Chapter 4 Evaluating the safety of geological disposal

4.1 Procedure for evaluating the safety of geological disposal

The safety of geological disposal of TRU waste was performed in accordance with the safety requirements discussed in Section 1.2. Here, a safety assessment methodology for geological disposal of TRU waste is described taking into account the characteristics of TRU waste.

In a 1991 report on safety assessment methods, the OECD/NEA stated that, in addition to deterministic consequence calculations, the approach to safety assessment should include, for example, uncertainty analysis and sensitivity analysis and the use of natural analogue data as input for establishing reliability (multiple methods and arguments). Furthermore, it was stated that the safety and performance assessments are applied to a wide range of activities with the aim of gaining the understanding of those persons affected by the disposal project (interested parties). The report reviewed the activities that are necessary to obtain an adequate evaluation result, such as verification and validation of model, quality assurance, critical reviews and international cooperation. However, there was insufficient consideration of “how to present and explain the results of safety assessments in a clear and comprehensive way to decision-makers and the public” (OECD/NEA, 1991).

When evaluating the safety of the geological disposal of TRU waste, it is essential to consider a generic geological environment, the existence of multiple types of waste and the temporal and spatial variations in the characteristics of barrier materials. Such considerations will inevitably involve the evaluation of multiple uncertainties. In order to gain the confidence of the public, rather than simply that of decision-makers (including experts) by considering such factors, it is important to take measures to review thoroughly the effects of these multiple uncertainties and to present them in a way that is easily understandable.

Here, we have employed an assessment system that aims to meet these goals. In Section 4.1.1 we present the main components of the system. In Section 4.1.2 we provide an overview of a newly developed top-down assessment approach, “a comprehensive sensitivity analysis method.” This method is capable of more thoroughly analyzing the effects of the uncertainties included in the system described in Section 4.1.1 and of presenting the robustness of the assessment in a way that is easily understandable.

4.1.1 Safety assessment system

In the 1991 report by the OECD/NEA mentioned above, a general approach to the long-term safety assessment of disposal systems was proposed (OECD/NEA, 1991). This approach comprises the activities shown below:

- Scenario development
- Model development and application
- Integrated assessment / uncertainty and sensitivity analysis / regulatory criteria for disposal
- Confidence building
The safety assessment approach employed in the present investigation is based on this conventional approach and is summarized in Fig 4.1.1-1.

Firstly, in order to present the scope of the assessment in an easily understandable manner, the following factors are set as initial or preconditions based on the characteristics of the disposal concept:

- The safety requirements (see Section 1.2);
- The geological environment (see Section 1.3);
- The amount of radioactivity in the waste (inventory) (see Chapter 2);
- The EBS design.

An aim of the present investigation is to consider how to evaluate a wide range of geological environments, as well as to improve understanding. Scenario development is performed in a manner similar to the conventional approach to safety assessment. Here, the characteristics of geological disposal of TRU waste are considered and a comprehensive scenario evaluation is performed, with reference to, the internationally proposed FEP list.

In the model development and application, the conditions of the disposal environment that are important for the safety assessment are specified. Model development and detailed investigation of individual phenomena, in which temporal and spatial changes in characteristics and associated uncertainties are considered, take into account the effect of factors such as cement, nitrates and gas generation, which are
typical for TRU waste disposal.

Integrated assessment, uncertainty and sensitivity analysis and regulatory criteria for disposal, are considered in the nuclide migration analyses and dose assessments. In addition to setting each analytical case according to the important environmental conditions of disposal (based on the investigation of individual phenomena), the relationship between the scenario and the various analytical cases is clearly specified to increase understanding of the analysis process. Furthermore, to assess the significance of uncertainties in the scenarios, models and parameters underlying each analytical case, alternative cases were evaluated using a deterministic method. Resulting dose is compared with regulatory guidelines in overseas PA reports and natural radiation levels in Japan.

For confidence building the results of a thorough investigation of one scenario are summarised. In addition to demonstrating the robustness of the safety assessment, these results highlight the issues that must be addressed in the future.

Investigating the uncertainties in the analysis will lead to increased credibility of the assessment. However, in order to thoroughly evaluate the effect of the uncertainties using a conventional deterministic consequence calculation method, a huge number of alternative analytical cases will be needed. This situation arises because it is necessary to consider the superimposition of multiple investigation cases and the variations in the individual parameters. It can be expected that the resulting large quantity of output will increase the difficulty of understanding the safety assessment result. Therefore, in the present work, a newly developed top-down assessment approach, “comprehensive sensitivity analysis method” is introduced and applied to evaluate the effects of the uncertainties of individual parameters and the superimposition of parameter combinations. The comprehensive sensitivity analysis is developed to complement the conventional deterministic consequence calculations, and make it possible to extract the conditions of alternative options, in addition to presenting quantitatively the effects of the uncertainties and the safety margins. It is also possible to define the issues that should be addressed in the future.
<table>
<thead>
<tr>
<th>General approach to safety assessment</th>
<th>Items corresponding to implementation of the safety assessment, and their contents</th>
<th>Location in report</th>
</tr>
</thead>
<tbody>
<tr>
<td>OECD/NEA (1991)</td>
<td>Summary of initial conditions</td>
<td>4.2</td>
</tr>
<tr>
<td></td>
<td>· Safety requirements</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Geological environment conditions</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Inventory</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Specified conditions</td>
<td></td>
</tr>
<tr>
<td>Scenario development</td>
<td>Scenario development</td>
<td>4.3</td>
</tr>
<tr>
<td></td>
<td>· Production of a comprehensive FEP list</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· FEP classification</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· FEP screening considered in safety assessment</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Classification of scenarios</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Scenario description</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Important repository environment conditions for safety assessment</td>
<td></td>
</tr>
<tr>
<td>Model development and application</td>
<td>Establishing conditions in the disposal environment for safety assessment</td>
<td>4.4</td>
</tr>
<tr>
<td></td>
<td>· Chemical condition of groundwater</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Effect of alteration of the engineered barrier</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Hyperalkaline alteration of host rock around the disposal facility</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Hydraulic conditions of the near-field</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Effect of colloids / organic materials / microbes</td>
<td></td>
</tr>
<tr>
<td>Integrated assessment</td>
<td>Radionuclide transport analysis and dose assessment</td>
<td>4.5</td>
</tr>
<tr>
<td>Uncertainty and sensitivity analysis</td>
<td>· Analytical cases</td>
<td></td>
</tr>
<tr>
<td>Regulatory criteria for disposal</td>
<td>· Analysis of the Reference Case</td>
<td></td>
</tr>
<tr>
<td></td>
<td>* Model / data selection</td>
<td></td>
</tr>
<tr>
<td></td>
<td>* Analysis / evaluation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Analysis of alternative cases in the base scenario</td>
<td></td>
</tr>
<tr>
<td></td>
<td>* Model / data selection</td>
<td></td>
</tr>
<tr>
<td></td>
<td>* Analysis / evaluation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Evaluation of uncertainty in the base scenario</td>
<td></td>
</tr>
<tr>
<td></td>
<td>* Comprehensive sensitivity analysis</td>
<td></td>
</tr>
<tr>
<td></td>
<td>* Specification of parameter variation ranges</td>
<td></td>
</tr>
<tr>
<td></td>
<td>* Analysis / evaluation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Analysis of perturbation scenario</td>
<td></td>
</tr>
<tr>
<td></td>
<td>· Analysis of isolation failure scenarios</td>
<td></td>
</tr>
<tr>
<td>Confidence building</td>
<td>Summary of disposal safety</td>
<td>4.6</td>
</tr>
<tr>
<td></td>
<td>· Summary of the results of the safety evaluation, assertion of the robustness of the evaluation and presentation of issues to be followed up</td>
<td></td>
</tr>
</tbody>
</table>
4.1.2 Methods for evaluating the influence of uncertainties

Previously, the influence of uncertainties that must be considered in safety assessments was evaluated by, for example, comparing the analytical results of a Reference Case with the results of a number of alternative cases. These cases have alternative values for some parameters that affect uncertainty of the results (JNC, 2000; TRU Coordination Team, 2000). Potentially, the adequacy of the uncertainty evaluation depends on the parameter ranges and the number of parameter combinations. However, a complete evaluation would require a huge number of cases to be analyzed which is considered difficult to explain.

In this report, to complement the existing deterministic analytical methods, a comprehensive sensitivity analysis is employed to extract combinations of parameter values (defined as “a successful condition”) that result in doses less than the target value. These values are given for parameters that are identified to be of relatively high importance. The importance of the parameters is determined by a statistical analysis of the results obtained when individual parameters are sampled randomly. This complementary approach uses a model that, as far as possible, comprehensively incorporates the various phenomena that occur within the repository.

Figure 4.1.2-1 shows the characteristics of the comprehensive sensitivity analysis adopted for the evaluation described in this report.

The parameters considered to be important are indicated by the extent of variation in dose within the specified parameter variation ranges and used to extract the successful conditions defined by combinations...
of parameter values (threshold values) within the variation ranges of parameter values that would give a
dose below a specified target value.

By adopting this approach, it is possible to give the information below:

1. Quantification of the influence of uncertainty and demonstration of the adequacy of safety
   assessments;
2. Quantification of safety margin to safety criteria and of parameter tolerance to changes in parameter
   values;
3. Presentation of alternative planning options and of the prospect on the treatment of unresolved
   problems;
4. Presentation of important issues to be researched.

By adopting this method, it is possible to effectively answer questions assumed from the results of the
deterministic consequence calculations such as whether or not there is greater parameter variation, or
whether other parameter combinations occur.

Up till now, estimating overall uncertainty has been attempted through the definition and calculation of
many analytical cases considering the wide range of parameter variations and parameter combinations. In
contrast, the comprehensive sensitivity analysis achieves this through a comprehensive presentation of
results given by random sampling. Also, it is possible to simplify the definition of the analytical cases and
improve understanding of results. Furthermore, it is possible to understand system performance
based on the successful condition deduced from key parameters.

In this method, all the parameters are treated individually. However, the importance of inter-relationships
among parameter values, for example solubilities, distribution coefficients, porosity, diffusion coefficients
and hydraulic conductivities is pointed out by expert judgment. If correlations between parameters for
different nuclides in the same decay chain are not taken into account, it is possible that many results will be
based on geochemically unreasonable parameter combinations and be highly misleading. For this reason, it
is important to investigate thoroughly how correlations are introduced between combinations of parameter
values in cases when a nuclide in a decay series is important in the evaluation.

In the existing evaluation (TRU Coordination Team, 2000), the dominant nuclides contributing to the
dose from TRU waste are I-129 and C-14. In cases when these nuclides are dominant, it is considered that
the importance of consideration of correlations on combinations of parameter values is relatively small.
Therefore, under these conditions, to avoid the effects of new uncertainties connected with establishing
correlations between parameters, all the parameters are treated individually. The introduction of parameter
correlations is a key issue in cases when decay chain nuclides become important in the assessment.

The analytical results used in this method are described in Section 4.5.4 in this chapter.
4.2 Summary of initial conditions

In this section, safety requirements, geological environment conditions, inventory and specified (EBS) conditions described in Sections 1.2, 1.3 and Chapters 2 and 3 are revised and summarized as pre-conditions for a safety assessment.

4.2.1 Safety requirements

The safety requirements, etc considered in this report, specified in Section 1.2, as requirements for the safety assessment are shown in Table 4.2.1-1. The ways in which these requirements can be addressed when carrying out a safety assessment are evaluated.

<table>
<thead>
<tr>
<th>General item</th>
<th>Requirement</th>
<th>Requirement No. in DS154</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i) Common requirements for technical evaluation</td>
<td>- Specific demonstration of disposal facility safety and level of reliability of safety</td>
<td>Requirement 12</td>
</tr>
<tr>
<td></td>
<td>- Consideration of temporal and spatial variations</td>
<td>Requirement 12</td>
</tr>
<tr>
<td></td>
<td>- Showing that there is no problem that might compromise safety</td>
<td>Requirement 12</td>
</tr>
<tr>
<td></td>
<td>- Presentation of unsolved problems</td>
<td>Requirement 12</td>
</tr>
<tr>
<td></td>
<td>- Ensuring adequate documentation (justification, tracking performance, clarity)</td>
<td>Requirement 13</td>
</tr>
<tr>
<td></td>
<td>- Exchanging opinions with internal and external reviewers</td>
<td>Requirement 13</td>
</tr>
<tr>
<td></td>
<td>- Quality management (including models used, data and verification and validation of codes)</td>
<td>Requirement 23</td>
</tr>
<tr>
<td>(iv) Safety assessment requirements</td>
<td>- Ensuring that the results of the safety assessment are sufficiently reliable</td>
<td>Requirement 6</td>
</tr>
<tr>
<td></td>
<td>- Understanding the characteristics and processes that contribute to safety; identification and understanding of phenomena and processes that might be detrimental to safety</td>
<td>Requirement 6</td>
</tr>
<tr>
<td></td>
<td>- Considering of uncertainty in the safety assessment</td>
<td>Requirement 6</td>
</tr>
<tr>
<td></td>
<td>- Checking adequacy of research scope (assessment timescale, assessed events/scenarios, analytical case)</td>
<td>Requirement 12</td>
</tr>
<tr>
<td></td>
<td>- Application of multiple arguments based on the results of sensitivity analysis, analysis of the significance of uncertainty, “what if” analysis, reserve FEPs, stylized approach, adopting complementary safety indicators and natural analogue research</td>
<td>Requirement 9 Requirement 12</td>
</tr>
</tbody>
</table>

4.2.2 Geological environment conditions

As described in Section 1.3, typical geological environment conditions for use in safety assessment are presented. The analyses carried out in the safety assessment correspond to these various geological environment conditions. Table 4.2.2-1 shows geological information that is used in safety assessments.
Table 4.2.2-1 Geological information used in assessments

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geography</td>
<td>Inland</td>
<td>Inland</td>
<td>Coast</td>
<td>Coast</td>
</tr>
<tr>
<td>Topographic features</td>
<td>Plain (hills, mountains)</td>
<td>Plain (hills, mountains)</td>
<td>Plain</td>
<td>Plain</td>
</tr>
<tr>
<td>Lithology</td>
<td>Sedimentary rock</td>
<td>Crystalline rock</td>
<td>Sedimentary rock</td>
<td>Crystalline rock</td>
</tr>
<tr>
<td>Groundwater origin</td>
<td>Precipitation</td>
<td>Precipitation</td>
<td>Oceanic</td>
<td>Oceanic</td>
</tr>
<tr>
<td>Transmissivity**1 (m² s⁻¹)</td>
<td>10⁻¹⁰ (10⁻⁹, 10⁻¹¹)</td>
<td>10⁻¹⁰ (10⁻⁹, 10⁻¹¹)</td>
<td>10⁻¹⁰ (10⁻⁹, 10⁻¹¹)</td>
<td>10⁻¹⁰ (10⁻⁹, 10⁻¹¹)</td>
</tr>
<tr>
<td>Hydraulic conductivity (m s⁻¹)</td>
<td>10⁻⁹ (10⁻⁸, 10⁻¹⁰)</td>
<td>10⁻⁹ (10⁻⁸, 10⁻¹⁰)</td>
<td>10⁻⁹ (10⁻⁸, 10⁻¹⁰)</td>
<td>10⁻⁹ (10⁻⁸, 10⁻¹⁰)</td>
</tr>
<tr>
<td>Hydraulic gradient</td>
<td>0.01 (0.05)</td>
<td>0.01 (0.05)</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Host rock type</td>
<td>SR-C</td>
<td>HR</td>
<td>SR-C</td>
<td>HR</td>
</tr>
<tr>
<td>Effective porosity (−)</td>
<td>0.3</td>
<td>0.02</td>
<td>0.3</td>
<td>0.02</td>
</tr>
<tr>
<td>Uniaxial compressive strength (MPa)</td>
<td>15</td>
<td>115</td>
<td>15</td>
<td>115</td>
</tr>
<tr>
<td>Disposal depth (m)</td>
<td>500, (300)</td>
<td>1,000, (500)</td>
<td>500, (300)</td>
<td>500, (300)</td>
</tr>
<tr>
<td>Biosphere</td>
<td>River water</td>
<td>River water</td>
<td>Seawater</td>
<td>Seawater</td>
</tr>
</tbody>
</table>

Values in parentheses ( ) are variant parameter values.

4.2.3 Inventory

The radionuclide inventory for safety assessment is presented, as described in Section 2. Safety assessment involves considering the characteristics of the waste package (radionuclide leaching characteristics, etc.) and carrying out the evaluation corresponding to the characteristics of each waste package group. For this purpose, it is important to present the inventory for each waste container type and waste package group. Therefore, firstly, Table 4.2.3-1 shows the classification of waste packages in each container group considered by the safety assessment.

Table 4.2.3-1 Classification of the waste packages in each waste package group

<table>
<thead>
<tr>
<th>Waste container group</th>
<th>Included container</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group 1</td>
<td>200L Drum (steel and stainless steel)</td>
<td>Gr1-D</td>
</tr>
<tr>
<td>Group 2</td>
<td>Stainless steel canister</td>
<td>Gr2-C</td>
</tr>
<tr>
<td></td>
<td>BNNS package (stainless steel)</td>
<td>Gr2-B</td>
</tr>
<tr>
<td>Group 3</td>
<td>200L drum (steel and stainless steel)</td>
<td>Gr3-D</td>
</tr>
<tr>
<td></td>
<td>Square package</td>
<td>Gr3-X</td>
</tr>
<tr>
<td></td>
<td>BNNS package (stainless steel)</td>
<td>Gr3-B</td>
</tr>
<tr>
<td>Group 4</td>
<td>200L drum (steel and stainless steel)</td>
<td>Gr4-D</td>
</tr>
<tr>
<td></td>
<td>Square package</td>
<td>Gr4-X</td>
</tr>
<tr>
<td></td>
<td>BNNS package (stainless steel)</td>
<td>Gr4-B</td>
</tr>
</tbody>
</table>

4-8
Additionally, the temporal variation in the radionuclide inventory in each type of waste container is shown in Figure 4.2.3-1 and numerical values are given in Table 4.2.3-2.

Figure 4.2.3-1 Temporal variation in radioactivity
Table 4.2.3-2 Model inventory for each waste package type used in safety assessment
(after 25 years of storage) (Bq)
C-14

Half-life*

Gr1-D

Gr2-C

Gr2-B

Gr3-D

Gr3-X

Gr3-B

Gr4-D

Gr4-X

Gr4-B

5.73E+03

0.0E+00

5.0E+14

3.3E+13

5.6E+12

7.0E+10

2.4E+13

8.4E+11

7.5E+09

4.0E+09

Cl-36

3.01E+05

0.0E+00

8.5E+12

1.8E+08

2.7E+11

1.4E+09

3.6E+04

1.3E+10

1.5E+08

4.3E+07

Co-60

5.27E+00

9.5E+04

5.7E+16

1.8E+15

1.9E+12

2.9E+11

1.8E+12

6.0E+13

3.1E+10

9.1E+13

Ni-59

8.00E+04

4.2E+03

7.0E+15

2.3E+14

8.6E+07

1.3E+09

0.0E+00

1.6E+12

1.4E+08

0.0E+00

Ni-63

9.20E+01

5.4E+05

9.6E+17

2.5E+16

9.9E+09

1.6E+11

0.0E+00

2.1E+14

1.8E+10

0.0E+00

Se-79

6.50E+04

3.0E+05

2.2E+12

0.0E+00

2.2E+09

6.4E+10

0.0E+00

4.4E+11

5.8E+09

0.0E+00

Sr-90

2.91E+01

2.8E+10

2.4E+17

1.6E+15

7.2E+14

5.8E+15

4.6E+11

7.8E+16

6.2E+14

2.8E+15

Zr-93

1.53E+06

1.4E+06

2.8E+14

1.6E+13

1.0E+10

2.8E+11

0.0E+00

6.1E+12

3.0E+10

0.0E+00

Nb-94

2.03E+04

2.5E+06

2.5E+15

9.2E+13

5.7E+05

2.0E+07

0.0E+00

5.0E+11

2.2E+06

0.0E+00

Mo-93

3.50E+03

2.9E+01

5.2E+13

0.0E+00

2.3E+06

8.7E+07

0.0E+00

1.2E+10

9.4E+06

0.0E+00

Tc-99

2.13E+05

0.0E+00

6.1E+14

7.0E+11

9.7E+10

2.0E+12

2.4E+08

4.0E+13

2.1E+11

2.5E+11

Pd-107

6.50E+06

8.0E+04

5.1E+11

0.0E+00

2.8E+08

1.6E+10

0.0E+00

1.6E+10

1.5E+09

0.0E+00

Sn-126

1.00E+05

5.7E+05

3.6E+12

0.0E+00

3.6E+09

1.1E+11

0.0E+00

2.4E+12

1.2E+10

0.0E+00

I-129

1.57E+07

5.1E+13

1.7E+11

1.2E+09

9.1E+11

4.8E+09

9.0E+10

2.9E+10

5.1E+08

4.6E+08

Cs-135

2.30E+06

3.3E+05

2.3E+12

1.0E+11

2.3E+09

6.6E+10

5.3E+06

8.8E+11

7.1E+09

6.4E+09

Cs-137

3.00E+01

4.0E+10

2.9E+17

1.2E+16

6.5E+14

8.2E+15

6.8E+11

1.1E+17

8.8E+14

9.3E+15

Cm-244

1.81E+01

6.1E+08

2.9E+15

1.1E+13

9.1E+12

6.9E+13

6.3E+09

6.2E+14

2.8E+12

8.1E+12

Pu-240

6.54E+03

2.8E+08

1.6E+15

2.5E+13

1.2E+13

3.3E+13

7.7E+09

1.5E+15

1.4E+12

1.5E+14

U-236

2.34E+07

1.9E+05

9.1E+11

1.5E+10

4.8E+09

2.2E+10

3.9E+06

2.1E+11

8.3E+08

4.7E+09

Th-232

1.41E+10

2.4E-04

4.9E+04

1.8E+01

6.8E+00

2.7E+01

4.8E-03

2.7E+02

1.0E+00

5.8E+00

Ra-228

6.70E+00

1.5E-04

4.7E+04

1.2E+01

4.7E+00

1.7E+01

3.1E-03

1.7E+02

6.6E-01

3.7E+00

Th-228

1.91E+00

1.1E+07

2.7E+12

1.0E+01

9.5E+09

6.5E+10

2.6E-03

2.5E+11

2.5E+09

3.1E+00

Cm-245

8.50E+03

1.7E+05

7.6E+11

0.0E+00

3.3E+09

1.9E+10

0.0E+00

1.9E+11

7.7E+08

0.0E+00
6.8E+16

Pu-241

1.44E+01

1.3E+11

7.1E+17

1.1E+16

5.5E+15

1.5E+16

3.5E+12

6.6E+17

6.2E+14

Am-241

4.32E+02

2.3E+09

1.1E+16

1.4E+14

1.1E+14

4.1E+14

5.2E+10

7.0E+15

4.0E+13

4.4E+14

Np-237

2.14E+06

1.3E+04

1.2E+12

1.1E+10

6.0E+09

3.0E+10

4.2E+06

1.2E+12

1.3E+09

6.5E+09

U-233

1.59E+05

7.8E+00

4.8E+09

1.2E+06

8.9E+05

4.0E+06

4.4E+02

1.5E+08

1.6E+05

5.6E+05

Th-229

7.34E+03

6.9E-02

1.4E+07

1.4E+03

2.4E+03

1.2E+04

5.1E-01

2.4E+05

4.5E+02

6.1E+02

Cm-246

4.73E+03

0.0E+00

4.0E+08

0.0E+00

1.9E+08

0.0E+00

0.0E+00

3.2E+08

0.0E+00

0.0E+00

Pu-242

3.87E+05

1.2E+06

6.7E+12

0.0E+00

2.0E+10

1.4E+11

0.0E+00

3.7E+12

5.8E+09

1.9E+11

U-238

4.47E+09

1.6E+05

7.6E+11

3.2E+10

1.2E+10

1.8E+10

4.6E+06

2.5E+11

6.9E+08

6.7E+09

U-234

2.45E+05

2.2E+06

5.5E+12

2.8E+11

6.6E+10

1.1E+11

4.8E+07

4.5E+12

4.6E+09

1.6E+11

Th-230

7.70E+04

1.6E+02

1.8E+08

2.9E+07

5.8E+06

2.6E+06

4.1E+03

3.1E+08

1.1E+05

7.6E+06
3.7E+04

Ra-226

1.60E+03

8.3E-01

9.4E+05

1.6E+05

3.9E+04

1.1E+04

2.2E+01

1.7E+06

4.4E+02

Pb-210

2.23E+01

1.8E-01

2.1E+05

3.4E+04

1.0E+04

2.1E+03

4.7E+00

3.7E+05

8.2E+01

7.7E+03

Am-243

7.38E+03

1.3E+07

1.9E+14

4.1E+11

1.5E+11

1.5E+12

2.2E+08

1.5E+13

6.2E+10

2.1E+11

Pu-239

2.41E+04

1.8E+08

9.8E+14

2.3E+13

8.9E+12

2.1E+13

5.0E+09

1.3E+15

8.4E+11

1.0E+14

U-235

7.04E+08

1.1E+04

5.4E+10

3.5E+09

1.2E+09

1.3E+09

2.9E+05

5.2E+10

4.8E+07

4.1E+08

Pa-231

3.28E+04

6.0E+00

3.2E+07

1.9E+06

7.9E+05

6.7E+05

1.5E+02

2.9E+07

2.5E+04

2.2E+05

Ac-227

2.18E+01

1.9E+00

1.1E+07

5.8E+05

3.0E+05

2.1E+05

4.8E+01

9.7E+06

7.8E+03

6.7E+04

* Half-life (years): Library data of ORIGEN2.1 used

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4.2.4 Specified conditions

The design of the disposal system is as described in Chapter 3.

Table 4.2.4-1 shows parameters describing the features of the waste disposal facility for each waste package group and Figure 4.2.4-1 shows the cross-sections of the disposal tunnel that is specified as a reference.

Table 4.2.4-1 Parameters describing the features of the disposal facility for each waste package group

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Length of disposal tunnel (m)</th>
<th>Fixed length of section for waste package (m)</th>
<th>Diameter excluding tunnel support (m)</th>
<th>Tunnel support thickness (m)</th>
<th>Initial volume of waste package (m$^3$)</th>
<th>Surface area (m$^2$)</th>
<th>Filled volume (m$^3$)</th>
<th>Buffer thickness (m)</th>
<th>Buffer surface area (m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gr1-D</td>
<td>28</td>
<td>24</td>
<td>12</td>
<td>0.1</td>
<td>318</td>
<td>624</td>
<td>672</td>
<td>1.0</td>
<td>905</td>
</tr>
<tr>
<td>Gr2-C</td>
<td>734</td>
<td>720</td>
<td>9.3</td>
<td>0.1</td>
<td>5573</td>
<td>13824</td>
<td>11016</td>
<td>1.0</td>
<td>21036</td>
</tr>
<tr>
<td>Gr2-B</td>
<td>167.3</td>
<td>165.3</td>
<td>9.3</td>
<td>0.1</td>
<td>1159</td>
<td>3042</td>
<td>2332</td>
<td>1.0</td>
<td>4830</td>
</tr>
<tr>
<td>Gr3-D</td>
<td>264</td>
<td>264</td>
<td>12</td>
<td>0.1</td>
<td>5645</td>
<td>9953</td>
<td>24213</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Gr3-X</td>
<td>11.2</td>
<td>11.2</td>
<td>12</td>
<td>0.1</td>
<td>390</td>
<td>422</td>
<td>877</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Gr3-B</td>
<td>5.7</td>
<td>5.7</td>
<td>12</td>
<td>0.1</td>
<td>140</td>
<td>215</td>
<td>505</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Gr4-D</td>
<td>423</td>
<td>423</td>
<td>12</td>
<td>0.1</td>
<td>9018</td>
<td>15947</td>
<td>38822</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Gr4-X</td>
<td>80</td>
<td>80</td>
<td>12</td>
<td>0.1</td>
<td>3178</td>
<td>3016</td>
<td>5870</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Gr4-B</td>
<td>43.7</td>
<td>43.7</td>
<td>12</td>
<td>0.1</td>
<td>1221</td>
<td>1647</td>
<td>3721</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>
### Cross-section of disposal tunnel

<table>
<thead>
<tr>
<th>Group</th>
<th>Disposal tunnel size</th>
<th>Thickness of support</th>
<th>Type of waste package</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group 1</td>
<td>Internal diameter 12 m</td>
<td>0.1 m</td>
<td>1. 200L drum</td>
</tr>
<tr>
<td>Group 2</td>
<td>Internal diameter 9.3 m</td>
<td>0.1 m</td>
<td>2. Canister, 3. BNGS package</td>
</tr>
<tr>
<td>Group 3</td>
<td>Internal diameter 12 m</td>
<td>0.1 m</td>
<td>1. 200L drum, 5. Square package, 6. BNGS package</td>
</tr>
<tr>
<td>Group 4</td>
<td>Internal diameter 12 m</td>
<td>0.1 m</td>
<td>7. 200L drum, 8. Square package, 9. BNGS package</td>
</tr>
</tbody>
</table>

Figure 4.2.4-1 Cross-sections of disposal tunnels specified as a reference
4.3 Scenario development

Generally, scenario development means describing the long-term behaviour of the repository, based on a summary and integration of the basic scientific and technical information that is needed for safety assessment. FEPs, (Features, Events and Processes) are abstracted from this important basic information, giving consideration to the characteristics of the waste packages that are to be disposed of, repository design and the geological conditions around the repository. By screening the comprehensively extracted FEPs, the FEPs to be considered in the safety assessment are obtained. From this reduced set of FEPs, the scenarios to be considered in the safety assessment is constructed.

The individual work steps involved in scenario development, according to the work flow adopted by this report, are described below. Figure 4.3-1 shows the work flow involved in scenario development, with reference to the OECD/NEA report (OECD/NEA, 1991) and the H12 report (JNC, 2000).

**Figure 4.3-1 Flow of scenario development**

**4.3.1 Production of a comprehensive FEP list**

A comprehensive FEP list has been developed for the geological disposal of TRU waste and is shown in Table 4.3.1-1. This list was obtained with reference to the H12 report (JNC, 2000) and the OECD/NEA International FEP database (OECD/NEA, 2000), and by taking into account the individual phenomena that are characteristic for TRU waste. Following the approach in the H12 report, this table classifies the FEPs
according to the locations within the multibarrier system to which they apply (across each row) and their related phenomena or functions (down each column).

[ Classification of location ]
- Waste
- Filler
- Structural framework
- Bentonite
- Plug / grout / support / backfill
- Host rock

[ Classification of phenomena ]
- Thermal phenomena / characteristics
- Hydraulic phenomena / characteristics
- Mechanical phenomena / characteristics
- Chemical phenomena / characteristics
- Radiological phenomena / characteristics
- Nuclide migration phenomena / characteristics
- Phenomena that may potentially disturb the system (initial defects / natural phenomena / human activities)

If this classification is compared to that in the H12 report, the organisation is essentially the same for locations beyond the bentonite. However, taking into account the structure of the engineered barrier system for the geological disposal of TRU waste, the classification is specified differently for the waste packages and their surroundings.

Nevertheless, in the organization of phenomena, there is some overlap with the H12 report: ① Phenomena connected with environmental conditions described as T (Thermal), H (Hydrological), M (Mechanical), C (Chemical) and R (Radiological) that are shown on a phenomena classification diagram; ② nuclide migration phenomena; and ③ system disturbances. Detailed FEPs that are classified as ① environmental conditions and ② nuclide migration phenomena include phenomena that are characteristic of the geological disposal of TRU waste (e.g. influences of cementitious materials, radionuclide migration in gaseous form, etc.)
**Table 4.3.1-1 Comprehensive FEP list for the geological disposal of TRU waste**

<table>
<thead>
<tr>
<th>Waste</th>
<th>Filler</th>
<th>Structural framework</th>
<th>Buffer material</th>
<th>Plug-and-grout/Support/Backfill</th>
<th>Host rock</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Phenomena Characteristics</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WT-01 Waste package’s thermophysical properties</td>
<td>MT-01 Filling materials’ thermophysical properties</td>
<td>ST-01 Structural framework’s thermophysical properties</td>
<td>BT-01 Buffer materials’ thermophysical properties</td>
<td>XT-01 Secondary devices’ thermophysical properties</td>
<td>RT-01 Host rocks’ thermophysical properties</td>
</tr>
<tr>
<td>WT-02 Waste package’s temperature</td>
<td>MT-02 Filling materials’ thermal expansion</td>
<td>ST-02 Structural framework’s thermal expansion</td>
<td>BT-02 Buffer materials’ thermal expansion</td>
<td>XT-02 Secondary devices’ thermal expansion</td>
<td>RT-03 Host rocks’ thermal expansion</td>
</tr>
<tr>
<td>WT-03 Waste package’s thermal expansion</td>
<td>MT-03 Heating by absorption of γ-rays from the waste package</td>
<td>ST-03 Heating by absorption of γ-rays from the waste package</td>
<td>BT-03 Heating by hydration</td>
<td>XT-04 Heating by hydration</td>
<td></td>
</tr>
<tr>
<td>WT-04 Production of radioactive decay heat</td>
<td>MT-04</td>
<td>ST-04</td>
<td>BT-04</td>
<td>XT-05</td>
<td></td>
</tr>
<tr>
<td>Hydrologic Phenomena Characteristics</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WM-01 Waste package’s hydraulic properties</td>
<td>MM-01 Filling materials’ hydraulic characteristics</td>
<td>SH-01 Structural framework’s hydraulic characteristics</td>
<td>BM-01 Buffer materials’ mechanical properties</td>
<td>XH-01 Secondary devices’ mechanical properties</td>
<td>RH-01 Host rocks’ mechanical properties</td>
</tr>
<tr>
<td>WM-02 Waste package’s saturation</td>
<td>MB-02 Filling materials’ saturation</td>
<td>SH-02 Structural framework’s saturation</td>
<td>BM-02 Buffer materials’ saturation</td>
<td>XH-02 Secondary devices’ saturation</td>
<td>RH-02 Host rocks’ saturation</td>
</tr>
<tr>
<td>WM-04 Deformation of solid asphalt</td>
<td>MM-04 Fracturing of filling material</td>
<td>SH-04 Structural framework’s corrosion expansion of reinforcing steel</td>
<td>BM-02 Buffer materials’ stress/deformation</td>
<td>XH-04 Fracturing of secondary devices</td>
<td>RH-04 Shrinkage</td>
</tr>
<tr>
<td>WM-05 Release from solid asphalt</td>
<td>MM-05</td>
<td>SH-05 Structural framework’s corrosion expansion of reinforcing steel</td>
<td>BM-03 Swelling of buffer material</td>
<td>XH-05 Release from secondary devices</td>
<td>RH-05 Swelling of secondary devices</td>
</tr>
<tr>
<td>WM-06 Fracturing of solid asphalt</td>
<td>MM-06</td>
<td>SH-06 Structural framework’s corrosion expansion of reinforcing steel</td>
<td>BM-03 Swelling of buffer material</td>
<td>XH-06 Fracturing of secondary devices</td>
<td>RH-06 Swelling of secondary devices</td>
</tr>
<tr>
<td>WM-07 Waste package movement/setting</td>
<td>MM-07</td>
<td>SH-07 Structural framework’s corrosion expansion of reinforcing steel</td>
<td>BM-03 Swelling of buffer material</td>
<td>XH-07 Fracturing of secondary devices</td>
<td>RH-07 Swelling of secondary devices</td>
</tr>
<tr>
<td>WM-08 Corrosion expansion of metal waste</td>
<td>MM-08</td>
<td>SH-08 Structural framework’s corrosion expansion of reinforcing steel</td>
<td>BM-03 Swelling of buffer material</td>
<td>XH-08 Fracturing of secondary devices</td>
<td>RH-08 Swelling of secondary devices</td>
</tr>
<tr>
<td>WM-09 Damage to external container</td>
<td>MM-09</td>
<td>SH-09 Structural framework’s corrosion expansion of reinforcing steel</td>
<td>BM-03 Swelling of buffer material</td>
<td>XH-09 Fracturing of secondary devices</td>
<td>RH-09 Swelling of secondary devices</td>
</tr>
<tr>
<td>WM-10 Corrosion expansion of external container</td>
<td>MM-10</td>
<td>SH-10 Structural framework’s corrosion expansion of reinforcing steel</td>
<td>BM-03 Swelling of buffer material</td>
<td>XH-10 Fracturing of secondary devices</td>
<td>RH-10 Swelling of secondary devices</td>
</tr>
<tr>
<td>Chemical Phenomena Characteristics</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WC-01 Waste package’s chemical characteristics</td>
<td>MC-01 Filling materials’ chemical characteristics</td>
<td>SC-01 Structural framework’s chemical characteristics</td>
<td>BC-01 Buffer materials’ chemical characteristics</td>
<td>XC-01 Secondary devices’ chemical characteristics</td>
<td>RC-01 Host rocks’ chemical characteristics</td>
</tr>
<tr>
<td>WC-02 Soluble transport in waste packages</td>
<td>MC-02 Soluble transport in structural framework</td>
<td>SC-02 Structural framework’s soluble transport</td>
<td>BC-02 Soluble transport in buffer materials</td>
<td>XC-02 Secondary devices’ soluble transport</td>
<td>RC-02 Host rocks’ soluble transport</td>
</tr>
<tr>
<td>WC-04 Chemical alteration of waste packages</td>
<td>MC-04 Chemical alteration of structural framework</td>
<td>SC-04 Chemical alteration of structural framework</td>
<td>BC-04 Chemical alteration of buffer materials</td>
<td>XC-04 Chemical alteration of secondary devices</td>
<td>RC-04 Chemical alteration of host rocks</td>
</tr>
<tr>
<td>WC-05 Effect of organics in waste packages</td>
<td>MC-05 Effect of organics in filling materials</td>
<td>SC-05 Effect of organics in structural framework</td>
<td>BC-05 Effect of organics in buffer materials</td>
<td>XC-05 Effect of organics</td>
<td>RC-05 Effect of organics in host rocks</td>
</tr>
<tr>
<td>WC-06 Effect of micros in waste packages</td>
<td>MC-06 Effect of microbes in filling materials</td>
<td>SC-06 Effect of microbes in structural framework</td>
<td>BC-06 Effect of microbes in buffer materials</td>
<td>XC-06 Effect of microbes</td>
<td>RC-06 Effect of microbes in host rocks</td>
</tr>
<tr>
<td>WC-07 Effect of colloids in waste packages</td>
<td>MC-07 Effect of colloids in filling materials</td>
<td>SC-07 Effect of colloids in structural framework</td>
<td>BC-07 Effect of colloids in buffer materials</td>
<td>XC-07 Effect of colloids</td>
<td>RC-07 Effect of colloids in host rocks</td>
</tr>
<tr>
<td>WC-08 Effect of nitrate in waste packages</td>
<td>MC-08 Effect of nitrate in filling materials</td>
<td>SC-08 Effect of nitrate in structural framework</td>
<td>BC-08 Effect of nitrate in buffer materials</td>
<td>XC-08 Effect of nitrate</td>
<td>RC-08 Effect of nitrate in host rocks</td>
</tr>
<tr>
<td>WC-10 Effect of gas production in waste packages</td>
<td>MC-10 Effect of gas production in filling materials</td>
<td>SC-10 Effect of gas production in structural framework</td>
<td>BC-10 Effect of gas production in buffer materials</td>
<td>XC-10 Effect of gas production in secondary devices</td>
<td>RC-10 Effect of gas production in host rocks</td>
</tr>
<tr>
<td>WC-11 Effect of salt accumulation in waste packages</td>
<td>MC-11 Effect of salt accumulation in filling materials</td>
<td>SC-11 Effect of salt accumulation in structural framework</td>
<td>BC-11 Effect of salt accumulation in buffer materials</td>
<td>XC-11 Effect of salt accumulation in secondary devices</td>
<td>RC-11 Effect of salt accumulation in host rocks</td>
</tr>
<tr>
<td>Radiological Phenomena Characteristics</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WR-01 Radionuclide decay/deposition in the waste package</td>
<td>MR-01 Radiolodine decay/deposition in the filling material</td>
<td>SR-01 Radiolodine decay/deposition in the structural framework</td>
<td>BR-01 Radionuclide decay/deposition in buffer materials</td>
<td>XR-01 Radionuclide decay/deposition in secondary devices</td>
<td>RR-01 Radionuclide decay/deposition in host rocks</td>
</tr>
<tr>
<td>WR-02 Radioactivity of waste package’s porewater</td>
<td>MR-02 Radioactivity of the filling material’s porewater</td>
<td>SR-02 Radioactivity of the structural framework’s porewater</td>
<td>BR-02 Radioactivity of buffer materials’ porewater</td>
<td>XR-02 Radioactivity of secondary devices’ porewater</td>
<td>RR-02 Radioactivity of host rocks’ porewater</td>
</tr>
<tr>
<td>WR-03 Radiation damage of waste packages</td>
<td>MR-03 Radiation damage of filling materials</td>
<td>SR-03 Radiation damage of structural framework</td>
<td>BR-03 Radiation damage of buffer materials</td>
<td>XR-03 Radiation damage of secondary devices</td>
<td>RR-03 Radiation damage of host rocks</td>
</tr>
<tr>
<td>Nuclear migration Phenomena Characteristics</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WN-02 Nucleide release from porous matrix</td>
<td>MN-02 Nucleide advection/dispersion</td>
<td>SN-02 Nucleide advection/dispersion</td>
<td>BN-02 Nucleide advection/dispersion</td>
<td>NN-02 Nucleide advection/dispersion</td>
<td>NN-02 Nucleide advection/dispersion</td>
</tr>
<tr>
<td>WN-03 Nucleide release from the exterior surface of waste packages</td>
<td>MN-03 Nucleide diffusion</td>
<td>SN-03 Nucleide diffusion</td>
<td>BN-03 Nucleide diffusion</td>
<td>NN-03 Nucleide diffusion</td>
<td>NN-03 Nucleide diffusion</td>
</tr>
<tr>
<td>WN-04 Nucleide release from the interior surface of waste packages</td>
<td>MN-04 Nucleide sorption</td>
<td>SN-04 Nucleide sorption</td>
<td>BN-04 Nucleide sorption</td>
<td>NN-04 Nucleide sorption</td>
<td>NN-04 Nucleide sorption</td>
</tr>
<tr>
<td>WN-05 Nucleide precipitation/dissolution</td>
<td>MN-05 Nucleide precipitation/dissolution</td>
<td>SN-05 Nucleide precipitation/dissolution</td>
<td>BN-05 Nucleide precipitation/dissolution</td>
<td>NN-05 Nucleide precipitation/dissolution</td>
<td>NN-05 Nucleide precipitation/dissolution</td>
</tr>
<tr>
<td>WN-06 Nucleide release in gaseous form</td>
<td>MN-06 Nucleide migration in gaseous form</td>
<td>SN-06 Nucleide migration in gaseous form</td>
<td>BN-06 Nucleide migration in gaseous form</td>
<td>NN-06 Nucleide migration in gaseous form</td>
<td>NN-06 Nucleide migration in gaseous form</td>
</tr>
<tr>
<td>WN-07 Nucleide release in colloidal form</td>
<td>MN-07 Nucleide migration in colloidal form</td>
<td>SN-07 Nucleide migration in colloidal form</td>
<td>BN-07 Nucleide migration in colloidal form</td>
<td>NN-07 Nucleide migration in colloidal form</td>
<td>NN-07 Nucleide migration in colloidal form</td>
</tr>
<tr>
<td>WN-08 Nucleide release in liquid form</td>
<td>MN-08 Nucleide migration in liquid form</td>
<td>SN-08 Nucleide migration in liquid form</td>
<td>BN-08 Nucleide migration in liquid form</td>
<td>NN-08 Nucleide migration in liquid form</td>
<td>NN-08 Nucleide migration in liquid form</td>
</tr>
<tr>
<td>WN-09 Nucleide release in solid form</td>
<td>MN-09 Nucleide migration in solid form</td>
<td>SN-09 Nucleide migration in solid form</td>
<td>BN-09 Nucleide migration in solid form</td>
<td>NN-09 Nucleide migration in solid form</td>
<td>NN-09 Nucleide migration in solid form</td>
</tr>
<tr>
<td>WN-10 Nucleide release in amorphous form</td>
<td>MN-10 Nucleide migration in amorphous form</td>
<td>SN-10 Nucleide migration in amorphous form</td>
<td>BN-10 Nucleide migration in amorphous form</td>
<td>NN-10 Nucleide migration in amorphous form</td>
<td>NN-10 Nucleide migration in amorphous form</td>
</tr>
<tr>
<td>Phenomenon that may potentially disturb the system</td>
<td>WQ-01 Production/manufacturing faults in waste packages</td>
<td>MQ-01 Production/manufacturing faults in filling material</td>
<td>SQ-01 Production/manufacturing faults in structural framework</td>
<td>EQ-01 Production/manufacturing faults in buffer material</td>
<td>QX-01 Failure of boring and tunnel seals due to deterioration</td>
</tr>
</tbody>
</table>
4.3.2 FEP classification

Using combinations of the comprehensive FEPs summarized in the preceding paragraphs, it is possible to describe the future behavior of the geological disposal system for TRU waste. Considering the expected function of each barrier and the main influences of these functions, as well as the final system classification etc, the FEPs are classified and summary descriptions are given of the FEPs belonging to each category.

The FEPs are classified into the following 5 categories.

- FEPs connected with safety requirements, geological environment condition, inventory and EBS design
- FEPs connected with the assumed or specified safety functions of the disposal system
- FEPs that potentially influence the assumed or specified safety functions of the disposal system
- FEPs that potentially harm the assumed or specified safety functions of the disposal system
- FEPs that potentially refute the assumed or specified safety functions of the disposal system

FEPs connected with the assumed or specified safety functions of the disposal system basically comprise those concerned with the expected long-term safety performance of the disposal system. FEPs that inherently cause the safety function to be inhibited are included in this category. These FEPs are connected with the diversity of TRU waste, the radionuclides and, at the same time, organic matter and nitrate that are unavoidably included in the waste packages. The FEPs connected with pre-conditions and FEPs connected with the assumed or specified safety functions of the disposal system are used to construct the Reference Scenario (and also the Reference Case) of the Base Scenario described below.

FEPs that potentially influence the assumed or specified safety functions of the disposal system comprise those that are major factors inherent in the engineered barrier system that may act as important initiators of phenomena that could potentially influence the disposal system’s safety functions. However, it is uncertain whether these phenomena actually produce these effects. Additionally, the phenomena that are considered may produce a relatively small influence. In the Base Scenario described below, scenarios (alternative scenarios) other than the Reference Scenario are constructed using FEPs in this category.

FEPs that potentially harm the assumed or specified safety functions of the disposal system comprise FEPs that are major perturbing factors external to, and independent of, the engineered barriers. The included FEPs are important initiating phenomena that may potentially inhibit the disposal system from exhibiting adequate safety functions. Fundamentally, these are FEPs connected with natural phenomena, those connected with future human activities and those connected with engineering measures to rectify initial defects. The Perturbation Scenarios described below are constructed using FEPs in this category.

FEPs that potentially refute the assumed or specified safety functions of the disposal system also comprise FEPs are major perturbing factors external to, and independent of, the engineered barrier system. However, these FEPs have the potential to undermine the safety function of the repository system connected with nuclide migration on groundwater scenario primarily. These FEPs are used to construct the Isolation Failure Scenario described below.

Individual comprehensive FEPs that belong to each FEP category and integrated FEPs and the
corresponding relationships are shown in Table 4.3.2-1. In the table, each comprehensive FEP is related to one corresponding integrated FEP, although it is considered that, in reality, many comprehensive FEPs are related to several integrated FEPs.

Table 4.3.2-1 Integration of comprehensive FEPs for the purpose of classification

<table>
<thead>
<tr>
<th>Integration FEP</th>
<th>Corresponding FEP (example)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[FEPs connected with pre-conditions]</td>
<td></td>
</tr>
<tr>
<td>Thermal environment</td>
<td>WT-01 MT-01 ST-01 BT-01 XT-01 RT-01</td>
</tr>
<tr>
<td>Hydrology</td>
<td>RH-01 RH-02 RH-03</td>
</tr>
<tr>
<td>Mechanical stability of rock mass</td>
<td>RM-01 RM-02 RM-03</td>
</tr>
<tr>
<td>Mechanical stability of plug/grout, support, backfill materials</td>
<td>XM-01 XM-02 XM-03 XM-05</td>
</tr>
<tr>
<td>Groundwater chemistry</td>
<td>RC-01 RC-02 RC-03</td>
</tr>
<tr>
<td>Radiolysis/radiation damage</td>
<td>WR-01 WR-03 WR-05 MR-01 MR-02 MR-03 SR-01 SR-02 SR-03</td>
</tr>
<tr>
<td>[FEPs connected with the assumed or specified safety functions of the disposal system]</td>
<td></td>
</tr>
<tr>
<td>Mechanical stability of engineered barrier materials</td>
<td>WM-01 WM-02 MM-01 MM-02 SM-01 SM-02 BM-01 BM-02</td>
</tr>
<tr>
<td>Internal hydrogeology of engineered barrier</td>
<td>WH-01 WH-02 WH-03 MH-01 MH-02 MH-03 SH-01 SH-02 SH-03</td>
</tr>
<tr>
<td>Swelling of buffer material</td>
<td>BH-01 BH-02 BH-03 XH-01 XH-02 XH-03</td>
</tr>
<tr>
<td>Poroswater chemistry</td>
<td>BC-01 BC-02 BC-03 XC-01 XC-02 XC-03</td>
</tr>
<tr>
<td>Nuclide release from waste packages</td>
<td>WN-02 WN-03 WN-04 WC-01 WC-02 WC-03 MC-01 MC-02 MC-03 SC-01 SC-02 SC-03</td>
</tr>
<tr>
<td>Precipitation/dissolution</td>
<td>WN-05 MN-05 SN-05 BN-05 XN-05 RN-05</td>
</tr>
<tr>
<td>Sorption</td>
<td>WM-03 MN-04 SN-04 BN-04 XN-04 RN-04</td>
</tr>
<tr>
<td>Diffusion and advection/dispersion</td>
<td>MN-02 MN-03 SN-02 SN-03 BN-02 BN-03 XN-02 XN-03 RN-02 RN-03</td>
</tr>
<tr>
<td>Nuclide migration within the engineered barrier</td>
<td>WN-01 MN-01 SN-01 BN-01 XN-01</td>
</tr>
<tr>
<td>Nuclide migration within the host rock</td>
<td>RN-01</td>
</tr>
<tr>
<td>Organics</td>
<td>WC-01 WC-02 WC-03 MC-01 MC-02 MC-03 SC-01 SC-02 SC-03</td>
</tr>
<tr>
<td>Nitrates</td>
<td>WN-03 MN-03 SN-03 BN-03 XN-03 RN-03</td>
</tr>
<tr>
<td>[FEPs that potentially influence the assumed or specified safety functions of the disposal system]</td>
<td></td>
</tr>
<tr>
<td>Microbes</td>
<td>WC-07 MC-06 SC-06 BC-06 XC-06 RC-06</td>
</tr>
<tr>
<td>Colloid production/transport</td>
<td>WC-08 MC-07 SC-07 BC-07 XC-07 RC-07</td>
</tr>
<tr>
<td>Non-radioactive gas</td>
<td>WN-01 MN-06 SN-06 BN-06 XN-06 RN-06</td>
</tr>
<tr>
<td>Radioactive gas</td>
<td>WC-11 MC-10 SC-10 BC-10 XC-10 RC-10</td>
</tr>
<tr>
<td>Salt accumulation</td>
<td>WN-08 MN-07 SN-07 BN-07 XN-07 RN-07</td>
</tr>
<tr>
<td>Alkali alteration of host rock</td>
<td>WC-12 MC-11 SC-11 BC-11</td>
</tr>
<tr>
<td>Alteration of buffer</td>
<td>BC-04</td>
</tr>
<tr>
<td>Alteration of cementitious material and fracture production</td>
<td>MC-04 SC-04 XC-04 MM-04 SM-04 SM-06 XM-06</td>
</tr>
<tr>
<td>Decrease in density of buffer material</td>
<td>BM-05</td>
</tr>
<tr>
<td>Corrosion expansion of engineered barrier materials</td>
<td>WM-06 WM-07 SM-06 XM-07</td>
</tr>
<tr>
<td>Movement and settling of the structural framework/waste package</td>
<td>WM-07 SM-05</td>
</tr>
<tr>
<td>[FEPs that potentially harm the assumed or specified safety functions of the disposal system]</td>
<td></td>
</tr>
<tr>
<td>Natural phenomena</td>
<td>NP-01 NP-02 NP-05</td>
</tr>
<tr>
<td>Initial defect connected with engineering measures</td>
<td>WQ-01 MQ-01 SQ-01 BQ-01 XQ-01 RQ-01</td>
</tr>
<tr>
<td>Future human activities</td>
<td>HA-02 HA-03 HA-04 HA-05</td>
</tr>
<tr>
<td>[FEPs that potentially refute the assumed or specified safety functions of the disposal system]</td>
<td></td>
</tr>
<tr>
<td>Natural phenomena</td>
<td>NP-01</td>
</tr>
<tr>
<td>Future human activity</td>
<td>HA-01</td>
</tr>
<tr>
<td>Criticability</td>
<td>RN-09</td>
</tr>
</tbody>
</table>

4.3.3 FEP screening considered in safety assessment

To ensure comprehensiveness of the performance assessment, all relevant FEPs were assembled and added to the comprehensive FEPs shown in Section 4.3.1. When the geological environmental conditions, repository construction, and waste package characteristics were considered, even FEPs with a small
probability of occurrence were abstracted. However, to identify FEPs aimed at the practical operation of Performance Assessment, screening of FEPs (and also scenarios) was carried out, as has been done widely in previous scenario development in various countries (OECD/NEA, 1999). Here, the methodology in the H12 report (JNC, 2000) was followed. According to this methodology, the comprehensive FEPs were screened according to the following reasons:

1. It is judged that the effects can be avoided by site selection.
2. It is judged that the influence can be avoided by engineering measures.
3. It is judged that there is an extremely low probability of occurrence.
4. It is judged that there is only a small influence on the disposal system.

Explanations of the reasons for screening and the results are given in Table 4.3.3-1.

From the point of view of appropriate site selection, engineering measures and probability of occurrence, the FEPs shown below can possibly be excluded:

- Earthquakes and active faulting (NP-01)
- Volcanoes and magmatic activity (NP-02)
- Initial defects connected with engineering measures (WQ-01/MQ-01/SQ-01/BQ-01)
- Future human activity: utilization of underground cavities (HA-03)
- Meteorite impact (NP-05)
- Criticality (RN-09)

Additionally, the FEPs listed below were judged to have a negligible or small influence on the disposal system to be screened out

- Thermal expansion (*T-03) (*: represented by W, M, S, B, X, R)
- Salt accumulation (WC-12/MC-11/SC-11/BC-11)
- Precipitation/dissolution of nuclides in the host rock (RN-05)
- Future human activity: surface environment (HA-02)

For each FEP corresponding to the influence of colloids in the disposal facility (WC-08 etc.), gas phase nuclide migration (WN-08 etc.), defects connected with sealing (XQ-01/RQ-01) and future human activity: deep drilling (HA-01), an explanation for address in the safety assessment is given of either its rejection or justification for its inclusion. Either explanation is the result of a standardised, rational judgment. The treatment of these FEPs is not discussed here.

Table 4.3.3-2 shows two arguments connected with FEPs for which judgment is reserved.
Table 4.3.3-1 FEPs that can potentially be excluded from the safety assessment

(1) FEPs that can potentially be excluded from the viewpoint of appropriate site selection, engineering measures and probability of occurrence (Reasons ①–③)

<table>
<thead>
<tr>
<th>Excluded FEP</th>
<th>Grounds for exclusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Earthquake/ active faulting NP-01</td>
<td>Fault activity for a period in the order of 100,000 years into the future can be considered as a continuation of activity that has occurred up to the present. Consequently, by maintaining an appropriate distance between individual active faults and the disposal facility, it is considered that the critical effects can be avoided. Furthermore, in Japan the probability of fault development in rocks without existing planes of weakness is small. For example, in the case where a new fault is produced, because the initial fault grows gradually as a belt of small-scale ruptures, there is a low probability that a large fault will grow rapidly, producing a large displacement. Even if it is assumed that such extremely low-probability active faulting will affect the geological disposal system, from trial risk calculations it is considered that the effect will be less than the upper limit proposed in other countries (JNC, 2000).</td>
</tr>
<tr>
<td>Volcanic/ magmatic activity NP-02</td>
<td>It is considered possible to evaluate the locations of future volcanic activity over timescales in the order of 10^5 years, based on the spatial and temporal variations in volcanic activity during past timescales in the order of 10^5 to 10^6 years. Therefore, if a repository is a suitable distance from present volcanic areas, it is considered possible to avoid large influences of volcanic activity. Trial risk calculations show that the probability of volcanic activity influencing the disposal system is extremely small. It is considered to be below the upper limit of influences proposed in other countries (JNC, 2000).</td>
</tr>
<tr>
<td>Initial defects connected with engineering measures WQ-01, MQ-01, SQ-01, BQ-01</td>
<td>By suitable quality management, it is considered possible to detect and rectify any defects that might arise from the methods employed in the manufacture of waste packages and bentonites. Therefore, initial defects due to engineering measures are considered to be very unlikely.</td>
</tr>
<tr>
<td>Future human activity (using underground excavations) HA-03</td>
<td>If the repository is constructed at an appropriate depth in a location with no natural resources, the possibility for direct human contact is small. It is considered that the utilization of underground spaces for mining, underground storage, geothermal resources, etc. can be avoided by suitable site selection.</td>
</tr>
<tr>
<td>Meteorite impact NP-05</td>
<td>Meteorite impact is a phenomenon that occurs randomly at the surface of the earth. According to the evaluations that have been performed to date, the frequencies of meteorite impacts that may have a direct effect at the depth of a HLW disposal facility range from 1.5×10^{-13} [km^{-2} y^{-1}] (Goodwin et al., 1994) to 5×10^{-10} [km^{-2} y^{-1}] (Diebold and Mueller, 1984). Consequently, it is considered that the possibility for the disposal system to be affected is extremely small.</td>
</tr>
<tr>
<td>Criticality RN-09</td>
<td>It has been pointed out that there is the possibility for criticality to develop autocatalytically if geological disposal of weapons-grade Pu is carried out (Bowman and Venneri, 1995). However, for such criticality to occur, various other processes are also necessary and the probability of these occurring is negligibly small. Provisionally, the energy released by criticality would be extremely small and it is judged that there would be no effect on the performance of the geological disposal system (Parks et al., 1995; Konynenburg, 1995). Furthermore Ahn et al. (1998) has discussed the possibility of criticality when geological disposal of solidified vitrified waste is undertaken. From the results, it is possible to evaluate the possibility of criticality if 40,000 vitrified waste packages are placed in an underground repository and it is assumed that all the released nuclides accumulate at a single locality. In the case where it is difficult for U to move within the medium, it has been shown that the accumulated quantity of U would be at most in the order of several moles, which is negligibly small. Provisionally, in the case where the accumulated U can move, and the host rock is granite with a porosity of more than 30%, the possibility of criticality phenomena can in reality be ruled out. From the above, the occurrence of criticality is considered unlikely.</td>
</tr>
</tbody>
</table>
(2) Influences on the disposal system that are judged to be negligibly small (Reason ①)

<table>
<thead>
<tr>
<th>Excluded FEP</th>
<th>Grounds for exclusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal expansion</td>
<td>Thermal expansion that would influence the functioning of the engineered and natural barriers is considered unlikely, because the repository is designed such that temperature conditions are appropriate for cementitious and bentonite materials.</td>
</tr>
<tr>
<td>Thermal expansion *T-03</td>
<td></td>
</tr>
<tr>
<td>Salt accumulation</td>
<td>It is considered that, after initial backfilling, there will be a period where the temperature gradient in the unsaturated bentonite is large. Salt accumulation, with local changes in chemical conditions, will occur (Karnland and Pusch, 1995). However, after the buffer has saturated with water and the temperature gradient has decreased, the accumulated salt will be dissolved as a contaminant and lost by diffusion.</td>
</tr>
<tr>
<td>Salt accumulation WC-12/MC-11/SC-11/BC-11</td>
<td></td>
</tr>
<tr>
<td>Precipitation or dissolution of nuclides in the host rock RN-05</td>
<td>Basically, there is a very large decrease in radionuclide concentrations towards the outside of the package and thereafter with increasing distance in the waste package vicinity. Furthermore, daughter nuclides may form by radioactive decay of parent nuclides. For the daughter nuclides to precipitate, they must have lower solubilities and distribution coefficients than the parent nuclides. Therefore it is considered that even if there is precipitation, the amount will be small. For these reasons the possibility that precipitation will have a large influence on radionuclide precipitation is considered to be small.</td>
</tr>
<tr>
<td>Future human activity (surface environment) HA-02</td>
<td>Because the repository will be constructed at a suitable depth where there are no natural resources, even though quarrying and trench excavation, etc. may be undertaken at the surface there will be no effect on the repository. Variations in the biosphere may possibly occur at the same time as variations in the surface environment, but it is considered that these can be included in the conceptual biosphere model using a stylized approach.</td>
</tr>
</tbody>
</table>
Table 4.3.3-2 Two arguments concerned with FEPs for which judgment is reserved

<table>
<thead>
<tr>
<th>FEPs for which judgment is reserved</th>
<th>Grounds for reservation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Influence of colloids in the disposal facility</td>
<td>[Explanation for selection]</td>
</tr>
<tr>
<td>WC-08/MC-07/SC-07/BC-07/XC-07 WN-07/MN-06/SN-06/BN-06/XN-06</td>
<td>In the case where a layer of bentonite exists</td>
</tr>
<tr>
<td></td>
<td>(Dependent on the influence of variations in alkali conditions) in the case where smectite dissolution and decrease in abundance is assumed, the expected filtration by the layer of bentonite may be compromised. There is then a possibility that colloids produced in the engineered barriers will penetrate.</td>
</tr>
<tr>
<td></td>
<td>In the case where a layer of bentonite does not exist</td>
</tr>
<tr>
<td></td>
<td>There is a significant quantity of colloids in the cement pore water. Furthermore, because colloids are produced by disturbances to the groundwater, in this situation (for example, influences of excavation, etc.), the production of colloids caused by repository construction cannot be ruled out.</td>
</tr>
<tr>
<td>Nuclide migration in gaseous form</td>
<td>[Explanation for exclusion]</td>
</tr>
<tr>
<td>WN-08/N-07</td>
<td>At a fixed point in time, volatile nuclides are not considered to exist within the waste packages in the repository. Following closure, during the process of migration the form of dissolved nuclides will change. Even though there will be volatilization, the quantity is considered to be extremely small.</td>
</tr>
<tr>
<td>Problems connected with sealing</td>
<td>[Explanation for exclusion]</td>
</tr>
<tr>
<td>XQ-01, RQ-01</td>
<td>It is considered that, during the manufacture and installation of sealing systems in waste tunnels, connecting tunnels and access tunnels, quality can be controlled in the same way as during the production and emplacement of waste packages and bentonites, etc. For this reason, the occurrence of defects connected with sealing is considered unlikely.</td>
</tr>
<tr>
<td>Future human activity (deep boring)</td>
<td>[Explanation for exclusion]</td>
</tr>
<tr>
<td>HA-01</td>
<td>It is considered that unintentional human intrusion will usually involve borehole drilling. In this case, it is difficult to provide information about the disposal site characteristics and design that is useful for analyzing risks from the transport of material to the surface, to the people involved and to the public. There is no technical basis on which to judge the possibility of human intrusion into the repository (NAS, 1995).</td>
</tr>
</tbody>
</table>

4-21
4.3.4 Classification of scenarios

The classification of scenarios is shown in Figure 4.3.4-1. Scenarios concerned with safety assessment are constructed from FEPs that were not excluded by screening (see Table 4.3.4-1). Additionally, the safety assessment scenarios are classified into groundwater scenarios and isolation failure scenarios. In the former, radionuclides may be transported to the human environment by media such as groundwater and gas etc, resulting in a radiological impact. In the isolation failure scenarios, the decreasing physical distance between the radioactive waste and the human environment results in a radiological impact. In contrast with HLW, TRU waste includes some radionuclides (eg. C-14 etc.) that have the possibility of volatilisation. A scenario describing the migration of these isotopes in a gaseous form is classified as one of the groundwater scenarios here.

