase
 N_α = unit vector normal to the fluid-solid interface
 $\langle \rangle$ = the average of the quantity enclosed
 $\wedge$ = the local fluctuations of the quantity.

The first term in the general continuity equation is the accumulation term. The next term accounts for concentration changes caused by changes in porosity; this term is useful for unsaturated conditions. The third term accounts for convection of species by movement of the fluid. The following term is the divergence of the average of the product of the local fluctuations of the mass concentration and pore velocity. This represents hydrodynamic dispersion, as defined by Bear (1972). The last term on the lefthand side and the first term on the right in Equation (3.3) relate to the effect of geometry on diffusive flux (tortuosity) and the diffusive flux, respectively. The last two terms relate to interphase mass transport and chemical production, respectively.

Simplifying Assumptions

Equation (3.3) represents a completely general transport equation; however, not all the terms in Equation (3.3) are easily quantified given present technology. Several simplifying assumptions are necessary to obtain a usable formulation:

1. The effect of changing atmospheric pressure is assumed to be negligible.
2. A velocity field is required for input to the model. This data can be obtained from a hydrologic model or from analysis of data produced from a field study program. In either case, the flow field is calculated before computing the mass transport simulation. Inherent in this procedure is the assumption that the flow patterns are independent of the chemical composition or temperature of the groundwater solution. This assumption is sound if the system is nearly isothermal and all solutes are at relatively low concentrations. For radionuclide transport from a geologic repository, the concentrations of solute are not high enough to affect the viscosity or density of the solution. Near the waste repository the thermal

buoyancy effect influences the travel path and pore velocity within the vicinity of the repository, but does not in the far-field.

Thus, the isothermal condition seems appropriate for the Site module of the SAS development effort.

The above assumption allows decoupling of the mass transport equations from the flow equations and heat transport equations, enabling simulation of each phenomenon separately rather than simultaneously.

Resolution of the flow patterns below a certain scale in a regional aquifer usually is not feasible, if not impossible. This small-scale uncertainty in the flow field results in the term "mechanical or hydrodynamic dispersion" (Bear 1972).

Schwartz (1977) subdivided hydrodynamic dispersion by scale and called it microscopic, macroscopic, or megascopic dispersion. Each term represents the scale of heterogeneity in the ground-water system. At the microscopic scale, dispersion occurs because the complex network of interconnected passages that compose the soil structure causes continuous division and redivision of the flowing fluid. On the macroscale, local variations in lithologic units are responsible for dispersion. Regional variations in lithology account for megascopic dispersion. In any case, the variation in hydraulic conductivity accounts for mechanical dispersion.

The two larger-scale dispersions are made of microscopic dispersion and have results similar to molecular diffusion. In fact, Bear (1972) concluded that after a sufficiently long period of time hydrodynamic dispersion could be modeled as molecular diffusion. Therefore, for the SAS(82), it was assumed that hydrodynamic dispersion processes can be included with molecular diffusion on the relative flux term. Furthermore, the relative mass flux can be assumed to be adequately described by expressions of the form of Fick's first law. Thus,

$$J_{\alpha} = -\rho \bar{D} \nabla W_{\alpha} \quad (3.4)$$

where

ρ = total mass density of the solution

$\bar{\bar{D}}$ = hydrodynamic dispersion tensor

W_α = mass fraction of species α (ρ_α/ρ).

Incorporating this assumption into Equation (3.1) results in:

$$\epsilon \frac{\partial \langle \rho_\alpha \rangle}{\partial t} + \langle \rho_\alpha \rangle \frac{\partial \epsilon}{\partial t} + \nabla \cdot (\langle V \rangle \langle \rho_\alpha \rangle) = \nabla \cdot (\rho \bar{\bar{D}} \Delta W_\alpha) + \epsilon (R_\alpha)^f \quad (3.5)$$

Incorporated into Fick's first law are the assumptions that the mixture is an ideal solution and that only binary interactions at the molecular level are significant. The hydrodynamic dispersion tensor, $\bar{\bar{D}}$, is assumed to be a function of the media alone (i.e., we are considering transport where the solute is not subject to sorption effects).

The convective term can be expanded giving:

$$\nabla \cdot \rho_\alpha V = \rho_\alpha (\nabla \cdot V) + (V \cdot \nabla) \rho_\alpha \quad (3.6)$$

The pore velocity, V , can be expressed as q/ϕ where q is the Darcy velocity and ϕ is the effective porosity for saturated flow. The assumption here is that Darcy's Law holds for description of saturated ground-water flow.

Expanding Equation (3.6) results in:

$$\nabla \cdot \rho_\alpha V = \rho_\alpha \frac{q}{\phi^2} + \frac{\rho_\alpha}{\phi} (\nabla \cdot q) + V \cdot \nabla \rho_\alpha \quad (3.7)$$

If the transporting medium is assumed incompressible, which is valid except near the boiling point of water, then:

$$\nabla \cdot q = 0 \quad \text{for saturated systems,} \quad (3.8)$$

and

$$\nabla \cdot q = - \frac{\partial \phi}{\partial t} \quad \text{for unsaturated systems.} \quad (3.9)$$

For the SAS(82) the only region that would invalidate the above assumption would be near the nuclear waste repository and then for only a relatively short time after emplacement of the waste. Incorporating the preceding assumptions and assuming that the total mass density of the mixture is relatively constant, Equation (3.3) becomes:

$$\frac{\partial \rho_{\alpha}}{\partial t} + \nabla \cdot \nabla \rho_{\alpha} = \nabla \cdot \bar{\bar{D}} \nabla \rho_{\alpha} + r_{\alpha} \quad (3.10)$$

for saturated systems.

