JAERI-Research
95-046

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June 1995

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編集兼発行　日本原子力研究所
印　　刷　いばらき印刷㈱

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Source Term Modeling and Analysis for Vault/Trench Facilities Located in an Unsaturated Zone

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(Received May 24, 1995)

This report outlines an analytical work on the third test case, Test Case 2b, specified by the IAEA sponsored co-ordinated research programme on the safety assessment of near-surface radioactive waste disposal facilities (NSARS). Test Case 2b focuses on a source term modeling of a disposal facility in an unsaturated soil layer. This report includes an analytical method used, groundwater flow analyses, a screening approach used, and transport calculations carried out, for two types of facilities:

(1) a concrete vault with grout backfill around the waste, and

(2) an open trench with soil backfill around the waste.

Optional infiltration barrier test cases for two types of facilities are also analyzed. The results of the Test Case 2b are presented in this report, and show that the effectiveness of the concrete vault to reduce the infiltration rate to the facilities. Furthermore, in order to examine the suitability of an assumption that a soil layer is saturated, which is often used in safety analyses to avoid a complexity of analyzing an unsaturated-saturated groundwater flow, various conceptual models are applied for the evaluation of the source term. The results show that the assumption of the saturated condition does not always give enough conservative results and then it is important to simulate the unsaturated flow velocity.

Keywords: Safety Assessment, Screening Analysis, Radioactive Waste, Near-surface Disposal, Disposal Facility, Trench, Vault, Transport, Unsaturated Zone

不飽和土壌中に位置するボールト・トレンチ処分施設からのソースターム評価におけるモデル化と解析

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（1995年5月24日受理）

本報告書は、「放射性廃棄物浅地層処分施設の安全評価」に関するＩＡＥＡ協力研究プログラムで提案された標準問題、テストケース２ｂ、に関する解析結果を取りまとめたものである。テストケース２ｂは処分施設からの核種放出のモデル化の問題である。本報告書には、以下に示す２つのタイプの処分施設に対して使用した解析手法、スクリーニング手法、地下水流解析、核種移行解析を記述した。

(1)廃棄体の周囲をグラウトで充塡したコンクリートピット構造

(2)廃棄体の周囲を土で充塡したトレンチ構造

また、上記の構造に降雨浸透バリアを持った構造についても解析を行った。解析の結果、コンクリートピット構造は降雨浸透量を減少させるという有効性が示された。さらに、浅地層処分施設の安全評価において飽和－不飽和浸透流解析の困難さを回避するために用いられることの多い、土壌が飽和状態であるとの仮定の適切性を検討するため様々な概念モデルを用いてソースターム評価を行った。その結果、飽和状態を仮定することが必ずしも保守的な結果になるとはいえず、不飽和浸透流解析の重要性が示された。

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1. INTRODUCTION

The International Atomic Energy Agency (IAEA) Coordinated Research Programme (CRP) on The Safety Assessment of Near-surface Radioactive Waste Disposal Facilities (NSARS) has one of its main objectives to improve the reliability of safety assessment methodologies for a near-surface radioactive waste disposal facility by conducting exercises on model intercomparison or validation. The JAERI is participating in NSARS aiming at the validation of the safety assessment methodology which was developed to evaluate radiological consequences associated with shallow land disposal of low-level radioactive waste (LLW).

The first intercomparison exercise (Test Case 1)[1] in this respect was based on the near-surface disposal leading to leaching of activity to a saturated sand aquifer with exposures resulting from aquifer use via a well and from intrusion in to a repository. Simple repository concept in combination with an arbitrary geosphere was used to calculate exposure to man with respect to some typical radionuclides.

Based on the experience of Test Case 1, it was decided that the second intercomparison exercises (Test Case 2) would consider real-site conditions incorporating hydrogeology of an existing site, realistic source term, and detailed biospheric modeling. Test Case 2 has been divided into subdomains to address specific parts of the analysis (e.g., source term, geosphere, biosphere, etc.) rather than grouping all of the different parts of the problem into a single analysis. The first subdomain considered was real-site groundwater flow and transport through the geosphere using a specified source term (Test Case 2a). Individual dose was modeled for receptors at a well and a spring. The second subdomain considered is source term and engineered features of the disposal facility (Test Case 2b).

Source term and engineered features influence on release rates which provide the basis for all subsequent calculations in support of a safety assessment of the near-surface radioactive waste disposal facility. In Test Case 2b, the emphasis is placed on this near-field modeling. The test case specifically addresses waste form release, subsequent flow and transport through the facility (in the case of a concrete vault), and flow and transport through an unsaturated zone.

This test case is intended to mirror the approach that would be taken in an actual safety assessment. This test case requires how to screen the insignificant radionuclides as the first step. Then, conservative assumptions will be made regarding lifetimes of the engineered materials and more detailed analyses will be conducted for the most significant radionuclides after the screening.

This report describes analytical methodologies used here, i.e., modeling approaches for disposal systems to be analyzed, screening approaches for important radionuclides to be used in the subsequent analyses and computer codes for numerical analyses, and results and discussions of water flow and radionuclide transport calculations carried out for the two types of facilities:

(1) a concrete vault with grout backfill around the waste (vault scenario), and

(2) an open trench with soil backfill around the waste (trench scenario).

In addition, optional infiltration barrier test cases for two types of facilities are also analyzed (vault with cover scenario and trench with cover scenario). The results are presented in a standard form specified by the IAEA. Furthermore, the evaluations of source term are carried out by using four different conceptual models, to examine the suitability of the assumption of a soil layer being saturated.

2. SPECIFICATION OF TEST CASE 2B

Specifications for Test Case 2b are provided in this chapter.

2.1 Radionuclides and Waste Form

A list of 13 radionuclides is provided. Their half-lives and inventories to be used are specified in Table 1. The initial inventory of daughters is assumed to be zero (Table 2). The radionuclides were selected to represent common radionuclides with a variety of combinations of half-life, distribution coefficient, and radiotoxicity.

Table 1 Radionuclide half-lives and inventories.

Radionuclide	Half-life[2]	Inventory (Bq)
H-3	12.35 a	1.0E11
C-14	5730 a	1.0E10
Co-60	5.3 a	1.0E11
Ni-59	75,000 a	1.0E7
Ni-63	100 a	1.0E12
Se-79	65,000 a	1.0E7
Sr-90	28.8 a	1.0E12
Tc-99	2.13E5 a	1.0E7
Ru-106	1.08 a	1.0E10
I-129	1.57E7 a	1.0E7
Cs-134	2.06 a	1.0E7
Cs-137	30.2 a	1.0E12
Th-230	77,000 a	1.0E9

Table 2 Half-lives for daughter radionuclides.

Daughter radionuclide	Half-life[2]
Ra-226	1,600 a
Rn-222	3.82 d
Po-218	3.05 min
Pb-214	26.8 min
Bi-214	19.9 min
Po-214	1.6E-4 s
Pb-210	22.3 a
Bi-210	5.01 d
Po-210	138.4 d
Pb-206	Stable

It is assumed that all wastes are homogenous with flow and transport properties as defined and specified in Table 3 and radionuclides are instantaneously available for release. Properties in Table 3 are assumed to represent a mixture of the waste and backfill material used in the facility. This is a simplifying assumption as the wastes will actually be comprised of a variety of different materials with vastly different physical and chemical properties. The assumption is based on the concept that water will pass through the soil or grout as it migrates from the facility; as thus, transport will be impacted by the properties of the soil or grout. The values in Table 3 are assumed based on the expert judgment because the detailed data regarding the waste forms are not available. Also, the time-dependent material properties for the waste forms are assumed in Table 3. The waste forms are assumed to be converted to sand chemically behaves like the waste forms at 500 years.

Table 3 Assumed flow and transport properties for waste and backfill.

Parameter / Material	θ_s	θ_r	k_{sat} (cm/s)	β	α (cm^{-1})	$D^{*)}$ (cm^2/s)	α_L (cm)	α_T (cm)	ρ_b (g/cm^3)
Grouted waste (0-200 yr)	0.50	0.40	1E-8	1.57	7E-7	5E-9	5	2	0.5
Grouted waste (200-500 yr)	0.50	0.30	1E-6	1.7	0.075	5E-9	5	2	1.3
Grouted waste (> 500 yr)**)	0.38	0.04	5E-3	2.43	0.155	5E-6	10	2	1.9
Trench waste	0.30	0.07	1E-3	1.08	6.03E-3	5E-6	10	2	0.5

*): Effective diffusion coefficient (includes tortuosity and moisture content effects but does not include the effects of sorption).
**): The waste forms are assumed to be converted to sand that chemically behaves like the waste forms (The values for the grouted waste after 500 years are the same as those for the sand in Table 4).

Definition of Terms for Table 3 and Table 4:
θ_s; saturated moisture content; θ_r; residual saturation, α, β; fitting parameters for Van Genuchten equations [3], α_L, α_T; longitudinal and transverse dispersivities, ρ_b; dry bulk density.

2.2 Site Characteristics

The LLW disposal facility is located in the Atlantic Coastal Plain. The surrounding areas are characterized by gently rolling hills with no usual topographic features that significantly influence the general climate. The climate is characterized as being humid-subtropical.

Mean annual rainfall within the region is 120.2 cm/a. The mean annual evapotranspiration rate is 78 cm. Subtracting the mean annual evapotranspiration rate from the mean annual precipitation rate yields the mean annual infiltration rate of 42.2 cm/a.

2.3 Groundwater Hydrology and Geology

The unsaturated zone is comprised of eolian sands, and is characterized by light clayey sand at the top to dark red sandy clay at the base. The thickness of the unsaturated zone in the vicinity of the disposal facility varies from 10 m to 14 m. An average of 12 m will be assumed. Soil is assumed to be used as backfill around the engineered features of the vault facility and as backfill around the waste in the trench facility.

The characteristic curves describing the relationship between pressure head and water saturation are described by the expression developed by van Genuchten [3], which is

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\{1 + (\alpha|\psi|^\beta)\}^m} \qquad \text{(Eq. 1)}$$

where θ ; moisture content

θ_r ; the residual moisture content
θ_s ; the saturated moisture content
ψ ; the suction head (m)
α (1/m), β, $m = 1 - 1/\beta$; empirical constants.

The unsaturated hydraulic conductivity as calculated by the van Genuchten relationship is expressed as a function of the saturated conductivity and effective saturation, which is

$$K(\theta) = k_{sat}\sqrt{S}\{1-(1-S^{1/m})^m\}^2 \qquad \text{(Eq. 2)}$$

where $S = (\theta - \theta_r)/(\theta_s - \theta_r)$; the effective saturation [3] and
k_{sat}; the saturated hydraulic conductivity (cm/s).

The properties of the soils (clayey sand and sandy clay, clay and sand) are listed in Table 4, together with the values for engineered features. The hydraulic conductivities of soils are assumed based on the slug test data performed in the site. Also, the time-dependent material properties for the concrete are assumed based on the expert judgment in Table 4. The concrete is assumed to increase in permeability for 500 years and then turn to sand that chemically behaves like concrete, and thus the values for the concrete after 500 years are identical to those for the sand.

Table 4 Assumed flow and transport properties for soils and engineered features.

Parameter / Material	θ_s	θ_r	k_{sat} (cm/s)	β	α (cm^{-1})	$D^{*)}$ (cm^2/s)	α_L (cm)	α_T (cm)	ρ_b (g/cm^3)
Clayey Sand and Sandy Clay (native soil)	0.30	0.07	1E-5	1.7	0.075	5E-6	10	2	1.6
Clay	0.39	0.11	1E-8	1.33	8E-4	1.5E-6	5	2	1.6
Concrete (0-200 yr)*)	0.15	0.12	1E-8	1.57	7E-7	5E-9	5	2	1.3
Concrete (200-500 yr)*)	0.15	0.12	1E-6	1.7	0.075	5E-9	5	2	1.3
Concrete (>500 yr)**)	0.38	0.04	5E-3	2.43	0.155	5E-6	10	2	1.9
Sand	0.38	0.04	5E-3	2.43	0.155	5E-6	10	2	1.9

*): The time-dependent concrete properties are assumed based on the expert judgment.
**): The concrete is assumed to be converted to sand that chemically behaves like the concrete. The values for the concrete after 500 years is the same as that for the sand.

2.4 Geochemistry Data

Element-specific distribution coefficients for the different material types are provided in Table 5. For use in modeling, sorption is often simulated as a distribution coefficient, K_d, which represents the relative amount of the radionuclide sorbed to the soil and in solution. The retardation coefficient can be approximated using [4]:

$$R_d = 1 + \frac{\rho_b K_d}{\theta} \qquad \text{(Eq. 3)}$$

where R_d ; the retardation coefficient
ρ_b ; the soil dry bulk density (g/cm^3) and
K_d ; the distribution coefficient (cm^3/g).

2.5 Screening Calculations

Radionuclide inventories for LLW disposal facilities can contain 100 or more radionuclides. It is neither cost-effective nor necessary to consider all of the radionuclides in a detailed analysis. Thus, a simplified approach is needed to remove radionuclides of minimal or no consequence from further consideration in a safety assessment. In a safety assessment for a disposal facility it will likely be necessary to actually calculate doses during the screening to demonstrate that the doses are below regulatory limits for radionuclides that will be removed from consideration. It is suggested that the six most significant radionuclides will be considered in the comparison of the detailed analyses.

In general, screening approach should emphasize site characteristics as opposed to modeling of performance of an engineered facility. So that the data for the native soil was used for our screening calculations. Two additional parameters that may be of use in screening are discussed in this section: ingestion dose factors and groundwater travel time to the well. Table 6 includes conversion factors for ingestion dose for all radionuclides and daughters in the inventory based on ICRP 30 [7]. A conservative groundwater travel time of 5 years through the aquifer can be assumed. This value is based on assuming a pore velocity of roughly 100 m/a and a distance to the well of roughly 500 m (the travel time through the vadose zone requires more assumptions to defend, and thus ignored in screening). Although a 5 year travel time is likely to be an underestimate, it can be used as a conservative input for a screening exercise. It is important to specify that this is a conservative value for use in screening and is not intended to be an actual estimate of the groundwater travel time.

Table 5 Distribution coefficients (cm^3/g) assumed for different materials and solubilities1).

Element	Clayey sand and trench waste form2)	Clay [5]3)	Sand [5]3	Concrete and vault waste form [4]3)	Solubility (M) [6]5)
H	0	0	0	0	
C	2	1	5	5,000	
Co	10	500	15	24)	1.0E-2
Ni	9	600	400	5,000	1.0E-2
Se	5	700	150	24)	
Sr	8	100	15	2	
Tc	0.5	1	0.1	1	
Ru	100	800	50	304)	
I	5	1	1	30	1.0E-2
Cs	100	2,000	300	2	
Th	1,500	6,000	3,000	5,000	1.0E-46)
Ra	100	9,000	500	24)	1.0E-8
Pb	300	500	300	24)	
Po	100	3,000	150	14)	

1): Values are for use in this comparison. The values should not be assumed to be generally applicable for use in actual assessments. Some values have been rounded off.
2): Values are assumed for the trench waste. These values should also be used for the screening calculations.
3): Generic values from literature.
4): Assumed values based on expert judgment.
5): Several values are not provided in the specification.
6): Values selected from conservative end of range.

Table 6 Ingestion dose conversion factors [7].

Radionuclide	Adult ingestion dose per unit intake (Sv/Bq)
H-3	1.7E-11
C-14	5.7E-10
Co-60	7.3E-9
Ni-59	5.7E-11
Ni-63	1.5E-10
Se-79	2.35E-9
Sr-90	3.6E-8
Tc-99	3.95E-10
Ru-106	7.4E-9
I-129	7.4E-8
Cs-134	2.0E-8
Cs-137	1.35E-8
Th-230	1.5E-7
Ra-226	3.1E-7
Pb-210	1.4E-6
Po-210	4.4E-7

2.6 Engineered Facility

A schematic cross-section of the engineered concrete vault facility is provided in Fig. 1. For the purpose of this comparison, it is assumed that the interior length of the facility in the third dimension is 100 m. This does not include wall thickness at the ends of the facility. The walls at the ends of the facility not shown in Fig. 1 are assumed to be the same thickness as the wall shown in figure (60 cm). To facilitate drainage, the roof and floor of the facility in Fig. 1 are assumed to have a two percent slope with peaks at the plane of symmetry. Fig. 2 is a schematic cross-section of the trench facility. The dimensions of the trench are the same as the interior dimensions of the concrete vault. Thus, the interior length of the trench is also 100 m in the third dimension. No slopes are assumed for the trench. Detailed descriptions of the site configuration are given in the specification of Test Case 1 [1].

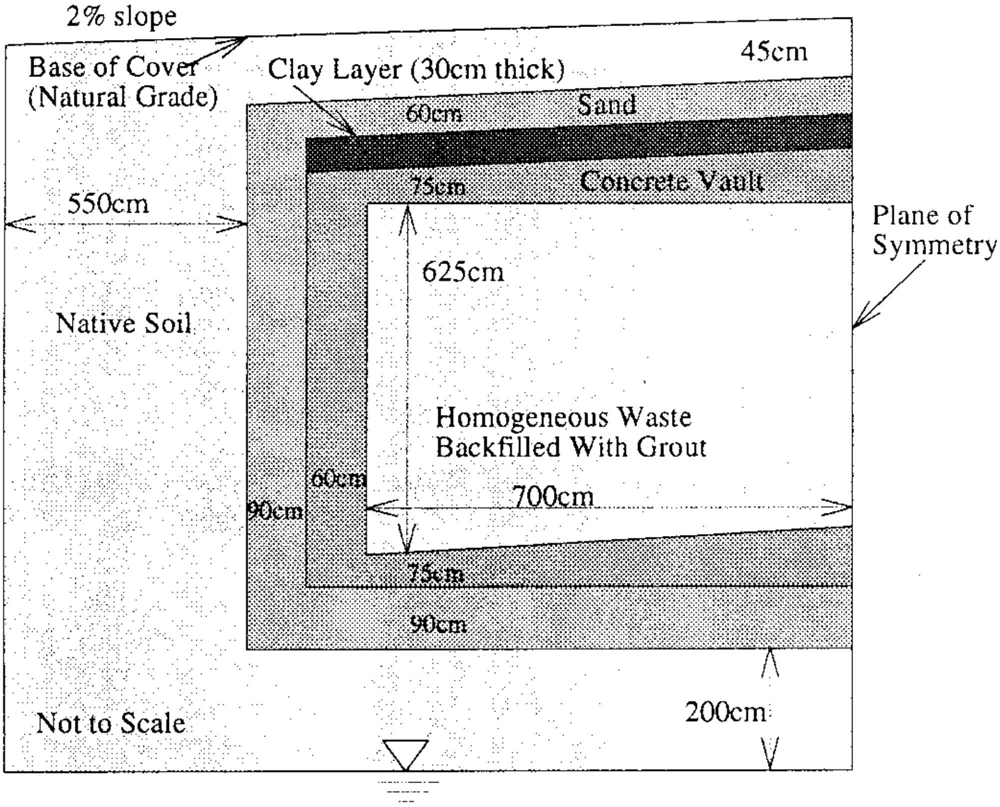


Fig. 1 Schematic cross-section of vault and surrounding soils.

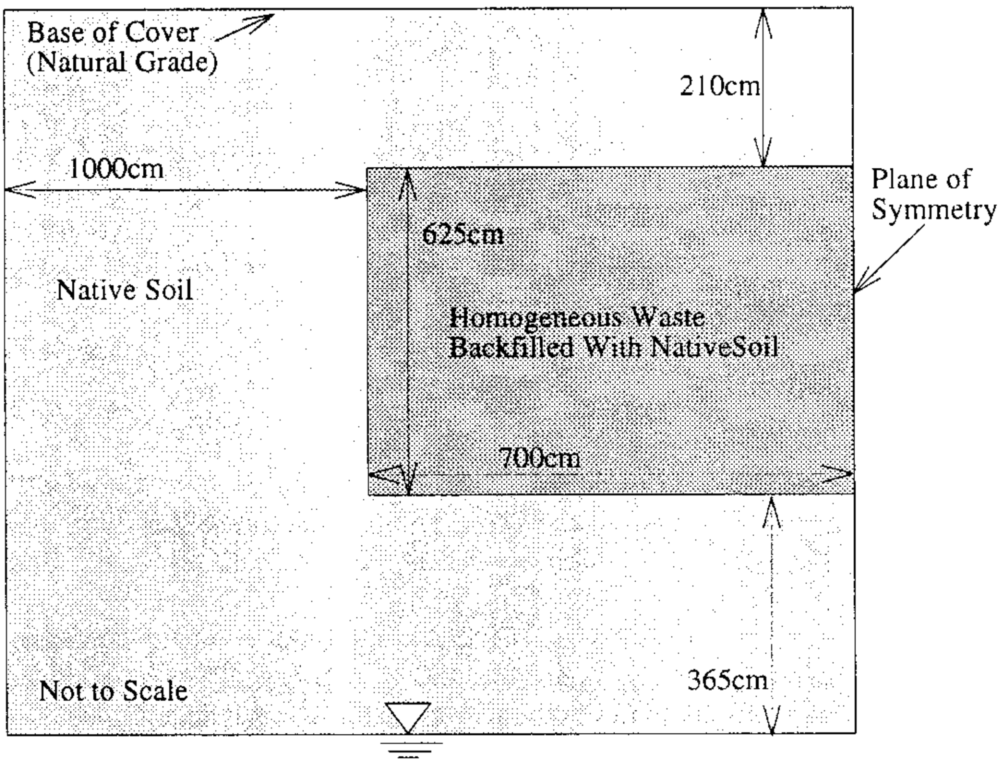


Fig. 2 Schematic cross-section of trench and surrounding soils.