Furthermore, the groundwater scenarios are sub-divided into a Base Scenario and Perturbation Scenarios. In the Base Scenario, it is assumed that the present geological conditions and surface environment will continue in the future. As described in Section 4.3.2, this scenario consists of a Reference Scenario and alternative scenarios. The Reference Scenario is based on FEPs connected with initial conditions and FEPs connected with the assumed /specified safety function of the disposal system. The alternative scenarios are based on FEPs that could possibly influence the safety function of the assumed/specified disposal system.

Accordingly, in the Perturbation Scenarios future changes in the geological environment and surface environment due to natural and anthropogenic phenomena are considered. In addition, consideration is also given to assumed initial defects in engineered components. In these scenarios, as described in Section 4.3.2, initiating phenomena are FEPs that could potentially harm the assumed/specified disposal system to lose its safety function.

In the isolation failure scenario, the physical separation between radioactive waste and the human environment decreases, thereby causing a radiological impact. This scenario is based on FEPs that could possibly be detrimental to the functioning of the assumed/specified disposal system. This scenario includes the exposure of the repository at the surface due to uplift and erosion and human intrusion. Furthermore, in this evaluation, scenarios that could be produced by FEPs that were excluded during screening are classified as hypothetical scenarios. These scenarios correspond to “what-if” scenarios in research conducted in other countries (Nagra, 2002). They are outside the scope of scenarios considered by safety assessments. The results of evaluating these scenarios do not influence the establishment of the geological disposal system, but aim to confirm that the system is robust.
4.3.5 Scenario description

4.3.5.1 Base Scenario

In the Base Scenario of the groundwater scenario, the present geological conditions of the host rock are assumed to continue into the future without change.

In the initial stages following repository closure, the conditions of the disposal tunnels and their surroundings are generally in a transitional state. More specifically, unsaturated conditions will continue in the environment around the heat-producing waste canisters until heat production ceases and for the short period until the repository resaturates. Furthermore, during the period until the remaining oxygen is consumed, an oxidizing environment will exist. Nuclides might be released through perforations in the canisters caused by corrosion during this period. Any release that occurs during this phase would be under conditions of relatively high temperature, non-saturation and oxidization. However, if release occurs after the transitional period has ended, then temperatures will be lower, and the environment saturated and reducing.

Any nuclides released from the waste would be retarded by the low-hydraulic conductivity matrix and equilibrium sorption in the surrounding medium. An example of the former is the retention of radionuclides in activated metal, while the latter would occur in the cement that forms the solid matrix and mortar. Furthermore, nuclides released from a waste package would migrate through the mortar and bentonite in the engineered barrier by repeated sorption and desorption.

Fundamentally, in disposal tunnels containing bentonite nuclide migration would be controlled by diffusion. In tunnels without bentonite, migration would be controlled by diffusion and advection depending on the hydraulic characteristics of the host rock. These migration properties will be influenced by any alteration of the barrier materials. In particular, there is a possibility that there will be effects from cementitious materials, etc in other barrier components. Reactions with groundwater will cause temporal...
variations in pore water characteristics, pore structure and mineral formation, resulting in temporal variations in the characteristics of nuclide migration in the engineered barrier system.

Nuclides released from the engineered barriers may migrate into the host rock via the excavation disturbed zone. Groundwater and mass transport in the host rock can be divided into the case where hydraulically conductive fractures are present (fractured medium) and cases where matrix porosity prevails (porous medium). These media have different retention mechanisms. In a fracture network, nuclide migration occurs by advection and the main retention mechanisms are sorption onto fracture-filling minerals and diffusion into the matrix of the host rock (matrix diffusion). In the case of nuclide transport by advection through the matrix porosity, retention is by sorption of nuclides on the surfaces of mineral grains.

From the hydrogeological conditions at the site, it is conjectured that nuclides will migrate through the host rock to the biosphere, via faults etc that connect to the GBI (Geosphere-Biosphere Interface). Hence, humans will be affected by radiological exposure. There is uncertainty concerning the assumed pathways in the biosphere that result in human exposure. A stylised approach whereby present environmental conditions and lifestyles are extrapolated into the future (ICRP, 1999) is considered to be appropriate for specifying biosphere models.

Based on the descriptions of the scenarios outlined above, and considering the previously mentioned FEPs connected with initial and FEPs connected with the supposed/specified safety functions of the disposal system, a reference scenario is specified. This scenario describes the probable future evolution of the geological disposal system for TRU waste as follows:

① With the precondition that the repository is designed to rule out any effect of temperature on the barrier materials, when radionuclides begin to escape from the waste containers, the transitional conditions of the near-field have already past and saturated, reducing conditions have returned. The scenario where radionuclide release begins during the period of transitional conditions is considered by the next alternative scenario.

② In other technical fields (mechanics, chemistry, radiation fields), near-field behavior that is considered to be of high probability is assumed. In particular, in the field of geochemistry, reactions between groundwater that flows into the repository and barrier materials (cementitious materials, bentonite materials, etc.) are considered.

③ Nitrate and organic matter contained in the waste react with the barriers and groundwater.

④ In highly fractured media with conductive fractures, nuclides that migrate through the host rock are retarded by sorption onto fracture-filling minerals and by diffusion into the rock matrix (matrix diffusion).

A wide range of materials are contained in the waste packages and engineered barriers. The characteristics of these materials vary with time and the future evolution of the disposal system for TRU waste is thus fundamentally complicated. Therefore, the base scenario is not entirely fixed. In order to evaluate uncertainties concerned with the degree of influence of the phenomena included in the reference scenario, as well as the effects of phenomena that are not included in the reference scenario, an alternative
scenario was specified. This alternative scenario considered the previously mentioned FEPs that may influence the safety function of the assumed/specified disposal system. The characteristics of the alternative scenario are summarized here:

⑤ The ability of the bentonite to retard water and its swelling characteristics are affected by the alteration caused by cementitious materials.
⑥ The ability of the surrounding host rock to retain radionuclides is affected by the alteration of cementitious materials.
⑦ In the case where radionuclide release begins while the near-field is in a transitional state, nuclide migration is influenced by the transitional conditions (high temperature, unsaturated, oxidizing conditions).
⑧ The nuclide migration is influenced by colloids, organic matter (natural) and microbes.
⑨ Nuclide migration is influenced by gas, etc.

4.3.5.2 Perturbation scenarios

In the Base Scenario, a precondition is that the present geological conditions and surface environmental conditions do not vary in future. In contrast, in the Perturbation Scenarios it is assumed that the geological environment and the surface environment are affected by natural phenomena and future human activity. Furthermore, also included in the Perturbation Scenarios are scenarios in which there are initial defects in engineered components. It is assumed that these initial defects are unnoticed and remain, so that they may significantly influence the disposal system.

The phenomena that initiate these Perturbation Scenarios are obtained from FEP screening and are given below:

Natural Phenomena
- Uplift, erosion
- Climate, sea level change
Initial defects in engineered components
- Seal failure, etc.
Future human activity
- Drilling wells and water extraction
- Variations in pathways for nuclide migration caused by drilling water wells

4.3.5.3 Isolation failure scenarios

In the isolation failure scenarios, the physical separation between the radioactive waste and the human environment may decrease, resulting in a radiological impact. The phenomena that may initiate these scenarios have been obtained by FEP screening. Among the natural phenomena, there is the case where uplift and erosion continue over long time periods, causing the disposal system to be exposed at the surface.
Among the phenomena related to future human activity, drilling may result in accidental penetration of the repository.

Issues to be considered in the selection of a general investigation area for the geological disposal of HLW, where the disposal depth is assumed to be greater than 300 m, are given in NUMO (2002). The same conditions (3 mm y⁻¹ limit) are applied to the geological disposal of TRU waste. If the present tectonic conditions can be extrapolated into the future, a scenario can be developed for the exposure of the repository due to uplift and erosion several tens of thousands of years into the future. On the other hand, development of an appropriate scenario for accidental penetration of the repository by drilling at least considers the period after institutional management and after loss of information concerning the existence of the repository.

4.3.6 Important repository environment conditions for safety assessment

Undertaking a safety assessment requires a basic understanding of environmental phenomena that affect the behaviour of the disposal system (thermal, hydraulic, mechanical, chemical, radiological). As a basis for judging the level of understanding connected with these phenomena, the understanding of separate phenomena that are characteristic of the disposal system is presented. In the case of geological disposal of TRU waste, for example, the influence of nitrate and organic matter in the waste is considered. Nuclide migration analysis and dose evaluation are carried out by initially carrying out analyses of environmental conditions and individual phenomena. To carry out the safety assessment, it is essential to have a sufficient understanding of these environmental conditions and individual phenomena (environmental conditions of the disposal environment). In Figure 4.3.6-1, a hierarchy of phenomena connected with safety assessment and examples of phenomena that must be considered by safety assessment are presented.

To carry out a safety assessment, important phenomena are extracted from the characteristics ①–⑨ of the base scenario of the groundwater scenario presented in Section 4.3.5. Here, a summary is given of important repository environment conditions for safety assessment. Table 4.3.6-1 shows the types of FEPs and summary FEPs, scenarios and important repository environment conditions for safety assessment.

![Figure 4.3.6-1 Hierarchy of phenomena connected with safety assessment](image-url)
Table 4.3.6-1 Types of FEPs, summary FEPs, scenarios and repository conditions that are important for safety assessment

<table>
<thead>
<tr>
<th>FEP Type</th>
<th>Summary FEPs</th>
<th>Scenario Type</th>
<th>Scenario sub-type</th>
<th>Scenario sub-sub-type</th>
<th>Important environmental conditions etc for safety assessment</th>
<th>Corresponding report section</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal environment</td>
<td>Hydrogeology</td>
<td>Mechanical stability of the host rock</td>
<td>Mechanical stability of plugs etc</td>
<td>Mechanical stability of engineered barrier materials</td>
<td>Temperature influence</td>
<td>3.2, 3.3</td>
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<tr>
<td></td>
<td></td>
<td>Swelling of the buffer</td>
<td>Decrease in density of the buffer</td>
<td>Corrosion expansion of engineered barrier materials</td>
<td>Hydraulic field (re-flooding)</td>
<td>4.4</td>
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<tr>
<td></td>
<td></td>
<td>Waste packages/structural members movement and settling</td>
<td>Groundwater chemistry/porewater chemistry</td>
<td>Radiological analysis/radiation damage</td>
<td>Mechanical conditions</td>
<td>3.3.2</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Groundwater chemistry</td>
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<td></td>
<td></td>
<td>Radiological effects</td>
<td>4.4.8</td>
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<td></td>
<td>Effects of organic matter (Contained in waste)</td>
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<td></td>
<td></td>
<td></td>
<td>Effects of nitrate</td>
<td>4.4.9</td>
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<td></td>
<td></td>
<td></td>
<td>Nuclide migration</td>
<td>4.5.2</td>
</tr>
<tr>
<td>Organic matter (included in the waste)</td>
<td>Nitrate</td>
<td>Release of nuclides from the waste</td>
<td>Precipitation and dissolution</td>
<td>Sorption</td>
<td>Effects of alteration of engineered barrier materials</td>
<td>4.4.2</td>
</tr>
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<td></td>
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<td></td>
<td></td>
<td></td>
<td>Alkaline alteration of surrounding host rock</td>
<td>4.4.3</td>
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<td>Hydrogeological conditions of the near field (influence of geochemical alteration)</td>
<td>4.4.4</td>
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<td></td>
<td>Effects of colloids</td>
<td>4.4.5</td>
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<td></td>
<td></td>
<td></td>
<td>Effects of organic matter (natural)</td>
<td>4.4.6</td>
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<td></td>
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<td></td>
<td>Effects of microbes</td>
<td>4.4.7</td>
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<td></td>
<td></td>
<td>Effects of gas and nuclides in gaseous form</td>
<td>4.4.10</td>
</tr>
<tr>
<td>Alteration of buffer material</td>
<td>Alteration and fracturing of cementitious materials</td>
<td>Alkaline alteration of the host rock</td>
<td>Hydrogeology of the engineered barrier</td>
<td>Production and migration of colloids</td>
<td>Natural phenomena scenario</td>
<td>4.4.11</td>
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<td></td>
<td></td>
<td>Hypothetical scenario Volcanoes, Magmatism</td>
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<td></td>
<td></td>
<td>Magma intrusion</td>
<td>4.5.6</td>
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<td></td>
<td></td>
<td>Effects of gas and nuclides in gaseous form</td>
<td>4.4.10</td>
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<td>Uplift and erosion</td>
<td>4.5.6</td>
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<td></td>
<td>Climate change, Sea level change</td>
<td>4.5.6</td>
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<td></td>
<td>Well drilling and water extraction</td>
<td>4.5.6</td>
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<td>Formation of new migration paths by boring</td>
<td>4.5.6</td>
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<tr>
<td>Unradioactive gas/radioactive gas</td>
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<tr>
<td>Natural phenomena</td>
<td>Initial defects connected with engineered components</td>
<td>Future human activity</td>
<td>Scenario concerned with initial defects</td>
<td>Scenario concerned with future human activities</td>
<td>Natural phenomena scenario</td>
<td>4.5.6</td>
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<td></td>
<td>Hypothetical scenario Volcanoes, Magmatism (Magma intrusion)</td>
<td>4.5.6</td>
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<td>Future human activity scenario</td>
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<td>Future accidental human intrusion</td>
<td>4.5.6</td>
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</tbody>
</table>
4.4 Establishing conditions in the disposal environment for safety assessment

As described in Section 4.3.6, when carrying out a nuclide migration analysis and dose assessment, it is important to understand environmental (Thermal/Hydraulic/Mechanical/Chemical/Radiological (THMCR)) conditions and to analyse closely related phenomena that are characteristic of the disposal system. This chapter specifies those environmental conditions needed to analyse nuclide migration and radiation exposure. The environmental conditions and phenomena that are important for safety assessment are evaluated.

In Section 4.3.6, the environmental conditions and discrete phenomena are arranged hierarchically. However, the definition of the hierarchy is complicated by the fact that these conditions and phenomena are inter-related. For example, groundwater chemistry is affected by interactions with repository materials and the original composition of groundwater in the disposal facility.

In this section, the descriptions of environmental conditions and phenomena take these relationships into account.

4.4.1 Chemical condition of groundwater

4.4.1.1 Reference composition of groundwater

In the H12 report (JNC, 2000), fresh, alkaline groundwater (FRHP) and saline alkaline groundwater (SRHP) were used as a reference groundwater (Yui et al., 1999a). FRHP was chosen as a reference groundwater for geological disposal of TRU waste and SRHP was also considered because of the existence of saline groundwater in Japan. However it was considered important to set the chemical composition of the reference water by taking into account relevant factors for the safety of TRU waste disposal. In particular pH, Eh, CO$_3^{2-}$, HCO$_3^-$, Cl$, SO_4^{2-}$, Mg$^2+$, silicate ion and aluminate ion were considered to be the important factors which have the potential to affect the safety of geological disposal of TRU waste.

4.4.1.2 Geochemical variations of groundwater caused by interaction with repository materials

The chemistry of groundwater in the TRU repository will be affected significantly by chemical reactions with cementitious materials. The main feature of cementitious material is that its pore water is hyperalkaline, due to the dissolution of NaOH and KOH, portlandite (Ca(OH)$_2$) and calcium silicate hydrates (C-S-H gels).

The chemistry of the cement pore water will change with time from Region I (> pH 13) in Figure 4.4.2-1 (Atkinson, 1985), where Na and K contents are high due to the dissolution of Na/KOH-rich phases, to Region II, which is characterized by equilibrium with portlandite. Subsequently, in Region III, the chemistry of the pore water is affected by dissolution of CSH gels. Eventually, the chemical conditions of the pore water become similar to those of the surrounding groundwater. The occurrence of these chemical changes is supported by numerous models and laboratory experiments (see 4.4.2.2). It is generally considered that chemical interactions between groundwater and cementitious material will include reaction with CO$_3^{2-}$ in the groundwater to precipitate calcite, reaction with SO$_4^{2-}$ to precipitate ettringite and gypsum,
and reaction with Cl\(^-\) to form Friedel salt. Additionally, in cases where there are relatively high Mg\(^{2+}\) concentrations, as in seawater, it is considered that reactions involving Mg\(^{2+}\) will cause the precipitation of Mg(OH)\(_2\) and magnesium silicate hydrates. By including these reactions, it is possible to carry out a simulation of the pore water chemistry in cementitious material assuming equilibrium between the major cement hydrates and groundwater (RWMC, 2005) and so the chemical conditions of pore water in the waste and filling material regions can be estimated.

The hyperalkaline leachates from the cement affect the dissolution and precipitation of the primary and secondary minerals that compose the bentonite. As a result, the chemical conditions of the pore water in the buffer are expected to change rapidly. For example, pH decreases owing to the dissolution of montmorillonite and chalcedony and, consequently, the concentrations of silicate ions increase, thereby influencing the precipitation of secondary minerals. The chemical conditions in the bentonite will also depend on the type of secondary minerals that are generated, as well as spatio-temporal variations in the chemical characteristics of the bentonite. Considering the uncertainty concerning the kinds of secondary mineral etc, it is not possible to decide the chemical conditions of the pore water in the bentonite following reaction with the leachates. Hence, in cases where the effects of chemical and mineralogical variations in the bentonite are evaluated as part of the nuclide migration analysis, it is problematic to specify the solubility and sorption distribution coefficients of radionuclides in altering bentonite.

**4.4.2 Effect of alteration of the engineered barrier**

Chemical conditions in the TRU disposal facility and the mass transport properties of the cementitious material change with time. High-pH pore water formed by the dissolution of cementitious material, enters the adjacent bentonite buffer. As a result, the chemical conditions of the pore water in the *bentonite* change. There is a possibility that the resulting alteration of the bentonite will cause the mass transport properties of the buffer to change. It is important that these phenomena are reflected in evaluations of nuclide migration. In this chapter, the spatio-temporal changes in chemical conditions in the engineered barrier and transport properties of the material are evaluated.

**4.4.2.1 Evaluation of long-term engineered barrier performance**

Various interactions between cement material and bentonite may occur. These alteration phenomena are promoted by nonlinear coupled processes with positive and negative feedbacks (development of a complex system; Metcalfe and Walker, 2004). It is not an entirely valid approach to understand such a complex system by rigorously evaluating hypothetical, idealised, individual phenomena. Instead, it is necessary to consider the effects of interactions between non-ideal phenomena globally. However, in this case, it is extremely difficult to understand every process accurately. In many cases, the behaviour of the whole system can be understood by evaluating the effects of combinations of all the component parts, not just those processes that have similarly strong relationships. Of course, a gap in theoretical understanding may exist. However, to address this complexity, realisations based on reasonable limiting cases can be used as a basis for engineering judgments (Saito, 1998).

In this case, it is important to take appropriate measures to choose reasonable limits. In the case where
long-term variations in the engineered barrier are considered, consideration should be given to the mutual influences between the various factors that contribute to the overall complexity, as follows:

- How far can the behaviour of the system be understood from current knowledge?
- In response to the above limits in understanding, what kind of conservative measures must be adopted?

4.4.2.2 Effect of cement-bentonite interactions on long-term performance

As described in 4.4.2.1, it is difficult to estimate the overall effects of interactions between cementitious materials and bentonites, since these constitute a nonlinear coupled system. However, there is considerable chemical information concerning the most important aspects of the degradation behaviour of these two engineered barrier components. By combining this information, it is possible, based on the present level of knowledge, to predict ranges of probabilities for the effects of these interactions. In this section, before making engineering decisions, knowledge concerning interactions between cementitious material and bentonite, is summarised.

(1) Alteration of cementitious material

It is anticipated that cementitious material will be used in disposal tunnels, as a support, in the structural framework and in filling material. Additionally such material might be used to fill waste packages. There will be physical evolution, such as the opening and clogging of cracks, as well as chemical evolution when the disposal facility is saturated with groundwater, such as changes in groundwater composition (including pH), dissolution of initial minerals, and precipitation of secondary minerals, accompanied with reactions among groundwater, wastes and cement hydrates.

This section mainly considers the alteration of cementitious materials on chemical condition in the disposal facility. The effects of cracking are considered elsewhere, in an evaluation that does not consider cementitious materials to have low hydraulic conductivities. In the manufacturing of cementitious material, several types of cement are used, depending on the application and required properties. This section mainly describes the alteration and the effects of alteration of OPC.

a. Hydration of cementitious material

Cement is hydrated and hardened. The time scale for a performance assessment is significantly longer than that of cement hydration. Hence, when carrying out an evaluation of long-term alteration of cementitious material, it is assumed that hydration has already proceeded sufficiently at the starting point of analysis.

Cement hydrates are composed of many hydrates, represented by portlandite (Ca(OH)$_2$), C-S-H gel, ettringite, monosulphate and hydrotalcite (e.g. Taylor, 1997). By focusing on these hydrates it is possible to model the dissolution behaviour of cementitious material, such as the generally used OPC, which is mainly composed of Ca(OH)$_2$ and C-S-H gel (ref. Table 4.4.2.2-1). However, mass transport in an actual disposal environment occurs very slowly, and the alteration is spatially inhomogeneous. For these reasons reprecipitation might occur when solutes in pore water that has been equilibrated with the cement hydrates migrate into adjacent areas. It is necessary to consider the effect of minor hydrates, taking into account the
local concentration of particular minerals by reprecipitation. In the cases of cementitious materials that incorporate specialised cement and mixed cement such as fly ash cement, difference of the major hydrates from those of OPC should be noted.

b. Leaching of cement material

Soluble components are leached from cementitious material by contact with groundwater. As a result, the groundwater’s composition, including its pH, changes, and the compositions of hydrates also vary.

In cases where OPC is used, the dissolution of Na and K occurs initially, and pH reaches levels above 13. However, subsequently, the liquid phase becomes dominated by Ca and is equilibrated with Ca(OH)$_2$, which maintains the pH at about 12.5. Later, after leaching of Ca(OH)$_2$ is completed, the Ca/Si ratio in the C-S-H gel decreases by selective leaching of Ca. A consequence of these processes is that pH in the liquid decreases continuously, as shown in Figure 4.4.2.2-1 (Atkinson, 1985).

As described previously, the compositions of hydrates in the cementitious materials used in specialised cement and mixed cement such as fly ash cement are different from that of OPC. Hence the leachates have different compositions. For example, in the case of fly ash cement, it is known that only low amounts of relatively soluble Ca(OH)$_2$ are generated (RWMC, 2005). As a result, the amounts of leachable Ca are decreased. However, it is possible to evaluate the degradation of cement hydrates for fly ash cement by using the same model as for OPC.

The chemical evolution of cement hydrates depends on the composition of groundwater. The variation of hydrates caused by contact with meteoric water type synthetic groundwater are almost the same as those caused by contact with deionised water (Iriya et al., 1999; RWMC, 2005). However, when synthetic groundwater of which composition is similar to that of seawater contacts with cement hydrates, the pH and hydrates show different variations and it is assumed that Friedel’s salt and brucite are formed (RWMC, 2005).

c. Reactions with chemical components that are assumed to occur in the disposal environment

In addition to reaction with groundwater, cementitious material might react with constituents that are eluted from waste and bentonite. In this section, reactions with the chemical components which may affect the alteration process among possible chemical components in groundwater, waste and bentonite are described. The selected chemical components were NaNO$_3$, carbonate, sulfate and chloride.
Table 4.4.2.2-1 Concrete and mortar components for evaluation

<table>
<thead>
<tr>
<th>Solid phase*</th>
<th>Concrete [mol/m³]</th>
<th>Mortar [mol/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₃AH₆ (Hydrogarnet)</td>
<td>134</td>
<td>215</td>
</tr>
<tr>
<td>C₃FH₆ (Iron hydrogarnet)</td>
<td>49</td>
<td>79</td>
</tr>
<tr>
<td>MH (Brucite)</td>
<td>147</td>
<td>237</td>
</tr>
<tr>
<td>C₆As₃H₃₂ (Ettringite)</td>
<td>25</td>
<td>40</td>
</tr>
<tr>
<td>C₄AsH₁₂ (Monosulphate)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>KOH</td>
<td>36</td>
<td>58</td>
</tr>
<tr>
<td>NaOH</td>
<td>23</td>
<td>37</td>
</tr>
<tr>
<td>C-S-H gel (Ca/Si mole ratio = 1.8)</td>
<td>1,938</td>
<td>3,121</td>
</tr>
<tr>
<td>CH (Portlandite)</td>
<td>879</td>
<td>1,415</td>
</tr>
<tr>
<td>Cl</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Solid phase in Sugiyama model</td>
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<td></td>
</tr>
<tr>
<td>C-S-H (CH)</td>
<td>2,817</td>
<td>4,536</td>
</tr>
<tr>
<td>C-S-H (S)</td>
<td>1,078</td>
<td>1,735</td>
</tr>
<tr>
<td>C/S mole ratio in whole solid phase (−)</td>
<td>2.61</td>
<td>2.61</td>
</tr>
<tr>
<td>Void ratio (−)</td>
<td>0.13</td>
<td>0.19</td>
</tr>
</tbody>
</table>

*The following form is followed except for KOH, NaOH. C: CaO, A: Al₂O₃, H: H₂O, M: MgO, S: SiO₂, s: SO₃ (ref. Appendix of Chapter 3: assumed specifications and analytical values for cementitious material)

Figure 4.4.2.2-1 Variation in the pH of the cement leachate (Atkinson, 1985)
(a) Nitrate salt (NaNO₃)

The effects of NaNO₃ on the mechanical and hydraulic characteristics and alteration of cementitious material has been evaluated (Takei et al., 2002, 2003; Fujita et al., 2003; Kaneko et al., 2004) and the results are described below.

It is known that leaching of Ca(OH)₂ is promoted by aqueous NaNO₃ solution. The effects of NaNO₃, including the influence on Ca(OH)₂ solubility, were evaluated by carrying out equilibrium calculations using the Pitzer model for correction of activity coefficients. The calculations explain the dissolved Ca concentrations under Region II conditions attained during a flow-through experiment using 1 mol (dm³)⁻¹ NaNO₃. These equilibrium calculations showed that, when the concentration of NaNO₃ was varied through a range of 0−6 mol (dm³)⁻¹, a maximum Ca(OH)₂ solubility was attained when the NaNO₃ concentration was 1 mol (dm³)⁻¹ of NaNO₃. This maximum solubility of Ca(OH)₂ was about 1.5 times of that in deionised water. Furthermore, it was found that monosulphate and carbono-monosulphate phases were changed into NaNO₃-monosulphate phases. However, monosulphate phases and carbono-monosulphate phases are not major hydrates in cement paste and no other mineralogical changes were identified. These findings are consistent with the relationships between porosity and unconfined compressive strength regarding to solidified cement paste flushed by NaNO₃ solutions can be explained by the empirical equation which is derived from experimental data acquired using the cement paste flushed by deionised water. It is recognized that dominant hydrates contributing to compressive strength were not degraded significantly.

However, flushing with NaNO₃ solution case, despite NaNO₃ promoting Ca dissolution, the hydraulic conductivity increase is more moderate than that which occurs when flushed with deionised water. Although the precise cause has not been identified, it is plausible that Na is connected with moderating the hydraulic conductivity increase, since Na is concentrated in those solid phases from which Ca has been leached. Immediately after switching the flushing solution from NaNO₃ solution to deionised water, the hydraulic conductivity increases rapidly. It is suggested that this increase possibly reflects the promotion of Ca dissolution combined with the loss of Na from the solids in which it has been concentrated.

Formation of NH₃ by reduction of NO₃⁻ has not been found to affect the hydrate compositions, hydraulic characteristics and mechanical strength of cementitious material (Osawa et al., 2004).

(b) Carbonate

CO₃²⁻ and HCO₃⁻ are chemical species that cause neutralization (carbonation) of the cementitious material. Calcite (CaCO₃) is generated by reactions between HCO₃⁻ and CO₃²⁻ in the groundwater and Ca(OH)₂ and C-S-H in the cement. A consequence could be that the strength of the hardened solid increases. However, it is also possible that the strength of the hardened solid might decrease owing to the disruption of binding between C-S-H phases. Previous work has reported that CaCO₃ formation causes the high-pH period to shorten (Atkinson and Guppy, 1988) and hydraulic conductivity to decrease (Shibata et al., 2000).

(c) Sulfate

SO₄²⁻ is a chemical species that causes the formation, in cement paste, of expanding secondary minerals,
such as ettringite and thaumasite (CaSiO$_3$, CaSO$_4$, CaCO$_3$, 15H$_2$O), leading to cracking and decrease in strength. Aluminate hydrates, such as monosulphate phases that are incorporated into cementitious material, react with SO$_4^{2-}$ and form ettringite. Additionally, dihydrate gypsum is generated by reaction with portlandite. It is reported that, in the initial stages, formation of ettringite fills cavities and clogs cracks (Onishi et al., 1998). However, it is also reported that formation of this mineral causes failure by expansion (e.g. Japan Society of Civil Engineers, 2003).

Additionally, a decrease in the strength of the cementitious material due to the formation of thumasite of which structure is similar to that of ettringite has been reported when carbonate coexists with sufficient concentration of sulphate. (e.g. Ujike, 2002). It is also reported that thaumasite can be formed by reactions with hydrates of cementitious material such as C-S-H and portlandite, if conditions, a low environmental temperature, the inflowing water supplies CO$_3^{2-}$ continuously and contains high sulfate concentrations are fulfilled (Yoshida and Yamada, 2005).

(d) Chloride

There are many reports that chloride promotes the corrosion of rebar within reinforced concrete (e.g. Japan Cement Association, 1993). Chloride also affects the alteration of hardened cementitious material, by reacting with aluminate hydrate to form Friedel’s salt. Additionally, it has been reported that pH may increase when Friedel’s salt is formed by reactions between Cl$^-$ and hydrogarnet (Glasser et al., 1998).

(e) Reaction with other chemical components

Other chemical components that are considered to affect the alteration of cementitious material are Mg in groundwater that is derived from seawater, and Si and Al components produced by dissolution of bentonite in alkaline condition. In cases where there are high Mg concentrations in the liquid phase which contacts the cement material, it is reported that Mg(OH)$_2$ is formed by exchange of Ca for Mg in the cementitious material, leading to a drop in pH (RWMC, 2005). It is considered that Si and Al components may generate C-S-H and C-A-S-H phases by reacting with Ca ions supplied from the cementitious material.

d. Crystallization of cementitious material

(a) Crystallization by thermal alteration

Temperatures above 80°C may cause thermal alteration of the cement phases so the repository is designed in such a way so as to prevent this temperature threshold from being exceeded. (ref. 3.2.2.2).

(b) Long-term maturation into stable crystals

Since the time scale considered for TRU waste disposal is very long, it is impossible to determine all the mineral alteration by experiment. However the following alteration is considered to occur.

- Crystallization of gels to more stable minerals
- Decreasing surface areas of solid phases

Bradbury and Sarott (1995) described the phenomena as follows:

① Based on research into natural analogues of cementitious materials, partial crystallization of C-S-H gel
might occur over long time scales. However, this crystallization does not cause large changes in the chemical environment, such as large decreases in pH. Furthermore, decreases in pH are not considered to have a significant effect on sorption until a pH of 10 is reached.

② The sorption distribution coefficients of Pu and Am for synthesized crystalline calcium-silicate are higher than those of unaltered cementitious material.

③ The decrease in contributing surface areas for sorption accompanied with crystallization is also considered. However, no saturation of sorption sites is considered to occur, since the concentrations of radionuclides are generally low. In any case, the effect on nuclide sorption seems to be small, perhaps because the decrease in surface area is countered by potential nuclide uptake into the crystal structure during the crystallization process.

Additionally, as described above, the temperature is regulated so as to prevent thermal alteration hence is unlikely to affect nuclide retardation in the cementitious material.

e. Model for dissolution and precipitation of cement hydrates

In the interaction between cementitious material and bentonite, the cementitious material is a source term for cations and OH. The leaching of these components also causes alteration and degradation of the cement material. Hence, it is important to understand the relationship between cement alteration and changes in the concentrations of aqueous components. C-S-H gel is the main hydrate that is generated by cement hydration, and is generally of low crystallinity, though not completely amorphous. The crystals have atoms arranged in short cycles (Arai, 1991). Many experimental studies of C-S-H gel dissolution have been reported (Greenberg et al., 1965; Fujii et al., 1981; Kalousek, 1954; Atkinson et al., 1987) and thermodynamic dissolution models have been proposed to reproduce the experimental results. Berner (1992), presented 2 solid phase models: Ca(OH)₂ and CaH₂SiO₄, in the case where the Ca/Si ratio of the C-S-H gel is above 1; and SiO₂ and CaH₂SiO₄ in the case where the Ca/Si ration of the C-S-H gel is below 1. The equilibrium constant for dissolution of each solid phase was varied until a fit to the experimental results was obtained.

Reardon (1992) proposed that, assuming the chemical composition of C-S-H gel is $x$CaO•SiO₂•xH₂O, experimental results can be used to express the equilibrium constant for the dissolution reaction as a function of the Ca/Si ratio. Glasser et al. (1998) also proposed a similar model. Additionally, Atkinson et al. (1987) assumed that the C-S-H gel can be treated as a solid solution of Ca(OH)₂ and hypothetical solid phase of same composition as tobermorite in the case that the Ca/Si ratio is above 0.833. In the case that the ratio is lower than this value, they considered the gel to be a solid solution of SiO₂ and this hypothetical solid phase. They used the Gibbs free energy of each solid phase to calculate the Gibbs free energy of the C-S-H gel. Solid solution models by Börjesson et al. (1997) and Rahman et al. (1999a, 1999b) express the dependency of Ca(OH)₂ and CaH₂SiO₄ or SiO₂ and CaH₂SiO₄ on the Ca/Si ratio using a Magules type treatment of solid solution. These models reproduce the variations in Ca/Si of a liquid that is equilibrated with the cement, but they do not consider the precipitation behaviour and variations in Ca/Si when the fluid that contacts the C-S-H gel is not at equilibrium.
Sugiyama et al (2001) suggested a model based on a fact that the structure of the C-S-H gel can be considered that Ca and H$_2$O are located between the chains of SiO$_4$ tetrahedra. They assumed that the cement could be modelled as a non-ideal solid solution of Ca(OH)$_2$ and SiO$_2$ in spite of Ca/Si ratio. Consequently, precipitation can be taken into account easily. They also proposed an extendable model in which C-A-S-H gel is generated by taking up Al. In these models, log K for the dissolution reactions of the various solid phases are expressed according to a Guggenheim mixing model proposed by Glynn (1991). The parameter values are established by fitting the results of cement paste dissolution experiments. The dependency of equilibrium constant of each model solid which is an end member of the solid solution on the Ca/Si ratio is shown in Table 4.4.2.2-2. With this model it is possible to reproduce the dependence of the pH, Ca and Si concentrations of the liquid phase on the solid’s Ca/Si ratio. It was considered that this model is potentially applicable to the experiments other than single-system experiments by applying the model to the experiments in which Ca precipitates as a result of the solution equilibrated with Ca(OH)$_2$ contacting C-S-H gel, or in which ettringite coexists with C-S-H gel in dissolution experiment.

Additionally, as shown in Table 4.4.2.2-1, cementitious material includes hydrates other than C-S-H gel and soluble components. It is possible to explain the results of liquid exchange experiments and mortar flow-through experiments by supposing that the initial hydrates and secondary minerals in the cementitious material are those shown in Table 4.4.2.2-3 (RWMC, 2005; Yamada et al., 2005). Hence, it is considered that the initial hydrates and secondary minerals to be considered in evaluations of engineered barrier alteration are those shown in Table 4.4.2.2-3. The effect of calcite generation by carbonate, ettringite generation by sulfate, Friedel’s salt generation by chloride and brucite generation by Mg are reflected in the following analysis. In addition, thaumasite, formed when sulfate and carbonate coexist under low-temperature conditions (it is stable at $< 15^\circ$C, and is formed particularly at a temperature lower than about 5°C), is not taken into account since the temperatures at the disposal depths of 300–1,000m is considered to be 24°C–45°C (JNC, 2000).
Table 4.4.2.2-2 Equilibrium constants for model solid solutions as functions of Ca/Si ratios (based on the model of Sugiyama et al. (2001) and using the database JNC-TDB.TRU (Arthur et al., 2005)).

<table>
<thead>
<tr>
<th>Ca/Si ratio</th>
<th>Conditional log $K_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 &lt; Ca/Si ≤ 0.400</td>
<td>$\log K_s = \log [K_{s0} \cdot \frac{1}{(Ca/Si) + 1}]$</td>
</tr>
<tr>
<td></td>
<td>$\log K_c = \frac{(Ca/Si)}{1 + (Ca/Si)} \log K_{c0} - \frac{(Ca/Si)}{1 + (Ca/Si)} \log \left[1 - \frac{(Ca/Si)}{1 + (Ca/Si)} \right]$</td>
</tr>
<tr>
<td></td>
<td>$+ \left[ \frac{(Ca/Si)}{[1 + (Ca/Si)]^2} \right] \left[ 36.902 - 37.015 \cdot \frac{(Ca/Si) - 1}{1 + (Ca/Si)} + 163.21 \cdot \frac{(Ca/Si) - 1}{1 + (Ca/Si)}^2 \right]$</td>
</tr>
<tr>
<td>0.400 &lt; Ca/Si ≤ 0.833</td>
<td>$\log K_s = \frac{1}{1 + (Ca/Si)} \log K_{s0} - \frac{1}{1 + (Ca/Si)} \log \left[1 - \frac{(Ca/Si)}{1 + (Ca/Si)} \right]$</td>
</tr>
<tr>
<td></td>
<td>$+ \left[ \frac{(Ca/Si)}{[1 + (Ca/Si)]^2} \right] \left[ -18.908 - 57.821 \cdot \frac{1 - (Ca/Si)}{1 + (Ca/Si)} - 58.779 \cdot \frac{1 - (Ca/Si)}{1 + (Ca/Si)}^2 \right]$</td>
</tr>
<tr>
<td>0.833 &lt; Ca/Si &lt; 1.686</td>
<td>$\log K_s = \frac{1}{1 + (Ca/Si)} \log K_{s0} - \frac{1}{1 + (Ca/Si)} \log \left[1 - \frac{(Ca/Si)}{1 + (Ca/Si)} \right]$</td>
</tr>
<tr>
<td></td>
<td>$+ \left[ \frac{(Ca/Si)}{[1 + (Ca/Si)]^2} \right] \left[ -18.933 + 49.633 \cdot \frac{1 - (Ca/Si)}{1 + (Ca/Si)} + 24.582 \cdot \frac{1 - (Ca/Si)}{1 + (Ca/Si)}^2 \right]$</td>
</tr>
<tr>
<td>1.686 ≤ Ca/Si</td>
<td>$\log K_s = -7.835$</td>
</tr>
<tr>
<td></td>
<td>$\log K_c = 22.71 \quad (= \log K_{c0})$</td>
</tr>
</tbody>
</table>

$\log K_{s0} = -2.639 \quad (JNC-TDB.TRU) \quad \log K_{c0} = 22.71 \quad (JNC-TDB.TRU)$
The dissolution of cement hydrate is faster than the mass transport in the disposal facility by diffusion etc. From this reason, the dissolution model and the mass transport model can be coupled by assuming that equilibrium is always established at each time and location (Fujita et al., 2002). RWMC (2005) and Yamada et al. (2005) suggest that experimental results can be explained by coupling the mass transport process with the assumption that dissolution and precipitation of C-S-H gel, other cement hydrates and secondary minerals are at instantaneous equilibrium. Hence, in the evaluation of engineered barrier alteration, the Sugiyama model is used for the dissolution and precipitation of C-S-H gel (including the dissolution and precipitation of portlandite). Compared to other models, this model has been verified by comparison with experimental results obtained over a wide range of conditions. It is also assumed that the initial hydrates and secondary minerals shown in Table 4.4.2.2-3 are at instantaneous equilibrium. The thermodynamic data of components other than C-S-H gel, are taken from the thermodynamic database JNC-TDB.TRU (Arthur et al., 2005).

Table 4.4.2.2-3 Initial hydrates and secondary mineral considered in the chemical model of cementitious material

<table>
<thead>
<tr>
<th>Initial hydrate</th>
<th>Secondary minerals</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca(OH)₂ (Portlandite)</td>
<td>C₃ASH₄</td>
</tr>
<tr>
<td>C-S-H gel</td>
<td>C₄AH₁₃</td>
</tr>
<tr>
<td>C₃AH₆ (Hydrogarnet)</td>
<td>C₄AH₁₉</td>
</tr>
<tr>
<td>C₆As₃H₃₂ (Ettringite)</td>
<td>C₂ASH₄ (Gehlenite hydrate)</td>
</tr>
<tr>
<td>MH (Brucite)</td>
<td>Kaolinite</td>
</tr>
<tr>
<td>NaOH*¹</td>
<td>Pyrophylite</td>
</tr>
<tr>
<td>KOH*¹</td>
<td>Sepiolite</td>
</tr>
<tr>
<td></td>
<td>Friedel’s salt</td>
</tr>
<tr>
<td></td>
<td>Monosulphate</td>
</tr>
<tr>
<td></td>
<td>Calcite</td>
</tr>
<tr>
<td></td>
<td>MH (Brucite)</td>
</tr>
<tr>
<td></td>
<td>Analcite</td>
</tr>
<tr>
<td></td>
<td>Laumontite</td>
</tr>
<tr>
<td></td>
<td>Hydrotalcite</td>
</tr>
</tbody>
</table>

(*¹: assumed to be highly soluble)

**g. Mass transport properties of the altered cementitious material**

**(a) Effective diffusion coefficient**

The effective diffusion coefficient was determined from the results of tritium diffusion tests on various mortar samples. The mortar was produced from cement samples that had a wide range of water/cement ratios, and that had undergone changes in porosity due to Ca leaching during flow-through tests (Yasuda et al., 2002). Based on the results, the effective diffusion coefficient is expressed as a function of the porosity, ε, and the diffusion coefficient \( D^* \) in free water (Mihara and Sasaki, 2005).

\[
De = D^* \varepsilon^{3.05}
\]  

(4.4.2.2-1)

**(b) Coefficient of hydraulic conductivity**

A relationship between hydraulic conductivity and porosity (ref. 4.4.4) was obtained from the results of
flow-through tests using hardened cement paste (Mihara et al., 2003). This function was obtained for a porosity greater than 0.5, but is also consistent with the results of flow-through tests using mortar samples having lower porosities (Yasuda et al., 2002).

(2) Analysis of alteration behaviour in a disposal facility without bentonite

This section evaluates the mineralogical and chemical transitions in a disposal facility without bentonite, based on the repository tunnel cross-sections for waste Group 3 and 4 in Section 3.2.2.2. A coupled, 1-dimensional mass transport-chemical reaction model with a simulated length of 10 m was used. In this case, mortar is specified for the analysis despite the fact that different components, such as supports, structural framework and filling materials have different compositions. As an external boundary condition of the facility, a fixed groundwater composition of FRHP or SRHP is assumed.

The analysis takes into account the influence of cracking caused by the corrosion of metals used in the structural framework, on the hydraulic conductivity of the facility (mortar) and natural barrier. In the case of crack generation, the effects of water from the surrounding host rocks entering the facility are also considered. In the case that, owing to alteration, the hydraulic conductivity of the buffer increases to a level similar to sand an increased flow rate is specified. The results of the analysis in Section 4.4.4.4 showed that the Darcy flow velocity of groundwater in the engineered barrier increased by a maximum of about 2.5 times. Referring to these results, here the flow rate in the facility is specified to be 2 times that of the natural barrier. Two extreme cases are specified in Table 4.4.2.2-4.

Table 4.4.2.2-4 Specifications for an analysis of variations in hydraulic conductivity in a disposal facility without bentonite

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Fractured near-field</th>
<th>Non-fractured near-field</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic conductivity of the facility (mortar)</td>
<td>Impermeability is not considered and the hydraulic conductivity is considered to be as large as that of sand, 4×10^{-6} [m s^{-1}] (ref. 4.4.4.2(2)c).</td>
<td>Effectively impermeable properties are specified by using an empirical formula, which relates the coefficient of hydraulic conductivity to the porosity.</td>
</tr>
<tr>
<td>Effective diffusion coefficient of the facility (mortar)</td>
<td>Diffusion coefficient is specified to be the same as that in free water multiplied by the porosity.</td>
<td>A low diffusion coefficient is specified using a relationship between the diffusion coefficient in free water and the porosity.</td>
</tr>
<tr>
<td>Approach to representing the hydraulic conductivity of the natural barrier</td>
<td>To consider the inflow of water from the surrounding host rock, the flow rate in the repository is specified to be 2 times greater than the natural barrier.</td>
<td>The hydrological gradient is specified to be 0.01.</td>
</tr>
</tbody>
</table>
An example of the simulated variations in the chemical environment is shown in Figure 4.4.2.2-2. The pH in the facility decreases with time, and the change in the outermost part is faster than that of the central part (this is a general trend for all cases). The time scales for which different chemical conditions (Region I and Region II) are maintained, based on the calculation results, are shown in Table 4.4.2.2-5. The tabulated cases show different combinations of hydraulic conductivities (whether the cement is fractured or not) and groundwater compositions (FRHP and SRHP). Region II conditions can be maintained for about 1,000 years when the cementitious material is fractured and about 10,000–20,000 years when there are no fractures. The estimated period until start of Region III depends on the location in the repository (centre or the outermost part) but is estimated to be about 1,000–10,000 years in the fractured repository and more than 70,000–100,000 years when there are no fractures. The decrease of pH is faster in the cases of SRHP than in those of FRHP. With SRHP, the period for which Region II is maintained when the cement is fractured is half that in the case where the water is FRHP. Moreover, as shown in Section 4.4.2.2(1)c, the solubility of Ca(OH)$_2$ increases by up to 1.5 times in waste group 3, which includes NaNO$_3$, so decreasing the maintenance period for Region II may shorten up to 2/3 in the base case (above).

Figure 4.4.2.2-2 Evaluation result for chemical environment in disposal facility without bentonite (FRHP–with fractured cement)
Table 4.4.2.2-5 Examples of the times for which specified chemical conditions occur, based on the analysis of alteration in a disposal facility without bentonite

<table>
<thead>
<tr>
<th>Combination of groundwater composition and permeability</th>
<th>Region I period</th>
<th>Region II period</th>
</tr>
</thead>
<tbody>
<tr>
<td>FRHP−fractured</td>
<td>ca. 1×10³ years</td>
<td>ca. 8×10³ years</td>
</tr>
<tr>
<td>SRHP−fractured</td>
<td>ca. 1×10³ years</td>
<td>ca. 4×10³ years</td>
</tr>
<tr>
<td>FRHP−non-fractured</td>
<td>ca. 1×10⁴ years</td>
<td>ca. 7×10⁴ years</td>
</tr>
<tr>
<td>SRHP−non-fractured</td>
<td>ca. 2×10⁴ years</td>
<td>ca. 7×10⁴ years</td>
</tr>
</tbody>
</table>

*: The increase of pH in the SRHP case occurred owing to the formation of Friedel’s salt.

(3) Alteration of buffer material

The buffer material is composed of Na-type bentonite and silica sand and is expected to be capable of retarding radionuclides by diffusion, sorption and colloid filtration, and providing a hydraulic barrier. These capabilities may be affected by any mineralogical changes and/or ion exchanges of the interlayer cation of montmorillonite (major component of bentonite) that may occur due to varying environmental conditions. The long-term mineralogical stability of the bentonite has been reported in many cases. For example, Shibata (2004) considered that reactions with groundwater alone would not cause a significant mineralogical change at temperatures below 100°C within timescales of interest to the safety assessment. However, in a TRU waste repository, cementitious material will be used and, in such cases, hyperalkaline leachates arising from the cementitious material might cause dissolution of bentonite components and precipitation of secondary minerals such as C-S-H gels and zeolites. Additionally, the early hyperalkaline leachates will contain a high concentration of K originating in the cement, and consequently montmorillonite, which is major component of bentonite, might change into a non-swelling layered silicate mineral such as illite. Accordingly, when evaluating alteration of the buffer in highly alkaline conditions, the dissolution of bentonite components, precipitation of secondary minerals and the ion exchange should be considered. To help better understand the potential ion exchanges in the bentonite and thereby changes in the expected capabilities of buffer, it is possible to use a presently available ion-exchange reaction model (Oda and Shibata, 1999) and empirical equations among mass transport parameters, mechanical properties and the ratio of exchangeable Na to the cation exchange capacity (Mihara et al., 1999; Ito, 2005).

a. Dissolution of the bentonite components

As shown in 4.4.1.2, it is considered that cement leachate chemistry will continuously evolve. To understand alteration processes of the buffer in these conditions, experiments were undertaken in which bentonite was reacted with alkaline solutions having a wide range of pH, varying from hyperalkaline (pH > 13) with abundant Na and K, via solutions that were equilibrated with Portlandite (pH 12.5) to solutions that had pH < 12.5. A major aim was to determine the dissolution rates of montmorillonite which is the
main component of bentonite under these conditions because the function of bentonite attribute to the nature of montmorillonite.

(a) Dissolution reaction of montmorillonite

The dissolution reaction of Na-montmorillonite is shown as follows (Wolery, 1992).

\[
\text{Na}_{0.33}\text{Mg}_{0.33}\text{Al}_{1.67}\text{Si}_4\text{O}_{10}(\text{OH})_2 \rightarrow \\
0.33\text{Na}^+ + 0.33\text{Mg}^{2+} + 1.67\text{Al}^{3+} + 4\text{SiO}_2(\text{aq}) - 6\text{H}^+ + 4\text{H}_2\text{O}
\]

Under high pH (13 > pH > 10) conditions, chemical species of Al and Si undergo hydrolysis and dissolution should be formulated by:

\[
\text{Na}_{0.33}\text{Mg}_{0.33}\text{Al}_{1.67}\text{Si}_4\text{O}_{10}(\text{OH})_2 + 6.68\text{H}_2\text{O} \rightarrow \\
0.33\text{Na}^+ + 0.33\text{Mg}^{2+} + 1.67\text{Al(OH)}_4^- + 4\text{HSiO}_3^- + 4.68\text{H}^+
\]

According to equation 4.4.2.2-3, dissolution of montmorillonite progresses increases in pH. Moreover, in a closed system, the concentrations of soluble chemical species gradually increase if there is no precipitation of secondary minerals. In such conditions, it is considered that dissolution will eventually attain equilibrium when the concentrations of these species become sufficiently high. Lasaga (1998) proposed the following general formula of rate law that takes into account the saturation state of the mineral phase in the dissolution reaction:

\[
\text{Rate} = k_0 \cdot A_{\text{min}} \cdot e^{-\frac{E_{\text{app}}}{RT}} \cdot a_H^{n_H} \cdot \prod_i a_i^{n_i} \cdot g(I) \cdot f(\Delta G_r)
\]

Where, \( k_0 \), \( A_{\text{min}} \), \( E_{\text{app}} \), \( R \), \( T \) are, respectively, a constant, the reactive surface area of the mineral, the apparent activation energy of the overall reaction, the gas constant and the absolute temperature. Additionally, \( a_i \) and \( a_H^+ \) denote the activity of the soluble chemical species, \( i \) and the activity of \( \text{H}^+ \) respectively. The terms \( n_i, n_H^+ \), \( g(I) \) and \( f(\Delta G_r) \) represent the reaction orders, a function of the ionic strength (I) and an expression for the change of the Gibbs free energy, respectively.

\[
ed^{-\frac{E_{\text{app}}}{RT}}
\]

represents the effect of temperature, \( a_H^{n_H} \) represents the effect of pH, \( \prod i \) represents the effect of ions that have either a catalytic or inhibiting effect, other than \( \text{H}^+ \) and \( \text{OH}^- \), and \( g(I) \) and \( f(\Delta G_r) \) represent the influences of the ionic strength and the departure from equilibrium on the dissolution rate respectively.

a) Dissolution rate under far-from-equilibrium conditions

The dissolution rate of montmorillonite in a system that is far from equilibrium becomes a minimum at near neutral conditions, and increases under acidic and alkali conditions (Huertas et al., 2001). However, previous experiments have been carried out using different methods (batch experiment or flow through experiments), samples (pure montmorillonite, natural bentonite and bentonite after manufacturing, etc.) and temperatures. Sato et al. (2004) measured the dissolution rate of montmorillonite by means of a flow...
through experiment with purified Na-montmorillonite at various temperatures (30°C − 70°C) and pH conditions (8 − 13). In addition to evaluating the dissolution rate from the varying composition of the experimental fluids, the rate determined by the flow through experiment was confirmed by the in-situ observation of montmorillonite particles dissolving, using atomic force microscopy. Moreover, by the in-situ observation, it was found that the dissolution of montmorillonite under hyperalkaline conditions occurs selectively at edge surfaces. As the result, it was showed that the dissolution rate of montmorillonite as a function of temperature and pH can be modelled assuming two parallel reaction paths, as proposed by Cama et al. (2002), and the following equation was given.

\[
Rate = \frac{4.74 \times 10^{-6} \cdot e^{-\frac{3957}{RT}} \cdot 177 \cdot e^{\frac{2037}{RT} \cdot a_{\text{off}}} + 1.70 \cdot e^{-\frac{6067}{RT} \cdot a_{\text{off}}}}{1 + 177 \cdot e^{\frac{2037}{RT} \cdot a_{\text{off}}} + 0.0297 \cdot e^{\frac{2353}{RT} \cdot a_{\text{off}}}} \cdot A_{\text{min}}
\]

(4.4.2.2-5)

\(Rate\): Dissolution rate of montmorillonite [mol/s]

\(A_{\text{min}}\): Reacted surface area of mineral [m²]

\(T\): Absolute temperature [K]

\(R\): Gas constant [kJ/K/mol]

The dissolution rate given by Sato et al. (2004) under sufficiently far from equilibrium conditions is considered to correspond to the rate equation 4.4.2.2-4 when the term \(f(\Delta G_f)\) is 1.

b) Dissolution rate in a near-equilibrium system

In an open system, soluble chemical species are supplied into a solution by the dissolution of solid phases and transported into the system, removed by precipitation of secondary minerals and transported out of the system. The balance of the rates of these processes determines the concentration of the solutes. If the rates for removing solutes exceed the supplying rates, the dissolution reaction proceeds under far-from-equilibrium conditions. However, the effect of saturation cannot be neglected in the conditions of large surface area/liquid volume ratio (SA/V) as in the bentonite buffer because the concentrations of solutes easily rise in such conditions. Therefore it is important to evaluate the dependency of dissolution rate of montmorillonite on the degree of saturation.

The variation in the dissolution rate of montmorillonite as a function of the saturation degree with respect to montmorillonite has been investigated by means of a flow-through experiment by Cama et al. (2000). They attempted to interpret the dependency of the dissolution rates on the degree of saturation in the following ways:

① Model based on transition state theory (TST)

In the transition state theory (TST) model, the Gibbs free energy function \(f(\Delta G_f)\) in 4.4.2.2-4 is formulated as follows:

\[
f(\Delta G_f) = 1 - \exp\left(\frac{\Delta G_f}{\sigma RT}\right)
\]

(4.4.2.2-6)
\( \Delta G_r \): Variation of the Gibbs free energy [kJ/mol]

\( \sigma \): Temkin stoichiometry coefficient

Although this model is based on transition state theory, experimental data can be reproduced only in the limiting case where the rate-controlling step for dissolution is a single reversible step.

2) Nonlinear model

A nonlinear model uses a more flexible empirical formula including 2 variables \((m, n)\) than the TST equation (in the case where \(m = n = 1\) it is equivalent to the TST equation).

\[
f(\Delta G_r) = 1 - \exp\left( m \left( \frac{\Delta G_r}{RT} \right)^n \right)
\]  \hspace{1cm} (4.4.2.2-7)

This model has been used to reproduce the dissolution rate of montmorillonite, gibbsite and albite in the weakly alkaline or acidic region (Cama et al., 2000; Metz et al., 2002; Nagy and Lasaga, 1992; Burch et al., 1993; Carroll et al., 1998; Nagy et al., 1999). It provides a better agreement to the experimental results, though the theoretical reasons for this are unclear. The empirical formula given by fitting of equation 4.4.2.2-7 to experimental data for the dissolution rate of montmorillonite at pH = 8.8 are shown in 4.4.2.2-8 (Cama et al., 2000). However, it is uncertain whether the equation is applicable under hyperalkaline conditions and, if so, what variable parameter values should be used.

\[
f(\Delta G_r) = 1 - \exp\left( -6 \cdot 10^{-10} \cdot \left( \frac{\Delta G_r}{RT} \right)^6 \right)
\]  \hspace{1cm} (4.4.2.2-8)

3) Silica inhibition model

\[
Rate = \frac{a}{1 + bC_{Si}}
\]  \hspace{1cm} (4.4.2.2-9)

This model expresses the dependency of the dissolution rate of montmorillonite on Si concentration \((C_{Si})\) in the solution and assumes that OH\(^{-}\) promoted dissolution reaction is inhibited by the absorption of Si onto the same site on the surface in which OH\(^{-}\) adsorbed (i.e. \(a\) and \(b\) are constants). This model is also able to reproduce the experimental data (Cama et al., 2000).

c) Dissolution rate law for montmorillonite used in the evaluation of buffer alteration

Among the options for modelling the dissolution rate of montmorillonite, the TST model is difficult to apply because montmorillonite dissolution reported by Cama et al. (2000) shows a nonlinear dependency with respect to the degree of saturation. The multioxide silicate model (Oelkers et al., 2001), which is the basis of the silica inhibition model (equation 4.4.2.2-9), expresses the dissolution behaviour in the far-from-equilibrium system, therefore it is considered to be difficult to use this model to evaluate
dissolution behaviour near to equilibrium. Instead, the nonlinear model is appropriate in such a case.

The dissolution rate \([\text{mol s}^{-1}]\) of montmorillonite used in the evaluation of the buffer alteration was therefore calculated using equation 4.4.2.2-10 (note that this rate is defined for the half unit cell formula for montmorillonite). This equation is a combination of the dissolution rate formula of Sato et al. (2004) (4.4.2.2-5) and the empirical formula describing dependency on saturation degree given by Cama et al. (2000) (4.4.2.2-8).

\[
\text{Rate} = \frac{4.74 \times 10^6 \cdot e^{3957/RT} \cdot a_{\text{OH}}}{1 + 177 \cdot e^{3507/RT} \cdot a_{\text{OH}}} + 1.70 \cdot e^{6067/RT} \cdot a_{\text{OH}} - 0.0297 \cdot e^{3535/RT} \cdot a_{\text{OH}} \cdot A_{\text{min}} \cdot \{1 - \exp(-610^{10} \cdot (2 \cdot \Delta G/RT))\}
\]

(4.4.2.2-10)

Both the nonlinear model and the TST model predict amounts of dissolved montmorillonite that exceed those observed in the experiment at 80°C using a compacted mixture of purified Na-bentonite (Kunipia F) and silica sand, with the latter model predicting a greater excess than the former model (RWMC, 2002). The experimental data also shows that quartz, the major component of silica sand, dissolves prior to montmorillonite, as predicted by the nonlinear model whereas the TST model predicts dissolution of montmorillonite is faster than that of quartz. Hence, the nonlinear model would appear to be more appropriate for the evaluation of the buffer alteration.

(b) Treatment of ion exchange reactions in the dissolution of montmorillonite

The exchangeable cation in the bentonite is mainly composed of Na and ion exchange reactions with Ca and K in the cement leachate will occur. Since ion exchange is considered to be a faster process than mass transport, the ion exchange reaction between pore water and montmorillonite was assumed to reach instantaneous local equilibrium. Additionally, the dissolution rate of each type of montmorillonite (i.e. Na-type, Ca-type, K-type and Mg-type) was given according to its degree of saturation.