In ground-water systems, the source/sink term, r_{α} , is usually a complex function of several variables including soil or rock type, temperature, pressure, and concentration of all species found at any point in the system. The function is normally represented by a complex rate expression. However, for most problems of practical interest these expressions probably are not known; and because of very difficult experimental problems, these expressions probably will not be obtained before a waste repository is put into operation. Fortunately, most ground water moves slowly and reaction kinetics are rapid enough to allow the assumption that most constituents in ground-water systems are at or near chemical equilibrium at all times.

In one dimension, Equation (3.10) reduces to

$$\frac{\partial \rho_{\alpha}}{\partial t} + \nabla \frac{\partial \rho_{\alpha}}{\partial x} = \frac{\partial (\bar{\bar{D}} \frac{\partial \rho_{\alpha}}{\partial x})}{\partial x} + r_{\alpha} \quad (3.11)$$

where

x = spatial position

t = time

$\rho_\alpha = \rho_\alpha(x,t)$ = mass concentration of radionuclide- α

$V = V(x,t)$ = ground-water pore velocity (no sorptive effects)

$D = D(x,t)$ = longitudinal dispersion (no sorptive effects)

$r_\alpha = r_\alpha(x,t)$ = radionuclide- α source/sink.

(Sorptive effects for one-dimensional transport are discussed later.)

The one-dimensional transport approach was followed for the SAS(82) primarily for computational efficiency; however, considering radionuclide transport in fractured bedrock to be primarily one-dimensional along fractures is not unreasonable. The travel time of a radionuclide in the host bedrock constitutes essentially the entire travel time to the biosphere.

TRAVEL-TIME FORMULATION

Let the interval $0 \leq x \leq L$ denote the travel path from the repository to the biosphere. The left end-point (0) indicates the repository and the right end-point (L) indicates the discharge point to the biosphere. Assume a particle is released from the repository, and the arrival time (T) to the discharge point (L) is to be calculated. (For this case assume no decay or sorption). Using Equation (3.11) with $r_\alpha(x,t) = 0$ (no source or sink within the travel path) the arrival time (T) of the individual particle is a random quantity because of longitudinal dispersion.

For the case where $D(x,t) = \text{constant}$ and $V(x,t) = \text{constant}$, Equation (3.11) reduces to the classical convective-dispersion equation

$$\frac{\partial \rho_\alpha}{\partial t} + V \frac{\partial \rho_\alpha}{\partial x} = D \frac{\partial^2 \rho_\alpha}{\partial x^2} \quad 0 < x < L \quad (3.12)$$

that yields a Fickian travel-time distribution for a particle to traverse the distance L. The density function for the Fickian travel time distribution is given by:

$$f_L(t) = \frac{b}{\sqrt{\pi a}} \frac{\exp[-(t-b)^2/at]}{t^{3/2}} \quad (3.13)$$

where

$$a = 4D/V$$

$$b = L/V$$

The expected value and standard deviation of the travel time (T) is given by

$$E(T) = b = L/V \quad (3.14)$$

$$\sigma^2(T) = ab/2 = 2DL/V^3 \quad (3.15)$$

Notice that the expected travel time is distance divided by velocity.

In general, the pore velocity $V(x,t)$ and the longitudinal dispersion coefficient $D(x,t)$ are spatially and temporally varying quantities affected by radioactive decay and sorption. Let the travel path $0 \leq x \leq L$ be partitioned into segments

$$0 = x_0 < x_1 < x_2 \dots < x_n = L \quad (3.16)$$

such that when the particle is within a segment $x_{i-1} < x \leq x_i$, the pore velocity $V_\alpha(x,t)$ and dispersion coefficient $D_\alpha(x,t)$ of a radionuclide- α are constant. Thus, the arrival time (T) is given by

$$T = \sum_{i=1}^N \Delta T_i \quad (3.17)$$

where ΔT_i is the travel time of the particle across the segment $x_{i-1} \leq x \leq x_i$ which may be simulated from a Fickian travel time distribution with the proper dispersion coefficient and pore velocity.

The SAS(82) has been coded assuming a Fickian travel time distribution. Evidence indicates that the classical convection-dispersion Equation (3.12) provides an inappropriate description of mass transport in a natural hydrologic system (Gelhar, Gutjahr and Naff 1979; Smith and Schwartz 1980; Matheron and De Marsily 1980; Dagan and Bresler 1979; Simmons 1981). Simmons (1981) has suggested that a log-normal arrival time distribution (that corresponds to

log-normal hydraulic conductivity distributions) would be more appropriate for one-dimensional transport. The log-normal arrival time density is given by

$$f_L(t) = \frac{1}{\sqrt{2\pi} a} \frac{\exp[-(\ln t - b)^2 / 2a^2]}{t} \quad (3.18)$$

where b is the mean value and a is the standard deviation of the underlying Gaussian process [i.e., $\ln(T)$ is Gaussian with mean b and standard deviation a]. The expected value and variance of a log-normal arrival time distribution are given by

$$E(T) = \exp(b + a^2/2) \quad (3.19)$$

$$\sigma^2(T) = E(T) [\exp(a^2) - 1] \quad (3.20)$$

Simmons (1981) has shown that the log-normal density function approximates a Fickian density if the coefficient of variation of the travel-time distribution is less than one, that is,

$$\left| \frac{\sigma(T)}{E(T)} \right| < 1 \quad (3.21)$$

Equating the first two moments of the Fickian density [Equations (3.14) and (3.15)] with those of the log-normal density yields the parameters a and b of the log-normal density that correspond to a Fickian density with pore velocity (V) and dispersion coefficient (D)

