

Uncertainty in Scenarios and Its Impact on Post Closure Long Term Safety Assessment in a Potential HLW Repository

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Abstract

In assessing the long term post closure radiological safety assessment of a potential HLW repository in Korea, three categories of uncertainties exist. The first one is the scenario uncertainty where series of different natural events are translated into written statements. The second one is the modeling uncertainty where different mathematical models are applied for an identical scenario. The last one is the data uncertainty which can be expressed in terms of probabilistic density functions. In this analysis, three different scenarios are selected; a small well scenario, a radiolysis scenario, and a naturally discharged scenario. The MASCOT-K and the AMBER, probabilistic safety assessment codes based on connection of sub-modules and a compartment theory respectively, are applied to assess annual individual doses for a generic biosphere. Results illustrate that for a given scenario, predictions from two different codes fairly match well each other. But the discrepancies for the different scenarios are significant. However, total doses are still well below the guideline of 2 mRem/yr. Detailed analyses with model and data uncertainties are underway to further assure the safety of a Korean reference disposal concept.

Key Words : HLW disposal, safety assessment, uncertainty, scenario, MASCOT-K

1. Introduction

Uncertainties in dose assessment of a HLW repository come from three different areas; scenarios, mathematical formulations for a given scenario, and data to be applied for a specific assessment case. The first source of uncertainties in scenarios is generated during the translation of

natural phenomena into specific words. For example, in the SKB studies for a deep repository project[1], five categories of scenarios are identified. The base scenario, the canister defect scenario, climate change scenario, tectonics/earthquake scenario, and scenarios based on human actions are assessed in the SR97 studies. In the base scenario, the present day biosphere is

assumed to be prevailed throughout the time frame of assessment. In reality, the climate can be changed in one case a little bit and in another cases significantly. However, the base scenario neglects any potential climate change so that it creates an uncertainty in translating a natural event into a stylized scenario.

The same is true to the scenario studies in H12[2] where natural disruptive events are the major concerns. As shown in Figure 1, thirty seven cases are quantitatively assessed in the H12 study. Among them, four different scenarios such as base, uplift/erosion, initial defect of the engineered barriers, and no natural barrier ones are mainly assessed. Then, as illustrated in Figure 2, the annual individual doses from many international studies are compared.

The same approach to develop scenarios is adopted to assure the safety of a potential HLW repository in Korea. At first, major scenarios are identified from the combination of the screened FEP[3]. All needed computational tools[4] and associated input data are collected from laboratory and field experiments as well as literature surveys. In this study three base scenarios are selected for the performance assessment.

The likelihood of the base scenarios can be summarised as:

- 1) The expected initial state of the components at the closure of a repository is defined based on the selection of barrier materials and the design of a repository as well as the characteristics of the waste and the site.
- 2) The development of the ecosystem different from present day conditions is not considered; however, reasonable further developments, based on the specific conditions of a site, can be included in the base and alternative scenarios.
- 3) The boundary conditions to the system, e.g.

climate factors, etc, at the time of repository closure are also rather well known.

- 4) The trend in future climate evolution for the coming several 1,000 years is less clear. In contrast, there is a rather well established consensus for the development of glacial conditions etc over longer time periods. The H12 studies state that within the next 100,000 years, the North-east Asia will be under the strong influence of the glaciation. For the nearest 2,000 years, different short term trends such as global warming and global cooling compete each other.

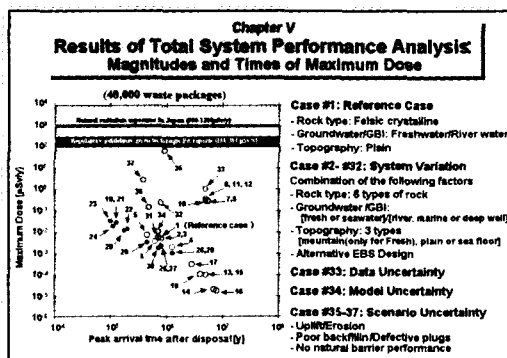


Fig. 1. Maximum Doses from Scenario Assessment in H12

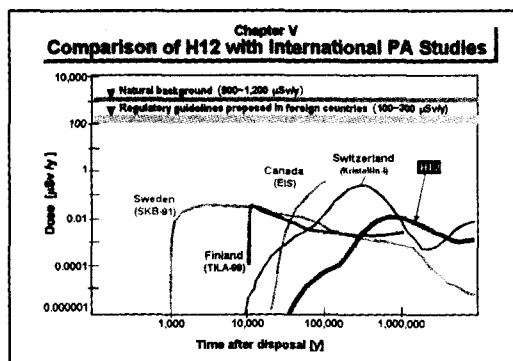


Fig. 2. Dose Comparison among International Studies

2. Uncertainties in Scenarios

The argument on the base scenario is quite plausible and a corner stone in the safety assessment of a potential HLW repository in Korea. Under the categories of the base scenario, three different scenarios are developed.