Two different facilities are considered for the purposes of Test Case 2b. The first facility is the engineered concrete vault with a surrounding cocoon of high permeability material. The second facility is assumed to be the pit excavated in the native soil with the same interior dimensions as the concrete vault. The two facilities are also assumed to be at the same depth beneath the ground surface and containers are assumed to be 2 m tall and stacked 3 high in the facility.

The time-dependent material properties for the waste form and facility are provided in Table 3 and Table 4, respectively. The following assumptions are specified for this test case based on the expert judgment.

1. The concrete is assumed to increase in permeability for 500 years and then turn to sand that chemically behaves like concrete.
2. The waste form also is converted to sand at 500 years similar to the concrete facility.
3. The cover is also assumed to function effectively for 500 years. For the purposes of this test case, the cover is assumed to reduce the natural infiltration rate to an average of 1 cm/a. Thus, the participants should assume constant infiltration of 1 cm/a through the upper boundary of the domain illustrated in Fig. 1 and Fig. 2 until 500 years. After 500 years, participants should assume the average infiltration rate through the upper boundary as though no cover were present.
4. The clay layer above the vault is assumed to fail when the roof fails. This assumption is made because the roof is considered to provide support for the clay. As the roof fails, the support no longer exists, and thus, the clay is compromised. It is assumed that the clay behaves like native soil after failure.
5. Geochemical properties can be expected to persist for much longer times than the physical stability of the facility. Thus, the geochemical properties in Table 5 are assumed constant.

In addition, for the vault and trench with cover scenario,

1. Cover failure is assumed to correspond with failure of the structural stability of the concrete facility in the vault with cover scenario. At failure, the cover is assumed to change into native soil.
2. The cover is also assumed to fail at 500 years for the trench with cover scenario.
3. The properties for the Clayey Sand and Sandy Clay should be used for the Clay on the roof of the vault/trench after 500 years.

2.7 Output Requirements

The participants are asked to prepare a table listing the relative doses calculated for each of the thirteen radionuclides based on the screening calculations. The participants should also briefly discuss the rational for selecting the six radionuclides to be considered in the more detailed analyses.

Two tables are requested listing the maximum flux rates (Bq/a) to the water table for each of the six radionuclides considered in the detailed analyses (and daughters, as appropriate) and the time of maximum with one table for the concrete vault and the other for the trench. The flux should be calculated across a plane 2 m below the lowest point in the waste for both facilities (i.e., in the native soil beneath the vault and sand). Tables are also requested listing the maximum concentrations (Bq/cm^3) outside of the facilities and times of maximum for each radionuclide and daughter for each facility. Concentrations should be reported at the point of maximum concentration along a plane 2 m below the lowest point in the waste.

A figure for time dependent flux rates and a figure for time dependent concentrations are sought that include all radionuclides and daughters for each of the facilities. These results should be reported at the same locations as discussed previously. A total of four figures should be provided.

The participants are requested to assess the results of the simulations and discuss lessons learned and difficulties encountered. The participants are also requested to discuss the appropriateness of the parameter values assumed for the waste from and concrete facility. The general formulation of the time dependent material properties should also be discussed, including a discussion of potential changes in the geochemistry with time.

Furthermore, the participants are requested to discuss potential areas where conservatism could be reduced if the results of an assessment using these models were to indicate releases in excess of acceptable levels. For example, (1) Would it be easier to defend less conservative assumptions related to facility, container, or waste form lifetime ? or (2) How could conservatism be reduced ? These consideration form the basis for the iterative nature of safety assessments, as well as, emphasizing the radionuclide-specific nature of assumptions for detailed analyses.

2.8 Cover Design - Optional Case

The engineered cover is assumed to be placed immediately above the domain specified for the vault and trench simulations illustrated in Fig. 1 and Fig. 2. The configurations for the vault and trench simulations with the cover are provided in Fig. 3 and Fig. 4. The influence of the root zone is assumed to end at the drainage (gravel) layer in the cover as reflected in Fig. 3 and Fig. 4. The calculations will be used to represent evapotranspiration. These calculations yield a percolation rate of 42 cm/yr beneath the root zone based on averaged evapotranspiration rates of 78 cm/yr. This can be used as the flux boundary condition at the top of the model.

A two layer cover comprised of a gravel drainage layer and a clay barrier layer is assumed. The slope of the layers is assumed to be 2 % which is the same as the slope of the roof and floor of the vault. For the purposes of this comparison, the participants may also assume that the trench is sloped in the same manner. The cover is assumed to extend to a gravel drain which is assumed to be the same material as the drainage layer. Some leakage will occur through the base of the drain. Assumptions regarding the representation of the drain in the models will be left to the participants.

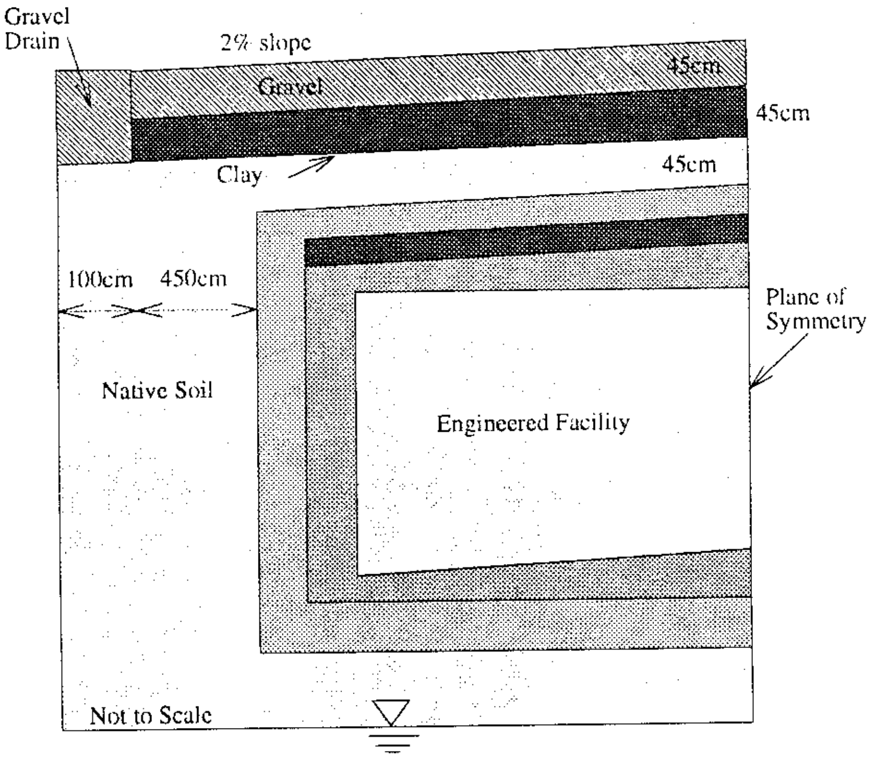


Fig. 3 Schematic cross-section of vault, surrounding soils, and cover.

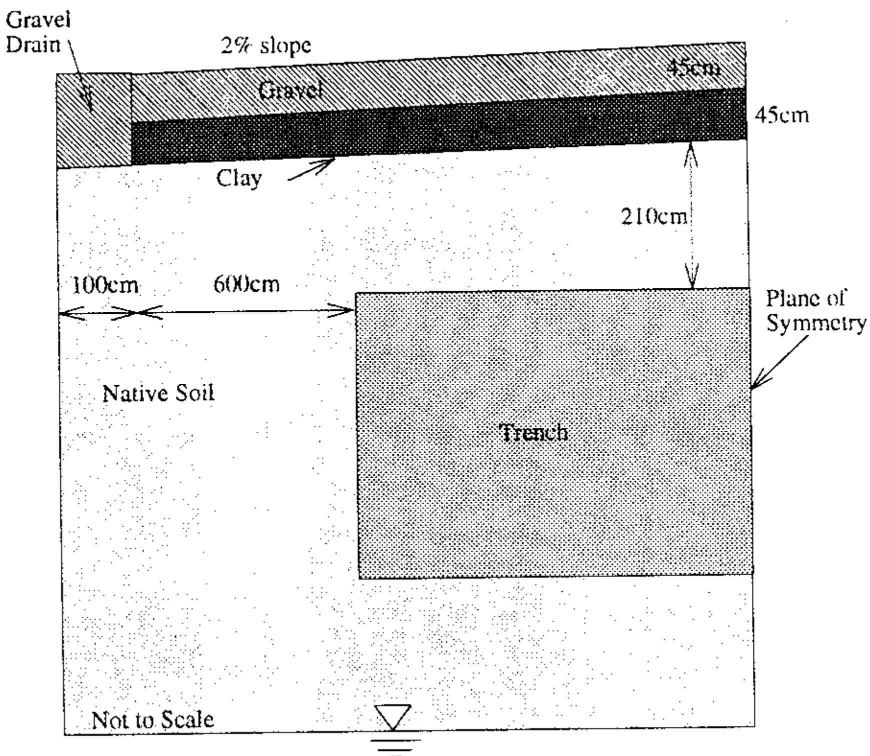


Fig. 4 Schematic cross-section of trench, surrounding soils, and cover.

2.8.1 Material Properties

Properties were specified in Table 3 - Table 5 for all materials except the gravel. Properties for the gravel are provided in Table 7 and Table 8. The values in Table 7 are representative of pea gravel. Distribution coefficients in Table 8 are based on the values of those for sand. This was assumed to be adequate given the minimal transport expected to occur through the gravel. The engineered cover is assumed to fail when the facility fails completely at 500 years. For the purposes of this simulation, the cover over the trench will also be assumed to fail at 500 years. At failure, the participants should assume that the cover materials are converted to the natural backfill soil (clayey sand and sandy clay), as defined in Table 4. This assumption is adopted because flow will be controlled by the backfill soils beneath the cover as moisture moves downward regardless of the cover properties.

Table 7 Assumed flow and transport properties for pea gravel[1].

Parameter / Material	θ_s	θ_r	k_{sat} (cm/s)	β	α (cm^{-1})	D[2] (cm^2/s)	α_L (cm)	α_T (cm)	ρ_b (g/cm^3)
Pea Gravel	0.30	0.07	1E-5	1.7	0.075	5E-6	10	2	1.6

1): Variables defined in Table 3 and Table 4.
2): Effective diffusion coefficient.

Table 8 Distribution coefficients (cm^3/g) assumed for different radionuclides[1].

Element	Pea Gravel [8][2]
H	0
C	5
Co	15
Ni	400
Se	150
Sr	15
Tc	0.1
Ru	50
I	1
Cs	300
Th	3,000
Ra	500
Pb	300
Po	150

1) Values are for use in this comparison. The values should be assumed to be generally applicable for use in actual assessments.
2) Generic values for sand from literature. Assumed to be adequate because minimal transport is assumed to occur in the gravel drain.

2.8.2 Output Requirements

The output requirements from section 2.7 should be used for the optional cover simulations too. Furthermore, the participants should discuss the appropriateness of the cover design, parameter values, and assumptions regarding degradation of the cover.

3. SCREENING CALCULATIONS

Radionuclide inventories for LLW disposal facilities can contain 100 or more radionuclides. It is neither cost-effective nor necessary to consider all of the radionuclides in a detailed analysis. Thus, it is needed to remove radionuclides of minimal or no consequence from further consideration in a safety assessment. Often a simplified, conservative approach can be used to compute doses to demonstrate that many of the radionuclides in the inventory are of minimal consequence. Test Case 2b requires to reduce the number of radionuclides to be considered in detailed analysis by screening.

3.1 Screening Approach

A screening calculation was done to determine the most important radionuclides for analysis. We used the following assumptions.

1. All of the radionuclides are released into the aquifer from the vault/trench instantaneously and they arrive a well by 5 years through a pipe having unit cross-section. (see Fig. 5)
2. Dispersion is neglected, travel time and decay-loss are taken into account.
3. Lead times for the initiation of radionuclide release from the vault/trench are (a) 0 year, (b) 100 years, (c) 200 years.
4. Intake rate of drinking water is 2,000 cm^3/day.

Based on the above assumptions, the equation used to calculate the individual dose D (Sv/a) is

$$D = DCF \times IW \times \frac{I \exp\{-\lambda(5R_f + t_{lead})\}}{VA(\varepsilon + \rho_{bulk} K_d)} \qquad \text{(Eq. 4)}$$

where
DCF ; dose conversion factor (Sv/Bq)
IW ; annual intake of drinking water (m^3/a)
I ; nuclide inventory (Bq)
λ ; decay constant (1/a)
t_{lead} ; lead time (a)
V ; Darcy velocity (30 m/a)
A ; cross-section of pipe (1 m^2)
ε ; porosity of native soil and
ρ_{bulk} ; dry bulk density of native soil (kg/m^3).

2.8.2 Output Requirements

The output requirements from section 2.7 should be used for the optional cover simulations too. Furthermore, the participants should discuss the appropriateness of the cover design, parameter values, and assumptions regarding degradation of the cover.

3. SCREENING CALCULATIONS

Radionuclide inventories for LLW disposal facilities can contain 100 or more radionuclides. It is neither cost-effective nor necessary to consider all of the radionuclides in a detailed analysis. Thus, it is needed to remove radionuclides of minimal or no consequence from further consideration in a safety assessment. Often a simplified, conservative approach can be used to compute doses to demonstrate that many of the radionuclides in the inventory are of minimal consequence. Test Case 2b requires to reduce the number of radionuclides to be considered in detailed analysis by screening.

3.1 Screening Approach

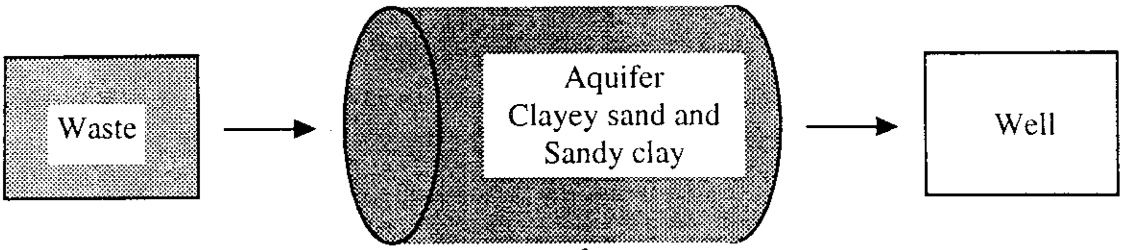
A screening calculation was done to determine the most important radionuclides for analysis. We used the following assumptions.

1. All of the radionuclides are released into the aquifer from the vault/trench instantaneously and they arrive a well by 5 years through a pipe having unit cross-section. (see Fig. 5)
2. Dispersion is neglected, travel time and decay-loss are taken into account.
3. Lead times for the initiation of radionuclide release from the vault/trench are (a) 0 year, (b) 100 years, (c) 200 years.
4. Intake rate of drinking water is 2,000 cm^3/day.

Based on the above assumptions, the equation used to calculate the individual dose D (Sv/a) is

$$D = DCF \times IW \times \frac{I \exp\{-\lambda(5R_f + t_{lead})\}}{VA(\varepsilon + \rho_{bulk} K_d)} \qquad \text{(Eq. 4)}$$

where
DCF ; dose conversion factor (Sv/Bq)
IW ; annual intake of drinking water (m^3/a)
I ; nuclide inventory (Bq)
λ ; decay constant (1/a)
t_{lead} ; lead time (a)
V ; Darcy velocity (30 m/a)
A ; cross-section of pipe (1m^2)
ε ;porosity of native soil and
ρ_{bulk} ; dry bulk density of native soil (kg/m^3).



Density; 1.6g/cm^3, Porosity;0.30,
Darcy velocity; 30.0 m/a,
Travel time for 500 m to a well; 5 years

Fig. 5 Concept for screening calculations.

The radionuclide which have large value of D is significant in this test case.

It should be noted that the dose values are for hypothetical conceptualization of a disposal system, and have therefore no absolute significance; moreover a number of simplifications were made to facilitate the screening.

3.2 Results of Screening

Table 9 shows the results of screening calculations. We calculated three cases changing with the lead time; 0, 100, 200 years. Also, Table 9 shows a ranking of radionuclides with respect to individual dose, for each cases. The top 6 radionuclides are typed bolded. It is clear that four radionuclides, Co-60, Ru-106, Cs-134 and Cs-137, have no radiological significance, because they will decay out before they reach the well from which drinking water is supplied. This is mainly due to their large K_d values and short half-lives. The results show that ranking of the radionuclides changes with the lead time. H-3 has a high ranking for the lead time of 0 year and 100 years, but it becomes insignificant for 200 years lead time. We selected the following six radionuclides for detailed analysis.

H-3, C-14, Ni-63, Sr-90, I-129, Th-230 and daughters

Note that this approach would cause some of the longer-lived radionuclides like as Se-79 and Tc-99 not to be considered. Also, no comparison is made to an actual dose standard. Although the ranking of dose is useful for this test cases, an actual screening approach would need to consider several calculations of individual dose and a comparison to a standard value in order to ensure that no potentially significant radionuclides are screened. With in mind that the ranking depends on the values of parameters, e.g., the lead time, we should select the adequate and conservative parameter values in the screening.

Table 9 Results of screening calculations.

Nuclide	Individual dose (Sv/a) Lead time 0year	rank	Lead time 100years	rank	Lead time 200years	rank
H-3	1.04E-1	2	3.80E-4	6	1.39E-6	8
C-14	3.93E-2	4	3.89E-2	1	3.84E-2	1
Co-60	4.05E-16	10	8.46E-22	10	1.77E-27	10
Ni-59	9.41E-7	9	9.41E-7	9	9.40E-7	9
Ni-63	4.54E-2	3	2.27E-2	3	1.14E-2	2
Se-79	6.88E-5	8	6.87E-5	8	6.86E-5	7
Sr-90	3.49E-1	1	3.15E-2	2	2.34E-3	3
Tc-99	8.74E-5	7	8.73E-5	7	8.73E-5	6
Ru-106	0.0	-	0.0	-	0.0	-
I-129	2.17E-3	5	2.17E-3	4	2.17E-3	4
Cs-134	0.0	-	0.0	-	0.0	-
Cs-137	4.79E-27	11	4.83E-28	11	4.87E-29	11
Th-230	1.06E-3	6	1.06E-3	5	1.06E-3	5

4. DESCRIPTION OF CONCEPTUAL MODEL

4.1 Governing Equations

In the modeling of groundwater flow and radionuclide transport, the following three basic equations are used.

1. The continuity equation which expresses mass conservation of fluid.
2. The Darcy's law for porous media which expresses momentum conservation.
3. The radionuclide transport equation which expresses mass conservation of solute.

Mass conservation of fluid

The continuity equation in a porous medium can be written.

$$\frac{\partial}{\partial t}(\theta\rho_w)+div(\rho_w\mathbf{u})=Q_f \qquad \text{(Eq. 5)}$$

where ρ_w ; the fluid density (kg/m^3)
$\mathbf{u}$; the Darcy velocity (m/sec)
t ; time (sec) and
Q_f ; the source or sink strength of fluid (kg/m^{3}sec).

The first term of Eq. 5 can be rewritten as the follows using pressure head h_p (m)

$$\frac{\partial}{\partial t}(\theta\rho_w)=\rho_w[C+S\rho_0 g(\alpha+\varepsilon\beta)]\frac{\partial h_p}{\partial t}\equiv\rho_w C'\frac{\partial h_p}{\partial t} \qquad \text{(Eq. 6)}$$

Table 9 Results of screening calculations.

Nuclide	Individual dose (Sv/a)					
	Lead time 0year	rank	Lead time 100years	rank	Lead time 200years	rank
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Co-60	4.05E-16	10	8.46E-22	10	1.77E-27	10
Ni-59	9.41E-7	9	9.41E-7	9	9.40E-7	9
Ni-63	4.54E-2	3	2.27E-2	3	1.14E-2	2
Se-79	6.88E-5	8	6.87E-5	8	6.86E-5	7
Sr-90	3.49E-1	1	3.15E-2	2	2.34E-3	3
Tc-99	8.74E-5	7	8.73E-5	7	8.73E-5	6
Ru-106	0.0	-	0.0	-	0.0	-
I-129	2.17E-3	5	2.17E-3	4	2.17E-3	4
Cs-134	0.0	-	0.0	-	0.0	-
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$$C' = C = \varepsilon \frac{\partial S}{\partial h_p} \quad \text{(unsaturated case)} \tag{Eq. 7}$$

$$C' = S_w = S\rho_0 g(\alpha + \varepsilon\beta) \quad \text{(saturated case)} \tag{Eq. 8}$$

where
C ; the specific moisture capacity (1/m)
S ; the saturation rate of water
ρ_0 ; the fluid density at a reference temperature (kg/m^3)
g ; gravitational acceleration (m/sec^2)
α ; the compressibility of rock (m^2/N)
β ; the compressibility of water (m^2/N)
ε ; the porosity of porous media and
S_w ; the specific storage (1/m).

The specific moisture capacity C is zero for the saturated case because the saturation rate S is constant for an increment of pressure head h_p. The effect of water and rock/soil compressibilities on the storage of water under the unsaturated conditions are usually small compared to the effect of changes in S, and therefore the specific storage S_w can be neglected for the unsaturated case.