$$a = \sqrt{\ln [1 + 2D/(LV)]} \quad (3.22)$$

$$b = \ln(L/V) - 0.5 \ln [1 + 2D/(LV)] \quad (3.23)$$

RADIOACTIVE DECAY

The SAS(82) is a radionuclide transport code with direct (Monte Carlo) simulation where atomic particles are released directly to a one-dimensional

hydrologic system so that the arrival times to a discharge point are simulated from a probability distribution (e.g., Fickian). The SAS(82) models first-order chain decay

$$\begin{array}{ccccccc} \alpha_1 & \rightarrow & \alpha_2 & \rightarrow & \dots & \rightarrow & \alpha_s \\ & & \tau_{\alpha_1} & & \tau_{\alpha_2} & & \tau_{\alpha_s} \end{array} \quad (3.24)$$

where α_1 represents a parent element, $\alpha_2 \dots, \alpha_{s-1}$ represent daughters, α_s represents a nonradioactive stable element, and $\tau_{\alpha_1}, \dots, \tau_{\alpha_s}$ represent the decay times from one element to the next.

The decay times $\tau_{\alpha_1}, \dots, \tau_{\alpha_s}$ are random quantities governed by stochastically independent exponential random variables with decay constants $\lambda_{\alpha_1}, \dots, \lambda_{\alpha_s}$. The probability density function (PDF) of an exponential random variable with decay constant λ is given by

$$\lambda \exp(-\lambda t) \quad , \quad t > 0 \quad (3.25)$$

The half life (HL) of a radioactive particle with decay constant λ is given by the median of the exponential distribution

$$HL(\lambda) = \ln(2)/\lambda \quad (3.26)$$

Given a particle α_1 to be released from the repository at time τ_0 , the decay times $\tau_{\alpha_1}, \dots, \tau_{\alpha_s}$ may be simulated by drawing stochastically independent variates $\tau'_{\alpha_1}, \dots, \tau'_{\alpha_s}$ from exponential- $\lambda_{\alpha_1}, \dots, \lambda_{\alpha_s}$ populations according to

$$\begin{aligned}\tau_{\alpha_1} &= \tau_0 + \tau'_{\alpha_1} \\ \tau_{\alpha_2} &= \tau_0 + \tau'_{\alpha_1} + \tau'_{\alpha_2} \\ &\vdots \\ \tau_{\alpha_s} &= \tau_0 + \tau'_{\alpha_1} + \dots + \tau'_{\alpha_s}\end{aligned}$$

To generate an exponential- λ variate (τ) from a uniformly distributed variate (v) on the interval $0 < x < 1$ [uniformly distributed (0,1) random number generators exist on all computers] let

$$\tau = -\ln(v)/\lambda \quad (3.28)$$

SORPTION

When considering sorption of the radionuclides by the porous media through which the radionuclide and water are flowing, Equation (3.12) becomes for one-dimension and first-order decay:

$$\frac{\partial \rho_{\alpha}}{\partial t} + \frac{Bd}{\phi} \frac{\partial S_{\alpha}}{\partial t} = D \frac{\partial^2 \rho_{\alpha}}{\partial x^2} - V \frac{\partial \rho_{\alpha}}{\partial x} - \lambda_{\alpha} \left(\rho_{\alpha} + \frac{Bd}{\phi} S \right) \quad (3.29)$$

where

Bd = bulk density of the media

ϕ = effective porosity

S_{α} = mass concentration of α sorbed to the porous media

λ_{α} = decay constant

Because the concentration of radionuclide is assumed to be small, the sorption equilibrium curve should be nearly linear and is described by

$$S_{\alpha} = Kd_{\alpha} \rho_{\alpha} \quad (3.30)$$

where, Kd_α is the distribution coefficient. Thus, by substituting Equation (3.30), the last term in Equation (3.29) becomes $\lambda_\alpha (1 + \frac{Bd}{\epsilon} Kd_\alpha) \rho_\alpha$. Since sorption is assumed to occur rapidly with respect to ground-water movement, Equation (3.30) becomes:

$$\frac{\partial S_\alpha}{\partial t} = Kd_\alpha \frac{\partial \rho_\alpha}{\partial t} \quad (3.31)$$

when differentiated with respect to time. Thus, Equation (3.29) becomes

$$R_\alpha \frac{\partial \rho_\alpha}{\partial t} = D \frac{\partial^2 \rho_\alpha}{\partial x^2} - V \frac{\partial \rho_\alpha}{\partial x} - R_\alpha \lambda_\alpha \rho_\alpha \quad (3.32)$$

after substituting Equation (3.31); R_α is the retardation coefficient to $1 + \frac{Bd}{\epsilon} Kd_\alpha$. Dividing Equation (3.32) by R_α yields.

$$\frac{\partial \rho_\alpha}{\partial t} + V_\alpha \frac{\partial \rho_\alpha}{\partial x} = D_\alpha \frac{\partial^2 \rho_\alpha}{\partial x^2} - \lambda_\alpha \rho_\alpha \quad (3.33)$$

which is similar to Equation (3.12) except for the $(-\lambda_\alpha \rho_\alpha)$ decay induced sink term and the radionuclide pore velocity (V_α) and dispersion coefficient (D_α) given by

$$V_\alpha = V/R_\alpha \quad (3.34)$$

$$D_\alpha = D/R_\alpha \quad (3.35)$$

4.0 NUMERICAL IMPLEMENTATION OF SAS(82)

The SAS(82) is a direct (Monte Carlo) simulation transport code that generates the arrival times of radionuclides released from a repository to a discharge point in the biosphere. In this section of the report, the internal programming and file structure of the SAS(82) will be described.

