A Numerical Approach for the Analytical Solution of the General Temperature Field for the Final Disposal of High-Level Radioactive Waste

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***Abstract*—After numerous years of international research and development, there is a broad technical consensus that deep geological disposal is the method for the management of High-Level Radioactive Waste (HLRW). Deep geological disposal offers relatively enough space to accommodate the large volume of HLRW accumulated over the years will provide safety of to humankind and the environment for now and far into the future. This paper presents the methodology that the analytical solution of the general temperature field of the HLRW underground disposal repository can be approximately obtained by performing the calculations of Gaussian numerical integration and Gaussian quadrature. The process of the calculations has been compiled to the MATLAB codes by the authors. The verification of the results confirms that the method of this study is feasible and accurate.**

***Index Terms*—The analytical solution of the general temperature field, deep geological disposal, Gaussian quadrature, the thermal conductivity of host rock.**

I. INTRODUCTION

When considering the High-Level Radioactive waste (HLRW), it is a serious issue for any government. In Taiwan, there are three nuclear power plants, two of them are considered as the most dangerous nuclear power plants on the planet in 2011 [1]. The three nuclear plants comprise two Westinghouse pressurized water reactors [2] and four General Electric boiling water reactors [3]. As the policy of decommissioning of the nuclear power plants, there will be numerous HLRW which must be disposed of by the deep geological barrier for long-term safety and security [4]. As a result, Taiwan government is one of the many that are seeking for a viable method to implement a deep geological repository [5]. For the method of deep geologic disposal of HLRW, one of the most advanced companies, Swedish Nuclear Fuel and Waste Management Company (SKB), has been chosen as the standard process of this paper.

In the concept of the strategy of SKB for vertical deposition holes, KBS-3V [6], the copper canisters with a cast iron insert containing the fuel are surrounded by bentonite clay for isolation and mechanical protection and are deposited in vertical deposition holes in the floor of horizontal tunnels at 400 m to 700 m depth below ground surface in a crystalline rock mass [7]. The heat generated by the spent nuclear fuel will increase the temperature of all components of the repository: canisters [8], engineered barriers, deposition tunnel backfills [9], tunnel seals, top seal below ground surface, arrangements for sealing off investigation boreholes and the host rock itself. For the bentonite buffer surrounding the canisters, the peak temperature must not exceed 100 ℃ for any of the deposition holes or the buffer will lose the ability to block the radioactive substance [10].

A strategy report [11] which concerns the temperature criterion was presented as follow.

The process of the report is as follows:

1) Construction of a thermal site descriptive model.
2) Estimation of model and data uncertainties [12].
3) Determining the temperature margin and establishing a corresponding temperature threshold.
4) Obtaining canister and tunnel spacing by the use of the analytical solution [11], [13].
5) For the numerical temperature calculations, a model is produced with the thermal properties distribution.
6) With lowest thermal conductivity in the central part of a tunnel, the peak buffer temperature is calculated. The canister spacing in the model is obtained by the step 4.
7) If the chosen trial value cannot meet the temperature threshold of bentonite (100 ℃ after adding the margin), the selection of canister spacing will be redone and the numerical analysis will be performed with the same distribution of the rock domain.
8) If the selected canister spacing is approved as the dimensioning rock domain spacing, it will be applied to the repository design.

The basic concept of the report [11] is to determine the maximum temperature of bentonite buffer. By adding two parts [14], the peak buffer temperature can be obtained. The first is the rock wall temperature at mid-height of the canister, which is obtained by the analysis solution with the heat decay function [15]. The second is the temperature difference between the surrounding rock wall at canister mid height and top of the canister, which is obtained by

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experiment results and heat transfer estimations [16]. Therefore, the purpose of this study is to reproduce the calculation of analytical solution to obtain the temperature of the rock wall temperature at mid-height of the canister through a self-written Gaussian quadrature program in MATLAB, and verified with [11] and a self-developed numerical model in $FLAC^{3D}$ [17].