Momentum conservation

The Darcy's equation is commonly adopted for the motion of groundwater flow in a porous medium

$$\mathbf{u} = -\mathbf{K}_f[\nabla(h_p + h_e) - \mathbf{e}_z \frac{\rho_w - \rho_0}{\rho_0}] \tag{Eq. 9}$$

where
$\mathbf{K}_f$; the hydraulic conductivity tensor (m/sec)
h_e ; the elevation head pressure (m) and
$\mathbf{e}_z$; an unit vector in a gravitational direction.

Note that $\mathbf{K}_f$ is generally the function of temperature and is also the function of pressure head in the unsaturated cases. In theory we must consider a corresponding equation for the motion of air in the unsaturated porous media. However, if we assume that the air is stationary or its movement can be ignored, Eq. 9 is valid for the unsaturated porous media. Therefore, Eq. 9 is adopted for this test case.

Mass conservation of solute

Transport of a chain of decaying solute species is described by the following equation considering advection, dispersion and adsorption on the surface of a solid:

$$\begin{aligned}\nabla(\mathbf{D}\nabla C_k - \mathbf{u}C_k) &= \frac{\partial}{\partial t}[\theta C_k + \rho_s(1-\varepsilon)C_{S,k}] + \lambda[\theta C_k + \rho_s(1-\varepsilon)C_{S,k}] \\ &\quad - \sum_{m=1}^{k-1} \xi_{km}\lambda_m[\theta C_m + \rho_s(1-\varepsilon)C_{S,m}] - Q_k\end{aligned} \tag{Eq. 10}$$

$$D_{ij} = D_T|\mathbf{u}|\delta_{ij} + (D_L - D_T)\frac{u_i u_j}{|\mathbf{u}|} + \theta D_d \tau \delta_{ij} \qquad \text{(Eq. 11)}$$

where
- $\mathbf{D}$; the hydrodynamic dispersion tensor (m^2/sec)
- C_k ; the concentration of radionuclide k in groundwater (kg/m^3)
- ρ_s ; the density of solid (kg/m^3)
- $C_{S,k}$; the adsorbed concentration of radionuclide k (kg/m^3)
- λ_k ; decay constant of radionuclide k (1/sec)
- ξ_{km} ; the mass fraction of radionuclide m (parent) transforming to k (daughter)
- Q_k ; source term of radionuclide k (kg/m^3sec)
- D_L ; longitudinal dispersion length (m)
- D_T ; transverse dispersion length (m)
- D_d ; the molecular diffusion coefficient in a free-water (m^2/sec) and
- τ ; tortuosity.

Assuming that a linear equilibrium isotherm describes the relation of the concentration of a specific solute in a solid and solution, Eq. 10 can be expressed as

$$\begin{aligned}\nabla(\mathbf{D}\nabla C_k - \mathbf{u}C_k) &= \frac{\partial}{\partial t}[\theta(1+\frac{\rho_s(1-\varepsilon)K_{dk}}{\theta})C_k] + \lambda_k[\theta(1+\frac{\rho_s(1-\varepsilon)K_{dk}}{\theta})C_k] \\ &\quad -\sum_{m=1}^{k-1}\xi_{km}\lambda_m[\theta(1+\frac{\rho_s(1-\varepsilon)K_{dm}}{\theta})C_m] - Q_k\end{aligned} \qquad \text{(Eq. 12)}$$

where K_{dk}; is the equilibrium constant.

Eq. 12 reduces to

$$\nabla(\mathbf{D}\nabla C_k - \mathbf{u}C_k) = \frac{\partial}{\partial t}(\theta R_k C_k) + \lambda_k \theta R_k C_k - \sum_{m=1}^{k-1}\xi_{km}\lambda_m \theta R_m C_m - Q_k \qquad \text{(Eq. 13)}$$

where R_k; is the retardation factor defined as following equation.

$$R_k = 1 + \frac{\rho_s(1-\varepsilon)K_{dk}}{\theta} \qquad \text{(Eq. 14)}$$

4.2 Modeled Domain

A cross-section of a conceptual model used in simulating the flow and radionuclides transport for the vault scenario is presented in Fig. 1 and for the trench scenario is presented in Fig. 2. It is assumed that the interior length of the facility in the third dimension is 100 m. In the cover scenario, an engineered cover which consists of a gravel drainage layer and a clay layer is placed over the vault/trench (see Fig. 3 and Fig. 4, respectively). The slope of the layers is assumed to be 2 %, which is the same as the slope of the roof and floor of the vault. The cover is extended to a gravel drain which is designed to divert the drainage water away from the facility. The thickness of the roof and floor of the vault are kept constant. A clay layer is placed on the top of the roof with permeable sand layer around the vault. The waste contained in the engineered vault is considered to be homogeneous, and radionuclides are instantaneously available for release.

We chose the modeled domain like as Fig. 1, Fig. 2, Fig. 3 or Fig. 4 in each scenario, respectively. We enlarged the modeled domain to 1 m under the water table. Thus, the lower boundary was placed in aquifer.

4.3 Degradation of the Material Properties

The time-dependent material properties for the waste form and facility are provided in Test Case 2b specification (see Table 3 and Table 4). After 200 years the concrete starts to degrade. After 500 years the concrete turns to sand, but keeps its original chemical characteristics. The clay layer above the vault is assumed to fail when the roof fails after 500 years. This is because the roof is considered to provide support for the clay. As the roof fails, the support no longer exists, and then the clay is compromised and changes to the native soils. The waste form degrades in the same manner as the concrete dose, turning to sand after 500 years. The engineered cover only lasts for 500 years, after which the cover soils change to the native soil in the region.

The cover is assumed to reduce the natural infiltration rate to an average of 1 cm/a in the vault and trench scenarios. We assume the constant infiltration of 1 cm/a through the upper boundary of the domain illustrated in Fig. 1 and Fig. 2 until 500 years in vault and trench scenarios. After 500 years , we assume the natural infiltration rate (42.2 cm/a) through the upper boundary as though no cover was present. In the cover scenarios, we assume the constant natural infiltration rates through the upper boundary of the domain illustrated in Fig. 3 and Fig. 4 during the time period for analysis. Table 10 shows the infiltration rates assumed in four scenarios. We divided the time period for analysis into three; (i) 0-200 years, (ii) 200-500 years, (iii) after 500 years in the vault and vault with cover scenarios, taking into account for the degradation of material properties. In the trench scenario, we assumed two time periods; (i) 0-500 years, (ii) after 500 years considering changes of the infiltration rate.

In this study, we assumed that the unsaturated steady state flow field in each time period is established, i.e. the time dependent changes of flow velocities are assumed as the step functions of the sequential unsaturated steady state flow velocities.

Table 10 Infiltration rates assumed in four scenarios. Values are in m/a.

Time	Vault	Trench	Vault with cover	Trench with cover
time < 500 a	0.01	0.01	0.422	0.422
time > 500 a	0.422	0.422	0.422	0.422

4.4 Numerical Method

The Test Case 2b problem was analyzed by using the MIG2DF code [9]. The MIG2DF is a two-dimensional, finite element code simulating the saturated-unsaturated groundwater flow and radionuclide transport in porous media for the safety evaluation of radioactive waste disposal. The equation of groundwater flow is discretized by using the Galerkin finite element method. The equation of radionuclide transport is discretized by using the Bubnov-Galerkin finite element method. Simulations can be performed in a vertical or horizontal cross-section, or an axisymmetric configuration. In flow analysis, many types of boundary conditions can be accommodated; (i) water table conditions, (ii) atmospheric conditions associated with seepage boundaries and infiltration, (iii) pumping and injection wells. For radionuclide transport analysis, (i) flux conditions, (ii) constant concentration (iii) source and sink conditions can be accommodated. The MIG2DF takes into account of advection, hydrodynamic dispersion, equilibrium sorption and decay chain in the transport analysis. Arbitrary release-pattern of radionuclides from sources can be handled.

The finite element grid used in the vault with cover scenario is presented in Fig. 6. It consists of 7808 rectangular elements and 7998 nodal points. We used 7320 elements and 7502 nodal points in the vault scenario, 5226 elements and 5372 nodal points in the trench with cover scenario, and 4950 elements and 5092 nodal points in the trench scenario, respectively.

Test Case 2b requires to calculate the release rates (Bq/a) which cross a plane 2 m below the lowest point in the waste for the concrete vault and for the trench. Since the MIG2DF code was designed to calculate solute concentrations, the time dependent release rates through the element i on the monitoring plane, q_i, was calculated as follows:

$$q_i = u_y C_i - \varepsilon D_y \frac{dC_i}{dy} \qquad \text{(Eq. 15)}$$

where u_y ; a vertical component of Darcy velocity (m/a)

D_y ; the vertical component of the dispersion coefficient (m^2/a) and

C_i ; the concentration of element i (Bq/m^3).

The total release rate Q (Bq/a) from the vault/trench can be defined as:

$$Q = 2 \times L \times \sum q_i \qquad \text{(Eq. 16)}$$

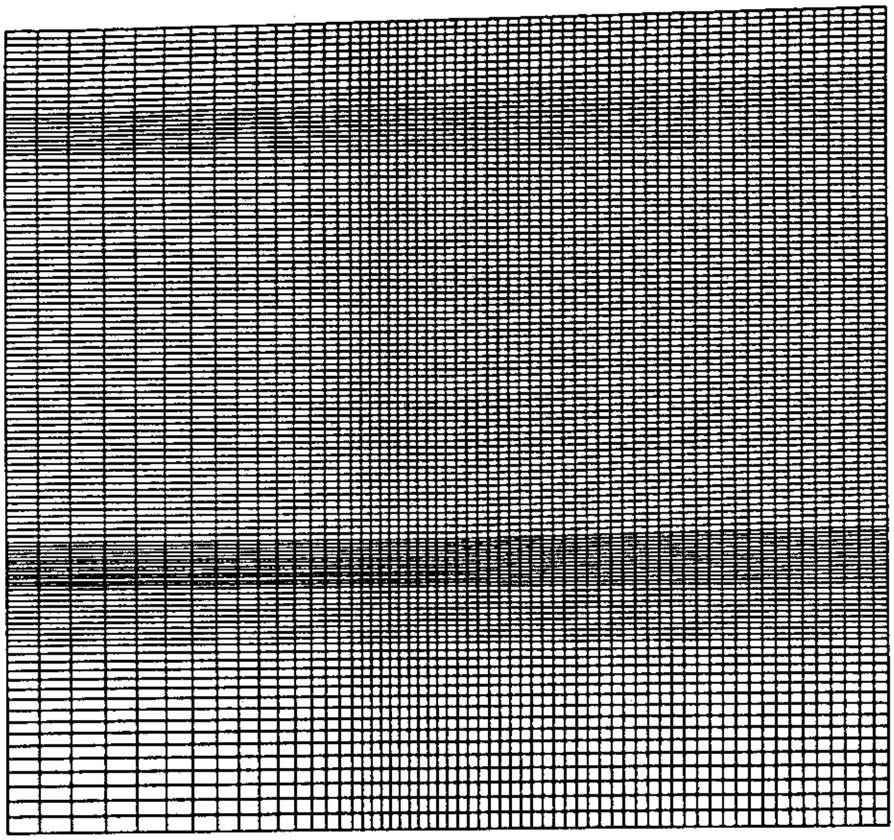


Fig. 6 Finite element grid used in the vault with cover scenario. The number of elements are 7808 and the number of nodes are 7998.

where L is interior length of the vault/trench in the third dimension (100 m).

4.5 Boundary and Initial Conditions

The groundwater flow analysis was performed by assuming steady state conditions in the each time period considering the degradation of the material properties. The radionuclide transport analysis was performed based on the steady-state flow fields calculated in the each time period. The same kinds of boundary conditions were applied for the each time period. In flow analysis, the boundary conditions at the top of the region were prescribed flux conditions, and left-side and bottom boundaries were prescribed as seepage boundaries to account for the right-side drainage of groundwater. In the transport analysis, the boundary condition at the left-side of the modeled domain was assumed to be zero flux boundary. The boundary condition at the bottom of region was set as that the gradient of concentration was zero. The specified boundary condition was the top of the modeled domain, where a zero concentration was assumed. The initial concentration was zero except the waste disposal unit. Figure 7 and Fig. 8 show the sketches of the boundary and initial conditions defined here.

In the cover scenarios, we need to consider the leakage through the base of the drain and the water traveling in the third dimension with the drain (the longitudinal drain direction). The two dimensional code, the MIG2DF, dose not deal with the flow in the third dimension. Therefore, we applied flux condition to the boundary of the drain for the cover simulations. We used the assumption that the 69 % of precipitated water from the top of the facility ran out through the boundary of the drain during the period before 500 years, because the cover layer and the drain is assumed not to fail during this period. This assumption is based on the surface run-off factor, 0.69, observed typically in Japan [10]. Thus, this value of the run-off factor is very conservative. We can not judge whether this assumption is adequate or not for these scenario in this test case. The run-off factor should be needed to measure from the field observations in real safety assessment. Figure 9 shows the sketch of the boundary conditions for flow simulations in the cover scenarios. The boundary and initial conditions for transport simulations in the cover scenarios are same as that of the no cover scenarios.

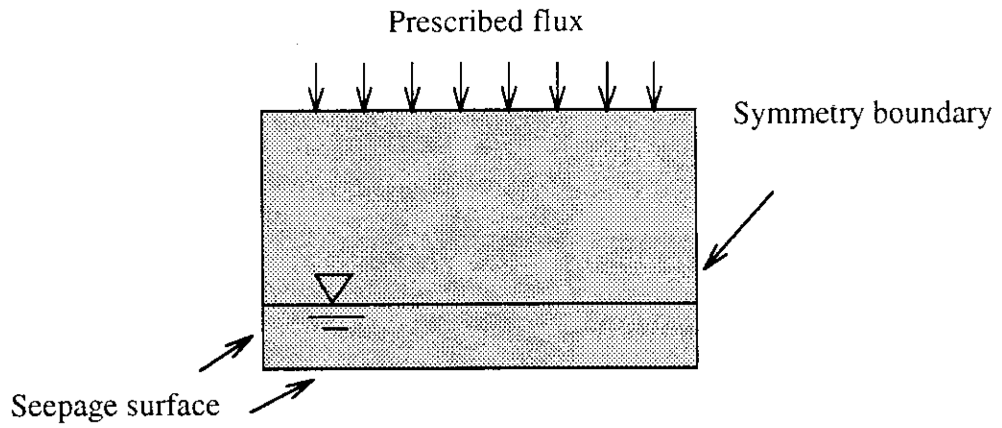


Fig. 7 Boundary conditions in flow analysis.

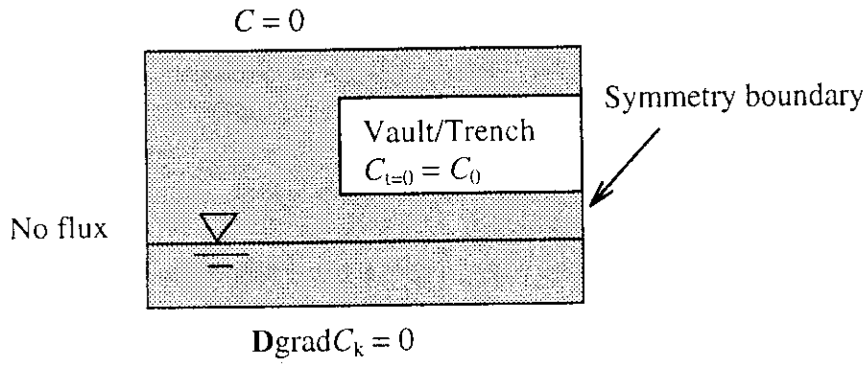


Fig. 8 Boundary and initial conditions in transport analysis.

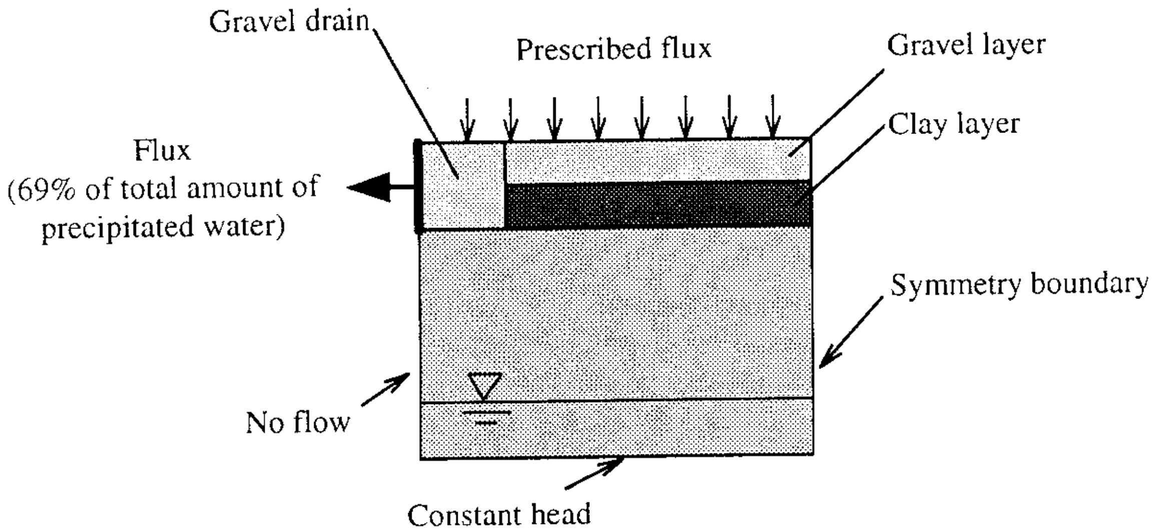


Fig. 9 Boundary conditions for the cover scenarios in flow simulations.

5. RESULT OF TEST CASE 2B

5.1 Results for the Flow Simulations

The primary purpose of the flow simulation is estimating the flow rate and moisture content in and around the waste. These values are necessary for the evaluation of the transport of radionuclides below the waste down to the water table. Due to the failure of the engineered cap on the top of the vault and the degradation of concrete and the waste form, the results of the flow analyses can be divided into the three time periods; 0-200 years, 200-500 years and after 500 years, in the vault and vault with cover scenarios. Also, in the trench and trench with cover scenarios, the analyses can be divided into the two time periods; before 500 years and

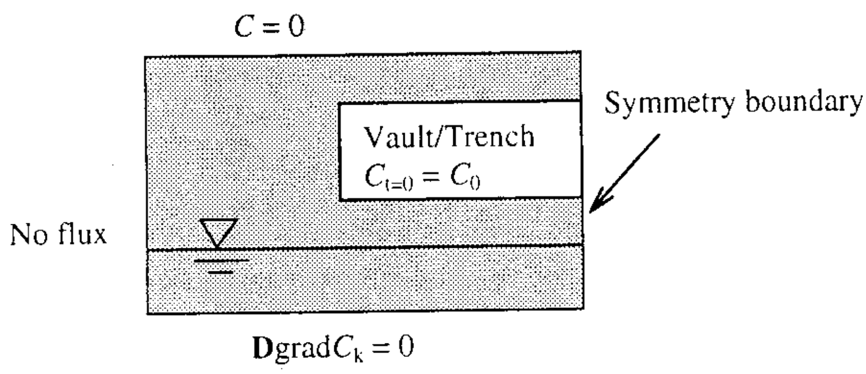
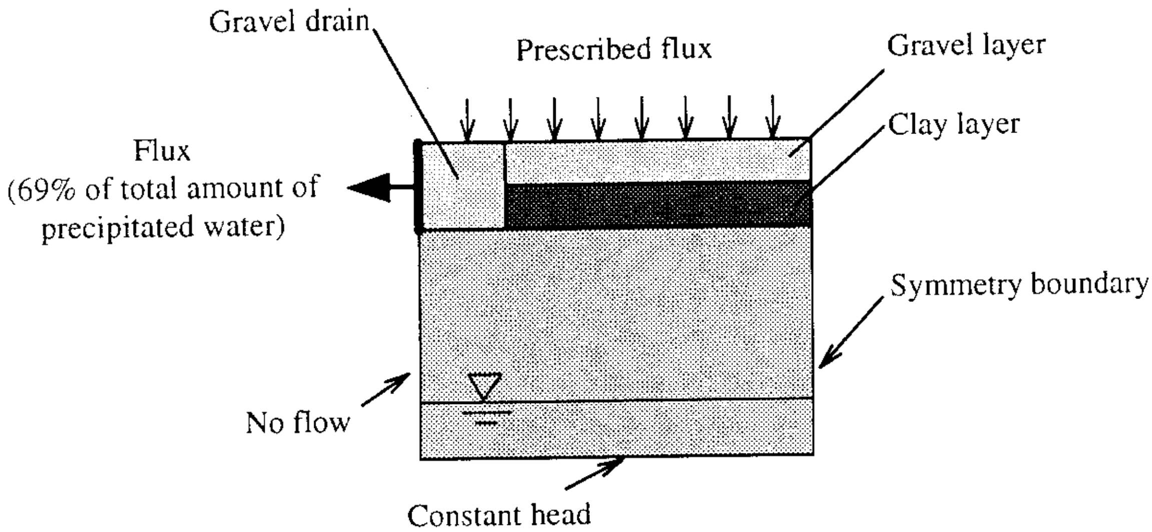


Fig. 8 Boundary and initial conditions in transport analysis.



