Journal of the Korean Nuclear Society
Volume 32, Number 3, pp.244~253, June 2000

Thermal Analysis of High Level Radioactive Waste Repository Using a Large Model

Jeong-Hwa Park, Jung-Eui Kuh, Sangki Kwon, and Chul-Hyung Kang

Korea Atomic Energy Research Institute
150 Dukjin-dong, Yusong-gu, Taejon 305-353, Korea
njhpark@kaeri.re.kr

(Received October 29, 1999)

Abstract

A Simple Large Model (SLM), which can be used to make thermal calculation for a deep geological repository with finite number of HLW canisters, was developed. In order to develop the SLM, a Simple Basic Model (SBM), which will be a unit of the SLM, was optimized first. The SBM was optimized to achieve the same maximum buffer temperature as that of the Detailed Basic Model (DBM) representing the real geometric aspects of the repository. In contrast to the models with the assumption of infinite number of canisters which cannot consider boundary effect, the SLM can model the real repository with finite number of canisters and thus consider the boundary effect. Thermal results from the SLM can be used to evaluate the reliability of the models, which do not consider boundary effect. This model can also be used to simulate the thermal layout design and to analyze the thermal safety of a deep geological repository as well as an underground laboratory.

Key Words : thermal analysis, high level radioactive waste repository, maximum temperature of buffer, layout of canister, deep geological repository

1. Introduction

1.1. General

Thermal analysis for a deep geological repository can provide temperature distribution, which is required for repository design as well as for the evaluation of the thermal integrity of the materials in near field of the repository. Especially, the maximum temperatures of the inner container and the buffer filling the space between the container and rock mass are usually considered as the most critical parameters for repository design. For instance, when bentonite is used as buffer material as Swedish repository concept, the maximum temperature required to preserve the integrity of buffer needs to be determined first as a thermal criterion. After then the container layout and thermal loading from spent fuel, which do not violate the thermal criterion, can be suggested.

For the thermal calculation to determine the temperatures of the major components such as container and buffer in a deposit hole, it is typical to treat the model as symmetric with the assumption of that there are unlimited number of containers in the horizontal plane of the repository. In such a model, however, the heat sink from the boundaries of the repository cannot be considered and the results from the thermal calculation should be different from the results using actual limited container layout.

In computer simulation of a real repository, it is usually recommended to refine the model mesh for the major components in near field. However, this will result too many elements are required to model the whole repository.

It is, therefore, recommended to use simple model for calculating the general trend of the whole repository. However, it can not be obtained the accurate temperature of the major components. If it is required to calculate the temperature of the major components accurately in order to determine whether the repository design satisfies the thermal criterion or not, the submodel function in ABAQUS can be used. In this study, a Simple Large Model (SLM), which can consider boundary effect, was developed to calculate the temperature distribution for the whole repository. Then the thermal calculation for the major components in a deposit hole was carried out using the submodel[1]. The core part mesh of the Detailed Basic Model (DBM) representing the real geometric aspects of the repository was the mesh of the submodel. And the thermal boundary conditions for the submodel were given from the results of the SLM.

1.2. Basic Algorithm for Thermal Calculation

The differential expression of heat transfer is

$$\frac{\partial}{\partial \underline{x}} \cdot \underline{q} + r = \rho c \frac{\partial T}{\partial t} \tag{1}$$

where

- $\underline{q}$: heat flux vector per unit area crossing surface
- r : heat flux per volume generated within body
- ρ : density of material mass
- c : specific heat of material mass
- T : temperature
- t : time

In ABAQUS, the term in the right hand side is expressed as material rate of change of U (the internal energy per unit mass) per time and density($\rho\dot{U}$).