II. METHODOLOGY

A. Analytical Solution

The rock wall temperature at mid-height of the canister can be solved by the thermal analytical solution that was reported in [13].

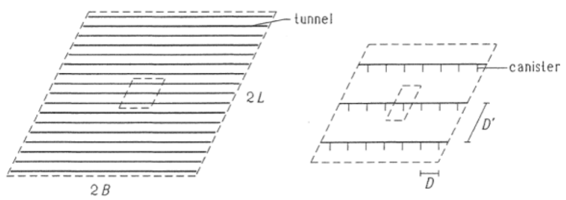

Figure 1. Schematic graphic of the repository of the report. Where D is the spacing of canisters, and D' is the spacing of tunnels [13].

Fig. 1 shows the schematic graph of the repository. The location of the canister at the center of the repository, is defined as (0, 0, 0), and the repository has the size that $-L < x < L$, $-B < y < B$, and $z = 0$ m. The range between the top boundary (z =500 m) and the bottom boundary (z=-500 m) is defined homogeneous with a thermal conductivity λ (W/(m·K)), volumetric heat capacity ρc ($J/m^3 \cdot K$). The thermal diffusivity is $\gamma = \lambda/\rho c$ (m^2/sec). Based on [18], the description of the temperature field is as (1):

$$(1/\gamma)\cdot(\partial^2 T)/(\partial t) = (\partial^2 T)/(\partial x^2) + (\partial^2 T)/(\partial y^2) + (\partial^2 T)/(\partial z^2) + Q(x,y,z)/\lambda \tag{1}$$

Briefly, by defining a window which contains point sources, line sources, compound sources, and the remaining area being a rectangular heat sink, the local thermal field can be described [11]. In the Fig. 2, the heat sink – q(t), which is denoted by a negative source, is to balance the heat. Then, applying the method of superimposing and the quadrature process [19], the global temperature solution of can be derived from the local field. The analytical description for the general temperature field is shown in (2):

$$T_{global}(x,y,z,t) = \int_0^t Q(t')\cdot(px\cdot py)^{-1}\cdot f\cdot h dt' \tag{2}$$

$$f = (\rho c)^{-1}\cdot[4\pi\cdot\gamma(t-t')]^{-0.5}\cdot\left[e^{-z^2/[4a(t-t')]} - e^{-(z-2H)^2/[4a(t-t')]}\right]$$

$$h = (1/4)\cdot\left\langle erf\{(L+x)/4a(t-t')\}^{0.5} + erf\{(L-x)/4a(t-t')\}^{0.5}\right\rangle \cdot\left\langle erf\{(B+y)/4a(t-t')\}^{0.5} + erf\{(B-y)/4a(t-t')\}^{0.5}\right\rangle$$

where the tunnels and deposition holes are separated by distances *py* and *px*, respectively.

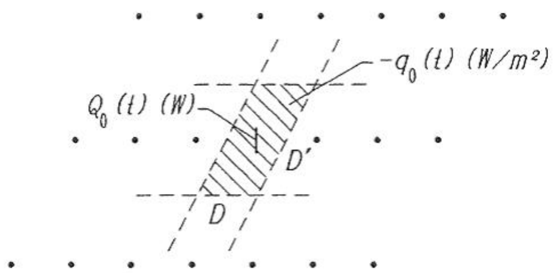

Figure 2. The local thermal field. Rectangular grid DD' with canister heat source Q_0 (t) and a balancing plane source $-q_0$ (t) [13]

B. Decay Function

According to the [13], the decay function which is defined that the heat release can be used for the actual local temperature field of a canister when all other canisters are considered as point heat sources Q_0 (t) on the z = 0 m plane, was adopted. The heat release can be represented by two exponentially decaying components that are shown in (3):

$$Q_0(t) = Q_1 e^{-t/t_1} + Q_2 e^{-t/t_2} \tag{3}$$

where $Q_0(t)$ is the heat release from each canister. The value of the first component, Q_1 is 700 W, and t_1 is 46 years. In the second component, Q_2 is 250 W, and t_2 is 780 years.