(c) Dissolution reaction of bentonite accessory minerals

The bentonite buffer considered in this report is compacted mixture of bentonite and silica sand as shown in Table 4.4.2.2-6. Table 4.4.2.2-7 shows mineralogical composition of the bentonite. The pH buffering effect of pyrite due to sulfate production accompanied with pyrite oxidation was neglected because the period of oxidizing condition is considered to be negligibly short in comparison with the period of interest. However, under the hyperalkaline conditions, chalcedony and quartz will all react and buffer the pH. Additionally, calcite in the buffer is an important source of carbonate, and reprecipitation of calcite near the interface between buffer and cementitious material might be caused by reaction with Ca that is supplied from the cement. This redistribution of calcite might affect mass transport which occurs through the interface between buffer and cementitious material. The evaluation of buffer alteration was focused on montmorillonite, calcite and chalcedony which has a greater reactivity than quartz. Calcite and chalcedony dissolution and precipitation reactions were assumed to be instantaneous local equilibrium.
Table 4.4.2.2-6 Specification of buffer material (based on the evaluation in Section 3.2.1.2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Set value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dry density</td>
<td>$1.6 \times 10^3$</td>
<td>Kg m$^{-3}$</td>
</tr>
<tr>
<td>Bentonite content</td>
<td>70$^*$1</td>
<td>wt%</td>
</tr>
<tr>
<td>Silica sand content</td>
<td>30$^*$1</td>
<td>wt%</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.40</td>
<td>–</td>
</tr>
</tbody>
</table>

$^*$1: Bentonite is 80 wt%, silica sand is 20 wt% in seawater system.

Table 4.4.2.2-7 Mineralogical composition of bentonite$^*$1

<table>
<thead>
<tr>
<th>Mineral name</th>
<th>Compositional formula</th>
<th>Formula weight</th>
<th>Set value$^*$1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Montmorillonite$^*$2</td>
<td>Na$<em>{0.33}$Mg$</em>{0.33}$Al$_{1.67}$Si$<em>4$O$</em>{10}$(OH)$_2$</td>
<td>369.0</td>
<td>48.0 wt%</td>
</tr>
<tr>
<td></td>
<td>Ca$<em>{0.165}$Mg$</em>{0.33}$Al$_{1.67}$Si$<em>4$O$</em>{10}$(OH)$_2$</td>
<td>368.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>K$<em>{0.33}$Mg$</em>{0.33}$Al$_{1.67}$Si$<em>4$O$</em>{10}$(OH)$_2$</td>
<td>374.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mg$<em>{0.165}$Mg$</em>{0.33}$Al$_{1.67}$Si$<em>4$O$</em>{10}$(OH)$_2$</td>
<td>365.4</td>
<td></td>
</tr>
<tr>
<td>Quartz</td>
<td>SiO$_2$</td>
<td>60.1</td>
<td>0.6 wt%</td>
</tr>
<tr>
<td>Chalcedony</td>
<td>SiO$_2$</td>
<td>60.1</td>
<td>38.0 wt%</td>
</tr>
<tr>
<td>Plagioclase</td>
<td>(Na,Ca)(Al,Si)$_4$O$_8$</td>
<td>262.2</td>
<td>4.7 wt%</td>
</tr>
<tr>
<td>Calcite</td>
<td>CaCO$_3$</td>
<td>100.1</td>
<td>2.4 wt%</td>
</tr>
<tr>
<td>Dolomite</td>
<td>MgCa(CO$_3$)$_2$</td>
<td>184.4</td>
<td>2.4 wt%</td>
</tr>
<tr>
<td>Analcime</td>
<td>NaAlSi$_2$O$_5$H$_2$O</td>
<td>238.2</td>
<td>3.3 wt%</td>
</tr>
<tr>
<td>Pyrite</td>
<td>FeS$_2$</td>
<td>120.0</td>
<td>0.6 wt%</td>
</tr>
</tbody>
</table>

$^*$1: Based on the analytical value in Ito et al. (1993)

$^*$2: The ratio of Na-type, Ca-type, K-type and Mg-type is given to correspond to the composition of exchangeable cations (the initial ratio of Na to CEC is 86%)

b. Precipitation of secondary minerals

If bentonite components dissolve under alkaline conditions, the concentrations of aqueous species such as Si, Al and Mg will increase and pH will be buffered. As a consequence of local enrichments of Al, Si etc in solution, and depending on the pH, various secondary minerals may precipitate in the buffer.

The amounts and types of secondary mineral can potentially affect the degree of buffer material alteration by affecting the rate of montmorillonite dissolution through the change of solution chemistry. In addition, the precipitation of secondary minerals can change the porosity of the buffer which affects mass transport processes. Hence, it is important that plausible secondary minerals through the alteration of buffer material are identified.
Using evidence from laboratory experiments and related natural systems, Oda et al. (2005) investigated the mineralogical changes that could possibly occur when the hyperalkaline leachates interact with bentonite. They considered that the chemical conditions in the buffer evolve over the long term, and that from a thermodynamic viewpoints, mineral reactions in the buffer depend on chemical conditions which vary with time and space. As a result, potential major products of interaction between bentonite and cement leachate are summarised (Table 4.4.2.2-8).

Table 4.4.2.2-8 Potential products of the interaction of bentonite with hyperalkaline fluids (Oda et al., 2005)

<table>
<thead>
<tr>
<th>Condition</th>
<th>Metastable phase*1</th>
<th>Stable phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-(Na,Ca,Mg-)Al-Si-H2O</td>
<td>Phillipsite (K+Na&gt;Ca), erionite (K)</td>
<td>Illite, K-feldspar</td>
</tr>
<tr>
<td>Na-(K,Ca-)Al-Si-H2O</td>
<td>Phillipsite (Na,Ca,K), chabazite (Na+K&gt;Ca), clinoptilolite (Na+K&gt;Ca)</td>
<td>Analcime (Na)</td>
</tr>
<tr>
<td>Ca-(Na,K-)Al-Si-H2O</td>
<td>Chabazite (Ca&gt;Na+K), clinoptilolite (Ca&gt;Na+K)-heulandite (Ca&gt;Na+K)</td>
<td>Laumontite (Ca)</td>
</tr>
<tr>
<td>Ca-(Al-)Si-H2O</td>
<td>C-S-H gel, C₃ASH₄ (3(CaO) Al₂O₃ SiO₂ 4(H₂O))</td>
<td>Tobermorite, jennite, awfillite</td>
</tr>
<tr>
<td>Ca-Al-(SO₄,Cl-)H₂O</td>
<td>Ettringite, monosulfate, Friedel’s salt</td>
<td></td>
</tr>
<tr>
<td>Mg-Al-CO₃-H₂O</td>
<td>Hydrotalcite</td>
<td></td>
</tr>
<tr>
<td>Mg-Si-H₂O</td>
<td>Sepiorite</td>
<td></td>
</tr>
<tr>
<td>Ca, Mg-OH</td>
<td>Portlandite, brucite</td>
<td></td>
</tr>
<tr>
<td>Ca, Mg-CO₃</td>
<td>Calcite, dolomite</td>
<td></td>
</tr>
</tbody>
</table>

*1: ( ) shows composition of alkali and alkaline earth elements in zeolite.

While, mineral parageneses in natural systems suggest that kinetics as well as thermodynamic stability is important in controlling their occurrence. Dibble and Tiller (1981) shows that thermodynamically metastable minerals can form instead of more stable minerals due to the kinetic balance, and kinetic controls can operate to delay the attainment of equilibrium by imposing a series of metastable reactions on the overall reaction path, and then metastable minerals remain over the long term in natural systems.

Since relevant kinetic data are unavailable and it is difficult to evaluate the kinetic aspect quantitatively, Oda et al. (2005) proposed that the effects of uncertainties in kinetic models and parameters should be approximated by assuming different sets of precipitating minerals in various simulations of the buffer material alteration as follows:

The bentonite components and the potential secondary minerals shown in 4.4.2.2-8 were classified into: (1) primary minerals in the buffer (2) secondary minerals, such as C-S-H gels which can form in the short term, (3) illite, which is more stable than montmorillonite under alkaline conditions, (4) metastable zeolite...
and (5) thermodynamically stable zeolite and K-feldspar. Mineralogical evolution paths of aluminosilicate minerals were summarised as shown in Fig.4.4.2.2-3 on the basis of the evidence from laboratory experiments and related natural systems. Based on the pathways shown in Fig.4.4.2.2-3, the correlation among five mineral groups was defined as shown in Fig.4.4.2.2-4. In other words, multiple scenarios for mineralogical evolution of the buffer material were considered, for a case where formation of relatively metastable phases may be dominant for long periods, a case where metastable phases may change to more stable phases rapidly so that metastable phases disappear quickly, a case where the transformation proceeds so slowly that metastable phases can exist with stable phases and a case where local thermodynamic equilibrium may be attained in relatively short periods.

To demonstrate hypothetical kinetic driving forces in the simulations, at first, instantaneous equilibrium was assumed for all precipitation reactions of the secondary minerals mentioned above. This assumption corresponds to infinite precipitation rates for all secondary mineral groups. On the other hand, if secondary mineral groups were removed from the analytical system, it assumes that there were zero precipitation rates for secondary minerals. By taking this approach, the impacts of mineral paragenetic uncertainty on the evaluation of the buffer material alteration over the long term were bounded.

Hence, combinations of mineral groups assumed in the analyses for the buffer alteration were given according to the scenarios as shown in Fig.4.4.2.2-4.

On the other hand, smectite minerals other than montmorillonite may form as a result of reactions among groundwater, cementitious material and bentonite. For example, the possibility that high-Mg saponite might precipitate has been suggested (Inoue, 2004). The transformation of montmorillonite to beidellite under highly alkaline and saline conditions has also been reported (Karnland et al., 2004). However, the swelling properties and low permeability of saponite is equal to or better than those of montmorillonite (Villar and Rivas, 1994). Additionally, the swelling properties of the Ca-type bentonite of which the main component is beidellite are equal to or better than those of the Ca-type bentonite of which main component is montmorillonite (Huang and Chen, 2004). Therefore, it is not plausible that mineral variations within the smectitic mineral group will cause a significant degradation of the functions of buffer material. Hence, in this report smectitic minerals other than montmorillonite were not specified as secondary minerals.

Figure 4.4.2.2-3 Outline of the mineralogical consequences of aluminosilicate mineral (Oda et al., 2005)
c. Summary of chemical models used in the evaluation of buffer material alteration

The chemical models used in the evaluation of buffer alteration are described below. The following assumptions are made:

- The dissolution reaction of montmorillonite follows the dissolution rate law (4.4.2.2-10).
- The ion exchange reaction of montmorillonite achieves instantaneous local equilibrium.
- Dissolution and precipitation reactions of chalcedony and calcite attain instantaneous local equilibrium.
- The equilibrium constant for dissolution and precipitation reactions of chalcedony is applied to that for the reactions of silica sand.
- The combinations in Figure 4.4.2.2-4 are employed as the secondary mineral assemblages and instantaneous local equilibrium is imposed on the dissolution and precipitation of secondary minerals.

d. Mass transport characteristics of altered buffer material

(a) Effective diffusion coefficient

The change of effective diffusion coefficient accompanied with alteration of the buffer were handled using the change of montmorillonite content and porosity. Using measured De values of tritium in compacted Na-type bentonite (Kunigel VI) or mixtures of silica sand and Kunigel VI (PNC, 1994; Kato et al., 1995; Shimura et al., 1995; Sato, 2002), Mihara and Sasaki (2005) showed that the De in bentonite...
depends on the porosity, $\varepsilon$ and the montmorillonite content, $f_s$ ($f_s$ of Kunigel V1 is equal to 0.48 according to Table 4.4.2.2-7):

$$De = 2.27 \times 10^{-9} \varepsilon^n$$

$$n = 2.22f_s^{0.13} + 1$$

Equation 4.4.2.2-11 is consistent with the measured $De$ for purified Na-bentonite (Kunipia F) containing 95% montmorillonite. From a diffusion experiment using Ca-type bentonite (prepared from Kunigel V1), it was found that the $De$ in Ca-type bentonite is similar to that in Na-type bentonite (Mihara et al., 1999). Hence, change in the type of exchangeable cation of montmorillonite does not affect the $De$ in the buffer.

(b) Hydraulic conductivity

The hydraulic conductivity of altered buffer is given by an empirical equation (ref. 4.4.4) that includes terms for the exchangeable Na ratio to the CEC of montmorillonite, the volume ratio of porosity to the montmorillonite and the equivalent ionic concentration of solution.

(4) Phenomenon at the interface between buffer and cementitious material

Components of the engineered barrier may not be altered uniformly in the whole region of the materials. As the composition of the pore water is different in various regions of the buffer and cementitious material, chemical reactions will occur selectively at the interface between these materials in accordance with solute transport that is driven by chemical gradients. It may be caused by local alteration at the interface where the initial mineral content decreases and the abundances of secondary minerals increase forming a third transition layer. Moreover, in order for alteration of the buffer and cementitious material to continue, it is necessary for solutes to be transported through the transition layer. For example, a study on the boundary between bentonite slurry and mortar over a period of 7 years revealed that Ca dissolution in the inner mortar was restricted by the formation of a calcite layer at the surface (RWMC, 2001). Hence, this alteration layer may exert an important influence on solute transport.

(5) Analysis of alteration behaviour in the buffer and cementitious material of the disposal facility

A quantitative analysis of the alteration of engineered barrier was performed. This analysis combined the above chemical reaction model for dissolution and alteration of buffer and cementitious material, with the above mass transport models. The uncertainty in the analysis is discussed in the next Section 4.4.2.3.

a. Analytical model

(a) Analysis system

A disposal concept of largest quantity ratio of cement/bentonite was selected among the repository tunnel cross sections specified in 3.2.2.2. The concept was approximated by the shape of a concentric circle
as a reference concept. The thickness of buffer was conservatively determined as 1 m. The thickness of the cementitious material in a one dimensional analysis system was defined as 2.5 m for the half of central region containing waste, containers and structures and 0.6 m for the tunnel support (Figure 4.4.2.2-5). These values were calculated from the amount of cement per unit area of the interface between the buffer and cementitious materials on the basis of the reference concept. The waste, waste container and structure were assumed to be composed of mortar, and the support was composed of concrete (note that waste container and structure will be composed of concrete, although they were considered as mortar with higher content of OH⁻ than concrete in this analysis to overestimate the influence of cement on the buffer alteration).

Figure 4.4.2.2-5 One dimensional analysis model (The mesh increments are also shown.)

(b) Chemical reaction model

• The chemical reactions responsible for altering the buffer and cementitious material were considered to include dissolution of the initial minerals, formation of secondary minerals and ion exchange reaction of montmorillonite as described in 4.4.2.2(1) and 4.4.2.2(3).

• Ion exchange was treated using the same selectivity coefficients for the ion exchange reaction as those given in the H12 report.

• Several scenarios were considered, with different combinations of potential secondary minerals which can form in the buffer. The probabilities of their occurrence cannot be evaluated. Here, in this section, the mineral variation scenario shown in Figure 4.4.2.2-4 that includes formation of both metastable and stable phases (Case 6) was assumed. The uncertainty concerning secondary minerals is then described in 4.4.2.3.

• The groundwater was assumed to be FRHP, and the initial composition of pore water in the buffer was defined by equilibrium between this groundwater and minerals in the buffer.

Thermodynamic data for minerals and soluble chemical species which are relevant to the chemical reactions involved in the alteration of engineered barrier were taken from the thermodynamic database JNC-TDB.TRU (Arthur et al., 2005).
(c) Mass transport model

Only diffusion was considered as the mechanism for mass transport due to the following reason. Using experimental data and the empirical formula (4.4.4), the hydraulic conductivity of the hypothetically degraded buffer (montmorillonite has all converted into Ca-type and about 60% of it has disappeared) is estimated to be less than 10^{-10} \text{ m s}^{-1}. De values of the buffer with such degradation are estimated to be in the order of 10^{-10} \text{ m}^2 \text{s}^{-1} from equation 4.4.2-11. In this case, assuming the hydrological gradient of 0.01 for “Reference Case,” the Darcy flow velocity in the region of the buffer is estimated to be 10^{-12} \text{ m s}^{-1}. In the case that the representative length of the buffer is 1 m, the Peclet number becomes 10^{-2}. Therefore diffusion is the dominant mechanism for mass transport.

The variation of De in the engineered barrier caused by alteration of buffer and cementitious material was expressed by the empirical formula described in (1) and (3). The mechanical phenomena were not included and the porosity change was calculated only from the change in volume of each mineral caused by the chemical reactions. The mechanical effects are considered in 4.4.2.3.

(d) Boundary condition

The realistic exterior boundary condition includes heterogeneity and uncertainty in hydrogeological characteristics of the natural barrier. For example, there may be heterogeneity of permeability place by place even in same site. Owing to a lack of information, essentially site-specific average hydraulic conductivities and in-situ hydraulic conductivities, cannot be determined. The following extreme conditions were given analytical cases for bounding the impact of uncertainty relevant to the exterior boundary conditions on the evaluation of the engineered barrier alteration:

- A case in which it is assumed that there is a highly permeable zone such as a fracture zone and that the boundary condition has a constant concentration fixed at the surrounding groundwater composition.
- A case in which it is assumed that the host rock is of extremely low hydraulic conductivity giving a zero flux boundary condition.

Additionally, a case where there is a significant increase of hydraulic conductivity in a concrete tunnel support by its degradation, the degraded support may become the prevailing flow path for groundwater. In this case, the pH of the pore water in the support may remarkably drop and degree of alteration of buffer from outside may be decreased. By contrast, the alteration of buffer from inside may not be affected by the elevation of hydraulic conductivities in support region because dominant mass transport mechanism within buffer may remain diffusion. Hence, such an effect is not considered in the analysis.

This section describes the analytical results in the case where there is a constant concentration fixed at the groundwater concentration (FRHP) as the exterior boundary condition. The case where there is a zero flux at the boundary is describe in 4.4.2.3.

b. Analytical results

The temporal variation of pH, porosity and the distribution of mineral components in the engineered barrier after 100,000 years, is shown in Figures 4.4.2.2-6 to 4.4.2.2-8.
Figure 4.4.2.2-6 Temporal variation of pH distribution

Figure 4.4.2.2-7 Temporal variation of porosity distribution
Figure 4.4.2.2-8 Calculated mineral distribution (after 100,000 years) 
(SiO$_2$(CSH) and Ca(OH)$_2$(CSH) in the figure are the C-S-H gel end members defined in the Sugiyama model (Sugiyama et al., 2001). The initial total amount of montmorillonite is 1,465 mol m$^{-3}$)

As shown in Figures 4.4.2.2-6, the pH in the buffer lay around 11.5 from a time several 100 years after the start, until 100,000 years. It appears to be controlled by a balance between the transport of OH$^-$ from the cementitious materials into the buffer, the consumption of OH$^-$ by hydrolysis of soluble species such as Si that is released into pore water by dissolution of buffer constituents (montmorillonite and chalcedony, etc.), and the consumption and/or production of OH$^-$ by relevant mineral precipitation. Furthermore, in this case, concentration of soluble Al species in the buffer adjacent to the interface with cementitious material were considered to be low by precipitation of potassium feldspar and zeolites. This phenomenon promotes the dissolution of montmorillonite adjacent to the waste region by a lowering of the degree of saturation of montmorillonite. The secondary mineral assemblage that was finally precipitated in the buffer region was dominated by potassium feldspar and heulandite, though analcime and sepiolite were also formed.

At the interface between the buffer and the cementitious materials, secondary C-S-H gels and calcite were abundantly precipitated so that the pores of the cementitious materials immediately adjacent to the interface were filled with these minerals by 10,000 years. The precipitation of C-S-H gels was caused by supply of Si from the buffer due to the dissolution of montmorillonite and chalcedony and Ca from portlandite. Redistribution of calcite appeared to be attributed to the steep change in the solubility of calcite due to the steep change of pore water pH over the interface.

The mass transport throughout the engineered barrier was significantly limited by the filling of pores at
the interface. As a result, the chemical condition of the waste region lay between Region I and II for 100,000 years.

Na-type was dominantly montmorillonite for several ten thousand years since the concentration of competitive Ca species in the pore water decreased by the consumption due to the precipitation of secondary minerals such as Ca-rich zeolite in the buffer. In addition, this was attributed to that supply of Ca from the cementitious region was limited by the filling of pores at the interface.

c. Effects on nuclide confinement

The results from b. show that after 100,000 years, about 80% of the montmorillonite is preserved in the buffer over the two central cells divided into irregular sizes, which correspond to 68 cm thickness of the 100 cm buffer. Furthermore, a significant porosity increase in the buffer was calculated in the parts near to the interface. However, the porosities in most other parts of the buffer were not changed, since the overall amount of dissolution was small and the volume of the solid phase was compensated by the precipitation of secondary minerals. This result means that the volume ratio of porosity to montmorillonite was kept so low as the equivalent hydraulic conductivity of the buffer lay within the order of $10^{-12}$ [m s$^{-1}$] for the long term. Hence, it is indicated that the effective function of the buffer as a hydraulic barrier can be maintained after 100,000 years.

On the other hand, there is a concern for cementation. If precipitated secondary minerals bind the particles of primary minerals of bentonite buffer, the buffer may be cemented by secondary minerals and lose the plasticity and swelling property. The cementation has been considered as a critical process since it may reduce or eliminate the key properties of bentonite buffer as mentioned above. Measurements of the swelling capacity of artificially degraded bentonite which was prepared under highly alkaline and high temperature conditions, have revealed that the swelling capacity is not lost in case where the proportion of preserved montmorillonite is above 70% (Ichige and Honda, 2005).

From the analytical result, it seems that the precipitation of secondary minerals such as C-S-H gels does not affect the capabilities of the whole buffer material since they precipitate locally near the interface. The analysis shows that potassium feldspar and zeolites precipitated. However 80% of montmorillonite preserved in most regions of the buffer even after 100,000 years, hence the swelling capacity of the buffer is not expected to be lost according to the results of the previous experiments. Considering these results, the possibility of cementation and its impact on the functions of the buffer was neglected in this report.

From the above evaluation, it is considered that the degree of alteration of the buffer will be so slight after 100,000 years as to maintain the function as the hydraulic barrier. Therefore diffusion continuously dominates the nuclide migration process within the engineered barrier for 100,000 years. It is shown that alteration causes significant pore filling, which improves the barrier performance of nuclides confinement. However, it should be noted that these results include uncertainties accompanied with several hypotheses.
4.4.2.3 Uncertainty in current knowledge and treatment of uncertainty in the nuclide migration analysis

Predictions of the effects of engineered barrier alteration on barrier performance as described in 4.4.2.2, include uncertainty because there are several assumptions which have not yet been confirmed. In such cases, based on the evaluation results, appropriate measures should be taken.

(1) Information about uncertainty

a. Dissolution rate law of montmorillonite

As described previously, it is considered that reliable data are available from current studies for the dissolution rates of montmorillonite in far-from-equilibrium conditions with high liquid-solid ratios. A decrease in the dissolution rate near to equilibrium has been observed at pH 8.8, and this result shows that assumptions of both instantaneous equilibrium and TST type saturation dependency are too pessimistic for evaluating the dissolution kinetics of montmorillonite. Under the current conditions, it is appropriate to use a reproducible nonlinear experimental rate law. Furthermore, a model based on transition state theory and an instantaneous equilibrium model were applied to the assessments as hypothetical model options in order to bound the uncertainty.

b. Types of secondary minerals

There are large uncertainties in the type of secondary minerals that occur and their transitions over the relevant time scales. Hence the probability of the mineral combinations existing in the scenarios described in Section 4.4.2.2(3) cannot be evaluated. In Section 4.4.2.2, an analysis is performed assuming the formation of metastable zeolite and stable phases (stable zeolite and K-feldspar). The analysis also assumed the general co-existence of minerals such as C-S-H gels ((1) and (2) group in Figure 4.4.2.2-4). In contrast, in this section, the following scenarios were supposed and the same kind of analyses as that in Section 4.4.2.2 were carried out:

- Metastable zeolite and stable phases are formed at an extremely slow rate, and generally co-existent minerals such as C-S-H gel and illite are formed relatively rapidly (Case 1 in Figure 4.4.2.2-4).
- It is assumed that stable phases and illite are produced relatively rapidly and metastable zeolite does not coexist or does exist for only a short time. In other words, the cases of stable phase formation and those of the formation of both stable phases and illite in addition to general co-existent minerals such as C-S-H gels (Case 3 and 5 in Figure 4.4.2.2-4) were assumed.
- It is assumed that the formation of stable phases are extremely slow and that the existence of metastable zeolites is sustained over a long term from the initial stage. The formation of general co-existent minerals such as C-S-H gels were also assumed (Cases 2 and 4 in Figure 4.4.2.2-4).

Among previous cases, Cases 1, 3 and 5 (the cases for no formation of metastable zeolite) resulted in insignificant quantities of montmorillonite being dissolved during a period of 100,000 years. The result suggests that the bentonite was more stable in the cases for no formation of metastable zeolite than in those
for formation of metastable zeolite.

The spatial distributions of minerals after 100,000 years in the case where metastable zeolite is formed, but stable zeolite and K-feldspar are not formed, is shown in Figure 4.4.2.3-1 (Case 4). The temporal changes of pH for the same case are shown in Figure 4.4.2.3-2. In this case, significant quantities of phillipsite and heulandite appeared, and the dissolution of montmorillonite was promoted. The amount of dissolution during 100,000 years was higher than the analytical result in 4.4.2.2. In this case, effective impermeability will be maintained for 100,000 years because more than 70% of the montmorillonite remained in 50 cm of the bentonite (and more than 60% of montmorillonite remained in 70 cm) even after 100,000 years.

The calculated changes in chemical conditions show that the region of the waste could maintain the states of Region I−Region II of cementitious material for 100,000 years and the condition of pH > 11 could be maintained in the pore water of bentonite buffer from several 100 to 100,000 years. The change of ion type in the montmorillonite was classified into 2 cases: cases (Cases 3 and 5) where Ca-type was formed early (in the order of 10,000 years) since Ca-rich metastable zeolite was not produced; and cases (Cases 1, 2 and 4) where Na type was dominant for 100,000 years because of the consumption of Ca by the formation of meta-stable zeolite (Cases 2 and 4) or no consumption of Na by the formation of zeolite minerals (Case 1). The results suggest the kinds and quantities of secondary minerals may affect the spatio-temporal variation of interlayer cation of montmorillonite. However, from the extent of the evaluation of both in Section 4.4.2.2 and in this section, it can be stated that the effectively impermeable characteristics of bentonite buffer will be maintained for 100,000 years even if Ca-type montmorillonite forms at an early time.

As in the cases in Section 4.4.2.2, the pore space in the region near the interface between cementitious material and the bentonite was almost filled by the precipitation of secondary mineral in all the assumed cases, improving the performance of the engineered barrier for retaining nuclides.
Figure 4.4.2.3-1 Mineral distribution in the case that assumes that stable zeolites and K-feldspar are not formed (Case 4 in Figure 4.4.2.2-4: after 100,000 years)

Figure 4.4.2.3-2 Time change of pH distribution in the case assuming that stable zeolites and K-feldspar are not formed

c. Precipitation rates of minerals

The concentration of aqueous species in the actual local pore water is controlled by a balance between a supply by dissolution of solid phases, mass transport to and from the system and a consumption by
precipitation reactions. However, in the analysis here, the dissolution and precipitation of secondary minerals is assumed to be at instantaneous equilibrium, and the actual reaction rates are not established. In this analysis, the dissolution reaction of montmorillonite, which is the main mineral in the bentonite, reflects the measured reaction rates. This dissolution reaction is the main process that supplies material to the liquid phase. Hence, it is considered that, neglecting the dissolution reaction of chalcedony, a realistic rate is used for the mass supplying process to the liquid phase. It has been confirmed that even if the actual rate is used for the dissolution reaction of chalcedony (Plettinck et al., 1994), mineralogical changes in the bentonite region and the chemical conditions of the pore water are not significantly affected (Sasaki et al., 2005). This result is no different to the case where instantaneous equilibrium is assumed because the primary dissolution reaction is itself very fast. In this analysis, the main role of dissolution and precipitation processes of secondary minerals is considered to be the consumption of aqueous species by precipitation of secondary minerals. To assume instantaneous equilibrium of secondary mineral dissolution and precipitation reactions is almost equal to the precipitation of a secondary mineral at an infinitely fast rate until equilibrium is reached. Hence, actual value is setup for mass supply rate into liquid phase, while the removal rate of solute from liquid phase assumes infinitely large rate. Therefore, in many cases, the concentrations of soluble chemical species are estimated to be lower than the actual conditions, if instantaneous equilibria of dissolution and precipitation reactions of secondary minerals are assumed.

The kinetics of the dissolution reaction of montmorillonite is expressed by a formula of ion product for aqueous species which is produced in the reaction. The ion product is smaller (concentrations of the aqueous species are smaller) and the dissolution rate is estimated to be larger. Hence, in this analysis, the dissolution rate of montmorillonite is evaluated to be conservative by comparing the case that actual precipitation rate is employed. The information of various precipitation rate of secondary mineral is necessary in order to perform more realistic evaluations.

d. Thermodynamic data

The equilibrium constant for montmorillonite dissolution used in the analysis in Section 4.4.2.2, is the value in the EQ3/6 database (Wolery, 1992). However, there are several methods for obtaining equilibrium constants and different methods may give different results. The larger constants will give the larger dissolution rate because the saturation index of montmorillonite becomes lower in calculations. In order to test this effect, the same analysis as in Section 4.4.2.2 was conducted by using the largest equilibrium constant among those evaluated with different methods. The result shows that the larger equilibrium constant brings about the earlier loss of the impermeable function of bentonite buffer within several 1,000 years. Another analysis that uses this large equilibrium constant do not show long-term stability of montmorillonite in saline groundwater (Sasaki et al., 2005). However this result is inconsistent with previous work (Kamei et al., 1992) that has shown bentonite to exist stably in an environment similar to seawater which has been cooled down from 160°C to 100°C over a period of 2 million years. Hence, the evaluation using this large equilibrium constant is not appropriate for judging the alteration of engineered barriers.

There is still uncertainty in knowledge concerning thermodynamic data for minerals and aqueous species.
However, there is little necessity for using data that gives an excessively conservative evaluation of the alteration of the engineered barrier.

e. Stability of pore filling secondary minerals

The analytical results of Sections 4.4.2.2 and 4.4.2.3(1)b, show that pore filling by secondary minerals occurs on the mortar side of the interface. The porosity increases in a limited zone of the bentonite side where the increase of porosity due to dissolution of initial minerals exceeds decrease of porosity due to the precipitation of secondary minerals. These results suggest the possibility that the alteration phase is not mechanically stable. In addition to this, if release of the gas generated in the waste region and water flow in cracks which are formed by gas pressure etc. are also taken into account, it is considered that the pore-fillings will be intermittent. Reactions between natural cement, groundwater and host rocks in Maqarin, Jordan are considered to have resulted in repeated closure and opening of fractures (Alexander and Smellie, 1998). Hence, filling of pores by secondary minerals does not always limit mass transport. Intermittent solute and nuclide migration can occur because of repeated partial destruction and re-clogging of defect formed by the destruction. For bounding the uncertainty arising from the consequence of the partial destruction and re-clogging of the engineered barrier, an analysis is carried out assuming that the effective diffusion coefficient does not decrease with a decrease in porosity. The results are shown in Figure 4.4.2.3-3 (the specification of secondary minerals is the same as Case 6).

In the analysis in Section 4.4.2.2, the OH-, Na+ and K+ ions were effectively confined in the cementitious material by pore-filling over the long term. In contrast, OH- easily migrated into bentonite buffer in this analysis and therefore the amount of dissolved montmorillonite was greater than that in Section 4.4.2.2. Ca-type was dominant montmorillonite in a wider region of buffer in this analysis than in Section 4.4.2.2, since competitive Na and K had migrated to the outside of the system and after which Ca was supplied continuously by cement minerals.

In this case, 70% of the montmorillonite remained in the 70 cm of bentonite buffer after 100,000 years. There is considered to be a negligible increase in permeability, even though Ca-type montmorillonite forms and the gel density of montmorillonite decreases (weight of montmorillonite in unit volume of buffer per sum of volumes of bentonite and pore in unit volume of buffer). It is also considered that the buffer does not lose its swelling capability as a result of cementation as mentioned in 4.4.2.2(5)c. Hence the effectively impermeable characteristics of the bentonite will be little affected, and it is considered that they will be maintained for 100,000 years. The pH change in the engineered barrier progressed more rapidly than in the analytical case that considered pore filling. In the absence of pore filling, it was estimated that in the waste, the duration of Region I is approximately several 1,000 years, while the duration of Region II is approximately several 10,000 years (after 100,000 years Region III is distributed around 20 cm from the outer edge of the waste region). In the bentonite region, pH of more than 11 was maintained until several 10,000 years and the pH decreased below 11 after 100,000 years.
f. Uncertainty concerning the exterior boundary condition

In the analysis in Section 4.4.2.2, the exterior boundary condition is fixed at the composition of FRHP. As described in Section 4.4.2.2(4)a, the same analysis is performed with a zero flux boundary, so as to evaluate uncertainty included in the boundary condition. It is revealed that there is no significant difference between the two cases except the maintenance of the Region I-II for 100,000 years in the region of the support in the case of zero flux boundary. In the case that the phenomenon of pore filling occurs at the boundary of cementitious material and bentonite buffer, it is estimated that the effects of the exterior boundary condition on chemical and mineralogical transitions in both waste and bentonite buffer regions are small for 100,000 years.

Figure 4.4.2.3-3 Mineral distribution in the case that assumes that the porosity does not change (after 100,000 years)

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g. Mechanical effects

This section describes analyses of coupled mass transport-chemical reactions by using a one dimensional model which does not perform coupling with mechanics. Mechanical effects are evaluated in Section 3.3.2.2, and use the evaluation of host rock creep obtained below.

A mechanical analysis is carried out using a two-dimensional model assuming the highly evolved condition of an engineered barrier. The creep of host rock is estimated to be several cm. However, even if the displacement of host rock is tentatively assumed to be 15cm, the deformation of the bentonite is estimated to be less than 10cm. The compression of the disposal facility by host rock creep and the
deformation are considered to be relatively small. Therefore, the effects on the porosity of the bentonite buffer and the partial density of montmorillonite can be neglected.

If spatial heterogeneity of smectite gel density due to smectite dissolution occurs, redistribution of smectite gel density by displacement is considered to occur for achieving stress balance because swelling pressure of buffer is a function of smectite gel density. Okutsu et al., (2005) assessed the mechanical impacts of the partial drop of smectite gel density due to the dissolution of the smectite.

The assessment shows the displacement and redistribution is not significant because of deformation resistance of buffer material. However there is no experimental evidence.

Both “redistribution neglecting case” and “case of perfect homogenization of smectite gel density” were employed for bounding the uncertainty arising from the redistribution of smectite gel density. The analyses show there is no significant difference in terms of permeability between previous cases for $10^5$ years. However, if the area of altered bentonite expands more, the permeability for “case of perfect homogenization” can show the significantly higher value than that for “redistribution neglecting case.”

(2) Treatment of nuclide migration

The long-term evolution of chemical environment of a disposal facility without bentonite is evaluated in Section 4.4.2.2(2). In this part, the conditions for a radionuclide migration analysis in the facilities with bentonite is determined by reflecting the previous evaluations on the evolution of engineered barrier due to the interaction between cementitious materials and bentonite. The evaluated plausible extent of the behaviour of the cement-bentonite system and their associated uncertainty were taken into account for the determination.

① Plausible case on the basis of available information (Realistic case); There is sufficient montmorillonite remaining in the 70cm central part of the bentonite, the effectively impermeable characteristics of the bentonite are expected to be maintained for at least 100,000 years. Moreover, because the precipitation of pore-filling secondary minerals occurs near the interface between cementitious material and bentonite, nuclide migration is significantly prevented in this area. From these results, it is considered that the alteration of the engineered barrier has a positive effect on the radionuclide retention function. However, it is necessary to note that there may be effects from fractures formed by external factors and inhomogeneous reactions.

② Conservative case; It is assumed that the pore filling effect of the secondary minerals in the interfacial altered layer will not restrict diffusion because of mechanical instability of altered zone. This means that the initial effective diffusion coefficients of the cementitious material and bentonite will be constant in future. In this case, the effectively impermeable characteristics of the bentonite will be guaranteed for at least 100,000 years since sufficient montmorillonite remains.

③ Hypothetical case; The following conditions are considered to have low probabilities:
montmorillonite dissolution is promoted by constantly unsaturated conditions because the equilibrium constant for montmorillonite solubility is larger than that present in the standard database; the dissolution of montmorillonite is promoted since the dissolution rate law for montmorillonite under highly alkaline conditions follows the instantaneous equilibrium model. In these hypothetical cases, the effective impermeability of the bentonite will be lost after several 1,000 years.

4.4.2.4 Summary
There are various uncertainties concerning alteration of the engineered barrier resulting from interactions between cementitious material and bentonite. However, based on present knowledge, the alteration will possibly improve the nuclide retention function, while not adversely affecting the long-term performance of the geological repository for TRU waste. One conservative assumption from the nuclide migration analysis is that the bentonite prevents significant advective water flow for at least 100,000 years. Under these circumstances, in accordance with the initial effective diffusion coefficient in the bentonite and cement material, it is adequate for nuclide migration analyses that nuclide release from the engineered barrier is assumed to continue for the period. There are various uncertainties in current knowledge concerning the alteration process of the engineered barrier system because the process is non-linear coupled system consists of various elementary processes. Evaluations of hypothetical cases, such as where the buffer loses its capability to prevent significant water flow after several 1,000 years, help to respond to these uncertainties.

4.4.2.5 Future issues
In order to reduce the uncertainty inherent in the present evaluation and to improve its reliability, it is important to address the following issues:

◆ Increase in knowledge on thermodynamic data and reaction rates, and incorporating this knowledge in the evaluation.

◆ Increase knowledge on the changes in barrier characteristics that may occur during alteration, including alteration of cement material and bentonite, taking into account the variety of chemical environments and barrier specifications.

The details of the former task are;

- Improve understanding of mineral dissolution and precipitation rates, including experimental verification of the reaction rate laws for montmorillonite dissolution under near-equilibrium conditions, and reflecting this knowledge in the evaluation.

- Improvement of the reliability of thermodynamic data for aqueous chemical species, primary minerals composing the engineered barrier and secondary minerals under hyperalkaline conditions.

- Increase knowledge on solution chemistry in small pores, such as those within the engineered barrier, in which pore water is strongly influenced by the solid surface, and reflecting this knowledge in the evaluation.
Detailed issues of the latter task are;

- Improved understanding of the influence of groundwater chemistry and specification of engineered barrier system (materials and construction conditions) on interactions between groundwater and engineered barriers.
- Variations in the hydraulic and mechanical characteristics of the components of the engineered barrier caused by alteration (e.g. cementation of bentonite, fracturing of cement material and filling of fractures by mineral precipitation).

4.4.3 Hyperalkaline alteration of host rock around the disposal facility

As described in Section 4.4.2, the pH of pore water in a disposal facility that incorporates cement reaches 12 to 13. Additionally, the Ca concentration becomes high as a result of the dissolution of hydrates that comprise the cement. The concentrations of Na and K are also high initially, owing to cement alteration. This pore water will move into the surrounding host rock and will change the groundwater composition, resulting in a region within the host rock that contains high-pH groundwater or a high pH plume. Chemical reactions between the surrounding rock and this high-pH plume include the dissolution of primary minerals and the precipitation of secondary minerals. It is reported that this alteration may affect nuclide migration, since the dissolution and alteration of the surrounding basement rock might change the groundwater composition, the chemical environment, the capacity to sorb radionuclides and the pore structure (Rochelle et al., 1992; Savage et al., 1992; Adler et al., 1999).

As a contribution to the analysis of radionuclide migration, this section promotes an understanding of the alteration of the surrounding rocks by a high-pH plume flowing from the disposal facility.

4.4.3.1 Types of surrounding host rock

The evaluation in this report is aimed to be applicable for a wide range of geological environments ranging from crystalline to sedimentary rocks (see Table 1 in the Executive Summary). Information about mineral and chemical compositions is required for these rocks. However, each of the rock types can show a range of mineral compositions. Therefore, the evaluation was carried out by assuming the rocks to contain mineral proportions that refer to those appearing in the classification diagram for igneous rocks (The Association for the Geological Collaboration in Japan, 1996) of the International Union of Geological Sciences (IUGS). Additionally, the concentrations of the main chemical constituents of the rocks are given for standard rock materials by the Geological Survey of Japan (The Association for the Geological Collaboration in Japan, 1996).

4.4.3.2 Knowledge of the chemical alteration of surrounding host rocks by a high-pH plume

The experimental investigation of hyperalkaline alteration of the surrounding rock has been carried out mainly for silica and silicate minerals, etc. (Savage et al., 1998ab). Leaching experiments using Ca(OH)₂
solutions, mixed solutions of NaOH・KOH・Ca(OH)₂ and various rock forming minerals (quartz, feldspar, mica, etc.) have been performed and the alteration behaviour has been observed. As a result of immersion in Ca(OH)₂ solutions, decreases in Ca concentrations and pH, leaching of silica and precipitation of secondary minerals, including C-S-H phases, was observed. The precipitation of C-S-H phase was also observed on the surfaces of initial minerals such as quartz and albite.

Additionally, using granite, batch-type hyperalkaline alteration tests have been performed by Owada et al. (2000) and column-type alteration tests have been carried out by Kato et al. (2000). The batch-type test used synthetic Ordinary Portland Cement leachate with pH 13 (AW) and 12.5 (CW), synthetic leachate from low-alkali cement (LW) and distilled water (DW). The batch type experiment was carried out at 80°C for granodiorite (under 250 µm) from Kamaishi mine. In the tests using synthetic leachates (AW, CW), Si and Al were observed to be leached from the feldspar in the granite and C-S-H phases from were found to precipitate. In the test using the synthetic low pH leachate (LW), leaching of rock constituents was not observed, but the concentrations of Si and Ca in the liquid phase were observed to decrease, suggesting the generation of secondary minerals such as C-S-H and C-A-S-H phases. These results suggest that changes in the disposal environment, such as permeability changes due to rock dissolution and precipitation of secondary minerals, and changes in the distribution coefficients describing nuclide sorption, could occur during a relatively short period.

Additionally, column experiments were performed using a large column of 4 m length, a flow rate of 0.1 mL min⁻¹ and a temperature of 80°C. These experiments were carried out in order to evaluate the spatial-temporal variations caused by the high-pH plume, though secondary minerals formed at 80°C should be different from that at a temperature in a disposal site (e.g. ettringite will be absent from the secondary minerals at 80°C). On the up-stream side, calcite and C-S-H phases precipitated on the surfaces of crushed granite. C-S-H phases also precipitated at from midstream to downstream, showing that the high-pH plume affects in the whole 4 m region.

Moreover, Nakazawa et al. (2004) performed immersion experiments using a fluid leached from Ordinary Portland Cement, pumice sandstone and pumiceous tuff. The matrix in the pumiceous sandstone was volcanic glass, micro- or non-crystalline minerals, and the rock included lots of grains of plagioclase and pumice. Generation of C-S-H phases by dissolution of non-crystalline materials such as volcanic glass was observed. However, in the case of pumice sandstone, no changes were observed in grains of crystalline minerals (plagioclase and augite, etc.).

From analyses of liquids and the surfaces of solid phases, variations in Ca concentrations after leaching were observed. The Ca concentrations in the liquid phase decreased while those in the solid phase increased. These results suggest that in the presence of Ca solutions, C-S-H phases are generated by reactions involving Si from non-crystalline materials such as volcanic glass and pumice.

These experiments showed that in a high-pH plume, especially in the hyperalkaline zone containing high concentrations of Na and K, some of the minerals in the rock surrounding the disposal facility might be partially altered by dissolution.
4.4.3.3 Impact analysis for hyperalkaline alteration of rocks surrounding a facility

As described previously, alkali components that are transported from cement in a disposal facility might cause the following effects by reactions with the natural barrier surrounding the disposal facility.

A change in the pore structure might occur as a result of mineral dissolution of mineral within the host rock and the generation of secondary minerals. Consequently the coefficient of hydraulic conductivity and the diffusion coefficient may be affected. Moreover, changes in groundwater composition and the mineralogical composition of host rocks may affect the sorption coefficient of nuclides. Variations in groundwater compositions may affect the solubility of nuclides.

In this report, it is difficult to specify specific mineral compositions since it is aimed to consider general geological conditions. Hence, to evaluate the influence of alkalis, specifications for the nuclide migration analysis were based on the above investigation results and past experimental results. Minerals that are highly reactive with alkalis were selected.

(1) Analytical conditions

In this evaluation, disposal tunnels for waste group 4, without bentonite components, were evaluated. A disposal tunnel with a circular cross-section of 12 m diameter (Figure 4.2.4-1) was evaluated using a one dimensional model. In this evaluation it was considered that the hyperalkaline plume broadens downstream from the disposal tunnel. Therefore, the simulation extended from the host rock 30 m upstream of the repository to 200 m downstream of the disposal facility. The composition and groundwater head at the upstream and downstream boundaries were considered to be constant. The modelled region is shown in Figure 4.4.3-1.

In this evaluation, the host rock is assumed to composed of silica minerals that may easily react with the hyperalkaline leachate. Several types of silica mineral were considered, such as amorphous silica and the crystalline minerals quartz, cristobalite and chalcedony. However, from these minerals, the relatively crystalline mineral chalcedony was selected for the analysis, since this mineral is considered to occur in the fresh groundwater system and to exist in bentonite. Additionally, amorphous silica and clay minerals were also considered to be fracture-filling minerals that may undergo reactions with the leachate. Chalcedony was assumed to comprise 10 wt% of the host rock. In contrast, the amount of fracture-filling amorphous silica was considered to be trivial and was set to 0.1 wt%. However, since tuff contains large quantities of amorphous materials such as volcanic glass, a case was implemented in which the amount of amorphous silica was increased from 0.01 wt% to 10 wt%. The quantity of clay minerals was assumed to be 0.1 wt%, and the evaluation was performed using data for montmorillonite. The minerals considered in each barrier are summarized in Table 4.4.3-2. Here, it is considered that the reactivity of minerals other than those that react with alkalis is extremely low. Since the dissolution of crystalline minerals in the host rock is slow and when the flow velocity of groundwater is fast, equilibrium will not be achieved and it was considered that the quantity dissolved would be controlled by the dissolution rate. Hence, the dissolution rate was considered in the case of chalcedony. On the other hand, since amorphous silica has a high reactivity, it was treated as being at instantaneous equilibrium. Similarly, the model regarded montmorillonite dissolution to
reach equilibrium instantaneously.

In this evaluation concerning the spreading of an alkali plume from the disposal facility, both crystalline and sedimentary type host rocks were considered. Both rock types were treated as porous media, but each rock type was considered to have a different porosity. Furthermore, an evaluation case was implemented for groundwater with the same composition as sea water, as in the evaluation described in Section 4.4.2. The parameters used in this analysis, including the hydraulic characteristics of the engineered barrier and host rock, are shown in Table 4.4.3-3.

Figure 4.4.3-1 System for the analysis of hyperalkaline alteration in the surrounding host rock
### Table 4.4.3-1 Minerals considered in each barrier material

<table>
<thead>
<tr>
<th>Barrier material</th>
<th>Initial mineral</th>
<th>Secondary mineral</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cement material</td>
<td>Portlandite</td>
<td>C₃ASH₄</td>
</tr>
<tr>
<td></td>
<td>C-S-H gel</td>
<td>C₂ASH₈</td>
</tr>
<tr>
<td></td>
<td>C₃AH₆</td>
<td>C₃AS₃</td>
</tr>
<tr>
<td></td>
<td>Ettringite</td>
<td>Kaolinite</td>
</tr>
<tr>
<td></td>
<td>Brucite</td>
<td>Pyrophylite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Friedel salt</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Calcite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Chalcedony</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Analcite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Laumontite</td>
</tr>
<tr>
<td>Host rock</td>
<td>Chalcedony</td>
<td>C-S-H gel</td>
</tr>
<tr>
<td></td>
<td>Amorphous silica</td>
<td>C₃ASH₄</td>
</tr>
<tr>
<td></td>
<td>Calcite</td>
<td>C₂ASH₈</td>
</tr>
<tr>
<td></td>
<td>Montmorillonite</td>
<td>C₃AS₃</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Brucite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Analcite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Laumontite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cristobalite</td>
</tr>
</tbody>
</table>

### Table 4.4.3-2 Physical properties and parameters values used in the analyses of alkali constituents

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Crystalline rock</th>
<th>Sedimentary rock</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability coefficient</td>
<td>m s⁻¹</td>
<td>4×10⁻⁶</td>
<td></td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>m² s⁻¹</td>
<td>8×10⁻¹⁰</td>
<td>1.2×10⁻⁹</td>
</tr>
<tr>
<td>Effective diffusion coefficient in the cement</td>
<td>m² s⁻¹</td>
<td>8×10⁻¹¹</td>
<td></td>
</tr>
<tr>
<td>Effective diffusion coefficient in the host rock</td>
<td>m² s⁻¹</td>
<td>1.2×10⁻⁹</td>
<td></td>
</tr>
<tr>
<td>Engineered barrier shape</td>
<td>Target disposal facility</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Natural barrier</td>
<td>Coefficient of hydraulic conductivity</td>
<td>m s⁻¹</td>
<td>1×10⁻⁹</td>
</tr>
<tr>
<td></td>
<td>Porosity</td>
<td>–</td>
<td>0.02</td>
</tr>
<tr>
<td></td>
<td>True density</td>
<td>kg m⁻³</td>
<td>2,700</td>
</tr>
<tr>
<td></td>
<td>Hydraulic gradient</td>
<td>m m⁻¹</td>
<td>0.01</td>
</tr>
</tbody>
</table>

*1: The coefficient of hydraulic conductivity of the cementitious material is based on the case in Section 4.4.4.2(2)c that considered fractured concrete.

### Analytical results

(2) Analytical results

For the case in which the groundwater is assumed to be fresh water and the rocks are taken to be crystalline, after 10,000 years the spatial distribution of solutes, and the volumetric fractions of solid phases are as shown in Figures 4.4.3-2 and 4.4.3-3, respectively. The pH variations are shown in Figure 4.4.3-4, and the spatio-temporal variations in pH and porosity are shown in Figure 4.4.3-5.
Cristobalite was generated as a secondary mineral during the alteration of the host rock. Additionally, in the host rock near the disposal facility, C-S-H gel with a low Ca/Si ratio (Ca/Si = 0.4) was formed under conditions in which amorphous silica was dissolved. In the area where amorphous silica disappeared, chalcedony dissolved and the Ca/Si ratio gradually increased, and C-S-H gel with Ca/Si = 0.9 was precipitated.

When the alkali constituents Na and K were transported, the pH in the host rock attained a value of about 11 as shown in Figure 4.4.3-2. However, when Na and K had dissipated after several 10s of thousands of years, the pH fell to 10.0 owing to equilibration with the C-S-H gel (Ca/Si = 0.4) that was generated during amorphous silica dissolution. In the area where amorphous silica disappeared, the pH became 10.8 owing to the fluid equilibrating with the C-S-H gel (Ca/Si = 0.9) that was generated during chalcedony dissolution. A change in porosity, owing to the different molar volumes and densities of these minerals, was calculated to occur only near the cement/host rock boundary, but this change was found to be insignificant.

The following results were given by analyses using different groundwater types (meteoric-type groundwater and saline ground water cases), rock types (crystalline rocks and sedimentary rocks) and quantities of amorphous silica (0.01 wt%–10 wt%). In the case with saline groundwater, after the free alkali component with high Na concentrations had dissipated, analcite was formed near the disposal facility owing to cristobalite dissolution. In the sedimentary rock case, the secondary minerals were also generated on the upstream side. The reason is that diffusive transport became prominent, because the porosity is large and the flow velocity of groundwater becomes small. (In the sedimentary rock case, because the actual groundwater flow rate was different, dispersive transport became prominent and secondary minerals were also generated on the upstream side.)

![Figure 4.4.3-2 Predicted distribution of solutes in the liquid phase after 10,000 years](image)

(freshwater type groundwater, crystalline rock)
Figure 4.4.3-3 Predicted variations in the volumetric fractions of solid phases after 10,000 year (freshwater type groundwater; crystalline rock)  Note 1: C-S-H gel is denoted by CSH (Ca/Si ratio).

Figure 4.4.3-4 Variation of pH (freshwater type groundwater, crystalline rock)
4.4.3.4 Summary

In order to evaluate the alkali alteration of the host rock surrounding the disposal facility, the reactivity of the rock to hyperalkaline leachates was investigated using published literature and experimental results. Additionally, the alteration of host rock and the dispersion of the alkali region were evaluated by a coupled analysis of chemical reactions and mass transport. The investigation showed the possibility that poorly crystalline minerals would dissolve and that secondary minerals such as C-S-H gel would form. The results that are most relevant for facilitating coupled simulations of chemical reactions and nuclide transport are those that show the production of C-S-H phases and secondary minerals in the rocks surrounding the repository. These minerals have a high capacity to sorb nuclides. Furthermore, it is considered that significant variations in porosity occur only near to the disposal facility. A decrease in porosity might occur in the region where there is selective precipitation of secondary minerals.

From these results, it is considered that overall, in the host rock surrounding the disposal facility, alkali constituents do not significantly influence pathways for nuclide migration. However, there is insufficient knowledge about variations in sorption coefficients in the surrounding host rocks, constraints on the matrix diffusion of nuclides, and constraints on mass transport owing to porosity reduction. Hence, additional evaluations of these issues are needed in future.

4.4.3.5 Future issues

In the analysis carried out during the present evaluation, there are uncertainties due to insufficient knowledge and due to issues receiving insufficient consideration. Consequently, issues that are considered to be important for future evaluations are given below:
• The adequacy of the mineral alteration scenario, such as the specification of initial and secondary minerals in the host rock, should be evaluated.
• The inhomogeneity of the geological medium should be considered, particularly the effects of alkali-host rock reactions on the fractured media model. In situ experiments have been carried out to investigate the effects of hyperalkaline leachates on fractured media (Mäder et al., 2004). Further, similar evaluations are necessary in future to improve confidence and provide more detailed information.
• In order to evaluate the variations in pore structures that are caused by mineral alteration in the surrounding rocks, the long-term mechanical creep behaviour of the host rock should also be considered.
• Changes in the pore structure of the geological medium that are caused by hyperalkaline leachate alteration should be confirmed. Mass transport parameters should be obtained.

4.4.4 Hydraulic conditions of the near-field

The hydraulic conditions in the near-field are important for evaluating nuclide migration, groundwater chemistry and engineered barrier alteration. Just after closure, the surrounding groundwater will saturate the disposal facilities. Ando et al. (2005) evaluated this re-saturation by using a 2 phase flow, gas-liquid, model. They reported that the disposal facility in the reference geological condition would be saturated by groundwater within 500 years after closure. The effects of re-saturation on nuclide migration are evaluated in Section 4.5.

The Darcy flow rate of groundwater in the facility and the groundwater flow volume from the excavated damage zone, EDZ, were estimated. The estimated values were used in the nuclide migration analysis 4.5.

4.4.4.1 Analytical assumptions

The preconditions of the analysis are described below.

• Modelling of host rock:

  Most rocks in Japan are fractured. Moreover, Neogene sedimentary rocks can be broadly divided into fractured and porous host rock. A fracture network model which considers heterogeneous fracture directions, sizes, frequencies, spatial distributions, and permeabilities was used to evaluate the hydraulic field (JNC, 2000). The average of logarithmic transmissivity was specified up to $10^{-10} \text{m}^2 \text{s}^{-1}$, as given in Section 1.3. The hydraulic conductivity of fractured host rock in the reference case of the H12 report was approximated as $2 \times 10^{-10} \text{m s}^{-1}$ (Sawada et al., 1999). The groundwater flow volume in the EDZ was estimated using a 2-D homogeneous steady-state groundwater flow model.

• Direction of groundwater flow:

  The direction of groundwater flow will not change after closure of the disposal facility.
Consideration of alteration of the EBS:

Cementitious material is used in the disposal facility. The changes in the hydraulic characteristics of the cementitious material are considered. For groundwater flow calculation, parameters are selected considering the alteration of the EBS. Time dependency of parameters are not considered in the calculation.

4.4.4.2 Model and data for hydrogeological analyses

(1) Mathematical modeling

a. Governing equations

In the general hydraulic analysis, the tunnels of the disposal facility are assumed for simplicity to be of circular cross-section. Hence, a cylindrical 2 dimensional mathematical model is used.

The equation for steady-state groundwater flow is as follows, where the Darcy flow velocity, $v$ of the groundwater is based on Darcy’s Law:

$$v = (v_r, v_\theta) = K \left( \frac{\partial P}{\partial r}, \frac{1}{r} \frac{\partial P}{\partial \theta} \right)$$

(4.4.4.2-1)

$$\frac{1}{r} \frac{\partial}{\partial r} (rv_r) + \frac{1}{r} \frac{\partial}{\partial \theta} (v_\theta) = 0$$

(4.4.4.2-2)

Here, $K$ is the hydraulic conductivity and $P$ is the hydraulic head. $P$ is a function of $\theta$ and $r$.

b. Boundary conditions

The boundary condition is specified as follows if the centre of the disposal facility is the origin and the disposal tunnel has a circular cross-section.

• Centre of disposal tunnel ($r = 0$)

$$P = 0$$

• Furthest distance from disposal facility ($r >> \text{radius of repository tunnel}$)

$$P = -hr \cos(\theta)$$

Here, $h$ is the hydraulic gradient.

c. Analysed groundwater flux and average Darcy flow velocity in each area

The following analysis is given for the above hydraulic head, $P$ in the governing equations. Here, $A$ and $B$ are constants which depend on the radius of the disposal tunnels, the coefficient of hydraulic conductivity and the hydraulic gradient.

$$P(r, \theta) = \left[ Ar + B \frac{1}{r} \right] \cos(\theta)$$

(4.4.4.2-3)

The groundwater flow volume $Q$, which passes through each area is given by the following formula:
\[
Q_r = k \int_{-\pi/2}^{\pi/2} \frac{dP(r, \theta)}{dr} r \, d\theta
\]  
(4.4.2-4)

In this analysis, the value of \( Q_r \) is for 1/2 the internal surface area of each region (the external surface area of the waste packages in the part with waste packages), and is regarded as an average Darcy flow.

(2) Data

a. Hydrological gradient

A hydraulic gradient of 0.01 in the plane of the model is used. The hydraulic gradient has a linear relationship with respect to the Darcy flow velocity of groundwater.

b. Radius of repository tunnels in the disposal facility

In current repository designs being considered in Japan tunnel diameters range from 9 to 12 m. Here, 12 m is used as this would have a large groundwater flow volume.

c. Hydraulic conductivity

- Host rock

A hydraulic conductivity of \( 2 \times 10^{-10} \text{ m s}^{-1} \) is specified, based on the fracture network model described before.

- Cementitious material

The cementitious material is gradually leached over a long time period, and simultaneously its hydraulic conductivity changes. In order to evaluate the long-term variation, Mihara et al. (2003) examined the relationship between the hydraulic conductivity \( (K \text{ [ms}^{-1}] \) and porosity \( (\theta [-]) \), based on flow-through experiments using hardened cement samples. If the porosity of a sample that has been altered by flowing water is known, the hydraulic conductivity can be specified. The observed relationship which is reported by Mihara et al. is shown in Figure 4.4.4-1.
It is assumed that the porosity of cementitious material is 0.19 in Section 4.4.2 (Table 4.4.2.2-1) and the hydraulic conductivity of $5 \times 10^{-11}$ ms$^{-1}$. However, this hydraulic conductivity is appropriate for non-fractured cement mortar. Over a long period, the porosity is considered to become 0.46 when the paste component of the cement mortar has been leached away. In this case, the hydraulic conductivity is specified to be $10^{-5}$ ms$^{-1}$, which is in the same order as that of very fine-grained sand (e.g. Imai, 1985). Moreover, in the case where there is some fracturing of the initial cement mortar, a hydraulic conductivity of $4 \times 10^{-6}$ ms$^{-1}$ is assumed in order to keep the actual flow velocity of groundwater in the cement mortar uniform. Actually, in cases where there are large amounts of Ca(OH)$_2$ or C-S-H gel, and calcite precipitation is caused by reaction with carbonate ions in the groundwater, these fractures may self-heal. However, this process cannot be evaluated quantitatively at present and therefore the hydraulic conductivity is assumed to be the same as that of sand.

The hydraulic conductivity described above are summarised in Table 4.4.4-1.