The SAS(82) is composed of four data files (CONTROL, STATIC HISTORY, VELOCITY, and ARRIVAL TIME) and three routines (RELEASE, FLOW, and DENSITY); Figure 2 contains the flow diagram for the SAS(82). In summary,

- RELEASE generates the STATIC HISTORY file that contains the radio-nuclide type, the release time, and the decay times for each particle to be released to the hydrologic system.
- FLOW reads the STATIC HISTORY file and generates the particle arrival times that are stored in the ARRIVAL TIME file. Arrival time distributions are determined from hydrologic parameters stored in the VELOCITY file.
- DENSITY reads the ARRIVAL TIME file and produces an arrival-time distribution for an output device (e.g., line printer or plotter).

The CONTROL file is used as input to execute any of the three routines; the SAS(82) was designed so that RELEASE, FLOW, or DENSITY may be executed independently of each other if the proper data files exist. For example, the same STATIC HISTORY file corresponding to a particular release scenario may be used as input to several different FLOW executions corresponding to different hydrologic travel paths. The SAS(82) was developed in a modular fashion so that it might incorporate waste-package and repository modules as simplified process models become available. A more detailed discussion of the internal structure of the SAS(82) is given below.

CONTROL FILE

CONTROL file is required as input to execute the RELEASE, FLOW, or DENSITY routines. CONTROL file contains the following information:

- the title of the analysis

FIGURE 2. SAS(82) Information Flow Diagram

- the number of radionuclides (s) in the linear decay chain

$$\alpha_1 \Rightarrow \alpha_2 \Rightarrow \dots \Rightarrow \alpha_s \quad (4.1)$$

and the radionuclide names and half-lives (years)

- the number of leaching time intervals, beginning and ending times for each interval (years), and the number of particles of each radionuclide type to be released in each interval
- the names of the STATIC HISTORY, VELOCITY, and ARRIVAL TIME files.

RELEASE ROUTINE

RELEASE creates the STATIC history file that contains the radionuclide type, release time, and decay times for each particle to be released to the hydrologic system. The RELEASE internal logic is as follows:

1. RELEASE reads from the CONTROL file the linear decay chain with half-lives, the leaching time intervals, the number of particles to be released per radionuclide type for each leaching time interval, and the STATIC HISTORY file name.
2. The particles to be released during a leaching time interval, $t_l \leq t \leq t_u$, are given random release times (τ_0) that are drawn from a uniform probability distribution with a range equal to the leaching interval, that is, with a probability density function given by

$$f(t) = \begin{cases} \frac{1}{t_u - t_l} & , \quad t_l < t < t_u \\ 0 & , \quad \text{otherwise} \end{cases} \quad (4.2)$$

3. The decay times for each radionuclide particle to be released to the hydrologic system are drawn from stochastically independent exponential probability distributions according to Equation (3.27).
4. RELEASE writes to the STATIC HISTORY file the particle type α_i , the release time τ_0 , and the decay times $\tau_{\alpha_i}, \tau_{\alpha_{i+1}}, \dots, \tau_{\alpha_S}$.

FLOW ROUTINE

FLOW is the transport routine of the SAS(82). For each particle to be released into the hydrologic system, FLOW calculates the arrival time to the discharge point and logs it into the ARRIVAL TIME file.

FLOW is based on one-dimensional radionuclide transport. The travel path is divided into N segments of possibly differing widths

$$0 = x_0 < x_1 < \dots < x_N = L \quad (4.3)$$

where x_0 represents the repository and $x_N = L$ is the discharge point. Figure 3 gives a representation of a three-dimensional travel path parameterized to one dimension. To allow for temporal variability, the time period for the simulation is partitioned into M time periods of possibly different lengths

$$0 = t_0 < t_1 < \dots < t_M = SL \quad (4.4)$$

SL represents the simulation length.

The spatial and temporal variability of the pore velocity and dispersion coefficients for a radionuclide- α are modeled as

$$\begin{aligned} V_{\alpha}(x, t) &= V_{ij\alpha} \quad \text{for } x_{i-1} \leq x < x_i \quad \text{and} \quad t_{j-1} \leq t < t_j \\ D_{\alpha}(x, t) &= D_{ij\alpha} \end{aligned} \quad (4.5)$$

FIGURE 3. A Three-Dimensional Travel Path Parameterized to One-Dimension

This means that the pore velocity and dispersion coefficient are homogeneous within the two-dimensional blocks of the displacement-time partition of Equations (4.2) and (4.3). The pore velocity and dispersion coefficient for a radionuclide- α are related to the ground-water pore velocity and dispersion coefficients according to Equations (3.34) and (3.35).

The FLOW internal logic is as follows:

1. FLOW reads from the CONTROL file the linear decay chain and the names of the STATIC HISTORY, VELOCITY, and ARRIVAL TIME file.
2. FLOW reads from the VELOCITY file
 - a) travel path length (L)
 - b) travel path partition $\{x_i\}$, $i = 1, \dots, N$
 - c) simulation length (SL)
 - d) the simulation time period partition $\{t_j\}$, $j = 1, \dots, M$
 - e) $V_{ij\alpha_k}$, $D_{ij\alpha_k}$, $i = 1, \dots, N$, $j = 1, \dots, M$,
and $k = 1, \dots, S$

Notice that retarded pore velocities and dispersion coefficients are read directly into FLOW from the VELOCITY file for each of the radionuclides of the decay chain.