Since such a differential form as Equation (1) represents thermal equilibrium at a point in a body, the following numerical formula can be obtained by averaging over the finite volume.

$$\int_V \delta T \rho \dot{U} dV - \int_V \frac{\partial T}{\partial \underline{x}} \cdot \underline{q} dV = \int_S \delta T q dS + \int_V \delta T r dV \tag{2}$$

If heat flux $\underline{q}$ in Equation (2) is expressed by Fourier's law, the following finite element approximation can be obtained for the thermal energy balance of transient analysis from Galerkin approach:

$$\frac{1}{\Delta t} \int_V \rho (U_{t+\Delta t} - U_t) dV + \int_V \frac{\partial N^N}{\partial \underline{x}} \cdot \underline{k} \,|_{t+\Delta t} \cdot \frac{\partial N^N}{\partial \underline{x}} dV \overline{T}^M_{t+\Delta t} - \int_V N^N r \,|_{t+\Delta t} - \int_S q \,|_{t+\Delta t} dS = 0. \tag{3}$$

If Equation (3) is nonlinear due to the time dependency of heat source, ABAQUS uses Newton's iteration method to solve the equation. The detailed algorithm is described in reference[2].

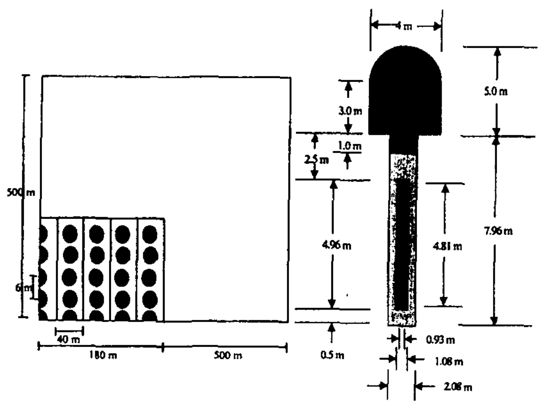


Fig. 1. Schematic Diagram of 9 Pitch by 9 Tunnel Layout and Borehole Type Repository Concept

2. Thermal Analysis for a Deep Underground Repository

2.1. Basic Concept of Underground Repository

KAERI proposed a reference concept of deep geological high level nuclear waste repository, in which the waste is disposed in vertical deposition holes[3]. It is, however, a quite preliminary repository design mainly for evaluating the feasibility of the design and for safety analysis.

In this study, it is assumed that the repository is located at 500m below surface in a granite rock mass. In the whole repository for SLM, there are nine horizontal tunnels with 40m spacing. In each deposition tunnel, nine vertical deposition holes are drilled in the floor. The length of each deposition hole is 7.96m and the borehole spacing is 6m. One container of 1.08m diameter and 4.96m length is placed in the borehole and buffer fills the space of 0.5m between the container and rock. In each container, four spent fuel assemblies of 40 year cooling time are inserted. The schematic diagram of borehole layout is shown in Fig.1.

Bentonite, which will be used as buffer material, can prevent ground water from penetrating into the container surface with its low permeability. Also it can retarded the migration of nuclides by adsorbing the nuclides leaked from damaged containers. If the temperature is over 100℃, bentonite will reduce its functional capabilities with phase change. Because of that, the repository should be design to maintain the buffer temperature below 100℃[4]. This is the most critical thermal constraint for repository design, if bentonite is considered as buffer matierial.

2.2. Modelling

Modelling described in this section implies the process for generating model mesh to solve the heat transfer equation, equation (3), by using ABAQUS.

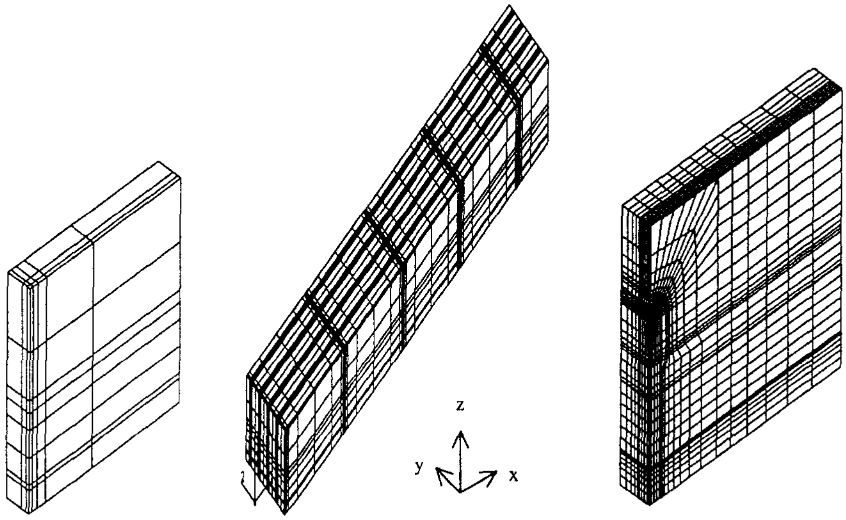
In the DBM, spent fuel, container, buffer, and backfill material in a deposition hole and rock mass are included with similar dimensions and shapes as actual design. The DBM can be used as a unit to build a large model for the whole repository. However, this will result too many meshes in the model and not allow efficient thermal calculation. It is, therefore, strongly recommended to simplify the model for the whole repository.