2.1. Small Well Scenario

The first one is the small well scenario. This is a deterministic case including a whole repository as illustrated in Figure 3. There are two types of spent nuclear fuel, PWR and CANDU to be emplaced in steel canisters. There are 11,375 PWR canisters and 2,529 CANDU canisters to accommodate 36,000 MTU of spent nuclear fuel from reactors to be in operation before 2015. Each canister is 4.96 m long and has a radius of 0.4 m. Once a steel container fails, radionuclides start to be released. The radionuclide inventory is split into two parts. The "gap" fraction consists of radionuclides stayed in a void volume between a cladding and a spent fuel matrix as well as those in a grain boundary of a uranium dioxide matrix as shown in Figure 4. The instantly released fractions of these nuclides are below 2-6 percents of their whole inventories in general[1]. The gap nuclides which have fairly high solubility limits dissolve into

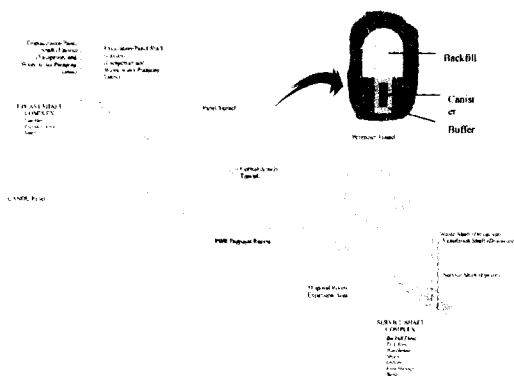


Fig. 3. Korean Reference Disposal Concept

intruding groundwater at the time of canister failure and diffuse out to a bentonite buffer and migrate further through a fracture intersecting a repository by advection and dispersion. The remainder is released congruently as the fuel dissolves, being controlled by the solubility limit of Uranium.

Each canister is surrounded by an annular bentonite buffer, 0.38 m thick. There is also bentonite above and below the canister. The canister and bentonite occupy holes drilled into the floor of repository tunnels and so the bentonite is in contact with the natural rock. The host rock is a fractured granite. Paths through this granite eventually lead to an aquifer from which water is extracted via a well. The water is used for potable water that can lead to human doses[5]. Transport through the granite is via fractures with the radionuclides diffusing into the "rock matrix". Biosphere processes are taken to be fully specified by dose conversion factors (Sv/year per Bq/yr leaving the fractures). The length of a fracture is assumed to be 100 meter, which is very conservative compared with other international studies.

2.2. Radiolysis Scenario

Differences between the first and this scenario are summarised as:

- 1) One percent of total canisters fail at the repository near to a fracture zone after 500 years since emplacement
- 2) There are a 30 meter fracture and a MWCF(Major Water Conducting Feature), a 800 meter fracture zone in contact with a biosphere.
- 3) The chemical alteration for the first 5,000 years after the failure of a waste container increases the dissolution rate of a uranium dioxide matrix to 10^{-7} per year and then decreases it to 10^{-8} per year after that as described in Figure 5.
- 4) The natural biosphere is applied.

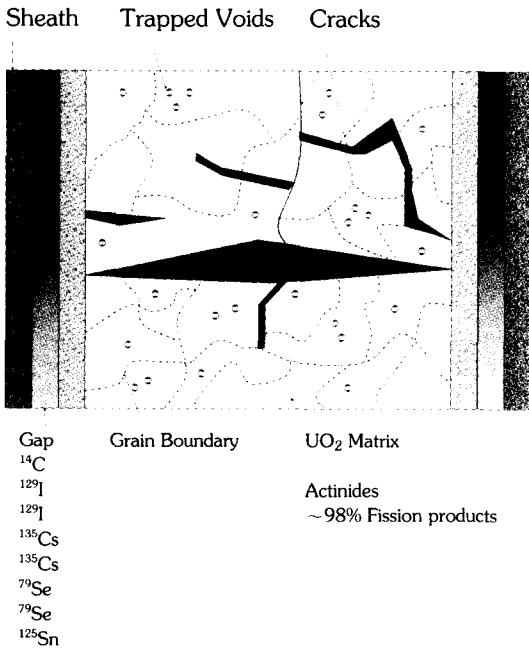


Fig. 4. Location of IRF Nuclides in a Spent Nuclear Fuel

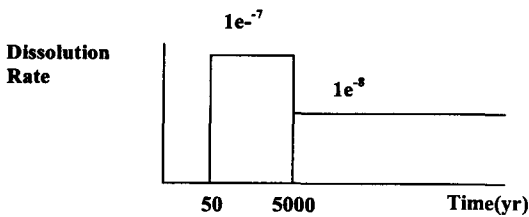


Fig. 5. Change of a Dissolution Rate of Uranium Matrix by Radiolysis

These assumptions are used in the Swedish SR97 study conducted by SKB as a part of its deep repository project. The redox front at early time increases the release rate of a Uranium dioxide matrix by one order. This phenomenon happens when the alpha radiolysis is dominant to decompose of water molecules into radicals and hydrogens. The radicals certainly increase the amount of free oxygens in intruding groundwater, which transform the Uranium dioxide to more

soluble U_3O_8 . The released nuclides enter a fracture via bentonite buffer and eventually reach a porous medium which is connected to a biosphere. The reference biosphere to be considered is a river[5] which in turn contaminates various compartments such as river sediments, agricultural lands, coastal water, coastal sediments, etc.