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5.1.1 Flow Simulation of Vault Scenario

Using the conceptual model as discussed in the previous chapter and parameters described in the specification, the distribution of steady state total head for the period 0-200 years in the vault scenario is shown in Fig. 10 (a). This figure shows that the engineered cover of disposal unit successfully diverts the precipitated water away from the disposal unit, so that the precipitated water flows downward through the sand drain along the left boundary of the unit. Thus, the flow velocity within the waste are smaller than the infiltration rate which is 0.01 m/a. The average flow velocities and moisture contents are presented in Table 11 for five layers: (1) concrete layer over the waste, (2) the waste, (3) concrete layer below the waste, (4) sand layer below the concrete layer and (5) native soil below the sand layer. The average flow velocity in vertical direction and moisture content within the waste are 3.48E-5 m/a and 0.500 (almost saturated), respectively. The general direction of water movement is downwards, except for the sand layer over the clay layer (infiltration barrier) and the bottom of the disposal unit.

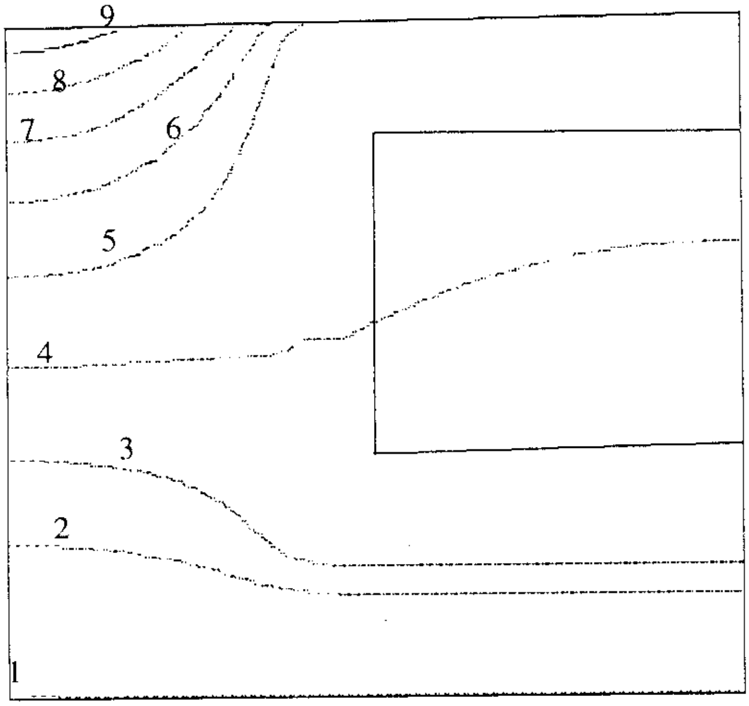
Table 11 Average flow velocity in vertical direction and moisture content of each layer in the vault scenario.

Flow	**Velocities**	**(m/a)**			
Time period (a)	Concrete over the waste	Waste	Concrete below the waste	Sand below the concrete	Native soil below the sand
0 - 200 a	2.65E-5	3.48E-5	4.43E-5	6.51E-3	1.25E-2
200 - 500 a	5.36E-5	1.44E-4	2.09E-5	6.59E-3	1.26E-2
after 500 a	0.435	0.559	0.563	0.541	0.525
Moisture	**content**				
Time period (a)	Concrete over the waste	Waste	Concrete below the waste	Sand below the concrete	Native soil below the sand
0 - 200 a	0.150	0.500	0.150	0.180	0.217
200 - 500 a	0.137	0.449	0.137	0.180	0.217
after 500 a	0.179	0.179	0.180	0.180	0.284

(a) 0 - 200 years
Vault scenario
Contour levels

1	0.000E+00
2	4.444E-01
3	8.889E-01
4	1.333E+00
5	1.778E+00
6	2.222E+00
7	2.667E+00
8	3.111E+00
9	3.556E+00

Total head (m)



(b) after 500 years
Vault scenario
Contour levels

1	0.000E+00
2	5.000E-01
3	1.000E+00
4	1.500E+00
5	2.000E+00
6	2.500E+00
7	3.000E+00
8	3.500E+00
9	4.000E+00

Total head (m)

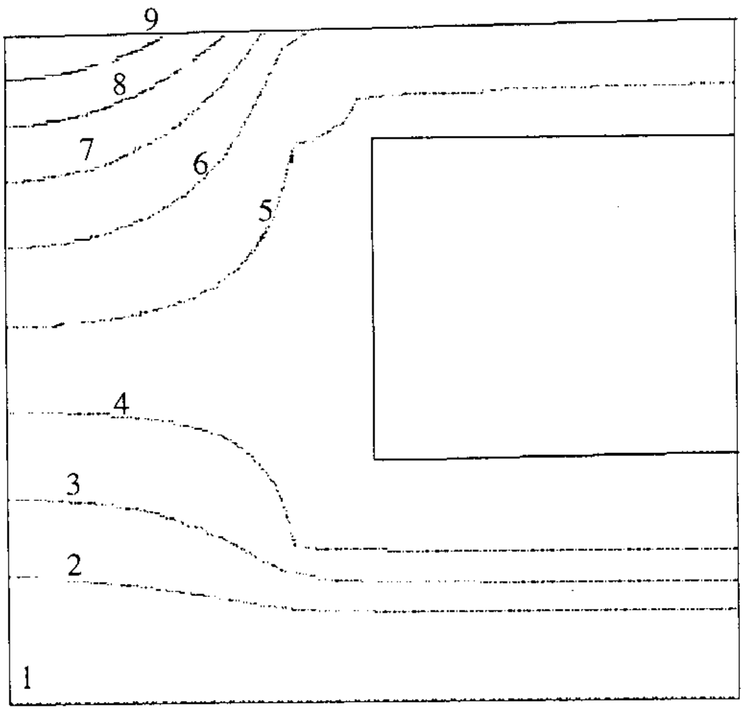


Fig. 10 Total head distribution for the time periods (a) 0-200 and (b) after 500 years in the vault scenario. Solid line shows the boundary of the waste.

After 200 years, the concrete vault starts to degrade resulting in a change in the flow properties of the concrete and waste form. The distribution of total head , not shown here, is almost similar as that during the time period 0-200 years, but the average flow velocity and moisture content change slightly due to the degradation. The average flow velocity and moisture content within the waste are 1.44E-4 m/a and 0.449, respectively.

After 500 years, the engineered cover placed on the top of the disposal facility fails completely, so that the infiltration rate becomes large (0.422 m/a). The concrete vault, as well as the clay layer placed on the top of the vault, also fails. The cover and clay layer change to the native soil, whereas the concrete and waste form change to the sand that chemically behaves like concrete. The steady state condition of the total head distribution during the time period after 500 years are shown in Fig. 10 (b). The average flow velocity within waste is higher than that of native soil located at the left side of the disposal unit because the permeability of the degraded concrete and waste form is higher than that of native soil. The average flow velocity in vertical direction and moisture content within the waste are 0.559 m/a and 0.179, respectively. The flow velocity is higher than the infiltration rate(0.422 m/a), this means that the degraded vault facility is the flow path if the permeability of vault is higher than that of native soil.

5.1.2 Flow Simulation of Trench Scenario

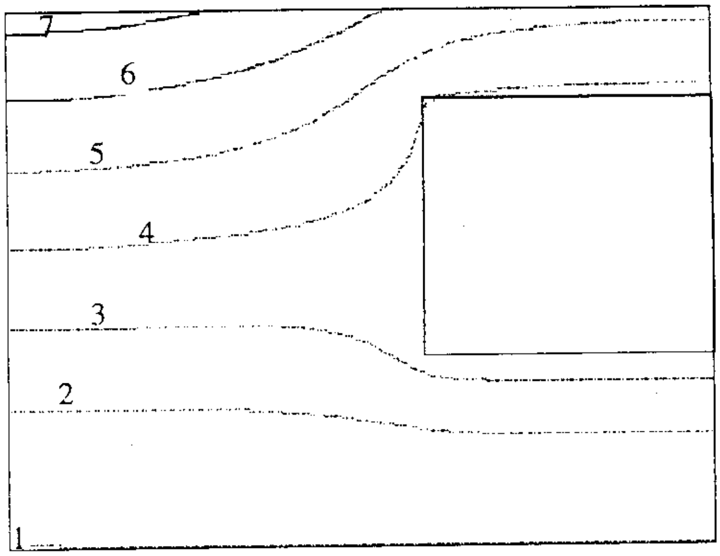
Figure 11 (a) shows the distribution of steady state total head for the time period 0-500 years in the trench scenario. It is clear that the general groundwater movement is downwards, except for the left upper and lower corner of the trench waste. It is observed that the infiltrated water within the native soil near the left upper corner of the waste moves into the waste and the water goes out from the lower corner of the waste, because the permeability of trench waste is higher than that of the native soil. The average moisture content and flow velocity in vertical direction in the trench are 0.281 and 1.45E-2 m/a, respectively. The flow velocity is slightly higher than the infiltration rate (0.01 m/a). Table 12 shows the average moisture contents and flow velocities of three layers (over, within and below the trench waste) for the time periods 0-500 and after 500 years.

The failure of the engineered cover after 500 years causes the change in the moisture content and total head. Figure 11 (b) shows the distribution of steady state total head for the time period after 500 years. The property of the trench waste is constant for all time. The general direction of water flow velocity is downwards. The average moisture content and

Table 12 Average flow velocities in vertical direction and moisture contents in the trench scenario.

	Flow velocity	**(m/a)**	
Time period (a)	Native soil over trench waste	Trench waste	Native soil below trench waste
time < 500 a	1.08E-2	1.45E-2	1.23E-2
time > 500 a	0.440	0.509	0.473
	Moisture Content		
Time period (a)	Native soil over trench waste	Trench waste	Native soil below trench waste
time < 500 a	0.179	0.281	0.210
time > 500 a	0.269	0.291	0.278

(a) 0 - 500 years
Trench scenario
Contour levels
1 0.000E+00
2 1.000E+00
3 2.000E+00
4 3.000E+00
5 4.000E+00
6 5.000E+00
7 6.000E+00
Total head (m)



(b) after 500 years
Trench scenario
Contour levels
1 0.000E+00
2 1.000E+00
3 2.000E+00
4 3.000E+00
5 4.000E+00
6 5.000E+00
7 6.000E+00
8 7.000E+00
9 8.000E+00
10 9.000E+00
Total head (m)

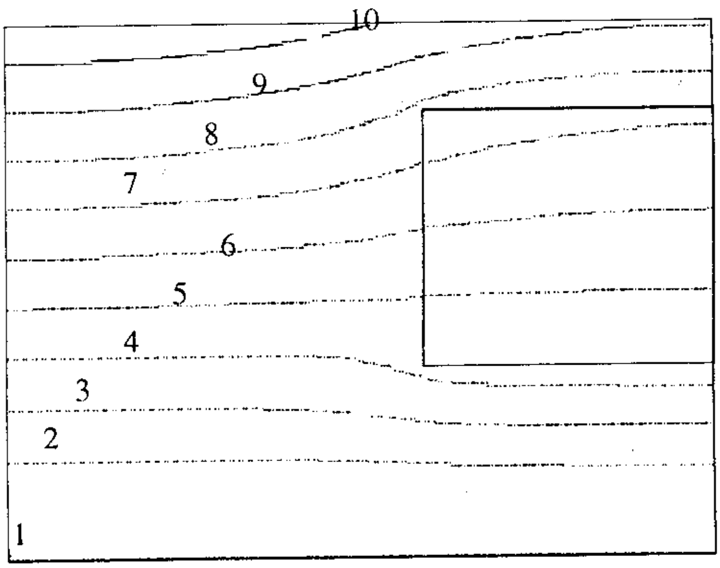


Fig. 11 Total head distribution for the time period (a) 0-500 and (b) after 500 years in the trench scenario. Solid line shows the boundary of the waste.

flow velocity in the trench are 0.291 and 0.509 m/a, respectively. The flow velocity is slightly higher than the infiltration rate(0.422 m/a).

5.1.3 Flow Simulations of Scenarios with Cover

Based on the vault and trench scenarios, we also simulate the vault and trench with cover scenarios. The result is given in Fig. 12 which shows that the total head distribution for the time period before 200 years. It is clear that the water infiltrated from the top surface flows toward the drain above the clay layer and most of water flow away through the left side boundary. Also, this figure shows that the residual water infiltrates to native soil through the bottom of the drain, and flow toward the vault. The distributions of steady state total and pressure head for the time period 200-500 years are almost identical to those for the time period 0-200 years. After 500 years, the distributions of total and pressure head are the same as those of the vault scenario because it is assumed that cover materials are converted to the natural backfill soil (clayey sand and sandy clay), and the concrete and grouted waste are converted to the sand that chemically behaves like a concrete. Table 13 shows the average moisture contents and flow velocities of the each layer for the each time period. The average flow velocity obtained with this scenario is seven times for the period before 200 years, and nine times for the time period 200-500 years, higher than that obtained with the vault scenario, respectively. The average moisture content in the vault with cover scenario is almost the same as that in the vault scenario. The flow velocity in this scenario is highly dependent on the assumption how to treat the drainage water. We assume the run-off factor observed in Japan (0.69, for natural soil layer) at the boundary of the drain. The realistic run-off factor may be larger than this value because the cover of facility is made of artificially compacted soil layer. If we will use a larger run-off factor like as 0.99, the flow velocity will decrease. In order to verify the results of the flow velocity, we need a more realistic data of the run-off factor.

Figure 13 shows the distribution of steady state total head for the time period 0-500 years in the trench with cover scenario. The pattern of total head distribution is analogous to that for the vault with cover scenario. Table 14 shows the average moisture contents and flow velocities of each layer during the each time period. It should be noted that any comparison of the results of water flow analyses between the scenarios with and without the cover is not justified because the both scenarios use completely different boundary conditions (water infiltration conditions) with each other. This means that such the comparison never gives any scientific basis to indicate the effect of the cover on the reduction of the flow velocity in the waste domain.

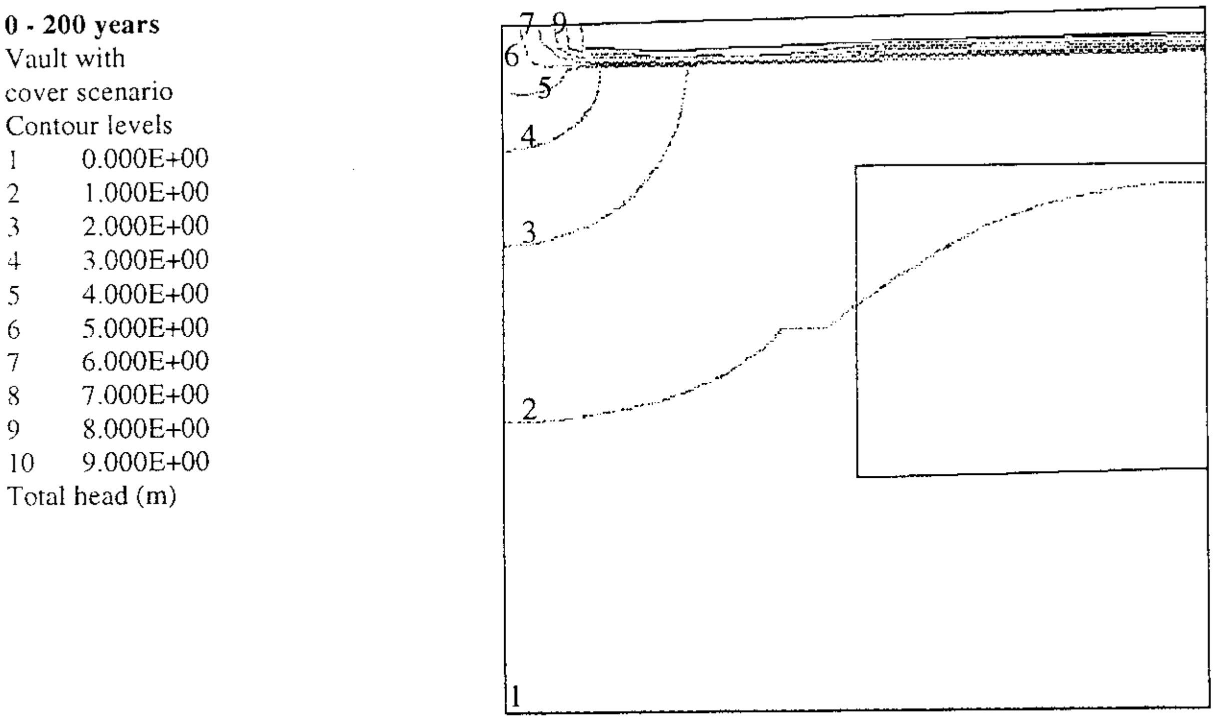


Fig. 12 Total head distribution for the time period 0-200 years in the vault with cover scenario. Solid line shows the boundary of the waste.

Table 13 Average flow velocity and moisture content of each layer in the vault with cover scenario.

Flow	**Velocities**	**(m/a)**			
Time period (a)	Concrete over the waste	Waste	Concrete below the waste	Sand below the concrete	Native soil below the sand
0 - 200 a	1.82E-4	2.38E-4	4.43E-5	6.24E-2	0.123
200 - 500 a	3.74E-4	1.25E-3	2.09E-5	6.32E-2	0.123
after 500 a	0.445	0.565	0.563	0.543	0.527
Moisture	**content**				
Time period (a)	Concrete over the waste	Waste	Concrete below the waste	Sand below the concrete	Native soil below the sand
0 - 200 a	0.150	0.500	0.150	0.180	0.282
200 - 500 a	0.137	0.449	0.137	0.180	0.282
after 500 a	0.179	0.179	0.180	0.180	0.284

0 - 500 years
Trench with
cover scenario
Contour levels
1 8.382E-01
2 1.680E+00
3 2.510E+00
4 3.350E+00
5 4.190E+00
6 5.030E+00
7 6.710E+00
8 7.540E+00
9 8.380E+00
a 9.220E+00
Total head (m)

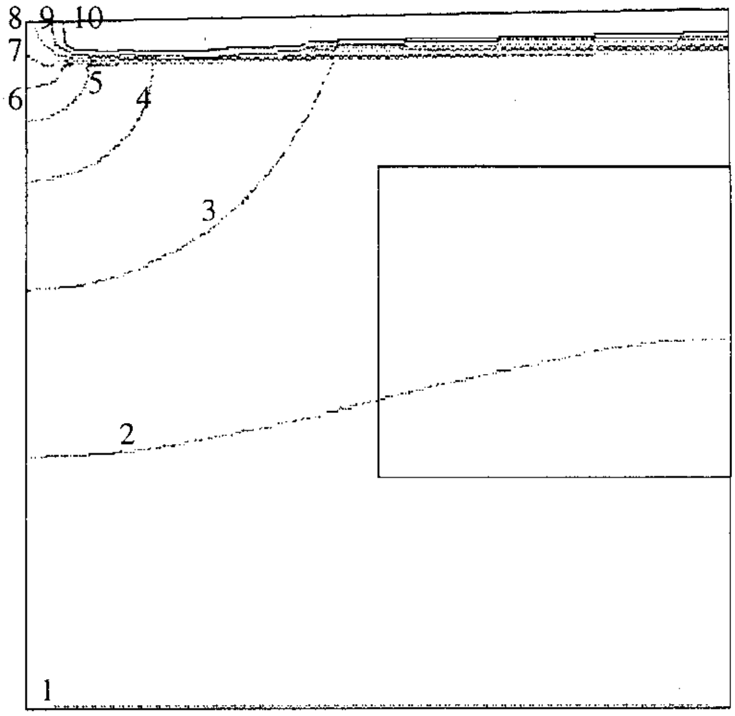


Fig. 13 Total head distribution for the time period 0-500 years in the trench with cover scenario. Solid line shows the boundary of the waste.

Table 14 Average moisture contents and flow velocities in the trench with cover scenario.

	Flow velocity	**(m/a)**	
Time period (a)	Native soil over trench waste	Trench waste	Native soil below trench waste
time < 500 a	6.04E-2	0.106	0.121
time > 500 a	0.436	0.466	0.449
	Moisture Content		
Time period (a)	Native soil over trench waste	Trench waste	Native soil below trench waste
time < 500 a	0.273	0.290	0.281
time > 500 a	0.274	0.290	0.282

5.2 Results of the Transport Simulations

Six radionuclides (H-3, C-14, Ni-63, Sr-90, I-129 and Th-230 with daughters) selected by the screening calculations are assumed to behave independently each other in the transport medium. Transport is assumed to occur exclusively in the aqueous phase; gaseous transport is neglected. All of the inventory is assumed to be immediately available for the transport. Radionuclides are partitioned between adsorbed and aqueous phases within the vault by using a linear reversible adsorption isotherm. The distribution coefficients for each element and associated material type are described in the test case specification (see Table 5 and Table 8).