To build a simplified large model, a Simple Basic Model (SBM), which will be used as a unit for the large model, should be developed first. In the SBM, the number of meshes was reduced by representing the real cylinder shape of container and buffer as rectangular elements. Since the outer shell of container is thin, it was not considered as a separated part but simply included in the heat source.

In the Simple Large Model (SLM), the geometry of repository is assumed to be symmetric in x and y directions on the base of the center line of the deposition hole in the center of the model. It is,

Table 1. Description of Each Model

Basic	Simple	Detailed
Basic	• rectangular elements are used for heat source, container, and buffer. • less mesh numbers • infinite number of containers • used as a unit model for the simple large model	• mesh shapes for heat source, container, and buffer are similar to the real shapes. • more mesh numbers • infinite number of containers • the core part mesh of the detailed model is used for the submodel mesh
Large	• represents the whole repository • built from many of simple basic models • finite number of containers • Effective way for describing the whole repository, because of less mesh numbers than detailed large model	• represents the whole repository • built from many of detailed basic models • finite number of containers • Ineffective way for describing the whole repository, because of too many mesh numbers.



Simple Basic Model　　Simple Large Model　　Detail Basic Model

Fig. 2. Finite Element of Core Part Around a Bore Hole in Three Different Models

therefore, possible to represent the whole repository by using one fourth of it. In this study, four and half tunnels were included in the SLM in x direction. The model boundaries in x and y directions are set up at 680m from the center of the model. Its validity will be discussed in the sensitivity analysis in section 2.6. Figure 2 shows the SBM, SLM, and DBM. Only the central part of 20 m around the repository horizon of each model was shown in Figure 2. The general description of each model is listed in Table 1.

2.3. Boundary Condition and Initial Condition

The boundaries on xz plane and yz plane in the SLM were assumed to be adiabatic. Zero heat flux was assumed to be along the symmetric plane of

Table 2. Material Data for Thermal Analysis

Parameter	Granite	Mixture (sand/bentonite)	Buffer	Canister	Spent Fuel
• Density (kg/m^3)	2,700	2,100	2,100	8,000	10,960
• Heat Conductivity (W/m.K)	3.6	2.0	1.2	15.2	7.0
• Specific Heat (J/Kg.K)	815	800	1,000	504	275

the center line. It was also assumed that natural air convection transfers heat from the ground surface to the atmosphere and the air temperature at the ground surface is assumed to be constant as 20℃. The bottom of the model is set up at the depth where the heat from the repository and geothermal heat are on equilibrium condition. Such a depth may vary with time and heat intensity. If thermal calculation for 2000 years is made, the temperature variation with decay heat can be ignored, because the thermal equilibrium between the heat source and geothermal heat can be achieved at 1500m below surface[1]. The boundary condition at this depth, therefore, can be fixed as geothermal temperature.

The typical geothermal gradient of 3℃/100m was used to calculate the initial geothermal temperature distribution in the model.

2.4. Input Data

As heat source for heat loading, PWR spent fuel is considered. In a PWR spent fuel assembly, there is 440Kg uranium in 17×17 rods and the burn up (4.0% reached U) is 45,000 Mwd/MtU. When the spent fuel is discharged from a reactor, its decay heat with time can be numerically predicted by the following equation[5]:

$$
\begin{aligned}
P(t) &= 852.34\exp(1/(0.2642+0.130889t)) , && 1 < t < 30 \\
P(t) &= 14548.7\, t^{-0.76204} , && 30 \leq t \leq 10^6
\end{aligned}
\tag{4}
$$

where, P is volumetric heat generation per ton of uranium, and t is cooling time(year).