Table 4.4.4-1 Hydraulic conductivity specified for cement mortar

<table>
<thead>
<tr>
<th></th>
<th>Intact cement mortar</th>
<th>Fractured cement mortar</th>
<th>Cement mortar from which cement paste has been leached</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity (−)</td>
<td>0.19</td>
<td>0.19</td>
<td>0.46</td>
</tr>
<tr>
<td>Hydraulic conductivity (m s$^{-1}$)</td>
<td>$5 \times 10^{-11}$</td>
<td>$4 \times 10^{-6}$</td>
<td>$10^{-5}$</td>
</tr>
</tbody>
</table>
• Bentonite

The backfill is assumed to be a Na bentonite initially. However, Ca-type bentonite might be formed owing to the influence of cementitious material. Additionally, in the long term, smectite in the bentonite might dissolve. Hence, it is assumed that, in cases where Ca-type smectite is altered, dissolved smectite is replaced by another mineral of the same density. Ito et al (2005) specified the hydraulic conductivity ($K$ [ms$^{-1}$]) using the following formula, which includes the equivalent ion concentration of pore water ($C_i$ eq dm$^{-3}$), exchangeable Na proportion in bentonite (ESP [−]), and smectite void ratio ($e_{sme}$ [−]). Using this formula, the hydraulic conductivity was specified for Na bentonite using an ESP of 0.85, and for Ca bentonite using an ESP of 0.15. The specified coefficients of hydraulic conductivity are shown in Table 4.4.4.2. In the following formula, when the smectite in the bentonite dissolves ($e_{sme}$ becomes large), the hydraulic conductivity becomes $10^{-5}$ ms$^{-1}$.

\[
K = 10^{1.30C_i + 3.48C_i} K_0
\]

\[
K_0 = \begin{cases} (0.91 - 1.57 \cdot ESP + 2.00 \cdot ESP^2) \times 10^{-13} \times e_{sme}^{7.44-5.69-ESP} \cdot \ldots \cdot e_{sme} \leq 7.0 \\ (0.91 - 1.57 \cdot ESP + 2.00 \cdot ESP^2) \times 10^{-13} \times 7.0^{7.44-5.69-ESP} \left(\frac{e_{sme}}{7.0}\right)^{11.4} \cdot \ldots \cdot 7.0 < e_{sme} \end{cases}
\]

Table 4.4.4.2 Values specified for the hydraulic conductivity of the backfill

<table>
<thead>
<tr>
<th></th>
<th>Initial value</th>
<th>Ca-type bentonite</th>
<th>Dissolution of smectite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity (−)</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>Hydraulic conductivity (ms$^{-1}$)</td>
<td>$10^{-12}$</td>
<td>$2 \times 10^{-11}$</td>
<td>$10^{-5}$</td>
</tr>
</tbody>
</table>

• EDZ

In the H12 report, it is assumed that the repository tunnels are excavated using a tunnel boring machine. In this case, based on actual measurements, the hydraulic conductivity of the host rocks in the region affected by drilling is estimated to increase by about one order of magnitude. In the disposal of TRU waste, it is assumed that the NATM (New Austrian Tunnelling Method) will be used, because it produces a repository tunnel with a large cross-section. In this case, rock bolts are used in the tunnels, and the hydrogeological variations in the region affected by excavation become complex. The sensitivity of the groundwater flux to these variations was investigated by assuming that the coefficient of hydraulic conductivity in the excavated area is between 0.1–10,000 times that of the host rocks. The results are shown in Figure 4.4.4.2. If the increase in hydraulic conductivity is more than 100 times, the sensitivity of
the flux becomes small. Hence, the hydraulic conductivity in the region affected by tunnelling was specified to be 100 times that of the host rocks.

![Figure 4.4.4-2 Relationship between the groundwater flux and the increase in hydraulic conductivity of the region affected by excavation](image)

(The hydraulic conductivity of the host rock is assumed to be $2 \times 10^{-10}$ m s$^{-1}$ and the width of the region affected by excavation is assumed to be 3 m)

d. Analysed geometry

The radius of the repository tunnel is 6m as described previously. It is assumed that a layer of 1m of bentonite backfill will be present in the disposal concept. Cement mortar is present in the inner part with a radius of $< 5$ m. In the disposal concept without bentonite backfill, it is assumed that the inside of the repository tunnel is cement mortar. It is also assumed that the rock bolts are 3m long and extend for the width of the zone affected by excavation. Each analysed geometry is shown in Figure 4.4.4-3.
(3) Analytical cases

The specifications for the analytical cases are summarized in Table 4.4.4-3. In these cases, the average Darcy flow rates and the groundwater fluxes in the region affected by excavating a repository shaft of unit length, were calculated.

Table 4.4.4-3 Summary of analytical cases

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Cement mortar</th>
<th>Bentonite backfill</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-1</td>
<td>Intact cement mortar</td>
<td>Initial emplacement</td>
</tr>
<tr>
<td>1-2</td>
<td></td>
<td>Ca type formation</td>
</tr>
<tr>
<td>1-3</td>
<td></td>
<td>Smectite dissolution</td>
</tr>
<tr>
<td>2-1</td>
<td>Fractured cement mortar</td>
<td>Initial emplacement</td>
</tr>
<tr>
<td>2-2</td>
<td></td>
<td>Ca type formation</td>
</tr>
<tr>
<td>2-3</td>
<td></td>
<td>Smectite dissolution</td>
</tr>
<tr>
<td>3-1</td>
<td>Degraded (leached) cement mortar</td>
<td>Initial emplacement</td>
</tr>
<tr>
<td>3-2</td>
<td></td>
<td>Ca type formation</td>
</tr>
<tr>
<td>3-3</td>
<td></td>
<td>Smectite dissolution</td>
</tr>
<tr>
<td>1</td>
<td>Intact cement mortar</td>
<td>Concept without</td>
</tr>
<tr>
<td></td>
<td></td>
<td>bentonite backfill</td>
</tr>
<tr>
<td>2</td>
<td>Fractured cement mortar</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Degraded (leached) cement mortar</td>
<td></td>
</tr>
</tbody>
</table>
4.4.4.3 Analytical results

The analytical results are summarised in Table 4.4.4-4. Here, values are selected by considering the long-termed alteration of cement mortar and bentonite backfill. The groundwater flux in the region affected by excavation is shown to be about 0.0022 m$^3$/y/m in each case. Based on Table 4.4.4-4, Figure 4.4.4-4 shows the relationships between Darcy flow velocities in the cement mortar and bentonite backfill, and the permeabilities of the backfill. For reference, the Darcy flow velocity in the host rocks is also shown. In most cases, the Darcy flow velocity in both materials increases with increasing permeability of the bentonite. If the hydraulic conductivity of the cement mortar and bentonite becomes similar to sand (10$^{-5}$ m s$^{-1}$), the Darcy flow velocity is about 3 times that in the host rocks. However, if the hydraulic conductivity of the cement mortar is 5×10$^{-11}$ ms$^{-1}$ and that of the bentonite is 10$^{-5}$ ms$^{-1}$, the Darcy flow velocity of cement mortar becomes as low as 10$^{-9}$ ms$^{-1}$. It is unexpected that, as the hydraulic conductivity of the bentonite becomes large, that of the cement mortar becomes small. Possibly, the existence of a high permeability zone outside the repository tunnel means that the Darcy flow velocity in the repository tunnel might decrease. A disposal concept in which gravel ballast with high permeability is placed outside the repository tunnel, has been evaluated in other researchers (McKinley et al., 2001).

<table>
<thead>
<tr>
<th>Region affected by drilling</th>
<th>Hydraulic conductivity (ms$^{-1}$)</th>
<th>Darcy flow velocity (ma$^{-1}$)</th>
<th>Flux (m$^3$ a$^{-1}$ m$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Cement mortar</td>
<td>Backfill material</td>
<td>Cement mortar</td>
</tr>
<tr>
<td>1-1</td>
<td>5.0×10$^{-11}$</td>
<td>1.0×10$^{-12}$</td>
<td>1.3×10$^{-7}$</td>
</tr>
<tr>
<td>1-2</td>
<td>5.0×10$^{-11}$</td>
<td>2.0×10$^{-11}$</td>
<td>9.0×10$^{-7}$</td>
</tr>
<tr>
<td>1-3</td>
<td>5.0×10$^{-11}$</td>
<td>1.0×10$^{-5}$</td>
<td>5.7×10$^{-9}$</td>
</tr>
<tr>
<td>2-1</td>
<td>4.0×10$^{-6}$</td>
<td>1.0×10$^{-12}$</td>
<td>1.5×10$^{-7}$</td>
</tr>
<tr>
<td>2-2</td>
<td>4.0×10$^{-6}$</td>
<td>2.0×10$^{-11}$</td>
<td>2.9×10$^{-6}$</td>
</tr>
<tr>
<td>2-3</td>
<td>4.0×10$^{-6}$</td>
<td>1.0×10$^{-5}$</td>
<td>1.4×10$^{-4}$</td>
</tr>
<tr>
<td>3-1</td>
<td>1.0×10$^{-5}$</td>
<td>1.0×10$^{-12}$</td>
<td>1.5×10$^{-7}$</td>
</tr>
<tr>
<td>3-2</td>
<td>1.0×10$^{-5}$</td>
<td>2.0×10$^{-11}$</td>
<td>2.9×10$^{-6}$</td>
</tr>
<tr>
<td>3-3</td>
<td>1.0×10$^{-5}$</td>
<td>1.0×10$^{-5}$</td>
<td>1.7×10$^{-4}$</td>
</tr>
<tr>
<td>1</td>
<td>5.0×10$^{-11}$</td>
<td>–</td>
<td>1.1×10$^{-6}$</td>
</tr>
<tr>
<td>2</td>
<td>4.0×10$^{-6}$</td>
<td>–</td>
<td>1.7×10$^{-4}$</td>
</tr>
<tr>
<td>3</td>
<td>1.0×10$^{-5}$</td>
<td>–</td>
<td>1.7×10$^{-4}$</td>
</tr>
</tbody>
</table>
In the case that soft rocks are assumed, the configuration of the disposal tunnels might change owing to long-term creep deformation. This kind of host rock deformation is considered in Section 3.3.2.2. However, the effect of deformation of disposal facility on the Darcy flow velocity in the engineered barrier is assumed to be small.

4.4.4.4 Summary

To consider the long-term alteration of engineered barrier materials, data for alteration have been assumed. The effects of this alteration on the hydraulic characteristics of the near-field have been evaluated using a 2 dimensional stationary hydrogeological model.

The results are summarized as follows.

- The Darcy flow velocity of groundwater in the engineered barrier increases as the capacity of the bentonite backfill to prevent water flow decreases. Even if the bentonite changes to Ca-type, the Darcy flow velocity of groundwater in the engineered barrier is 1 order lower than that of the host rock. Additionally, in the case that the permeability of the bentonite becomes similar to that of sand owing to alteration, the Darcy velocity of groundwater in the engineered barrier reaches 2.5 times of that in the host rock.
- The groundwater flux in the region affected by tunnel excavation is about $0.002 \text{ m}^3\text{a}^{-1}\text{m}^{-1}$ even if considering the long-term alteration of the engineered barrier.
4.4.4.5 Future issues

This evaluation used a simple model, based on knowledge from the H12 report. In order to evaluate the hydrogeology of the near-field in more detail, the following is needed:

- Evaluation the groundwater fluxes in regions affected by excavation in various other rock types (i.e. not just the rock types examined in this report).
- Further evaluations for TRU waste disposal taking into account progress with hydrogeological research at Tono (crystalline rocks) and Horonobe (sedimentary rocks).

4.4.5 Effects of colloids

Colloids exist in all natural waters (e.g. McCarthy et al., 1993) and it is assumed that colloids will be produced by EBS components and wastes and as a result of chemical disturbances. It is assumed that the migration of radionuclides that are bound to colloids will be quite different from the migration of radioactive nuclides are present in groundwater as ions. This migration process is called Colloid-Facilitated Transportation (hereafter, “CFT”) (e.g. Ryan et al., 1996).

This section evaluates the effects of colloids that have been generated in the engineered barrier and natural barrier of a disposal facility. Considerable information concerning nuclide migration analysis is summarised.

4.4.5.1 Effect of colloids in the EBS

The types of colloids that are generated by constructing the disposal facility and waste emplacement are summarised here. The behaviour of colloids in the EBS is evaluated by means of nuclide migration analysis modelling.

(1) Colloids generated/pre-existing in the EBS

The main types of colloids that are generated or pre-existing in the EBS are as follows (Avogadro et al., 1984; Ramsay, 1988; Fujita et al., 1997):

1. true colloids such as actinides, etc.
2. corrosion products of metals and glass
3. clay minerals such as bentonite
4. cement colloids

It is assumed that organic polymers such as cellulose and its decomposition products in the waste may form complexes with radionuclides and affect transport in a similar fashion to colloids. These effects are described in Section 4.4.6. Additionally, it is also considered that similar effects are caused by microbes and metabolic materials produced by microbes. These effects are described in Section 4.4.7.
(2) Colloid behaviour in the EBS and an assessment of its consequences

In the EBS, the types of colloids are limited and the chemical and hydraulic features of the EBS can be understood. Hence, the behaviour of colloids in the EBS was evaluated for plausible colloids generated during construction of the disposal facility and waste emplacement. The effects on nuclide migration were estimated.

Degueldre et al. (1993) reported that the significance of the CFT effect is determined by the following conditions: ① whether or not colloids are generated or pre-existing and whether their concentrations are significant or not, ② whether the colloids are stable or not, ③ whether the colloids are migratory or not, and ④ whether the colloids adsorb the radionuclides or not. The CFT effect is important when all these conditions apply.

The features of colloids and the media within which they occur (materials composing the EBS and the far-field) are varied and complex. However, if any of the above conditions do not apply, it is assumed that colloids would have insignificant effects on radioactive waste disposal. Taking these criteria into account, about the understanding of colloid behaviour in the EBS is described and the importance of the effects of colloids is assessed.

a. Colloid mobility

As shown in Section 3.2.2 in the geological repository for TRU waste two types of disposal concept are evaluated: a case with and without bentonite buffer material. In the former, it is expected that the bentonite buffer acts as a barrier to colloid migration. Colloids are filtered because the bentonite pores are smaller than the colloids. In this case, colloids are not considered to affect nuclide migration because they become immobile in the buffer. Filtration experiments using compacted bentonite showed that the colloids can be filtered if the buffer material is composed of bentonite with a dry density greater than 800 kg/m³, as shown in Figure 4.4.5-1 (Kurosawa et al., 1997, 1999a).

![Figure 4.4.5-1 Filtration effects of buffer on colloids (Kurosawa et al., 1999a)](image-url)

Figure 4.4.5-1 Filtration effects of buffer on colloids (Kurosawa et al., 1999a)
The case where the bentonite buffer material has been altered in a high-pH environment has also been evaluated (Kurosawa et al., 2002). Under highly alkaline conditions (a mixed solution of NaOH-KOH-Ca(OH)$_2$ with a pH of about 14, which is similar to the initial liquid from cementitious material), bentonite buffer material is altered by dissolution of smectite and generation of secondary minerals. Hence, depending on the change in pore structure of the bentonite and fracture generation, the filtration of colloids may decrease. However, as shown in Section 4.4.2, there is only a low possibility that all the bentonite buffer material will be altered and retention of some degree of filtration is therefore expected.

b. Generation, stability and concentration of colloids

In the disposal concept without a layer of bentonite buffer material, the above colloid filtration effect will not occur. In this case, it is considered that pre-existing colloids that originate in the cementitious material and the generation of new colloids is important. The stability and concentration of these colloids must be considered. Fujita et al. (2003) reported that colloids are destabilised as Ca concentrations increase and that, consequently, colloid concentrations decrease. Wieland and Van Loon (2003) investigated the relationship between ionic strength and colloid mass concentration in the groundwater (Figure 4.4.5-2). In accordance with previous work on colloid stability, their results indicated that colloid mass concentrations decrease with increasing ionic strength. This trend is consistent with the report of Fujita et al. (2003). Moreover, they reported that the upper limit of colloid mass concentration in the cement pore water is $1 \times 10^{-4}$ kg/m$^3$ (this value is for synthetic cement pore water with pH 13.3, which simulates cement pore water during the early
stages of emplacement, see above). Natural colloid concentrations of $0.6 - 1.9 \times 10^{-4} \text{ kg/m}^3$ were observed in a highly alkaline groundwater environment at Maqarin, Jordan (Wetton et al., 1998).

There are also reports that colloids were not observed when cementitious phases such as C-S-H and ettringite were leached experimentally for three months (Iwaida et al., 1999). However, there are other reports that disagree and that state that colloids may originate in highly alkaline cement. Hence, there is a need to evaluate this in future. However, it was assumed that colloid concentrations would be low due to the relatively high ionic strength of the cement pore water. Hence an upper limit of $1 \times 10^{-4} \text{ kg/m}^3$ was assumed. Additionally, when emplacing the layer of bentonite buffer material, colloids might be formed by the dispersion of montmorillonite and accompanying minerals into the groundwater. Based on experimental results, it is assumed that, for colloids to be generated from unaltered bentonite material due to the shear stress exerted by groundwater flow, the groundwater flow rate must be more than $10^{-5} - 10^{-4} \text{ m s}^{-1}$ (Pusch, 1987; Kurosawa et al., 1999b; Kanno and Matsumoto, 1997). However, following a recent evaluation (Matsumoto and Tanai, 2005), it was estimated that the critical flow rate for erosion to occur is smaller than $2 \times 10^{-6} \text{ m s}^{-1}$ under fresh groundwater conditions. In groundwater that is similar to seawater, the critical flow rate is estimated to be greater than $8 \times 10^{-6} \text{ m s}^{-1}$. The conditions under which colloids may be generated from bentonite are strongly dependent on the composition of the fluid phase. Hence, the possibility that colloids will be generated from the bentonite used as a buffer material cannot be ruled out.

The colloids that are generated in the bentonite are treated in the same way as colloids in the natural barrier. This approach is taken since the colloids are generated at the boundary between the bentonite layer and the surrounding host rock and are transported into the natural barrier.

c. Influence of nuclide sorption on colloids

There is little information about the composition and sizes of colloids that may sorb radionuclides. Hence, it is difficult to specify a range of distribution coefficients for each radionuclide. In order to calculate the effect of colloids on sorption on mineral surfaces, the distribution coefficient in the presence of colloids is defined by (Wieland, 2001)

$$R_{d, eff} = \frac{R_d}{1 + R_c m_c} = \frac{R_d}{F_{red}} \text{ [m}^3/\text{kg]}$$  (4.4.5.1-1)

Here, $R_d$ is the distribution ratio [m$^3$/kg] for radionuclides that are sorbed on the solid phase under conditions where there are no colloids. $R_c$ is the distribution ratio [m$^3$/kg] between the colloid and liquid and $m_c$ is the mass concentration [kg/m$^3$] of colloids. Using this formula, the effect of colloids on nuclide sorption is presented using a coefficient describing the decrease in sorption or sorption reduction factor ($F_{red}$). The relationship between the colloid mass concentration and the sorption reduction factor is shown in Figure 4.4.5-3. From these results, if an upper colloid mass concentration in cement pore water of $10^{-4}$ kg/m$^3$ is assumed, the effect on the distribution ratio is very limited.
As described previously, there is insufficient knowledge about colloid behaviour in the EBS and available knowledge has not been summarised systematically. However, based on the above appraisal, during barrier construction in a TRU waste disposal facility the following colloid effects are expected. It is considered that colloids that are generated within the barrier system will be prevented from being transported by filtration. A significant decrease in filtration due to alteration of smectite is not expected to occur. It is predicted that cement pore water will have low concentrations of colloids owing to its relatively high ionic strength. Furthermore, considering the sorption of radionuclides onto colloids, the effects of colloids on nuclide transport are assumed to be limited.

4.4.5.2 Effects of colloids in the natural barrier

The chemical composition, geometric shape, configuration and grain size of colloids in groundwater depend significantly on the geology and geochemical conditions of the aquifer. Hence, it is difficult to discuss the effects of colloids quantitatively before selecting a disposal area and geological environment. Moreover, since the disposal facility will be constructed in a deep underground, there will be chemical perturbations that will include steep gradients of pH and Ca concentration. This disturbance will affect the generation of colloids, but a quantitative evaluation cannot be performed at the present stage. Hence, in this section, the method for handling the effects of colloids in the natural barrier is evaluated by summarising available information on colloidal material in groundwater.
(1) Plausible colloids in the natural barrier

Natural colloids in groundwater are classified into inorganic colloids, organic colloids such as humic materials and biocolloids. Inorganic colloids are composed of clay minerals, such as the aluminosilicates kaolinite, gibbsite and illite, and oxides of iron and manganese (Ryan et al., 1996). Humic materials are metabolites of plants and microbes. Humic materials are acidic, owing to the presence of carboxyl and phenol groups, and they form complexes with high valence cations. The average molar weight is from several tens of thousands to several hundred thousand. Metabolic materials are generated by microbes and may behave as colloids, but there is little information. It is reported that most of the colloids sampled from natural groundwater (especially in crystalline rocks) are inorganic. Hence, the evaluation of colloids is performed by considering inorganic colloids (JNC, 2000). There is an alternative view that the effects of organic colloids, such as chemically active humic materials, should also be evaluated (Ryan et al., 1996; Kim, 1993). However, it is important to consider how to specify conditions for the radionuclide migration analysis, taking into account the fact the colloids will depend on the actual geological environment and chemical conditions. Therefore, a reported colloid concentration of $0.01 - 1 \times 10^{-3} \text{ kg/m}^3$ in a geological aquifer spring in Switzerland is used to support the specification of conditions (Figure 4.4.5-2).

Except for the pre-existing colloids in the disposal area, it is reported that colloids are generated by chemical perturbations (changes in ionic strength, pH, etc.) and physical disturbances (pumping and increasing groundwater flow in fractures, etc.; McCarthy et al., 1993). Hence, it is not possible to rule out the possibility that colloids will be generated by such disturbances during the construction of a disposal facility in a geological formation. As described in Section 4.4.5.1, there is a possibility that colloids will be generated from bentonite by erosion (Matsumoto and Tanai, 2005). The effects of these colloids in the natural barrier close to the disposal facility need to be evaluated. It is also considered that there will be steep gradients in the concentrations of constituents such as OH$^-$ and Ca, which are leached from cementitious material near the disposal facility. Secondary minerals will also be generated. It is considered that these factors will influence colloids and should be considered in more detailed evaluations in the future.

(2) Concept for assessing the effects of colloids in the natural barrier

It is considered that the effects of colloids in the natural barrier should be evaluated in basically the same way as in the EBS. The effects of colloid generation, concentrations, stability, mobility and nuclide sorption capability should be considered. However, various types of colloid could plausibly occur in the natural barrier, depending on the geological conditions. Hence, the effects should be evaluated taking into account site information.

Numerous laboratory and field investigations of colloid migration have been undertaken and there has been extensive modelling of colloid transport. Investigations of filtration, sorption of colloids on fracture surfaces and physical trapping of colloids in fractures have also been carried out. However, these evaluations contain significant uncertainties since the chemical, physical and hydraulic characteristics of
host rocks are site-specific and depend on the geological environment conditions and their heterogeneities. Due to the considerable range of colloidal characteristics, lack of information and heterogeneities in the chemical/physical/hydraulic properties of the medium for colloid transport, quantitative evaluations of colloid behavior in natural barriers cannot be performed at present.

The effects of colloids on nuclide migration are estimated by considering the CFT effect, since colloids behave as radionuclide carriers in a different way to ions. For example, in the H12 report (JNC, 2000), the evaluation assumed that colloid transportation occurred without effects such as matrix diffusion and sorption onto fracture surfaces. Uncertainty is inevitable in any evaluation of the effects of colloids in natural barriers. However, it is possible to estimate the colloid effect in the natural barrier by taking these uncertainties into account.

4.4.5.3 Summary
The effects of colloids on nuclide migration are classified into effects within the EBS and effects within the natural barrier. The treatment is based on a summary of information about colloid behaviour and a summary of information that must be considered by a nuclide migration analysis. The effects of colloids in the EBS are estimated to be small, owing to filtration by bentonite, low concentrations and small influences on sorption on the rock. The effects of colloids in the natural barrier are difficult to evaluate due to the wide variety of colloid characteristics and a lack of information about the transport properties and heterogeneity of the geological medium. However, although the transport behaviour of colloids and its effects cannot be determined precisely, it is possible to estimate the effects of CFT on transport.

4.4.5.4 Future issues
As described previously, there is uncertainty in the evaluation of colloid behaviour in the natural barrier because of insufficiency of knowledge. In future, the following issues should be considered.

- Clarification of the conditions under which colloids are generated in groundwater near the disposal facility
- Accumulation of information about colloids in natural barriers, understanding their behaviour and development of an evaluation model
- Acquisition of sorption distribution coefficients for colloids and data on the irreversibility of sorption
4.4.6 Effects of organic materials

Sources of organic material in a TRU waste disposal facility are waste, groundwater and EBS material. Organic materials affect solubility and sorption distribution coefficients of nuclides by complexation with organic materials and its decomposing products. Hence, assessments of nuclide migration must take into account the possibility that organic materials affect these parameters.

Organic materials also affect gas generation and EBS materials (e.g. CO₂ gas generation and neutralisation of cementitious material). Such effects are described in the sections on gas and microbes below.

4.4.6.1 Organic materials considered

Organic material is not included in Group 1 TRU waste. A certain amount of organic material (mainly cotton waste, etc.) is included in Group 2 waste of JAEA. A separation procedure is used to remove this organic material, but it is assumed that 0.1% will remain in the waste (Kurakata et al., 1996). The waste in Group 3 includes low-level liquid waste from Tokai reprocessing plant of JAEA that has been solidified in bitumen. Also included in this group is bituminised waste that will be returned by AREVA (France). The total amount of bitumen that will be disposed of in a geological repository is estimated to be 2.60×10⁶ kg. It is considered that Group 4 waste will not include organic material since incineration treatment will be applied. Additionally, cement chemical admixtures (mainly water reducing agents) may include organic material. Such admixtures are used in both the construction of cementitious filling materials and the structural framework. The amount of the water-reducing agent is estimated to be about 0.3 - 3% of the cement weight (Japan Concrete Admixture Association, 2003). According to a reported analysis of water-reducing agent, the proportion of total organic carbon in the agent is estimated to be about 9 wt% (Iriya et al., 2000). In addition to organic material in waste compounds and construction materials in the disposal facility, natural organic material in groundwater such as humic materials is included.

4.4.6.2 Effects of organic materials from waste

(1) Effect of cotton waste in Group 2 waste

Greenfield et al. (1992) measured the solubility of Pu in leachates of various organic materials in the presence of cementitious material. In the leachates from organic materials such as nylon and polystyrene, no increase in solubility was observed. However, in the leachate from cellulose solubility increased by about seven orders of magnitude. Therefore, Iso-Saccharinic Acid (ISA) which is a degradation product of cellulose is considered to be an important organic material in the assessment of nuclide migration. Additionally, Bradbury and Sarott (1994) estimated a solubility enhanced factor (SEF) and a sorption reducing factor (SRF) for use in nuclide migration analyses. SEF and SRF depend on the ISA concentration and nuclide type. A conservative value for nuclide solubility can be calculated by multiplying its solubility in the absence of ISA by SEF. Similarly, a conservative value for nuclide sorption coefficient can be calculated by dividing the coefficient’s value in the absence of ISA by the SRF. In the case where the ISA concentration is less than 1×10⁻⁶ mol/dm³, SEF and SRF are 1 for each nuclide, and increase in solubility
while decreases in sorption coefficients do not occur. As described before, the main component of organic material in Group 2 waste is cellulosic material such as cotton waste. Hence, Honda and Mihara (2004) evaluated the effect by assuming that organic material in Group 2 waste is all cellulose that decomposes fully into ISA. The effect of ISA was re-evaluated using the latest estimated waste inventory because the previous evaluation was based on the amount of material in the 1st TRU progress report. According to the case for no release of ISA from the repository in the previous evaluation, the concentration of ISA in the pore water of the facility was evaluated assuming the sorption of ISA onto cement hydrates. This case gave the highest concentration of ISA because the transport of ISA to the outside was neglected and all the cellulose was assumed to be broken down to ISA. This approach gave a maximum estimate of $5 \times 10^{-6}$ mol/dm$^3$, which is more than the $1.0 \times 10^{-6}$ mol/dm$^3$ limit noted above. Therefore the effect of ISA should be considered by the nuclide migration analysis.

(2) Effect of bitumen in Group 3 waste

If bitumen is degraded in the disposal environment and changes to soluble organic species, the species might affect nuclide migration. Greenfield et al. (1997) performed leaching tests on bitumen for a period of 2 years. They used a liquid:solid ratio of 20:1, a low oxygen atmosphere and a liquid temperature of 80°C. There were various environmental conditions with and without cementitious material and with NaNO$_3$ concentrations of 0 - 3 mol/dm$^3$. It was observed that the concentration of total organic carbon (TOC) in the leachate was not dependent on the leaching time, suggesting that the leached organic compounds did not result from the progressive decomposition of bitumen. The co-existence of concrete and NaNO$_3$ did not promote the decomposition of bitumen. A solubility test was performed using the leachate. The solubility of Pu was not affected by the soluble organic species in the leachate, of which concentration reached to several tens of ppm as TOC. Therefore they concluded that effective ligands for Pu are hardly generated in reducing and alkaline environment. These results suggest that significant degradation of bitumen would not occur in the disposal facility and that the impact of degradation of bitumen on nuclide solubility would not be significant. Greenfield et al. (1997) also tested the degradation of bitumen by $\alpha$-radiation. Under low-oxygen conditions with co-existing cement, the solubility of Pu in the leachate from degraded bitumen was measured and was found to be only $2 \times 10^{-11} - 8 \times 10^{-9}$ mol/dm$^3$ and the effect of the leachate can therefore be ignored. Additionally, Van Loon and Kopajtic (1990) performed a bitumen degradation test using $\gamma$-emitters. They reported that the chemical form of soluble nuclides is not significantly changed. Considering these findings, the chemical impact of bitumen degradation on nuclide migration is considered to be small.

(3) Effect of solvent waste included in Group 3 waste

Bituminised waste classified in the Group 3 are solidified solvents that are used in reprocessing, including TBP and its degradation products (DBP and MBP). These components may form complexes with radionuclides and might affect nuclide solubilities and sorption distribution coefficients. Hence, complex formation with these solvent components and their degradation materials have been evaluated (Shibata et
al., 2005). The evaluation of the effects of these waste solutions considers that complexes with U(IV) and Pu(IV) in DBP are stronger than those with TBP in dilute nitric acid solution (1.0×10^{-2} mol/dm³). It is also considered that the amounts of TBP and MBP in that waste are less than the amount of DBP. Therefore DBP was employed as a representative among TBP and its degradation products. The concentration of these components in the waste solution is evaluated as 1.4×10^{-2} mol/dm³ and all of them are assumed to be DBP. Using the JAEA thermodynamic database, the solubilities of Ni(II), Am(III), Pu(IV), Th(IV) and U(IV) were calculated over the range of DBP concentration of 10^{-6} - 1 mol/dm³ in cement pore fluid. However, in this region no effect on solubility was observed and the dominant chemical species were hydroxyl species. The similar calculation was done for the outside of the disposal facility, using fresh groundwater (FRHP). It was found that only the solubility of Ni increased when the DBP concentration was above 10^{-2} mol/dm³. However, this DBP concentration corresponds to the concentration in pore water within the waste packages. The concentration in the natural barrier will be lower than that in pore water in waste packages and consequently is ignored. Max and Keiling (1989) measured the solubility of NaU₂O₇, NpO₂(OH), Pu(OH)₄, AgI and CsNO₃ in solutions that were saturated with TBP or DBP and equilibrated with halite, cement degradation materials and Fe-oxyhydroxide. They confirmed that the existence of TBP and DBP do not significantly affect the solubility. These experimental results also support the results of the solubility calculations described previously.

4.4.6.3 Effect of cement additives

The main cement additive used in the disposal facility is considered to be a water-reducing agent. This agent was evaluated since it is a surface-active agent and can form complexes with radionuclides. Greenfield et al. (1998) measured the solubilities of Pu, U, Am and Tc using cementitious leachate to which a diluted high performance AE water-reducing agent was added. They reported that the solubility of each nuclide increases with increasing concentration of high performance AE water-reducing agent (naphthalenesulfonic acid system and polycarboxylate system). On the other hand, Ewart et al. (1991) measured the sorption distribution coefficient of Pu using a cementitious solid phase to which one of four types of water-reducing agents (naphthalenesulphonate, melamine formaldehyde, sodium lignosulphonate and sodium gluconate) had been added. The results showed that the addition of these water-reducing agents does not affect the sorption distribution coefficient of Pu.

The observations of Greenfield et al. (1998) and Ewart et al. (1991) gave different trends, which may possibly have been caused by the differing chemical characteristics of the different agents used. However, it is considered that this result may partly reflect different experimental conditions, i.e. Greenfield et al. (1998) added water-reducing agent after the solid phase had been removed from the solution. However, Ewart et al. (1991) added water-reducing agent during cement hydration and used leachate from the solidified cement. Another difference is that Greenfield et al. (1998) performed solubility measurements without a cement solid phase being present, while Ewart et al. (1991) measured sorption distribution coefficients in the presence of a co-existing cementitious solid phase.
For the case where the added water-reducing agent is sodium gluconate, Bradbury and Van Loon (1998) calculated the concentration of the agent in cement pore water assuming the sorption of gluconic acid on hardened cement paste. Since gluconic acid is sorbed onto the cement paste, the concentration in the pore water was estimated to be $3 \times 10^{-5}$ mol/dm$^3$.

Generally, water-reducing agents commonly show a high degree of sorption onto solid cement phases because of their original function. This explains why the experiments of Ewart et al. (1991) did not show any significant effects of admixing. Moreover, the organic components that are leached from hardened cement paste, to which a high performance AE water-reducing agent had been added, have quite different molecular mass distributions from those of the original high performance AE water-reducing agent. The latter is replaced by organic materials with lower molecular masses (Iriya et al., 2000). This phenomenon also explains why the experimental results of Greenfield et al. (1998) and Ewart et al. (1991) are different. Actually, the experimental conditions of Ewart et al. (1991) are more similar to conditions in a repository than those of Greenfield. Based on their results, the effects are estimated to be small. Additionally, if the difference of the results attributes to the difference of agents, the one that shows the smallest effect should can be chosen, as demonstrated by the experimental results of Ewart et al. (1991).

### 4.4.6.4 Effects of natural organic material

The types and concentrations of natural organic materials in groundwater are considered to depend on location and the geological environment. However the geological conditions of the disposal site have not been determined. Therefore the magnitude of the effect of natural organic material was understood from the results of nuclide migration analyses which were conducted using a conservative distribution coefficient based on actual examples of measurements as done in H12 report (JNC, 2000).

### 4.4.6.5 Summary

Natural organic material was treated as in the H12 report and engineered organic materials (bitumen, waste solutions, cellulose and cement additives) were evaluated. The following results were obtained:

- From the current data, the effects of bitumen on the solubilities and sorption behaviour of nuclides are small.
- The impacts of waste solvents (TBP and DBP) on solubilities and sorption distribution coefficients, are small.
- It is estimated that the effects of cement additives in disposal facilities containing solid cement phases are small. Additionally, it is possible to select admixing agents that would have only small effects on nuclide behavior.
- It is assumed that all the inseparable organic material in hulls and ends change into ISA. The evaluation of nuclide migration is considered to be conservative if it is assumed that the
concentration of ISA in pore water in the disposal facility is $5 \times 10^{-6}$ mol/dm$^3$.

4.4.6.6 Future issues
The following issues are considered to be important for future consideration:

- Improvement of knowledge about the decomposition behaviour of organic materials present in waste and concrete and the impacts of their degradation products on both barrier material and behaviour of nuclides.
- Evaluation of the promotion of redox reactions between bitumen and nitrate by the catalytic action (e.g. microbial action).

4.4.7 Effects of microbes
The anaerobic condition of the geological repository and the presence of cement will maintain a highly alkaline environment (> pH 12.5) for a long period. Previously, it was considered that microbes would not be active in such an environment but recent studies have revealed that, even at several hundred metres depth, various microbes can be active under anaerobic conditions in neutral to mildly alkaline pH conditions (Sasamoto et al., 1996; Murakami et al., 2003). Moreover, there have been reports of microbes that are active in aerobic, highly alkaline environments (Horikoshi and Akiba, 1993) and extremely anaerobic alkaline microbes that are active at pH 8.5 - 12.5 (Takai et al., 2001). Additionally, there are reports that microbes which are active in neutral to alkaline environments adapted to higher alkaline conditions with pH 12.5 (Fujiwara and Kawashima, 2002). Hence, the effects of microbial activity in a geological repository for TRU waste cannot be ignored.

At present, research into the effects of microbes in waste repositories is being carried out in various countries. A classification of these effects is summarized in Table 4.4.7-1. However, not all microbes would affect all locations within a disposal facility for TRU waste. Instead, specific microbial activity would occur only over certain periods and locations under which suitable environmental conditions for specific microbes occur.

The factors that influence microbial activity in geological environments can be divided into primary environmental factors of deep underground (microbe types, redox conditions, temperature, pressure, etc.) and external factors (waste characteristics, structure of the disposal facility, organic material in the disposal facility, etc.). The types of microbe that are active in the disposal environment depend strongly on the geological environment of the disposal site. It is also considered that the external factors might change, depending on the site characteristics. Hence, at present it is difficult to determine the above influencing factors and to evaluate the microbial activities.

In Japan and in other countries, in order to evaluate the effects of microbes quantitatively, the rate of gas generation and geochemical conditions have been modelled (Arter et al., 1991; Agg, 1993; Yim et al.,
However, as described previously, it is difficult to decide on the input parameters at present because of uncertainty concerning the influencing factors. Hence, the qualitative estimations based on the estimated environmental conditions and an evaluation based on the material balance under conservative assumptions were conducted in this section.

<table>
<thead>
<tr>
<th>Effect on solubility and sorption</th>
<th>Process</th>
<th>Phenomenon</th>
<th>Degree of influence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Complex formation</td>
<td></td>
<td></td>
<td>N</td>
</tr>
<tr>
<td>Colloid formation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>pH change</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxidation-reduction reaction</td>
<td></td>
<td></td>
<td>N, P</td>
</tr>
<tr>
<td>Sorption/incorporation of nuclides</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| Effect on EBS (direct effect)     |          |            |                     |
| Cementitious material alteration  |          |            | N                   |
| Metal corrosion                   |          |            |                     |
| Bitumen alteration                |          |            |                     |
| Bentonite alteration              |          |            |                     |

| Effect on engineered and natural barriers (indirect effect) |          |            |                     |
| Closure of pores                      |          |            | P                   |
| Others                                |          |            |                     |
| Gas generation                        |          |            |                     |

N: Possibility that the process has negative impact on the safety of the disposal facility.
P: Possibility that the process has positive effect on the safety of the disposal facility.
4.4.7.1 Microbial activity in a geological repository for TRU waste

The materials which form the nutrients for microbial activity in each waste group are: cellulose in Group 2 waste (in JAEA waste about 0.1 wt% cotton; Kurakata et al., 1996), bitumen (waste solidification matrix), nitrate salt (from fluids produced by the PUREX reprocessing method), TBPs (TBP and its degradation products (DBP and MBP)) in Group 3 waste, and cement additives (water-reducing agents, etc.), natural organic materials (humic substances, etc.) and inorganic salts (nitrate salts, sulfate salts etc.) from groundwater in all the waste groups.

It is estimated that the accumulated inflow of humic substances from groundwater over a period of about 100,000 years will only be as much as about 1/10 (Groups 1 and 2) to about 1/25 (Groups 3 and 4) of the amounts in the cement additives, even if it is assumed that the disposal facility becomes more permeable. Additionally, humic substances are the final decomposition products of microbial activity. Thus, it is considered that humic substances are difficult for microbes to metabolise and decompose (e.g. EIC net, 2005). Furthermore, if humic substances are metabolised and decomposed, the effects would be similar to those induced by microbial metabolism of the cement additives, etc. Hence, if the effects of microbial metabolism of cement additives, etc. are considered, the effects of microbial metabolism of the humic substances can be ignored.

The studies of denitrifying bacteria, sulphate-reducing bacteria (SRB) and methanogens, etc. deep underground have been reported (Motamedi and Pedersen, 1998; Kotelnikova et al., 1998; Chang et al., 2001; Naganuma et al., 2002). It is considered that denitrifying bacteria, SRB, methanogens, and bacteria that can decompose cement additives, cellulose, bitumen and TBPs, would be important in a geological repository for TRU waste. The substrates and microbial activities in a geological repository are summarised in Table 4.4.7-2.
Table 4.4.7-2 Substrates and microbial activities in a geological repository

<table>
<thead>
<tr>
<th>Gr.</th>
<th>Waste Facility / groundwater</th>
<th>Substrates in waste group</th>
<th>Microbial activities</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Not included</td>
<td>Cement additives, Humic substances, Inorganic salts</td>
<td>Cement additive decomposing bacteria*¹, Sulphate-reducing bacteria, Methanogens</td>
</tr>
<tr>
<td>2</td>
<td>Cellulose</td>
<td>Cement additives, Humic substances, Inorganic salts</td>
<td>Cement additive decomposing bacteria<em>¹, Cellulose decomposing bacteria</em>¹, Sulphate-reducing bacteria, Methanogens</td>
</tr>
<tr>
<td>3</td>
<td>Bitumen, Nitrate salt, TBP group</td>
<td>Cement additives, Humic substances, Inorganic salts</td>
<td>Cement additive decomposing bacteria<em>¹, Bitumen decomposing bacteria</em>¹, TBPs decomposing bacteria*¹, Denitrifying bacteria, Sulphate-reducing bacteria, Methanogens</td>
</tr>
<tr>
<td>4</td>
<td>Not included</td>
<td>Cement additives, Humic substances, Inorganic salts</td>
<td>Cement additive decomposing bacteria*¹, Sulphate-reducing bacteria, Methanogens</td>
</tr>
</tbody>
</table>

*¹: The classification is not based on microbiology, but is a descriptive term that is adequate for the evaluation.

4.4.7.2 Effect on nuclide solubility and sorption
(1) Effect on pH variations

For assessing the drop of pH due to metabolic products of microbes, the assumption that microbial degradation of organic materials generates CO₂ is more conservative rather than the assumption that the process generates C1 carboxylic acids in terms of stoichiometry. Hence, the decrease in pH is evaluated, by making the assumption that organic material is completely decomposed to CO₂.

In the waste Groups 1, 2 and 4, the amounts of hydrated Ca in cementitious material are one to two orders of magnitude higher than the amount of CO₂ generated from the organic materials (Kato et al., 2005). Hence, if all the organic material in these waste groups within a disposal facility is decomposed into CO₂ by microbial activity, the CO₂ generated would be neutralized by the Ca-hydrates. Consequently, the effect of organic material decomposition on pH is considered to be small. In Group 3 waste there is considerable amounts of bitumen. Like humic substances, the bitumen is difficult for microbes to decompose. If all the saturated and aromatic compounds in the bitumen were to be completely decomposed to CO₂, the amount of CO₂ generated would reach about 60% (mole ratio) of the amount of Ca hydrate in the cementitious material. However, it is considered that the pH-buffering characteristics of the remaining Ca hydrate would
be maintained (Kato et al., 2005). Additionally, the activity of TBPs-degrading bacteria might cause
generation of free phosphoric acid. However, phosphoric ion is precipitated as insoluble hydroxyapatite
\( \text{[Ca}_{10}(\text{PO}_{4})_{6}(\text{OH})_{2}] \), causing the ion’s concentration in pore water to decrease to about \( 10^{-6}\text{mol/dm}^3 \) (Takei
et al., 2002). The amount of phosphoric acid that is released by microbial decomposition of TBPs is about 5
orders of magnitude lower than the amount of Ca hydrate the cementitious material. Hence, changes in the
amount of phosphoric acid that is generated by TBPs composition, is considered to have only a small effect
on pH.

(2) Effect on complex formation

The metabolic products of bacteria such as decomposed cement additives, cellulose, bitumen and TBPs,
might act as complexing agents. However, there is little knowledge about the microbial metabolism of
organic material in a repository. Consequently, the evaluation of complex formation between radionuclides
and metabolic products of microbes is difficult. Complex formation with organic material that originates
from cotton in Group 2 waste is evaluated by assuming that the all the organic material is cellulose and that
it is completely decomposed to ISA. The results are reflected in the analysis of nuclide migration (Section
4.4.6).

Hence, the formation of complexes between nuclides and microbial metabolites of organic materials,
except for cellulose, is an issue for future consideration.

(3) Effects of colloid formation, nuclide sorption and incorporation

In a disposal facility where buffer material is used, colloids will be formed by microbial activity
(including microbes that sorb or contain nuclides) have no negative influence by filtration effect of buffer
material during the period while a buffer performance is maintained. In contrast, there is little knowledge
concerning colloid generation by microbes when the buffer material is altered and the filtration capability is
lost. There is also little knowledge about the effects of colloids produced by microbes in disposal facilities
without buffer material. Evaluation of these matters is difficult. Hence, the effects of colloid formation by
microbial activity are an issue for future consideration.

(4) Effects of changing redox conditions

The disposal environment becomes anaerobic owing to the activity of aerobic microbes and the
consumption of oxidized chemical species by metal corrosion etc. after the facility’s closure. After the
establishment of an anaerobic environment, suitable microbes for the temporal redox condition will
dominate the microbial activity in the repository during period of time in which the original redox
condition deep underground is recovered. Microbial activities can promote the recovery of the reducing
condition by consuming oxidising species but do not generate an oxidising condition. Therefore the
negative impact of microbial activity on the solubility and sorption of nuclides by changing the redox
condition is considered to be negligible.
4.4.7.3 Effects on the engineered and natural barriers

(1) Effect of alteration of cementitious material

As described above in Section 4.4.7.2(1), for all the waste groups, the total amount of CO₂ which is generated from included organic material is smaller than the amount of Ca hydrate in cementitious material. Additionally, phosphoric ions in Group 3 is precipitated as insoluble hydroxyapatite. Such neutralization and precipitation reactions result in leaching of Ca. However, except for Group 3 waste, the amount of Ca hydrate in the cementitious material is more than 1 or 2 orders larger than the amounts leached. Hence, the influence on the alteration of cementitious material is considered to be small except in the disposal tunnels for Group 3 waste. The metabolism and decomposition of bitumen by microbes does not occur over a short period. As described before, these are considered to be long-term reactions because the bitumen consists of organic material that cannot be used easily by microbes. However, eventually about 60% (mole ratio) of the Ca hydrates in cementitious material can combine with CO₂ generated from bitumen (Kato et al., 2005). It is considered that this process will affect significantly the use of cementitious material as a general construction material. However, since the required capabilities of cementitious material for long-term are pH buffering and nuclide sorption, predictive evaluations were performed for the case where CO₂ is generated from bitumen quickly. The results showed that cementitious material from which 60% of Ca is leached and is precipitated as CaCO₃ by reacting with CO₂ originating from bitumen, keeps pH within Region III. The dose was almost the same as that of the reference case even when the nuclide migration analysis was performed with Region III conditions maintained throughout (Kato et al., 2005). Hence, these effects on nuclide migration are considered to be small.

(2) Effect on metal corrosion

It is considered that the effects of organic acid and phosphoric acid on metal corrosion are small since these acids, which are generated by microbes, are neutralized by Ca hydrates in cementitious material. Additionally, the activity of SRB is inhibited in compacted bentonite (Nishimura et al., 1999).

Moreover, in experimental simulations, there is no difference in the corrosion rate of carbon steel when there is H₂S gas purging (the simulation case in which SRB are active) or when there is nitrogen gas purging (the simulation case in which SRB are not active; Taniguchi et al., 2001). Hence, if SRB activity is assumed to occur, it is considered that the effects on metal corrosion and gas generation resulting from corrosion are small.

(3) Effect on bitumen alteration

There is little knowledge concerning the effect of microbes on the nuclide containment properties of bitumen, which is used as a matrix to solidify radioactive liquid waste. It is therefore difficult to evaluate the significance of this alteration.

(4) Effect on bentonite alteration

It is considered that organic cations that are generated by microbial activity enter into the inter-layer of
smectite. Since smectite is the main mineral composing the bentonite, the bentonite’s capabilities are changed. Organic cations are mostly nitrogen compounds, and especially, amine compounds (Kagaku-Daijiten-Henshu-Linkai, 1987). However, Group 1 and 2 wastes in disposal facilities that include bentonite buffer materials, contain only small amounts of organic matrices, and nitrogen compounds are not taken into the repository. Moreover, it is reported that the concentrations of natural nitrogen-bearing organic material in groundwater is small (Nagao, 1995; JNC, 2000). Furthermore, cement additives that do not contain nitrogen compounds can be selected. Hence, there is considered to be little possibility that organic cations generated by microbes enter into the inter-layer of smectite and change the capabilities of the bentonite. Moreover, as described in Section 4.4.7.2(1), extreme pH variations are not caused by microbes. Therefore there is also little possibility that there will be alteration of bentonite owing to microbially mediated pH changes.

(5) Effect on porosity filling

The formation of biofilms and CaCO$_3$ can fill the pores of the disposal system. There is also a possibility that this process would restrict the transportation of groundwater. Hence, void sealing by microbial activity works dominantly to enhance the confinement function of disposal system.

4.4.7.4 Effect on gas generation

The main gases generated by microbial activity in the disposal environment are CO$_2$ (total microbial activity) and N$_2$ (activity of denitrifying bacteria). In the repository environment CO$_2$ is fixed as CaCO$_3$. Since the amount of Ca hydrate in the cementitious material is larger than the amount of CO$_2$ generated (Kato et al., 2005), the effect of CO$_2$ generation on the disposal system in terms of impacts of gas generation is considered to be small. Additionally, there is a possibility that CH$_4$ is generated. The impacts of the previous gas generation process by microbial activities is included in evaluation of both the effects of the gas generation (Section 4.4.10) and the nitrate salt effect (Section 4.4.9.).

In the case that methanogens are present, it is possible that radioactive gas species containing $^{14}$C ($^{14}$CH$_4$) are generated. A nuclide migration analysis for the case in which all the C-14 becomes CH$_4$ is described in Section 4.4.10.

4.4.7.5 Summary

It is considered that the following effects of microbial activity have little impact on the safety of the geological repository for TRU waste: the effects of pH variation; redox reactions; alteration of cementitious materials; metal corrosion; bitumen alteration; bentonite alteration; void sealing; and gas generation (except for $^{14}$CH$_4$ generation). The impacts of complexation with metabolic products on solubility and sorption behaviour of nuclides, colloid formation (including the colloidal behaviour of microbes) and the generation of radioactive gases containing $^{14}$C are considered to be issues for future consideration.
4.4.7.6 Future issues
To improve the reliability of assessments of microbial effects in geological disposal systems for TRU waste, it is necessary to clarify the metabolism of organic materials by microbes (decomposition of bitumen, $^{14}$CH$_4$ generation, etc.) and the effects of the metabolites (the formation of complexing agents and colloid, etc.). Specifically, the following research and development are necessary:

- Clarification of the scheme for organic metabolism
  The microbial metabolism scheme for cement additives (especially, low molecular organic material dissolved in pore water), cellulose and bitumen should be clarified. An improved understanding of the formation of complexing agents and colloids is necessary. Cement additives and bitumen are important organic material in terms of amount.

- Understanding of the effect of C-14
  It is necessary to understand the processes that generate radioactive gases ($^{14}$CH$_4$), the rates of radioactive gas generation, and to establish an evaluation method.

Additionally, since there is little knowledge about microbial activity and its impacts in a geological disposal environment, improved data and expansion of knowledge are necessary through experiments and investigation both in laboratory and field.

4.4.8 Effects on the radiation field
Since the initial quantities of radioactive substances are small in a geological repository for TRU waste compared to that in a repository for HLW, the radiation field in a TRU waste repository will be relatively moderate in most cases. However, considering that overpack of HLW delays nuclide leakage and has a shielding effect that decreases short half life nuclides, the radiation field in a geological repository from some TRU wastes with no shielding is expected to be higher.

This section analyses the radiation field in a geological repository for TRU waste, focusing on specific waste conditions and the EBS design conditions. Based on the results, damage of the EBS material is evaluated and the effect for geochemical environment by radiolysis of pore water in EBS is evaluated.

4.4.8.1 Radiation field in the EBS considering the shielding effect
(1) Evaluation method
Group 2 waste (hulls and end-pieces) is evaluated. This is the most radioactive and heat-producing waste among the waste groups considered. The characteristics of hulls and end-pieces produced by each reprocessing facility are different. However, here, hulls and end-pieces that are produced by private sector reprocessing plants were evaluated because they have large abundances. In the evaluation, the linear nuclide transportation code ANISN (Engle, 1967) was used.

The concentration of radioactive substances in hulls and end-pieces that are generated from private sector reprocessing plants were calculated by ORIGEN2 under the combustion condition of spent fuel. The
quantities of radioactive substances used in the shielding calculation, were based on a storage period of 25 years. The following items were included in the modelled region.

- **Canister**
  - The fragmented cladding (hulls and end-pieces) is compressed into a disk. In 1 canister, 5-7 compressed disks are emplaced. After emplacement, a clearance void that is not filled remains in the canister.

- **Waste package B (Ref. Table 3.2.1.1-1)**
  - 4 canisters are stored in a waste package B (box type) then transported and emplaced. The clearance is filled with cement mortar after canister emplacement.

- **Steel structural framework**
  - The steel structural framework is made of carbon steel.

- **Buffer material**
  - Buffer material is made by mixing 70% of bentonite and 30% of sand.

Figure 4.4.8-1, shows the modelled system used in the shielding calculation. Based on the specifications of waste emplacement (vertical cross-section of disposal tunnel) in crystalline rock, 4 waste packages and a buffer material layer are modelled. A steel structural framework is established on the sides and bottom, but not on the upper side. Therefore, the shielding capability of the steel structural framework is not considered in the shielding calculation.

Figure 4.4.8-1 Model system used in shielding calculations
(2) Evaluation result

The spatial distributions of the air-kerma rate in the model system at 1 year and 1,000 years are shown in Figure 4.4.8-2. Though the shielding calculation is aimed at primary $\gamma$-rays, secondary $\gamma$-rays and neutron radiation, the contribution by primary $\gamma$-rays is most significant. When the air-kerma rate after 1,000 years is compared with that at 1 year in the same figure, it is seen that there is no significant change in spatial distribution, though a decrease of 2 orders of magnitude. Moreover, in the model system in which 4 waste packages of type B are included, the air-kerma rate in each waste package B is almost the same and the 4 packages show almost the same air-kerma rate distribution.

A comparison between the absorbed dose rate on the surface of 19 cm thick overpack surrounding HLW canister (JNC, 2000) and that on the surface of waste package B, without overpack, is shown in Table 4.4.8-1. Although the HLW has greater quantities of included radioactive substances, the lack of overpack means that hulls and end-pieces in TRU waste give a $\gamma$-ray absorbed dose rate that is 3 orders of magnitude higher.

| Table 4.4.8-1 Comparison of absorbed dose rate on waste surfaces [Gy/y] |
|-----------------------------|-----------------------------|
|                            | HLW                         | TRU waste                   |
| $\gamma$-ray               | $\sim 3 \times 10^3$        | $\sim 4 \times 10^4$        |
| Neutron radiation          | $\sim 4 \times 10^{-1}$     | $\sim 5 \times 10^{-1}$     |

HLW condition: 50 years storage, thickness of overpack 19cm, value at overpack surface

TRU waste condition: 25 years storage, without overpack, value at surface of waste package B
Figure 4.4.8-2 Air-kerma rate in the model system
4.4.8.2 Exposure damage to EBS material

(1) Cementitious material

From experimental results, the radiation effect on cementitious material which is used as a solidified matrix or grout is reported to be 9-12 MGy of $\gamma$-exposure as follows (Wilding et al., 1991):

- In most samples significant changes were not observed.
- In some samples, discoloration on surfaces was observed.
- In the case of BFS/OPC grout, denudation, fracturing and deformation were observed.

In addition, from experimental results, the radiation effect on cementitious material which is used in reinforced concrete is reported to be a maximum of $1.7 \times 10^8$ Gy of $\gamma$-exposure as follows (Yamada et al., 1984).

- There is a decrease of about 10% in compressive strength under heating conditions. However, there is no significant difference between experimental heating and heating by $\gamma$-exposure. Hence, the decrease of compressive strength owing to heating is more significant than the decrease caused by exposure damage.
- Since the elastic modulus is sensitive to the effect of temperature and moisture content, the dynamic elastic modulus is decreased more due to the effect of air curing or heating than as a result of $\gamma$-exposure.
- From the measurement of neutralization depths, there is no difference in the degree of neutralization with and without of $\gamma$-exposure.
- The pore sizes of cement pastes with 55% of water/cement ratio which undergo air curing and $\gamma$-exposure shows almost the same the distribution and there is no significant difference in the amounts of all pore sizes.

From existing knowledge, it is considered that exposure damage is insignificant. The amount of absorbed dose by the cement mortar is almost the same or more smaller than that of the total amount of radiation in the current study (ca. 30 MGy in 1,000 years, ref. Figure 4.4.8-3). Even if the exposure is continued for the long term, the overall cement mortar performance will be maintained though there may be some local changes near the surfaces of canisters.

(2) Bentonite material

The radiation effect on the smectite structure of bentonite material generally does not result in significant structural alteration (e.g., Ewing, 1984).

Pusch et al. (1993) report that, in exposure experiments using Co-60 and MX-80, there is no significant change in the smectite structure (until $3.27 \times 10^7$ Gy). However, the loss of feldspar and the alteration of small montmorillonite grains are also reported.

Based on $9.5 \times 10^7$ Gy $\gamma$-exposure experiments, it is reported that there is no significant effect on the hydrogeological properties of bentonite (Grauer, 1986). It is also reported that the ion exchange capacity of montmorillonite is increased during experimental exposure to $\gamma$-rays, using Co-60, until a maximum of
$10^8$Gy (Spitsyn et al., 1982).

The exposure damage effect is not significant and the radiation absorption of the buffer material is almost the same or more smaller than that of the radiation amount in the current study (ca. 2MGy in 1,000 years, ref. Figure 4.4.8-4). Therefore, even if the exposure is continued for the long term, significant changes to the smectite structure will not occur. The possibility that the buffer material will be significantly damaged by exposure to radiation is considered to be small.

Figure 4.4.8-3 Radiation absorption rate and adsorption dose in cement mortar (part adjacent to canister)

Figure 4.4.8-4 Radiation absorption rate and adsorption dose in buffer material (inside boundary)
4.4.8.3 Radiolysis of pore water

H₂ and H₂O₂ were included as molecular decomposition products of water radiolysis. However, in the case that H₂ is dispersed as gas or transported rapidly in liquid, it is reported that an oxidizing atmosphere is produced by the remaining H₂O₂ (e.g. Grenthe et al., 1983). Here, the possibility that such an oxidizing atmosphere will form by water radiolysis is evaluated.

(1) Specification of G value

The amount of oxidizing agent generated by radiolysis is calculated by multiplying the absorption dose and G value. The absorption dose of α-ray is calculated by assuming the average energy of α-ray to be 5MeV and by calculating the total amount of α-emission from the amounts of radioactive substances that contain α-emitting nuclides (McKinley, 1985). The adsorption doses of γ-rays and neutrons in pores within a canister are derived from the shielding calculations whose results are shown in Section 4.4.8.1. A conservative G value of H₂O₂ is specified in the current studies and the values for α, γ and neutron radiation, are 0.985, 0.72, 1.145 [molecule/100eV], respectively (Christensen and Bjergbakke., 1982; Bjergbakke et al., 1984; Sunaryo et al., 1994).

(2) Effect of oxidizing agents generated in canisters

The main feature of radiolysis in canisters is the generation of oxidizing agents by α-rays. The corrosion of metal waste and canisters proceeds by consuming surrounding oxidizing agents. Therefore, the possibility of an oxidizing atmosphere being produced can be estimated by comparing the corrosion rates and amounts of metal that exist, with generation rates or amounts of oxidizing agents.

A comparison between the generation rate of oxidizing agents by radiolysis and the generation rate of reducing agents produced by corrosion, is shown in Figure 4.4.8-5. Activated metal and canisters are considered to be the corroded metals. Oxidizing corrosion and reducing corrosion are considered individually. It is considered that corrosion undergoes a transition from oxidizing corrosion to reducing corrosion, when the supply rate of reducing agents exceeds the generation rate of oxidizing agents. Actually, if it is considered that there is a the delay in the rate of corrosion owing to the time taken for resaturation, and a decrease in the amount of α-emission within a canister owing to nuclide leakage, the supply rate of reducing agents might exceed the generation rate of oxidizing agents after 10,000 years.

The abundance of metallic materials in canisters determines the reducing capacity. The relationships between the accumulated amounts of oxidizing agents produced by water radiolysis and the reducing capacity provided by metallic materials are shown in Figure 4.4.8-6. The generated quantities of oxidizing agents are evaluated by considering different time delays (10 years, 100 years and 1,000 years) until the canister is resaturated, since initially there is no water that may undergo radiolysis in the pores of the canister. In the same figure, it can be seen that continuation of the radiation effect for a long period, more than 10⁷ years, is necessary in order for the reducing capacity of the canister (9.5×10⁸ mol) to be exceeded.
Figure 4.4.8-5 Generation rates of oxidizing agents and the supply rates of reducing nuclides in the canister

Figure 4.4.8-6 Cumulative amounts of oxidizing agents generated in the canister and reducing volume of the canister
(3) Effects of oxidizing agent generation in mortar and buffer material

Oxidizing agents generated by γ-ray penetration are the main feature of radiolysis of mortar and buffer material. The space-time distributions of concentrations of oxidizing agents in these areas are shown as follows:

(Mortar: \( 0 \leq x < L_m \))

\[
\frac{\partial C(x,t)}{\partial t} = D_m \frac{\partial^2 C(x,t)}{\partial x^2} + R_m(t) \cdot \exp(-\lambda_m x) \tag{4.4.8-1}
\]

(Buffer material: \( L_m < x \leq L_m + L_b \))

\[
\frac{\partial C(x,t)}{\partial t} = D_b \frac{\partial^2 C(x,t)}{\partial x^2} + R_b(t) \cdot \exp(-\lambda_b x) - \frac{15}{4} k' \frac{SA}{V} C(x,t) \tag{4.4.8-2}
\]

\[
R_i(t) = \frac{\varepsilon_i G E_i(t)}{100 Av} \quad (i = m, b) \tag{4.4.8-3}
\]

(Boundary condition)

\[
C(x,t) = 0 \quad \text{at} \quad x = 0, L_m, L_m + L_b \tag{4.4.8-4}
\]

- \( C(x,t) \): Concentration of oxidizing agent [mol/m³]
- \( D_i \): Effective diffusion coefficient of the medium \( i \) [m²/s]
- \( \lambda_i \): Linear absorption coefficient at medium \( i \) [1/m]
- \( k' \): Rate constant for oxidizing agent loss by pyrite oxidation [m/s]
- \( SA \): Surface area of pyrite [m²]
- \( V \): Volume of pore water [m³]
- \( \varepsilon_i \): Porosity of medium \( i \) [m³/s]
- \( G \): G value of oxidizing agent generation [molecule/100eV]
- \( E_i(t) \): Absorption dose of pore water in medium \( i \) [eV/(m³ s)]
- \( Av \): Avogadro's number [molecule/mol]

In the area of the buffer material, loss of pyrite by oxidation is considered as well as diffusion migration of the oxidizing agent and generation of oxidizing agents by γ-ray penetration.