3. For each particle to be released to the travel path
 - a) FLOW reads from the STATIC HISTORY file the radionuclide type α_i , the release time τ_0 , and the decay times $\tau_{\alpha_i}, \dots, \tau_{\alpha_{S-1}}$.
 - b) FLOW propagates the particle along the travel path to the discharge point L and records the arrival time and radionuclide type (it could change because of decay) in the ARRIVAL TIME file.

Stable particles (α_S) are not counted in the ARRIVAL TIME file.

Details on the FLOW calculation of particle arrival times to the discharge point are given below.

Let T denote the arrival time of a particle at the discharge point $x_N = L$. T is given by

$$T = \tau_0 + \sum_{i=1}^N \Delta T_i \quad (4.6)$$

where ΔT_i is the travel time of the particle across the path segment $x_{i-1} \leq x \leq x_i$. Because of the random nature of the decay times and longitudinal dispersion, ΔT_i , $i=1, \dots, N$ are random quantities and are simulated from travel-time probability distributions.

To simulate the travel time across the path segment $x_{i-1} \leq x \leq x_i$ let T_i be the 'present' time of a radionuclide - α_k particle at position x_{i-1} .

$$T_i = \tau_0 + \sum_{i'=1}^i \Delta T_{i'} \quad (4.7)$$

A travel time $\Delta T_{i'}$ is drawn from a Fickian travel time distribution corresponding to a displacement $\Delta x_i = x_i - x_{i-1}$, pore velocity = $V_{ij\alpha_k}$, and dispersion coefficient $D_{ij\alpha_k}$. The integer j indicates the position of the 'present' time T_i in the time grid [Equation (4.4)].

$$t_{j-1} < T_i \leq t_j \quad , \text{ for some } j = 1, \dots, M \quad (4.8)$$

If the particle velocity does not change in this time interval, that is,

$$T_i + \Delta T_{i'} \leq t_j \quad \text{and} \quad T_i + \Delta T_{i'} \leq \tau_{\alpha_{k+1}} \quad (4.9)$$

then $\Delta T_i = \Delta T_{i'}$ and $(T_i + \Delta T_i)$ is the 'new' time at spatial position x_i . The travel-time accumulation process then continues to the next travel path segment $x_i \leq x \leq x_{i+1}$.

If the particle pore velocity and/or dispersion coefficients change in the new time interval, that is,

$$T_i + \Delta T_{i'} > t_j \quad \text{or} \quad T_i + \Delta T_{i'} > \tau_{\alpha_{k+1}} \quad (4.10)$$

then the interval $x_{i-1} \leq x \leq x_i$ must be further divided to accurately estimate ΔT_i . Let ΔT be given by

$$\Delta T = t_j - T_i \quad \text{or} \quad \tau_{\alpha_{K+1}} - T_i \quad (4.11)$$

according to Equation (4.10). The distance traversed in time ΔT from position x_{i-1} is given by

$$\Delta x = \frac{\Delta T}{\Delta T_i} (\Delta x_i) \quad (4.12)$$

Thus, the particle is positioned at $x_{i-1} + \Delta x$ at time $T_i + \Delta T$. The original partition [Equation (4.3)] is modified (for this particle only) to

$$0 = x_0 < x_1 < \dots < x_{i-1} < x_{i-1} + \Delta x < x_i < x_{i+1} < \dots < x_N \quad (4.13)$$

The travel-time accumulation process then proceeds to the next travel path segment $x_{i-1} + \Delta x \leq x \leq x_i$.

For numerical simplicity the SAS(82) has implemented the log-normal approximation to the Fickian travel-time distribution [Equations (3.22) and (3.23)] because Gaussian random number generators are prevalent on most computer systems. An exponentiation of a Gaussian variate yields as log-normal variate.

DENSITY ROUTINE.

DENSITY is a data processing routine that analyzes the ARRIVAL TIME file and produces a smooth arrival-time density function from statistically irregular (noisy) histograms. DENSITY is based on the 'kernel' smoothing algorithm developed by E. Parzen and is described by Tapia et al. (1978).

Let $F(t)$ and $f(t)$ denote the cumulative distribution and density functions of a random variable T (arrival time)

$$F(t) = P [T \leq t] \quad (4.14)$$

$$f(t) = \frac{d F(t)}{dt} \quad (4.15)$$

Let $t_1, t_2, \dots, t_n$ be n independent observations of the random variable T . The empirical cumulative distribution of T corresponding to the random sample $t_1, t_2, \dots, t_n$ is the step-wise increasing function $F_e(t)$ given by

$$F_e(t) = \frac{1}{n} \times (\text{the number of } t_i \text{'s, } i = 1, \dots, n \text{ such that } t_i \leq t) \quad (4.16)$$

For example, $F_e(t) = 0$ for all t less than the minimum of $\{t_i\}$; $F_e(t) = 1$ for all t greater than or equal to the maximum of $\{t_i\}$. Figure 4 contains a plot of $F_e(t)$ for $n = 5$ sample values.