For the spent fuel after 40 years cooling, the heat flux can be calculated from Equation (4), which can be rearranged to a suitable form for ABAQUS using the user's subroutine HETVAL.

Container, buffer, and rock are assumed to be homogeneous and the thermal properties of them are listed in Table 2. Those properties were selected from a SKB technical report[6] and PNC data[7]. Since it is generally accepted that the thermal properties of them are more or less constant under the temperature 100℃, constant thermal properties are used.

2.5. Thermal Analysis by SLM

In order to compare the results from SBM and SLM with those from DBM directly, the location as well as the dimensions of core parts of each model need to be identical. It is, therefore, necessary to carry the submodel thermal analysis using the thermal boundary conditions obtained from the thermal analysis of SLM or SBM. The submodel used here is the same as the core model of DBM in Fig.2. This allows more or less direct comparison between the results from different models is available and more detailed temperature distribution can be achieved.

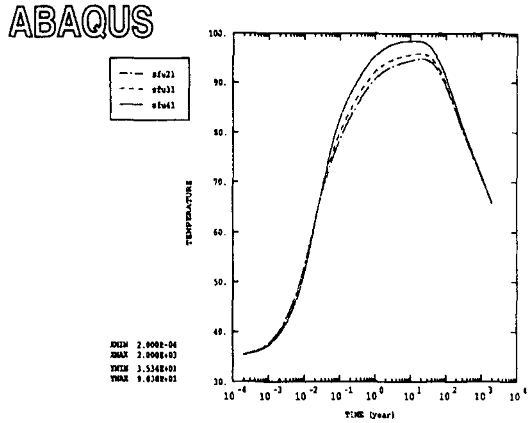


Fig. 3. Temperature Profiles As a Function of Buffer Thickness Calculated from Simple Basic Model(sfu21=44.3cm, sfu31=50, sfu41=60cm)

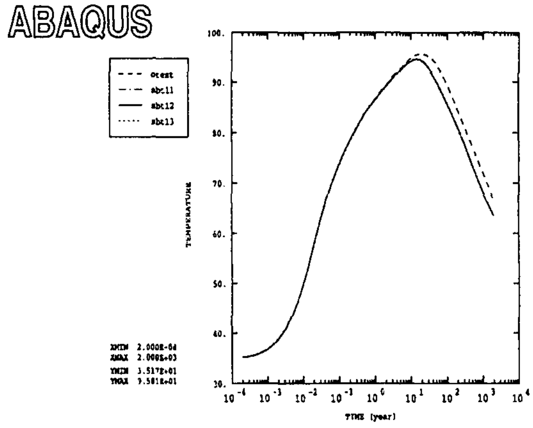


Fig. 4. Temperature Profiles As a Function of Buffer Thickness Calculated from the Submodel (otest=detailed model, sbt11=44.3cm, sbt12=50cm, sbt13=60cm)

2.6. Sensitivity Analysis

For the SLM, it is desirable to include tunnels and boreholes equal to these of the whole repository. If it is possible to include the more tunnels and boreholes in the modelling, the more reliable results can be obtained. There are, however, limitations on the number of tunnels and boreholes in a model, since the number of meshes of the model will be increased significantly with the increase of the number of tunnels and boreholes.

To make an optimized SLM, it is necessary to optimize first the SBM with fewer number of meshes and with little temperature difference from the DBM. If necessary, the components of repository needs to be minimized in order to reduce the number of meshes. In an extreme case, when the repository is assumed to be consisted of heat source and rock mass only, the number of mesh can be minimized, but it results inaccurate calculation.

Even though it is recommended to include all components in a deposition hole for the optimum SBM, container was not modeled as a separate component but included in heat source. This is acceptable because of its high thermal conductivity and small volume compared to other components. In order to develop the optimum SBM, sensitivity study was performed for the following parameters: (a) thickness of buffer; (b) mesh size of the top and bottom models; (c) dimensions of the model in x and y directions; and (d) size of repository.

- Thickness of Buffer

In the SBM, buffer is simplified by using rectangular elements instead of circular elements, even though the actual buffer shape is circular. Because of that, the thickness of buffer in the model is different from the actual thickness depending on location and hence the temperature at a specified point might not be the same as the DBM with circular elements. In order to find the influence of buffer thickness on the temperature at a specific point, sensitivity study was performed for three different buffer thicknesses of 44.3cm, 50.0cm and 60.0cm.