In this paper, another heat decay function is defined by [11], is shown in (4).

$$Q(t) = \sum_{i=1}^{7} A_i \exp(-t/t_i) \tag{4}$$

where A_i and t_i are listed in the following Table I.

TABLE I. DECAY FUNCTION COEFFICIENTS

i	A_i(non)	t_i(years)	i	A_i(non)	t_i(years)
1	0.060	20	5	0.025	2,000
2	0.705	50	6	-0.009	5,000
3	-0.055	200	7	0.024	20,000
4	0.250	500			

The heat decay function is an exponential expression, fitted to data from SVEA96 spent fuel to give the normalized canister power *Q*(*t*) after 37 years of interim storage [20]. The initial canister power is assumed to be 1,700 W.

C. Semi-analytical Solution and Numerical Model

In previous sections, the method of the analytical description for the general temperature field is obtained. As for solving (2) through analytical method, this model has some serious difficulties such as the temperature field differing with time, and the boundary conditions being nonhomogeneous which make it cannot be solved directly. Nevertheless, there is a possible way of handling this problem. This paper deals with this issue with Gaussian numerical integration and has developed a Gaussian quadrature program in MATLAB that can standardize the process of the analytical solution by combining several subroutines to achieve fast and accurate calculations.

The Gaussian integral is not limited to intervals divided into equal subintervals, making this method more suitable for various problems. To integrate the first term of (6), the numerical solution can be given by the approximation with the third term of (6), where w_i, i = 1…n represents the weight. The original function f(x) can be then rewritten to

$$f(x) = W(x) \cdot g(x) \tag{5}$$

Where $g(x)$ is an approximate function and $W(x)$ is a known weighting function, giving in (6):

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} W(x)g(x)dx \approx \sum_{i=1}^{n} w_i' \cdot g(x_i) \tag{6}$$

The analytical solution is a time-dependent problem. When using the Gaussian integration, the weighting function is in the form of

$$W(x) = e^{-x} \tag{7}$$

For the simplest Gaussian integral equation (6), the weighting function is $W(x)$ = 1 and the associative polynomial is a Legendre polynomial $P_n(x)$, which gives [21]:

$$w_i = 2 / (1 - x_i^2) \cdot [P_n'(x_i)]^2 \tag{8}$$

Where w_i is the i-th root of $P_n(x)$, where $P_n(x)$ is:

$$P_n(x) = \prod_{1 \le i \le n} (x - x_i) \tag{9}$$

By changing the original interval [a, b] to [-1, 1], an approximation can be obtained as (10):

$$\int_a^b f(x)dx \approx \tfrac{(b-a)}{2} \sum_{i=1}^{n} w_i f\left(\tfrac{b-a}{2} x_i + \tfrac{b+a}{2}\right) \tag{10}$$

Because of the development of the Gaussian quadrature program for the analytical solution, it is easier to discuss the problems of different conditions. In the Gaussian quadrature program, the thermal properties can be changed and are independent of the method of the solution. It is also possible to select specific points of times and have the code resolve the answer. This is a great advantage with cases of a large timescale, such as 1,000 years or more years, the results can found in a couple of minutes, while compared to numerical analysis programs such conditions may take up to a week to resolve the solution.

III. Verification of the MATLAB Program

The heat decay functions were first combined with (2), and the numerical process for the semi-analytical solution was programmed using MATLAB code. In this section, different heat decay functions which are (3) and (4), were adopted by the authors for data comparison in two cases.

A. *Case 1: the Decay Function From* [13]

In the case 1, the authors have set up semi-analytical method for the data comparison with [13] and numerical model. Eq. 3 is adopted as the heat decay function in the case 1. The parameters which are shown in Table II, were input into the Gaussian quadrature program and FLAC^{3D} model for an analysis of 8,000 years after the canisters are put into the repository.