These formulae are analyzed using the conditions in Table 4.4.8-2, and concentrations of oxidizing agents generated by radiolysis in mortar and buffer materials are evaluated. The results are shown in Figure 4.4.8-7.
### Table 4.4.8-2 Conditions specified for evaluating the behaviour of oxidizing agents in mortar and buffer material

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Mortar</th>
<th>Buffer material</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective diffusion coefficient of oxidising agent [m²/s]</td>
<td>Dᵢ</td>
<td>8×10⁻¹⁰</td>
<td>3×10⁻¹⁰</td>
<td>Ref. 4.5.2.1</td>
</tr>
<tr>
<td>G value of oxidising agent [molecule/100eV]</td>
<td>G</td>
<td>0.72</td>
<td></td>
<td>Bjergbakke et al., (1984)</td>
</tr>
<tr>
<td>Radiation absorption rate [eV]</td>
<td>Eᵢ(t)</td>
<td>Result of shielding calculation</td>
<td>Evaluation result until 10⁴ years</td>
<td></td>
</tr>
<tr>
<td>Porosity [volume/volume]</td>
<td>εᵢ</td>
<td>0.19</td>
<td>0.40</td>
<td>Reference common setting</td>
</tr>
<tr>
<td>Avogadro’s number [molecule/mol]</td>
<td>Av</td>
<td>6.023×10²³</td>
<td></td>
<td>—</td>
</tr>
<tr>
<td>Rate constant for decay of oxidizing species [m/s]</td>
<td>k’</td>
<td>—</td>
<td>1.46×10⁻⁹</td>
<td>Manaka et al., (2000)</td>
</tr>
<tr>
<td>Surface area of Pyrite [m²]</td>
<td>SA</td>
<td>—</td>
<td></td>
<td>Specific surface area of pyrite 0.03[m²/g], content 0.6wt%, specification corresponds to the analytical mesh</td>
</tr>
<tr>
<td>Volume of pore water [m³]</td>
<td>V</td>
<td>—</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Linear absorption coefficient [1/m]</td>
<td>λᵢ</td>
<td>13.9</td>
<td>8.78</td>
<td>Result of shielding calculation</td>
</tr>
<tr>
<td>Thickness [m]</td>
<td>Lᵢ</td>
<td>0.165</td>
<td>1</td>
<td>Design of EBS</td>
</tr>
</tbody>
</table>

(Additional character i = m,b: m means mortar and b means buffer material.)

The oxidizing agents in the pore water in the buffer material are consumed by redox reactions with pyrite. Consequently, the concentrations of the oxidizing agents are kept low. Moreover, a sufficiently low oxidizing agent concentration is shown after 100 years, though a significant amount of oxidizing agent remains in the pore water of the mortar during the initial stages after closure.
4.4.8.4 Summary

The shielding calculation shows that the surface radiation dose from waste package B, which stores hulls and end-pieces, becomes several orders greater than that from the overpack of HLW. This suggests that any measures for emplacing waste package B and for ensuring safety during closure phase should be required.

Considering existing experimental results, there would be no exposure damage that would inhibit the performance of cement material and bentonite material, even for the above surface radiation dose.

The possibility that an oxidizing atmosphere would form by radiolysis is evaluated for canister, mortar and buffer material, individually. In the canister, the supply rate of reducing agents by metallic corrosion is greater than the generation rate of oxidizing agents during an interval of several 10s of thousands of years. Additionally, since there is enough reducing capacity to consume the accumulative amount of oxidizing agent generated, the possibility of forming an oxidizing atmosphere is considered to be small. Besides that, existing experimental studies have revealed that coexisting H₂ under conditions of γ-exposure inhibits oxidation by oxidizing agents (King et al., 1999), supporting the above conclusion. In the mortar and buffer, space-time distribution of oxidizing agents produced by γ-ray was simulated. The results showed that the oxidizing agent is sufficiently consumed by redox reactions with pyrite in the buffer material, and that sufficiently low concentrations of oxidizing agents are maintained after about 100 years following closure. Actually, considering that there would be a period of 500 years until resaturation (Ando et al., 2005), the possibility that an oxidizing region is formed in the mortar and buffer material, is considered to be low.
4.4.8.5 Future issues

In order to ensure the evaluation of a geological repository system for TRU waste, the following issues concerning the effects of the radiation field should be considered.

① Radiation protection at construction, operation and closure

In the evaluation of disposal technology in Chapter 3 it was concluded that radiation protection during construction, operation and closure must be ensured by using remote handling technology. However, this conclusion is not based on the shielding calculation results, which consider the conditions of each kind of waste and the structures of the disposal facilities. In future, in order to ensure radiation protection during construction, operation and closure, a detailed shielding calculation should be performed to envisage more appropriate facility designs.

② Knowledge of radiolysis of actual water, considering the effects of coexisting components

The radiolysis of water is a complicated process, related to the concentrations of radicals, ions, excited molecules and various solutes. Actual pore water contains various coexisting components and the rate-determining process of radiolysis is not completely understood. Moreover, in this evaluation, based on experimental facts about radiolysis in a pure water system, G values of decomposition products are established. However, actual G values in real pore water might not always be consistent with the values specified above. Hence, the radiolysis characteristics of water in the presence of other components, is considered to be an important issue for future consideration.

4.4.9 Nitrate salt effects

4.4.9.1 Generation of nitrate with organic material inclusions and impact assessment

In Japan, the spent fuel from nuclear power plants is reprocessed and U and Pu are recovered. At present, the PUREX method is the mainstream reprocessing method, and is used in Japan. This method produces nitrate salt (mainly, NaNO₃) which would also be disposed of in a TRU waste disposal facility if special treatments are not performed. Such wastes that include nitrate salts is classified as Group 3 waste. The total amount of nitrate salts to be disposed of is estimated to be about 3.25×10⁶ kg.

Nitrate salt might affect the functions of components of the disposal facility and the behaviour of radionuclides. Hence, the presence of nitrate salts should be reflected in nuclide migration analyses. The NO₃⁻ might be reduced to N₂ and/or NH₃ by microbes and by reactions with reducing materials such as metal. Hence, an evaluation of the effects of nitrate should include the effects of chemical species that are produced from NO₃⁻. Consequently, in this section, the chemical transitions of NO₃⁻ are evaluated. Based on the results, the effects on cementitious material, the solubilites and the sorption distribution coefficients of radionuclides are evaluated.

4.4.9.2 Chemical transition of nitrate ions

NO₃⁻ might be reduced by existing reducing material (metal and organic material). However, in order to
promote the reduction of $\text{NO}_3^-$, catalytic effects, such as may occur on the surfaces of metals or iron hydroxides, are necessary (Sazarashi et al., 1999; Wada et al., 2002). Hence, the reduction process of $\text{NO}_3^-$ by metal is modelled as a combination of water reduction reactions, reduction of $\text{NO}_3^-$ to produce $\text{NO}_2^-$, reduction of $\text{NO}_2^-$ to produce $\text{NH}_3$ and dissolution of carbon steel (Honda et al., 2005). A rate parameter has been experimentally measured for each reaction. Moreover, since the reduction of $\text{NO}_3^-$ by denitrifying bacteria cannot be rejected, this bacterial effect is considered by the above chemical reaction model (Kato et al., 2005). This chemical model and one-dimensional material transportation process are combined and used as an assessment model.

Using this assessment model, $\text{NH}_3$ concentrations and the rates of gas generation ($\text{H}_2$ by corrosion and $\text{N}_2$ by the activity of denitrifying bacteria) in the disposal facility have been calculated (Masuda et al., 2005). In the case for giving the highest concentration of $\text{NH}_3$ (constant metal corrosion rate of 0.1µm/y, no increase of permeability by fracturing), the concentration of $\text{NH}_3$ reaches a maximum of 0.8mol/dm$^3$. The generation of $\text{H}_2$ by corrosion is inhibited by competition between the $\text{NO}_3^-$ reduction reaction and the $\text{H}_2$ generating reaction. However, the concentration of nitrate salt in the pore water of the disposal facility is decreased as the nitrate is transported out from the disposal facility over time. When the activity of pore water becomes appropriate (>0.94) for microbial activity, $\text{N}_2$ generation is started by denitrifying bacteria. Moreover, since the inhibition effect of nitrate to hydrogen gas generation will be diminished as the $\text{NO}_3^-$ concentration decreases, the total gas generation rate becomes larger than $\text{H}_2$ generation rate from metal corrosion in the absence of nitrate. However, the period when this occurs is limited, because after a certain decrease in $\text{NO}_3^-$ concentration occurs there is a decrease in the activity of denitrifying bacteria. The maximum rate of total gas generation becomes 1.4 times the $\text{H}_2$ generation rate by metal corrosion in the absence of nitrate.

4.4.9.3 Effect of nitrate salt on cementitious material

The effects of nitrate salt on the mechanical properties, hydraulic characteristics and alteration of cement have been evaluated (Takei et al., 2002; 2003; Fujita, 2003; Kaneko et al., 2004). From these evaluations, as described previously, there are insignificant impacts on variation of mineral assemblage of cementitious material, as described before (4.4.2.1). However, it has been revealed that the ionic strength is increased by dissolution of nitrate salt and that the solubility of portlandite is changed. The dissolution of Ca is promoted, depending on the concentration of nitrate salt. However, the greatest increased solubility is 1.5 times of that in ion-exchanged water.

The relationship between the porosity and unconfined compressive strength of cement paste, is the same when a NaNO$_3$ solution is passed through or when ion exchange water is passed through. The same formula can be used to explain the relationship in both cases. This fact also suggests that there is no significant mineralogical change in the cement paste. For $\text{NH}_3$, there was no observed effect on the mineralogical composition, hydraulic characteristics and mechanical strength of the cementitious material (Osawa et al., 2004).
4.4.9.4 Effect on solubility of radionuclides and sorption distribution coefficients

(1) Redox conditions

The inside of a disposal facility for Group 3 waste and its neighbourhood should be oxidizing, since NO$_3^-$ exists at a concentration near to saturation with NaNO$_3$. Hence, the oxidizing states of radionuclides might be different from those that would occur under the initial natural reducing conditions underground. The form of the solubility limiting solid phases and/or dominant soluble chemical species are changed. These changes might result in variations in solubilities and/or sorption distribution coefficients. Hence, in the nuclide migration analysis for a disposal facility for Group 3 waste, it is important to specify solubilities and sorption distribution coefficients assuming oxidizing condition.

(2) Effects of complex formation

In a disposal facility for Group 3 waste, NO$_3^-$ or NH$_3$ and radionuclides from NO$_3^-$ might form complexes. The solubility and sorption behaviour of radionuclides might be affected by these complexation.

Actinoid nuclides that are considered to have complexation tendency with NO$_3^-$ were evaluated to determine the effects of nitrate salt. Dominant soluble chemical species of actinoids with trivalent (Am) and tetravalent (Np, Pu and U) forms were evaluated using the JNC-TDB (Yui et al., 1999b) and the NEA-TDB (Guillaumont et al., 2003) because a significant increase in the solubility and decrease in sorption distribution coefficient did not occur if soluble nitric acid complexes became dominant soluble chemical species. All these nuclides were dominantly in the form of hydrolysed species under the pH conditions of cement pore water. Nitric acid complexes did not dominate the chemical speciation even at low pH values, if the total concentration of carbonic acid was that of the reference groundwater (about 10$^{-3}$mol/dm$^3$). Hence, inside and outside a disposal facility for Group 3 waste, the NO$_3^-$ effect on solubilities and sorption distribution coefficients of actinoids with trivalent and tetravalent species is considered to be small. The sorption distribution coefficient of Am and Th on hardened cement paste and tuff is not decreased by coexisting NO$_3^-$ (Morooka et al., 2004), supporting the above evaluation result.

Under the oxidizing conditions in which NaNO$_3$ is saturated, U(VI), Pu(VI) and Np(V) might dominate chemical forms. Hence, complexation with nitrate ions under highly oxidizing conditions was evaluated using the JNC-TDB. It was found that nitrate complexes did not dominate the chemical species in the disposal facility. However, NpO$_2$NO$_3$ was found to be a dominant chemical species in lower pH, if the NO$_3^-$ concentration was above 0.15mol/dm$^3$. This result suggests the possibility that the increase in solubility and decrease in sorption distribution coefficient of Np(V) might occur outside the facility. However, this chemical species is not selected in the NEA-TDB, and the pros and cons of this chemical species selection should be discussed.

The effect of NH$_3$ has been considered by a thermodynamic evaluation of amine complex formation with radionuclides (Ochs et al., 2003). NH$_3$ of Lewis base can form a complex with metal ion of Lewis acid. However, since NH$_3$ is a “soft” base, it is especially difficult for NH$_3$ to form complexes with lanthanoids or actinoids. Hence, it is considered that “soft” and/or “B” type cation forms amine complexes easily (e.g.
Stumm and Morgan, 1996). Additionally, Ochs et al. (2003) evaluate the effect of NH₃ concentration on the solubility of NiO (cr) by using a previously obtained stabilization constant. As a result, it is estimated that there is an increase in solubility of about 20% when 1 mol/dm³ is reached. The solubility becomes three orders of magnitude larger in solutions with a 5mol/dm³ NH₃ concentration. The solubility of Ni was evaluated by changing the NH₃ concentration in experiments (Miyamoto et al., 2005). A significant increase in solubility was observed in a 0.1mol/dm³ solution, and a 3-4 orders of magnitude solubility increase were observed in a 1mol/dm³ solution. Considering that the maximum NH₃ concentration in pore water of the disposal facility is 0.8 mol/dm³ (Ochs et al., 2003), there is a possibility that the solubilities and sorption distribution coefficients of Ni, Pd, Sn, Nb, Co and Pb, which have a tendency of forming amine complexes, can be affected.

(3) Effects on soluble elements

The sorption distribution coefficients of C (organic type (formaldehyde) and inorganic type), I, Cl and Cs, might be affected by nitrate salt and NH₃ by a different mechanism to the above soluble complex formation (e.g. competition with nitrate ion and its counter ion). The effect of nitrate solution and NH₃ on the sorption distribution coefficient of C (organic type (formaldehyde) and inorganic type), I, Cl and Cs on hardened cement paste and tuff has been evaluated (Morooka et al., 2004). The sorption distribution coefficient of Cs on hardened cement paste is not significantly affected by nitrate salt. However, for the organic carbon, Cl and I, a decrease in the sorption distribution coefficient by nitrate salt was observed. The sorption distribution coefficient of Cs on tuff shows a significant decrease by addition of NaNO₃, though the effect of nitrate salt was not observed for C (inorganic and organic), Cl and I. A decrease in the sorption distribution coefficient of organic C on tuff by NH₃ was observed. However, the effect is covered by considering the effect of nitrate salt. Moreover, the effect of nitrate salt on the sorption distribution coefficients of organic carbon on cementitious material (OPC and OPC/BFS=1/9) and sedimentary rock were evaluated, and supports the above result (Sasou et al., 2004).

4.4.9.5 Summary

・ The maximum NH₃ concentration in the disposal facility was estimated by modelling to be 0.8mol/dm³. An increase in solubility and a decrease in sorption distribution coefficients by amine complex formation cannot be neglected for elements that easily form complexes with NH₃.
・ In the early stages of disposal, the generation of H₂ by corrosion is inhibited by competition with the reduction reaction of NO₃⁻. However, in the period with the fastest gas generation rate, total gas generation rate (H₂ by metal corrosion + N₂ by microbial activities) exceeds H₂ gas generation rate by corrosion without nitrate. The total generation rate of gas in this case is 1.4 times faster than in the case that only H₂ is generated by metal corrosion.
・ If NaNO₃ solution is passed through cementitious material, Ca dissolution might be promoted; the dissolution rate of Ca is 1.5 times larger than that when ion-exchanged waste is used. The relationship between the unconfined compressive strength and porosity of hardened cement paste
through which NaNO₃ is passed, can be expressed by the same formula as that which is used when
the fluid is ion-exchanged water. Hence, the decreasing strength of the altered paste is explained by
an increase in porosity.

・ The setting of solubility and sorption distribution coefficients for oxidizing conditions is necessary
because the disposal facility for Group 3 waste and its surroundings are oxidized owing to the large
amount of NO₃⁻.

・ In order to evaluate the effect on solubilities and sorption distribution coefficients of nitric complex
formation, the dominant chemical species of actinoid elements were evaluated. However, for the
trivalent and tetravalent actinoids, nitrate complexes do not become dominant chemical species
under alkaline conditions. Moreover, in a sorption experiment using NaNO₃ solution (3mol/dm³), no
effects on sorption distribution coefficients in hardened cement paste and tuff were observed with
and without nitrate and ammonia. Considering the oxidizing conditions caused by NO₃⁻, Np(V), U
(VI) and Pu(VI) were evaluated by using the thermodynamic database JNC-TDB. As a result, it was
shown that there is no influence on the conditions in the disposal facility. However, the Np (V)
species NpO₂NO₃ become dominant in lower pH, suggesting that there may be an influence outside
the repository. However, in the current NEA-TDB thermodynamic database, this complex is not
selected.

・ A decrease in the sorption distribution coefficients of soluble C (organic type), Cl and I on hardened
cement paste were observed in the presence of nitrate salt.

・ A decrease in the sorption distribution coefficient of Cs on tuff was observed in the presence of
nitrate salt.

・ A decrease in the sorption distribution coefficient of soluble C (organic type) on hardened cement
paste was observed in the presence of nitrate salt. However, the extent of the effect is covered by
considering the effect of the nitrate salt.

4.4.9.6 Future issues

The following are considered to be areas that require further study:

・ changes in the chemical forms of NO₃⁻ in geological media and improving knowledge about the
effects on groundwater chemistry and the effects on nuclide oxidation states;

・ the evaluation of nitrate plumes in geological media, taking into account the chemical transitions of
NO₃ within the geological media;

・ Data acquisition for the solubilities and sorption distribution coefficients of nuclides in solutions
with high concentrations of NaNO₃ and clarification of the threshold concentration of nitrate salt,
under which the effect of nitrate salt on solubility and sorption of nuclides can be neglected.

Moreover, the following issue is considered to be important for future research.

・ An evaluation of the mechanical effect of swelling pressure due to the osmotic pressure on solidified
bitumen.
4.4.10 Quantification of gas effects and the behaviour of gaseous nuclides

The waste and structural components in repository tunnels generate gases by metal corrosion, microbial degradation of organic material and radiolysis. The pore pressure will rise and the pore water will be expelled from the disposal facility by displacement of generated gas. Hence, it might affect the long-term safety of the facility. In the 1st TRU report, the mechanical effects of pore pressure buildup in the barriers and enhanced release of contaminated pore water were considered to be evaluation targets among these potential effects. In this section, considering the accumulation of knowledge about gas transport and improvements in evaluation techniques, non-radioactive gas generation and migration analyses are clarified in Section 4.4.10.1 (Ando et al., 2005). The pore pressure distribution in the EBS are used to confirm the mechanical integrity of the barriers. The effect of forcing out of contaminated water is included in the safety evaluation. Based on international evaluations of the gas effect (OECD/NEA, 2001; Rodwell and Norris, 2003), the quantities of generated radioactive gas and the migration analysis of gaseous radionuclides (Ando et al., 2005) are also evaluated by considering those radionuclides that are transported in gaseous form. These results are also included in the safety evaluation.

4.4.10.1 Generation and migration of non-radiogenic gases

(1) Method for evaluating gas generation rate and data

In repository, various types of gas generation by reduction of groundwater caused by metal corrosion, microbial degradation of organic materials and radiolysis of groundwater or waste is expected. The evaluation method for gas generation and data which is considering these features is described below.

a. Method for evaluating gas generation rate

(a) Metal corrosion

The metals in the disposal facility that are considered, are carbon steel and stainless steel, which are used for drums and structures, and zircaloy and inconel, which are used for fuel assemblies. It is assumed that hydrogen gas is generated by corrosion of these metals under reducing conditions.

(b) Degradation of organic materials by microbes

Bitumen and cellulose are considered to be the representative organic materials in the disposal facility. It is expected that gas generation occurs by microbial degradation of these organic materials. As described in Section 4.4.7, the gases that are generated mainly by microbial activity in the disposal facility are CO₂ (almost all microbes), N₂ (denitrifying bacteria) and CH₄ (methanogens). In this report, it is assumed that all amounts of cellulose is decomposed into gas completely. It is also assumed that aliphatic and aromatic hydrocarbons without asphaltene and resin are the subjects of microbial attack in bitumen. The component of aliphatic and aromatic hydrocarbons in bitumen is assumed 56%, based on experimental data obtained by blown bitumen.
(c) Radiolysis

Pore water and organic materials in the wastes and the backfill will be decomposed by radiation from radionuclides in the waste, and gases such as hydrogen will be generated. In cases that organic materials are irradiated, C-H bonds of organic materials are split and hydrogen radicals are generated. These radicals can react with organic materials and with other hydrogen radicals to produce hydrogen gas. Moreover, H• and OH• are generated by the radiolysis of water, and water molecules emit electrons under the high-energy radiation. These electrons generate dipole momentum in water molecules, and stabilized as aqueous electrons (eaq). The reaction that produces hydrogen gas occurs between reactive H•, OH• and eaq (EPRI, 1998).

b. Data for evaluation

(a) Metal corrosion

The rates of gas generation by metal corrosion were specified based on experimental measurements (Mihara et al., 2002; Nishimura et al., 2003). The reported values are equivalent corrosion rates that were calculated from the measured hydrogen gas generation rates of carbon steel, stainless steel and zircaloy at 30~50°C under alkaline conditions.

An experimentally determined corrosion rate for carbon steel of 1.0×10⁻⁷m/y (experimental conditions: pH=10.5, Cl⁻ concentration 20,000 ppm at 35°C for 200-500 days) was used for the evaluation. In the case of stainless steel, an experimentally determined rate of 2.0×10⁻⁸m/y (experimental conditions: pH=12.4, Cl⁻ concentration=3,200ppm at 35°C for 600 days) was used. The value for stainless steel was also used for inconel. For zircaloy, a corrosion rate of 5.0×10⁻⁹m/y (experimental conditions: pH=12.4, Cl⁻ concentration=3,200ppm at 35°C for 600 days) was used.

(b) Microbial degradation of organic materials

The data concerning gas generation by microbial degradation of organic material under alkaline conditions is extremely limited. In this report, data specified for the evaluation of a low-level radioactive waste repository (SFR) in Sweden were used (Moreno et al., 2001). A rate of 8.9×10⁻⁵mol/g/y (2.0×10⁻⁶STPm³/g/y in ref.) was used for cellulose and bitumen.

(c) Radiolysis

G values for H₂ gas generation were estimated as input data for calculating the amount of gas generated by radiolysis of water and bitumen. These values were collected and classified by Müller et al. (1992). For water, values of 0.05 molecules/100eV were assumed for β γ-rays and 0.5 molecule/100eV for α-ray. Additionally, for bitumen, G values of 0.26 molecule/100eV for β γ-rays and 0.72 molecule/100eV for α-ray were assumed.

(d) Content and form of metals and organic materials

The quantities of gas source materials in the disposal facility were estimated by calculating the amounts of metal and organic matter in the wastes, structure materials, liner and EDZ in each waste group and in
The metals were assumed to have a plate shape. Materials with unknown thickness were treated as if their thickness were 1.6 mm, which is equivalent to the thickness of drums. The endpieces were treated as plates with estimated outer dimensions of 213.5mm×213.5mm, thickness of 22.9mm and height of 93.4mm. The thickness of the endpieces as the plate was estimated to be 18.4mm from the calculation: volume/(surface area/2). The hulls were taken to be 0.57mm thick, as most thin PWR fuel cladding. Steel (H-type steel) for liner was assumed to form plates, the thickness of which was assumed to be 9mm. Since rock bolts have a diameter of 25mm, equivalent thickness as the plate shape was estimated to be 12.5mm. All organic material except for cellulose and bitumen were evaluated as though it was cellulose.

c. Calculated gas generation rates

The rate of gas generation in the repository tunnels by metal corrosion, microbial degradation and radiolysis in each waste group, was calculated. As an example of crystalline bedrock, the maximum cumulative amount of generated gas and the maximum gas generation rate in 1m length of repository tunnels, are shown for each waste group in Figure 4.4.10.1-1. The case with the largest gas annual generation rate was for wastes contained in 200L drum in Group 4 waste, which included metal waste with a large specific surface area, and gave a rate of 98.0 mol/m/y. The rate of 57.4 mol/m/y given by Group 4 waste in square packages followed. Since the maximum gas generation rate affects pore pressure buildup and the volume of expelled pore water, for conservative assessment, the highest gas generation rate for each waste group was specified in the gas migration analysis. The rates were calculated for Groups 2, 3 and 4 wastes by specifying wastes contained in canisters, 200L drums and 200L drums, respectively. The largest cumulative amount of gas generation of 5.51×10⁶ mol/m, was given by waste form of Group 4 in square packages. This package contains the largest amount of metal waste. The next largest amount was 3.74×10⁶ mol/m, given by Group 3 wastes in square packages. Furthermore, lower gas production amount were given by wastes in 200L drums of Group 3 waste and wastes in canisters of Group 2 waste gave even lower gas production.
As an example, gas generation rates of various gas sources are shown for Group 2 waste (canister) in Figure 4.4.10.1-2. The maximum rate of gas generation of Group 2 waste (canister) was dominated by the radiolysis of pore water in the waste. That is, the contribution of radiolysis by $\alpha$-ray was large since the $\alpha$-ray intensity is higher than in other waste. The dominant nuclides were Pu-239, Am-241 and Cm-244. Since the half-lives are 87.7 years, 432 years and 18.1 years, respectively, the rate of gas generation decreases moderately over a period of several hundreds years. Owing to decreases in the abundances of these nuclides, corrosion of hulls becomes the largest contribution to the gas generation rate after about 600 years. It was found that there are only small contributions to gas generation by pore water radiolysis in cementitious backfill and microbial gas production from organic materials.
(2) Evaluation of gas migration  
a. Evaluation method for gas migration and data  

A TRU waste disposal facility will be composed of cementitious material, compacted bentonite and host rock, which form barriers with different characteristics. There are different gas migration mechanisms in each of these media. There are different pore structures and mechanical properties. Appropriate migration models are required for each kind of fluid transport properties. The evaluation models for gas migration in each barrier material are described below.

(a) Method for evaluating gas migration in each barrier material  

For cementitious materials and porous host rock such as sandstone, tuff or limestone, it is generally possible to apply a continuous two-phase flow model that is based on Darcy's Law. An evaluation performed by EU (Rodwell and Norris, 2003), giving consideration to discussion in workshop held by OECD/NEA (OECD/NEA, 2001), stated that conventional two-phase flow models of gas migration are generally regarded as applicable to these materials and two-phase flow parameters are considered to be determined adequately.

Figure 4.4.10.1-2 Variation of gas generation rates with time – Crystalline bedrock, Group 2 (canister)
The behaviour of gas migration in swelling clay material, such as bentonite, is characterised by a distinctive threshold gas entry pressure that depends on density and mineral composition of the clay (Tanai et al., 1999), the permeability changed by gas pressure and very small amount of expelled pore water by gas migration. Hence, it is not certain that conventional two-phase flow-models are properly applicable to the gas transport mechanisms operating in clay materials. (Horseman and Harrington, 1997; Rodwell and Norris, 2003). However, well established models to simulate gas transport mechanisms in swelling clay is not available at present. Therefore, some modelling efforts to reflect formation of a preferential pathway and permeability change that depends on gas pressure were carried out based on the continuous two-phase flow model. By the application of specified two-phase flow parameters to reproduce gas migration behavior in clay materials (Yamamoto et al., 1999), Kozeny-Carmen relationship for permeability determination, a model for pressure effects on permeability and a model for reproducing breakthrough/shut-in behavior, better reproducibility of the breakthrough pressure and the amount of expelled gas and water were achieved.

In the case of fractured rock, it was considered that migration pathways would form by displacement of pore water in fractures. In the migration analysis of two-phase flow, attempts were made to apply fracture bundle model (FBM) and fracture network model (FNM), but these are insufficiently practical. An application of continuous two-phase flow model in combination with dual porosity model or dual permeability model to fractured rock is practical in the field of oil resource engineering and geothermal dynamics. The specification of two-phase flow parameters and considering heterogeneity is discussed. However, based on the OECD/NEA discussion, an EU evaluation (Rodwell and Norris, 2003) reported that application of the current continuous gas-liquid two-phase flow model is appropriate.

(b) Mathematical model and analysis code

A continuous two-phase flow model based on Darcy's Law was used. The multi-component, multi-phase fluids flow simulator TOUGH2 (Pruess and Battistelli, 1999) was used since it has been evaluated sufficiently in the past studies (Nagra, 2002; Baker et al., 1997). The Kozeny-Carman relationship and models to simulate changes of permeability by stress and breakthrough/shut-in behaviours of transport pathways (Bentonite Domain Module (Tanai and Yamamoto, 2003) were incorporated into TOUGH2 code, in order to reproduce features of migration in preferential pathways.

(c) Analysis data

This analysis used parameters for buffer material that were specified using the Bentonite Domain Module of enhanced TOUGH2, based on gas injection experiments performed under conditions of drainage and constant volume (Yamamoto et al., 2004). Additionally, two-phase flow parameters of barriers other than buffer were specified using a conventional two-phase flow model that was implemented using the original TOUGH2 code (Yamamoto et al., 2000). Two-phase flow parameters for cementitious back fill and host rocks were specified by using a continuous two-phase flow model. As far as possible these parameter values were based on the results of gas injection tests and the capillary pressure tests on the drainage side.
b. Results of gas migration analysis

A gas migration analysis was performed for each waste group. Temporal changes in the pore pressure and quantities of expelled pore water from each disposal tunnel were calculated. The calculated pore pressure in repository tunnels at a depth of 1,000m in crystalline rock, and at a depth of 500m in sedimentary rock, are shown in Table 4.4.10.1-1.

<table>
<thead>
<tr>
<th>Geological conditions at the depth of the disposal facility</th>
<th>Waste Gr.</th>
<th>Maximum gas generation rate (mol/m/y)</th>
<th>Maximum pore pressure /time of appearance (MPa) at (year)</th>
<th>Maximum pore water drainage rate /time of appearance (m³/m/y) at (year)</th>
<th>Maximum cumulative amount of drainage (m³/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystalline bedrock 1,000[m]</td>
<td>1 (Spent silver absorbent)</td>
<td>10.6</td>
<td>11.2 at 850 years</td>
<td>0.26 at 1,180 years</td>
<td>2.5</td>
</tr>
<tr>
<td>2 (Canister)</td>
<td>40.1</td>
<td>11.3 at 120 years</td>
<td>0.17 at 150 years</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>3 (200L Drum)</td>
<td>28.8</td>
<td>10.6 at 220 years</td>
<td>0.007 at 42 years</td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>4 (200L Drum)</td>
<td>98.0</td>
<td>10.6 at 85 years</td>
<td>0.024 at 14 years</td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>Sedimentary rock 500[m]</td>
<td>1 (Spent silver absorbent)</td>
<td>12.2</td>
<td>6.3 at 480 years</td>
<td>0.46 at 480 years</td>
<td>1.9</td>
</tr>
<tr>
<td>2 (Canister)</td>
<td>67.8</td>
<td>6.5 at 72 years</td>
<td>0.25 at 85 years</td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>3 (200L Drum)</td>
<td>30.3</td>
<td>5.7 at 180 years</td>
<td>0.014 at 24 years</td>
<td>2.2</td>
<td></td>
</tr>
<tr>
<td>4 (200L Drum)</td>
<td>99.6</td>
<td>5.8 at 46 years</td>
<td>0.046 at 8 years</td>
<td>2.3</td>
<td></td>
</tr>
</tbody>
</table>

As an example of these temporal changes, the calculated result of pore pressure and discharge of pore water for waste group 2 (canister) is shown in Figure 4.4.10.1-3. In the waste emplacement area at about 10 years after closure of disposal facility, gas phase is formed because H₂ exceeds the solubility in groundwater and pore pressure starts to increase. About 15 years, gas phase is formed in steel structural framework. In the buffer layer, the generated gas penetrates into EDZ from liner layer after about 150 years. At this time, gas saturation in waste emplacement area shows about 15% in maximum. After the generated gas penetrates into buffer layer, the pore pressure in disposal facility is rapidly decreasing and it becomes steady state at about 10.6MPa of pore pressure in waste emplacement area.

The pore water flow into host rock from disposal facility start to discharge rapidly by gas generation after 10 years of facility closure and it will stop with 0.17m³/y/1m tunnel length after 150 years by entrance of gas phase into EDZ. By the rapid decreasing of pore pressure in disposal facility, groundwater start to flow into the disposal facility and it becomes steady state at about 300 years after the closure of facility. The discharge rate of pore water per 1m tunnel is estimated to be about 0.006 ～ 0.009m³/y, and it reaches about 0.17m³/y in very short term at gas penetrating of buffer layer.
Figure 4.4.10.1-3 Example results from a gas migration analysis –Crystalline bedrock, Group 2 (canister)
(Left: Variation of pore pressure in the disposal facility, Right: Variation of pore water drainage rate)

4.4.10.2 Generation and migration of radioactive gas

(1) Evaluation aimed at gaseous radioactive nuclides

In the GASNET of EU project (Rodwell and Norris, 2003), the effect of radioactive gas on safety assessment is shown as follows.

The production of radioactive gases is insignificant relative to non radioactive gases in terms of volume, but the possibility of the radiological effect should be considered. As radioactive nuclide in gaseous form, C-14, H-3, Rn-222, I-129 and Kr-87 were considered. And it was expected that only C-14 introduced the radiation hazard after repository closure from the potential gaseous chemical forms, half life, amount of radioactive substance. As plausible gas including C-14, CO₂ and CH₄ are considered. However, since CO₂ is highly soluble and it forms CaCO₃ by reaction with Ca in cement pore water, it is considered that this chemical form is not able to reach to the surface. Hence, CH₄ including C-14(¹⁴CH₄) was considered as gaseous radioactive material to be estimated in this evaluation.

To estimate effects of radioactive methane, waste groups with largest amount of C-14 and CH₄ generation were considered. Hence, the¹⁴CH₄ release rates for waste group 3 which has largest amount of bitumen and thus highest CH₄ generation and waste group 2 with highest C-14 content were evaluated in this section.
(2) Amounts of radioactive gas generated

a. Method for calculating amounts generated

(a) Waste Group 2

Group 2 waste consists of compacted hulls and end-pieces including highest C-14 content. It was assumed that all of C-14 contained is discharged as CH₄. In the case of hulls, it is known that 20% of C-14 content exists in the surface oxide layer and other 80% exists in bulk metal. Hence, it was assumed that C-14 in surface oxide layer is discharged as CH₄ instantaneously into pore water at the time of site closure. Moreover, it considers that C-14 in the bulk metal of hulls, end-pieces and other material (stainless steel and other metal parts) is released congruently with corrosion loss of each metal as CH₄ into pore water.

The evaluation for corrosion in waste group 2 is calculated for hulls (zircaloy), end-pieces (stainless steel) and other metal parts. (It assumed that corrosion rate is the same as that of stainless steel.) Their C-14 content was estimated to be 66% in hulls (zircaloy), 34% in stainless steel and other metal parts. It also assumed that the C-14 content per weight of stainless steel and other metal parts is the same and that it contains 0.22 in stainless steel and 0.12 in other metal parts. Gas generation rates and equivalent corrosion rates considered that the cathode reaction under the reducing atmosphere is dominated by reduction of water and H₂ generation. However for the zircaloy, 4 times of the equivalent corrosion rate was used since a certain quantity of produced H₂ is absorbed into the zircaloy (Honda et al., 2005).

(b) Waste Group 3

The waste group 3 is the group which includes bituminized waste thus has the highest content of organic materials. Since the CH₄ ratio in generated gases by microbial degradation of bitumen remains considerable uncertainty at present, it assumed that all of C-14 in the waste group 3 is released as CH₄ in proportion to microbial degraded amount of bitumen as a conservative approach.

b. Calculation amount generated

The calculated maximum release rate of C-14 and maximum generation rate of ¹⁴CH₄ per unit length of disposal tunnel for waste group 2 (canister), and waste group 3 (200L Drum) are summarized in Table 4.4.10.2-1. The maximum released rate of C-14 in waste group 2 and 3 in crystalline rock are about 10⁹ Bq/m/y and 7×10⁵ Bq/m/y respectively. Moreover, the maximum generation rate of ¹⁴CH₄ of waste group 2 and 3 in crystalline rock are about 4×10⁻² mol/m/y and 3×10⁻⁷ mol/m/y respectively. The discharge rate per unit tunnel length of waste group 2 is different depending on the host rock condition which causes difference of cross sectional area of disposal tunnel.
Table 4.4.10.2-1 Maximum C-14 release rate and maximum generation rate in the case that all C-14 is released as CH₄

<table>
<thead>
<tr>
<th>Host rock condition</th>
<th>Waste group</th>
<th>Maximum C-14 release rate (Bq/m/y)</th>
<th>Maximum ¹⁴CH₄ generation rate (mol/m/y)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystalline rock</td>
<td>2 (Canister)</td>
<td>9.2×10⁸</td>
<td>4.0×10⁻²</td>
</tr>
<tr>
<td></td>
<td>3 (200L Drum)</td>
<td>7.1×10⁵</td>
<td>3.1×10⁻⁷</td>
</tr>
<tr>
<td>Sedimentary rock</td>
<td>2 (Canister)</td>
<td>1.5×10¹¹</td>
<td>6.6×10⁻²</td>
</tr>
<tr>
<td></td>
<td>3 (200L Drum)</td>
<td>7.1×10⁵</td>
<td>3.1×10⁻⁷</td>
</tr>
</tbody>
</table>

For the waste group 2 (canister) in crystalline bedrock, variation of gas generation rates in 1m of repository tunnel length with time are shown in Figure 4.4.10.2-1. The total radioactive CH₄ was estimated under the assumption that all contained C-14 is released as the chemical form of CH₄. Generation rate of the non radioactive CH₄ is calculated under the assumption that all of generated gas by microbial degradation of organic materials is CH₄. Since C-14 in the surface oxide layer of hulls is released instantaneously after closure of disposal facility, the CH₄ release rate in the first year is 3 orders of magnitudes larger than that of after 2 years and later. However, the value of the gas generation rate is estimated to be 4×10⁻²mol/m/y, and it estimates about 1/1,000 of maximum gas generation rate (40.1mol/m/y) for non radioactive gas from waste group 2 (canister). 2 years after and later, it decreased into 1×10⁻⁵mol/m/y and it continued with constant rate depending on the amount of metal corrosion rate, but the release rate is decreasing by decay of C-14 after 1000 years of site closure.

For the waste group 3 (200L Drum) in crystalline bedrock, variation of gas generation rates in 1m of repository tunnel length with time are shown in Figure 4.4.10.2-2. The total radioactive CH₄ was estimated under the assumption that all contained C-14 is released as CH₄. Generation rate of the non radioactive CH₄ is calculated under the assumption that all of generated gas by microbial degradation of organic materials is CH₄. In waste group 3, C-14 is released depending on the decreasing of microbial degraded amount of bitumen just after the site closure. Hence, CH₄ is released by 3×10⁻⁷mol/m/y with constant rate. This is equal to about 1/10⁸ of maximum gas generation rate (28.8mol/m/y) for non radioactive gas in waste group 3 (200L Drum) as shown in Table 4.4.10.1-1. The generation rate of ¹⁴CH₄ is decreasing by decay of C-14 after 1,000 years of site closure.
Figure 4.4.10.2-1 $^{14}$CH$_4$ generation rate – Crystalline bedrock, Group 2 (canister)

Figure 4.4.10.2-2 $^{14}$CH$_4$ generation rate – Crystalline bedrock (Group 3: 200L drum)
(3) Evaluation of gas migration

a. Method and data for evaluating gas migration

The basic evaluation method of gas migration of $^{14}\text{CH}_4$ is same as that is used in non radioactive gas migration analysis. Since features of the CH$_4$ gas for migration analysis such as solubility are different in this case, TMVOC code (Pruess et al., 1999) which is improved TOUGH2 code was used. Since smaller amount of CH$_4$ dissolution on the pathway to surface is expected because of the shorter migration distance, the repository in the sedimentary rock at 500 m depth was evaluated.

b. Results of gas migration analysis

In the case of waste group 2 in sedimentary, rock, since all amount of generated CH$_4$ is dissolved into groundwater, gaseous CH$_4$ does not reach the surface. In the case of waste group 3, while so that the amount of C-14 is smaller than that of group 2, since the generated amount of CH$_4$ is much larger, gaseous CH$_4$ reaches to the surface. The variation of migration rate of $^{14}\text{CH}_4$ on surface with time is shown in Figure 4.4.10.2-3. The gaseous $^{14}\text{CH}_4$ reaches at surface $10^4$ years after site closure. Comparing with the generated amount of $^{14}\text{CH}_4$, the maximum value of migration rate is 1 order of magnitude smaller because of decreasing by methane gas dissolution into groundwater and decay of C-14 (half life 5,730 years). In this analysis, since CH$_4$ concentration in freshwater type groundwater is small ($10^{-9}$mol/dm$^3$), it is evaluated by considering that any CH$_4$ is not existed in initial groundwater. While, since CH$_4$ concentration is high ($10^{-2}$mol/dm$^3$) in the sea water type ground water (JNC, 2000), the dissolution of radioactive methane gas is expected to be smaller and the dilution effect by stable isotope might works in the sea water type groundwater. Hence, these effects should be evaluated in future.

![Figure 4.4.10.2-3 Migration rate of $^{14}\text{CH}_4$ on the surface (Group 3)](image-url)
4.4.10.3 Summary

For each waste group, the gas generation rates by metal corrosion, microbial degradation of organic materials and radiolysis were calculated. The maximum generation rate is estimated to be 7 to 100mol/m/y per 1m of repository tunnel, and it is revealed that the contribution of metal corrosion is the largest except for waste group 2 which shows the highest contribution of gas generation mechanism was radiolysis by $\alpha$-emitting nuclides.

The pore pressure build up from initial groundwater pressure in crystalline rock by gas generation shows 1.3 to 1.4MPa in waste group 1 and 2, and about 0.7MPa in waste group 3 and 4 which are constructed without buffer material. The mechanical stability of EBS is evaluated based on this result. The maximum discharge rate of pore water per 1m length of the disposal tunnel with buffer material of waste group 2 is 0.006 to 0.009m$^3$/m/y (0.17m$^3$/m/y in very short period). In the tunnel without buffer material, the maximum discharge rate of pore water in waste group 4 is 0.018 to 0.024m$^3$/m/y. These results were used as for one scenario in the safety assessment.

The calculated amount of radioactive gas based on the conservative assumption shows $4 \times 10^{-2}$mol/m/y for CH$_4$ in waste group 2 (canister) in crystalline rock and it is equal to about 1/1,000 of 40.1mol/m/y of non radioactive gas generation. After more than two years, it decreases to $1 \times 10^{-5}$mol/m/y. In waste group 3 (200L Drum), CH$_4$ is released with constant rate of $3 \times 10^{-7}$mol/m/y which is equivalent to about 1/10$^8$ of gas generation rate of non radioactive gases.

The results of migration analysis of radioactive gas for $^{14}$CH$_4$ show that in the case of waste group 2 the gaseous $^{14}$CH$_4$ does not reach to surface because of dissolution of methane gas into groundwater. Dissolution of all generated radioactive gas in aquifer was assumed as a reference for the evaluation of effect of gaseous radionuclides in EN2002 (Nagra, 2002). However, in the case of group 3, gaseous $^{14}$CH$_4$ reaches to the surface since the generated amount of methane gas is much larger. The maximum migration rate at surface is about $3 \times 10^{-8}$mol/m/y in this case.

4.4.10.4 Future issues

In the evaluation of gas generation rates, the gas generation rate from metal is held. In future, more realistic evaluations that consider the temporal change of metal corrosion rate, evaluation of gas generation rate by microbial degradation under repository conditions and development of long-term microbial gas generation models are needed.

In gas migration assessment, especially transport properties in clay material are affected by stress field, thus it is necessary to develope gas-liquid migration models combined with stress analysis models. Moreover, transport parameter values evaluated from different experimental conditions of effective clay dry density, chemical condition of groundwater, stress condition and saturation condition. In order to evaluate re-saturation process, data collection of two-phase flow parameters for inhibition processes including hysteresis feature of clay materials are necessary. It is also necessary to acquire two-phase flow parameter data for different rock types and to perform realistic assessment of gaseous radioactive migration to surface by development of gas migration model in fractured rock. Furthermore, more realistic evaluation is able to be achieved by development of analytical tool combined appropriate models for each transport
media and by the validation of the analysis tool using in-situ test results.

For the evaluation of radioactive gas generation rate, since it is assumed that all of contained C-14 in waste is released as CH₄ gas at the present time, it is necessary that acquisition of release rate data of C-14 as a gaseous chemical species and generation rate data of gaseous radioactive material from bituminized waste and investigation of radioactive gas generation model are performed. In the migration evaluation of radioactive gas, in the modeled mixed gas system of ¹⁴CH₄ and non radioactive gases, isotope dilution with dissolved gas is neglected conservatively, while the assumption of 0 initial concentration of dissolved non radioactive gas in groundwater is unconservative. Further examination of these assumptions is needed. Moreover, the model which is combined with the transition model of CH₄ to other chemical species assimilated by ecological system, such as CO₂, should be investigated and validated.

In this section, various environmental conditions important for safety assessment and the investigation of new insight, analysis and evaluation related to discrete phenomena were described. The evaluation results of the environmental (Thermal/Hydraulic/Mechanical/Chemical/Radiological) conditions and the discrete phenomena are summarized in Figures 4.4.10.4-1 and 4.4.10.4-2, respectively.
<table>
<thead>
<tr>
<th>Environmental condition</th>
<th>Evaluation results of environmental conditions</th>
</tr>
</thead>
</table>
| Temperature             | • A heat conduction analysis was performed for soft rock-type host rock (SR-C) and hard rock-type host rock (HR) for Group 2 waste. The temperature at the centre of the waste was specified to be below 80°C, considering the alteration of cementitious material.  
  • The temperature at the centre of the waste was estimated to be 79°C in soft rock-type host rock and was estimated to be 77°C in hard rock-type host rock. |
| Hydrological conditions | • There was an increase in the Darcy flow velocity of groundwater in the EBS as the barrier’s low-permeability characteristics were compromised. However, if the buffer material changed to a Ca type, the Darcy flow velocity of groundwater in the EBS was lower than that in the host rock. Moreover, if the hydraulic conductivity of the buffer material changed and became similar to that of sand, the Darcy flow velocity of groundwater in the EBS became 2.5 times higher than that in the host rock.  
  • Considering the long-term alteration of the EBS, the sensitivity of the amount of groundwater flow to the region affected by drilling was neglected and the flux was about 0.002 m³/y/m. |
| Mechanical conditions   | • For soft rock-type host rock (SR-C) and hard rock-type host rock (HR), the creep deformation during 1,000,000 years was estimated to be several cm. The deformation of the EBS caused by the swelling pressure of the buffer material was trivial.  
  • The effect of temperature, stress and gas pressure on the near-field was small.  
  • The decrease in density of the buffer material caused by extrusion into fractures was small. The effect on the mechanical stability of the near-field of out-flowing bentonite was small. |
| Chemical conditions     | • Freshwater-type groundwater, which is appropriate for the geological settings and rock types in Japan, is considered to be the reference groundwater.  
  • Seawater-type ground water is also considered, since there is groundwater that originated in sea water.  
  • In waste and backfilled regions, the chemical conditions of Regions I, II, III, which are decided by chemical equilibrium between cementitious material and groundwater components, are considered.  
  • In the buffer material region, dissolution of minerals forming the buffer material and precipitation of secondary minerals change over time. Hence, the chemical conditions of the pore water are also changed. |
| Radiation field         | • Since waste package B, which stores hulls and end-pieces, has no barrier such as overpack for shielding, the surface radiation dose becomes several orders higher than the radiation dose at the surface of overpack used for HLW. This shows that it is necessary to evaluate the radiation dose to secure safety during waste emplacement and closure work. From current knowledge, it is considered that exposure damage of bentonite material does not occur.  
  • The possibility that oxidizing species generated by radiolysis of water, may form an oxidizing atmosphere is considered to be low. This conclusion is based on an evaluation of: the supply rates and amounts of reducing agents in the canister; the generation of oxidizing species; and the migration behaviour of oxidized and reduced species in mortar and buffer material. |
<table>
<thead>
<tr>
<th>Discrete phenomena</th>
<th>Result of evaluating discrete phenomena</th>
</tr>
</thead>
</table>
| **Long-term behaviour of the EBS (4.4.2)** | • The alteration scenario for the EBS was analysed using a model that combines chemical reaction and mass transport, taking into account mineral transitions, dissolution rates of minerals and uncertainties in mass transport parameters. In most cases the results showed that pores on the cement side of the cement/bentonite boundary were closed.  
• Owing to pore closure, the transition region (> pH12.5) of the cement material is maintained for a long time (e.g. Region I is 10^5 years.).  
• Additionally, it was revealed that the capability of bentonite to prevent water flow is maintained for 10^5 years.  
• Considering the uncertainties in both thermodynamic data for minerals and the dissolution rate law, a loss of swelling cap ability by cementation is considered to be possible. If this is significant, the capability to prevent water flow will be lost after several 1,000 years. |
| **Hyperalkaline alteration of surrounding host rock (Section 4.4.3)** | • The experimental investigations of hyperalkaline reactions of minerals, showed the possibility that poorly crystalline minerals would dissolve and secondary minerals, such as C-S-H gel, would be formed.  
• Analyses of mineral chemical reactions and mass transport showed that secondary minerals such as C-S-H gel would be formed in host rock surrounding the disposal facility.  
• Additionally the overall long-term mechanical behaviour of host rock, which is affected by processes such as changes in pores caused by mineral dissolution and generation of secondary minerals, has not been established. The region that shows significant changes is limited, and the possibility of porosity decreasing is also considered in the locations where secondary minerals precipitate.  
• These results show that the effects of the alkaline component on the surrounding host rock occur near the disposal facility. There are no significant effects on the overall nuclide migration pathways.  
• There is not enough knowledge about changes in sorption distribution coefficients in the surrounding host rock, caused by generation of secondary minerals. Additionally, there is insufficient knowledge about constraints on matrix diffusion and mass transport of nuclides by decreasing porosity. Further evaluations of these matters are necessary. |
| **Effect of colloids (Section 4.4.5)** | • The effects of colloids in the EBS are considered to be small because of the filtration effect in bentonite. Additionally, colloids will have low concentrations and a small effect on sorption.  
• The effects of colloids in natural barrier cannot be determined. This is because there are considerable variations in colloid concentrations and properties and there is a lack of information about properties of the transport medium, including its heterogeneity. For these reasons, quantitative evaluations are difficult in present.  
• It is considered to be possible to estimate colloid effects by adding the effects of CFT into a nuclide migration analysis. |
| **Effect of organic materials (Section 4.4.6)** | • Natural organic material is treated in the same way as in the H12 report. Engineered organic materials (bitumen, TBP and its degradation products, cellulose and cement additives) are evaluated.  
• The effect on nuclide solubility and sorption behaviour of bitumen and the TBP and breakdown products of TDB that it contains, are considered to be small.  
• Organic material in hulls and end-pieces is evaluated by considering that it all changes into ISA. If the concentration of ISA in pore water in the disposal facility is assumed to be 5×10^{-6}mol/dm^3, the resulting nuclide migration analysis is shown to be conservative.  
• The cement additives in themselves result in increases in the solubilities of radionuclides. However, the effects on adsorption distribution coefficients of nuclides in cementitious materials are considered to be small, since additives have a strong adsorption capability in cement material and dissolved organic material is of low molecular mass. |
### Table 4.4.10-4-2 Summary results from an evaluation of discrete phenomena (2/2)

<table>
<thead>
<tr>
<th>Discrete phenomena</th>
<th>Result of evaluating discrete phenomena</th>
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</thead>
<tbody>
<tr>
<td><strong>Effect of microbes</strong></td>
<td>- Microbial activity in disposal facilities for each group of waste has been summarised. The evaluation covered: formation of complexes; pH changes; redox reactions; concrete alteration; metal corrosion; bentonite alteration; pore closure and microbial effects on gas generation.</td>
</tr>
<tr>
<td>(Section 4.4.7)</td>
<td>- Amounts of organic material/CO₂ generated from organic material and TBP, and amounts of nitrogen and phosphoric acid generated were evaluated. It was concluded that the generation of redox-sensitive species, colloid formation and the generation of radioactive gaseous chemical species might affect the disposal system. However, since uncertainties about microbial activity are significant and validation of specified parameters is difficult, these are issues for future consideration.</td>
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<tr>
<td></td>
<td>- Other microbial effects on the disposal system are considered to be small.</td>
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<tr>
<td><strong>Effect of nitrate salts</strong></td>
<td>- The calculated maximum ammonia concentration in the disposal facility is 0.8mol/dm³. An increase in metal solubility by formation of amine complexes cannot be neglected.</td>
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<tr>
<td>(Section 4.4.9)</td>
<td>- In the early stages of disposal, the generation of hydrogen by decomposition is limited. However, if NO₃⁻ concentration is decreasing and the activity of water is above 0.94, denitrifying bacteria are active and generate nitrogen. The total gas generation rate then increases.</td>
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<td></td>
<td>- The dissolution of Ca is promoted if NaNO₃ is transported. The relationship between unconfined compressive strength and the porosity of cement paste, in the case that the NaNO₃ solution is transported, is represented by a formula for the case where ion-exchanged water is present. That is, a decrease in strength of the altered part of the paste is explained by an increase in porosity.</td>
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<tr>
<td></td>
<td>- Using the current thermodynamic database, nitric acid complexes of actinoids are not calculated to dominate the chemical species under the alkaline conditions of Region I and II.</td>
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<td></td>
<td>- An experiment using NaNO₃ solution (3mol/dm³) revealed that the presence of nitric acid and ammonia have no effect on sorption distribution coefficients in OPC paste and tuff.</td>
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<td></td>
<td>- A decrease in the sorption distribution coefficients are observed for sorption of organic carbon in C1 and I cement paste and for sorption of Cs in tuff.</td>
</tr>
<tr>
<td><strong>Effect of gas</strong></td>
<td>- From the analyses of gas generation and migration, the increasing in pressure in the disposal facility is estimated to be 1.3 ~ 1.4MPa for Group 1 and 2 wastes in crystalline rock. The possibility of mechanical damage to the buffer material being caused by such a pressure increase is considered to be small.</td>
</tr>
<tr>
<td>(Section 4.4.10)</td>
<td>- In cases where tunnels contain buffer material, Group 2 waste shows the maximum pore water outflow rate from the EBS caused by gas generation. This rate is 0.006 to 0.009m³/y. In the case where a tunnel does not contain buffer material, waste Group 4 shows a maximum value of 0.018 to 0.024m³/y.</td>
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<td></td>
<td>- For Group 2 and 3 waste, the amount of gas reaching into the biosphere is analysed based on the hypothesis that all the C-14 is incorporated into CH₄. The amount of gas that reaches the biosphere was calculated. The results showed that the gas is substantially dissolved in the groundwater. Consequently, there is little possibility that gas will reach the biosphere. Additionally, for Group 3 waste, the greatest amount of CH₄ produced is 3 x 10⁸ mol/m/y (per unit length of tunnel).</td>
</tr>
</tbody>
</table>
4.5 Radionuclide transport analysis and dose assessment

TRU waste typically includes a wide variety of waste materials, such as metal, nitrates and organic material. I-129 and C-14 are the key radionuclides that dominate dose. The amounts of radionuclides (inventory) in TRU wastes are lower than those in high-level waste (HLW) and the heat generation of TRU waste is also lower than that of HLW. Hence in the disposal concept for TRU waste no overpack is required. Except for metal-containing waste belonging to Group 2, the waste packages are not expected to fulfil the function of restricting radionuclide release. Additionally, since heat generation is small, wastes can be emplaced together in tunnels with large cross-sections, with void spaces between wastes being filled with cement mortar.

The variety of materials used may have an impact on the disposal environment and this is a cause of uncertainty in safety assessments of TRU waste disposal. Considering the features of a geological repository for TRU waste in Japan, and the fact that the repository site has not yet been selected, in order to demonstrate safety, a conservative disposal analysis that takes into account various uncertainties is necessary.

An OECD/NEA report (OECD/NEA, 2004) suggests that the evaluation of uncertainty should be included in safety assessment in order to improve reliability. Hence, in this section, radionuclide transport analyses and dose assessments are performed using an existing deterministic approach (deterministic consequence calculation) (OECD/NEA, 1991) and a newly developed top-down assessment approach, “a comprehensive sensitivity analysis method” (Ooi et al., 2004), to complement the existing approach from the point of view of uncertainty.

The specifications and methods used in analytical cases based on the disposal environment conditions outlined in Section 4.4 are described in Section 4.5.1. The radionuclide transport database and the deterministic consequence calculation used in the Reference Case of the base scenario of the groundwater scenario in Section 4.5.1 is described in Section 4.5.2. The deterministic consequence calculation, which is also applied to the alternative cases of the base scenario (alternative scenario) of the groundwater scenario, is described in Section 4.5.3, and the results of comprehensive sensitivity analyses are described in Section 4.5.4. An analysis of the perturbation scenario of the groundwater scenario is described in Section 4.5.5, and the results of an assessment of the isolation failure scenario are described in Section 4.5.6.

4.5.1 Analytical cases

Analytical cases are specified based on analyses of individual phenomena described in Section 4.4 and take into account model and parameter uncertainties (Table 4.5.1-1). The reference scenario analytical case in the base scenario of the groundwater scenario is termed the Reference Case. Other analytical cases in the base scenario are termed alternative cases. The type of uncertainty/case and the assessment method used (deterministic consequence calculation or comprehensive sensitivity analysis) in each analytical case are
shown in Table 4.5.1-1. The type of uncertainty/case considered are as follows:

① Reference Case of the groundwater scenario
   Reference scenario analytical case in the groundwater scenario, which is based on the most likely phenomena in the TRU waste repository. This forms the base case, under the influence of uncertainty, against which alternative cases are compared.

② Groundwater scenario uncertainty
   Analytical case which considers possible phenomena that are not considered in the Reference Case.
   The range of possible phenomena affecting dose in the assessment is a source of uncertainty.

③ Groundwater scenario uncertainty (hypothetical setting)
   Analytical case taking into account possible phenomena for which knowledge or data is sparse. The use of hypothetical parameter values is a source of uncertainty.

④ Groundwater model/parameter uncertainty
   Uncertainty relating to selection of models and parameters used in assessments.