The maximum buffer temperatures for the cases with different buffer thicknesses were plotted with time as shown in Fig.3. As expected, the

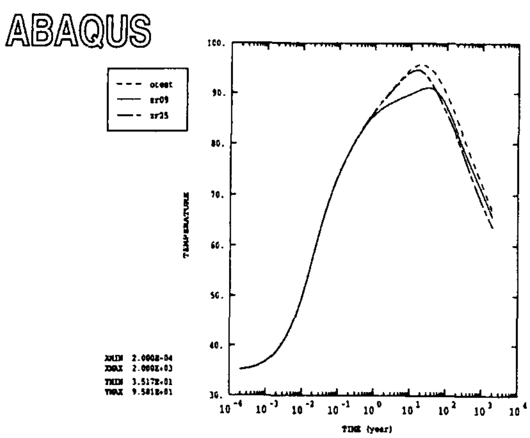


Fig. 5. Temperature Profiles As a Function of the Ratio of Mesh Length in Simple Basic Model (otest=1/16, zr09=1/9, zr25+1/25 : Ratio is L1/L2)

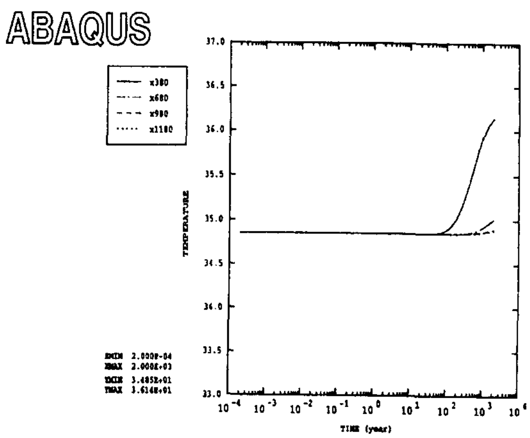


Fig. 6. Temperature Profiles As a Function of the Distance into the Rock along x Direction

maximum buffer temperature increases with the increase of buffer thickness as shown in Fig.3.

The maximum buffer temperatures calculated from the submodels and the DBM are plotted in Fig.4. Different boundary temperatures from the SBMs with different buffer thicknesses were used for each submodel. Each submodel used the same mesh as the core model of the DBM for direct comparison. As shown in Fig.4, the maximum buffer temperature from the submodel for the cases was not influenced by buffer thickness. This seems due to that the variation of the submodel boundary temperature with time is almost same in three cases, which are determined from the SBMs with different buffer thichnesses. It is, therefore, concluded that any of the three thicknesses can be used for the rectangular elements in order to obtain the submodel boundary temperature. The maximum buffer temperature from the DBM (otest) is about 2°C higher than that from the submodels.

- Mesh Size of the Top Model and Bottom Model

Top model represents the upper part of the model mesh from the top surface of the core part in Fig.2 to ground surface, while bottom model represents the lower part from the bottom surface of the core part to the bottom boundary. They were set up properly to carry accurate thermal analysis and efficient numerical calculation. In the case of DBM, each of the top and bottom model was divided into 5 elements vertically and the length along z direction of the mesh, which is closest to the core part, was enforced to be one sixteenth of the farthest mesh from the core part. In the case of SBM, each of the top and bottom models was divided into 3 elements vertically and various ratios of the farthest mesh to the closest one was used to find the optimum value. Optimum ratio means that the temperature calculated from the SBM with the ratio is similar to that from DBM.

The maximum buffer temperatures calculated from the DBM(otest) and from the two cases, in which the ratios of mesh lengthes (L1/L2 : L1 is the longest and L2 is the shortest) are 9(zr09) and 25(zr025), are presented in Fig.5. From this figure, it is possible to observe that the maximum buffer temperature from the SBM with the ratio of 25 is almost the same as that from the DBM. Using the ratio 25, it is possible to calculate similar temperature distribution as DBM by using SBM, which has less vertical elements than DBM.

- Dimensions of the Model in x and y Directions

The assumption setting the bottom boundary of the SLM at 1500m below surface, was proven to be valid from the sensitivity analysis, which was carried out for developing the DBM[1]. In this study, additional meshes were added to the SLM along the x and y directions to satisfy the assumption of adiabatic condition at the boundaries, to which the heat from the heat source can not reach during the period of calculation (here 2,000year).