2.3. Naturally Discharged Scenario

This scenario as depicted in Figure 6 is the combination of the near field of the first scenario and the far field and the biosphere from the second scenario. Here, the waste containment life time is set to be 1,000 years and the length of a fracture is assumed to be 100. The rest of a natural barrier and a biosphere are identical to those in a radiolysis scenario.

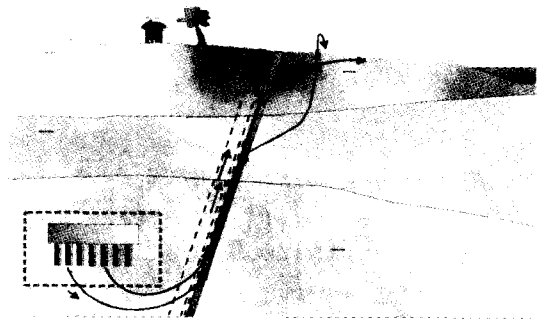


Fig. 6. Migration Pathway of a Radionuclide Naturally Discharged at the Biosphere

These different scenarios are assessed to understand their impacts on total system performance safety using different computational codes based on different mathematical theories.

3. Uncertainties in Modelling

It is interesting to apply different performance assessment softwares for an identical scenario

and to understand similarities and discrepancies of results. For this purpose, two different performance assessment codes, MASCOT-K by KAERI and AMBER by Quintessa are applied. KAERI and Quintessa in the United Kingdom set up a special project to assess long term post-closure radioactive safety of a repository for given scenarios. Throughout the project each institute proposes a scenario with given data set. Then for a given scenario, each party uses different software, MASCOT-K and AMBER and perform blind tests. After calculations, two organizations compare the results for a given scenario and identify the similarities and discrepancies of results. Finally, two groups try to understand the reasons for similarities and discrepancies and to draw future R&D directions on safety assessment. Two out of three scenarios described in the previous section are assessed by two institutes.

This approach is well known for confidence building for specific softwares developed for performance assessment and total system performance assessment of involved parties.

The MASCOT-K developed by KAERI, based on the MASCOT originally developed by SERCO in the United Kingdom, is capable of simulating dissolution mechanisms of spent nuclear fuels which are not in the original MASCOT[6]. It also handles the migration of radionuclide in the form of a pseudo-colloid in a fractured porous medium. The MASCOT-K predicts a flux and a concentration at a given time and a position. It is a network of analytic solutions[7] as illustrated in Figure 7 for each process and a barrier. For example, what happens in a geosphere is described in a series of sub-modules such as a fractured geosphere and a porous geosphere. The fractured geosphere sub-module handles migration of a radionuclide along a straight line type fracture with a certain aperture by advection, dispersion, sorption, kinetic actions as well as matrix diffusion.

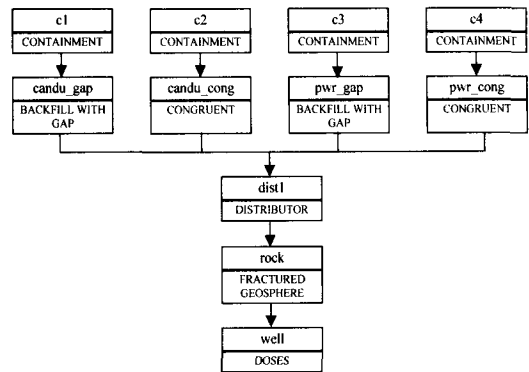


Fig. 7. MASCOT-K Model Network Structure Developed Simulating the Small Well Scenario

The porous geosphere sub-module describes migration of a radionuclide in an equivalent porous medium.

For a given scenario, the MASCOT-K and AMBER[8] use different approaches. For example, for a Small well scenario, radionuclides are released by gap and congruent types. The MASCOT-K explicitly handles two dissolution phenomena based on analytic solutions. In the case of congruent release, the concentration of a Uranium matrix is prescribed in a mathematical formula. There a Uranium matrix is dissolved under the control of its own solubility. The dissolution of other nuclides are controlled by the solubility limit of a Uranium matrix. Since the mathematical model is explicitly developed to describe this process in the MASCOT-K, there is no problem to apply the MASCOT-K for a small well scenario proposed by KAERI. However, the AMBER code which uses the compartment theory does not describe the dissolution mechanisms explicitly because all the interactions between compartments in the AMBER are expressed as the term of a "mass transfer coefficient". Therefore, the application of the AMBER for a Small well scenario needs careful arrangement to identify the mass transfer coefficient from a solid Uranium

matrix to the adjacent buffer barrier, which in turn gives the correct dissolution rates for other nuclides.