⑤ Analysis of perturbation scenarios
   Analytical cases that consider the impact of future human activity and alteration of the natural barrier over the long term

⑥ Analysis of the isolation failure scenario
   Case where the repository is penetrated by accidental drilling or is exposed at the surface due to uplift and erosion

In this section, the influence of these uncertainties is assessed using deterministic consequence calculations supplemented with a comprehensive sensitivity analysis for ② – ④
### Table 4.5.1-1 Relationship between scenarios, analytical cases and uncertainties

<table>
<thead>
<tr>
<th>Scenario classification</th>
<th>Important conditions etc</th>
<th>Supposed phenomenon</th>
<th>Treatment in analysis</th>
<th>Analytical case</th>
<th>Uncertainty /Case</th>
<th>Method</th>
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<tbody>
<tr>
<td><strong>Groundwater scenario</strong></td>
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<tr>
<td>Base scenario</td>
<td>Temperature influence</td>
<td>Disposal facility is designed such that temperature does not exceed 80°C</td>
<td>Not considered</td>
<td>Reference case</td>
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<td></td>
<td>Hydraulic field (resaturation and nuclide release)</td>
<td>Nuclide leakage starts at saturation after closure of facility</td>
<td>Nuclide migration data for host rock varies with alkali alteration</td>
<td>Ground water scenario uncertainty</td>
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<td></td>
<td>Mechanical conditions</td>
<td>Geochemical conditions have small influence on mechanical conditions</td>
<td>Mechanical stability is not considered</td>
<td>Ground water scenario uncertainty</td>
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<tr>
<td></td>
<td>Groundwater chemistry</td>
<td>Freshwater is assumed in underground environment</td>
<td>Nuclide migration data for host rock varies with alkali alteration</td>
<td>Ground water scenario uncertainty</td>
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<tr>
<td></td>
<td>Radiological effects</td>
<td>Radiological effects small</td>
<td>Nuclide migration data for host rock varies with alkali alteration</td>
<td>Ground water scenario uncertainty</td>
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<td></td>
<td>Effects of organic nuclides in waste</td>
<td>Organic material in group 2 is affected in disposal facility</td>
<td>Same treatment as alteration of engineered barrier material</td>
<td>Ground water scenario uncertainty</td>
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<td></td>
<td>Nitrates affect group 3 waste</td>
<td>For group 3, nuclide migration data is setup by considering an oxidizing condition caused by nitrates and high ion strength</td>
<td>Ground water scenario uncertainty</td>
<td>Ground water scenario uncertainty</td>
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<td></td>
<td>Nuclide migration</td>
<td>Dissolution/precipitation, sorption, diffusion, advection - dispersion, etc.</td>
<td>Same treatment as colloid effects</td>
<td>Ground water scenario uncertainty</td>
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<td>Alternative scenario</td>
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<td>Effects of alteration of surrounding host rock</td>
<td>Alteration of cement material and dissolution of anhydrate in buffer material occurs</td>
<td>Nuclide migration and hydraulic parameters vary by cement material and buffer material alteration with time</td>
<td>Ground water scenario uncertainty</td>
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<td></td>
<td>Alkaline alteration of surrounding host rock</td>
<td>Wide area of basement rock affected by alkali alteration</td>
<td>Nuclide migration data for host rock varies with alkali alteration</td>
<td>Ground water scenario uncertainty</td>
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<td>Hydrogeological conditions of the near field (influence of geochemical alteration)</td>
<td>Hydraulic condition of barrier material is affected by alteration of engineered barrier</td>
<td>Same treatment as alteration of engineered barrier material</td>
<td>Ground water scenario uncertainty</td>
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<td>Long term re-flooding does not terminate</td>
<td>Long term re-flooding does not terminate</td>
<td>Same treatment as alteration of engineered barrier material</td>
<td>Ground water scenario uncertainty</td>
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<tr>
<td></td>
<td>Effect of colloids</td>
<td>Colloids exist in natural barrier</td>
<td>Dissolution condition is maintained for a short time after closure and nuclide migration parameters varies with time</td>
<td>Ground water scenario uncertainty</td>
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<td>Natural organic matter affects nuclide migration</td>
<td>Natural organic matter affects nuclide migration</td>
<td>Nuclide migration data for host rock varies considering effects of natural organic matter (hypothetical values used)</td>
<td>Ground water scenario uncertainty</td>
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<td></td>
<td>Effects of microbes</td>
<td>Nuclides absorbed by microbes and migrate as colloids</td>
<td>Same treatment as that of colloid effects</td>
<td>Ground water scenario uncertainty</td>
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<td>Gas is generated by microbe activity</td>
<td>Gas is generated by microbe activity</td>
<td>Same treatment as that of gas migration and gaseous nuclide migration</td>
<td>Ground water scenario uncertainty</td>
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<td>Effects of gas and nuclides in gaseous form</td>
<td>Ground water in engineered barrier flows out by gas generation Nuclides migrate in gaseous form</td>
<td>Nuclide migration data for host rock varies with alkali alteration</td>
<td>Ground water scenario uncertainty</td>
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### Table 4.5.1-2 Relationship between scenarios, analytical cases and uncertainties (continued)

<table>
<thead>
<tr>
<th>Scenario classification</th>
<th>Important conditions etc</th>
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<tr>
<td>Baseline</td>
<td>Parameter of nuclide migration is set considering variation geological environment</td>
<td>Nuclide migration and hydraulic parameters vary by cement material and buffer material alteration with time</td>
<td>Nuclide migration data for host rock varies with alkali alteration</td>
<td>Ground water scenario uncertainty</td>
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<td>Data set considering uncertainty of natural barrier conditions</td>
<td>Data set considering uncertainty of natural barrier conditions</td>
<td>Same treatment as alteration of engineered barrier material</td>
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<td>Improved performance of waste</td>
<td>Improved performance of waste</td>
<td>Dissolution condition is maintained for a short time after closure and nuclide migration parameters varies with time</td>
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<td>Data set with various disposal facility designs</td>
<td>Data set with various disposal facility designs</td>
<td>Dissolution condition is maintained for a short time after closure and nuclide migration parameters varies with time</td>
<td>Ground water scenario uncertainty</td>
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<td></td>
<td>Porous media model is used as a nuclide migration model in the natural barrier</td>
<td>Porous media model is used as a nuclide migration model in the natural barrier</td>
<td>Nuclide migration data for host rock varies considering effects of natural organic matter (hypothetical values used)</td>
<td>Ground water scenario uncertainty</td>
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</table>

### Table 4.5.1-2 Relationship between scenarios, analytical cases and uncertainties (continued)

<table>
<thead>
<tr>
<th>Scenario classification</th>
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<th>Treatment in analysis</th>
<th>Analytical case</th>
<th>Uncertainty /Case</th>
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<td>Natural phenomenon</td>
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<td>Uplift and erosion</td>
<td>Uplift and erosion</td>
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<td>Initial defects connected with engineered components</td>
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<td>Sealing mistake</td>
<td>Analysis of perturbation scenario</td>
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<td>Future human activity</td>
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<td>Formation of migration pathway by drilling</td>
<td>New pathway created by drilling</td>
<td>New pathway created by drilling</td>
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### Table 4.5.1-2 Relationship between scenarios, analytical cases and uncertainties (continued)

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<th>Treatment in analysis</th>
<th>Analytical case</th>
<th>Uncertainty /Case</th>
<th>Method</th>
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<td><strong>Isolation Failure scenario</strong></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uplift and erosion</td>
<td>Uplift and erosion</td>
<td>Uplift and erosion</td>
<td>Uplift and erosion</td>
<td>Uplift and erosion</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Accidental future human intrusion</td>
<td>Exploratory drilling</td>
<td>Exploratory drilling</td>
<td>Exploratory drilling</td>
<td>Analysis of isolation failure scenario</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

4-134
4.5.2 Analysis of the Reference Case

The deterministic consequence calculation of the Reference Case is described in this section. The assumptions used in the calculation, radionuclide transport datasets, radionuclide transport analytical models, biosphere models and data, model chain, analytical results and summary are described in sections 4.5.2.1, 4.5.2.2, 4.5.2.3-4.5.2.5, 4.5.2.6, 4.5.2.7, 4.5.2.8 and 4.5.2.9, respectively.

4.5.2.1 Assumptions in the analysis

The disposal concept assumptions, radionuclide transport pathways and analytical results of the deterministic consequence calculations for the Reference Case are summarised below.

(1) Disposal concept

The depth of the disposal facility is assumed to be 1,000 m in crystalline rock (Figure 4.2.4-1). This ensures reducing groundwater conditions.

(2) Radionuclide transport pathway analysis

- Radionuclide transport pathway in the engineered barrier system:

  In the engineered barrier system, radionuclide leaching from the waste and migration through the buffer and filling materials into the host rock are analyzed. In the Reference Case, waste packages are present but their radionuclide containment capability is not taken into account. Hence, radionuclides are assumed to dissolve rapidly from the waste and migrate into the filling material, with the exception of activation products in stainless steel and ends such as zircaloy.

- Radionuclide transport pathways in the host rock:

  Radionuclide migration from the engineered barrier system into the host rock and faults is modelled based on the radionuclide transport analysis performed in H12 report (JNC, 2000). In this analysis, complex geological structures are not considered and the disposal facility is located at a distance of 100 m from a fault. It is assumed that radionuclides migrate in groundwater to the fault which is located downstream of the facility.

- Radionuclide transport pathways in faults:

  An analysis is performed of radionuclide transport through the host rock and into the biosphere (aquifer) via a fault. A sediment layer above the host rock is assumed to be 200 m thick and it is assumed that an aquifer is present between the sediment layer and the host rock.

  Since the disposal depth is assumed to be 1,000 m, the radionuclide transport distance through the fault is assumed to be 800 m.

- Radionuclide transport and dose in the biosphere:

  It is assumed that radionuclides that migrate from the disposal facility into the host rock will
eventually enter the biosphere (aquifer) via the fault (Figure 4.5.2-1).

Figure 4.5.2-1 Radionuclide transport pathway in the Reference Case

(3) Assessment period and output from analytical results
The output of analytical results are radionuclide transport rates (Bq/y) and dose (Sv/y) for each waste Group. In the H12 report, an assessment period of $10^7$ years was considered. In the evaluation in the 1st performance assemment report for TRU waste it was revealed that the maximum dose was reached after several 10,000 years and was not exceeded even after $10^7$ years. Hence, the time period for the analyses was set at $10^7$ years.

(4) Target radionuclides
Radionuclides with high toxicity are selected as target radionuclides for analysis, as in the 1st performance assemment report for TRU waste disposal and the H12 report. Radionuclides which can be treated as being in equilibrium with their parent radionuclides are considered in the biosphere assessment.

C-14, Cl-36, Co-60, Ni-59, Ni-63, Se-79, Sr-90, Zr-93
Nb-94 (Nb-93m), Mo-93, Tc-99, Pd-107, Sn-126, I-129, Cs-135, Cs-137
Cm-244→Pu-240→U-236→Th-232→Ra-228→Th-228
Cm-245→Pu-241→Am-241→Np-237→U-233→Th-229
Cm-246→Pu-242→U-238→U-234→Th-230→Ra-226→Pb-210 (Po-210)
Am-243→Pu-239→U-235→Pa-231→Ac-227
Note: The underlined radionuclides are target radionuclides used in radionuclide transport analyses. U-234 is taken as the parent radionuclide and Am-242m→Pu-238 is considered in the radionuclide transport analysis in the engineered barriers. U-234 is added to the radionuclides used in the analysis. Nb-93m and Po-210 are assumed to be in radioactive equilibrium with their parent radionuclides.

4.5.2.2 Dataset for radionuclide transport analysis (RAMDA: RADionuclides Migration DATaset)
Radionuclide solubilities, effective diffusion coefficients and sorption distribution coefficients (for cement mortar, bentonite and rock) were specified in a dataset for radionuclide transport analysis (RAMDA, Mihara and Sasaki (2005)). This dataset considers the chemical variations in the engineered barriers for TRU waste disposal. Data used in the Reference Case are taken from this database as outlined below.

(1) Solubilities ($C^s$)
Radionuclide solubilities are strongly affected by the chemical composition and pH of pore water in cement mortar. The pH of the pore water and the long-term chemical evolution in cement mortar are divided into 3 regions (Regions I, II and III in Figure 4.4.2.2-1). Based on calculations using a geochemical equilibrium model (JNC-TDB) (Yoshida and Shibata, 2005), the solubilities of elements for which there are insufficient thermodynamic data are defined by referring to chemical analogues and/or experimental data.

(2) Effective diffusion coefficients ($D^e$)
For cement mortar, the effective diffusion coefficient is specified as a function of porosity based on measurements of tritium. Moreover, for cracked cement mortar, the diffusion coefficient in pore water is set as being the same as that in free water. For buffer material, the effective diffusion coefficient is also specified as a function of porosity and amount of smectite, which is obtained from experimental data.

(3) Sorption distribution coefficients ($\alpha^s$)
Sorption distribution coefficients for each element in cement mortar are specified for Regions I, II and III as described in (1). Pore spacing in the cement mortar is considered to be much larger than that in the buffer material. The specific surface area is kept roughly constant and does not depend on the degree of granulation of hardened cement paste (Bradbury and Sarott, 1994). The measured values obtained from batch-type sorption experiments are applied.

For buffer material, the sorption distribution coefficients are specified for bentonite below pH 11, bentonite above pH 11 and altered bentonite above pH 11. Since it has been reported that pore water in the buffer material has different properties to those of free water (e.g. Torikai et al., 1996), the sorption distribution coefficient is not applied directly in the radionuclide transport assessment. As in the H12 report, the
sorption distribution coefficient is specified from the diffusion coefficient of radionuclides in compacted bentonite.

The sorption distribution coefficient of host rock is specified based on data for each rock type, ionic strength and redox conditions, and by referring to the H12 report.

Sorption distribution coefficients are obtained from experimental data. However, in cases where there are no experimental data, the values are estimated from radionuclides that have similar chemical properties.

4.5.2.3 Models and parameters of the engineered barriers
In the radionuclide transport analysis in the engineered barrier system, radionuclide dissolution from the waste, retardation and decay of radionuclides in the filling material and buffer material are evaluated. Radionuclides in the host rock that have penetrated the buffer and filling materials are then evaluated.

Here, a model concept for radionuclide transport analysis in the engineered barriers is described and a mathematical model is established.

(1) Radionuclide transport analysis model in the engineered barriers
The model outline, mathematical formulation and analysis code for radionuclide transport in the engineered barriers in the Reference Case are described here.

a. Model outline
In order to construct a model for radionuclide transport in the engineered barriers, the following assumptions are assumed.

- The temperature in the disposal facility remains below 80°C. Taking into account an envisaged 1,000 m disposal depth, the host rock temperature is estimated to be 45°C.
- The disposal facility is rapidly saturated by groundwater after repository closure.
- Radionuclides (activation products) in metal of Group 2 waste dissolve into the filling material due to metal corrosion. For other waste, the radionuclides dissolve rapidly into the filling material after closure of the repository.
- The pH of the pore water in the filling material remains above 12.5 (Regions I, II) over the long term due to the dissolution of cement hydrates.
- The composition of the pore water of the filling material is controlled by chemical equilibrium of cement hydrates and groundwater. In the case where buffer material is used, the solubility of radionuclides is based on the composition of pore water in the filling material. In the case where buffer material is not used, it is assumed that colloids will form.
- The concentration of radionuclides in the pore water of filling material is constrained by solubility.
Moreover, precipitation and dissolution are assumed to be instantaneous and reversible. If precipitation occurs, it is assumed that redissolution will also occur in order to maintain solubility. The solubility of stable elements is not considered.

- Radionuclides sorb on filling material and migrate into the buffer material. At present, radionuclide transport in the structure is ignored. Diffusion is the dominant transport mechanism for radionuclides in the buffer material and radionuclides are retarded by instantaneous sorption. Based on the evaluation in Section 4.4.1, radionuclide sorption in the buffer material is considered and restriction of solubility of radionuclides in the buffer material is ignored.

- Colloids are filtered by the fine pore structure of the buffer material.

- Radionuclides which penetrate into the buffer material are rapidly mixed with groundwater flowing through the excavation disturbed zone and it assumed all these radionuclides flow into cracks in the host rock. In the excavation disturbed zone, retardation effects such as sorption are not considered.

- A part of the waste in Group 2 affects the solubility and sorption of radionuclides in cementitious filling material because of the presence of organic material.

- Nitrate affects only Group 3 waste and not other waste Groups.

A one-dimensional concept for the radionuclide transport model in the engineered barriers is shown in Figure 4.5.2-2.

Figure 4.5.2-2 One-dimensional concept for the model for radionuclide transport analysis in the engineered barriers (example of Group 2 waste)
b. Mathematical modeling

(a) Waste area

As shown in Figure 4.5.2-2, radionuclides in the waste are dissolved and leach into the cementitious filling material. By setting the dissolution time \( T_n \) for the waste matrix, the leach rate of radionuclides can be specified. If the amount of radionuclide \( n \) in the waste matrix is estimated to be \( A_n \) mol, the time-dependence of \( A_n \) mol of radionuclides can be expressed by the following formula.

\[
\frac{\partial A_n}{\partial t} = -\lambda_n A_n + \sum_p \lambda_p A_p
\]  

(4.5.2.1-1)

where \( t \) is the period \([y]\) after waste emplacement and \( \lambda_n \) is the decay constant \([1/y]\) of radionuclide \( n \) \((=\ln(2)/T_{1/2,n}; T_{1/2,n} \) is the half-life \([y]\) of the radionuclide). \( \lambda_p \) and \( A_p \) are the decay constant and amount of the parent radionuclide, respectively. Assuming the case where waste is encapsulated in a strong package, the leach rate \( (W_n) \) of radionuclides into cementitious filling material is expressed as follows:

\[
W_n = \begin{cases} 
0 & (t < T_{cont}) \\
\frac{A_n}{T_n} & (T_{cont} \leq t \leq T_{cont} + T_n) \\
0 & (T_{cont} + T_n < t)
\end{cases}
\]  

(4.5.2.1-2)

where \( T_{cont} \) \([y]\) is the time period before the package is damaged. Radionuclide transport processes in the waste disposal area include molecular diffusion, advection/dispersion, precipitation/dissolution, sorption and decay of radionuclides. Here, it is assumed the waste contains \( N \) radionuclides and \( E \) elements. The concentration of a radionuclide \( n \) is expressed as \( c_d^n \) \([mol/m^3\text{-liquid}]\) radionuclides dissolved in the liquid phase, \( c_s^n \) \([mol/m^3\text{-solid}]\) radionuclides sorbed on the solid phase and \( c_p^n \) \([mol/m^3]\) radionuclides by precipitation. The overall concentration \( c^n \) \([mol/m^3]\) of nuclide \( n \) is expressed by the following formula:

\[
c^n = \theta c_d^n + (1-\theta)c_s^n + c_p^n
\]  

(4.5.2.1-3)

where \( \theta \) is porosity [-] of the waste. The total amount of radionuclides \( k^n \) \([mol]\) in volume \( V[m^3] \) of the waste becomes \( Vc^n \). The total amount of element \( e \) \( K^e \) \([mol]\) and its corresponding radionuclide \( n \) is expressed by the following formula.

\[
K^e = \sum_n k^n
\]  

(4.5.2.1-4)

The relationship between element concentration and concentration of its radionuclide is shown by the following formula.

\[
c_d^n = \gamma^n C_d^e, c_s^n = \gamma^n C_s^e, c_p^n = \gamma^n C_p^e
\]  

(4.5.2.1-5)

\[
C_d^e = \sum_n c_d^n, C_s^e = \sum_n c_s^n, C_p^e = \sum_n c_p^n
\]  

(4.5.2.1-6)

\[
\gamma^n = k^n / K^e
\]  

(4.5.2.1-7)

where \( C_d^e, C_s^e \) and \( C_p^e \) are element concentration \([mol/m^3\text{-liquid}]\) in the liquid phase, element
concentration \([\text{mol/m}^3\text{-solid}]\) in the solid phase and concentration of precipitated elements \([\text{mol/m}^3]\) respectively and \(\gamma^n[-]\) is the ratio of radionuclide and total amount of element \(K^e\) which is calculated by multiplying average thickness of the waste and cross-sectional area \(\gamma m^2\) in volume \(V\).

\[
K^e = V\left(\theta C^e_s + (1 - \theta) C^e_p + C^e_P\right) \quad (4.5.2.1-8)
\]

The element concentration in the solid phase is expressed by the following formula.

\[
C^e_s = \frac{\rho C^e_s}{1 + \beta C^e_d} \quad (4.5.2.1-9)
\]

Here, \(\rho\) is the true density \([\text{kg/m}^3]\) of the waste, \(\alpha^e\) and \(\beta^e\) are Langmuir constants of elements in the waste area. Assuming linear sorption, \(\beta^e\) is 0 \(\text{m}^3/\text{mol}\) and \(\alpha^e\) is equal to the sorption distribution coefficient \([\text{m}^3/\text{kg}]\). The effective retardation coefficient \(R_{\text{eff}}\) is defined by the following formula.

\[
R_{\text{eff}} = 1 + \frac{C^e_s}{C^e_d} = 1 + \frac{\rho \alpha^e}{1 + \beta^e C^e_d} \quad (4.5.2.1-10)
\]

The element precipitation concentration \(C^p_s\) is related to the element solubility \(C^s_e\) [\text{mol/m}^3]. The amount of precipitation (maximum value of element amount in liquid phase and solid phase at precipitation) \(K^e_s\) [mol] is defined by the following formula.

\[
K^e_s = V\left(\theta C^e_s + (1 - \theta) \frac{\rho \alpha^e C^e_s}{1 + \beta^e C^e_d}\right) \quad (4.5.2.1-11)
\]

The amount of element precipitation in waste can be expressed by the following formula.

\[
VC^e_p = \max(K^e - K^e_s, 0) \quad (4.5.2.1-12)
\]

Here, \(C^e_p > 0\), the concentration of radionuclide \(n\) in the liquid phase \(c^p_d\) [\text{mol/m}^3] is expressed by the following formula.

\[
c^p_d = \frac{k^n}{K^e} C^e_d \quad (4.5.2.1-13)
\]

If \(C^e_p \leq 0\) there is no precipitation and the concentration of radionuclide \(n\) in the liquid phase \(c^p_d\) [\text{mol/m}^3-liquid] is expressed by the following formula.

\[
c^p_d = \frac{k^n}{\theta W R_{\text{eff}}} \quad (4.5.2.1-14)
\]

The temporal exchange of total amount \(k^n\) [mol] of radionuclide \(n\) at \(x\) [m] in the waste is expressed by the following formula (since the waste area is expressed as 1 cell, the radionuclide concentration in the waste is homogeneous).

\[
\frac{\partial k^n}{\partial t} = \alpha^e \frac{\partial^2 \left(\frac{k^n}{C^e_d}\right)}{\partial x^2} - \frac{\partial \left(\frac{k^n}{C^e_d}\right)}{\partial x} + \sum_{p} \frac{k^n}{p} \xi^p \kappa^n \quad (4.5.2.1-15)
\]
The first term on the right side of the equation corresponds to inflow/outflow of radionuclide n by diffusion/dispersion over distance x and the second term represents inflow/outflow of radionuclide n by migration. The third term represents the amount of daughter radionuclide n and the fourth term reduction of radionuclide n through decay.

\[ k_p^n \] is the total amount [mol] of parent radionuclide of radionuclide n.

\[
D^e = D_p^e + \frac{d_e q}{\theta} \quad (4.5.2.1-16)
\]

Where \( D^e \) is the dispersion coefficient of element e in pore water \([m^2/y]\), \( D_p^e \) is the diffusion coefficient of element e in pore water \([m^2/y]\) (the relationship \( \theta D_p^e = D^e \) exists. \( D^e \) is the effective diffusion coefficient of element e), \( d_e \) is the dispersion length \([m]\) and \( q \) is the Darcy flow velocity \([m/y]\).

**b) Engineered barrier area**

The radionuclide transport processes considered in the engineered barriers are the same as those considered in the waste area, i.e. molecular diffusion, advection/dispersion, precipitation/dissolution, sorption and decay of radionuclides. The mathematical models are also the same. The boundary condition in the waste and the engineered barriers is expressed using a mixing cell with flow \( Q [m^3/y] \) as illustrated in the following formula.

\[
\frac{\partial k^n}{\partial t} = -\theta D^e \frac{\partial^2 (Vc^e_n)}{\partial x^2} \bigg|_{x=x_{in, in}} + \frac{\partial (Vc^e_n q_v^n)}{\partial x} \bigg|_{x=x_{in, in}} + \sum_p \lambda_p k^n_p - \lambda_n k^n \quad (4.5.2.1-17)
\]

The boundary condition of the engineered barriers and the mixing cell condition are expressed by the following formula.

\[
\frac{\partial k^n}{\partial t} = -\theta D^e \frac{\partial^2 (Vc^e_n)}{\partial x^2} \bigg|_{x=x_{in, out}} + \frac{\partial (Vc^e_n q_v^n)}{\partial x} \bigg|_{x=x_{in, out}} - Q e_n + \sum_p \lambda_p k^n_p - \lambda_n k^n \quad (4.5.2.1-18)
\]

**c) Excavation disturbed zone (mixing cell)**

At the boundary between the engineered and natural barriers, a mixing cell is specified and the total amount of radionuclide n is expressed by the following formula.

\[
\frac{\partial k^n}{\partial t} = -Q e_n + \sum_p \lambda_p k^n_p - \lambda_n k^n \quad (4.5.2.1-19)
\]

**c. Analysis code**

The TIGER code (orthogonal 1-D coordinate(s), finite difference method), which can be used to solve several decay series and to solve the amount of precipitation and dissolution of each isotope (Mihara and Ooi, 2004), is applied for modeling the radionuclide transport processes in the engineered barriers (Figure 4.5.2-2). This code has the same capability as the MESHNOTE code (Wakasugi et al., 1999) used in the
H12 report and outputs from both are compared (Mihara and Ooi, 2004).

(2) Data

a. Cross-sectional shape of the disposal tunnel
The emplacement density of waste in the disposal tunnel depends on the shape of the package for each waste type. Hence, in the radionuclide transport analysis in the engineered barrier system, several disposal tunnel cross-sections are used (Table 4.2.4-1 in Section 4.2.4).

b. Inventory
The inventory described in Section 4.2.3 is used. Since there is the possibility that some C-14 is organic (Yamaguchi et al., 1999), the chemical form of some C-14 is also treated as organic in the model. The low-level waste (Gr3-B) of BNGS in Group 3 is assumed to be inorganic since C-14 exists as BaCO3.

c. Containment function of the waste package
The radionuclide containment function of the waste package is not taken into account. Hence, it is assumed that waste comes into contact with groundwater after closure.

d. Radionuclides in metal in Group 2 waste
As described in Section 4.5.2.3(1)a, it is assumed that the radionuclides in metal in this waste group dissolve with metal corrosion. Hence, the percentage of radionuclides in the metal should be specified. For each metal in Group 2 waste, the percentage of C-14, Cl-36, Co-60, Ni-59, Ni-63, Se-79, Zr-93, Nb-94 and Mo-93 is specified. Representative metals considered in Group 2 waste are zircaloy used as an insulator for fuel rods, stainless steel upper and lower nozzles in fuel assemblies and inconel lattice supports of fuel rods. The radionuclide percentages in these metals are summarized in Table 4.5.2-1. It has been reported that 20% of an insulator (zircaloy) of spent fuel is oxidized (Yamaguchi et al., 1999) and that 20% of activation products exist the oxidized film.
Table 4.5.2-1 Radionuclide ratio in metals of Group 2 waste

<table>
<thead>
<tr>
<th>Radionuclide</th>
<th>Sticked ratio</th>
<th>Zircaloy*</th>
<th>Stainless steel, Inconel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Oxidized film</td>
<td>Base material</td>
</tr>
<tr>
<td>C-14</td>
<td>0.00</td>
<td>0.13</td>
<td>0.53</td>
</tr>
<tr>
<td>Cl-36</td>
<td>0.01</td>
<td>0.20</td>
<td>0.79</td>
</tr>
<tr>
<td>Co-60</td>
<td>0.01</td>
<td>0.04</td>
<td>0.18</td>
</tr>
<tr>
<td>Ni-59</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Ni-63</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Se-79</td>
<td>0.98</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Zr-93</td>
<td>0.04</td>
<td>0.19</td>
<td>0.77</td>
</tr>
<tr>
<td>Nb-94</td>
<td>0.00</td>
<td>0.01</td>
<td>0.02</td>
</tr>
<tr>
<td>Mo-93</td>
<td>0.00</td>
<td>0.01</td>
<td>0.02</td>
</tr>
</tbody>
</table>

*: Rounded to two decimal places.

e. Leaching period of radionuclides in Group 2 waste

It is assumed that radionuclides in metal of Group 2 waste are dissolved into the filling material by metal corrosion and the corrosion rate of metal (zircaloy, stainless steel and inconel) is therefore specified (Section 4.4.10) from the viewpoint of hydrogen generation due metal corrosion; especially for zircaloy, the corrosion rate is equivalent to the generation rate of hydrogen based on the assumption of occluded hydrogen. It is assumed that 75% of hydrogen generated by corrosion reactions is absorbed into zircaloy (Honda et al., 2005) and the corrosion rate is assumed to be 0.02 μm/y. For zircaloy, the infiltration period is specified from the effective wall thickness and corrosion rate, and for stainless steel and inconel the infiltration period is specified from the thickness of the structural elements and corrosion rate. The leaching of C-14 from zircaloy is concordant with the corrosion of zircaloy. The infiltration period for radionuclides from each metal of Group 2 is shown in Table 4.5.2-2.

Table 4.5.2-2 Radionuclide dissolution period in Group 2 waste

<table>
<thead>
<tr>
<th>Metal</th>
<th>Radionuclide leaching period (y)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zircaloy</td>
<td>11,400</td>
</tr>
<tr>
<td>Stainless steel/inconel</td>
<td>8,500</td>
</tr>
</tbody>
</table>

f. Solubility increase and lowering of sorption distribution coefficient

As described in Section 4.4.6, organic material is included in Group 2 waste. In the case where organic material is assumed to be cellulose, the concentration of Iso-Saccharinic Acid (ISA) in the pore water of the
filling material does not exceed 10^{-5} \text{ mol/dm}^3 \) (cf. Section 4.4.6.2). Solubility enhancement factors (SEF) for actinides and Tc (Bradbury and Sarott, 1994) are shown in Table 4.5.2-3. If the concentration of ISA is 10^{-5} \text{ mol/dm}^3, the solubility of tetravalent and trivalent actinides increases by a factor of 20.

Table 4.5.2-3 Solubility enhancement factors (SEF) for actinides and Tc (Bradbury and Sarott, 1994)

<table>
<thead>
<tr>
<th>ISA concentration \text{ (mol/dm}^3)</th>
<th>Pu(IV)</th>
<th>Am(III)</th>
<th>Th(IV)</th>
<th>U(VI)</th>
<th>Np(IV)</th>
<th>Tc(IV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^{-6}</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>10^{-5}</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>10^{-4}</td>
<td>500</td>
<td>500</td>
<td>500</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>10^{-3}</td>
<td>20,000</td>
<td>20,000</td>
<td>20,000</td>
<td>100</td>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td>10^{-2}</td>
<td>1,000,000</td>
<td>1,000,000</td>
<td>1,000,000</td>
<td>5,000</td>
<td>5,000</td>
<td>500</td>
</tr>
</tbody>
</table>

Based on these results, for the actinides with tetravalent and trivalent bonds, the SEF is set to a conservative value of 20. The effect of ISA is ignored as this has previously been reported as being small (Bradbury and Sarott, 1994). Bradbury and Sarott (1994) reports that the sorption reduction factor (SRF) is assumed to be equal to SEF; SEF and SRF are specified as shown in Table 4.5.2-4.

Table 4.5.2-4 Specified values for solubility enhancement factor (SEF) and sorption reduction factor (SRF)

<table>
<thead>
<tr>
<th>Element</th>
<th>SEF and SRF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pu, Th, U, Np, Pa</td>
<td>20</td>
</tr>
<tr>
<td>Am, Cm, Ac</td>
<td>20</td>
</tr>
<tr>
<td>Zr, Sn</td>
<td>20</td>
</tr>
<tr>
<td>Other elements</td>
<td>1</td>
</tr>
</tbody>
</table>

g. Solubility

Alkaline (pH >12.5) conditions in the filling material are maintained over the long term as described in Section 4.4.2. For setting the solubility in Region I (pH 13.2) and Region II (pH 12.5) in the radionuclide migration dataset, RAMDA, large values are used. The solubility of Groups 1 and 2 is considered for parts with cementitious filling material and it is assumed that not all radionuclides are precipitated in buffer material, as described in Section 4.5.2.3(1)a. For Groups 3 and 4, buffer material is not used, radionuclides do not precipitate and the effects of colloid formation are considered from a conservative point of view. The solubilities of each element are shown in Table 4.5.2-5.
Table 4.5.2-5 Solubility of specified elements (maximum value for Region I (pH 13.2) and Region II (pH 12.5)) (unit: mol/dm³)

<table>
<thead>
<tr>
<th>Element</th>
<th>Group 1</th>
<th>Group 2</th>
<th>Groups 3, 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>C (inorganic)</td>
<td>1×10⁻⁴</td>
<td>1×10⁻⁴</td>
<td></td>
</tr>
<tr>
<td>C (organic)</td>
<td>soluble</td>
<td>soluble</td>
<td></td>
</tr>
<tr>
<td>Cl</td>
<td>soluble</td>
<td>soluble</td>
<td></td>
</tr>
<tr>
<td>Co</td>
<td>5×10⁻⁴</td>
<td>5×10⁻⁴</td>
<td></td>
</tr>
<tr>
<td>Ni</td>
<td>5×10⁻⁴</td>
<td>5×10⁻⁴</td>
<td></td>
</tr>
<tr>
<td>Se</td>
<td>5×10⁻⁴</td>
<td>5×10⁻⁴</td>
<td></td>
</tr>
<tr>
<td>Sr</td>
<td>5×10⁻¹</td>
<td>5×10⁻¹</td>
<td></td>
</tr>
<tr>
<td>Zr</td>
<td>5×10⁻⁵</td>
<td>1×10⁻⁵</td>
<td></td>
</tr>
<tr>
<td>Nb</td>
<td>5×10⁻⁵</td>
<td>5×10⁻⁵</td>
<td></td>
</tr>
<tr>
<td>Mo</td>
<td>1×10⁻⁵</td>
<td>1×10⁻⁵</td>
<td></td>
</tr>
<tr>
<td>Tc</td>
<td>1×10⁻⁶</td>
<td>1×10⁻⁷</td>
<td></td>
</tr>
<tr>
<td>Pd</td>
<td>soluble</td>
<td>soluble</td>
<td></td>
</tr>
<tr>
<td>Sn</td>
<td>5×10⁻¹</td>
<td>soluble</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>soluble</td>
<td>soluble</td>
<td></td>
</tr>
<tr>
<td>Cs</td>
<td>soluble</td>
<td>soluble</td>
<td></td>
</tr>
<tr>
<td>Pb</td>
<td>5×10⁻⁴</td>
<td>5×10⁻⁴</td>
<td></td>
</tr>
<tr>
<td>Ra</td>
<td>1×10⁻⁶</td>
<td>1×10⁻⁶</td>
<td></td>
</tr>
<tr>
<td>Ac</td>
<td>5×10⁻¹⁰</td>
<td>1×10⁻⁸</td>
<td></td>
</tr>
<tr>
<td>Th</td>
<td>1×10⁻⁸</td>
<td>2×10⁻⁸</td>
<td></td>
</tr>
<tr>
<td>Pa</td>
<td>5×10⁻⁵</td>
<td>1×10⁻⁵</td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>5×10⁻⁶</td>
<td>1×10⁻⁶</td>
<td></td>
</tr>
<tr>
<td>Np</td>
<td>5×10⁻⁷</td>
<td>1×10⁻⁷</td>
<td></td>
</tr>
<tr>
<td>Pu</td>
<td>1×10⁻¹⁰</td>
<td>2×10⁻⁷</td>
<td></td>
</tr>
<tr>
<td>Am</td>
<td>5×10⁻¹⁰</td>
<td>1×10⁻³</td>
<td></td>
</tr>
<tr>
<td>Cm</td>
<td>5×10⁻¹⁰</td>
<td>1×10⁻³</td>
<td></td>
</tr>
</tbody>
</table>

Precipitation not considered

h. Effective diffusion coefficient

(a) Filling material (cement mortar)

When setting effective diffusion coefficients for radionuclides in cement mortar in the Reference Case, it is assumed that cracks will form in the cement mortar and the diffusion coefficient of pore water is the same as that of free water. The diffusion coefficient of water is calculated by multiplying porosity and diffusion coefficient in free water (Mihara and Sasaki, 2005). Considering the temperature of the disposal facility (45°C - 80°C), the largest value of 4×10⁻⁹ m²/s for diffusion coefficients in free water at 60°C (Sato et al., 1992) is taken as the diffusion coefficient for radionuclides in free water. Also, if the porosity of cement mortar is assumed to be 0.19 (cf. Section 4.4.2.2), the effective diffusion coefficient is estimated to be 8×10⁻¹⁰ m²/s.

(b) Buffer material (compacted bentonite)

Several Japanese researchers have published effective diffusion coefficients for Kunigel VI using tritium (Kato et al., 1995; Shimura et al., 1995; Sato, 2002; Kato et al., 1999; PNC, 1994). The relationship between the effective diffusion coefficient, porosity and smectite inclusions in bentonite is sought from experimental data (Mihara and Sasaki, 2005):
Here, $\theta$, $f_s$ and $D^*$ are porosity (-), smectite inclusion ratio (-) and diffusion coefficient (m$^2$/s) of radionuclides in free water, respectively. If the smectite concentration decreases to 0, the effective diffusion coefficient is obtained by multiplying porosity and diffusion coefficient of radionuclides in free water. The effective diffusion coefficient for compacted bentonite with a typical cation, e.g. Cs, and a typical anion, e.g. I, is reported (Mihara et al., 1999). These effective diffusion coefficients are quite different to those using tritium. The effective diffusion coefficient of compacted bentonite with Cs and I is shown as follows (Mihara and Sasaki, 2005).

\[
D_{e}^{\text{HTO}} = \theta \times (\theta^{2.226^{0.13}} )D^* \tag{4.5.2.1-20}
\]

If the porosity, smectite inclusion ratio and radionuclide diffusion coefficient in free water are assigned, Cs and I are $4 \times 10^{-10}$ m$^2$/s and $4 \times 10^{-11}$ m$^2$/s, respectively. These values are specified for typical cations and anions in pore water. The established values for effective diffusion coefficients are summarized in Table 4.5.2-6.

<table>
<thead>
<tr>
<th>Neutral radionuclide</th>
<th>Cation radionuclide (Cs)</th>
<th>Anion radionuclide (Inorganic C, Cl, I, Se, Mo)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3 \times 10^{-10}$</td>
<td>$4 \times 10^{-10}$</td>
<td>$4 \times 10^{-11}$</td>
</tr>
</tbody>
</table>

**i. Dispersion length**

The dispersion length is specified as 1/10 of the system length as described in Section 4.5.2.4(2) c (a).

**j. Sorption distribution coefficient**

(a) Cement mortar

The sorption distribution coefficient in each Group used for the Reference Case analysis is specified using RAMDA as follows:

Group 1: Minimum values for Regions I and II of RAMDA are used. For Iodine, if the total amount of radionuclide in the waste is dissolved into the filling material, the concentration results in a high value (0.1 mol/dm$^3$). Considering high concentration of Iodine in waste area, the sorption distribution coefficient of I is estimated to be 1/10 (Mine et al., 1997).

Group 2: Minimum values for Regions I and II of RAMDA are used based on the effects of organic material.
Group 3: Minimum values for Regions I and II of RAMDA are used considering the effects of nitrates and an oxidizing environment of seawater type groundwater.

Group 4: Minimum values for Regions I and II of RAMDA are used.

Sorption distribution coefficients for cement mortar are summarized in Table 4.5.2-7.
Table 4.5.2-7 Sorption distribution coefficients for elements in cement mortar (unit: m³/kg)

<table>
<thead>
<tr>
<th></th>
<th>Group 1</th>
<th>Group 2</th>
<th>Group 3</th>
<th>Group 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>C (inorganic)</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>C (organic)</td>
<td>0.00025</td>
<td>0.00025</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Cl</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Co</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
</tr>
<tr>
<td>Ni</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
</tr>
<tr>
<td>Se</td>
<td>0.0025</td>
<td>0.0025</td>
<td>0</td>
<td>0.0025</td>
</tr>
<tr>
<td>Sr</td>
<td>0.00125</td>
<td>0.00125</td>
<td>0.00125</td>
<td>0.00125</td>
</tr>
<tr>
<td>Zr</td>
<td>2.5</td>
<td>0.125</td>
<td>2.5</td>
<td>2.5</td>
</tr>
<tr>
<td>Nb</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Mo</td>
<td>0.0025</td>
<td>0.0025</td>
<td>0.00025</td>
<td>0.0025</td>
</tr>
<tr>
<td>Tc</td>
<td>2.5</td>
<td>2.5</td>
<td>0</td>
<td>2.5</td>
</tr>
<tr>
<td>Pd</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
</tr>
<tr>
<td>Sn</td>
<td>2.5</td>
<td>0.125</td>
<td>2.5</td>
<td>2.5</td>
</tr>
<tr>
<td>I</td>
<td>0.000125</td>
<td>0.00125</td>
<td>0</td>
<td>0.00125</td>
</tr>
<tr>
<td>Cs</td>
<td>0.0025</td>
<td>0.0025</td>
<td>0.0025</td>
<td>0.0025</td>
</tr>
<tr>
<td>Pb</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
<td>0.0125</td>
</tr>
<tr>
<td>Ra</td>
<td>0.00125</td>
<td>0.00125</td>
<td>0.00125</td>
<td>0.00125</td>
</tr>
<tr>
<td>Ac</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>Th</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>Pa</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>U</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.025</td>
<td>0.25</td>
</tr>
<tr>
<td>Np</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>Pu</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.025</td>
<td>0.25</td>
</tr>
<tr>
<td>Am</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>Cm</td>
<td>0.25</td>
<td>0.0125</td>
<td>0.25</td>
<td>0.25</td>
</tr>
</tbody>
</table>

(b) Buffer material (compacted bentonite)

For the sorption distribution coefficient of each element used for analysis in the Reference Case, the minimum value for the sorption distribution coefficient for bentonite (< pH 11 and > pH 11) is selected from the RAMDA data. The selected sorption distribution coefficients are summarized in Table 4.5.2-8.
Table 4.5.2-8 Sorption distribution coefficient for elements in the buffer material (unit: m³/kg)

<table>
<thead>
<tr>
<th>Element</th>
<th>Sorption distribution coefficient</th>
<th>Element</th>
<th>Sorption distribution coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0</td>
<td>I</td>
<td>0</td>
</tr>
<tr>
<td>C (organic)</td>
<td>0</td>
<td>Cs</td>
<td>0.05</td>
</tr>
<tr>
<td>Cl</td>
<td>0</td>
<td>Pb</td>
<td>0.05</td>
</tr>
<tr>
<td>Co</td>
<td>0.05</td>
<td>Ra</td>
<td>0.001</td>
</tr>
<tr>
<td>Ni</td>
<td>0.05</td>
<td>Ac</td>
<td>1</td>
</tr>
<tr>
<td>Se</td>
<td>0</td>
<td>Th</td>
<td>5</td>
</tr>
<tr>
<td>Sr</td>
<td>0.001</td>
<td>Pa</td>
<td>5</td>
</tr>
<tr>
<td>Zr</td>
<td>1</td>
<td>U</td>
<td>5</td>
</tr>
<tr>
<td>Nb</td>
<td>0.1</td>
<td>Np</td>
<td>5</td>
</tr>
<tr>
<td>Mo</td>
<td>0</td>
<td>Pu</td>
<td>5</td>
</tr>
<tr>
<td>Tc</td>
<td>1</td>
<td>Am</td>
<td>1</td>
</tr>
<tr>
<td>Pd</td>
<td>0.05</td>
<td>Cm</td>
<td>1</td>
</tr>
<tr>
<td>Sn</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

k. Darcy flow velocity of groundwater inside outside the engineered barrier system (excavation disturbed zone)

Hydraulic conductivities based on evaluated results of Darcy flow velocity in the filling material, buffer material, excavation disturbed zone and host rock are shown in Table 4.5.2-9 (see also Section 4.4.4.) In the Reference Case, it is assumed that cracks occur in cement mortar and that bentonite converts to Na type.

Table 4.5.2-9 Hydraulic conductivities used in the EBS and host rock

<table>
<thead>
<tr>
<th>Group</th>
<th>Filling material</th>
<th>Buffer material</th>
<th>Excavation disturbed zone</th>
<th>Host rock</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group 1</td>
<td>4×10⁻⁶ m s⁻¹</td>
<td>2×10⁻¹¹ m s⁻¹</td>
<td>2×10⁻⁸ m s⁻¹</td>
<td>2×10⁻¹⁰ m s⁻¹</td>
</tr>
<tr>
<td>Group 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Group 3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Group 4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*This analytical case is the same as analytical cases 2-2 & 2 in Section 4.4.4.

Based on the values in Table 4.5.2-9, groundwater flow velocities used in the analysis of the Reference Case are as follows:
For the disposal concept where buffer material is envisaged (namely for Group 1 and 2 wastes), a maximum value of $3 \times 10^{-6}$ m/y ($2.9 \times 10^{-6}$ m/y in the analysis) for groundwater flow (Darcy flow) is used in the filling material and buffer material zones.

Flow in the excavation disturbed zone set to 0.0025 m$^3$/y/m based on the analytical result (0.0022 m$^3$/y/m) in Section 4.4.4.

In the disposal concept which does not use buffer material (namely for Group 3 and 4 wastes), groundwater flow velocity in the cement mortar is assumed to be $2 \times 10^{-4}$ m/y ($1.7 \times 10^{-4}$ m/y in the analysis).

For the disposal facility where buffer material will not be used, a large groundwater flow velocity is assumed. In the excavation disturbed zone, groundwater flux is calculated by multiplying the groundwater flow velocity in the engineered barriers ($2 \times 10^{-4}$ m/y) by the surface area and length of the disposal tunnel (37.7 m$^2$ in the case of a tunnel 12 m in diameter).

The established values are summarized in Table 4.5.2-10.

<table>
<thead>
<tr>
<th></th>
<th>Groundwater flow velocity in the engineered barriers (m/y)</th>
<th>Groundwater flux in the excavation disturbed zone (m$^3$/y/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group 1</td>
<td>$3 \times 10^{-6}$</td>
<td>0.0025</td>
</tr>
<tr>
<td>Group 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Group 3</td>
<td>$2 \times 10^{-4}$</td>
<td>0.0075</td>
</tr>
<tr>
<td>Group 4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

4.5.2.4 Radionuclide transport data and models in the host rock

(1) Analytical model of radionuclide transport in the host rock

a. Model concept

One-dimensional multipathway and parallel-plate models are used for modelling radionuclide transport in the host rock. It is assumed that the migration distance to a fault downstream from the disposal facility is 100 m and that the host rock does not delay the migration of radionuclides. It has been shown that the one-dimensional multipathway model produces similar results to a three-dimensional fracture network model (Sawada et al., 1999) in modelling radionuclide transport in fractured host rock. Preliminary dose assessments of the important radionuclides C-14 and I-129 using the one-dimensional multipathway model and the three-dimensional network model also produced broadly similar results.

Here, the one-dimensional parallel-plate model and the one-dimensional multipathway model are described
(JNC, 2000).

(a) One-dimensional parallel-plate model

The one-dimensional parallel-plate model is widely used in performance assessments of geological repositories by modelling radionuclide transport in fractured host rocks. In this model, the flow in the rock matrix is ignored and radionuclide transport by advection/dispersion in cracks, diffusion (matrix diffusion) into the rock matrix from cracks and sorption onto the surface of mineral grains in the rock matrix are considered. The concept of the one-dimensional parallel-plate model is shown in Figure 4.5.2-3.

![Figure 4.5.2-3 Conceptual illustration of the one-dimensional parallel-plate model](image)

The model simplifications are as follows:

- The representation of mechanical dispersion by a fracture network structure is characterised by length of dispersion.
- Sorption on mineral surfaces in the rock matrix is assumed to be rapid/reversible.
- Since secondary minerals were observed in fractures at the Kamaishi mine, radionuclide transport retardation through sorption on such minerals is expected. In the model, this is not considered to be conservative since the quantitative evaluation of infill minerals in fractures is difficult.
- Retardation by diffusion in fractures without groundwater flow is conservatively ignored.
- Since there is insufficient knowledge of the effects of colloids, organic material and microbes on radionuclide transport, these are not considered in the Reference Case and are evaluated in alternative cases.
- The effects of density-driven flow due to thermal convection and the marine-meteoric water interface are not considered.
(b) One-dimensional multipathway model

This model is used to determine the radionuclide release rate \( g_n(t) \) by summing the radionuclide release rates in discretized segments and weighting with a probability distribution function of transmissivities in the host rock (Sawada et al., 1999). The radionuclide release rate in each segment is calculated using the one-dimensional parallel-plate model.

\[
g_n(t) = p_1 h_n(T_1, t) + p_2 h_n(T_2, t) + p_3 h_n(T_3, t) + \ldots + p_I h_n(T_I, t)
\]

Where \( I \) : total number of segments \([-]\) (= number of node points)
\( p_j \) : probability distribution of \( j \)th fracture \([-]\)
\( h_n(T_j, t) \) : radionuclide release rate from \( j \)th fracture in time \( t \) [moles/y] \( T_j \) : median value of transmissivity in segment \( I \) [m²/s] \( t \) : time [y]

The suffixes \( n \) and \( i \) represent radionuclide and segment number, respectively. The same transmissivities are obtained from the one-dimensional multipathway model when discretization is above 12 segments (Sawada et al., 1999). Hence, 12 segments are used in order to determine transmissivity using the one-dimensional multipathway model.

b. Mathematical formulation

(a) Governing equation

Similar radionuclide transport processes to those in the engineered barrier area are considered in the natural barrier and fault area. However, matrix diffusion of radionuclides from fracture surfaces is considered because of the fracturing properties of the host rock. Hence, radionuclide transport is given by the following formula.

\[
\frac{\partial k^n}{\partial t} = \Theta D^n \frac{\partial^2 \{V_q e_d^n \}}{\partial x^2} - \frac{\partial \{V_q e_d^n \}}{\partial x} + \sum_{p} \lambda_{p} k^n - \lambda_n k^n + \delta F^n
\]

Where \( \delta \) is matrix diffusion area [m²/m³] per volume of a single fracture. \( F^n \) [mol/y] of radionuclide \( n \) diffuses into the matrix from the fracture as follows.

\[
F^n = D^{n,e} \theta^n \frac{\partial k^n}{\partial y} \bigg|_{y=0}
\]

Here \( y \) : perpendicular distance from the fracture surface into the matrix [m]
\( k^n_m \) : total amount of radionuclide \( n \) in matrix [mol]
\( D^{n,e} \) : diffusion coefficient of element \( e \) in pore water in matrix [m²/y]
\( \theta^n \) : porosity in matrix [-]
\[ \frac{\partial k_m^n}{\partial t} = \Theta^n D^{\nu - \varepsilon} \frac{\partial^2 \{ V_{C,d}^n \}}{\partial x^2} + \sum_p \lambda_p^n k_p^n - \lambda_d^n k_d^n \]  
(4.5.2.1-26)

(b) Boundary conditions

The initial concentration of radionuclides in fracture and matrix is set to 0. Also, radionuclide transport from the engineered barriers in each waste group is given as an initial condition.

The initial condition in the fracture surface is shown in equation 4.5.2.1-25 and the initial condition with matrix diffusion at maximum depth \( d \) [m] is expressed as follows.

\[ \left. \frac{\partial c_y}{\partial y} \right|_{y=d} = 0 \]  
(4.5.2.1-27)

c. Analytical code

The mathematical model based on the radionuclide transport processes in the natural barrier is shown in Figure 4.5.2-3. The analysis can be carried out using the TIGER code as described before. It is shown that radionuclide transport in the geosphere can be modeled more correctly with TIGER compared with the MATRICS code (Shirakawa et al., 2000; Mihara and Ooi, 2004).

(2) Data

a. Hydraulic gradient

Few data exist for defining deep hydraulic gradients. In H12, the highest frequency value (0.01) of published groundwater gradients was selected for the Reference Case. Based on actual measurements around the Tono mine, it is revealed that the hydraulic gradient at 500 m or deeper is smaller than that near the surface.

In this report, 0.01 is also selected for the Reference Case.

b. Fracture parameters

(a) Transmissivity distribution \( f(x) \) of fractures

Based on in situ hydraulic tests at the Kamaishi mine, Sawada et al. (1999) showed that transmissivity could be modeled using a normal distribution (equation 4.5.2.1-28). In this evaluation, \( \log (x) \) of transmissivity follows a normal distribution and the mean log value of transmissivity is -8.99 and the standard deviation \( (\sigma) \) is 1.07. In the H12 report, the depth of the disposal facility was assumed to be 1,000 m and the log mean value \( (\mu) \) is considered to be -9.99 by considering the depth dependence of hydraulic conductivity. In this report, this transmissivity distribution is used and \( 3\sigma \) is considered to be the range of transmissivity. Hence, the maximum value of transmissivity is estimated to be \( 10^{-7} \) m²/s.

\[ f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{(x - \mu)^2}{2\sigma^2}\right) \]  
(4.5.2.1-28)
(b) Darcy flow velocity of groundwater in fractures

Using discretized transmissivities \( T_n [m^2/s] \), the Darcy flow velocity \( v_n [m/s] \) and matrix diffusion area/fracture volume ratio \( \delta [m^2/m^3] \) in fractures are calculated using equations 4.5.2.1-29 and 30 below (Sawada et al., 1999).

\[
v_n = 0.5 \sqrt{T_n} \times i \tag{4.5.2.1-29}
\]

\[
\delta_n = 0.5 \left( \frac{1}{v_n} \right) \times \Omega \times i = \frac{1}{\sqrt{T_n}} \times \Omega \tag{4.5.2.1-30}
\]

where \( i \) is the hydraulic gradient (0.01[-] is specified) and \( \Omega \) is the matrix diffusion area ratio[-].

c. Radionuclide transport parameters

(a) Macroscopic dispersion length

Macroscopic dispersion is observed in heterogeneous rock masses and generally exhibits a longitudinal dispersion length that increases as the transport distances increases. The longitudinal dispersion length for transport distances of 10-1,000 m was assumed to be 1/10 of the transport distance (PNC, 1992). 1/10 of the transport distance was also assumed in the H12 report and again here. In other words, for 100 m transport distance in the host rock, the dispersion length is 10 m.

(b) Matrix diffusion depth

The heterogeneity of the rock matrix and the coating of fracture surfaces with altered minerals complicate the modeling of diffusion from fractures into the matrix (Sawada et al., 1999). From limited natural analogue studies, the depth of matrix diffusion is estimated to be 0.03 - 0.1 m. However, matrix diffusion depths estimated from natural analogue research are considered to be minimum values and a conservative value of 0.1 m was used for the radionuclide transport analysis in H12 (JNC, 2000). This conservative value is also used in this report.

(c) Proportion of fracture surface from which radionuclides can diffuse into the matrix

The H12 report shows that the proportion of fracture surface from which radionuclides can diffuse into the matrix varies depending on the vertical stress on the fracture surface. It was reported that the percentage of accessible surface area was 0.85-0.92, 0.58-0.85 and 0.58-0.70 for vertical stresses of 3 MPa, 33 MPa and 85 MPa, respectively (Pyrak-Nolte et al., 1987). The vertical stress on the fracture surfaces around the disposal facility at 1,000 m depth depends on the origin and orientation of the fracture. If stress due to the rock overburden is 27 MPa (density of granite 2.7 Mg/m^3 × 1,000 m), the effective fracture area ratio would be 0.58-0.7. The lower value is specified and 0.5 is considered in this evaluation.
(d) Porosity
Based on a literature review by Sato et al. (1992), the average porosity of granite is considered to be around 0.019. The average porosity around unaltered fractures in the Kamaishi mine is 0.023 and 0.032, and the porosity around fractures is relatively large (Sato et al., 1997). In this report, a constant value of 0.02 is used for matrix porosity including unaltered zones and surrounding parts of fractures.

(e) Dry density
An average value for crystalline rock (acid rock) of 2.64 Mg/m³ (Taniguchi et al., 1999) is assumed. The calculated true density using the porosity above is 2.7 Mg/m³.

(f) Effective diffusion coefficient
The effective diffusion coefficient of granite is known to be dependent on pore size, connectivity and flection. Here the same value as that used in H12 \((3\times10^{-12}\text{ m}^2/\text{s})\) is assumed.

(g) Sorption distribution coefficients
The sorption distribution coefficients in the RAMDA database for each element in granite are used for Group 1, 2 and 4 wastes. Since some of the wastes in Group 3 have large amounts of soluble nitrates, data in RAMDA that include ionic strength and oxidizing effects are used. The assumed values for sorption distribution coefficient are summarized in Table 4.5.2-11.
Table 4.5.2-11 Sorption distribution coefficients of elements in the host rock (unit: m³/kg)

<table>
<thead>
<tr>
<th>Element</th>
<th>Groups 1, 2, 4</th>
<th>Group 3</th>
<th>Element</th>
<th>Groups 1, 2, 4</th>
<th>Group 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.0001</td>
<td>0</td>
<td>I</td>
<td>0.0001</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0.0001</td>
<td>0</td>
<td>Cs</td>
<td>0.05</td>
<td>0.005</td>
</tr>
<tr>
<td>Cl</td>
<td>0.0001</td>
<td>0</td>
<td>Pb</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Co</td>
<td>0.01</td>
<td>0.001</td>
<td>Ra</td>
<td>0.5</td>
<td>0.05</td>
</tr>
<tr>
<td>Ni</td>
<td>0.01</td>
<td>0.001</td>
<td>Ac</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Se</td>
<td>0.01</td>
<td>0</td>
<td>Th</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Sr</td>
<td>0.5</td>
<td>0.05</td>
<td>Pa</td>
<td>1</td>
<td>0.005</td>
</tr>
<tr>
<td>Zr</td>
<td>0.1</td>
<td>0.1</td>
<td>U</td>
<td>1</td>
<td>0.005</td>
</tr>
<tr>
<td>Nb</td>
<td>0.1</td>
<td>0.1</td>
<td>Np</td>
<td>1</td>
<td>0.005</td>
</tr>
<tr>
<td>Mo</td>
<td>0.0001</td>
<td>0</td>
<td>Pu</td>
<td>1</td>
<td>0.05</td>
</tr>
<tr>
<td>Tc</td>
<td>1</td>
<td>0</td>
<td>Am</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Pd</td>
<td>0.1</td>
<td>0.1</td>
<td>Cm</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Sn</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

4.5.2.5 Radionuclide transport analysis model in faults and associated data

(1) Radionuclide transport model for a fault

a. Model concept

The one-dimensional parallel-plate model is used for modeling a fault, as in the H12 report. The following simplifications are made:

- The radionuclide transport distance in the fault is 80 m
- The thickness of the sedimentary layer above the host rock is 200 m
- Heterogeneity in the inner fault is not considered
- Radionuclide transport retardation due to diffusion and sorption in clay in the fault is not considered.

b. Mathematical formulation

The same mathematical formulation is used as that in Section 4.5.2.4(1)b.

c. Analytical code

The TIGER code is selected as the analytical code, as in Section 4.5.2.4(1)c (Mihara and Ooi, 2004).
(2) Data

a. Radionuclide release rate

It is assumed that all radionuclides released into the host rock enter the fault.

b. Transmissivity and Darcy flow of groundwater in fractures

The transmissivity of the fault is set to a maximum value of $10^{-7}$ m$^2$/s. Based on the formula in equation 4.5.2.1-29, the Darcy flow velocity of groundwater in a fracture is calculated as 50 m/y.

c. Dispersion length

As in the H12 report, the dispersion length is set to 1/10 of the migration distance (80 m).

A list of the parameter values used in the Reference Case for the host rock is summarized in Table 4.5.2-12.

<table>
<thead>
<tr>
<th>Table 4.5.2-12 Summary boundary conditions in the Reference Case model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
</tr>
<tr>
<td>Rock type</td>
</tr>
<tr>
<td>Groundwater</td>
</tr>
<tr>
<td>Hydraulic gradient</td>
</tr>
<tr>
<td>Radionuclide release rate input</td>
</tr>
<tr>
<td>Migration distance (m)</td>
</tr>
<tr>
<td>Transmissivity (m$^2$/s)</td>
</tr>
<tr>
<td>Darcy flow velocity of groundwater in fracture (m s$^{-1}$)</td>
</tr>
<tr>
<td>Dispersion length (m)</td>
</tr>
<tr>
<td>Proportion of fracture surface from which radionuclides can diffuse into the matrix (–)</td>
</tr>
<tr>
<td>Diffusion depth (m)</td>
</tr>
<tr>
<td>Porosity (–)</td>
</tr>
<tr>
<td>Dry density (Mg/m$^3$)</td>
</tr>
<tr>
<td>Effective diffusion coefficient(m$^2$/s)</td>
</tr>
<tr>
<td>Sorption distribution coefficient</td>
</tr>
</tbody>
</table>
4.5.2.6 Biosphere model and data
The biosphere model considers a plain topography and a fresh water system which is evaluated by applying the same compartment model as used in the H12 report. The dose conversion factors for farming, freshwater fishing and marine water fishing exposure groups are estimated. The radionuclides that are relevant for TRU waste that were not considered in the H12 report were added to the biosphere model and dose conversion factors for each radionuclide are summarized in Table 4.5.2-13. From this, the farming group is identified as the dominant group. These dose values are used in the radionuclide transport analysis described below. In the calculation of dose conversion factors, the effects of naturally occuring stable isotopes are not considered. These need to be evaluated in future biosphere assessments.
<table>
<thead>
<tr>
<th>Radionuclide</th>
<th>Farming group</th>
<th>Freshwater fishing group</th>
<th>Marine fishing group</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-14</td>
<td>6.4×10^{-17}</td>
<td>3.5×10^{-17}</td>
<td>2.4×10^{-17}</td>
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<tr>
<td>Cl-36</td>
<td>4.5×10^{-17}</td>
<td>6.0×10^{-18}</td>
<td>2.9×10^{-21}</td>
</tr>
<tr>
<td>Co-60</td>
<td>1.3×10^{-16}</td>
<td>1.2×10^{-16}</td>
<td>2.1×10^{-17}</td>
</tr>
<tr>
<td>Ni-59</td>
<td>3.7×10^{-18}</td>
<td>4.1×10^{-19}</td>
<td>1.1×10^{-19}</td>
</tr>
<tr>
<td>Ni-63</td>
<td>5.0×10^{-18}</td>
<td>9.8×10^{-19}</td>
<td>2.6×10^{-19}</td>
</tr>
<tr>
<td>Se-79</td>
<td>3.2×10^{-15}</td>
<td>3.2×10^{-17}</td>
<td>3.4×10^{-17}</td>
</tr>
<tr>
<td>Sr-90</td>
<td>1.1×10^{-15}</td>
<td>2.0×10^{-16}</td>
<td>2.4×10^{-19}</td>
</tr>
<tr>
<td>Zr-93</td>
<td>9.6×10^{-18}</td>
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<td>4.5×10^{-19}</td>
</tr>
<tr>
<td>Nb-93m</td>
<td>2.3×10^{-18}</td>
<td>8.5×10^{-19}</td>
<td>9.8×10^{-20}</td>
</tr>
<tr>
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<td>7.5×10^{-16}</td>
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<td>3.7×10^{-19}</td>
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<td>Tc-99</td>
<td>2.6×10^{-17}</td>
<td>4.8×10^{-18}</td>
<td>5.5×10^{-19}</td>
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<tr>
<td>Pd-107</td>
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<td>3.1×10^{-20}</td>
</tr>
<tr>
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<td>1.0×10^{-15}</td>
<td>1.2×10^{-16}</td>
<td>9.9×10^{-16}</td>
</tr>
<tr>
<td>I-129</td>
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<td>7.3×10^{-16}</td>
<td>2.3×10^{-17}</td>
</tr>
<tr>
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<td>3.7×10^{-19}</td>
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<td>2.8×10^{-18}</td>
</tr>
<tr>
<td>Cm-244</td>
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<td>7.8×10^{-16}</td>
<td>2.9×10^{-16}</td>
</tr>
<tr>
<td>Pu-240</td>
<td>3.8×10^{-15}</td>
<td>1.5×10^{-15}</td>
<td>5.4×10^{-16}</td>
</tr>
<tr>
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<td>2.9×10^{-16}</td>
<td>1.4×10^{-18}</td>
</tr>
<tr>
<td>Th-232</td>
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<td>1.4×10^{-15}</td>
<td>5.5×10^{-14}</td>
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<tr>
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<td>6.5×10^{-16}</td>
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<tr>
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<tr>
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<td>2.9×10^{-17}</td>
<td>4.2×10^{-18}</td>
</tr>
<tr>
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<td>1.5×10^{-15}</td>
<td>4.3×10^{-16}</td>
</tr>
<tr>
<td>Np-237</td>
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<td>7.6×10^{-16}</td>
<td>2.4×10^{-17}</td>
</tr>
<tr>
<td>Pu-233</td>
<td>1.8×10^{-17}</td>
<td>6.6×10^{-18}</td>
<td>1.2×10^{-19}</td>
</tr>
<tr>
<td>U-233</td>
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<td>3.2×10^{-16}</td>
<td>2.8×10^{-18}</td>
</tr>
<tr>
<td>Th-229</td>
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<td>3.7×10^{-15}</td>
<td>5.1×10^{-15}</td>
</tr>
<tr>
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<td>1.5×10^{-15}</td>
<td>7.2×10^{-16}</td>
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<tr>
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<td>3.0×10^{-16}</td>
<td>1.7×10^{-18}</td>
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<tr>
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<td>2.1×10^{-18}</td>
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<tr>
<td>Th-230</td>
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</tr>
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<td>3.9×10^{-15}</td>
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<td>1.5×10^{-15}</td>
<td>2.3×10^{-15}</td>
</tr>
<tr>
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</tr>
<tr>
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<td>2.9×10^{-16}</td>
<td>4.0×10^{-18}</td>
</tr>
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<td>1.8×10^{-14}</td>
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<td>9.2×10^{-15}</td>
<td>3.8×10^{-16}</td>
</tr>
</tbody>
</table>
4.5.2.7 Safety assessment model chain
The model chain used in the analysis of the Reference Case is summarized here. Initial conditions, boundary conditions and parameters used in the radionuclide transport analysis are described in sections 4.5.2.3 and 4.5.2.6. Figure 4.5.2-4 illustrates the model chain and main data flow for the radionuclide transport analysis used for the Reference Case calculations.