Fig.6 shows the temperature variation with time at a point on a boundary surface of the SLM with different boundary lengths in x and y directions, 380m(×380), 680m(×680), 980m(×980), and 1,180m(×1180). When the boundary length is 380m, there is a considerable temperature increase at the point about 200 years after emplacement. When the boundary length is over 680m, however, the temperature increase at the point is negligible.

- Size of Repository

Generally, the thermal calculation of the repository layout with unlimited containers can be simplified by using the symmetric characteristics of the model. The number of containers in a real repository, however, is limited. In this study, it was assumed that there are only 9 tunnels and 9 boreholes per each tunnel as shown in Fig.1, even though thousands of containers are usually emplaced in a repository. This was required because of the calculation capacity (especially ram memory) and running time of computer.

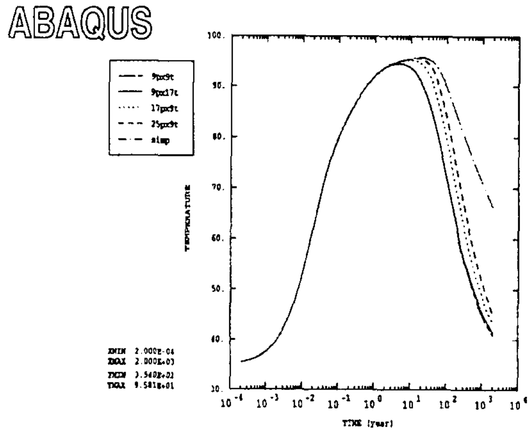


Fig. 7. Temperature Profiles As a Function of Canister Number

In the case of limited layout, four cases with different number of tunnels and boreholes were developed as following: (a) 9 tunnels and 9 boreholes in each tunnel (9p×9t); (b) 17 tunnels and 9 boreholes in each tunnel(9p×17t); (c) 9 tunnels and 17 boreholes in each tunnel(17p×9t); and (d) 9 tunnels and 25 bore hole in each tunnel(25p×9t).

The maximum buffer temperatures of the limited and unlimited container layouts are presented in Fig.7. The maximum buffer temperatures of the limited canister layout were determined from submodel of the center position of repository using the boundary temperature, which was roughly calculated from different SLMs. The temperature for unlimited container layout was calculated by using DBM.

From Fig. 7, it was found that the variation of the maximum buffer temperature was small, even though the number of tunnels was increased twice. In contrast, the number of boreholes in a tunnel influences significantly on the maximum buffer temperature. With increase of the number of boreholes, the maximum buffer temperature approaches to that from the unlimited layout.

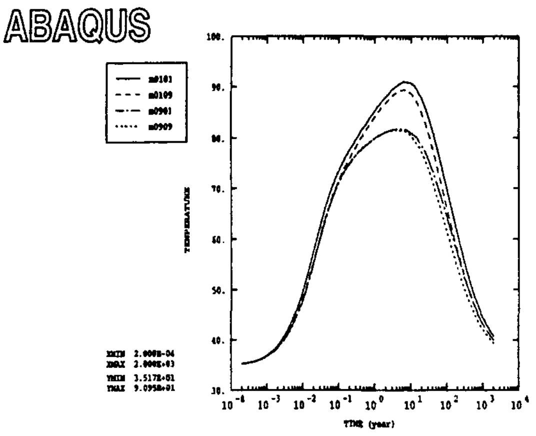


Fig. 8. Buffer Temperature Profiles for the Corner Holes in the Simple Large Model

2.7. Discussion of Thermal Analysis

A SLM was generated by using the optimized SBM as a unit model. Various sensitivity studies were performed to develope the optimized SBM, which results similar temperature distribution to the DBM.

Since the influence of buffer thickness of SBM on maximum buffer temperature is negligible, when a submodel is used to determine the temperature of buffer, as shown in Fig.4, it is reasonable to determine the thickness of rectangular buffer from the volume of actual circular buffer.