5.2.1 Transport Simulation of Vault Scenario

The calculated maximum release rates and concentrations for each radionuclide are shown in Table 4.(a) in appendix. Among the radionuclides analyzed here, Po-210 gives the highest concentration and Ni-63 does the lowest, in this scenario. The fastest peak time is obtained for H-3 at 100 years. The ranking with respect to peak concentrations thus obtained is:

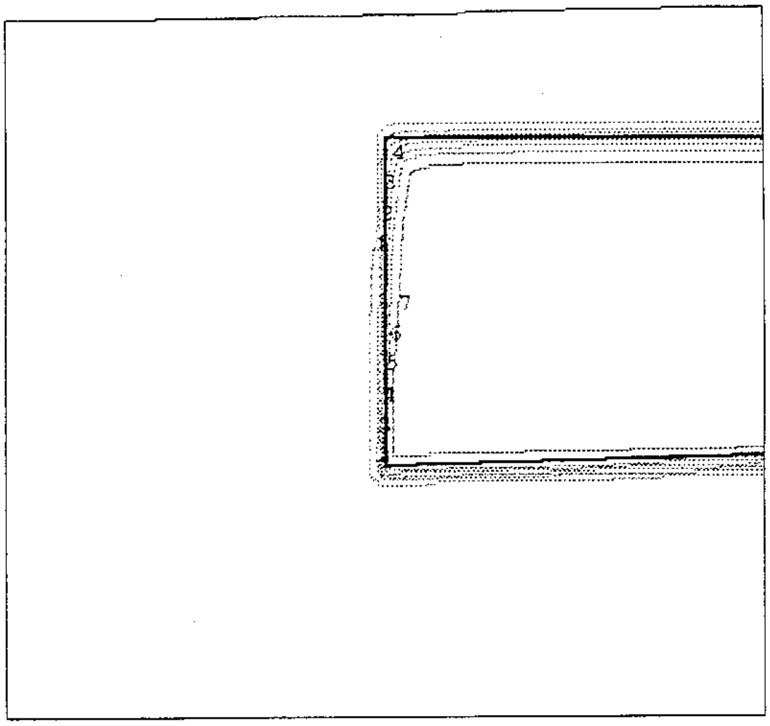
Po-210 > Ra-226 > Pb-210 > C-14 > I-129 > Sr-90 > Th-230, H-3 > Ni-63.

The time dependent release rates and the concentrations are shown in Fig. 5.(a)-1 and 2 in appendix. The short-lived radionuclide, H-3, disappears from the figure due to decay in the vault scenario. No significant release from the vault takes place during the first 500 years indicating that a vault concept holds promise to confine radionuclides within the facility.

(a) 2,000 years
Vault scenario
Contour levels

1	5.000E-5
2	1.000E-4
3	1.500E-4
4	2.000E-4
5	2.500E-4
6	3.000E-4
7	3.500E-4

Concentration of C-14
(Bq/cm^3)



(b) 7,000 years
Vault scenario
Contour levels

1	5.000E-5
2	1.000E-4
3	1.500E-4

Concentration of C-14
(Bq/cm^3)

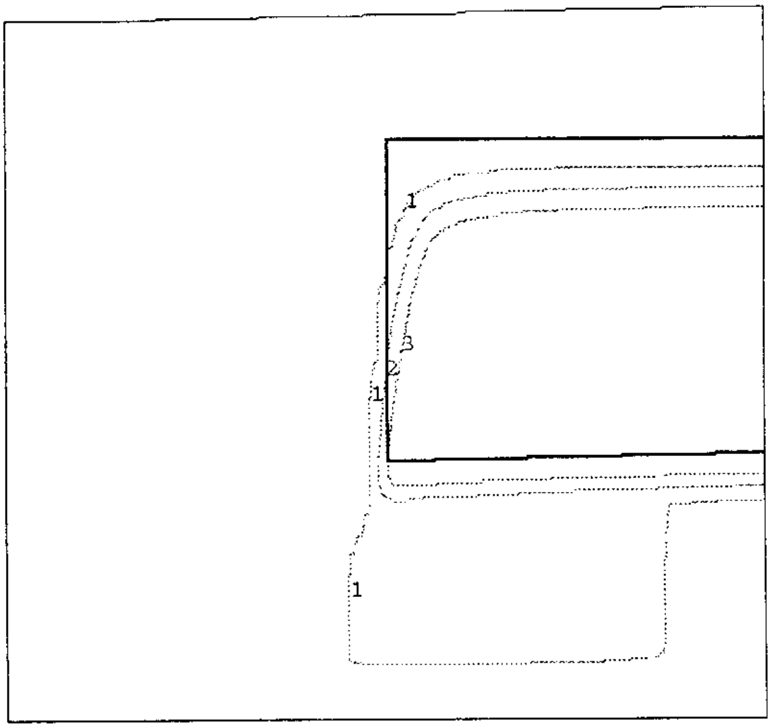


Fig. 14 The distribution of the concentration of C-14 at (a) 2,000 and (b) 7,000 years in the vault scenario. Solid line shows the boundary of the waste (initial concentration C_0 = 4.6E-4 Bq/cm^3).

Figure 14 shows the distributions of the concentration of C-14 at (a) 2,000 and (b) 7,000 years. The values in the figure indicate the concentration of C-14 in the liquid phase (Bq/mL). The solid line is the boundary of the waste backfilled with grout. It is obtained that the plume of radionuclide does not move significantly from the initial location until 2,000 years due to slow water velocity and a large distribution coefficient. Horizontal dispersion is negligible compared with vertical dispersion due to a small transverse dispersion length (0.02 cm) used in these calculations. The maximum concentration is obtained at a point from 6.8 m away from the vault center line and 2 m below the waste for the C-14 case.

5.2.2 Transport Simulation of Trench Scenario

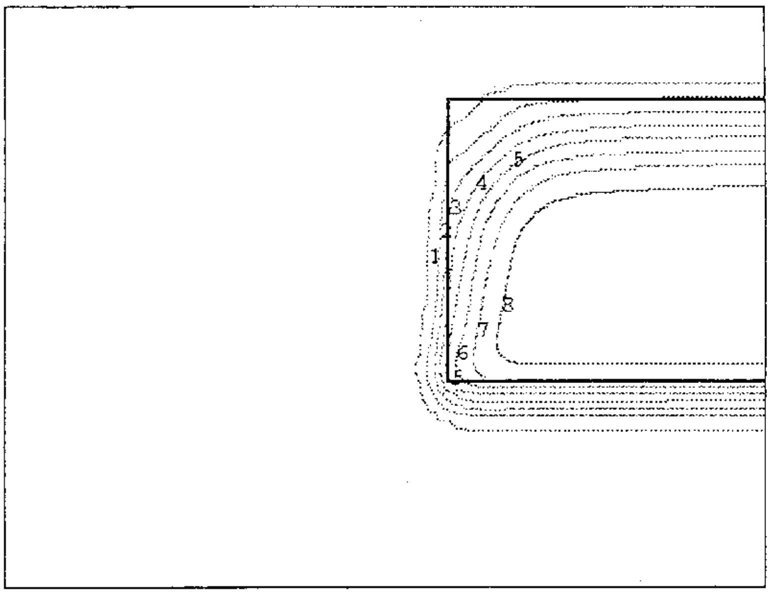
The maximum release rates and concentrations for each radionuclide are given in Table 4.(b) in appendix. The tables shows that all radionuclides except H-3, which has the shortest half-life and 0 distribution coefficient, reach their maxima after 500 years. The table also shows that only Th-230 reaches the maximum concentration beyond 15,000 years due to its large distribution coefficient. The ranking of radionuclides with respect to the peak concentrations obtained is:

H-3 > C-14 > Ni-63 > Ra-226 > Po-210 > I-129 > Pb-210 > Th-230 > Sr-90.

The time dependent release rates and concentrations are shown in Fig. 5.(b)-1 and 2 in appendix. The figure shows that significant releases of C-14, Ni-63, Sr-90 and I-129 take place during the time period from 200 years to 800 years. The values of the maximum release rates and the concentrations of radionuclides are larger than those in the vault scenario due to the fast flow velocity.

Figure 15 shows the distributions of concentration for C-14 at (a) 100 and (b) 505 years. This figure indicates that the radionuclide moves quickly toward the groundwater table in the trench facility. Horizontal dispersion is negligible as compared with vertical dispersion due to transverse dispersion length as small as that used in the vault scenario. An increasing flow velocity has more significant effect on the movement of the plume than those in the vault scenario. Therefore, it is more important to estimate the flow velocity in the trench scenario than in the vault scenario. The maximum concentration is obtained at the point 0.2 m away from the center line and 2 m below the waste for the C-14 case.

(a) 100 years
Trench scenario
Contour levels
1 1.000E-1
2 2.000E-1
3 3.000E-1
4 4.000E-1
5 5.000E-1
6 6.000E-1
7 7.000E-1
8 8.000E-1
Concentration of C-14
(Bq/cm^3)



(b) 505 years
Trench scenario
Contour levels
1 1.000E-1
2 2.000E-1
3 3.000E-1
4 4.000E-1
5 5.000E-1
6 6.000E-1
7 7.000E-1
8 8.000E-1
Concentration of C-14
(Bq/cm^3)

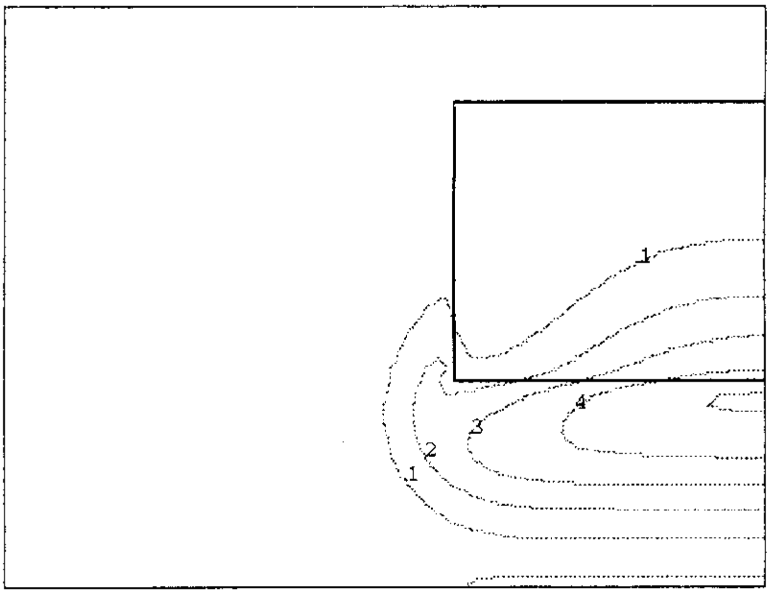


Fig. 15 The distribution of the concentration of C-14 at (a) 100 and (b) 505 years in the trench scenario. Solid line shows the boundary of the waste(initial concentration C_0 = 8.9E-1 Bq/cm^3).

5.2.3 Transport Simulation of Scenarios with Cover

The maximum release rates and concentrations for each radionuclide in the vault with cover scenario are given in Table 8.(a) in appendix. The table shows that all radionuclides except H-3 reach their maxima after 500 years. The table also show that C-14 and Th-230 reach the maximum concentration beyond 10,000 years due to their large distribution coefficients.

The time dependent release rates and concentrations are shown in Fig. 9.(a)-1 and 2, respectively, in appendix. The figure suggests that significant releases for Sr-90 and I-129 take place during the period from 500 years to 800 years and those of C-14 and Th-230 with daughters take place after 1,000 years. The maximum release rate of H-3 appears at 128 years and the curve of release rate for H-3 shows two peaks. This is caused by the changing to the fast water flow at 200 years. The values of maximum release rates and concentrations of the radionuclides are larger than those in the vault scenario. In the vault and vault with cover scenarios, the flow velocity has a great effect on the breakthrough curve of the radionuclides after 500 years. The flow velocities obtained with both scenarios for the period after 500 years are almost the same. Thus, the breakthrough curves of the radionuclides are also the same in the both scenarios. The ranking of the radionuclides in this scenario is identical to that of the vault scenario as follows.

Po-210 > Ra-226 > Pb-210 > C-14 > I-129 > Sr-90 > Th-230 > H-3 > Ni-63

The maximum release rates and concentrations for each radionuclide in the trench with cover scenario are listed in Table 8.(b) in appendix. The table shows that all radionuclides except Th-230 and its daughters, which have high distribution coefficients, reach their maxima before 250 years. The table also shows that only Th-230 reaches its maximum concentration beyond 16,000 years in the trench with cover scenario. It is clear that the change of the flow velocity during first 500 years has no effect on the breakthrough curve of Th-230. The ranking of the radionuclides in respect to the peak concentrations obtained is:

H-3 > Ni-63 > C-14 > Sr-90 > Ra-226 > Po-210 > I-129 > Pb-210 > Th-230.

The time dependent release rates and concentrations are shown in Fig. 9.(b)-1 and 2 , respectively, in appendix. The curve of release rate for Ni-63 shows the influence of the changing to the fast water flow at 500 years, and then the curve of Ni-63 shows the additional sharp peak at 500 years. The curves of Sr-90 and I-129 show the additional peaks also. The figures suggest that the precise estimation of the flow velocity is essential to obtain trustworthy results of safety analysis, at least for mobile radionuclides e.g. C-14, Ni-63, Sr-90 and I-129.

5.3 Discussions

The two-dimensional flow simulation by using the MIG2DF indicates that the complex flow fields are formed in each time stage corresponding to the degradation of material properties. The water velocities have significant effects on the results of radionuclides transport analyses. Therefore, it is needed to estimate the more precise infiltration rates and hydraulic conductivities to obtain realistic flow fields.

In addition, we have to evaluate the effects of boundary conditions by changing them, so as to define reasonable boundary conditions. For example, in the specification of the cover scenario the boundary conditions are arbitrarily given, and are completely independent of those of the corresponding scenario without cover. As a result of this, the results of analyses gave the conclusion that the flow velocity through the waste domain is higher in the scenario with cover than those without cover. Even though the test problem proposed by the IAEA does not intend to evaluate the effect of cover on the flow rate, the boundary condition should be defined based on reasonable scientific basis. Otherwise there are possibilities of drawing grotesque conclusions from this kind of analyses.

The unsaturated flow simulations indicate that the concrete and clay layer in the vault scenario and the cover on the top surface with gravel drain in the cover scenarios are much effective for the reduction of the vertical flow velocity through the disposal unit. Also, it suggests that the values of the flow velocity within the vault/trench after the complete degradation of the materials are larger than that of the infiltration rate in all scenarios. The precipitated water from the surface flows selectively through the vault/trench, in other words, the vault/trench becomes the flow path due to the high permeable properties after the material degrades completely. This situation of flow field is undesirable to realize safe disposal of LLW. Off course, the results obtained in this study depend on the assumptions of the degradation of material. Therefore, the unsaturated flow simulation by using a reasonable assumption of the degradation of material, which should be derived from the experimental or natural analogue study, is required to obtain a reliable flow velocity in future work.

In the transport simulation of the vault and vault with cover scenarios, the effects of the concrete layer can be seen in the breakthrough curves of many of the radionuclides. If the physical and chemical properties of degraded vault facility are assumed to be the same as those of trench facility, the maximum release rate of C-14 in the vault with cover scenario would be 3 orders in magnitude lower than those in the trench with cover scenario. Also, the maximum release rate of Ni-63 is 9 orders lower. The comparison between the results of vault and trench with cover scenario indicates the effectiveness of suitable backfill and sorbing barriers to reduce the release rate of C-14 and Ni-63. It was also suggested through the comparison that the use of the concrete in the design of disposal facility is effective to reduce a flow velocity during first some hundreds of years. A simpler and more conservative analysis may be possible by assuming completely degraded state as an initial condition of the vault.

Several limitations associated with numerical techniques used here existed in the flow and transport analysis of this test case. It was difficult to obtain converged results using the specified hydraulic properties in the unsaturated flow simulations. It is well known that the numerical solution of a non-linear partial differential equation is beset with the difficulties related to stability and convergence, particularly when material heterogeneities exist [11]. Thus, the flow simulation have to be performed iterativly in order to obtain a better convergence result. In the transport simulations, we used fine grids and small time steps to avoid numerical dispersion due to a weak-dispersion, so that the simulation needed a long computing time. The stability criterion given by Price et al [12] was used in this study, i.e., the grid Peclet number $P_c = Udx/D < 2$ (dx ; the size of the grid in the direction of the velocity, D ; the dispersion coefficient and U ; the velocity). Additional criterion used here was the grid current number $C_0 = (U/n)(dt/dx)$ be on the order of 1, smaller than 1/3 [13], where dt is the time step and n is porosity. All simulations for Test Case 2B satisfied the above criteria (the grid Peclet numbers are about 0.81 and the grid current numbers are about 0.3 within the waste of vault scenario after 500 years).

6. CONSERVATIVENESS OF THE OBTAINED RESULTS

Comparisons between a result calculated from realistic models and that from simple models like one-dimensional models will give important information on the conservativeness of models. In addition, a knowledge of suitability of the assumptions, applying in the conceptualization of the model, is obtained. It is important to assess the conservativeness of models and the suitability of the assumptions applying in the models in order to improve the reliability of the obtained results.

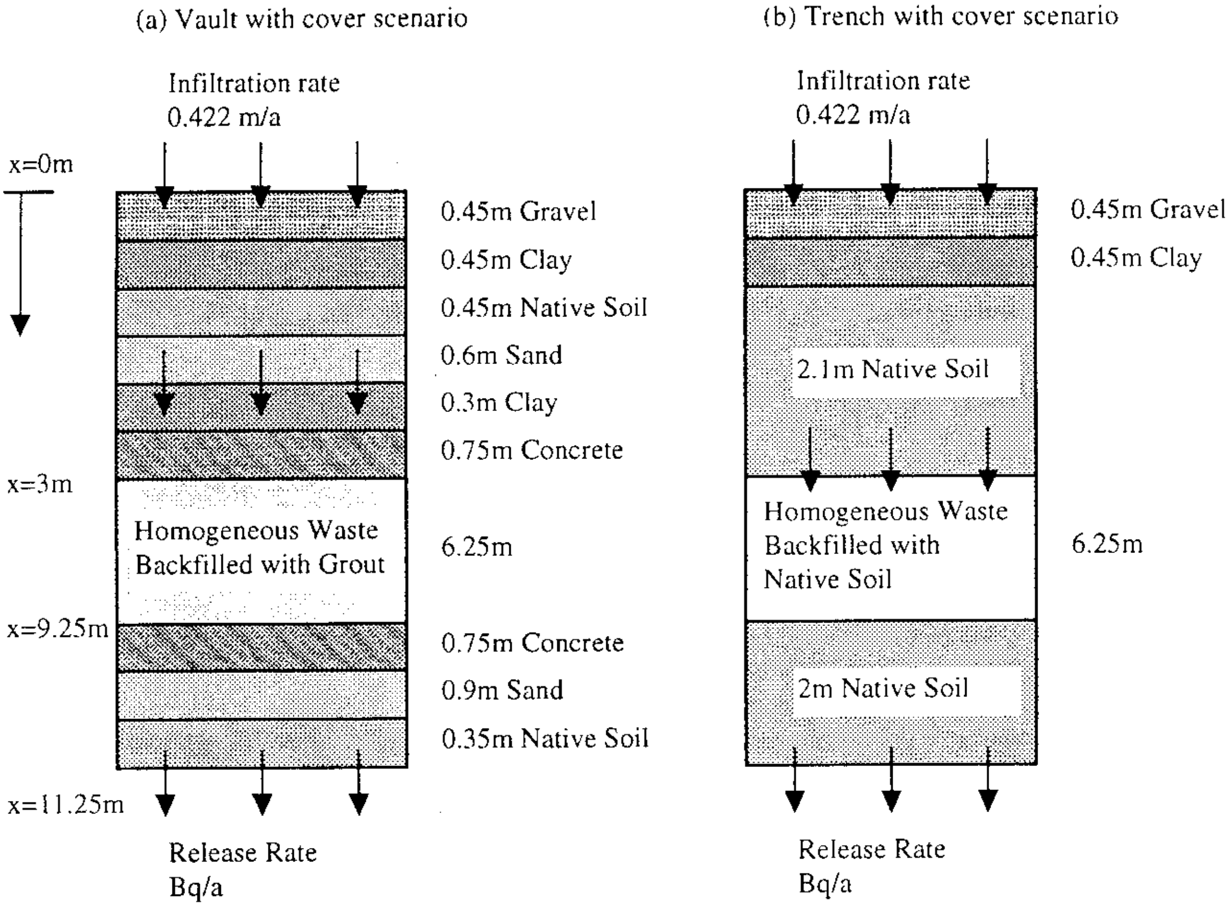
The assumption of a saturated soil layer is often used in safety analyses to avoid a complexity of analyzing an unsaturated-saturated groundwater flow. In general, an unsaturated soil layer is less permeable than a saturated soil layer, and the water velocity under the saturated conditions is regarded as the conservative water velocity (fast water velocity) in transport analysis. Therefore, conceptual models using the saturated conditions are recognized to be conservative. However, there is no evidence that conceptual models using the saturated conditions are conservative for this test case, in which the facility has a complex structure and materials would degrade with time.

We investigate the difference in the results which are derived from various models and simplifying assumptions associated with the flow velocity in the transport analysis. The results obtained from the two-dimensional computer program, MIG2DF, are compared with those from the three one-dimensional models using different concepts of the flow field within the disposal facility. The three one-dimensional transport models and the discussions of the conservativeness of the obtained results are described in the following sections.

6.1 One-dimensional Transport Models using Different Conceptualizations

In order to discuss the conservativeness of transport models and the suitability of the assumption of a soil layer being saturated, we consider the following three one-dimensional models based on different concepts of the flow field for modeled domain in the vault and trench with cover scenarios.