4.5.2.8 Analysis results
(1) Radionuclide release rates from the engineered barrier
Release rates of radionuclides from the engineered barriers in each waste Group and release rates for each radionuclide are shown in Figures 4.5.2-5 and 4.5.2-6, respectively. For Group 3 and 4 where there is no buffer material, the radionuclide release rates reach a maximum just after closure of the disposal facility. Group 4 waste show the highest release rates from the engineered barriers. Group 2 has the largest amount of radioactive material, but the radionuclide release rates are reduced by the buffer material. Group 3 shows the same level of release rates as Group 2 if no buffer material is used. Group 1 has low volumes of radioactive material and has the lowest release rates.

Sr-90, Cs-137 and Pu-241 are the dominant radionuclides and all belong to Group 4. The dominant radionuclide during the early stage is C-14 (organic) from Group 3 and then C-14 from metal in Group 2 dominates release rates. The radionuclide release rate in Group 1 is controlled by I-129.
Figure 4.5.2-5 Radionuclide release rates from engineered barriers for each waste group

Figure 4.5.2-6 Release rate of each radionuclide from the engineered barriers
(2) Radionuclide release rates from the host rock and the fault

a. Release rates from the host rock

Radionuclide release rates from each group are shown in Figure 4.5.2-7 and individual radionuclides are shown in Figure 4.5.2-8. Group 2 shows the maximum total radionuclide release. As pointed out above, although the maximum release rate for Group 4 from the engineered barriers is large, the release rate is significantly decreased by the host rock and is one order of magnitude less than for Group 3. For individual radionuclides (Fig. 4.5.2-8), the dominant radionuclides are C-14 (organic material), I-129 and Tc-99 since the sorption distribution coefficient of these radionuclides in the host rock is small. In the case of Tc-99 (included in Group 3), since oxidizing conditions in the engineered barriers and the geosphere are assumed, the dissolved chemical form becomes anionic and the sorption distribution coefficient is decreased. On the other hand, radionuclides such as Sr-90 and Cs-137, which have short half-lives of about 30 years, do not reach the host rock.

Figure 4.5.2-7 Release rate from the host rock (for each waste group)
b. Radionuclide release rates to the biosphere via the fault

Radionuclide release rates to the biosphere via the fault from each group are shown in Figure 4.5.2-9 and release rates of individual radionuclides are shown in Figure 4.5.2-10. The maximum rate shows the same value as that for the host rock. Since groundwater flow velocity in the fault is large (50 m/y), no decrease in radionuclide release rates through the fault is observed. However, the release rates are delayed.

The nuclide release rates from the engineered barriers, host rock and fault are shown in Figure 4.5.2-11. Compared with the radionuclide release rates from the engineered barriers and radionuclide transport from the host rock and fault, the difference is significant up to several 100 years after disposal. The difference between the two values is about 1 order of magnitude after 100 years. The radionuclide release rates in the host rock and the fault are almost the same after several 100 years.
Figure 4.5.2-9 Radionuclide release rates for each waste group to the biosphere via the fault

Figure 4.5.2-10 Release rates to the biosphere via the fault
Figure 4.5.2-11 Release rates from each barrier component

(3) Dose from radionuclide release rates to the biosphere

The dose is calculated by multiplying the release rate to the biosphere (via the fault) in (2)b by the effective dose conversion factor in the biosphere in Section 4.5.2.6. The result for each group and radionuclide are shown in Figures 4.5.2-12 and 4.5.2-13. The safety standards in foreign countries and natural background radiation levels in Japan are also shown. The waste group which has the largest effect on dose is Group 1, with a maximum value of about 2 µSv/y per 10,000 years. The next is Group 3, then Group 2 and, finally, Group 4. Since the influence of nitrates in Group 3 is considered and it is not anticipated that I and C are sorbed by materials in the engineered barriers and the geosphere, the maximum dose from Group 3 (0.5 µSv/y) peaks before that of Group 1.

According to Figure 4.5.2-13, the dominant radionuclide after disposal and up to $10^7$ years is I-129. This is followed by C-14, Se-79 and Tc-99. In particular, Se-79 and Tc-99, which belong to Group 3, control dose due to the influence of nitrates.
Figure 4.5.2-12 Results of dose assessment (for each waste group)

Figure 4.5.2-13 Results of dose assessment (for each radionuclide)
4.5.2.9 Summary

The analytical results for the Reference Case can be summarized as follows:

- The maximum dose in the Reference Case is about 2 µSv/y after about 10,000 years and is below the national safety standard of 100~300 µSv/y. The dominant radionuclide is I-129 in Group 1 waste.
- Group 3 waste contributes the next largest maximum dose. This dose takes into account the effect of nitrates in Group 3 waste. Specifically, the dose is due not only to I-129 and C-14 under oxidizing and high ionic strength conditions, but is also due to the sorption distribution coefficients of Se-79 and Tc-99 being decreased in the engineered and natural barriers.
- The third largest influence on dose is given by Group 2 waste. In this case, C-14 (in organic material) dominates the dose.
- In the case of Group 4 waste, the proportion of radionuclides that migrate from the engineered barriers is high, but the contribution to dose is small because sorption in the host rock retards the radionuclides.

4.5.3 Analysis of alternative cases in the base scenario

In Section 4.5.2, the parameters used in the Reference Case and the results of the radionuclide transport analysis were described. In this section, a number of alternative cases are considered and compared with the Reference Case in order to understand the sensitivity of the system to system variations. Changes in disposal system design, variation in waste behavior and variations in the natural barrier are evaluated by means of a comprehensive sensitivity analysis in Section 4.5.4.

The alternative cases considered are as follows:

- Effects of alteration of engineered barrier materials
- Alkaline alteration of surrounding host rock
- Influence of initial oxidizing conditions
- Effect of colloids
- Effects of natural organic material
- Effect of gas and nuclides in gaseous form
- Variation in the geological environment
- Variation in natural barrier data

In Section 4.5.3.1 below, the parameters used in the analysis of alternative cases in Section 4.5.3.2 are established and the analytical results are presented in Section 4.5.3.3. A summary and future issues are discussed in sections 4.5.3.4 and 4.5.3.5, respectively.
4.5.3.1 Model expansion necessary for analysing the alternative cases

Radionuclide transport analyses are carried out for each of the above-mentioned alternative cases and the basic analytical model used in the Reference Case is expanded by including the following individual phenomena (Ooi et al., 2004):

1. Temporal variation in hydraulic and chemical degradation of the engineered barriers
2. Colloids in the natural barrier
3. Expulsion of groundwater in the engineered barriers through gas generation

(1) Alteration of engineered barrier materials over the long term

In order to consider the degradation of cementitious material and alteration due to the reaction between a high-pH plume and the buffer material, the temporal variation of the cement filling and the buffer material are modelled and incorporated into a radionuclide transport analysis. Sorption distribution coefficients, effective diffusion coefficients, porosity, solubility in the cement filling material, the hydraulic conductivity of the filling material and the buffer material are treated as time-dependent parameters. When calculating the permeability of cement filling material, high permeabilities and cracks are conservatively assumed. This parameter is not time-dependent.

(2) Colloid model

Radionuclide sorption on colloids in fracture groundwater is incorporated into the radionuclide transport analysis model. The effect of colloids is analyzed using the model in the H12 report (JNC, 2000), in which radionuclide sorption on colloids is assumed to be linear, instantaneous and reversible.

(3) Gas model

Metal waste corrodes in water and this continues in a reducing atomosphere, producing hydrogen gas. It is also expected that gas will be produced as a result of radiolysis of groundwater by waste and by microbes. Some of the gas generated in the waste is transferred to the outer engineered barriers by dissolution in groundwater. In the case where gas generation is large, gas forms and forces out the same volume of groundwater. In the disposal system with buffer material, gas might also create a pathway in the buffer material. A simple model is developed where groundwater in the engineered barriers is displaced by gas generation, resulting in increased flow velocity in the engineered barriers. This is then incorporated into the radionuclide transport analysis model (Ooi et al., 2004).

(4) Analytical environment and assumptions

OZONE (Takase et al., 2002) was selected as the analytical code for modeling colloids and gas since it has the same function as TIGER, in addition to being very versatile. Output from OZONE has been verified by Miki et al. (2003) by comparison with output from TIGER using the same dataset, and again here in this report by comparison with the output for the Reference Case. In the evaluation of the alternative cases,
I-129, C-14, Cs-137 and the Am-241 series including Np-23 and Th-229 (Am-241, Np-237, U-233, Th-229) are considered. $10^7$ years is assumed as the assessment period, as in the Reference Case.

### 4.5.3.2 Parameters used in alternative cases

(1) Effects of alteration of engineered barrier materials

In the analysis of alteration of cementitious material and buffer material by a high-pH plume (cf. Section 4.4.2), it is suggested that, if the uncertainty in thermodynamic data for minerals, dissolution rates and loss of swelling of the buffer material due to cementation is significant, the low permeable function of buffer material might be lost after several thousands years. Under realistic conditions, it is assumed that the low permeable function of the buffer material is maintained during $10^5$ years. If alteration of the buffer material is assumed, the uncertainty in the pore water composition in Section 4.4.1 is taken into account and solubility limits and sorption are ignored. Based on these assumptions, the following cases are assumed as alternative cases:

1. The low permeable function is lost at 1,000 years and the sorption distribution coefficients, solubilities and effective diffusion coefficients of cementitious filling material and buffer material change.
2. Loss of low permeable function of the buffer material and variation in sorption distribution coefficients occur after $10^4$ years.
3. Loss of low permeable function of the buffer material and variation in sorption distribution coefficients occur after $10^5$ years.
4. Loss of low permeable function of the buffer material and variation in sorption distribution coefficients occur after $10^6$ years.

The analytical cases and parameters are shown in Table 4.5.3-1.
Table 4.5.3-1 Summary of parameters in alternative cases for effects of alteration of the engineered barrier materials

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case</th>
<th>Alteration of engineered barriers</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility</td>
<td>mol/dm³</td>
<td>(Maximum value in Region I and II (RAMDA database* used))</td>
<td>Changes to soluble type</td>
<td>Considers decrease in low permeable function of buffer material</td>
</tr>
<tr>
<td>Sorption distribution coefficient of cementitious filling material</td>
<td>m³/kg</td>
<td>Data for Region I, II Minimum value of (RAMDA)</td>
<td>Minimum value in Region I, II and III (RAMDA)</td>
<td>-</td>
</tr>
<tr>
<td>Sorption distribution coefficient of buffer material</td>
<td>m³/kg</td>
<td>Data for pH &gt; 11, pH ≤ 11 Minimum value of (RAMDA)</td>
<td>Changes to 0</td>
<td>Considers dissolution of smectite in buffer material and assumes that the partition coefficient is 0 after dissolution of smectite</td>
</tr>
<tr>
<td>Hydraulic conductivity of cementitious filling material</td>
<td>m/s</td>
<td>4 × 10⁻⁶</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Hydraulic conductivity of buffer material</td>
<td>m/s</td>
<td>2 × 10⁻¹¹</td>
<td>Changes to 1 × 10⁻⁵</td>
<td>Considers the low permeable function of buffer material</td>
</tr>
<tr>
<td>Porosity of cementitious filling material</td>
<td>-</td>
<td>0.19</td>
<td>Changes to 0.46</td>
<td>Considers the outflow of cement paste</td>
</tr>
<tr>
<td>Porosity of buffer material</td>
<td>-</td>
<td>0.4</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Effective diffusion coefficient of cementitious filling material</td>
<td>m²/s</td>
<td>8 × 10⁻¹⁰</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Effective diffusion coefficient of buffer material</td>
<td>m²/s</td>
<td>(Group 1) 4 × 10⁻¹¹ (Group 2) 3 × 10⁻¹⁰</td>
<td>Changes to 2 × 10⁻⁹</td>
<td>Before alteration: The value for nuclide which contributes to dose is adopted After alteration: Considers smectite dissolution in buffer material</td>
</tr>
<tr>
<td>Start of parameter variation in engineered barrier</td>
<td>y</td>
<td>-</td>
<td>1 × 10³ 1 × 10⁴ 1 × 10⁵ 1 × 10⁶</td>
<td>Assumes parameter variation at time in left column</td>
</tr>
</tbody>
</table>

*RAMDA is radionuclide transport data set in Section 4.5.1 (Mihara and Sasaki, 2005).

For detailed solubility and sorption distribution coefficients, refer to Appendix 4A p2.

(2) Alteration of the host rock by a high-pH plume

In the analysis of alkaline effects on the host rock (cf. Section 4.4.3) it is assumed that the variation in porosity with mineral precipitation and dissolution is insignificant. It is also noted that the uncertainty regarding secondary mineral formation by hyperalkaline reaction of initial minerals in the host rock and the behaviour of the high-pH plume in fractured media are issues that need to be evaluated in the future. Hence, it is recognised that large uncertainties still surround the influence of high pH conditions on host rocks. It is also suggested that the precipitation of secondary minerals on fracture surfaces by the reaction between the high-pH plume and the host rock in fractured media results in a decrease in the effective diffusion coefficient of the matrix and a decrease in the proportion of fracture surface from which nuclides can diffuse into the matrix.
In the alternative cases, it is assumed that silicate minerals precipitate on the fracture surface, thus preventing diffusion of radionuclides into the host rock matrix. Variation in the proportion of fracture surface from which nuclides can diffuse into the matrix is also considered. Since there are not enough reliable data for a realistic evaluation, 1/10 of the diffusion used in the Reference Case is assumed. Moreover, the effect of precipitation of C-S-H gel with a high capacity for radionuclide sorption is not considered. The parameters are summarized in Table 4.5.3-2.

Table 4.5.3-2 Summary of parameters used in alternative cases for host rock data uncertainty

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case</th>
<th>Alternative case</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proportion of fracture surface from which nuclides can diffuse into the matrix</td>
<td>-</td>
<td>0.5</td>
<td>0.05</td>
<td>1/10 of Reference Case</td>
</tr>
</tbody>
</table>

(3) Effect of initial oxidizing conditions

After closure of the disposal facility, the groundwater chemical conditions in the engineered barriers change dynamically until all the initial oxygen and carbon dioxide from the atmosphere introduced during excavation of the facility are consumed. Variation in redox potential due to radiolysis by the waste might also occur. However, it is assumed that the possibility of variation of groundwater chemistry due to radiolysis is small since there is a sufficient volume of metal-reducing agents in waste (see section 4.4.8).

As an alternative case, after closure of the disposal facility an evaluation is performed that assumes an oxidizing environment in groundwater until complete resaturation. Hence, parameters are specified by assuming that an oxidizing atmosphere is maintained until resaturation. The analysis is performed by assuming that all parameters revert back to the original value in the Reference Case at the end of the period of oxidizing conditions.

It is difficult for spent silver absorbent, I-129 filter, to dissolve into groundwater in an oxidizing environment and hence release of I from waste might be restricted. However, this effect is not considered here. The parameters are summarized in Table 4.5.3-3. Since the required period for resaturation is assumed to be 500 years (see resaturation analysis in Section 4.4.4), a wide range of analytical values are used.
Table 4.5.3-3 Summary of parameters used in alternative cases on effects of initial oxidizing conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference case</th>
<th>Initial oxidizing case</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility</td>
<td>mol/dm³</td>
<td>Maximum value (RAMDA)* in Region I, II</td>
<td>Maximum value in RAMDA and oxidizing condition in Reference Case</td>
<td></td>
</tr>
<tr>
<td>Sorption distribution coefficient of cementitious filling material</td>
<td>m³/kg</td>
<td>Minimum value (RAMDA) in Region I, II</td>
<td>Minimum value in RAMDA and oxidizing condition in Reference Case</td>
<td></td>
</tr>
<tr>
<td>Sorption distribution coefficient of buffer material</td>
<td>m³/kg</td>
<td>Minimum value in (RAMDA) pH&gt;11, pH≤11</td>
<td>Minimum value in RAMDA and oxidizing condition in Reference Case</td>
<td></td>
</tr>
<tr>
<td>Continuous duration of oxidizing environment</td>
<td>y</td>
<td>—</td>
<td>1×10², 1×10³, 1×10⁴</td>
<td>Assumes that parameter varies with time in left column</td>
</tr>
</tbody>
</table>

*RAMDA is radionuclide transport data set in Section 4.5.1 (Mihara and Sasaki, 2005).

For detailed solubility and sorption distribution coefficients refer to Appendix 4A p3.

(4) Effect of colloids

In the evaluation of the behaviour of colloids (see Section 4.4.5) in the engineered barrier system, it assumed that the effect on radionuclide migration is small for Groups 1 and 2 due to the presence of buffer material. Hence, the effect of colloids in the engineered barriers is not considered. For Group 3 and 4 wastes, the effects of colloids are considered by excluding radionuclide precipitation.

Although there are currently no realistic data on the influence of colloids in the geosphere, an analysis was performed using the evaluation model and data in the H12 report in order to estimate the extent of influence of colloids on radionuclide migration.

A summary of the parameters for the alternative cases of effects of colloids is given in Table 4.5.3-4.
Table 4.5.3-4 Summary of parameters used in alternative cases on effects of colloids

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case</th>
<th>Colloid influence case</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>In host rock region, pseudo-colloid concentration \times diffusion coefficient into pseudo-colloid</td>
<td>-</td>
<td>-</td>
<td>1</td>
<td>Pseudo-colloid concentration set at 1ppm and diffusion coefficient at 1000 m$^3$/kg</td>
</tr>
<tr>
<td>In host rock region, advection rate of pseudo-colloid concentration used to calculate groundwater flow velocity</td>
<td>-</td>
<td>-</td>
<td>1.3</td>
<td>Maximum value in H12 report (Grindrod, 1993)</td>
</tr>
</tbody>
</table>

(5) Effect of organic material (natural)

In the Reference Case, the effects of cellulose in Group 2 were analysed. However, the effect on radionuclide behavior in the host rock from naturally occurring organic material was not considered. It is assumed that the existence of organic material depends on the geological environment and an evaluation in a generic geological environment thus requires some simplification. Here, it is assumed that a constant concentration of naturally occurring organic material exists in groundwater and the effect on radionuclide migration is evaluated hypothetically.

In the alternative case, it is assumed that the sorption distribution coefficient in the geological medium is affected. Here, the lower limit of data uncertainty in the analytical case in the H12 report is used. The parameters used in these alternative cases are summarized in Table 4.5.3-5.

Table 4.5.3-5 Summary of parameters used in alternative cases on effects of organic material

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case</th>
<th>Organic matter (natural)</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorption distribution coefficient of host rock matrix</td>
<td>m$^3$/kg</td>
<td>Granite data (RAMDA)*</td>
<td>Granite data and minimum uncertainty data value from H12 report</td>
<td>I and C selected assuming 0 m$^3$/kg for Se</td>
</tr>
</tbody>
</table>

*RAMDA is radionuclide transport data set in 4.5.1 (Mihara and Sasaki, 2005).

For detailed solubility and sorption distribution coefficients refer to appendix 4A-p4.
(6) Gas influence

In the gas influence case in Section 4.4.10, the possibility of mechanical deformation of the buffer and the excavation disturbed zone was considered to be small. The influence of gas generation on groundwater flow in the natural barrier was also considered to be small. In the groundwater migration scenario, nuclide migration is increased by the forcing out of groundwater from the engineered barrier system. Hence, the expulsion of contaminated water depending on gas generation from each waste group is used to evaluate gas influence (Table 4.4.10.1-1). The parameters are summarized in Table 4.5.3-6.

Migration analyses of radionuclides in gaseous form (see Section 4.4.10) for Groups 2 and 3, which have large amounts of gas generation, are used to evaluate the amount of gas which reaches the biosphere, assuming that the total amount of C-14 in waste is $\text{CH}_4(\text{g})$. The result of this analysis shows that, since $\text{CH}_4$ from Group 2 is almost completely dissolved into groundwater, there is only a small likelihood of $\text{CH}_4$ reaching the biosphere in gaseous form. Moreover, the maximum $\text{CH}_4$ generated from Group 3 is estimated to be $3 \times 10^{-8} \text{ mol/m/y}$ (per length of tunnel).

Assuming that such gaseous $\text{CH}_4$ reaches the biosphere and dissolves in the aquifer, the dose is calculated using dose conversion factors based on the river water/plain model. From this, the estimated dose for radionuclide migration in gaseous form is around $1 \times 10^{-8} \text{ Sv/y}$, which is significantly smaller than that for groundwater migration (around $2 \times 10^{-6} \text{ Sv/y}$).

Table 4.5.3-6 Summary of parameters used in alternative cases on gas influences

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case</th>
<th>Waste group</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Group 1</td>
</tr>
<tr>
<td>Total drainage</td>
<td>$\text{m}^3/\text{m}$</td>
<td>-</td>
<td>2.6</td>
</tr>
<tr>
<td>Maximum drainage velocity</td>
<td>$\text{m}^3/\text{m/y}$</td>
<td>-</td>
<td>0.26</td>
</tr>
<tr>
<td>Start time of drainage</td>
<td>$\text{y}$</td>
<td>-</td>
<td>1000</td>
</tr>
<tr>
<td>Drainage period</td>
<td>$\text{y}$</td>
<td>-</td>
<td>Total drainage/maximum drainage velocity</td>
</tr>
</tbody>
</table>

(7) Alternative geological environments

a. Alternative rock types

The same six generic rock types used in the H12 report are used again here. The radionuclide transport model in the natural barrier assumes a fractured sedimentary rock for the alternative case and the one-dimensional multipathway model is used. Effective porosity, effective diffusion coefficient and distribution coefficient are specified for each rock type. For Neogene rocks (hard), variation of disposal depth takes into account the length of nuclide transport along a fault, which is set at 300 m. The parameters
used in alternative rock types are summarized in Table 4.5.3-7.

Table 4.5.3-7 Summary of parameters for alternative geological environment cases

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case</th>
<th>Alternative rock type cases</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Case 1</td>
</tr>
<tr>
<td>Rock type</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Crystalline rock</td>
<td>-</td>
<td>Crystalline rock (acidic)</td>
<td></td>
</tr>
<tr>
<td>Pre-Neogene sandstone</td>
<td>-</td>
<td>Pre-Neogene sandstone</td>
<td></td>
</tr>
<tr>
<td>Neogene sandstone</td>
<td>-</td>
<td>Neogene sandstone</td>
<td></td>
</tr>
<tr>
<td>Neogene mudstone/tuff</td>
<td>-</td>
<td>Neogene mudstone/tuff</td>
<td></td>
</tr>
<tr>
<td>Effective porosity</td>
<td>-</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>Effective diffusion coefficient</td>
<td>m²/s</td>
<td>3×10^{-12}</td>
<td>9×10^{-14}</td>
</tr>
<tr>
<td>Matrix sorption diffusion coefficient</td>
<td>-</td>
<td>RAMDA* (granite)</td>
<td>RAMDA (basalt)</td>
</tr>
<tr>
<td>Length of fault</td>
<td>m</td>
<td>800</td>
<td>800</td>
</tr>
</tbody>
</table>

*RAMDA is radionuclide transport data set in Section 4.5.1 (Mihara and Sasaki, 2005).

For detailed solubility and sorption distribution coefficients refer to Appendix 4A p5.

b. Alternative types of groundwater

The alternative geological environments are not restricted to the rock-types above, but also include the chemical composition of groundwater (e.g. freshwater, seawater). Hence, as an alternative case seawater type groundwater is considered as an alternative to freshwater type groundwater with a high pH considered in the Reference Case. The parameters are summarised in Table 4.5.3-8. In the case where groundwater has a marine water composition, suitable site conditions in the biosphere model are also considered (e.g. coastal zone sedimentary layer model).
### Table 4.5.3-8 Alternative groundwater origin case

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case</th>
<th>Alternative groundwater origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical condition of groundwater</td>
<td>—</td>
<td>Fresh/high-pH groundwater</td>
<td>Sea/high-pH groundwater</td>
</tr>
<tr>
<td>Solubility</td>
<td>mol/dm³</td>
<td>Maximum value in Region I and II (RAMDA*)</td>
<td>Maximum value of data for sea water Region I, II (RAMDA) and reference value</td>
</tr>
<tr>
<td>Sorption distribution coefficient of cementitious filling material</td>
<td>m³/kg</td>
<td>Minimum value (RAMDA) in Region I, II</td>
<td>Minimum value of data for sea water Region I, II and reference value</td>
</tr>
<tr>
<td>Sorption distribution coefficient of buffer material</td>
<td>m³/kg</td>
<td>Minimum value (RAMDA) in range pH&gt;11, pH≤11</td>
<td>Minimum value of data for sea water in range pH&gt;11, pH≤11 and reference value</td>
</tr>
<tr>
<td>Sorption distribution coefficient of matrix</td>
<td>m³/kg</td>
<td>RAMDA granite</td>
<td>Minimum value of data for granite (RAMDA) and set value of reference case</td>
</tr>
<tr>
<td>Model for dose conversion factor</td>
<td>—</td>
<td>River water/plain model</td>
<td>Coastal zone sedimentary layer model</td>
</tr>
</tbody>
</table>

*RAMDA is radionuclide transport data set in Section 4.5.1 (Mihara and Sasaki, 2005).

For detailed solubility, sorption distribution coefficients and dose conversion factors refer to Appendix 4A-1.

(8) Alternative natural barrier data

In the Reference Case, the radionuclide retardation capability of the host rock is set to be the same as in the H12 report. However, in the case of TRU waste disposal, the hydraulic properties and radionuclide retardation properties of the host rock have a large influence on the result of dose assessment, as described in the 1st performance assessment report for TRU waste disposal. Hence, for parameters that strongly depend on geological properties, single sensitivity analyses are used to evaluate the sensitivity of dose to parameter variation. Table 4.5.3-9 shows parameter ranges used to evaluate parameter uncertainty.
Table 4.5.3-9 Sensitivity analysis of parameters in the natural barrier

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Reference Case value</th>
<th>Sensitivity range</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fracture transmissivity statistic</td>
<td>m²/s</td>
<td>$1 \times 10^{-10}$</td>
<td>$1 \times 10^{-11} - 1 \times 10^{-9}$</td>
<td>Mean logarithmic standard deviation of fracture transmissivity is set to 1.07</td>
</tr>
<tr>
<td>Hydraulic gradient</td>
<td>-</td>
<td>0.01</td>
<td>0.001 - 0.05</td>
<td>Coastal zone, plain, hills and mountains; considered to be 5 times the range of the Reference Case</td>
</tr>
<tr>
<td>Host rock matrix diffusion depth</td>
<td>m</td>
<td>0.1</td>
<td>0.01 - 1</td>
<td>Data uncertainty: region with 0.1 - 10 times of reference setting</td>
</tr>
<tr>
<td>Proportion of fracture surface from which radionuclides can diffuse into the matrix</td>
<td>-</td>
<td>0.5</td>
<td>0.05 - 1</td>
<td>Data uncertainty: region with 0.1 - 5 times of reference setting</td>
</tr>
<tr>
<td>Porosity of host rock matrix</td>
<td>-</td>
<td>0.02</td>
<td>0.003 - 0.5</td>
<td>Covers all rock types</td>
</tr>
<tr>
<td>Length of fault</td>
<td>m</td>
<td>800</td>
<td>1 - 1000</td>
<td>Large range</td>
</tr>
</tbody>
</table>

(9) Other effects
Other individual phenomena that may have adverse effects on the safety of the disposal system include gas generation by microbes. However, there is currently insufficient knowledge to allow development of meaningful analytical cases.

4.5.3.3 Analytical results

(1) Comparison of the Reference Case with alternative cases for the groundwater scenario
Here, groundwater scenario uncertainty is evaluated by comparing the results of the Reference Case with results from the alternative cases using the parameters described in (1) – (8) above (Fig. 4.5.3-1).

In the alternative case for the engineered barriers, which takes into account the degradation with time of cementitious filling material and buffer material, only a small increase in maximum dose is observed compared to that of the Reference Case if degradation commences $10^3$ years after closure.

In the case which considers radionuclide sorption on colloids in the geosphere, the maximum dose increases by a factor of two compared with that of the Reference Case.

The maximum dose in the gas influence case is almost the same as for the Reference Case and is not changed even if the transport of radionuclides in gaseous form from Groups 2 and 3 is included. In this alternative case, it is assumed that radionuclide migration increases as groundwater expulsion from the engineered barrier increases.

In the case where the duration of oxidizing condition is $10^4$ years and resaturation takes 500 years, the maximum dose is almost as in the Reference Case. In all cases, I-129 dominates the maximum dose.
in Groups 1, 3 and 4, which is the same as for the Reference Case, and C-14 controls the maximum dose for Group 2. Since I-129 and C-14 are soluble with low sorption capability in the engineered barriers, they are unlikely to affect the performance of engineered barrier system. Hence, significant changes in maximum dose are not seen.
Figure 4.5.3-1 Comparison of the Reference Case with alternative cases in the groundwater scenario
Comparison of the Reference Case with analytical cases using hypothetical parameters

Comparison of analytical cases using hypothetical parameters with the Reference Case is shown in Figure 4.5.3-2. In the alternative case that considers effects of organic material, the maximum dose is three times greater than the Reference Case dose. Also, in the case where host rock is altered by high-pH conditions, the maximum dose a factor of two larger than that of the Reference Case.

In the alternative cases that take into account effects of organic material and where the host rock is altered by high-pH conditions, it is assumed that a decrease in sorption distribution coefficient in the host rock is caused by precipitation, which, in turn, decreases the matrix diffusion area. However, due to a lack of knowledge, hypothetical parameters were used. A decrease in the radionuclide containment capability of the host rock was considered in both cases.

Figure 4.5.3-2 Comparison of results of Reference Case with alternative cases that use hypothetical parameters
(3) Comparison of the Reference Case and alternative cases where the geological environment is varied

Analytical results are shown in Figure 4.5.3-3. The dependence of maximum dose on rock type is small (around $2 \times 10^{-6}$ Sv/y in every case).

If seawater-type groundwater is assumed and applied to the river water/plain model in the biosphere model, the maximum dose is three times greater than that of the Reference Case. However, if seawater-type groundwater is applied to a coastal zone sedimentary layer model, the resulting maximum dose to the atmosphere is one order of magnitude less than that of the Reference Case. In this case, the dominant nuclide controlling maximum dose is C-14 from Group 2.

* For comparison with other cases, dose conversion factors for river water are used.

Figure 4.5.3-3 Analytical results for the geological environment alteration case
(4) Validation of data for the natural barrier
Here, some parameters are varied individually, while others are fixed to reference values in order to understand their impact/effect on maximum dose. The parameters that are varied individually are the log-mean of fracture transmissivity, hydraulic gradient, host rock matrix diffusion depth, proportion of fracture surface from which radionuclides can diffuse into the host rock matrix, host rock matrix porosity and fault length (cf. Table 4.5.3-9). All these parameters are found to significantly affect maximum dose, except for fault length.

The impact of the log-mean of host rock transmissivity for each Group is shown in Figure 4.5.3-4. The maximum dose in Groups 1, 3 and 4 is proportional to the log-mean of host rock transmissivity. However, the maximum dose decreases by two orders of magnitude in Group 2 if the log-mean of host rock transmissivity is below $10^{-10}$ m$^2$/s. As described in Section 4.5.3.3(2), I-129 is the key radionuclide in Groups 1, 3 and 4 in the Reference Case and C-14 dominates dose in Group 2. The sensitivity of the log-mean of host rock transmissivity to dose in Group 2 is due to C-14 having a shorter half-life than I-129.

The influence of transmissivity on maximum dose is shown in Figure 4.5.3-5. The dose varies with transmissivity by almost same amount as with the log-mean of transmissivity. However, C-14 contributes significantly to maximum dose when transmissivity is below 0.01. The influence of host rock matrix diffusion depth and proportion of fracture surface from which radionuclides can diffuse into the host rock matrix are shown in Figures 4.5.3-6 and 4.5.3-7. Maximum dose increases as these parameters are decreased.
Figure 4.5.3-5 Analytical results for transmissivity

Figure 4.5.3-6 Analytical results for the host rock matrix diffusion depth
Figure 4.5.3-7 Analytical results for proportion of fracture surface from which radionuclides can diffuse into the matrix

The influence of porosity in the host rock matrix and fault length are shown in Figures 4.5.3-8 and 4.5.3-9 respectively. The maximum dose from waste Group 3 changes by one order of magnitude as porosity is varied. This is due to the assumed oxidizing conditions in the geosphere for Group 3 waste, the sorption distribution coefficient of I being small and the radionuclide retention function of the host rock being strongly dependent on the porous features in the host rock matrix.

The length of the fault does not affect the maximum dose. In the case where flow velocity in fractures in the Reference Case is assumed to be 50 m/y, it is assumed that there is virtually no barrier function for long-lived radionuclides.
Figure 4.5.3-8 Analytical results for porosity of the host rock matrix

Figure 4.5.3-9 Analytical results for the length of faults
4.5.3.4 Summary

Alterations of the engineered barrier materials are a source of uncertainty, classified in Table 4.5.1-1 as “uncertainty in the groundwater scenario”. The analysis of this uncertainty considers the influence of initial oxidizing conditions, colloids and gases. When colloids are included, the maximum dose increases by a factor of 2 compared to the Reference Case. The increase in the maximum dose due to other effects was not significant. In these cases, the radionuclide contributing most to dose was I-129 in Group 1 waste.

Analyses of uncertainty in the groundwater scenario (hypothetical values) showed that, compared to the Reference Case, the maximum dose was increased by a factor of 2 in the case where the host rock was altered under highly alkaline conditions, and by a factor of 3 in the case where natural organic material was present.

Alternative cases aimed at the geological environment investigated uncertainties in the groundwater scenario model and parameters. There were no observed variations in the maximum dose due to differences in rock types. If the groundwater changes from freshwater-type to seawater-type, the proportion of radionuclides that migrate to the biosphere is increased. However, if dose conversion factors which are consistent with the seawater environment are used, the maximum dose is decreased by a factor of about 10. In this case, the radionuclide that contributed most to the dose was C-14 in Group 2 waste.

These alternative cases also revealed that variations in the maximum dose are caused by the log-mean of the host rock transmissivity and variations in transmissivity. If the log-mean of the host rock transmissivity is increased by a factor of 10 compared to the Reference Case, the maximum dose is also increased by a factor of 10. In all the analytical results, the radionuclide which contributed most to the maximum dose was I-129 in Group 1 waste.

In the above analyses, the impact/effect of each chosen parameter was evaluated by specifying an optional fixed value for the parameter, or by changing its value. The other parameter values were fixed to be the same as in the Reference Case. However, in order to evaluate the effects of uncertainties more robustly, more detailed analyses are needed to consider the effects of varying all parameter values in different combinations. The next Section, 4.5.4, describes robust results that were obtained from such a comprehensive analysis.

4.5.3.5 Future issues

- Model upgrade for alteration of the engineered barrier materials

The model used for evaluating alteration of the engineered barrier materials assumed that some parameters, such as sorption distribution coefficient and solubility, change abruptly at set time periods. In this analysis, since the radionuclides I-129 and C-14 which dominate dose are soluble and have low sorption in the engineered barriers, the sorption distribution coefficient and solubility of the engineered barrier materials
have no effect on the maximum dose. In future, in order to improve the reliability of the evaluation, refinement of the model and development of a method for selecting suitable input parameters is needed.

- Upgrading of colloid model and data acquisition
The colloid model in this report assumes linear instantaneous sorption of radionuclides by colloids. However, at present there is no reliable model for the effect colloids. Hence, integration of realistic models into the radionuclide transport analysis is necessary. In addition, the chemical forms of radionuclides that migrate from waste are not uniform. Hence, for assessing the effects of colloids, data for each radionuclide needs be accumulated and reflected in the radionuclide transport analysis.

- Treatment of host rock alteration in the presence of natural organic material and high pH
Depending on how these datasets are handled can lead to evaluations that are either under-conservative or over-conservative. Further investigations are needed for these datasets.

- Improving knowledge of I and C in the host rock
Parameters such as depth of matrix diffusion were taken from the safety assessment performed in the H12 report. However, the behavior of I and C in the host rock may be different from radionuclides relevant for HLW. Hence, further study is required of the behaviour of I and C in the host rock.
4.5.4 Evaluation of uncertainty in the base scenario
In the previous section (4.5.3), the influence of model and parameter uncertainty in the groundwater scenario on dose calculation was evaluated by comparing output from alternative cases (e.g. groundwater scenario uncertainty (cf. Section 4.5.1) etc) with that of the Reference Case.

Here in this section, the influence of overlap of scenarios and/or phenomena and the wide variation in parameters, including hypothetical parameter ranges, are evaluated using a comprehensive sensitivity analysis (Ooi et al., 2004). This method involves randomly sampling independent parameters and then using a statistical approach to identify parameters that have a large impact on dose and to extract combinations of parameter values (defined as “a successful condition”) that result in doses less than the target value.

As described in Section 4.5.3, total dose is predominantly controlled by I-129 in Group 1, which is soluble, has low sorption and does not form a decay chain. In order to reduce the number of computations in the evaluation, uncertainty concerned with the migration of I-129 mainly is evaluated quantitatively.

In this section the following is presented:
① Quantification of the influence of uncertainty and demonstration of the adequacy of safety assessments;
② Quantification of safety margin to safety criteria and of parameter tolerance to changes in parameter values;
③ Presentation of alternative planning options and of the prospect on the treatment of unresolved problems;
④ Presentation of important issues to be researched.
Section 4.5.4.1 describes the comprehensive sensitivity analysis method, Section 4.5.4.2 the variation range of parameters, Section 4.5.4.3 the results and Section 4.5.4.4 the conclusions.

4.5.4.1 Comprehensive sensitivity analysis
A large number of parameters that have an impact on dose are identified and the effects of each parameter on dose variation are investigated. Threshold parameter values (or parameter value combinations) that do not result in a target dose being exceeded are extracted. This condition is defined as a successful condition (see below).

(1) Identification of important parameters and their impact on dose
In this analysis, a number of parameters are given ranges that are considered to be conservative (see Section 4.5.4.2 below). Each parameter has its own unique range which is treated as a uniform distribution for simplicity. Parameter values are identified by random sampling of these uniform distributions. Multiple maximum doses that are regarded as being statistically significant are calculated using nuclide migration analyses using OZONE (see Section 4.5.3.1) for the randomly sampled parameter values. These results are
then plotted on a 2D distribution of maximum dose (vertical axis) versus parameter value (horizontal axis) (Figure 4.5.4-1) in order to identify parameters that have a large impact. The methodology can be summarised as follows:

1. Parameter ranges are divided into equal sub-divisions.
2. Average maximum dose in each sub-division is calculated and all averages (points) are fitted to a polynomial using the least squares approach.
3. Parameter importance is defined as the difference between maximum and minimum values of the fitted curve of the polynomial (see Figure 4.5.4-1).
4. Parameter influence (where influence equals importance divided by variability) is calculated using parameter importance and parameter variability (defined as the difference between maximum and minimum values).

An example of the quantification of parameter importance is shown in Figure 4.5.4-1. By comparing the results, parameters with the greatest importance are identified. The curve that shows the relationship between parameter variation and dose is useful information for understanding the effects of the parameter on dose variation.

![Figure 4.5.4-1 Identification of parameter importance (see text for definition)](image)

(2) Definition and extraction of the “successful condition”
The successful condition is defined here as the parameter value (or combination of parameter values) that
does not result in a maximum permitted dose (target dose) being exceeded. In order to extract this condition, parameters with a high level of importance are identified first.

The approach for extraction of this condition using parameters with large importance is described as follows.

a. Estimation of the successful condition
The curves are fitted to average values and $3\sigma$ calculated in each division. An intersection of the $3\sigma$ curve and target dose line is regarded as a candidate parameter value for a successful condition when $3\sigma$ does not exceed target dose. As an example, the relationship between host rock matrix diffusion depth and maximum dose is shown in Figure 4.5.4-2. If the target dose is set to 10 $\mu$Sv/y, then a host rock matrix diffusion depth of 0.5 m or above (indicated by arrow) would yield a successful condition.

![Figure 4.5.4-2 Depth of host rock matrix diffusion versus maximum dose (I-129 only)](image)

b. Identification of the successful condition
In order to identify the successful condition, the candidate parameter value identified above for the assumed successful condition is set and dose is calculated using deterministic consequence calculations (using OZONE), with all the other parameters set to conservative values (within plausible parametric ranges). If the target dose is exceeded, the candidate parameter value for the assumed successful condition
is varied within the assumed parameter range and the analysis is repeated again until a value is found where target dose is not exceeded.

c. Confirmation of adequacy of successful condition
The other parameters that were fixed in the calculations above are varied and an upper limit is confirmed based on deterministic consequence calculations used to identify the successful condition above. If the target dose is exceeded, the cause is identified and the conservative values of parameters in the identification of the successful condition are reviewed.

4.5.4.2 Specification of parameter variation ranges
A wide parameter range is used in the comprehensive sensitivity analysis based on existing experimental and literature data in order to cover the parameter values used in the deterministic consequence calculations. Example parameter ranges, sorption distribution coefficients (Kd) of cementitious filling material in Group 4 are shown in Figure 4.5.4-3, as well as the reference values from Section 4.5.3. Also, the parameter ranges and fixed values (Group 1) used in the comprehensive sensitivity analysis above are shown in Table 4.5.4-1.

![Parameter ranges of sorption distribution coefficients (Kd) of cementitious filling materials used in the comprehensive sensitivity analysis](image-url)
<table>
<thead>
<tr>
<th>No.</th>
<th>Classification</th>
<th>Parameter</th>
<th>Unit</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Design condition</td>
<td>Inventory of I</td>
<td>Bq</td>
<td>$5.11 \times 10^{12} - 5.11 \times 10^{14}$</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>Disposal amount of waste</td>
<td>m$^3$</td>
<td>318</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>Burial ratio of waste to volume</td>
<td>—</td>
<td>0.29</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>Height of waste emplacement area</td>
<td>m</td>
<td>5.5</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>Cross-section area of waste emplacement area</td>
<td>$m^2$</td>
<td>41.25/($LR$)</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>Total length of shaft</td>
<td>m</td>
<td>24 * ($LR$)</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>Tunnel length variation ratio ($LR$)</td>
<td>—</td>
<td>0.37 - 2</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td>Thickness of buffer material</td>
<td>m</td>
<td>0.1 - 3</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td>Thickness of excavation damaged zone (EDZ)</td>
<td>m</td>
<td>0.5 - 5</td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>True density of cementitious filling material</td>
<td>kg/m$^3$</td>
<td>2580</td>
</tr>
<tr>
<td>11</td>
<td></td>
<td>True density of buffer material</td>
<td>kg/m$^3$</td>
<td>2680</td>
</tr>
<tr>
<td>12</td>
<td></td>
<td>True density of rock</td>
<td>kg/m$^3$</td>
<td>2700</td>
</tr>
<tr>
<td>13</td>
<td>Geological environment</td>
<td>Hydraulic gradient</td>
<td>—</td>
<td>0.001 - 0.23</td>
</tr>
<tr>
<td>14</td>
<td></td>
<td>Log mean of fracture transmissivity</td>
<td>m/s</td>
<td>$1 \times 10^{-15} - 1 \times 10^{-4}$</td>
</tr>
<tr>
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<td>Standard deviation of logarithmic distribution of fracture transmissivity</td>
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<td>16</td>
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<td>Fracture aperture width coefficient ($\alpha$)</td>
<td>—</td>
<td>0.1 - 10</td>
</tr>
<tr>
<td>17</td>
<td></td>
<td>Fracture aperture width coefficient ($\beta$)</td>
<td>—</td>
<td>0.5</td>
</tr>
<tr>
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<td></td>
<td>Fracture internal effective diffusion coefficient</td>
<td>m/s</td>
<td>$4 \times 10^{-9}$</td>
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<tr>
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<td>Length of natural barrier</td>
<td>m</td>
<td>100</td>
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<td>Dispersion ratio in natural barrier</td>
<td>—</td>
<td>0.01 - 1.00</td>
</tr>
<tr>
<td>21</td>
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<td>Matrix diffusion depth</td>
<td>m</td>
<td>0.01 - 1</td>
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<td>Matrix diffusion area ratio (Proportion of fracture surface from which nuclides can diffuse into the matrix)</td>
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<td>0.1 - 1</td>
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<td>Porosity of Matrix</td>
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<td>0.003~0.5</td>
</tr>
<tr>
<td>24</td>
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<td>m/s</td>
<td>$6 \times 10^{-12} - 4 \times 10^{-11}$</td>
</tr>
<tr>
<td>25</td>
<td>Biosphere model</td>
<td>Dose conversion factor of I</td>
<td>Sv/Bq</td>
<td>$2.31 \times 10^{-9} - 1.59 \times 10^{-9}$</td>
</tr>
<tr>
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<td>Barrier characteristics</td>
<td>Start time of nuclide leaching from waste</td>
<td>y</td>
<td>0</td>
</tr>
<tr>
<td>27</td>
<td></td>
<td>Duration of nuclide leaching from waste</td>
<td>y</td>
<td>0 - 10</td>
</tr>
<tr>
<td>28</td>
<td></td>
<td>Hydraulic conductivity before alteration of cementitious filling material</td>
<td>m/s</td>
<td>$1 \times 10^{-15} - 1 \times 10^{-14}$</td>
</tr>
<tr>
<td>29</td>
<td></td>
<td>Hydraulic conductivity after alteration of cementitious filling material</td>
<td>m/s</td>
<td>$1 \times 10^{-15} - 1 \times 10^{-14}$</td>
</tr>
<tr>
<td>30</td>
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<td>Diffusion coefficient in pore water before alteration of cementitious filling material</td>
<td>m/s</td>
<td>$4 \times 10^{-10}$</td>
</tr>
<tr>
<td>31</td>
<td></td>
<td>Diffusion coefficient in pore water after alteration of cementitious filling material</td>
<td>m/s</td>
<td>$4 \times 10^{-10}$</td>
</tr>
<tr>
<td>32</td>
<td></td>
<td>Porosity of cementitious filling material before alteration</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>33</td>
<td></td>
<td>Porosity of cementitious filling material after alteration</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>34</td>
<td></td>
<td>Hydraulic conductivity of buffer material before alteration</td>
<td>m/s</td>
<td>$2 \times 10^{-13} - 2 \times 10^{-11}$</td>
</tr>
<tr>
<td>35</td>
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<td>Hydraulic conductivity of buffer material after alteration</td>
<td>m/s</td>
<td>$2 \times 10^{-17} - 1 \times 10^{-15}$</td>
</tr>
<tr>
<td>36</td>
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<td>Diffusion coefficient in pore water before alteration of buffer material</td>
<td>m/s</td>
<td>$6 \times 10^{-12} - 2 \times 10^{-11}$</td>
</tr>
<tr>
<td>37</td>
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<td>Diffusion coefficient in pore water after alteration of buffer material</td>
<td>m/s</td>
<td>$6 \times 10^{-12} - 4 \times 10^{-11}$</td>
</tr>
<tr>
<td>38</td>
<td></td>
<td>Porosity of buffer material before alteration</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>39</td>
<td></td>
<td>Porosity of buffer material after alteration</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>40</td>
<td></td>
<td>Increasing ratio of permeability at EDZ</td>
<td>—</td>
<td>10~1000</td>
</tr>
<tr>
<td>41</td>
<td></td>
<td>Increasing ratio of flow rate at EDZ</td>
<td>—</td>
<td>0.1~100</td>
</tr>
<tr>
<td>42</td>
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<td>Dispersion ratio in engineered barrier area</td>
<td>—</td>
<td>0.1</td>
</tr>
<tr>
<td>43</td>
<td></td>
<td>Sorption distribution coefficient of I before alteration of cementitious filling material</td>
<td>m$^3$/kg</td>
<td>—</td>
</tr>
<tr>
<td>44</td>
<td></td>
<td>Sorption distribution coefficient of I after alteration of cementitious filling material</td>
<td>m$^3$/kg</td>
<td>$1 \times 10^{-17} - 1 \times 10^{-13}$</td>
</tr>
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<td>Sorption distribution coefficient of I before alteration of buffer material</td>
<td>m$^3$/kg</td>
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<td>Sorption distribution coefficient of I after alteration of buffer material</td>
<td>m$^3$/kg</td>
<td>0</td>
</tr>
<tr>
<td>47</td>
<td></td>
<td>Sorption distribution coefficient of I of matrix</td>
<td>m$^3$/kg</td>
<td>$1 \times 10^{-4} - 1 \times 10^{-7}$</td>
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<td>48</td>
<td></td>
<td>Solubility of I</td>
<td>mol/l</td>
<td>Soluble</td>
</tr>
<tr>
<td>49</td>
<td></td>
<td>Flow velocity scale of colloid in filling material area</td>
<td>—</td>
<td>1~1.3</td>
</tr>
<tr>
<td>50</td>
<td></td>
<td>Colloid concentration in filling material * Sorption distribution coefficient into colloid</td>
<td>—</td>
<td>0~1</td>
</tr>
<tr>
<td>51</td>
<td></td>
<td>Flow velocity scale of colloid in buffer material area</td>
<td>—</td>
<td>1~1.3</td>
</tr>
<tr>
<td>52</td>
<td></td>
<td>Colloid concentration in buffer material * Sorption distribution coefficient into colloid</td>
<td>—</td>
<td>0~1</td>
</tr>
<tr>
<td>53</td>
<td></td>
<td>Flow velocity scale of colloid in fracture</td>
<td>—</td>
<td>1~1.3</td>
</tr>
<tr>
<td>54</td>
<td></td>
<td>Colloid concentration in fracture * Sorption distribution coefficient into colloid</td>
<td>—</td>
<td>0~1</td>
</tr>
<tr>
<td>55</td>
<td></td>
<td>Total drainage amount from engineered barrier by gas generation</td>
<td>m$^3$/m</td>
<td>0.02~2.6</td>
</tr>
<tr>
<td>56</td>
<td></td>
<td>Drainage velocity from engineered barrier by gas generation</td>
<td>m$^3$/m/y</td>
<td>0.26</td>
</tr>
<tr>
<td>57</td>
<td></td>
<td>Drainage start time from engineered barrier by gas generation</td>
<td>y</td>
<td>1000~10000</td>
</tr>
<tr>
<td>58</td>
<td></td>
<td>Alteration time of engineered barrier</td>
<td>y</td>
<td>$1 \times 10^{-8} - 1 \times 10^{0}$</td>
</tr>
<tr>
<td>59</td>
<td></td>
<td>Alteration duration of engineered barrier</td>
<td>y</td>
<td>0~0</td>
</tr>
</tbody>
</table>

Table 4.5.4-1 Parameter ranges and constant parameter values used in the comprehensive sensitivity analyses (for Group 1 waste)
4.5.4.3 Analytical results
The first step is to decide on a target dose. Here 10 µSv/y is chosen as the target dose (with I-129 in as the target radionuclide). A preliminary analysis is performed and linear relationships between dose conversion factor and dose, and between radionuclide inventory and dose are confirmed in Group 1.

Here, the radionuclide inventory and dose conversion factor are set to the reference value and other parameters with a high level of importance are identified and the successful conditions are extracted.

(1) Results of statistical analysis
The results of the statistical analysis and comparisons between level of importance and influence on maximum dose are shown in Figure 4.5.4-4. The result of the deterministic consequence analysis for the Reference Case shown in Section 4.5.2 and the results of alternative cases shown in Section 4.5.3 are illustrated in Figure 4.5.4-4. From Figure 4.5.4-4, it can be seen that the log-mean of fracture transmissivity, duration of nuclide leaching from waste, sorption distribution coefficient of I before alteration of cementitious filling material and hydraulic gradient significantly affect the maximum dose. These parameters have a high level of importance.

Figure 4.5.4-4 Results of the statistical analysis and comparisons between level of importance and influence on maximum dose

The successful condition is evaluated by focusing on the log-mean of fracture transmissivity. The relationship between log-mean and maximum dose is shown in Figure 4.5.4-5. From Figure 4.5.4-5, permitted dose (10 µSv/y) is exceeded if other parameters are varied. This shows that the log-mean of fracture transmissivity alone does not result in a successful condition.
In the comprehensive sensitivity analysis, if a single parameter with a high level of importance does not yield a successful condition, combinations of multiple parameters with a high level of importance are then investigated.

From the preliminary analysis, it was recognized that hydraulic parameters such as log-mean of fracture transmissivity (T) or hydraulic gradient (i) which express groundwater flow velocity (V) (cf. Section 4.5.2) in the geological environment have a high level of influence on dose.

In order to simplify the analysis, it is assumed that the variation range of the product of the log-mean of fracture transmissivity and hydraulic gradient is within the range of $10^{-13} - 10^{-11}$ m$^2$/s. The hydraulic gradient is then set to 0.01 and the log-mean of fracture transmissivity is changed to $10^{-11}$, $10^{-10}$ and $10^{-9}$ m$^2$/s. Furthermore, in the analysis, porosity of matrix is set to the reference value (0.02) in the reference geological environment for crystalline rock.

Successful conditions are extracted for cases where hydraulic gradient, porosity of matrix and log-mean of fracture transmissivity are 0.01, 0.02 and $10^{-10}$ m$^2$/s or $10^{-9}$ m$^2$/s, respectively.

Figure 4.5.4-4 shows that a discrete increase in maximum dose occurs after $10^3 - 10^6$ years (indicated by an ellipse). From statistical analyses, it is revealed that this is caused by accumulated radionuclides in the
engineered barriers being released over a short period. As the containment function of long half-life radionuclides before degradation of engineered barrier materials increases, the radionuclide release rate from the engineered barriers after degradation is increased. Under this condition, in order to perform a conservative evaluation with respect to extracting a successful condition, the performance of the engineered barrier should be set up for higher radionuclide containment. However if the engineered barrier system has a higher radionuclide containment function, the calculated (i.e. resulting) dose is not conservative. Therefore, it is difficult to make a confident evaluation with a high radionuclide containment function unless parameters relating to the radionuclide containment function are reliable and realistic. Assuming degradation of the engineered barrier materials, the analysis is performed using conservative values for rapid release and rapid degradation.

(2) Analytical result for hydraulic conditions in the geological environment of the Reference Case

In this evaluation, in addition to the log-mean of fracture transmissivity, hydraulic gradient and porosity of matrix which relate to the geological environment, radionuclide transport distance and fault length are set to reference values ($10^{10}$ m$^2$/s, 0.01, 0.02 and 100 m and 800 m respectively). Also, the thicknesses of the buffer material and the excavation damaged zone (EDZ) and increasing ratio of flow rate at EDZ are set to reference values. These parameters have low or controllable uncertainty. Considering barrier degradation, the sorption distribution coefficient of I of cementitious material and buffer material is assumed to be 0 at all times. Moreover, it is assumed that radionuclide release from waste is instantaneous. The results of statistical analyses and comparisons between parameter importance and influence on maximum dose for this analytical case are shown in Figure 4.5.4-6.

![Graph showing statistical analysis results and comparisons between parameter importance and influence on maximum dose](image)

Figure 4.5.4-6 Statistical analysis results and comparisons between parameter importance and influence on maximum dose
As shown in Figure 4.5.4-6, maximum dose can be decreased to several 10 µSv/y without regard to the variation of other parameters when geological environment parameters and some parameters which have controllable or low uncertainty are set to reference values. However, it should be noted that around 50% of statistical results have doses higher than 10 µSv/y. Moreover, based on sensitivity analyses, it is revealed that the host rock matrix diffusion depth, sorption distribution coefficients of the host rock matrix, the product of colloids concentration in fractures and the sorption distribution coefficients into colloids of I and the proportion of fracture surface from which radionuclides can diffuse into the matrix significantly affect maximum dose.

Based on these results, attention is focused on parameters with a high importance, namely matrix diffusion depth, sorption distribution coefficient of the host rock matrix of I and the proportion of fracture surface from which radionuclides can diffuse into the matrix. The successful condition is established through a combination of these parameters. Here, an analysis is carried out with the proportion of fracture surface from which radionuclides can diffuse into the matrix set to 0.2 and 0.5, while other parameters are varied. This result is summarized in Figure 4.5.4-7 and shows the relationship between matrix diffusion depth and sorption distribution coefficient of I in the host rock matrix. In Figure 4.5.4-7, the upper right region beyond the dotted line is estimated to represent a successful condition.

In order to confirm that this region represents a successful condition, matrix diffusion depth (example) is set to the reference value (0.1 m) while the sorption distribution coefficient of the host rock matrix of I is varied and the analysis is performed with other parameters set to conservative values. This result is shown in the figure.
in Figure 4.5.4-8. In the case where the proportion of fracture surface from which radionuclides can diffuse into the matrix is 0.5, the resulting dose remains below the target dose if the sorption distribution coefficient for the host rock of I is above $8 \times 10^{-5}$ m$^3$/kg.

![Figure 4.5.4-8 Confirming the successful condition](image)

Figure 4.5.4-8 Confirming the successful condition

Parameter ranges and reference values for this condition are shown in Table 4.5.4-2.

Table 4.5.4-2 Example of the successful condition

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Threshold range</th>
<th>Variation range</th>
<th>Reference value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inventory (Bq)</td>
<td>$\leq 5.11 \times 10^{13}$</td>
<td>$5.11 \times 10^{12} - 5.11 \times 10^{14}$</td>
<td>$5.11 \times 10^{13}$</td>
</tr>
<tr>
<td>Dose conversion factor (Sv/Bq)</td>
<td>$\leq 3.19 \times 10^{-15}$</td>
<td>$2.31 \times 10^{-17} - 1.59 \times 10^{-13}$</td>
<td>$3.19 \times 10^{-15}$</td>
</tr>
<tr>
<td>Log-mean of fracture transmissivity (m$^2$/s)</td>
<td>$\leq 1 \times 10^{-10}$</td>
<td>$1 \times 10^{-11} - 1 \times 10^{-6}$</td>
<td>$1 \times 10^{-10}$</td>
</tr>
<tr>
<td>Hydraulic gradient (-)</td>
<td>$\leq 0.01$</td>
<td>$0.001 - 0.23$</td>
<td>$0.01$</td>
</tr>
<tr>
<td>Porosity of host rock matrix (-)</td>
<td>$0.02 \leq$</td>
<td>$0.003 - 0.5$</td>
<td>$0.02$</td>
</tr>
<tr>
<td>Length of natural barrier</td>
<td>100</td>
<td>-</td>
<td>100</td>
</tr>
<tr>
<td>Length of fault</td>
<td>800</td>
<td>-</td>
<td>800</td>
</tr>
<tr>
<td>Thickness of buffer material (m)</td>
<td>$1 \leq$</td>
<td>0.1 - 3</td>
<td>1</td>
</tr>
<tr>
<td>Thickness of excavation disturbed zone (m)</td>
<td>$\leq 3$</td>
<td>0.5 - 5</td>
<td>3</td>
</tr>
<tr>
<td>Increase ratio of flow rate at EDZ (-)</td>
<td>$\leq 1$</td>
<td>0.1 - 100</td>
<td>1</td>
</tr>
<tr>
<td>Matrix diffusion depth (m)</td>
<td>$0.1 \leq$</td>
<td>0.01 - 1</td>
<td>0.1</td>
</tr>
<tr>
<td>Sorption distribution coefficient of I in host rock matrix (m$^3$/kg)</td>
<td>$8 \times 10^{-5} \leq$</td>
<td>$1 \times 10^{-7} - 1 \times 10^{-4}$</td>
<td>$1 \times 10^{-4}$</td>
</tr>
<tr>
<td>Matrix diffusion area ratio (-)</td>
<td>$0.5 \leq$</td>
<td>0.1 - 1</td>
<td>0.5</td>
</tr>
<tr>
<td>Other parameters</td>
<td>All possible ranges</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
It is expected that many values for the three parameters highlighted in yellow in Table 4.5.4-2 exist whereby dose is not exceeded. The parameter combinations in Table 4.5.4-2 result in one successful condition, even if uncertainty in the input range of all other parameters is taken into account. In Figure 4.5.4-9, the results of the statistical analysis using values in Table 4.5.4-2 are shown.

With the exception of the case relating to a change in groundwater origin, all other analyzed values from alternative cases fall within the statistical range. One reason why the change in groundwater origin case lies outside the statistical range is that the dose conversion factor used in this case was for a seawater model and not a river water model, as was used in all the other cases.

The scenarios that are considered to have an impact on parameter values in Table 4.5.4-2 are lowering of the sorption distribution coefficient of I in the host rock by natural organic material, lowering of matrix diffusion area ratio by a high-pH plume and decrease in matrix diffusion depth. Hence, improving the understanding of the degradation of the natural barrier due to these effects is important. Excluding parameters related to the design of the engineered barriers, conservative values are considered. Moreover, excluding parameters related to the design, conservative values are set for the parameters related to the engineered barriers in this analysis. If uncertainty can be reduced in these parameter settings, there is some leeway for these parameters in the obtained successful condition.

Figure 4.5.4-9 Successful condition below target dose and results of a statistical analysis
(3) Uncertainty in hydraulic features and performance target in alternative technologies

As described in Section 4.5.3, in the condition where the log-mean of fracture transmissivity is 10 times higher than the Reference Case and the hydraulic gradient is 0.01, the maximum dose slightly exceeds the target dose, even if other parameters are set to reference values. Hence, under the same conditions, in order to stay below target dose, other parameter values should be selected so that radionuclide containment increases. As a simple alternative, an increase in the thickness of buffer material is considered. However, in this section, the focus is on duration of nuclides leaching from waste with a high level of importance identified in Section 4.5.4.3(1) and related to advanced waste containment functions discussed in Chapter 7, and a successful condition which satisfies the target dose is evaluated.