The difference described above creates the uncertainties in the modelling. Results from the AMBER and MASCOT-K applications should bear some discrepancies in reality. The same is true to the second scenario, Radiolysis. In this scenario, the MASCOT-K cannot handle the release rate type boundary conditions and the time dependent release rates directly. However, careful step-wise assignment is created to simulate the scenario. At first, the proper solubility limit of a Uranium matrix for the annual release rate of 10^{-7} is deduced by trial and error. It is used as a key input for the MASCOT-K analysis. Then, the solubility limit for the annual release rate of 9×10^{-8} is assessed. For the case of the annual release rate of 10^{-7} the canister life time is assumed to be 500 years since emplacement. For the case of the release rate of 9×10^{-8} the canister life time is 5,000 years since emplacement which is the same as the end of the era of radiolysis. The real annual dose for a radiolysis scenario is the subtraction of the case of 9×10^{-8} release rate from the case of 10^{-7} release rate. In this simulation, uncertainties can be generated when identifying the solubility limits of Uranium matrix. There should be inherent uncertainties in each model approach.

For two scenarios different mathematical models are applied. At first, for the Small well scenario, the MASCOT-K, the AMBER, and the PICNIC[9] are applied for the blind test. The PICNIC code is in essence based on the identical compartment theory as the AMBER. Results in Figure 8-10 illustrate the similarities and discrepancies.

As noted, all three analyses indicate that the I-129 is the dominating species from the beginning up to more than a million years. However, the tails from different approaches are different because, the MASCOT-K is the diffusion

controlled approach, while the AMBER and STMAN/PICNIC treats the radionuclide migration in terms of simple mass transfer coefficients which strongly depend on the number of compartments and how to formulate mass transfer coefficients. Therefore, some discrepancies are inevitable.

The issues that arise as a result of the analysis of the Small well scenario can be split into three types: conceptual, mathematical and software.

Conceptual

In this section, three conceptual issues are discussed: fuel dissolution models; buffer-rock boundary conditions; and rock-matrix structure.

The fuel dissolution model in MASCOT-K is based on the concept of fuel dissolution being limited by the solubility of the Uranium in the water surrounding the fuel. This gives rise to a very slow dissolution rate of less than 10^{-9} per year.

The alternative conceptual model that has been widely used is that the fuel dissolves more rapidly under the influence of produced oxidants. In this case, the solubility of Uranium still limits release of the uranium isotopes, but other elements are limited by their own solubilities. This is an area of current research, and there is not a settled