(1) 1D unsaturated transport model; one-dimensional numerical transport simulation using averaged water contents and water flow velocities obtained from the unsaturated flow simulations for the vault and trench with cover scenarios. The values of averaged water contents and flow velocities used in this simulation are calculated from the results of the unsaturated flow simulations of the MIG2DF, and the values for each soil and concrete layer are listed in Table 13 and Table 14. The time dependent changes of material properties are considered as same as those used in the simulations by the MIG2DF, i.e. (i) grouted waste and concrete start to degrade after 200 years and degrade to sand after 500 years, but retain their chemical properties (reversible linear adsorption, K_d = constant), (ii) the cover materials and clay are converted to the native soil after 500 years, (iii) the degraded properties of material are given in Table 3 and 4. The conceptual sketch of 1D model A are shown in Fig. 16.



- 1D unsaturated transport model with no lateral dispersion
- Reversible linear adsorption is assumed (K_d = constant for all time).
- An averaged water velocities and water contents for each layer are used in this simulation. The values are calculated from the results of simulations of the MIG2DF, and are given in Table 13 and 14.
- The time dependent changes of material properties are considered as same as that used in the simulations by the MIG2DF (see Table 3 and 4).

Fig. 16 A conceptual sketch of 1D unsaturated transport model.

(2) 1D saturated transport model; one-dimensional numerical transport simulation using a saturated condition. The flow velocities are assumed to be time-independent and the value is assumed to be 0.422 m/a, which is based on the infiltration rate, and the saturated moisture contents are assumed. The reversible linear adsorption is assumed (the K_d model) for all time. The conceptualization is almost the same as that of 1D unsaturated transport model shown in Fig. 16, while the time dependent changes of materials being assumed in 1D unsaturated transport model. In this simulation the time dependent changes of material properties are ignored. The degraded properties of materials(concrete, grouted waste, the engineered cover and clay) are used. It should be noted that the significant difference between 1D unsaturated transport model and 1D saturated transport model is that the former simulation uses the values of water velocities and moisture contents which are calculated from the realistic unsaturated flow simulations, but the latter uses the values based on the infiltration rate and the saturated conditions.

(3) 1D analytical saturated transport model; one-dimensional analytical transport simulation using following assumptions; (i) the medium is saturated, isotropic and homogeneous, (ii) reversible linear adsorption (the K_d model) is assumed, (iii) the daughter products are not considered, (iv) the changes in material properties are ignored. Using these assumptions, the change in the amount of radioactivity in the disposal unit is given by the following equation:

$$\frac{dC_s}{dt} = -\left(\frac{u}{L(\theta + \rho_{bulk} K_d)} + \lambda\right) C_s \qquad \text{(Eq. 17)}$$

where C_s ; the total amount of the radioactivity in the disposal unit (Bq)
u ; the infiltration rate (m/a) and
L ; a thickness of the waste (m).

The solution of Eq. 17 is given by an exponential function of time. Thus, we obtain the time dependent concentration at the bottom of the disposal unit. After release from the waste, the radionuclide migrates through the concrete, sand and native soil (in vault with cover scenario) or native soil (in trench with cover scenario). The governing equation is given by

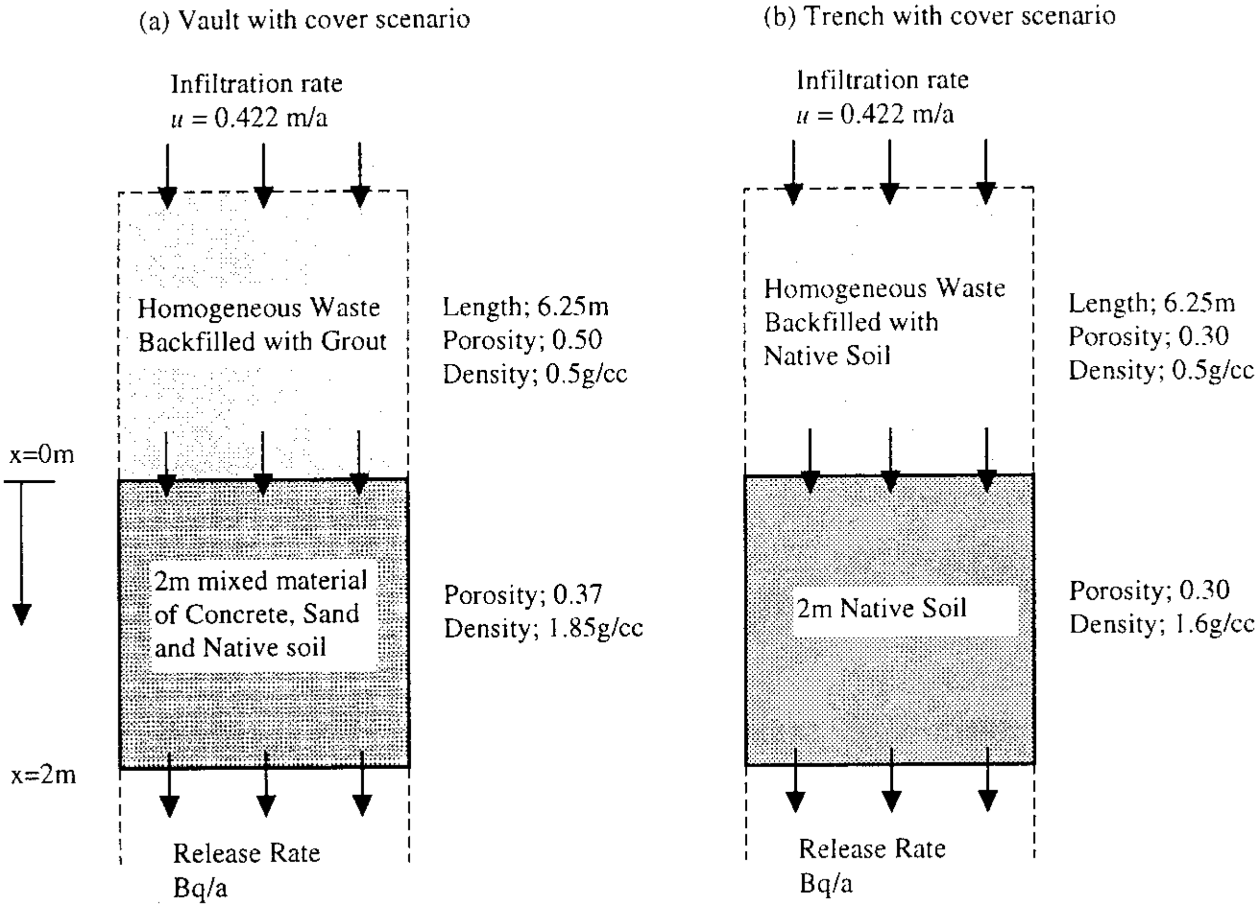
$$\theta R \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(uC - D\frac{\partial C}{\partial x}\right) - \theta R \lambda C \qquad \text{(Eq. 18)}$$

where C ; the concentration of radionuclide and
D ; dispersion coefficient (m^2/a).

An analytical solution of Eq. 18 is obtained by Harada et al. [14] for the following boundary condition and initial conditions.

$$\begin{aligned} &C = f(t)\,,\ x = 0, && f(t);\ \text{an exponential function} \\ &C = 0\,,\ x = \infty, && \text{for all } t \\ &C = 0\,,\ 0 < x < \infty, && \text{for } t = 0 \end{aligned} \qquad \text{(Eq. 19)}$$

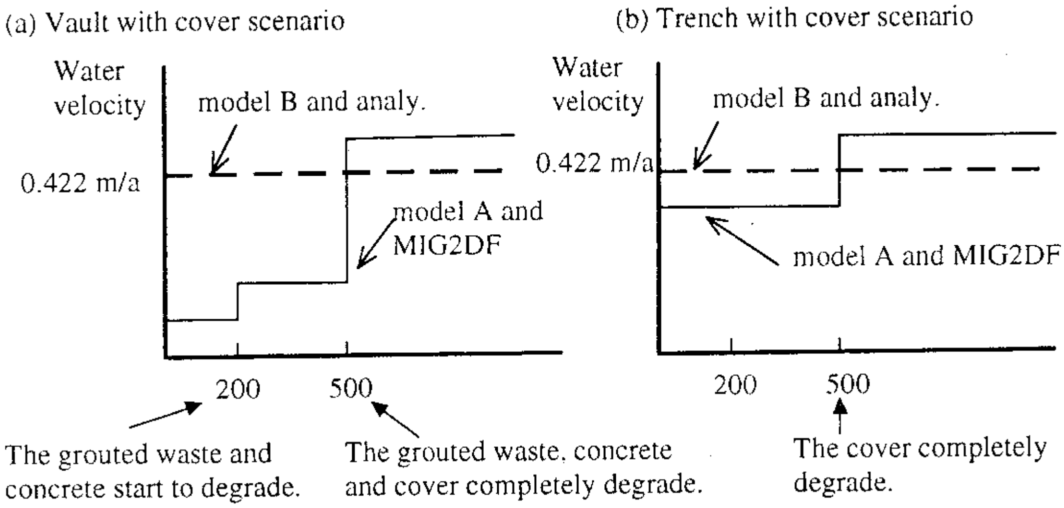
Input parameters used for simulations are the same as the data in the specification. Note that the analytical solution does not apply to multilayer system and time dependent changes of material properties. Thus, the multilayer system of the concrete, sand and native soil are assumed as a one layer of mixed material. So, we use the weighted average K_d values and saturated moisture contents for the mixed material in the vault with cover scenario. The time dependent changes of material properties are ignored, and the degraded properties of materials (concrete, grouted waste, the engineered cover and clay) are used in this simulation. The conceptual sketch of 1D saturated analytical model are shown in Fig. 17.



- 1D analytical saturated transport model with no lateral dispersion
- A multi layer system is reduced to one layer of mixed material in the vault with cover scenario.
- Revesivle linear adsorption is assumed
- The values of K_d are constant for all time, the weighted average values of K_d are assuemd for mixed material.
- The time dependent changes of material properties are ignored.

Fig. 17 A conceptual sketch of 1D analytical saturated transport model.

These three 1D transport models and the two-dimensional transport model (MIG2DF) are classified into two groups with respect to the major difference of the treatment of the flow velocity within the facility, in order to discuss the conservativeness of the result obtained from each simulation and the suitability of the assumption of a soil layer being saturated. The assumption is often used in safety analyses to avoid a complexity of analyzing the unsaturated-saturated groundwater flow. One group of the transport models uses the unsaturated flow velocities and moisture contents which are obtained from the detailed and realistic unsaturated flow simulations assuming the degradation of material properties. This group is composed of 1D unsaturated transport model and the two-dimensional transport model by the MIG2DF. The other group, which is composed of 1D saturated transport model and 1D analytical saturated transport model, uses the assumed flow velocities and moisture contents which are based on the infiltration rate, the saturated conditions and degraded material properties. Figure 18 shows the difference of the conceptualizations of the flow velocity within the disposal unit among the three 1D models in the vault and trench with cover scenarios. In this figure, 'model A' denotes the 1D unsaturated transport simulation,



Model B and analy. ; the water velocities are assumed based on the infiltration rate and saturated conditions.
Model A and MIG2DF ; the water velocities are obtained from the results of the MIG2DF. Sequential steady state condition is assumed.

Fig. 18 The difference of the conceptualizations of water flow velocities among the three 1D models in (a) the vault with cover scenario and (b) the trench with cover scenario. The terms of 'model A', 'model B', 'analy.' and 'MIG2DF' denote (i) 1D unsaturated transport model, (ii) 1D saturated transport model, (iii) 1D analytical saturated transport model and (iv) 2D unsaturated transport model, respectively.

'model B' denotes the 1D saturated transport simulation, 'analy.' denotes the 1D analytical saturated transport simulation and 'MIG2DF' denotes the 2D unsaturated transport simulation. Though a difference of the treatment of the multilayer system in the 1D analytical saturated transport model exist, we divide into the above two groups. The grouping is helpful to make clear the difference between the obtained results and the suitability of the assumptions being saturated.

6.2 Comparison of the Results

Figure 19 shows the time dependent release rates obtained by the three 1D models and 2D model(MIG2DF) in the vault with cover scenario. The figure shows that the maximum release rates of H-3 obtained by 1D saturated simulations assuming a constant flow velocity (model B and analy.) in the vault with cover scenario are significant larger than that by the unsaturated simulations using the time dependent flow velocity(model A and the MIG2DF). However, those of C-14, I-129 and Th-230 by 1D saturated simulations assuming a constant flow velocity are smaller than those by the unsaturated simulations using the time dependent flow velocity.

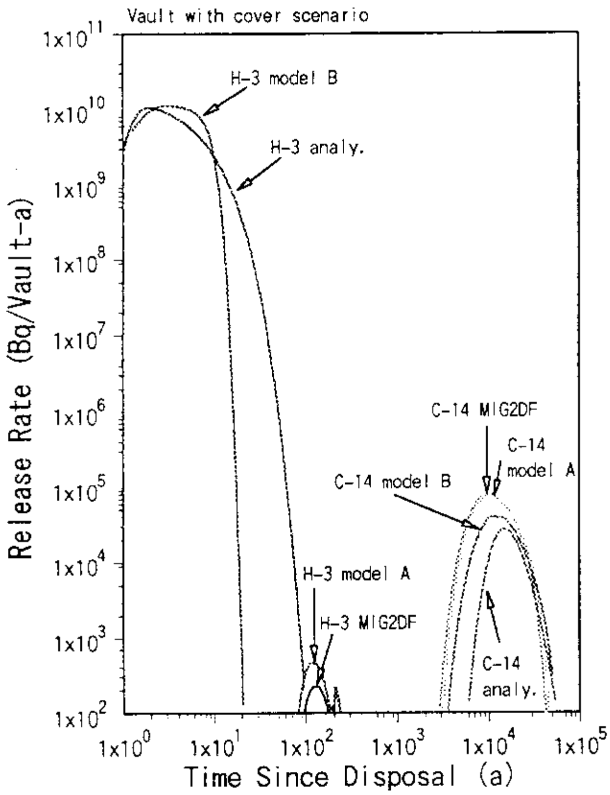
These are ascribed to that the values of the unsaturated flow velocities within the vault calculated by MIG2DF before 500 years are smaller than the assumed constant flow velocities in the saturated simulations, and the values after 500 years are larger than that. In other words, it is considered that the water flow velocities, which increase rapidly after 500 years in the unsaturated transport simulations, bring the high peak values of breakthrough curves of radionuclides. The time integrated release rate should be the same values for long-lived radionuclide in all simulations because the inventories of the radionuclides are assumed the same. The peak values of breakthrough curve will become large, if the width of breakthrough curve, which has strong correlation with the increased flow velocity after 500 years, will be narrow. The peak value increases with increasing the water flow velocity that narrows the breakthrough curve, as is the case for I-129 in Fig. 19 (b). In the unsaturated simulations, for the time period before 500 years the plume of I-129 moves downward slowly by diffusion due to the slow water flow, after 500 years it moves quickly by advection due to the fast water flow. As the results, the releases of the radionuclide for the unsaturated simulations become rapid releases and the peak values of the radionuclides release rates become larger than those for the saturated simulations.

The maximum release rate and the time of maximum obtained with the three 1D simulations and the 2D simulation in the vault with cover scenario are shown in Table 15. The huge differences in the values of peak release rate of H-3 case were observed between the unsaturated simulations and the saturated simulations. The values are in the range 2.3E+2 to 1.1E+10 Bq/a. This scatter are ascribed to the difference in the values of the flow velocity for the time period before 500 years. The flow velocities used in the saturated simulations are larger than those used in the unsaturated simulations, and thus there are no significant influences of decay on the obtained results of release rates for H-3 in the saturated simulations. There are significant influences of decay on those in the unsaturated simulation. It is said that the difference of the estimated release rates is caused by the different assumptions of the flow velocity. The saturated simulation tends to overestimate the release rate, in the early stage during which the materials keep the initial properties, especially for mobile and short-lived radionuclides.

In the case for C-14, the difference of the peak values of release rates are in the range of one order of magnitude in all simulations (2.7E+4 Bq/a - 7.7E+4 Bq/a). In the cases for I-129 and Th-230, the peak values are also in the range of one order. The times of maximum release rates for the cases of C-14, I-129 and Th-230 appear after 500 years due to retardation in all simulations. The differences of the estimated release rates have significant effects on the following transport calculations in geosphere and the individual dose calculations in biosphere. Therefore, it become important to estimate the precise release rate and to estimate the model robustness in order to ensure the conservativeness of the obtained results in the safety analysis.

Note that the values of the maximum release rate obtained with the saturated simulations are lower than those obtained with the unsaturated simulations for the radionuclides analyzed here. This result might be highly specific to analytical assumptions used here; the flow velocities used in the saturated simulations without taking account of the degradation of material properties are smaller than that used in the unsaturated simulations. It is said that the saturated simulations involve the possibility of giving underestimation for relatively immobile radionuclide during the time stage in which the materials completely degrade. This result suggests that the 1D saturated simulation should be optimized by 2D or 3D water flow analyses to estimate a reliable flow velocity in each domain involved. In other words, the transport simulation, which uses the flow velocity obtained from the detailed unsaturated flow simulation taking into account of time dependent material properties, should be performed in the safety analysis of LLW disposal adopting the vault system.

(a) H-3 and C-14



(b) I-129 and Th-230

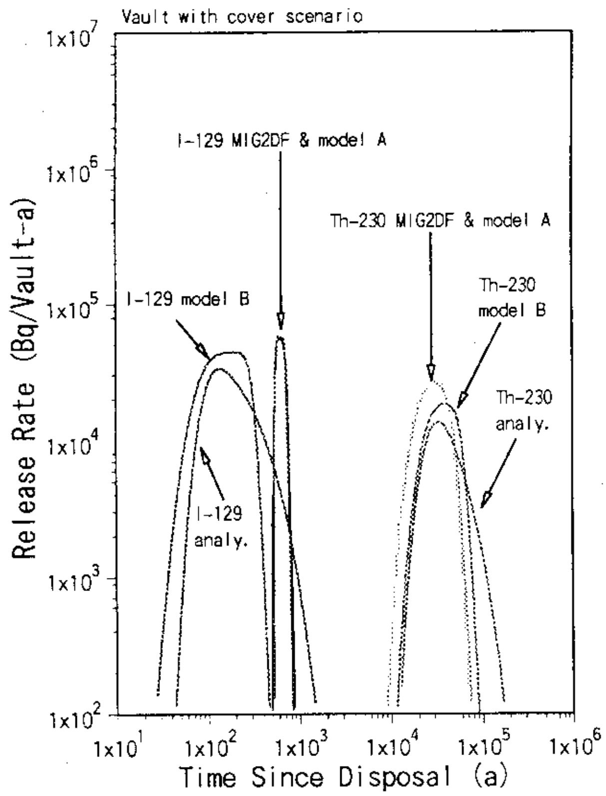


Fig. 19 The comparisons of time dependent release rates in the vault with cover scenario for (a) H-3 and C-14, (b) I-129 and Th-230. The terms of 'model A', 'model B', 'analy.' and 'MIG2DF' denote (i) 1D unsaturated transport model, (ii) 1D saturated transport model, (iii) 1D analytical saturated transport model and (iv) 2D unsaturated transport model, respectively.

Table 15 The maximum release rates and times of maximum for three 1D simulations and one 2D simulation in the vault with cover scenario.

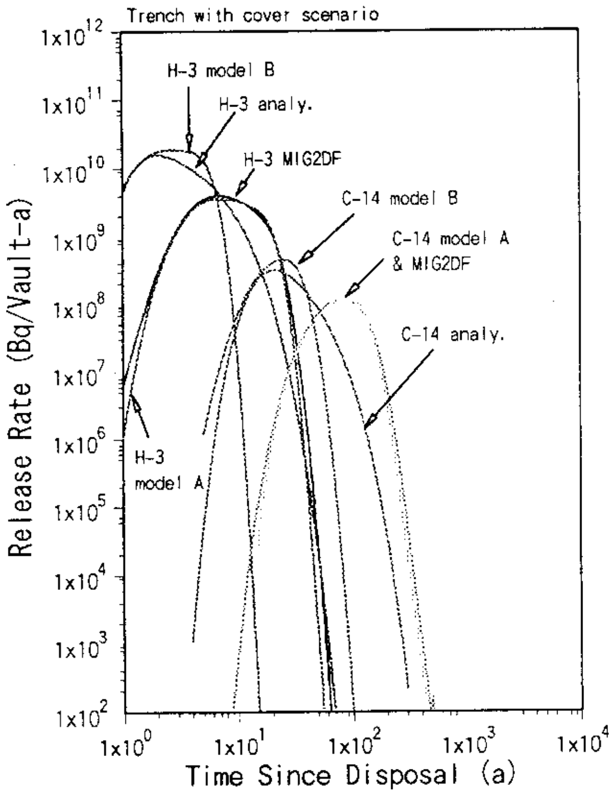
Nuclide / Model	H-3		C-14		I-129		Th-230	
	Maximum release rate (Bq/a)	Time of maximum (a)	Maximum release rate (Bq/a)	Time of maximum (a)	Maximum release rate (Bq/a)	Time of maximum (a)	Maximum release rate (Bq/a)	Time of maximum (a)
1D unsaturated transport model	4.8E+2	1.2E+2	7.7E+4	1.0E+4	5.9E+4	6.5E+2	2.6E+4	3.2E+4
1D saturated transport model	1.1E+10	3.1	4.1E+4	1.2E+4	4.4E+4	2.0E+2	1.8E+4	3.9E+4
1D analytical saturated model	1.1E+10	2.0	2.7E+4	1.5E+4	3.3E+4	1.4E+2	1.3E+4	3.4E+4
2D unsaturated transport model	2.3E+2	1.3E+2	7.6E+4	1.1E+4	5.7E+4	6.2E+2	2.6E+4	3.1E+4

Figure 20 shows the time dependent release rates obtained by the three 1D models and the 2D model in the trench with cover scenario. The maximum release rate and time of maximum are given in Table 16. The peak values of release rate in all simulations are in the range of one order. The difference among the peak values of release rate in the trench with cover scenario are smaller than that in the vault with cover scenario. The reason for this is that the difference of conceptualization decreases because the trench system has a simpler structure than the vault system. The saturated simulations assuming a constant flow velocity give conservative results for H-3, C-14 and I-129. However, the result of Th-230 is not enough conservative. This is the same reason as the vault with cover scenario case, because the times of maximum release rate of Th-230 in all simulations are about 15,000 years, until such time the cover materials have completely degraded. It might be said therefore that the assumption of the saturated condition is conservative for H-3, C-14 and I-129, but not enough conservative for Th-230 in the trench with cover scenario.