TABLE II: The Arrangement of Channels [13].

parameter	value	parameter	value
L	500 m	γ	1.62*10^6 m^2/s
B	500 m	Q_1	700 W
H	500 m	Q_2	250 W
D	6 m	t_1	46 years
D'	25 m	t_2	780 years
$T_{rep,0}$	15 °C	H_c	5 m
λ	3.5 W/(mK)	R_c	0.4 m
ρc	2.16*10^6 J/(m^3·K)	-	-

Where $T_{rep,0}$ is the temperature of the position of the repository, based on the assumption of [13].

In order to obtain the numerical solution for comparison, the group of the host rock was set to be homogeneous and isotropic. Also, the canisters are considered as homogeneous heat sources with the same decay function that was been displayed as (3). Notably, in the numerical model, the temperature data which has been recorded is the rock wall temperature at the mid height of the canister in the center of the repository.

The temperature increase is due to the global temperature field of the repository. The curve of time (years) and temperature increase for an analysis of 8,000 years of deposition time are shown in Fig. 3. To focus on the peak temperature the curve of an analysis of 1,000 years of deposition time is shown in Fig. 4. It can be seen that the results are in a good agreement.

For further verification, the comparisons of the vertical temperature field after 1,000, and 2,000 years of deposition time between the data from [13], the Gaussian quadrature program, and FLAC^{3D} simulation are shown in Fig. 5 and Fig. 6. To summarize the results throughout the 8,000 years of the elapsed time, the central rock wall temperature at different elapsed times are listed in Table III. The different rates are all lower than 0.1086 %, which means the Gaussian quadrature program shows significant agreement with the analytical solution and FLAC^{3D} simulation.

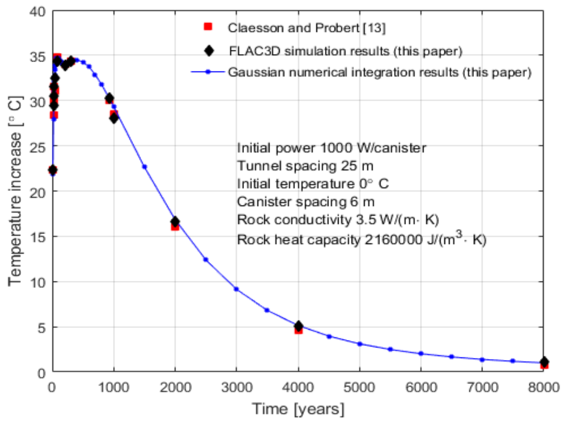

Figure 3. Comparison of the Gaussian quadrature program, FLAC^{3D}, and the analytical solution [13] of 8,000 years deposition time

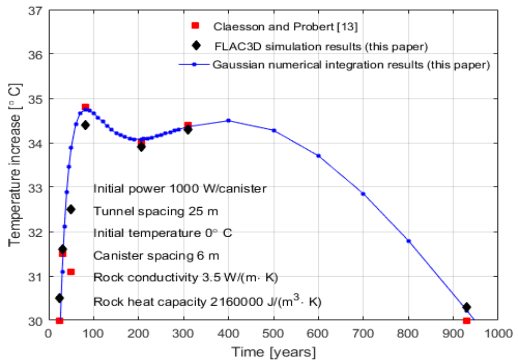

Figure 4. Comparison of the Gaussian quadrature program, FLAC^{3D}, and the analytical solution [13] of 1,000 years deposition time