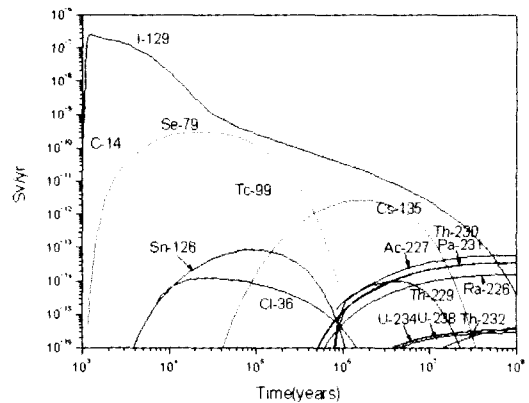


Fig. 8. Annual Individual Doses for the Small Well Scenario Using the MASCOT-K

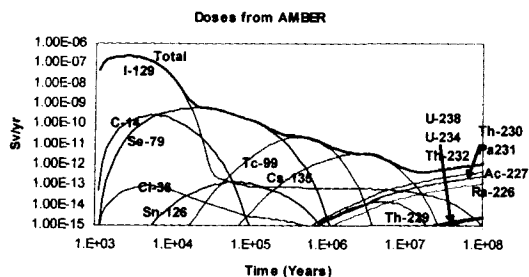


Fig. 9. Annual Individual Doses for the Small Well Scenario Using the AMBER

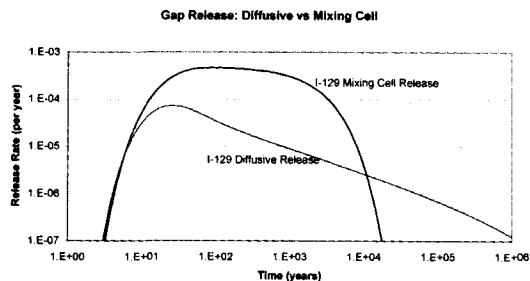


Fig. 11. Discrepancy in the Release Rate Between the MASCOT-K and the AMBER

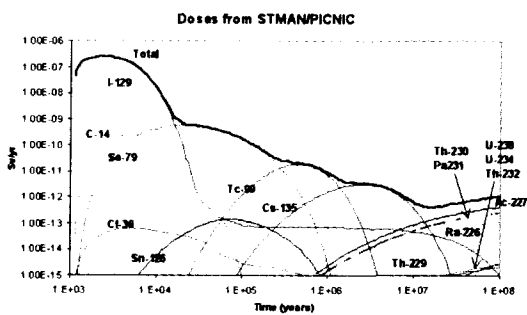


Fig. 10. Annual Individual Doses for the Small Well Scenario Using the STMAN/PICNIC

scientific view at present. The buffer-rock boundary condition is perhaps the key conceptual assumption in the MASCOT-K models. Therefore, it is worthwhile to explore its effects through the use of the analytic results. The I-129 is selected, since this is the dominant nuclide for dose. Given its lack of sorption and long half-life, its behaviour ought to be relatively easy to understand.

Comparing the diffusive (MASCOT-K) and Mixing-cell (AMBER) releases from the buffer for a unit gap inventory in the above Figure 11, the mixing-cell release is larger and more limited in time. Note that the impact of this difference is hidden in the final dose results because of the highly dispersive nature of the geosphere component. The results shown are for the data as used in the main comparison. The mixing-cell

result is obviously very sensitive to the effective flow rate chosen. The behaviour here is clearly controlled by the rate at which the I-129 moves away from the boundary - in the diffusive case this is a slow process whereas in the mixing-cell it is much faster.

For Tc-99 in Figure 12, which has significant sorption particularly in the rock, a rather different picture is drawn. Again, the dose results hide the difference, but now the diffusive releases are generally higher. This is a result for the high rock Kd value of Tc. The effect of a highly sorbing rock is to reduce the aqueous concentration at the buffer-rock interface and so enhance the release. This sensitivity of the model to this parameter implies that care must be taken in the selection of these properties.

Initially, for congruently released nuclides the models are identical because diffusion has not reached the far side of the buffer. The diffusive rate is always proportional to $t^{-\frac{1}{2}}$ and so the total release is proportional to $t^{\frac{1}{2}}$, and appears as a straight line on the log-log plot as shown in figure 13. The mixing cell release rate falls initially (as the concentration in the buffer builds up) but eventually reaches a steady-state which is higher than the diffusive value.

The conceptual model for the rock-matrix itself is important, because it leads to a significant delay

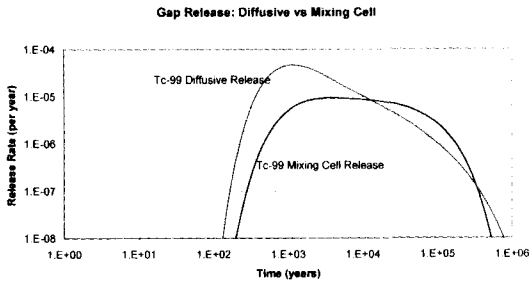


Fig. 12. Discrepancy of the Release Rate of Tc-99 from Two Different Codes, MASCOT-K and AMBER

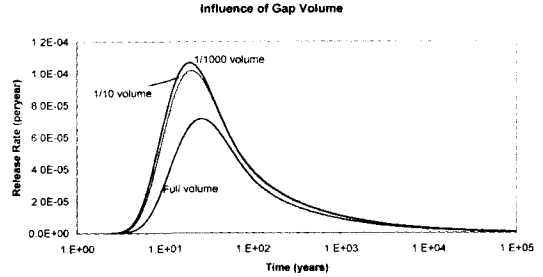


Fig. 14. Effect of the Gap Volume on the Release Rate

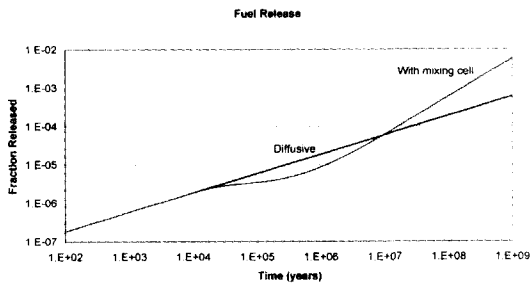


Fig. 13. Discrepancy in the Fractional Release Rates from Two Different Codes, MASCOT-K and AMBER