In the SBM, the ratio of the mesh lengths of the closest to and farthest from the core part influences on the buffer temperature as shown in Fig.5. When each of the upper and lower model is divided into three elements vertically, the mesh length ratio of 25 results closer temperature to that from the DBM than the case with the ratio of 9. Thus, 25 was selected as the ratio for further modelling.

Adding additional meshes to x and y directions was done for determining the outer boundary surfaces for the SLM. From Fig.6, it was found that the temperature increase at a point on boundary surface was negligible when the boundary length is over 680m and the calculation time is over 2,000 years. It is, therefore, recommended to use 680m long model to simulate the heat flux around an underground repository for 2,000 years.

From the sensitivity study related to the size of repository(to refer Fig.7), it was found that the maximum buffer temperature increases and approaches to that of unlimited layout with the increase of repository size, especially when the number of boreholes per unit tunnel length increases.

When the number of meshes of the SBM is minimized, the results from the submodel are similar to those from the DBM and the SLM built by the SBM simulates the whole repository effectively, the optimum SBM could be developed.

The thermal analysis using the SLM built by the optimum SBM was carried out in the whole repository, 9p × 9t. Fig.8 shows the maximum buffer temperatures at different boreholes in this model. The temperature is highest in the borehole at the center of the model (m0101), while much lower temperature is predicted in the borehole located at the end of the pitch direction (m0901). On the other hand, the temperature in the borehole at the end of the spacing direction is almost the same as that in the borehole at the center. The temperature in the borehole farthest from the center of the model in diagonal direction(m0909) is more or less the same or a little lower than the temperature at m0901.

3. Conclusions

It is usually assumed in modelling that there are unlimited number of canisters. In that case, the model can be simplified by introducing the symmetric characteristics of the model. In such a model, however, the temperature is expected to be a little higher than the actual, because the model cannot consider the heat sink from the boundaries of the repository. It is, therefore, recommended to develop a SLM, which can consider the influence of the boundaries of the repository with limited number of canisters.

In order to develop a SLM, which can be used for thermal analysis of an underground nuclear waste repository in deep location, an optimized SBM was used as a unit model. To optimize the SBM, thermal analysis using the submodel function in ABAQUS was carried out. The boundary temperature of the submodel, which has exactly same model mesh as the core part in the DBM, was derived from the rough calculation using SBM for different cases. By comparing the results from the submodel and the DBM, it was possible to develop the optimum SBM, in which the number of meshes is minimized without losing accuracy.

To determine the temperature distribution around the boreholes in important areas in the SLM, thermal analysis using the submodel were carried out. The boundary temperatures of the submodels for the boreholes in different locations were derived from the SLM. Like this, it is possible to perform thermal analysis for a repository with limited number of canisters by using the submodel.

Acknowledgement

This study has been carried out under the Nuclear R&D Program by Ministry of Science and Technology of Korea.

References

1. Jung-Eui Kuh,Chul-Hyung Kang,Jun Park, "Thermal Analysis for the Near Field of the High Level Radioactive Waste Repository using ABAQUS", ABAQUS Users' Conference Proceedings, May 26-28, (1999).
2. ABAQUS lecture note, "Heat Transfer and Thermal Stress Analysis", (1996).
3. Jongwon Choi,Chul-Hyung Kang,Sangki Kwon,Young-Sung Choi, "Technology Assessment of Disposal Alternatives to Determine a Reference Geological System for HLW", KAERI/TR-1361/99, (1999).
4. L.H.Johnson, J.C.Tait, D.W.Shoesmith, J.L.Crosthwaite and M.N.Gray, "The Disposal of Canada's Nuclear Fuel Waste: Engineered Barriers Alternatives", AECL-10718, COG-93-8, (1994).
5. J.W.Choi, C.H.Kang, W.I.Ko, Y.M.Lee, J.H.Park, Y.S.Hwang, "Reference Spent Fuel and Its Characteristics for the Concept Development of a Deep Geological Disposal System", KAERI/TR-914/97, (1997).
6. Lenmart B rgesson "Interaction between Rock, Bentonite Buffer and Canister. FEM Calculation of Some Mechanical Effects on the Canister in Different Disposal Concepts", SKB Technical Report 2-30, (1992).
7. PNC, "Research and Development on Geological Disposal of High-Level Radioactive Waste", PNC TN 1410, (1992).