The range of the product of the log-mean of fracture transmissivity and hydraulic gradient is assumed to be $10^{-13} - 10^{-11} \text{ m}^2/\text{s}$, and the maximum dose obtained from the analysis with varying other parameters is shown in Figure 4.5.4-10 against the nuclides leaching time. Furthermore, the maximum dose obtained from calculations with $10^{-10} \text{ m}^2/\text{s}$ (Reference Case) and $10^{-9} \text{ m}^2/\text{s}$ of log-mean of fracture transmissivity and with the same values as in the Reference Case of other parameters are shown in Figure 4.5.4-11 against the nuclide leaching time from waste.

![Figure 4.5.4-10 Results of a statistical analysis](image-url)
The solid lines in Figure 4.5.4-10 and the line expressing the multiplication of leach rate from waste and dose conversion factors in Figure 4.5.4-11 show the relationship between maximum dose calculated using leach rate with no engineered barriers and leaching duration. From this analysis, it is shown that the data which are plotted on the high dose side of the solid line in Figure 4.5.4-10 are caused by dissolution of radionuclides that accumulated in the engineered barriers and are then released by degradation of the engineered barriers over the short term. This means that, in the case that degradation of the engineered barriers occurs and a large amount of radionuclides are sorbed in the engineered barriers before degradation, the maximum dose is assumed to be above 10 µSv/y, even assuming 100,000 years of radionuclide leach time.

As shown in Figure 4.5.4-11, if it is not necessary to consider the radionuclide release relating to degradation of the engineered barriers, the maximum dose is below 10 µSv/y for about 20,000 years of nuclide release time regardless of hydrological conditions. If the nuclide release time is 100,000 years, the maximum dose is assumed to be around 2 µSv/y, which is the same as in the Reference Case. Hence, in order to improve the safety of disposal, different systems from those with emphasis the on radionuclide containment should be also evaluated.

However, it is difficult to consider short-term degradation after several 10,000 years (or several 100,000 years). Furthermore, in this analysis, the transition from a sound barrier to a degraded barrier was connected by discrete steps and such degradation modeling might lead to extremely conservative results.
Since there is insufficient knowledge about the temporal change in the engineered barriers, further work on improving understanding of temporal change is needed.

In addition to analyses of alternative cases using deterministic consequence analyses in Section 4.5.3, the result of the comprehensive sensitivity analysis which includes influence of change in design conditions (variation in thickness of buffer material), change in waste performance (effect of changing of radionuclide leach rate) was shown.

These analyses use a one-dimensional multipathway model in the natural barrier based on the 1D parallel-plate model. However, it is important to evaluate the effect of model uncertainty on dose. In this report, in evaluating the effect of model/parameter uncertainty, the assumption that the transport medium in the natural barrier is a porous medium is considered.

A comprehensive sensitivity analysis for a natural barrier with a porous medium has already been performed using the same parameters as above (e.g. inventory) (Ooi et al., 2004). From this result, it was shown that the successful condition could be extracted even in groundwater flow rate conditions (product of hydraulic conductivity and hydraulic gradient \((1.0 \times 10^{-9} \text{ m s}^{-1} \times 0.05)\)) that are 5 times higher than groundwater flow rate \((1.0 \times 10^{-9} \text{ m s}^{-1} \times 0.01)\) in the Reference Case for porous media in this study. Because of the different models, simple comparison appears difficult. However, the concept of TRU waste geological disposal in this report is considered to be a robust concept from the point of view of safety, even in the migration model for a porous medium natural barrier.

**4.5.4.4 Summary**

1. It has been confirmed that parameters describing geological environment conditions (hydrogeological parameters) significantly affect the maximum dose.
2. It has been confirmed that, when the geological environment conditions (log-mean transmissivity, hydraulic gradient, porosity of matrix), analytical conditions (length of natural barrier, length of fault) and design condition parameters were assumed to have the same values as in the Reference Case, even if the uncertainties are taken into account in all parameters except the above, the maximum dose was less than several 10s of \(\mu\text{Sv/y}\) and safety is not significantly compromised.
3. In the successful condition obtained from the comprehensive sensitivity analysis, it has been confirmed that, if it is assumed that the maximum acceptable target dose is 10 \(\mu\text{Sv/y}\), safety is not compromised by the effects of engineered barrier degradation, colloids, gases and initial oxidizing conditions. This result holds true even when the effects of these phenomena are considered together. Furthermore, concerning hypothetical uncertainty of natural organic material and alteration of host rock by high pH, if the sorption distribution coefficient of I, host rock matrix diffusion depth of I and surface area through which I may diffuse were the same as in the Reference Case, it was confirmed that safety is not compromised even when all other varied parameters are considered.
It has been confirmed that system safety will not be compromised in the case where the geological environment conditions are not as favorable as the reference conditions, due to improvements in the performance of waste packages. This result is true even when consideration is given to uncertainties in other phenomena.

4.5.4.5 Future issues

The reliability of the results obtained from the comprehensive sensitivity analysis depends on the conservativeness of analytical models for evaluating each phenomenon and parameter ranges. Hence, further study of the phenomena mentioned in Section 4.4 is necessary, in addition to developing a sensitivity analysis approach that can handle epistemic uncertainty (uncertainty due to ignorance and/or lack of understanding of a system). Moreover, since most parameters can be correlated with other parameters, development of a sensitivity analysis approach that can handle such parameter relationships is also a future issue.

4.5.5 Analysis of the perturbation scenario

4.5.5.1 Natural event impact case

Natural phenomena generic FEPs (earthquake/active faulting, volcanoes/magma activity, uplift/erosion, climate/sea-level change and meteorite impact) are considered here. However, based on FEP screening, only uplift/erosion and climate/sea-level change are chosen as important phenomena in the safety assessment for the geological disposal of TRU waste (cf. Section 4.3.3). If a suitable site is selected, the probability of occurrence and the impact on safety of the geological disposal system is considered to be negligible, hence, others phenomena (earthquake/active faulting, volcanoes/magma activity and meteorite impact) are excluded from the safety assessment.

(1) Uplift and erosion

a. Assumptions

If the disposal site shows evidence of long-term uplift and the rate of uplift/erosion is assumed to be the same, the disposal depth could become shallow. If the disposal site reaches the weathered zone (up to 100 m below the surface), many changes to the hydrogeology and chemical environment of the host rock may occur. The assumed geological environment of the disposal facility during uplift/erosion is shown in Figure 4.5.5-1.

If uplift and erosion continue over the long-term, the disposal facility will be exposed at the surface and together.

4. By adopting a comprehensive sensitivity analysis approach, it is possible to perform a comprehensive evaluation of the effects of uncertainty on system safety. It is considered that the method is able to present the characteristics of system performance in a way that is easy to understand by using key parameters and successful conditions.
radioactive material could be directly released into the biosphere without transport via groundwater. The influence of such a condition on the safety assessment is described in the isolation failure scenario below.

Figure 4.5.5-1 Geological environment in the uplift/erosion scenario

b. Conceptual model
The evaluation of the influence of each environmental THMCR condition is shown in Table 4.5.5-1. Transport pathway and dose assessment in the radionuclide transport analysis in the biosphere is shown in Table 4.5.5-2.

Table 4.5.5-1 Assumptions made in conceptual model of uplift/erosion

<table>
<thead>
<tr>
<th>Environmental condition</th>
<th>Assumptions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal</td>
<td>Ground temperature decreases due to decrease in depth.</td>
</tr>
<tr>
<td>Hydrology</td>
<td>Increase in transmissivity and porosity might be caused by decreasing earth covering. Range of hydraulic gradient increases due to influence of topography.</td>
</tr>
<tr>
<td>Mechanical</td>
<td>Rock stress decreases due to decrease in earth covering</td>
</tr>
<tr>
<td>Chemical</td>
<td>Mineral composition and rock porosity may change due to weathering. Pore water chemistry may change from reducing (deep groundwater condition) to oxidizing due to infiltrating meteoric water.</td>
</tr>
<tr>
<td>Radiation field</td>
<td>No significant change</td>
</tr>
</tbody>
</table>
Table 4.5.5-2 Transport pathway and specification of the biosphere in the uplift/erosion scenario

<table>
<thead>
<tr>
<th>Transport pathway/biosphere</th>
<th>Specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engineered barriers</td>
<td>If the TRU repository reaches the weathered zone, the corrosion rate of activated metal, solubility, sorption distribution coefficients and effective diffusion coefficients are set for oxidizing groundwater conditions.</td>
</tr>
<tr>
<td>EDZ</td>
<td>Same as for Reference Case.</td>
</tr>
<tr>
<td>Host rock</td>
<td>For the weathered zone, it is assumed that groundwater flow velocity is 10 times higher due to increasing of permeability, porosity and the influence of surface topography. The sorption distribution coefficient dataset is for oxidizing groundwater conditions.</td>
</tr>
<tr>
<td>Cataclastic zone</td>
<td>Not considered as a transport medium.</td>
</tr>
<tr>
<td>Biosphere</td>
<td>Same as for Reference Case (river water/plain model (agricultural group)).</td>
</tr>
</tbody>
</table>

c. Evaluation of uplift/erosion

In the open solicitation documents for selection of Preliminary Investigation Areas (PIAs) for the final disposal of HLW, it is stated that “areas where there is clear evidence of uplift amounting to more than 300 m during the last 100,000 years will be excluded from PIAs” (NUMO, 2002). The same site selection requirements for HLW are envisaged for the geological disposal of TRU waste i.e., uplift rate is less than 3 mm/y.

The result of the evaluation of uplift/erosion is shown in Figure 4.5.5-2 for constant uplift/erosion rates of 1 mm/y and 0.1 mm/y over 100,000 years. When the disposal facility reaches the weathered zone (after 900,000 years and 9,000,000 years respectively), the dose increases abruptly. However by this time the key radionuclides have already reached the biosphere. Maximum dose which is obtained 10,000 years after disposal is the same in as the Reference Case.
and the disposal facility. In the case of the inland zone, if permafrost formation over a wide area is assumed, depending on the relationship between the locations of talik (localized unfrozen ground), outflow zones and the groundwater flow conditions around the disposal facility will vary sporadically.

Case. Where talik appears, groundwater flow velocity is assumed to be 10 times that of the value in the Reference Case. In the case if permafrost forms over a wide region as a result of climate change, groundwater flow is generally inhibited and the groundwater flow conditions around the disposal facility will vary sporadically depending on the relationship between the locations of talik (localized unfrozen ground), outflow zones and the disposal facility. In the case of the inland zone, if permafrost formation over a wide area is assumed, groundwater flow is set to 1/10 of the groundwater flow velocity in the Reference Case. In the case where talik appears, groundwater flow velocity is assumed to be 10 times that of the value in the Reference Case.

Figure 4.5.5-2 Evaluation of the uplift/erosion scenario

(2) Climate/sea-level change

a. Assumptions
The periodical change in global climate and sea-level is considered to be one of the phenomena with high probability of occurrence. Based on historic records, the present time is considered to be just over halfway through an interglacial period. It is also assumed that the next ice age will occur after several 10,000 years.

b. Conceptual model
The assumed influence of climate/sea-level change on THMCR environmental conditions is shown in Table 4.5.5-3. The geological environment during climate/sea-level change is evaluated separately for inland and coastal zones, since the conditions are assumed to be quite different in each case (Fig.4.5.5-3). The transport pathway concept for the radionuclide transport analysis in the inland and coastal zones is shown in Table 4.5.5-4 and 5.

If permafrost forms over a wide region as a result of climate change, groundwater flow is generally inhibited and the groundwater flow conditions around the disposal facility will vary sporadically depending on the relationship between the locations of talik (localized unfrozen ground), outflow zones and the disposal facility. In the case of the inland zone, if permafrost formation over a wide area is assumed, groundwater flow is set to 1/10 of the groundwater flow velocity in the Reference Case. In the case where talik appears, groundwater flow velocity is assumed to be 10 times that of the value in the Reference Case.
For the coastal zone case, if the surrounding groundwater environment of the disposal facility changes to salt water as a result of marine transgression, static groundwater flow is assumed. On the other hand, if it is assumed that the salt/freshwater boundary exists near the disposal facility due to marine regression, the groundwater flow condition changes depending on the relationship between topographic gradient, location of outflow regions and the disposal facility (Hasegawa et al., 2001; Imamura et al., 2001). During marine transgression, if the disposal facility is located in a salt water zone, 1/10 of the groundwater flow velocity in the Reference Case is assumed. If the disposal facility is assumed to be near the salt/freshwater boundary, 5 times the groundwater flow velocity of the Reference Case is assumed.

The conceptual model for the biosphere in the Reference Case is based on the present-day mild climate. This is modified to model a cool-temperate climate or tundra climate and applied to the inland and coastal zones. The assumptions made to construct the conceptual model for the inland zone are a radionuclide release area in a river plain, a cool-temperate climate or tundra climate and a farming exposure group. If the disposal facility is located in the salt water region or near the salt/freshwater boundary, in the case of a coastal zone the assumptions made to construct the conceptual model are radionuclide release in a sedimentary layer, a cool-temperate climate or tundra climate and a marine fishing exposure group. If the disposal facility exists in a freshwater region due to marine regression, the assumptions made to construct the conceptual model are radionuclide release in a river water plain, a cool-temperate climate or tundra climate and a farming exposure group. The dose conversion factors used in the biosphere models are shown in Table 4.5.5-6.

It should be noted that rather short climate/sea-level change periodicity values are reported elsewhere (Dansgaard-Oeschger cycle, Dansgaard et al., 1993). Therefore, periodicity is not modeled continuously in this assessment, but rather as multiple snapshots of representative conditions of climate/sea-level change.
<table>
<thead>
<tr>
<th>Environment condition</th>
<th>Assumptions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal</td>
<td>Surface temperature changes</td>
</tr>
<tr>
<td>Hydraulic</td>
<td>A decrease in rainwater recharge and water table is assumed in the case of permafrost formation. Moreover, if permafrost forms over a wide area, groundwater flow is generally limited and periodically changes depending on the locations of talik, outflow regions and the disposal facility. If the salt/freshwater boundary migrates close to the disposal facility in the coastal zone, groundwater flow with a large variation is assumed. Also if the topographic gradient changes due to marine erosion, a variation in hydraulic gradient is assumed.</td>
</tr>
<tr>
<td>Mechanical</td>
<td>If permafrost forms on the surface, the stress condition around disposal facility may change.</td>
</tr>
<tr>
<td>Chemical</td>
<td>If the salt/freshwater boundary migrates close to the disposal facility in the coastal zone, the pore water periodically varies between salt and freshwater.</td>
</tr>
<tr>
<td>Radiation field</td>
<td>No significant variation.</td>
</tr>
</tbody>
</table>
Figure 4.5.5-3 Schematic diagrams of geological environments in the climate/sea-level scenario
Table 4.5.5-4 Transport pathway and biosphere specifications in the climate/sea-level change scenario
(inland zone)

<table>
<thead>
<tr>
<th>Transport pathway/biosphere</th>
<th>Specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engineered barriers</td>
<td>Same as in the Reference Case</td>
</tr>
<tr>
<td>EDZ</td>
<td>Depending on the hydraulic conditions of the host rock, 1/10 or 10 times the Reference Case value</td>
</tr>
<tr>
<td>Host rock</td>
<td>Consideration of reduced hydraulic conditions (1/10 of groundwater flow velocity) in the case where permafrost forms over wide areas and the effects of talik formation and changes in transport pathway and hydraulic conditions (10 times of groundwater flow velocity)</td>
</tr>
<tr>
<td>Cataclastic zone</td>
<td>Not considered as a transport medium</td>
</tr>
<tr>
<td>Biosphere</td>
<td>River water/plain model (farming exposure group; cool-temperate climate or tundra climate)</td>
</tr>
<tr>
<td>Pathway specification/biosphere</td>
<td>Specifications</td>
</tr>
<tr>
<td>--------------------------------</td>
<td>----------------</td>
</tr>
<tr>
<td>Engineered barriers</td>
<td>In the case where the disposal facility is located in a salt water region, the corrosion rate of activated metal, solubility, sorption distribution coefficient, effective diffusion coefficient and transmissivity of the buffer material are set for SRHP-type groundwater conditions.</td>
</tr>
<tr>
<td>EDZ</td>
<td>Depending on the hydraulic condition of host rock, 1/10, 5 and 10 times the value in the Reference Case</td>
</tr>
<tr>
<td>Host rock</td>
<td>If the disposal facility is in a freshwater region, groundwater flow velocity is 5 times the Reference Case value due to increase in topographic gradient through marine erosion. If the disposal facility is close to the salt/freshwater boundary, the groundwater flow velocity is increased by a factor of 10. If the disposal facility is located in a salt water region, groundwater flow velocity is 1/10 or less compared to the Reference Case value or static. If the disposal facility is located in a salt water region, sorption distribution coefficients are used and SRHP-type groundwater data are assumed.</td>
</tr>
<tr>
<td>Cataclastic zone</td>
<td>Not considered as a transport medium</td>
</tr>
<tr>
<td>Biosphere</td>
<td>In the case where the disposal facility is in a salt water region near the salt/freshwater boundary, a coastal zone sedimentary layer/plain model (marine fishing group) is assumed. In the case of a freshwater region, river water/plain model (farming group) is assumed. Cool-temperate and tundra climates are considered in each case.</td>
</tr>
</tbody>
</table>
Table 4.5.5-6 Dose conversion factors used in climate/sea-level change scenario

<table>
<thead>
<tr>
<th>Nuclide release</th>
<th>River water</th>
<th>Coastal zone sedimentary layer</th>
<th>Unit ([(Sv)/(y)/(Bq)/(y)])</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Warm climate</td>
<td>Cool-temperate climate</td>
<td>Tundra climate</td>
</tr>
<tr>
<td><strong>Application</strong></td>
<td><strong>Reference Case</strong></td>
<td><strong>Climate/sea-level change</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>Coastal location</strong></td>
<td><strong>Coastal location</strong></td>
</tr>
<tr>
<td></td>
<td></td>
<td>((at marine transgression))</td>
<td>((at marine transgression))</td>
</tr>
<tr>
<td>C-14</td>
<td>6.4E-17</td>
<td>1.3E-17</td>
<td>1.8E-16</td>
</tr>
<tr>
<td>Cl-36</td>
<td>4.5E-17</td>
<td>1.6E-17</td>
<td>1.2E-16</td>
</tr>
<tr>
<td>Co-60</td>
<td>1.3E-16</td>
<td>4.5E-17</td>
<td>6.0E-17</td>
</tr>
<tr>
<td>Ni-59</td>
<td>3.7E-18</td>
<td>1.0E-18</td>
<td>1.8E-18</td>
</tr>
<tr>
<td>Ni-63</td>
<td>5.0E-18</td>
<td>2.0E-18</td>
<td>4.1E-18</td>
</tr>
<tr>
<td>Se-79</td>
<td>3.2E-15</td>
<td>1.7E-16</td>
<td>7.5E-16</td>
</tr>
<tr>
<td>Sr-90</td>
<td>1.1E-15</td>
<td>3.9E-16</td>
<td>3.8E-16</td>
</tr>
<tr>
<td>Zr-93</td>
<td>9.6E-18</td>
<td>3.3E-18</td>
<td>2.3E-18</td>
</tr>
<tr>
<td>Nb-93m</td>
<td>2.3E-18</td>
<td>1.5E-18</td>
<td>9.0E-19</td>
</tr>
<tr>
<td>Nb-94</td>
<td>7.5E-16</td>
<td>2.0E-16</td>
<td>2.2E-17</td>
</tr>
<tr>
<td>Mo-93</td>
<td>5.5E-17</td>
<td>3.2E-17</td>
<td>3.2E-17</td>
</tr>
<tr>
<td>Te-99</td>
<td>2.6E-17</td>
<td>1.3E-17</td>
<td>1.8E-17</td>
</tr>
<tr>
<td>Pd-107</td>
<td>1.4E-18</td>
<td>5.4E-19</td>
<td>2.5E-19</td>
</tr>
<tr>
<td>Sn-126</td>
<td>1.0E-15</td>
<td>2.6E-16</td>
<td>5.9E-17</td>
</tr>
<tr>
<td>I-129</td>
<td>3.2E-15</td>
<td>2.0E-15</td>
<td>2.7E-15</td>
</tr>
<tr>
<td>Cs-135</td>
<td>1.2E-16</td>
<td>4.9E-17</td>
<td>6.2E-17</td>
</tr>
<tr>
<td>Cs-137</td>
<td>5.4E-16</td>
<td>2.2E-16</td>
<td>3.8E-16</td>
</tr>
<tr>
<td>Cm-244</td>
<td>2.4E-15</td>
<td>1.4E-15</td>
<td>8.2E-16</td>
</tr>
<tr>
<td>Pu-240</td>
<td>3.8E-15</td>
<td>2.1E-15</td>
<td>1.6E-15</td>
</tr>
<tr>
<td>U-236</td>
<td>8.8E-16</td>
<td>5.5E-16</td>
<td>3.5E-16</td>
</tr>
<tr>
<td>Th-232</td>
<td>1.5E-13</td>
<td>1.3E-14</td>
<td>2.2E-15</td>
</tr>
<tr>
<td>Ra-228</td>
<td>1.3E-14</td>
<td>7.2E-15</td>
<td>7.5E-15</td>
</tr>
<tr>
<td>Th-228</td>
<td>2.6E-15</td>
<td>1.5E-15</td>
<td>1.2E-15</td>
</tr>
<tr>
<td>Cm-245</td>
<td>1.1E-14</td>
<td>2.7E-15</td>
<td>1.4E-15</td>
</tr>
<tr>
<td>Pu-244</td>
<td>8.6E-17</td>
<td>3.9E-17</td>
<td>3.0E-17</td>
</tr>
<tr>
<td>Am-241</td>
<td>3.3E-15</td>
<td>1.7E-15</td>
<td>1.3E-15</td>
</tr>
<tr>
<td>Np-237</td>
<td>1.3E-15</td>
<td>9.5E-16</td>
<td>7.1E-16</td>
</tr>
<tr>
<td>Pu-233</td>
<td>1.8E-17</td>
<td>1.1E-17</td>
<td>5.8E-18</td>
</tr>
<tr>
<td>U-233</td>
<td>1.0E-15</td>
<td>6.0E-16</td>
<td>3.8E-16</td>
</tr>
<tr>
<td>Th-229</td>
<td>2.3E-14</td>
<td>6.8E-15</td>
<td>5.1E-15</td>
</tr>
<tr>
<td>Cm-246</td>
<td>7.4E-14</td>
<td>2.6E-15</td>
<td>1.4E-15</td>
</tr>
<tr>
<td>Pu-242</td>
<td>3.7E-15</td>
<td>2.0E-15</td>
<td>1.5E-15</td>
</tr>
<tr>
<td>U-238</td>
<td>9.0E-16</td>
<td>5.6E-16</td>
<td>3.6E-16</td>
</tr>
<tr>
<td>U-234</td>
<td>9.6E-16</td>
<td>5.9E-16</td>
<td>3.8E-16</td>
</tr>
<tr>
<td>Th-230</td>
<td>2.7E-14</td>
<td>4.6E-15</td>
<td>1.9E-15</td>
</tr>
<tr>
<td>Ra-226</td>
<td>3.2E-14</td>
<td>5.1E-15</td>
<td>3.5E-15</td>
</tr>
<tr>
<td>Pb-210</td>
<td>2.4E-14</td>
<td>1.3E-14</td>
<td>2.9E-14</td>
</tr>
<tr>
<td>Po-210</td>
<td>4.8E-15</td>
<td>2.7E-15</td>
<td>6.3E-15</td>
</tr>
<tr>
<td>Am-243</td>
<td>5.5E-15</td>
<td>1.8E-15</td>
<td>1.3E-15</td>
</tr>
<tr>
<td>Pu-239</td>
<td>3.9E-15</td>
<td>2.1E-15</td>
<td>1.6E-15</td>
</tr>
<tr>
<td>U-235</td>
<td>9.3E-16</td>
<td>5.6E-16</td>
<td>3.5E-16</td>
</tr>
<tr>
<td>Pa-231</td>
<td>6.5E-14</td>
<td>1.3E-14</td>
<td>4.8E-15</td>
</tr>
<tr>
<td>Ac-227</td>
<td>2.6E-14</td>
<td>1.6E-14</td>
<td>8.1E-15</td>
</tr>
</tbody>
</table>
c. Results

The evaluation in the case where the disposal facility is sited inland is shown in Figure 4.5.5-4. In a cool-temperate climate or tundra climate, dose is insignificant since the hydraulic features have a tendency to decrease dose. In this evaluation, even if dose does increase, the maximum value becomes approximately 10 µSv/y.

The case of a coastal region is shown in Figure 4.5.5-5. In the case where the surrounding environment of the disposal facility changes to a salt water region, radionuclide release into the biosphere is delayed by the low permeable environment and the conversion factor for I-129 becomes 2 orders of magnitude lower than that for the Reference Case in the coastal sedimentary layer/plain model (marine fishing group), as shown in Table 4.5.5-6. Hence, the maximum dose becomes significantly smaller than that of the Reference Case. In the case where the surrounding environment of the disposal facility changes to freshwater, the conversion factor for dose is the same as for the Reference Case in the cool-temperate climate or tundra climate (cf. 4.5.5-6), and the dose becomes larger than the Reference Case value because an increase in groundwater flow velocity is caused by marine erosion. The maximum value is about 10 µSv/y. In the case of the the salt/freshwater boundary located near the disposal facility, Cs-137 peaks tens of years after disposal and Nb-94 peaks 10,000s of years after disposal. This is due to the high groundwater flow velocity and also the dose conversion factor being set 1 to several orders larger than that of Reference Case (ref. Table 4.5.5-6). Both these peaks are about 100 µSv/y.

![Figure 4.5.5-4 Evaluation of the climate/sea-level scenario (inland location)](image-url)
4.5.5.2 Sealing defects in the engineered barrier system

(1) Sealing defects

a. Assumptions

It is intended that the access tunnel will be backfilled in order to create a similar barrier function to that of the surrounding host rock. Here, a hypothetical case is assumed where backfilling is not properly sealed, resulting in a radionuclide transport pathway through the access tunnel (Figure 4.5.5-6).
b. Conceptual model

The model concept is summarised in Table 4.5-7.

Table 4.5-7 Transport pathway and biosphere conceptualization in the sealing defect scenario

<table>
<thead>
<tr>
<th>Transport pathway/biosphere</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engineered barriers</td>
<td>Same as in Reference Case</td>
</tr>
<tr>
<td>EDZ</td>
<td>Increase in EDZ flow due to incomplete sealing (10 times)</td>
</tr>
<tr>
<td>Host rock</td>
<td>Access tunnel is a transport pathway; assumed that groundwater flow velocity is 10 times higher than that of the host rock.</td>
</tr>
<tr>
<td>Cataclastic zone</td>
<td>Not considered as a transport medium.</td>
</tr>
<tr>
<td>Biosphere</td>
<td>Same as in Reference Case. (river water/plain model (farming group))</td>
</tr>
</tbody>
</table>

c. Results

The dose calculations are shown in Figure 4.5-7. There are several types of disposal tunnel in a TRU waste repository, depending on the type of waste and shape of package. It is difficult to envisage that a sealing defect will occur in all disposal tunnels at the same time, hence one tunnel is considered here. The effect on increasing dose depends on which tunnel has the sealing fault. The influence of a sealing fault in a disposal tunnel for Group 1 is most significant to exceed 10µSv/y. On the other hand, a fault in a disposal tunnel for Group 4 waste would have higher dose compared to the Reference Case, but it does not exceed 1µSv/y.
4.5.5.3 Future human intrusion case

(1) Well drilling and water sampling scenario

a. Assumptions

Here, radionuclides released from the disposal facility contaminate deep well water and eventually enter water for human use (Figure 4.5.5-8).
**b. Conceptual model**

Radionuclide transport in the host rock is the same as in the base scenario. It is considered that the radionuclides contaminate the aquifer (deep well water). The model conceptualizations are shown in Table 4.5.5-8. The river water/plain model (farming group) used for the base scenario and the dose conversion factors for the deep well/plain model (farming group) used for the well drilling scenario are shown in Table 4.5.5-9.

<table>
<thead>
<tr>
<th>Transport pathway/biosphere</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engineered barriers</td>
<td>Same as in Reference Case.</td>
</tr>
<tr>
<td>EDZ</td>
<td>Same as in Reference Case.</td>
</tr>
<tr>
<td>Host rock</td>
<td>Same as in Reference Case.</td>
</tr>
<tr>
<td>Cataclastic zone</td>
<td>Same as in Reference Case.</td>
</tr>
<tr>
<td>Biosphere</td>
<td>Deep well/plain model (farming group)</td>
</tr>
</tbody>
</table>
Table 4.5.5-9 Dose conversion factors for river water/plain model and deep well/plain model

<table>
<thead>
<tr>
<th>Nuclide releases region</th>
<th>River water</th>
<th>Aquifer (deep well)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mild climate</td>
<td>Mild climate</td>
</tr>
<tr>
<td></td>
<td>Farming group</td>
<td>Fresh water fishing group</td>
</tr>
<tr>
<td></td>
<td>Reference Case</td>
<td>--</td>
</tr>
<tr>
<td></td>
<td>Well drilling/ water sampling case</td>
<td>--</td>
</tr>
</tbody>
</table>

| Application | C-14 | C-15 | Co-60 | Ni-59 | Ni-63 | Se-79 | Sr-90 | Zr-93 | Nb-93m | Nb-94 | Mo-93 | Te-99 | Pd-107 | Sn-126 | I-129 | Cs-135 | Cs-137 | Pu-240 | U-236 | Th-232 | Ra-228 | Th-236 | Cs-236 | Cs-238 | Ra-227 | Gd-157 | Ac-227 |
|-------------|------|------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|--------|-------|-------|--------|--------|-------|-------|-------|-------|-------|--------|-------|-------|
| Reference Case | 6.4E-17 | 4.5E-17 | 1.3E-16 | 3.7E-18 | 5.0E-18 | 3.2E-15 | 1.1E-15 | 9.6E-18 | 2.3E-18 | 7.6E-16 | 5.6E-16 | 2.6E-17 | 1.4E-18 | 1.0E-15 | 3.2E-15 | 1.2E-16 | 7.7E-16 | 3.2E-15 | 5.5E-16 | 3.1E-15 | 1.3E-15 | 1.1E-15 | 6.3E-17 | 2.6E-17 | 1.8E-17 | 2.4E-17 |
| Farming group | 3.5E-17 | 6.0E-18 | 2.1E-17 | 4.1E-19 | 9.8E-19 | 3.2E-17 | 2.0E-16 | 2.0E-18 | 8.8E-18 | 5.8E-15 | 1.1E-19 | 2.6E-16 | 4.5E-19 | 1.5E-15 | 7.7E-16 | 3.0E-17 | 2.8E-16 | 5.4E-16 | 2.9E-16 | 9.9E-16 | 1.1E-16 | 4.3E-16 | 6.3E-19 | 2.6E-19 | 4.5E-19 | 9.2E-20 |
| Fresh water fishing group | 2.4E-17 | 8.6E-21 | 2.3E-15 | 1.1E-19 | 2.6E-16 | 3.4E-17 | 2.7E-19 | 4.5E-19 | 8.9E-17 | 8.9E-17 | 2.7E-15 | 5.9E-20 | 3.1E-20 | 4.8E-16 | 1.4E-17 | 1.1E-16 | 6.1E-17 | 6.2E-19 | 4.2E-16 | 9.2E-17 | 1.1E-17 | 2.7E-18 | 5.4E-19 | 3.7E-19 | 9.2E-20 | 3.1E-20 |
| Marine fishing group | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
c. Results
The dose calculations are shown in Figure 4.5.5-9. Excluding dose calculation at the biosphere, the calculated release rate of radionuclides from natural barriers into biosphere is the same as for the Reference Case.

(2) Formation of new transport pathways by drilling
a. Assumed conditions
Here, it is assumed that the region near the disposal facility is accidentally penetrated by future deep drilling (geological survey or hot spring investigation), forming a new radionuclide migration pathway to the biosphere (Figure 4.5.5-10).

One legal requirement for final disposal of HLW in Japan is that no site will be considered where there is any record of mineral resources. Moreover, in the open solicitation documentation for Preliminary Investigation Areas (PIAs), it is stated that “areas expected to have significant thermal effects, highly acidic thermal waters or significant hydrothermal convection will also be excluded from PIAs” (NUMO, 2002). It is envisaged that the same site selection factors will be applied to the site selection for the TRU waste repository. Here, the very small possibility of well drilling for geological surveys or hot spring investigations are considered.
A similar and more severe condition where a borehole would directly penetrate the repository is evaluated in the isolation failure scenario, later.

![Diagram of borehole, oxidizing groundwater, and TRU waste disposal facility + EDZ]

Figure 4.5.5-10 Scenario for the creation of transport pathway by drilling

**b. Conceptualization**

Model conceptualizations for radionuclide transport analysis and dose conversion factors in the biosphere are shown in Table 4.5.5-10. It is assumed that oxidizing groundwater in atmospheric equilibrium will enter the disposal facility via the borehole. The groundwater flow rate in the EDZ increases by a factor of 10 due to drilling perturbation and that radionuclides that entered the EDZ from the EBS can reach the biosphere directly.

It is also assumed that drilling at the disposal site occurs after loss of information of the existence of the disposal facility. Since this will take some time to occur, 300 years and 1,000 years after closure of the facility are considered here.

**Table 4.5.5-10 Transport pathway and biosphere specifications for drilling near the disposal facility**

<table>
<thead>
<tr>
<th>Transport pathway/biosphere</th>
<th>Specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engineered barriers</td>
<td>Corrosion rate of activated metal, solubility, sorption distribution coefficient and effective diffusion coefficient for oxidizing groundwater conditions.</td>
</tr>
<tr>
<td>EDZ</td>
<td>EDZ flow increases by a factor of 10 due to drilling.</td>
</tr>
<tr>
<td>Host rock</td>
<td>Not considered as a transport medium.</td>
</tr>
<tr>
<td>Cataclastic zone</td>
<td>Not considered as a transport medium.</td>
</tr>
<tr>
<td>Biosphere</td>
<td>Same as for Reference Case (river water/plain model (farming group)).</td>
</tr>
</tbody>
</table>
c. Results

The dose calculations are shown in Figure 4.5.5-11.

As in the sealing defect scenario, the dose depends on the type of disposal tunnel affected by drilling. However, the effect on dose is much higher than for the sealing defect scenario.

In this drilling scenario, since the performance of the natural barrier which contributes to retarding I-129 is not considered, the dose from Group 1 is increased to about 100 µSv/y. Moreover, actinides which are insignificant in the base scenario contribute significantly to dose in Group 4 since there is no buffer material.
4.5.5.4 Summary of perturbation scenarios

Figure 4.5.5-12 shows the maximum doses for the perturbation scenarios, together with the doses calculated for the Reference Case (maximum 2 µSv/y). In many cases, the maximum dose is below 10 µSv/y. In the biosphere model for a cool climate, the dose conversion factors for several radionuclides are specified to be large. However, the evaluations gave an exposure of around 100 µSv/y for: the climate and sea-level change (coastal location, salt/freshwater boundary) scenario, which assumes relatively rapid groundwater flow rates; the well drilling and water sampling scenario, in which dilution effects in the biosphere are relatively small and the scenario in which radionuclides from Groups 1 and 4 reach the biosphere at an early stage via boreholes close to the waste tunnels. In any case, the calculated exposure is similar to, or lower than, the safety level specified in foreign countries (100–300 µSv/y) and is below the natural radiation level (900–1200 µSv/y) in Japan.

In this evaluation, the climate/sea-level change (coastal location, salt/freshwater boundary) scenario gave a relatively high dose. This was caused by an increase in the dose conversion factor for important
radionuclides, obtained from modeling radionuclide release into a coastal zone sedimentary layer under cool climatic conditions. However, many uncertainties still exist in the biosphere model that assumes a cool climate and it is important to exercise care when using the conversion factors. Moreover, in the same scenario it is conservatively assumed that, when the salt/freshwater boundary is near the disposal facility, there is an increase in the groundwater flow rate in the host rock, resulting in a relatively high dose. It is suggested that the groundwater flow conditions near the salt/freshwater boundary vary in a complex way, owing to changes in the topographic gradient, stratigraphy, location of the outflow and the behavior of marine regression and transgression (Imamura et al., 2001). Therefore, it is inevitable that there are still many uncertainties concerning changes in the groundwater flow velocity near the fresh/saline water interface.

In the well drilling/water sampling scenario and the scenario in which new transport pathways are formed by well drilling, doses are found to be relatively high. However, as in the accidental intrusion scenario described later, the initiating phenomena in these scenarios are considered to be unlikely. However, it is important that the probability of occurrence should be appropriately evaluated for each relevant scenario, using the risk theory. It is particularly important that, in the scenario where new transport pathways are formed by drilling, the effect can be reduced by engineering measures such as limiting the number of waste packages and dividing the repository tunnels into segments.
4.5.6 Analysis of isolation failure scenarios
4.5.6.1 Surface exposure of the disposal facility by uplift and erosion

(1) Assumptions
If uplift and erosion at the disposal site continue over a long period, the disposal facility could eventually be exposed at the surface. This scenario is considered here with human consumption not through groundwater transport to the surface but rather from soil contamination as result of direct exposure at the surface.

As described in Section 4.5.5, Japanese legislation states that the depth of a HLW repository must be more than 300 m below the surface and the disposal facility is not expected to be exposed at the surface for at least 100,000 years after final disposal. In this report, as the construction of the TRU repository is envisaged at 500 m (sedimentary rock) and 1000 m (crystalline rock), if the same site selection factors as for HLW final disposal are used the surface exposure of the TRU repository is also estimated to be at least 100,000 years after final disposal.

(2) Model conceptualization
The conceptual model is shown in Figure 4.5.6-1.
Here, it is assumed that surface exposure of the disposal facility occurs after 100,000 years and that a radionuclide plume around the disposal facility forms by radionuclide leaching from the facility.
In the surface exposure scenario of the disposal facility, it is difficult to construct the biosphere model in order to evaluate exposure to the public from contaminated soil. A methodology will be developed in future. By referring to the evaluation in the H12 report (JNC, 2000), the effect of radiolysis is discussed by comparing radionuclide flux as follows.

- Radionuclide flux from the repository:
  Caused by erosion of contaminated host rock in the disposal facility.
  Calculated from the radionuclide concentration in exposed contaminated host rock in the disposal facility (assumed to be concentration in disposal facility × homogeneous distribution at 20 m depth) and annual erosion rate.

- Natural radionuclide flux:
  The radionuclide flux generated by the erosion of a host rock such as granite or a uranium ore deposit which includes natural radionuclides.
  Calculated from the natural radionuclide concentration in the host rock and the annual erosion rate in the disposal area.

Uplift and erosion rates of 0.1 mm/y and 1 mm/y are assumed, which satisfies the site selection factors above.
(3) Results

The case of crystalline rock and an uplift/erosion rate of 1 mm/y is shown in Figure 4.5.6-2. The flux of U-238 which is generated by erosion of the exposed disposal facility is smaller than that from a naturally occurring uranium ore deposit.

1 Compared with the natural radiation flux in Appendix B-2, volume 3 of H12 report, the natural flux in Figure 4.5.6-2 shows a lower value. This is because the area of the TRU/disposal facility is smaller than that for HLW.
TRU waste disposal facility

Assuming leached nuclide forms uniform plume around disposal facility

\[300 \text{m} \times 300 \text{m} \times 300 \text{m}\]

Figure 4.5.6-1 Conceptual model of surface exposure due to uplift and erosion

**Figure 4.5.6-2** Surface exposure of the disposal facility

(crystalline rock with an uplift/erosion rate of 1 mm/y)
4.5.6.2 Accidental penetration of the repository by drilling

(1) Assumed dose pathway

If drilling occurs near the disposal facility, several radionuclide pathways to the human environment may be created. Although many pathways should be considered for a comprehensive evaluation, here a few plausible scenarios are modeled and uncertainties assessed. For the evaluation of human intrusion, it is recommended that “the consequences of one or more typical plausible stylised intrusion scenarios should be considered by the decision-maker to evaluate the resilience of the repository to potential intrusion.” (ICRP 1998).

Although an accidental penetration of repository scenario is not necessarily well stylized yet, here the following is based on other assessment reports on the intrusion scenario (JNC, 2000; JAERI, 2004).

Here, the following are evaluated (Table 4.5.6-1)
① Internal/external radiation exposure of drill core observer;
② Internal/external radiation exposure of drilling operator;
③ Internal/external radiation exposure of inhabitants.

<table>
<thead>
<tr>
<th>Radiation source</th>
<th>Target person in dose assessment</th>
<th>Dose pathway</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drill core</td>
<td>drill core observer</td>
<td>External dose</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Internal dose by dust inhalation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Internal dose by oral ingestion</td>
</tr>
<tr>
<td>Mixture of drilling mud and waste</td>
<td>drilling worker</td>
<td>External dose</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Internal dose by dust inhalation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Internal dose by oral ingestion</td>
</tr>
<tr>
<td>Mixture of contaminated drilling material</td>
<td>inhabitant</td>
<td>External dose</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Internal dose by dust inhalation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Internal dose by oral ingestion</td>
</tr>
</tbody>
</table>

(2) Calculation of radiation dose

External and internal exposure through inhalation and ingestion by a drill core observer, drilling worker and the general public are calculated using the following formula.
\[ D(t) = H_{\text{ext}}(t) + H_{\text{inh}}(t) + H_{\text{ing}}(t) \]

\[ H_{\text{ext}}(t) = \sum_{i} \eta_{i}^{\text{ext}} \cdot C_{i}(t) \cdot T_{\text{ext}} \]

\[ H_{\text{inh}}(t) = \sum_{i} \eta_{i}^{\text{inh}} \cdot C_{i}(t) \cdot f_{\text{dil}} \cdot \varepsilon \cdot B \cdot T_{\text{inh}} \]

\[ H_{\text{ing}}(t) = \sum_{i} \eta_{i}^{\text{ing}} \cdot C_{i}(t) \cdot f_{\text{dil}} \cdot M \cdot T_{\text{ing}} \]

\[ (4.5.6-1) \]

**D(t)** : radiation dose [Sv]

**\( H_{\text{ext}}(t) \)** : external dose [Sv]

**\( H_{\text{inh}}(t) \)** : internal dose by inhalation [Sv]

**\( H_{\text{ing}}(t) \)** : internal dose by oral ingestion [Sv]

**\( C_{i}(t) \)** : concentration of radionuclide i in waste at time t [Bq/g]

**\( \eta_{i}^{\text{ext}} \)** : conversion factor for dose for external dose of radionuclide i \([\text{Sv/h}/(\text{Bq/g})]^{2}\)

**\( \eta_{i}^{\text{inh}} \)** : conversion factor for dose for intake by inhalation of radionuclide i [Sv/Bq]

**\( \eta_{i}^{\text{ing}} \)** : conversion factor for dose for oral ingestion of radionuclide i [Sv/Bq]

**\( T_{\text{ext}} \)** : radiation exposure duration in the evaluation of external dose [h]

**\( T_{\text{inh}} \)** : radiation exposure duration in the evaluation by intake by inhalation [h]

**\( T_{\text{ing}} \)** : radiation exposure duration in the evaluation of oral ingestion [h]

**\( f_{\text{dil}} \)** : Dilution rate by mixing of drilled accumulated debris in the disposal facility [-]

**\( \varepsilon \)** : Dust concentration in air [g/m³]

**\( B \)** : Rate of respiration [m³/h]

**\( M \)** : Ingestion rate [g/h]

---

**3) Parameter specification for calculation of radiation doses**

The parameters used for calculating radiation dose are shown in Tables 4.5.6-2 to 4.5.6-4.

---

2 The external dose and radiation strength are calculated by linear radionuclide transport code ANISN for each radionuclide.
Table 4.5.6-2 Parameter settings for calculating external dose to drill core observers and drilling operators

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Name</th>
<th>Value</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of core</td>
<td>D</td>
<td>Core diameters (BQ:36 mm, NQ:48 mm, HQ: 64 mm) used for wireline method (Japan Geotechnical Consultant Association, 2004)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Length of core</td>
<td>L</td>
<td>Simulated setting from H12 report (infinite cylinder)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density of core</td>
<td>(\rho)</td>
<td>Waste density</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Distance from core surface</td>
<td>(r)</td>
<td>From H12 report</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 4.5.6-3 Parameter settings for calculating radiation doses to drill core observers

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Name</th>
<th>Value</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilution rate</td>
<td>(f_{dil})</td>
<td>0.01 (crystalline rock) 0.05 (sedimentary rock)</td>
<td></td>
<td></td>
<td>Thickness of waste layer is assumed to be 10 m. Core length is 1,000 m in crystalline rock, 500 m in sedimentary rock</td>
</tr>
<tr>
<td>Observation duration (external)</td>
<td>(T_{ext})</td>
<td>1</td>
<td>h</td>
<td>0.91 ((0.013 \text{ day for 1 m of core observation (Japan Geotechnical Consultant Association, 2004)} \times 7 \text{ h/day and 10 m of core length}))</td>
<td></td>
</tr>
<tr>
<td>Observation duration (inhalation/oral)</td>
<td>(T_{inh}, T_{ing})</td>
<td>100 (crystalline rock) 50 (sedimentary rock)</td>
<td>h</td>
<td>91 h ((45.5 \text{ h for 0.013 day per 1 m of core observation (Japan Geotechnical Consultant Association, 2004)} \times 7 \text{ h/day and 1000 m (crystalline rock) and 500 m (sedimentary rock) of core length}))</td>
<td></td>
</tr>
<tr>
<td>Dust concentration in air</td>
<td>(\varepsilon)</td>
<td>5.0(\times)10(^{-4})</td>
<td>g/m(^3)</td>
<td>Anticipated area ((1.0\times10^{-3} \sim 1.0\times10^{-4} \text{ g/m}^3)) in construction scenario of IAEA (1987)</td>
<td></td>
</tr>
<tr>
<td>Rate of respiration</td>
<td>(B)</td>
<td>1.2</td>
<td>m(^3)/h</td>
<td>IAEA (1987)</td>
<td></td>
</tr>
<tr>
<td>Ingestion rate</td>
<td>(M)</td>
<td>0.01</td>
<td>g/h</td>
<td>Assumptions: density of dust on finger, 0.5 g/cm(^3); thickness of dust 0.1 mm; surface area of finger 2 cm(^2); finger inserted in mouth once an hour (ISPN, 1992).</td>
<td></td>
</tr>
</tbody>
</table>
### Table 4.5.6-4 Parameter settings for calculating external dose to drilling operators

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Name</th>
<th>Value</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilution rate</td>
<td>$f_{dil}$</td>
<td>0.01 (crystalline rock) 0.05 (sedimentary rock)</td>
<td>0.01</td>
<td>--</td>
<td>Thickness of waste assumed to be 10 m. Total length of core 1,000 m in crystalline rock and 500 m in sedimentary rock.</td>
</tr>
<tr>
<td>Operation duration (external)</td>
<td>$T_{\text{ext}}$</td>
<td>20</td>
<td>h</td>
<td></td>
<td>15.6 h (drilling rate, 4.5 m/d (Japan Geotechnical Consultant Association, 2004); thickness of waste layer 10 m; operation duration, 7 h/day).</td>
</tr>
<tr>
<td>Operation duration (inhalation/oral)</td>
<td>$T_{\text{inh}}$, $T_{\text{ing}}$</td>
<td>800 (crystalline rock) 400 (sedimentary rock)</td>
<td>h</td>
<td></td>
<td>7 h/day (drilling rate, 4.5 m/d (Japan Geotechnical Consultant Association, 2004); drilling continues to 1,500 m in crystalline rock and 750 m in sedimentary rock.)</td>
</tr>
<tr>
<td>Dust concentration in air</td>
<td>$\varepsilon$</td>
<td>$5.0 \times 10^{-4}$ g/m$^3$</td>
<td></td>
<td></td>
<td>Center of envisaged construction area ($1.0 \times 10^{-3} - 1.0 \times 10^{-4}$ g/m$^3$) IAEA (1987).</td>
</tr>
<tr>
<td>Rate of respiration</td>
<td>$B$</td>
<td>1.2</td>
<td>m$^3$/h</td>
<td></td>
<td>IAEA (1987)</td>
</tr>
<tr>
<td>Ingestion rate</td>
<td>$M$</td>
<td>0.01</td>
<td>g/h</td>
<td></td>
<td>Assumptions: density of dust on finger 0.5 g/cm$^3$; thickness of dust 0.1 mm; surface area of finger 2 cm$^2$; finger inserted in mouth once an hour (ISPN, 1992).</td>
</tr>
</tbody>
</table>

### (4) Calculation of risk

Quantitative assessments of risk should be made for unlikely phenomena such as accidental human intrusion by drilling (e.g. ICRP, 1985). Here, the risk of accidental penetration of the repository by drilling is evaluated using the following formula:

$$ R_j(t) = \gamma \cdot S \cdot P \cdot H_j(t) $$  \hspace{1cm} (4.5.6-2)

- $R_j(t)$: annual risk by dose pathway $j$ in time $t$ [y$^{-1}$]
- $\gamma$: risk coefficient [Sv$^{-1}$]
- $S$: total projected cross-section area from above of regions occupied by waste [m$^2$]
- $P$: drilling frequency to depth of disposal facility [m$^2$y$^{-1}$]
- $H_j(t)$: radiation dose via dose pathway $j$ [Sv]

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For a drill core observer and drilling worker in crystalline rock, risk is calculated using equation (4.5.6-2) (Figure 4.5.6-3). The risk coefficient $\gamma$ is set to $5 \times 10^{-2}$ [Sv$^{-1}$] (ICRP, 1991). The projected cross-sectional area is set by considering the geometric shape of final waste emplacement for each waste form and length of disposal tunnel. The projected cross-sectional area in each disposal tunnel for each waste form used in the risk calculation is shown in Table 4.5.6-5. The frequency of drilling is $1.3 \times 10^{-9}$ [m$^2$y$^{-1}$], which is the same as that in the H12 report (JNC, 2000).

$10^{-6}$ to $10^{-5}$ [y$^{-1}$] is used as a safety standard, which is the same as in overseas countries. Assuming that the location of the TRU disposal facility is adequately recorded for 300 years, the risk assessment value is lower than safety standards in all cases.

Table 4.5.6-5 Projected cross-sectional area in the risk calculation for the disposal tunnels for each waste group

<table>
<thead>
<tr>
<th>Group</th>
<th>Projected cross section area [m$^2$]</th>
<th>Type of package</th>
<th>Shape of storage package</th>
<th>Emplacement method</th>
<th>Length of shaft [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group 1</td>
<td>210</td>
<td>200L Drum</td>
<td>$1.5 \times H1.1$</td>
<td>5 raw ($\times 5$ column)</td>
<td>28.0</td>
</tr>
<tr>
<td>Group 2</td>
<td>4404</td>
<td>Canister</td>
<td>$1.2 \times H1.6$</td>
<td>4 raw ($\times 3$column)</td>
<td>734.0</td>
</tr>
<tr>
<td></td>
<td>920</td>
<td>BNGS package</td>
<td>W1.1 x L1.9 x H1.4</td>
<td>4 raw ($\times 3$column)</td>
<td>167.3</td>
</tr>
<tr>
<td></td>
<td>5324</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Group 3</td>
<td>2376</td>
<td>200L Drum</td>
<td>$1.5 \times H1.1$</td>
<td>6 raw ($\times 7$column)</td>
<td>264.0</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>Square package</td>
<td>$1.6 \times H1.2$</td>
<td>5 raw ($\times 7$column)</td>
<td>11.2</td>
</tr>
<tr>
<td></td>
<td>56</td>
<td>BNGS package</td>
<td>W1.1 x L1.9 x H1.4</td>
<td>9 raw ($\times 6$column)</td>
<td>5.7</td>
</tr>
<tr>
<td></td>
<td>2522</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Group 4</td>
<td>3807</td>
<td>200L Drum</td>
<td>$1.5 \times H1.1$</td>
<td>6 raw ($\times 7$column)</td>
<td>423.0</td>
</tr>
<tr>
<td></td>
<td>640</td>
<td>Square package</td>
<td>$1.6 \times H1.2$</td>
<td>5 raw ($\times 7$column)</td>
<td>80.0</td>
</tr>
<tr>
<td></td>
<td>433</td>
<td>BNGS package</td>
<td>W1.1 x L1.9 x H1.4</td>
<td>9 raw ($\times 6$column)</td>
<td>43.7</td>
</tr>
<tr>
<td></td>
<td>4880</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: Meshed value used risk calculation. Each data is response to the design of disposal tunnel in crystalline rock.
Figure 4.5.6-3 Risk of accidental repository penetration by deep drilling

(1) Core observer

(2) Drilling worker
4.6 Summary of disposal safety
In order to examine the safety of the repository for TRU waste disposal, the individual factors that make up the structure of the safety assessment were established and a safety assessment system was constructed that focused on impact of uncertainty. Pre-conditions relating to the disposal environment and the concept for TRU waste disposal was compiled and the safety assessment that considered diverse uncertainty was carried out through a detailed evaluation of individual phenomena including the temporal and spatial variations in the characteristics of barrier material.

4.6.1 Method for conducting safety assessments of a geological repository
The key characteristics of the geological disposal system for TRU waste are the large variety of waste, including metals, nitrates and organic material, and the use of large amounts of cementitious material. This affects the evolution of the disposal facility and the possible spatio-temporal evolution of barrier materials. Furthermore, the geological disposal system for TRU waste is being developed for a generic geological environment as no actual site has been identified as yet. These factors are a source of uncertainty in the safety assessment.

OECD/NEA (2004) stipulates that investigations of uncertainty should be included in safety assessments in order to improve the reliability of the evaluation. In order to obtain the confidence of not only decision-maker and specialist but also the general public in the safety assessment, various uncertainties should be evaluated in detail and the results should be presented clearly.

Hence, a new safety assessment system was constructed that includes a comprehensive sensitivity analysis in order to evaluate uncertainty comprehensively, which the deterministic consequence calculations can not always treat sufficiently.

4.6.2 Summary of preconditions used in the safety assessment
Since the safety concept of the geological disposal of TRU waste is not decided as yet, it is important to define and to present safety requirements for clarifying the target and range of assessments in the safety evaluation. In this assessment, based on IAEA (DS154), safety requirements considered in the current stage of development were defined.

Since the development of a TRU waste repository is at a generic stage, the geological conditions were summarised by considering the research program of HLW. The inventories of radionuclides, taking into account future generation of TRU waste, were calculated and the design of the disposal facility for safety assessment based on TRU inventories was presented. These requirements and conditions were summarised as preconditions.
4.6.3 Scenario development
A comprehensive FEP list was constructed based on examples from Japan and abroad. Exhaustive scenario evaluations were performed by considering the features of geological disposal and the relationship between FEPs and scenarios. A base scenario of groundwater scenario including the reference scenario and the alternative scenario, perturbation scenario of groundwater scenario and isolation failure scenario were constructed. Furthermore, important repository environmental conditions in the safety assessment were identified.

4.6.4 Specification of environmental condition in the safety assessment
The repository environmental conditions which form an important part of the safety assessment were evaluated. In these conditions, the site conditions (thermal, hydraulic, mechanical, chemical, radiation field) and phenomena related to radionuclide transport and to organic material and nitrates in TRU waste were included. Furthermore, the conditions affected by alteration effects of the engineered barriers, alkaline alteration effects of the surrounding host rock, effects of the hydraulic field in the near-field, colloid effects, effects of natural organic material, effects of microbes and gaseous effects were included. In the evaluating these conditions, detailed individual phenomena were investigated by considering spatio-temporal variations and uncertainties in the barrier materials (cf. Section 4.4.11).

4.6.5 Radionuclide transport analysis and dose assessments
4.6.5.1 Specification of analytical cases
Based on an evaluation of important disposal environments in the safety assessment, analytical cases were set up. Analytical cases that considered model and parameter uncertainty were also established and the methodology used to evaluate the analytical cases was described.

4.6.5.2 Results of safety assessment for the base scenario of the groundwater scenario
In order to evaluate the safety of the TRU waste disposal concept, deterministic consequence calculations for the Reference Case were made. These showed that the maximum dose was about 2 µSv/y, which is well below the safety standard in overseas countries (100–300 µSv/ y ), natural background radiation level in Japan and the existing safety standards for shallow disposal in Japan (10 µSv/ y ).

In order to ensure the reliability of the safety assessment, alternative cases were analyzed and compared with the Reference Case in order to address uncertainties in scenario, models and data. In the alternative cases, potential impact of the phenomena which affect the safety of TRU waste disposal were investigated, deterministic consequence calculations and sensitivity analyses for key parameters were carried out with alternative values of key parameters set up based on the parameter ranges. The maximum dose in most cases was below the 10 µSv/y. However, the influence of transmissivity and hydraulic gradient showed a strong linear relationship with maximum dose, and the target value (10 µSv/y) was exceeded in some cases.
depending on the parameter values.

A complementary comprehensive sensitivity analysis was performed in order to evaluate the effects of uncertainty on maximum dose. The result showed that disposal safety is assured even with the existence of various uncertainties in the assumed parameters and models under the reference geological environment, except for cases based on hypothetical parameters due to lack of information.

Considering the uncertainty of the geological environment, disposal safety could be assured by including alternative technologies for reducing nuclide release from waste even in the presence of multiple uncertainties. These technologies are presently under development and are briefly described in Chapter 7.

The importance of the data relating to sorption of natural organic material in the host rock, the data relating to the proportion of fracture from which radionuclides can diffuse into matrix and the improvement of waste technologies which help prevent radionuclide release from waste was indicated through the assessment. In order to avoid excessively conservative assessment, and improve the reliability of the safety assessments, research should focus on these issues.

### 4.6.5.3 Results of the safety assessment of the perturbation scenario in the groundwater scenario

In the perturbation scenario, scenarios of natural phenomena, initial defects of engineered barriers and human intrusion were evaluated.

In the natural phenomena scenario, the effect of uplift/erosion and climate/sea-level change were considered. Based on site-selection factors for high-level waste (uplift and erosion below 300 m during 100,000 years), 0.1 mm/y and 1 mm/y for uplift and erosion rates were considered. The results show that the maximum dose is almost the same as that of the Reference Case. The controlling factor for this analysis is the rate of increase (10 times) in groundwater flow velocity and the time period over which the effects of uplift and erosion become significant (900,000 years and 9,000,000 years). From the evaluation of uncertainty in Section 4.5.4 (Figure 4.5.4.3-7), if an increasing groundwater flow velocity and uplift and erosion rate stay within the above values, disposal safety is not compromised, even taking into account parameter uncertainties related to an oxidizing environment.

Considering the effects of a cool climate or tundra climate, the variation was mainly affected by the differences in biosphere models or uncertainty of groundwater flow around the disposal facility. Hence in future, more realistic hydraulic conditions, biosphere models and relevant parameters for future climate change are required.
In the scenario of initial defects of engineered barriers, the effect of fault sealing was considered. The groundwater flow condition (10 times that of the host rock) and the increase in flow in the EDZ (10 times) due to incomplete sealing were established. The evaluation showed that the maximum dose was several 10 μSv/y in the case of Group 1.

In the human intrusion scenario, the formation of new radionuclide transport pathways by well drilling and water sampling was considered. In the drilling and water sampling scenario, it was assumed that contaminated pore water in the aquifer was used by general public directly. As a result of the analysis, the maximum dose was estimated to be about 100 μSv/y. For the formation of new radionuclide transport pathways by drilling, it was assumed that oxidizing groundwater enters the repository and flow in the EDZ increases by a factor of 10. It was also assumed that radionuclides at EDZ directly reach the biosphere. The analytical results show that the maximum dose for Group 1 reaches about 100 μSv/y.

Summarizing these results, the maximum dose for the perturbation scenario in the groundwater scenario is below 10 μSv/y in many cases. Otherwise, the scenario which considers the formation of new radionuclide transport pathways by well drilling and water sampling, different biosphere models and borehole drilling gives 100 μSv/y. Nevertheless, this level is the same as, or less than, the regulatory safety standard (100-300 μSv/y) in overseas countries.

### 4.6.5.4 Results of safety assessment for the isolation failure scenario

Exposure of the disposal facility at the surface by uplift and erosion and accidental penetration of the repository by drilling were evaluated as isolation failure scenarios.

In the case of surface exposure, taking into account site selection factors (uplift and erosion below 300 m during 100,000 years), this event only happens after 100,000 years. At this point, it is assumed that radionuclide was released forming a contaminated plume around the repository. In the evaluation, since the exposure pathway is different from the normal groundwater scenario, the U-238 conversion flux was chosen as a safety index for dose rate. The flux caused by erosion of repository was found to be smaller to that generated from erosion of granite and uranium ore deposits.

For accidental repository penetration by drilling, an evaluation was performed based on the evaluation method for the scenario by drilling in the H12 report (JNC, 2000) and the risk was found to be below $10^{-6}$ - $10^{-5}$ [y⁻¹], which is the safety standard in several overseas countries.

Among the phenomena which form the basis for the perturbation scenarios and isolation failure scenarios above, extremely unlikely phenomena such as drilling were also included. In order to evaluate such phenomena in detail, some form of risk-based reasoning that includes event probability is necessary in future.
4.6.6 Summary of safety

An exhaustive scenario evaluation for TRU specific waste disposal was carried out. A base scenario of the groundwater scenario, perturbation scenario and isolation failure scenario were constructed and evaluated. In the evaluation of the base scenario, a detailed evaluation of individual phenomena that considers the uncertainty relating to spatio-temporal changes in the barrier materials was performed based on current data and natural phenomena.

Based on these results, the analytical case for radionuclide transport and dose assessment was established and it was demonstrated that the TRU waste disposal concept in Japan is the safe concept with robustness by the combination of deterministic consequence calculations and a comprehensive sensitivity analysis. Based on the evaluation of perturbation/isolation failure scenarios, it was shown that risk was below $10^{-6} - 10^{-5}$ [y⁻¹], which is the indicated safety standard in severa overseas countries.

From these evaluations and analyses, an exhaustive safety assessment was carried out. Key areas for future research are summarised in Chapter 8.
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