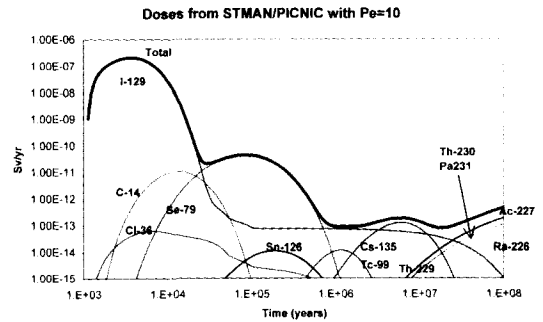


Fig. 15. Annual Individual Dose by STMAN/PICNIC for Higher Peclet Number, 10

in the transport of radionuclides. Two features of the model need to be considered carefully - the structure of the fracture pathways, and the rock-matrix diffusion depth. The model assumes that the pathways are planar features in the rock. This impacts the model through the effective surface area available for diffusion. If the flow was actually channelled then this area could be significantly less. The second aspect is the maximum diffusion distance. The value used is 50 cm, which is quite large. There is a need to justify this, as many experimental projects appear to suggest that diffusion takes place over much smaller distances.

Mathematical

The mathematical aspects that arise are: the use

of Cartesian coordinates; the treatment of the canister water volume in the congruent model; and the use of very low Peclet numbers. The MASCOT-K models use Cartesian coordinates rather than radial coordinates that would be geometrically more realistic. The impact of water volume in a canister, gap volume, can be explored by looking at how the releases for the gap model change when the volume is reduced to zero. Figure 14 shows the I-129 release for a range of volumes.

The difference between calculations with the full volume and a very small volume is at most 50%, with the small volume being conservative. So, the impact of ignoring the canister volume in the congruent model will be small.

The use of a very low Peclet number (2) in the

Table 1. Comparison of Peak Doses in International Programs

Study	Peak Dose Rate (Sv/yr)	Dominant Nuclide	Number of Canisters
H12	$5.0 \cdot 10^{-9}$	Cs135	40 000
SR97	$5.0 \cdot 10^{-8}$	I129	4 000
SPA - ENRESA	$1.4 \cdot 10^{-6}$	I129	3 600
SPA - GRS	$1.0 \cdot 10^{-5}$	I129	15 600
SPA - IPSN	$1.5 \cdot 10^{-6}$	Ra226	14 400
SPA - VTT	$2.7 \cdot 10^{-7}$	I129	1 400
MASCOT-K KAERI	$2.6 \cdot 10^{-7}$	I129	13 900
AMBER KAERI	$2.3 \cdot 10^{-7}$	I129	13 900
PICNIC/STMAN	$2.5 \cdot 10^{-7}$	I129	13 900

geosphere has the effect of spreading releases out. The major impact is that early releases are higher, which can be particularly important for radionuclides that have half-lives of the same order as their transport time. For these nuclides, the effect of the low Peclet number is to increase their consequences. For radionuclides that are not significantly decayed, the effect will be to reduce the peak release. Where matrix diffusion is important, the higher Peclet number allows more time for matrix diffusion and so has a generally lowering effect on breakthroughs. To demonstrate these effects, STMAN/PICNIC calculations with a Peclet number of 10 are performed as shown in Figure 15.

This shows a reduction in doses for most nuclides, due to the effectively longer travel time and increased matrix diffusion. So the low Peclet number is conservative and has little impact on the key I-129 release.

Software

A number of issues concerning the use of

MASCOT-K and AMBER arose and are discussed here. In the AMBER calculations, the main problem that arose was over the best way of discretizing the rock matrix. A great deal of care was necessary in order to arrive at a sensible approach. This is because of the large range of diffusion distances that are relevant across the range of radionuclides. This in turn arises from the range of sorption coefficients that is applied. Comparing the results against analytic calculations is recommended in order to ensure that a suitable discretization has been created. A second issue that must be addressed for AMBER is the number of compartments along the direction of flow. This is largely constrained by the Peclet number. The number of cells must be at least half the Peclet number if numerical dispersion is not to dominate. In the scenario treated here, with a Peclet number of 2, then a small number of compartments would be adequate. Five compartments are used to satisfy the scenario that has a Peclet number of 10.

Figures 8-10 show the annual individual dose as a function of time since emplacement. As shown the so called gap nuclides such as I-129, C-14, Se-