A smoothed estimate of the density function $[\hat{f}(t)]$ is derived from convolving the empirical distribution function $[F_e(t)]$ with a kernel or filtering function (K) .

$$\begin{aligned} f(t) &= \int_{-\infty}^{+\infty} K(t-z) dF_e(z) \\ &= \frac{1}{n} \sum_{i=1}^n K(t - t_i) \end{aligned} \quad (4.17)$$

To preserve the total mass of the arrival-time distribution, the kernel function must be normalized to unity in the L^1 -sense.

$$\int_{-\infty}^{+\infty} K(z) dz = 1 \quad (4.18)$$

FIGURE 4. Empirical Cumulative Distribution Function (n=5 Sample Values)

DENSITY uses symmetric kernel functions of the following form

$$K(z) = \frac{Q(z/h)}{h} \quad (4.19)$$

where Q may be one of these functions

$$Q_1(t) = \begin{cases} 1/2 & \text{for } -1 < t < 1 \\ 0 & \text{otherwise} \end{cases} \quad (4.20)$$

$$Q_2(t) = \begin{cases} 1 - |t| & \text{for } -1 < t < 1 \\ 0 & \text{otherwise} \end{cases} \quad (4.21)$$

$$Q_3(t) = \begin{cases} 15/16 (1 - t^2)^2 & \text{for } -1 < t < 1 \\ 0 & \text{otherwise} \end{cases} \quad (4.22)$$

Q_1 is known as a "box" kernel, Q_2 as a "triangle" kernel, and Q_3 as a "bell" kernel; Q_1 , Q_2 , and Q_3 are shown in Figure 5. The value h is known as the "window width" of the kernel and determines the degree of smoothing (large h = much smoothing). The window value may be estimated using the formula (Tapia et al. 1978)

FIGURE 5. a) "Box," b) "Triangle," and c) "Bell" Smoothing Kernels

$$h = \frac{1.07 \hat{\sigma}}{n^{(0.2)}} \quad (4.23)$$

where $\hat{\sigma}$ is the standard deviation of the random sample $t_1, t_2, \dots, t_n$.

The internal logic of DENSITY is as follows:

1. DENSITY reads the radionuclide types $\alpha_1, \dots, \alpha_{s-1}$ of the linear decay chain and the ARRIVAL TIME file name from the CONTROL file.
2. For each radionuclide $\alpha_K, K = 1, \dots, s-1$
 - a) DENSITY reads from the ARRIVAL TIME file the arrival-time data for α_K -particles,
 - b) DENSITY plots a histogram of the α_K -arrival time data,
 - c) DENSITY plots a smooth arrival-time density function. The user specifies the window width and the kernel function type ("box," "triangle," or "bell"). The default window width value is calculated from Equation (4.24) and the default kernel function is the "bell."

Examples of arrival-time density smoothing are contained in the next section of the report.

5.0 TEST CASES

In this section we describe two test cases that were run to check the numerics of the SAS(82). Case 1 involves the release of ^{129}I , considering only dispersive effects. Case 2 involves the point release of ^{248}Cm , considering only exponential decay effects. Analytical solutions exist for both test cases, permitting an evaluation of the direct-simulation approach to radionuclide transport modeling.

CASE 1

For CASE 1, the numerics of the Fickian travel-time distribution modeled within the SAS(82) were checked. The following parameter values were used for the analysis:

- radionuclide released-- ^{129}I , 1000 particles at time = 0
- half-life of $^{129}\text{I} = 1.72 \times 10^7$ years
- travel path length = 10,000 m
- number of travel path segments = 1
- ground-water pore velocity = 20 m/yr
- ground-water longitudinal dispersion coefficient = $2,000 \text{ m}^2/\text{year}$
- retardation coefficient of $^{129}\text{I} = 1.0$.

Because the expected arrival time (100 years) is short in comparison to the decay time (1.72×10^7 years) no decay is expected for the 200 particles that were released into the hydrologic system.

Using the log-normal approximation to the Fickian travel time distribution [Equations (3.22) and (3.23)], the parameter values of the log-normal density are $a = 0.14072$ and $b = 6.20471$. This results in an analytical solution arrival time density function

$$\frac{2.83501}{t} \exp [-(\ln t - 6.20471)^2 / (0.03961)] \quad (5.1)$$

Figure 6 contains plots of the DENSITY smoothed arrival-time density function and the analytical solution of the arrival-time density function. The

FIGURE 6. Plots of Analytical and DENSITY Smoothed Arrival Time Density Functions for ^{129}I

excellent agreement between the estimated and analytical density functions using 1000 particles indicates the strength of the direct travel-time simulation approach to radionuclide transport. (Default parameter values were used in DENSITY.)

CASE 2

For Case 2, the numerics of exponential decay were checked. The following parameter values were used in the analysis:

- radionuclide released— ^{248}Cm , 1000 particles at time = 0.
- decay chain $^{248}\text{Cm} \rightarrow ^{244}\text{Pu}$
- half-life of $^{248}\text{Cm} = 4.7 \times 10^5$ years
half life of $^{244}\text{Pu} = \text{infinite}$
- travel path length = 10,000 m

- ground-water pore velocity = 20.0 m/year
- ground-water longitudinal dispersion coefficient = 0 m²/year
- retardation coefficient of ²⁴⁸Cm = 1000
- retardation coefficient of ²⁴⁴Pu = 3000.

The half-life of ²⁴⁴Pu was assumed to be infinite so that an exact analytical solution of the ²⁴⁴Pu arrival time density could be calculated. No dispersion was allowed so that the exponential random decay effect could be isolated.

Let τ denote the exponentially distributed decay time associated with

Because the half-life of ²⁴⁸Cm equals 4.7×10^5 years, using Equation (3.26), the τ exponential density function is given by

$$\frac{1}{678,067} \exp\left(\frac{-t}{678,067}\right), \quad t > 0 \quad (5.2)$$

The ²⁴⁸Cm pore velocity equals 0.02 m/year, which implies that a ²⁴⁴Pu particle exits at the discharge point only if $\tau \leq 500,000$ years. The probability that $\tau \leq 500,000$ year is given by

$$\begin{aligned} P[\tau \leq 500,000] &= \frac{1}{678,067} \int_0^{500,000} \exp(-t/678,067) dt \\ &= 0.52164 \end{aligned}$$

that is, the proportion of ²⁴⁴Pu particles to pass through the discharge point is 52.164%.