Furthermore, Fig. 20 shows that the model A, 1D saturated transport simulation, is almost the same result as that of the 2D unsaturated transport simulation by using the MIG2DF. This brings about benefits in safety analysis of LLW disposal; a short computing time and simplification of the simulation. In the transport simulation, the simplifying assumptions, which were used in the 1D unsaturated transport simulation, are valid for the disposal facility adopting the vault and trench system. It is, however, necessary to simulate the precise flow velocity in the unsaturated zone using a two-dimensional unsaturated flow model. The reason for this is that the simulation assuming a constant flow velocity might not be suitable for the case in which materials change with time.

The results obtained here are reflected from the assumption given by the specification of NSARS. The specification of NSARS test case 2B is formulated based on a real site characteristics and is judged to be realistic, expect for the long-term degradation behavior of an engineered facility. The results of the study clearly indicate that the degradation of the engineered materials, e.g. concrete structure, affects a long-term hydrology inside and outside the facility. This study indicates that the conservativeness of any assumptions to be used in safety analysis should be carefully examined to ensure the robustness of the results, and that the unsaturated flow simulation taking account of the time dependent material properties should be performed in the safety analysis of LLW disposal located in the unsaturated zone.

(a) H-3 and C-14



(b) I-129 and Th-230

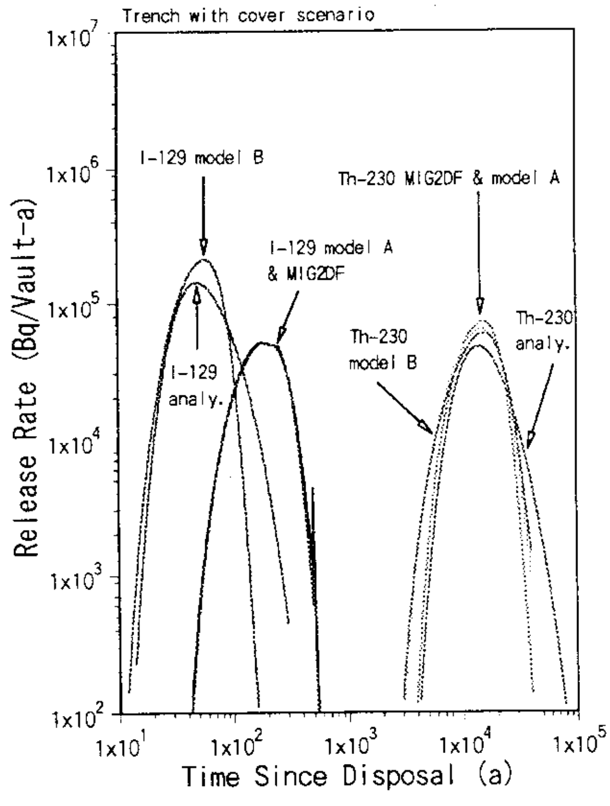


Fig. 20 The comparisons of time dependent release rates in the trench with cover scenario for (a) H-3 and C-14, (b) Ni-63, I-129 and Th-230. The terms of 'model A', 'model B', 'analy.' and 'MIG2DF' denote (i) 1D unsaturated transport model, (ii) 1D saturated transport model, (iii) 1D analytical saturated transport model and (iv) 2D unsaturated transport model, respectively.

Table 16 The maximum release rates and times of maximum for three 1D simulations and one 2D simulation in the trench with cover scenario.

Nuclide / Model	H-3		C-14		I-129		Th-230	
	Maximum release rate (Bq/a)	Time of maximum (a)	Maximum release rate (Bq/a)	Time of maximum (a)	Maximum release rate (Bq/a)	Time of maximum (a)	Maximum release rate (Bq/a)	Time of maximum (a)
1D unsaturated transport model	3.7E+9	7.1	1.2E+8	91	5.4E+4	2.1E+2	6.2E+4	1.5E+4
1D saturated transport model	1.9E+10	2.8	4.6E+8	26	2.1E+5	58	5.7E+4	1.5E+4
1D analytical saturated model	1.6E+10	2.0	3.2E+8	22	1.4E+5	50	4.6E+4	1.4E+4
2D unsaturated transport model	4.0E+9	7.0	1.1E+8	84	5.2E+4	2.0E+2	7.2E+4	1.5E+4

7. CONCLUSION

We performed an analytical work required by Test Case 2B of the NSARS; the screening calculation, the unsaturated flow simulation and transport simulation for two types of disposal facilities which located in the unsaturated zone. Also, we discussed the suitability of the assumption of a soil being saturated. The summary of our study is as follows;

1. The groundwater flow velocities have significant effects on the results of the radionuclides transport. It was recognized that estimations of a more precise infiltration rate and hydraulic conductivities are essential to obtain realistic results. Also, it is important how to treat the boundary conditions of the modeled domain to obtain a more realistic flow velocity.

2. The unsaturated analysis indicates that low permeable clay on the top surface with gravel drain will be much effective for the reduction of vertical flow through the vault/trench. It is also suggested that the vault facility can be the flow path after the materials completely degrade, if the assumptions for the degradation are suitable in the vault with cover scenario.

3. The transport simulations need fine grids and small time steps due to a weak-dispersion, and require long computing times. In Test Case 2b simulations, the results show that vault concept is much effective to reduce the release rate from the facility. The vault facility may introduce no significant release during the first 500 years.

4. From the comparison among different conceptual models, the one-dimensional unsaturated transport model using a realistic flow velocity obtained by the two-dimensional flow simulation gives enough realistic result which is the same as the result of the two-dimensional unsaturated transport model in the vault and trench with cover scenarios. Also, the comparison shows that the assumption of a constant flow velocity under the saturated condition, without taking account of the time dependent changes of the material properties, does not always give a conservative result for the disposal facility. It is necessary to simulate a flow velocity in the unsaturated zone using a two-dimensional model. Forthermore, it is important to estimate the model robustness in order to ensure the conservativeness of the obtained results in the safety analysis.

In future work, it should be clarified how the uncertainty of conceptual model affects the release rate from the disposal facility and the resulting dose in the integrated system (source term + geosphere + biosphere) for the safety assessment of LLW disposal.

ACKNOWLEDGMENT

The authors wish to thank to Mr. S. Shima, Mr. T. Takahashi and Mr. S. Takeda for their helpful discussions.

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2. The unsaturated analysis indicates that low permeable clay on the top surface with gravel drain will be much effective for the reduction of vertical flow through the vault/trench. It is also suggested that the vault facility can be the flow path after the materials completely degrade, if the assumptions for the degradation are suitable in the vault with cover scenario.

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In future work, it should be clarified how the uncertainty of conceptual model affects the release rate from the disposal facility and the resulting dose in the integrated system (source term + geosphere + biosphere) for the safety assessment of LLW disposal.

ACKNOWLEDGMENT

The authors wish to thank to Mr. S. Shima, Mr. T. Takahashi and Mr. S. Takeda for their helpful discussions.

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APPENDIX OUTPUT RESULTS OF NSARS TEST CASE 2B

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RESULTS FOR NSARS TEST CASE 2B (7)

4. TABLES FOR MAXIMUM RELEASE RATES AND CONCENTRATIONS

(a) Vault Scenario

- Release rate is Bq per vault-a, locations are specified in Specification.

Radionuclide (incl. daughters)	Maximum Release Rate (Bq/vault-a)	Time of Maximum (a)
H-3	3.2	107
C-14	6.9E+4	1.02E+4
Ni-63	2.0E-5	960
Sr-90	3.2E+4	549
I-129	5.7E+4	633
Th-230	2.5E+4	3.09E+4
Ra-226	2.2E+5	3.80E+3
Pb-210	7.8E+4	3.88E+3
Po-210	2.3E+5	3.88E+3

Radionuclide (incl. daughters)	Maximum Conc. (Bq/cm^3)	Time of Maximum (a)
H-3	1.9E-7	100
C-14	1.0E-4	9.11E+3
Ni-63	1.71E-12	1.30E+3
Sr-90	5.8E-5	552
I-129	7.3E-5	654
Th-230	3.2E-5	3.09E+4
Ra-226	3.0E-4	3.88E+3
Pb-210	1.0E-4	3.95E+3
Po-210	3.1E-4	3.95E+3

Table 4.(a) The maximum release rates and concentrations for each radionuclide in the vault scenario.

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RESULTS FOR NSARS TEST CASE 2B (8)

4. TABLES FOR MAXIMUM RELEASE RATES AND CONCENTRATIONS (Cont.)

(b) Trench Scenario

- Release rate is in Bq per vault-a, locations are specified in Specification.

Radionuclide (incl. daughters)	Maximum Release Rate (Bq/vault-a)	Time of Maximum (a)
H-3	1.1E+8	22.9
C-14	2.9E+8	511
Ni-63	2.3E+8	570
Sr-90	2.4E+4	550
I-129	1.9E+5	539
Th-230	7.6E+4	1.44E+4
Ra-226	3.5E+5	1.76E+3
Pb-210	1.2E+5	1.79E+3
Po-210	3.5E+5	1.79E+3

Radionuclide (incl. daughters)	Maximum Conc. (Bq/cm^3)	Time of Maximum (a)
H-3	4.3	26.4
C-14	4.6E-1	513
Ni-63	3.4E-1	576
Sr-90	3.2E-5	554
I-129	3.0E-4	543
Th-230	1.1E-4	1.53E+4
Ra-226	5.2E-4	1.79E+3
Pb-210	1.7E-4	1.82E+3
Po-210	5.2E-4	1.82E+3

Table 4.(b) The maximum release rates and concentrations foe each radionuclide in the trench scenario

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RESULTS FOR NSARS TEST CASE 2B (9)

5. FIGURES FOR TIME DEPENDENT RELEASE RATES

(a) Vault Scenario

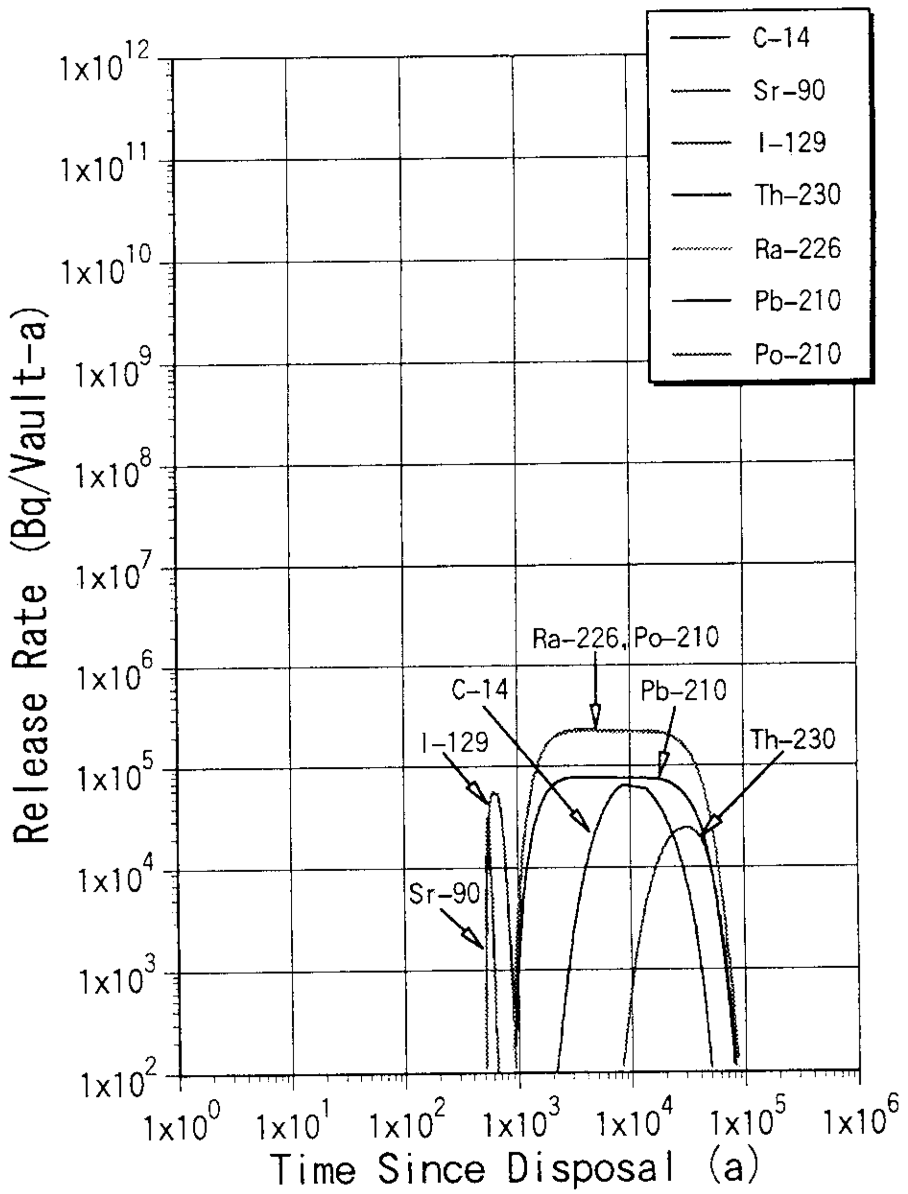

Fig 5.(a)-1 The time dependent release rates in the vault scenario.

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RESULTS FOR NSARS TEST CASE 2B (10)

5. FIGURES FOR TIME DEPENDENT RELEASE RATES (Cont.)

(b) Trench Scenario

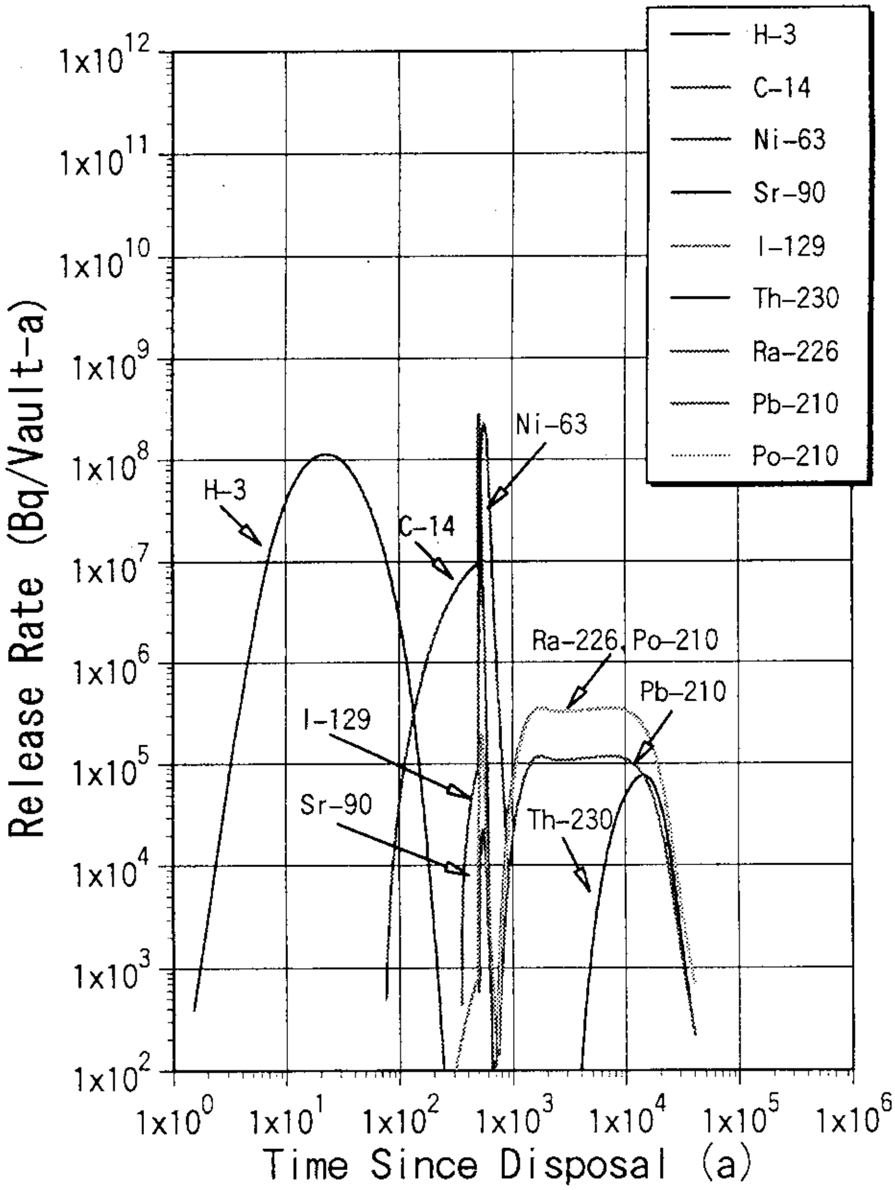

Fig. 5.(b)-1 The time dependent release rates in the trench scenario.

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RESULTS FOR NSARS TEST CASE 2B (11)

5. FIGURES FOR TIME DEPENDENT CONCENTRATIONS

(a) **Vault Scenario**

- Concentration at point where maximum concentration occurs.

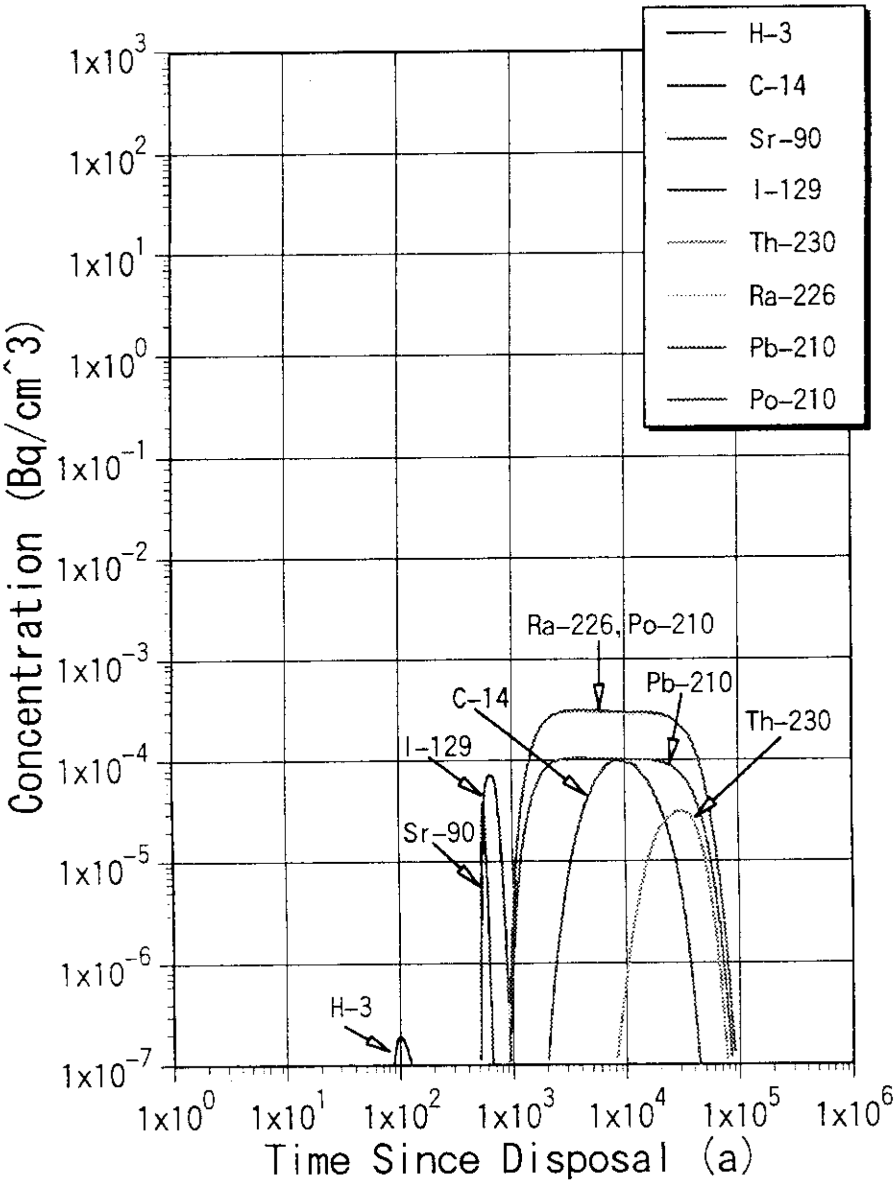

Fig. 5.(a)-2 The time dependent concentrations in the vault scenario.

