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PRELIMINARY SEABED DISPOSAL MODELING STUDIES

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ABSTRACT

In order to evaluate the fluid flow, heat transfer, and ion migration rates within a postulated sub-seafloor waste disposal site, preliminary calculations and computer aided simulations were performed. A base case site description was formulated and a representative set of physical parameters were defined. This information was used in an advanced transport computer code developed by Intera Environmental Consultants to simulate, in detail, site behavior. The simulation studies were divided into an initial "short term" heat transfer study (Case 1) followed by a "long term" ion migration simulation (Case 2). Results for the Case 1 heat transfer studies showed that very high canister surface temperatures were reached within a few days and that a convective flow cell was clearly established; however, its effect was minimal in lowering canister temperatures. In the second case, the calculations showed that the transient convective flow cell strongly influences ion migration rates; however, this effect decreases directly as the heat generation rate of the waste in the canister decays. This mechanism for ion transport becomes unimportant after about 1000 years.

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Introduction

Sandia Laboratories is currently investigating the concept of sub-seafloor disposal of radioactive nuclear waste from nuclear reactors. Three major reports are available which describe the overall project and its development.^{1,2,3} In December 1977, work was initiated to augment the modeling and mathematical efforts of this project. This decision led to a brief review of appropriate and available computer codes that would be capable of describing the fluid flow, heat transfer, and, especially, the ion migration aspects of sub-seafloor disposal. Comprehensive transport codes have been developed by Battelle⁴, Oak Ridge⁵, and Intera Environmental Consultants⁶. The Intera code, which is currently being used by Sandia personnel for the Waste Isolation Pilot Plant studies, was chosen for the preliminary sub-seafloor simulations because of its demonstrated capabilities.

The Intera code was used through an agreement with Intera Environmental Consultants of Houston, Texas. Two meetings followed with Lantz of Intera Environmental Consultants on February 3 and March 14, 1978. During these Houston work sessions, the problem was formulated, a basic geometry was defined, input parameters and boundary conditions were specified, the simulation objectives were clarified, and the computer runs were performed. The results from these simulation studies are presented in the following sections.

Description of the Simulations

Two types of simulations were performed using the Intera code. First, the short-term (10 to 100 yrs) period was simulated, followed by a simulation incorporating ion transport and extending the simulated time to about 1 million years. In this study, the waste was assumed to be held in storage

ten years prior to emplacement. In the first case studied, only the thermal aspects of the problem were treated and no waste ions were introduced into the system. The objective was to assess the effects of conductive versus convective heat transfer. In the second case, four general types of chemical species were introduced: a non-adsorbing tracer and three ionic species with differing adsorption coefficients. In this second case, the object was to assess the migration rate of ions from an implanted canister to the ocean floor and to assess the effect on migration rates of convective circulation within the sub-seafloor formation.

Geometry

The initial task in defining the simulations was to establish a geometry and scale for the disposal concept. A system was defined as 1 canister (0.3 m x 3 m) implanted vertically at a level of 30 meters in a sediment layer 60 meters thick. Representation of the disposal concept is illustrated schematically in Figure 1.

The cylindrical sedimentary region, surrounding the canister and bounded by the ocean floor on the top and the basalt zone on the bottom, was subdivided into a r-z grid for numerical representation within the simulation code. This grid spacing is illustrated in Figure 2. The coordinates (r-z) were defined with the origin at the sea floor, directly above the canister. As illustrated, the two-dimensional region is divided into ten horizontal layers and ten radial sections. The radial spacing was logarithmic and the thicknesses of the horizontal layers were chosen arbitrarily to provide a good definition of gradients near the canister. The grid spacings in feet and meters are given in Table 1. Other factors and boundary conditions relating to the geometric description are given in

Figure 1. Schematic Diagram of Seabed Disposal Concept

Figure 2. Grid System for the Seabed Simulations

TABLE I

Grid Spacings for Seabed Disposal SimulationsHorizontal Sections

<u>Layer No.</u>	<u>Thickness</u>		<u>Layer No.</u>	<u>Distance from Center of Canister to Center of Layer</u>	
	<u>(ft)</u>	<u>(m)</u>		<u>(ft)</u>	<u>(m)</u>
1	44	13.4	1	+77	+23.5
2	30	9.1	2	+40	+12.2
3	15	4.6	3	+17.5	+ 5.3
4	5	1.5	4	+ 7.5	+ 2.3
5*	5	1.5	5	+ 2.5	+ 0.76
6*	5	1.5	6	- 2.5	- 0.76
7	5	1.5	7	- 7.5	- 2.3
8	15	4.6	8	-17.5	- 5.3
9	30	9.1	9	-40	-12.2
10	44	13.4	10	-77	-23.5