The arrival-time distribution of ²⁴⁸Cm particles is a point mass at 500,000 years because the dispersion coefficient equals zero. Thus, 47.836% of all particles released will exit at the same time, 500,000 years, as ²⁴⁸Cm. The remaining 52.164% of particles will discharge as ²⁴⁴Pu with a smeared (nonpoint mass) distribution.

The arrival time of a ^{244}Pu particle (^{244}T) is given by

$$^{244}\text{T} = \Delta^{248}\text{T} + \Delta^{244}\text{T} \quad (5.3)$$

where $\Delta^{248}\text{T}$ is the ^{248}Cm travel time and $\Delta^{244}\text{T}$ is the ^{244}Pu travel time. Equation (5.3) is valid only if $\tau \leq 500,000$ years. Substituting τ , the ^{244}Pu pore velocity (0.00667 m/year), the ^{248}Cm pore velocity (0.02 m/year) into (5.3) yields

$$\begin{aligned} ^{244}\text{T} &= \tau + \frac{10,000 - \tau(0.02)}{0.00667} \\ &= 1.5 \times 10^6 - 2\tau \end{aligned} \quad (5.4)$$

The conditional density function for τ "given that $\tau \leq 500,000$ " is given by

$$\frac{\exp(-t/678,067)}{(678,067) P[\tau \leq 500,000)]} = \frac{\exp(-t/678,067)}{353,707} \text{ for } 0 < t < 500,000 \quad (5.5)$$

Therefore, the conditional density function of ^{244}T "given that $\tau \leq 500,000$ " is

$$\begin{aligned} &\frac{\exp\left(\frac{t - 1.5 \times 10^6}{2(678,067)}\right)}{353,707} \left(\frac{1}{2}\right) \\ &= \frac{\exp\left(\frac{t - 1.5 \times 10^6}{1.356 \times 10^6}\right)}{7.075 \times 10^5} \text{ for } 0.5 \times 10^6 < t < 1.5 \times 10^6 \end{aligned} \quad (5.6)$$

Figure 7 contains plots of the analytical solution density [Equation (5.6)] and a plot of the DENSITY smoothed arrival-time density using the default window width value [Equation (4.9)] and the "bell" kernel function (Q_3). The smoothed density does not accurately approximate the analytical solution in

FIGURE 7. Plots of Analytical and DENSITY Smoothed Arrival Time Density Functions for ^{244}Pu

those regions near the upper (1.5×10^6) and lower (0.5×10^6) limits of the arrival-time distribution because the smoothing window overlaps the range of Equation (5.6). However, DENSITY does accurately estimate the density in the region where the smoothing window does not overlap the range (e.g., $t = 1.0 \times 10^6$).

For most transport analyses, the default value smoothing of DENSITY is adequate for two reasons:

1. Most arrival-time density functions to be encountered have two "tails" that each gradually decrease to zero as t approaches the upper and lower limits of the distribution (e.g., the Fickian distribution of Case 1). The default value smoothing of DENSITY is inaccurate only when extremely truncated arrival-time distribution are encountered.

2. Radionuclide transport analyses would involve more than a point release of particles. Particle releases over a long time period (i.e., integrating point releases) yield an arrival-time distribution where the tail probabilities are an insignificant part of the total mass. The arrival time range would be large enough to permit accurate DENSITY smoothing for all but an insignificant part of the distribution.

6.0 HANFORD BASALT EXAMPLE

In this section, the SAS(82) simulation of radionuclide transport from a nuclear waste repository located within the Hanford basalts is discussed. Thus, the SAS approach to performance assessment of geologic nuclear waste isolation may be evaluated. The authors wish to acknowledge that the following description of the Hanford basalt geohydrology is largely a summary from the Basalt Waste Isolation Project paper of Baca et al. (1981).

HANFORD BASALT GEOHYDROLOGY

The basalt rock beneath the Hanford Reservation represents a stratiform or tabular geology characterized by sequences of individual basalt flows or layers that, in certain locations, are separated by pervious water-bearing horizons. The repository candidate basalt flow is known as the Umtanum and is located within the Grande Ronde Formation. The Umtanum flow is ~71 m thick and is laterally continuous across the basin. The basic geologic conceptual model consists of an alternating sequence of dense basalt flows and flow contacts.

Great differences in hydraulic properties between the dense basalt flows and flow contacts (hydraulic conductivity of dense basalt flow is $\sim 10^{-10}$ m/sec; hydraulic conductivity of flow top is $\sim 10^{-6}$ – 10^{-9} m/sec) causes a "stair-step" ground-water travel path from the Umtanum flow to a discharge point in the basalt outcrops. Under natural thermal conditions (i.e., assuming no repository heat), the ground-water travel path is predominantly horizontal with nominal upward ground-water movement through the basalt flows. The upward movement occurs because of an upward hydraulic gradient and a significant vertical anisotropy in the hydraulic conductivity for the dense basalt flows. Figure 8 contains a plot of a typical ground-water travel path through the Grande Ronde Formation, assuming no thermal effects from a nuclear waste repository located within the Umtanum flow.

Within the first 10,000 years after repository closure, the thermal plume affects travel paths by driving ground water upward from the repository to higher level basalt flows before the horizontal ground-water flow predominates. Figure 8 also indicates a ground-water travel path influenced by this thermal

FIGURE 8. Thermal Buoyancy Effects on Radionuclide Travel Paths in the Hanford Basalt

buoyancy effect. The difference in travel paths can result in significantly different radionuclide travel times to the biosphere.