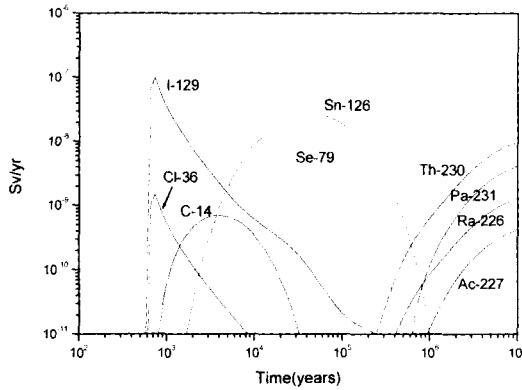


Fig. 16. Annual Individual Dose for a Radiolysis Scenario from MASCOT-K

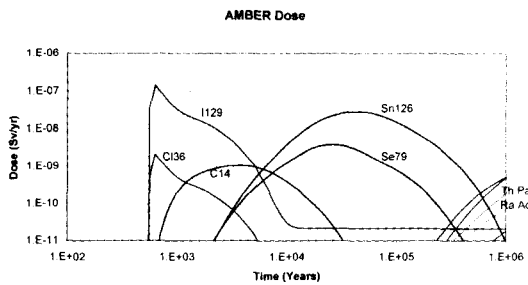


Fig. 17. Annual Individual Dose for a Radiolysis Scenario from AMBER

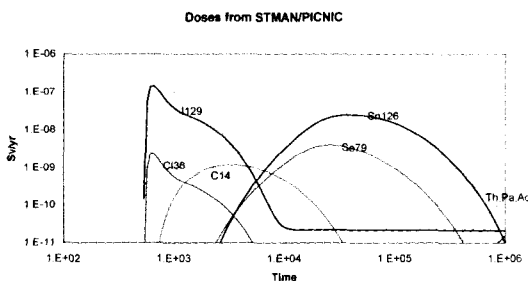


Fig. 18. Annual Individual Dose for a Radiolysis Scenario from STMAN/PICNIC

79 etc result in higher peaks at earlier times than congruently released ones. Results from this study are compared with those from international studies as well as that by the application of the MASCOT-K. The peaks predicted by the AMBER

and MASCOT-K are almost identical. Likely to other studies, the dominant nuclide is turned out to be I-129. The peak value from the AMBER application well suits in the range of values from other studies.

Figures 16-18 illustrate the doses from the radiolysis scenario using three TSPA codes. Results from different code applications are similar. The maximum dose mainly contributed by I-129 in this scenario is similar to that from the first scenario. However, the contribution of other nuclides for overall doses becomes more significant than the first scenario.

4. Uncertainties in Data

To understand the effect of uncertainty in data, the third scenario, Natural discharge one is developed. The near field dissolution model in this scenario is identical to that in the Small well scenario and the far field and the biosphere are the same as those in the Radiolysis scenario. Figure 19 illustrates the annual individual dose for the natural discharge scenario with reference data set. As expected, the gap nuclides dominate the dose. It is of interest to see what are the major input parameters significantly affecting the trend of this dose profile. Several major variables are selected to see their effects on the annual individual dose. Results can be used to prioritize the key parameters for the future PA program.

Three different categories are considered. The first group is the characteristics of the major water conducting features(MWCF's). If the effects of these parameters are significant, in the next R&D phase the more profound R&D activities to identify the characteristics of MWCF's are required. The second group is the characteristics of the chemistry such as retradation coefficients. Final group is the effect of the canister life time.

As shown in Figures 20 and 21, the

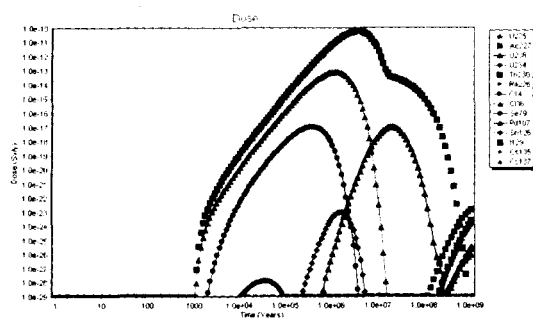


Fig. 19. Annual Individual Dose for a Natural Discharge Scenario

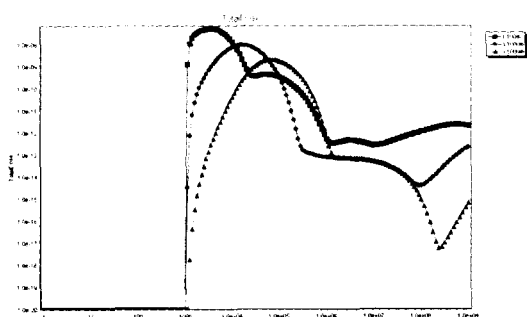


Fig. 20. Effect of the Data Uncertainty in the Length of a Fracture

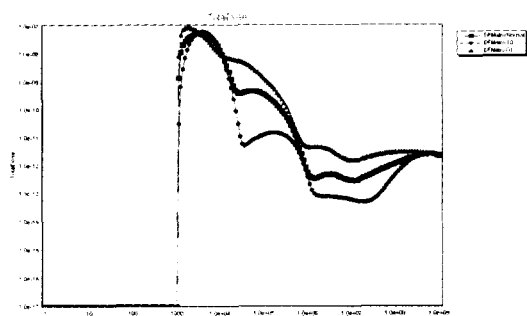


Fig. 21. Effect of the Data Uncertainty in the Diffusion Coefficient of a Rock Matrix