*canister

Radial Sections

<u>Section No.</u>	<u>Thickness(Δr)</u>		<u>Center of Section</u>	
	<u>(ft)</u>	<u>(m)</u>	<u>(ft)</u>	<u>(m)</u>
1	0.58	0.177	0.4	0.12
2	0.66	0.2	0.85	0.26
3	1.4	0.427	1.79	0.55
4	2.96	0.902	3.77	1.15
5	6.25	1.91	7.98	2.43
6	13.21	4.03	16.85	5.14
7	27.91	8.51	35.61	10.86
8	58.98	17.98	75.26	22.95
9	124.64	38.	159.03	48.48
10	263.39	80.3	336.06	102.46

Table II. Input parameters for the code are discussed in the next section.

Input Parameters

Input data for the Intera code consist of the system geometry, initial and boundary conditions, physical and chemical parameters, and many internal code setup parameters. Approximately 70 FORTRAN input data cards were required for the simulations. The data, format, and description of code options can be found in the User's Manual.⁶ The data setup and input for the current studies was performed in consultation with Lantz, Intera Environmental Consultants, Inc. A summary of the key simulation parameters is presented in Table III. These include thermal properties, physical properties, chemical data, heat generation rates, and system geometry. The results from the Intera code are presented in the following section.

Results

First, the thermal aspects were studied exclusive of ion migration. The simulated time period for this calculation was from 10 to 100 years and the age of the waste since reprocessing was assumed to be 10 to 100 years. Using this information and the data given in Table III, the resulting canister surface temperature history for this first case is:

<u>Time (days)</u>	<u>Temperature(surface canister)</u>		<u>Heat Rate (Kw/m³)</u>
	<u>(°F)</u>	<u>(°C)</u>	
0.28	298	148	34 - avg. 10-100 yr. waste
0.65	523	273	
1.0	667	353	
1.56	831	444	
2.74	1053	567	
5.63	1382	750	

TABLE II

<u>System Geometry Factors and Boundary Conditions⁶</u>	<u>SI</u>	<u>Intera</u>
Bed Thickness (canister at 30 m level)	~ 60 m	197 ft.
Canister	0.3 m OD x 3 m length	1.0 ft x 10 ft
External radius of simulated region	152.4 m	500 ft
Assumed 10 vertical layers and 10 radial positions		
Pressure (ref)	55,152 KPa	8000 psi
Temperature (ref)	274.65 °K	34.7 °F

TABLE III

Physical, Chemical, Thermal Data for the Seabed Simulations

<u>Thermal Properties</u> ³	<u>SI</u>	<u>Intera</u>
Thermal conductivity - porous medium	$7.8 \times 10^{-1} \frac{\text{W}}{\text{m}^\circ\text{K}}$	$10.82 \frac{\text{BTU}}{\text{ft}^\circ\text{F day}}$
Fluid Heat Capacity	$3.4 \times 10^3 \frac{\text{J}}{\text{Kg K}}$	$0.813 \frac{\text{BTU}}{\text{lb}^\circ\text{F}}$
Coefficient of Thermal Expansion	$2.6 \times 10^{-4} \text{K}^{-1}$	$1.44 \times 10^{-4} \text{F}^{-1}$
Solids Heat Capacity	$2.3 \times 10^3 \frac{\text{KJ}}{\text{m}^3^\circ\text{K}}$	$34.3 \frac{\text{BTU}}{\text{ft}^3^\circ\text{F}}$
Heat Generation Rates (see page 9) ³		
<u>Fluid and Seabed Properties</u>		
Fluid Density (@ 1.5°C)	$1.02 \times 10^3 \frac{\text{Kg}}{\text{m}^3}$	$63.65 \frac{\text{lb}}{\text{ft}^3}$
Solid Density ⁹	$2.77 \times 10^3 \frac{\text{Kg}}{\text{m}^3}$	$170 \frac{\text{lb}}{\text{ft}^3}$
Fluid Compressibility	$3.945 \times 10^{-7} \text{KPa}^{-1}$	$0.272 \times 10^{-5} \text{psi}^{-1}$
Hydraulic Conductivity ⁹	0.009 m/day	$0.00274 \frac{\text{ft}}{\text{day}}$
Porosity ⁹	0.75	0.75
Compressibility of Pore Structure	$4.35 \times 10^{-7} \text{KPa}^{-1}$	$0.3 \times 10^{-5} \text{psi}^{-1}$
Longitudinal Dispersivity Factor	6.1 m	20 ft.
Transverse Dispersivity Factor	0.61 m	2 ft.
Molecular Diffusivity ⁸	$1.16 \times 10^{-9} \text{m}^2/\text{s}$	$0.93 \times 10^{-5} \frac{\text{ft}^2}{\text{day}}$
Viscosity (see page 9)		