Example 1-- ^{99}Tc Transport

For this example, the thermally influenced ground-water path of Figure 8 was used. Table 1 contains all relevant hydrologic information. The hydrologic data of Table 1 correspond to thermally influenced flow paths 100 years after repository closure, as reported in Baca et al. (1981), with the exception of the dispersion coefficients. The dispersion coefficients were calculated using longitudinal dispersivity values of 5.0 and 10.0 m for the dense basalt and flow tops, respectively, within the Grande Ronde [from Table 7-4 of Arnett et al. (1980)]. The length of this travel path was specified to be ~1 mile to correspond to the boundary of a hypothetical buffer zone now being considered by regulatory agencies.

For this example, the performance of the host rock was assessed on the basis of a key radionuclide, ^{99}Tc , that has a large initial repository inventory (6.1×10^5 Ci) and a long half-life (2.1×10^5 yr). [The inventory

is based on ~47,000 tons of heavy metal corresponding to one-half of the nations spent-fuel projected to the year 2000; see Baca et al. (1981).] A nondisruptive event involves releasing 10^{-5} years of the entire initial repository inventory over 10,000 years. For the SAS(82) run, it was assumed that one percent of the radionuclides were transported along the travel path indicated in Table 1. A constant release rate of 10^{-5} years for the total "transportable" ^{99}Tc inventory ($6.1 \times 10^3 = 6.1 \times 10^5 \times 10^{-2}$ Ci) was assumed for 1000 years commencing 100 years after repository closure. The anionic form of ^{99}Tc accounts for relatively low sorptive properties in basalt; a retardation coefficient value of 1.0 was used.

TABLE 1. Hydrologic Parameters for Hanford Basalt: Example 1

Zone	Description	Length, m	Flow Direction	Ground-Water Pore Velocity, m/yr	Ground-Water Dispersion Coefficient m^2/y
1	Repository backfill	6	up	0.01	0.0
2	Umtanum dense basalt	20	up	1.5	0.0
3	Umtanum flow top	17	up	150	0.0
4	Dense basalt	50	up	0.5	0.0
5	Flow top	400	horizontal	0.5	5.0
6	Dense basalt	100	up	0.03	0.15
7	Flow top	1000	horizontal	1.0	10.0

Figure 9 is a plot of the ^{99}Tc activity distribution as a function of time; the dispersive effects of zones 5, 6, and 7 drop the peak activity level from 6.1×10^{-2} Ci/year in the near-field zones (1 to 4) to 0.01 Ci/year at the end of the travel path. Ten thousand ^{99}Tc particles were released into FLOW for this simulation; default smoothing parameters were used in DENSITY.

Example 2-- ^{99}Tc Transport with GSM Effects

The Geologic Simulation Model (GSM--Petrie 1981) has predicted up to a doubling in Darcian flow within the Grande Ronde Formation ~600 years in the future. The enhanced flow is a result of combined climatic and geomorphic effects on recharge and regional head gradients.

FIGURE 9. ⁹⁹Tc Activity for Hanford Basalt: Example 1

For this example, the far-field (zones 5, 6 and 7) pore velocities and dispersion coefficients were doubled (see Table 2). The travel path and near-field hydrology parameters were as in Example 1. This assumes that the thermal buoyancy effects have not appreciably changed in 500 years. The same release rate (6.1×10^{-2} Ci/year) and duration (1000 years) for ⁹⁹Tc will be used as in Example 1, with release commencing 600 years after repository closure.

Figure 10 is a plot of the ⁹⁹Tc activity distribution as a function of time. The peak activity observed is 0.037 Ci/year at the end of the travel path. The doubling of Grande Ronde Darcian velocity resulted in a 50% increase in peak activity; this shows the potential impact of geologic perturbations to nuclear waste repository performance. Ten thousand ⁹⁹Tc particles were released into FLOW for this simulation; default smoothing parameters were used in DENSITY.

TABLE 2. Hydrologic Parameters for Hanford Basalt: Example 2

Zone	Description	Length, m	Flow Direction	Ground-Water Pore Velocity, m/yr	Ground-Water Dispersion Coefficient, m ² /yr
5	Flow top	400	horizontal	1.0	10.0
6	Dense basalt	100	up	0.06	0.30
7	Flow top	1000	horizontal	2.0	20.0

FIGURE 10. ⁹⁹Tc Activity for Hanford Basalt: Example 2

DISCUSSION

Examination of radionuclide transport in basalt has revealed an inadequacy of the SAS modeling approach. The SAS(82)--and most one-dimensional models--assumes a fixed travel path for radionuclides throughout the simulation time

period. For the release durations commonly considered in nuclear waste isolation problems (10,000 years in the nondisruptive release scenario) the travel path for the ground water could change because of thermal buoyancy effects and geologic activity.

The thermal buoyancy effect drives radionuclides to upper basalt layers where the natural ground-water flow finally predominates. The position where the natural ground-water flow dominates thermal buoyancy effects is, by definition, the near-field/far-field boundary. For the SAS to adequately model the thermal buoyancy effects, the capability to calculate the quantity of radionuclide (as a function of time) to be delivered to a particular far-field travel path must be included in development of the SAS REPOSITORY module. The FLOW routine of the SAS(82) is an adequate far-field transport model, assuming fixed travel paths.

Geologic changes in far-field travel paths (e.g., as a result of tectonic activity) may be accommodated by simply running FLOW over a multitude of travel paths as predicted by the Geologic Simulation Model (Petrie 1981) the multi-travel path approach is commonly used to supply multidimensionality to one-dimensional analysis capabilities.

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