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RESULTS FOR NSARS TEST CASE 2B (12)

5. FIGURES FOR TIME DEPENDENT CONCENTRATIONS (Cont.)

(b) Trench Scenario

- Concentration at point where maximum concentration occurs.

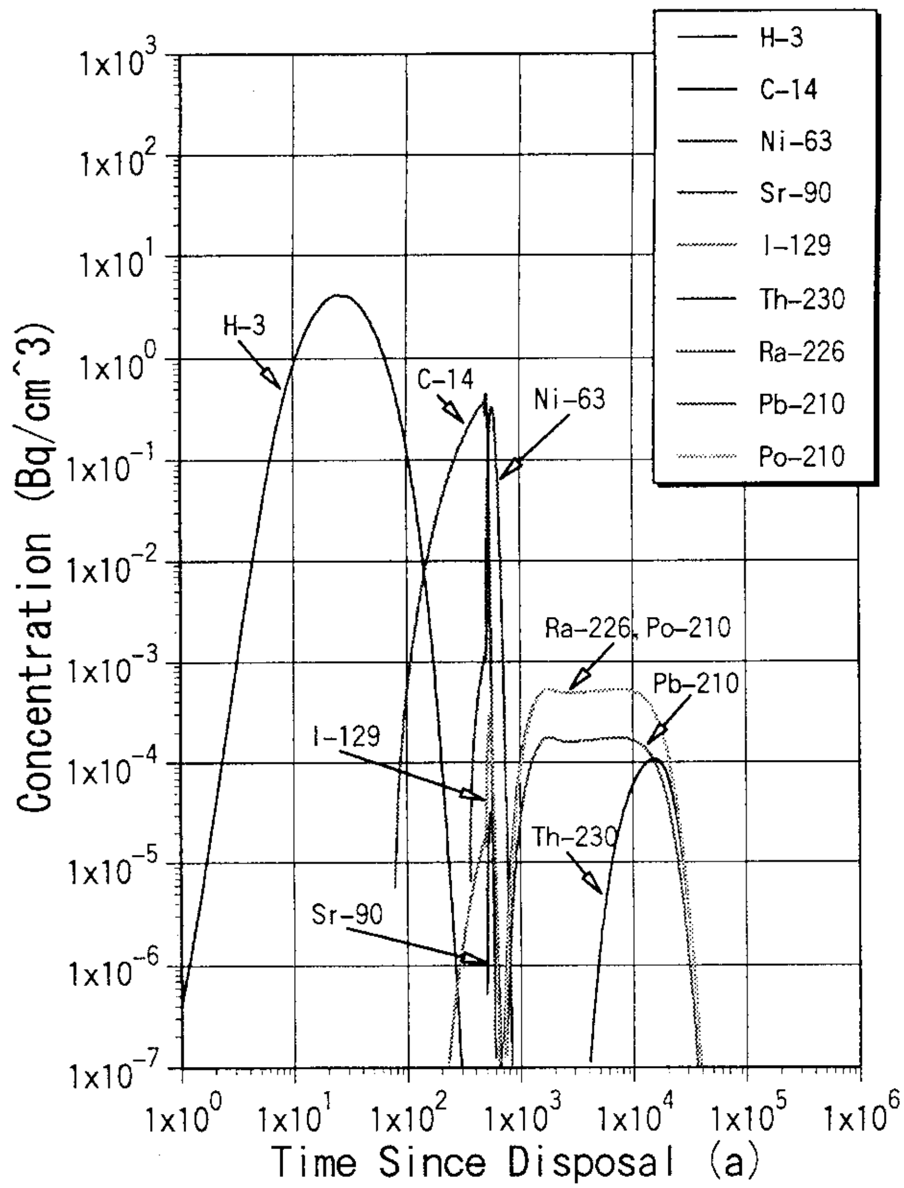

Fig 5.(b)-2 The time dependent concentrations in the trench scenario.

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RESULTS FOR NSARS TEST CASE 2B (15) - Optional

8. TABLES FOR MAXIMUM RELEASE RATES AND CONCENTRATIONS -Optional

(a) **Vault with Cover Scenario**

- Release rate is Bq per vault-a, locations are specified in Specification.

Radionuclide (incl. daughters)	Maximum Release Rate (Bq/vault-a)	Time of Maximum (a)
H-3	2.3E+2	128
C-14	9.8E+4	1.00E+4
Ni-63	0.41	1.60E+3
Sr-90	3.4E+4	549
I-129	5.7E+4	621
Th-230	2.6E+4	3.08E+4
Ra-226	2.1E+5	4.13E+3
Pb-210	8.6E+4	4.45E+3
Po-210	2.4E+5	4.37E+3

Radionuclide (incl. daughters)	Maximum Conc. (Bq/cm^3)	Time of Maximum (a)
H-3	7.1E-6	216
C-14	1.3E-4	1.00E+4
Ni-63	6.3E-9	1.58E+3
Sr-90	4.0E-5	552
I-129	7.4E-5	660
Th-230	3.3E-5	3.08E+4
Ra-226	3.0E-4	3.82E+3
Pb-210	3.0E-4	1.58E+4
Po-210	5.1E-4	1.58E+4

Table 8.(a) The maximum release rates and concentrations for each radionuclide in the vault with cover scenario.

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RESULTS FOR NSARS TEST CASE 2B (16) - Optional

8. TABLES FOR MAXIMUM RELEASE RATES AND CONCENTRATIONS -Optional (Cont.)

(b) Trench with Cover Scenario

- Release rate is Bq per vault-a, locations are specified in Specification.

Radionuclide (incl. daughters)	Maximum Release Rate (Bq/vault-a)	Time of Maximum (a)
H-3	4.0E+9	7.0
C-14	1.1E+8	84.4
Ni-63	4.3E+8	234
Sr-90	3.0E+7	146
I-129	5.2E+4	196
Th-230	7.2E+4	1.54E+4
Ra-226	3.6E+5	7.92E+3
Pb-210	1.2E+5	7.76E+3
Po-210	3.6E+5	7.76E+3

Radionuclide (incl. daughters)	Maximum Conc. (Bq/cm^3)	Time of Maximum (a)
H-3	23.8	7.4
C-14	0.80	104
Ni-63	2.4	244
Sr-90	0.15	148
I-129	3.7E-4	240
Th-230	1.1E-4	1.60E+4
Ra-226	5.7E-4	7.76E+3
Pb-210	1.9E-4	7.76E+3
Po-210	5.7E-4	7.76E+3

Table 8.(b) The maximum release rates and concentrations for each radionuclide in the trench with cover scenario.

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RESULTS FOR NSARS TEST CASE 2B (17) - Optional

9. FIGURES FOR TIME DEPENDENT RELEASE RATES -Optional

(a) Vault with Cover Scenario

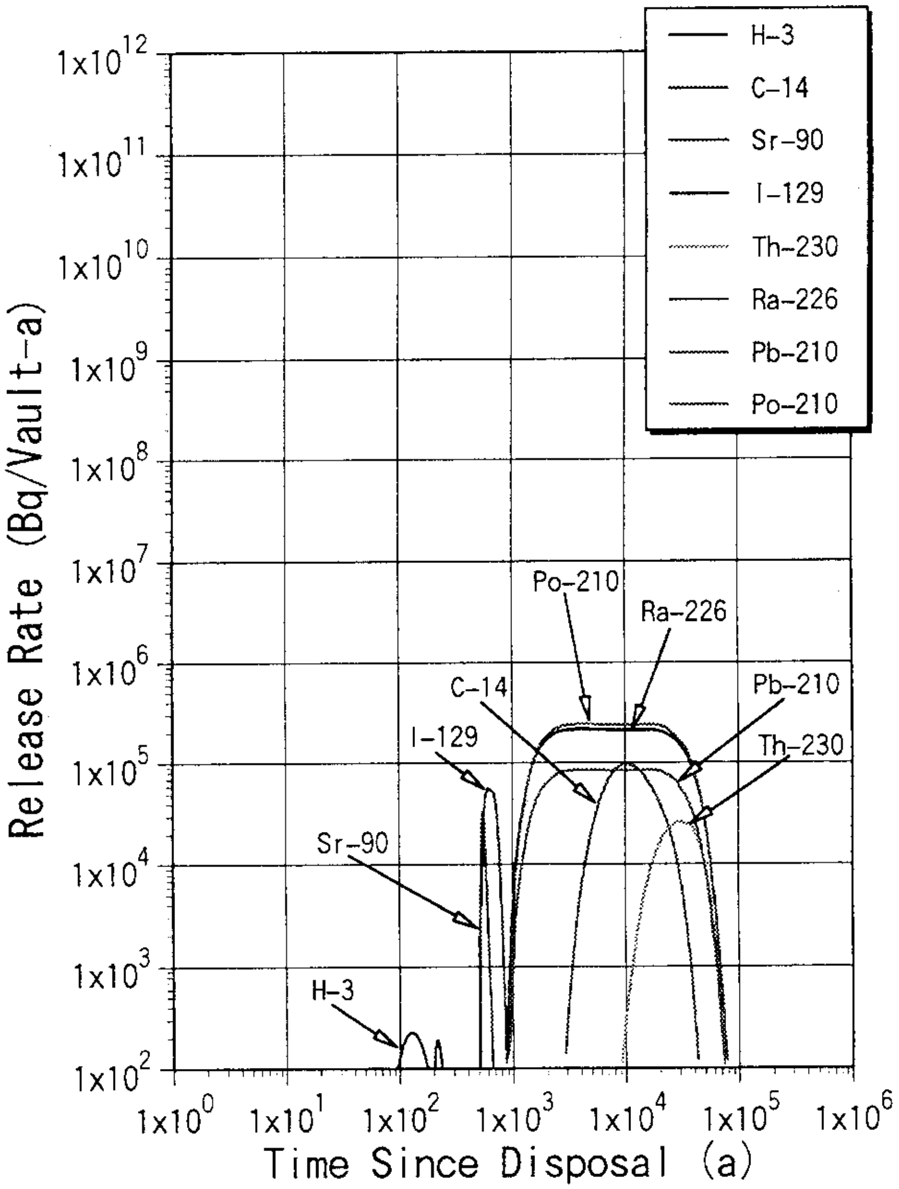

Fig 9.(a)-1 The time dependent release rates in the vault with cover scenario.

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RESULTS FOR NSARS TEST CASE 2B (18) - Optional

9. FIGURES FOR TIME DEPENDENT RELEASE RATES -Optional (Conts.)

(b) Trench with Cover Scenario

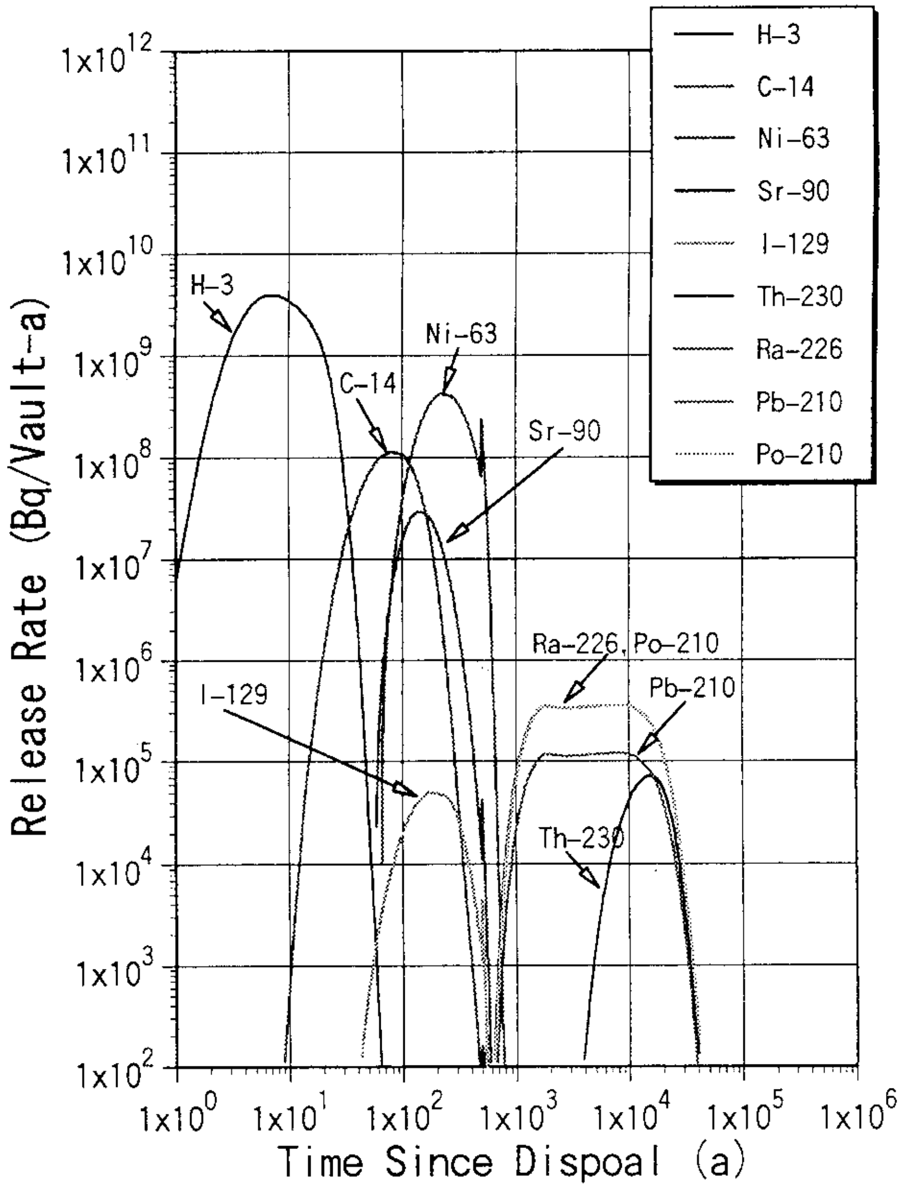

Fig 9.(b)-1 The time dependent release rates in the trench with cover scenario.

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RESULTS FOR NSARS TEST CASE 2B (19) - Optional

9. FIGURES FOR TIME DEPENDENT CONCENTRATION -Optional

(a) **Vault with Cover Scenario**

- Concentrations at point where maximum concentration occurs.

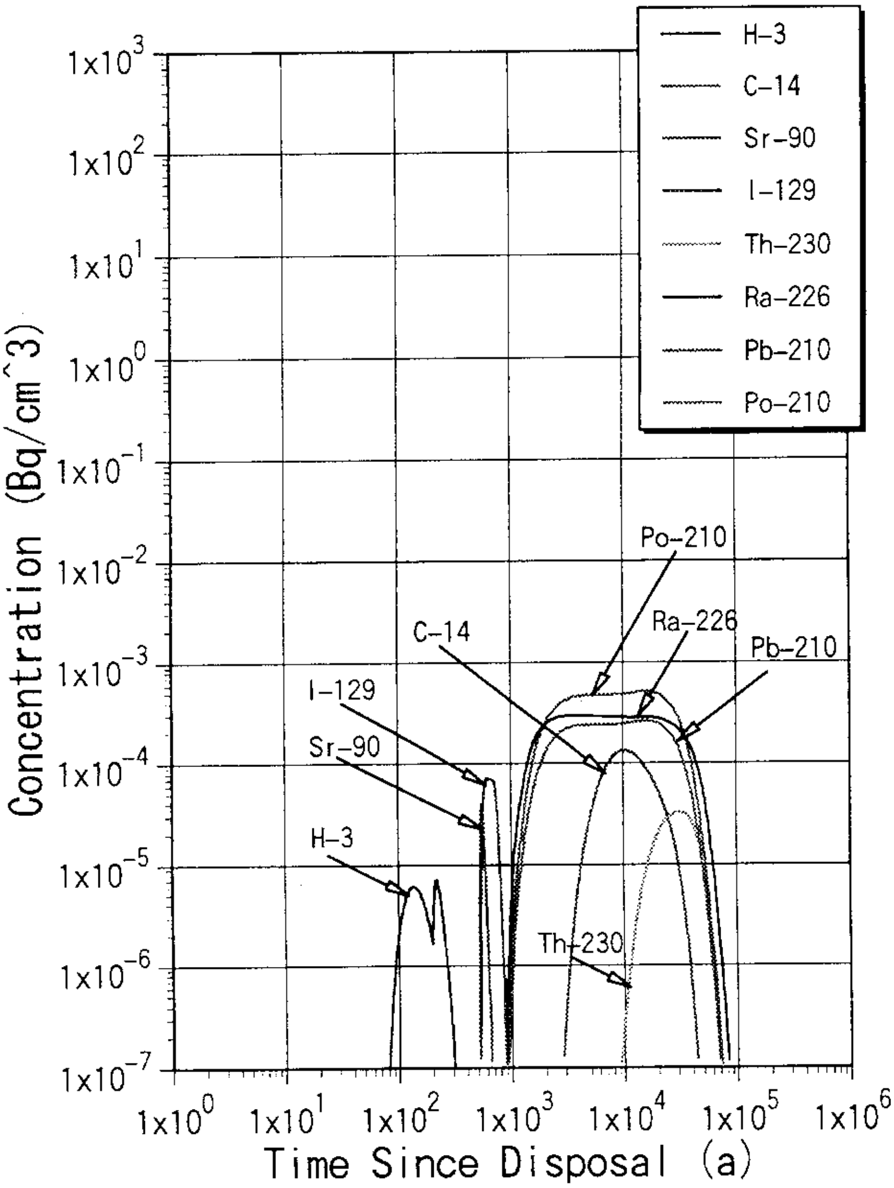

Fig. 9.(a)-2 The time dependent concentrations in the vault with cover scenario.

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RESULTS FOR NSARS TEST CASE 2B (20) - Optional

9. FIGURES FOR TIME DEPENDENT CONCENTRATION -Optional (Cont.)

(b) Trench with Cover Scenario

- Concentrations at point where maximum concentration occurs.

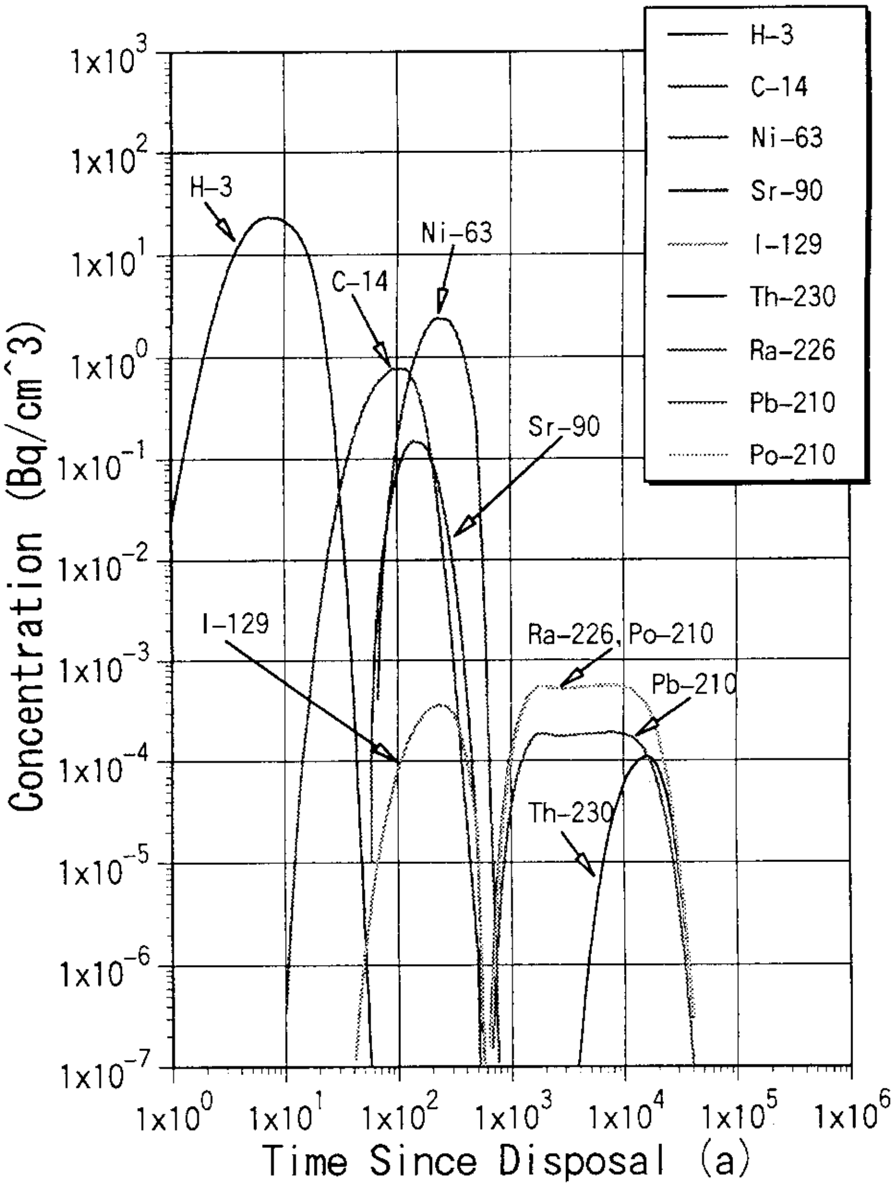

Fig. 9.(b)-2 The time dependent concentrations in the trench with cover scenario.