ComponentsComponent Adsorption Coefficients⁸

1. Tracer	0	0
2. Low (Kd)	$0.1 \text{ m}^3/\text{kg}$	$1.6 \text{ ft}^3/\text{lb}$
3. MED (Kd)	$10 \text{ m}^3/\text{kg}$	$160 \text{ ft}^3/\text{lb}$
4. HIGH (Kd)	$100 \text{ m}^3/\text{kg}$	$1600 \text{ ft}^3/\text{lb}$

TABLE III (cont.)

Viscosity versus TemperatureTemperature

$^{\circ}\text{F}$	$^{\circ}\text{C}$	SI N.s/m^2	Intera Cp
34.7	1.5	1.8×10^{-3}	1.8
212	100.0	0.3×10^{-3}	0.3
437	225.0	0.14×10^{-3}	0.14
705	373.9	0.024×10^{-3}	0.024
1382	750.0	0.02×10^{-3}	0.02

Heat Generation Rates⁽¹⁾

<u>Time (Years)</u>	<u>Volumetric Heat Generation Rate (KW/m³)</u>	<u>Heat Input Canister KW</u>	<u>Intera BTU/day</u>
0	487	108	8.85×10^6
3	88	19.6	1.6×10^6
10	49	10.9	8.96×10^5
100	3.5	0.78	6.4×10^4
1000	0.8	0.18	1.5×10^4

Case 1 $\dot{Q}$ = 6.3×10^5 BTU/day 10 - 100 yrs.

Case 2 $\dot{Q}$ = 6.3×10^4 BTU/day @ 100 yrs.

Canister Vol. = 7.85 ft^3 (0.223 m^3)

As indicated by these calculated results, the canister temperature rapidly becomes excessive. The objectives of these thermal analyses were to assess canister temperatures and to evaluate the effects of simultaneous conduction and convection in dissipating the heat. The conclusion is that natural convection plus conduction did not significantly dissipate the heat and thus did not maintain moderate canister temperatures (the calculated temperatures were extremely high).

In the second study (100 to 10^5 yrs) radioactive species were released and ion migration rates investigated. The effect of convective circulation was also studied and analytical models were used to better assess diffusion transport. The migration rates of four general types of ions were investigated using the Intera code. The four non-decaying ions were assigned equal initial concentrations and leaching rates but had distinctly different adsorption coefficients. These components and their corresponding K_d 's are listed in Table III. The enhanced migration rate due to convective transport during the first 1000 years was found to be about equal to that produced by diffusion. The average convective velocity between the canister and the sea floor for 100 year old waste was 5.6×10^{-3} m/yr. At this sustained rate, a non-adsorbing ion would migrate from the canister to the surface, 30 meters above, in about 5000 years. However, because of the decaying heat generation rate during the first 1000 years, the convective velocity becomes insignificant after 1000 years and, thus, after this period the ion migration becomes diffusion controlled.

Since the ion migration rates for times in excess of 1000 years are only diffusion controlled, several simplified analytical solutions were used to calculate approximate ion arrival times at the ocean floor. The following four cases were evaluated:

1. Continuous point source - spherical coordinates
2. Instantaneous point source - spherical coordinates
3. Instantaneous input to an infinite column - no flow
4. Instantaneous input to an infinite column - diffusion plus convective flow

These analytical solutions were for a non-adsorbing ion only. The breakthrough curve for the first calculation is given in Figure 3. As shown in this figure, the arrival time for the midpoint of this very wide breakthrough curve is about 28,000 years. In the second case, a pulse source was introduced and the resulting wave, 30 meters from this point source, was observed. This wave is also shown in Figure 3. In this case the maximum concentration occurred after about 4000 years. It should be noted that the arrival times are very strongly dependent upon the definition of breakthrough.