uncertainties in the characteristics of MWCF's influence the annual individual dose significantly. The length of a fracture is a key parameter as illustrated in Figure 20. The shorter the length is, the higher the annual individual dose. Also the lengthier fracture can be exposed to the matrix

diffusion more. Therefore, the length of a fracture affects the peak value of the annual individual dose and the arrival time of the peak. The effect of the matrix diffusion coefficient is also significant. The matrix diffusion is the mechanism to extract radionuclides from a faster moving channel, fracture and hold radionuclides in a surrounding rock matrix. Therefore, the higher value of the matrix diffusion coefficient reduces the peak of the annual individual dose and retards the migration velocity. The effect of a fracture aperture, even though not illustrated in this paper, is also important because it is related to the mass transfer area and the pore velocity of ground water in a fracture.

In summary the uncertainties of the characteristics of MWCF's are important so that more study is needed to identify these throughout the in-situ investigation.

The second category is the chemistry. In this paper, the effect of the uncertainty in retardation coefficients is investigated. As illustrated, the maximum dose is mainly contributed by I-129. However, I-129 is known to be not retarded in both engineered and natural barriers. Therefore, the effect of uncertainty in retardation coefficient of I-129 is not so significant. For among TRU's Ac-227 turns out to be the most significant species on the dose. However, as illustrated in Figure 22, the uncertainty of Ac-227 retardation coefficients is not so important, since the time of interest for Ac-227 is well beyond a million year. The same is true to one of the most dangerous nuclide, Pu-239 as shown in Figure 23. Therefore, for the final disposal of spent nuclear fuel in a fractured rock whose main dose contributors are gap nuclides such as the non-retarding I-129, the effect of retardation coefficients is not so significant.

The effect of the uncertainty in the canister life time shown in Figure 24 is interesting. As shown in the figure, the canister with a rather shorter

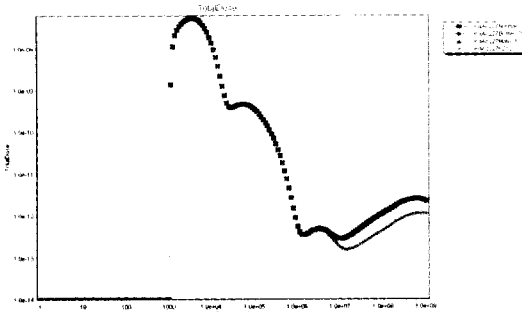


Fig. 22. Effect of Data Uncertainty in the Retardation Coefficient of Ac-227

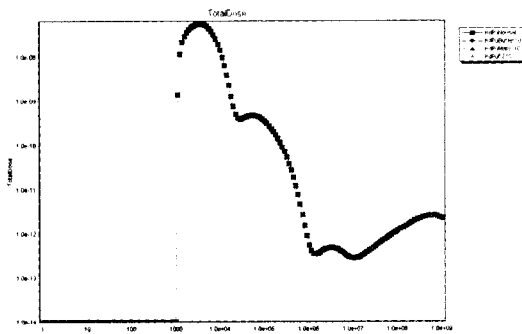


Fig. 23. Effect of Data Uncertainty in the Retardation Coefficient of Pu-239

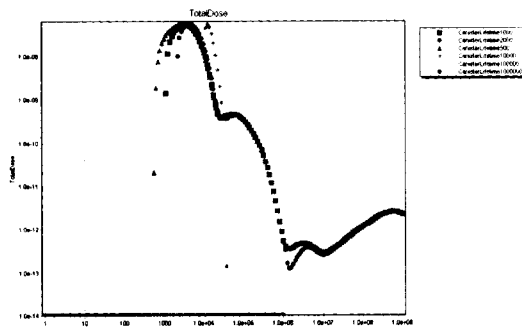


Fig. 24. Effect of Data Uncertainty in the Canister Lifetime

canister life time, i.e., less than 100,000 year does not affect the annual individual dose. If the primary function of the canister is to reduce the annual individual dose, then an appropriate canister material whose life time is more than

100,000 year should be selected. If the canister material with a less life time is allowed, the mechanical strength and the production cost are important for the material selection.

Conclusions

In this paper, the effects of uncertainties in scenarios, mathematical modeling, and input data are studied. To reduce the uncertainty in scenario development, more detailed FEP and scenario study is recommended. Two different scenarios of Small well and Radiolysis, predict different annual individual doses as expected. However, the uncertainties in the peak doses of two scenarios assessed from the mathematical models are not so significant even though two application codes, MASCOT-K and AMBER are based on the totally different mathematical approaches. Results can be used as a part of the confidence building on the TSPA code developed by KAERI, MASCOT-K. The uncertainties in the input data are important not only to assess the dose itself but also to prioritize the future R&D activities. The features of the MWCF's are more significant than those of retardation coefficients. Therefore, in the next R&D phase more efforts should be concentrated on the works for site investigation.

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