In the final two calculations column geometry was assumed rather than spherical geometry as in the previous cases. In these column calculations, a convective velocity was also added. The resulting curves are shown in Figure 4. The arrival time without flow was about 12,000 years as compared to about 4500 years with flow. However, as stated previously, the effect of flow diminishes very rapidly during the first 1000 years and we assumed a constant flow in this case equal to that for 100 year waste. Thus, the flow case arrival time is conservatively short. In the following section, future proposed studies are outlined.

Summary of Findings

1. The problem of seabed disposal seems to subdivide naturally into three time periods: 10 to 100 yrs, 100 to 10^3 yrs, and 10^3 —.

Figure 3. Point Source - Infinite Media (spherical coordinates)

Figure 4. Point Source - Infinite Media (1 D coordinate)

a. The period from 10 to 100 years cannot be simulated because of the high rate of heat generation and the simplicity of the model. Calculated canister temperatures during this period are in the thousands of degrees.

b. During the next time period, which is relatively short in terms of ion transport, the convective flow contribution is about equal to that of diffusion but becomes insignificant after about 1000 years.

c. The period beyond 1000 years is simply a diffusion problem with adsorption and radioactive decay.

2. From an analysis of the long time period problem (1000 years plus), it can be shown from the diffusion equation that the peak arrival time for ion migration from a pulse input is proportional to $(t = Z^2 K_D/D)$

a. distance squared, Z^2

b. adsorption coefficient, K_D

c. one over the molecular diffusivity, $\frac{1}{D}$.

This implies that the breakthrough times for ions to reach the ocean floor are quite sensitive to the canister emplacement depth.

3. It is felt that the long-term diffusion problem can be adequately modelled using spherical coordinates in an infinite media with a point source representation of the canister, though cylindrical coordinates (r-z) would be necessary to assess gradients near the canister and to treat the true boundary conditions. Also, if cylindrical coordinates were used, the problem would be much more difficult to solve.

4. For the cases studied, breakthrough began at about 1000 years, peaked for a pulsed point source at about 5000 years, and for a continuous

source reached the 50 percent level after 28,000 years. This was for a non-adsorbing species with the canister located 30 meters down into the sediment from the ocean floor.

Future Work

A study of arrival times (1000 yrs plus) and parameter sensitivities will be performed using a spherical coordinate diffusion model with adsorption and radioactive decay. Actual ionic species will be studied and actual waste concentrations included as an initial condition. The concentration history at the 30 meter level will be compared with available maximum permissible concentration, MPC, information. This will help identify ions of primary importance and elucidate the key factors affecting their escape.

References

1. W. P. Bishop, Editor, "Seabed Disposal Program, A First Year Report," December 1974, SAND74-0410.
2. Talbert, Daniel, Editor, "Seabed Disposal Program, Annual Report," January-December, 1975, SAND76-0256, 1976.
3. Talbert, Daniel, Editor, "Seabed Disposal Program, Annual Report Parts I and II," SAND77-120, 1976.
4. Lester, D. H., Jansen, G., Burkholder, H. C., "Migration of Radionuclide Chains Through Adsorbing Medium," BNWL-SA-5199, 1974.
5. Duguid, J. O. and Reeves, M., "Material Transport Through Porous Media: Finite-Element Galerkin Model," Environmental Sciences Division Publication 733, Oak Ridge National Laboratory, ORNL-4928, March 1976.
6. "Development of Radioactive Waste Migration Model," Intera Environmental Consultants, Inc., Document prepared for Sandia Laboratories, Sept. 1977.
7. Personal Communication with K. L. Erickson, Sandia Laboratories.
8. Personal Communication with D. M. Talbert, Sandia Laboratories.
9. Heath, G. Ross, G. Epstein and R. A. Prince, "Sea Disposal Program: Geochemical and Sedimentological Studies of North Pacific Sediments," Progress Report Jan. 1, 1976-Dec. 31, 1976, COO-26-89-6.

10. Crank, J., The Mathematics of Diffusion - 2nd Ed., Clarendon Press, Oxford, 1975.
11. Bear, Jacob, Dynamics of Fluids in Porous Media, American Elsevier Publishing Co., Inc. (1975).

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