TABLE III: THE COMPARISONS OF DIFFERENT ELAPSED TIMES

t (years)	Gaussian quadrature program	Claesson & Probert, [13]	Diff. rate	FLAC^{3D}	Diff. rate
10	21.8	22.3	-0.0224	22.3	-0.0224
20	27.9	28.4	-0.0176	29.4	-0.0510
25	29.7	30.0	-0.01	30.5	-0.0262
30	31.1	31.5	-0.0127	31.6	-0.0158
50	33.9	31.1	0.09	32.5	0.0431
82	34.8	34.8	0	34.4	0.0116
206	34.2	34.0	0.0059	33.9	0.0088
309	34.4	34.4	0	34.3	0.0029
930	30.2	30.0	0.0066	30.3	-0.0033
1000	29.3	28.5	0.0281	28.0	0.0464
2000	16.8	16.0	0.05	16.6	0.0120
4000	5.1	4.6	0.186	5.1	0.0000
8000	1.0	0.8	0.25	1.1	-0.0909

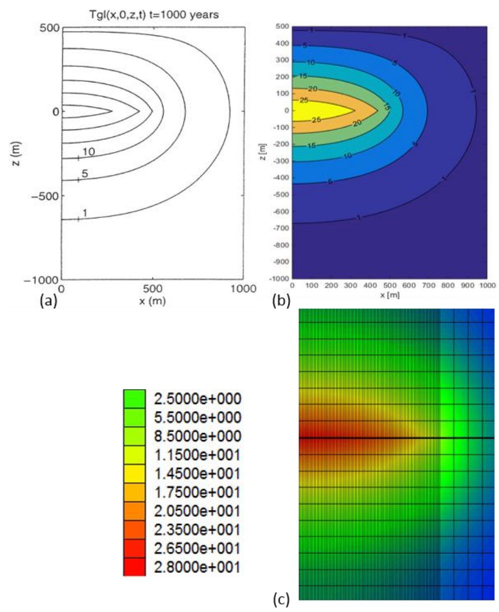

Figure 5. Comparison of the vertical temperature distribution after 1,000 years of deposition time. (a) The analytical solution [13]; (b) Gaussian quadrature program; (c) FLAC^{3D} simulation.

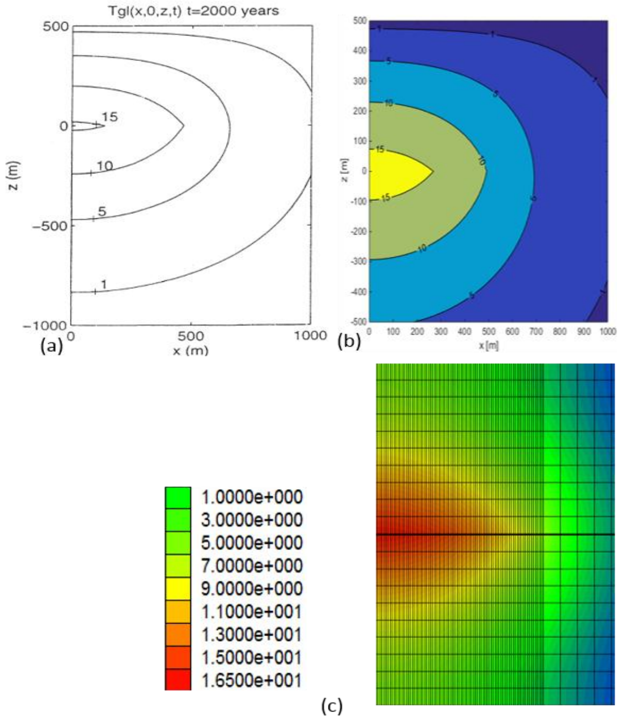

Figure 6. Comparison of the vertical temperature distribution after 2,000 years of deposition time. (a)The analytical solution [13]; (b) Gaussian quadrature program; (c) FLAC^{3D} simulation

B. Case 2: the Decay Function From [11]

In the case 2, the layout of the repository which is based on [11], was built. The repository contains 5 areas with the spacing of 70 m. Each area contains 29 tunnels with the spacing of 40 m. Each tunnel contains 41 canisters with the spacing of 6 m. The length of the tunnels is 246 m (x-axis). The length of the areas is 1,160 m (y-axis). A schematic of the repository is shown in Fig. 7.

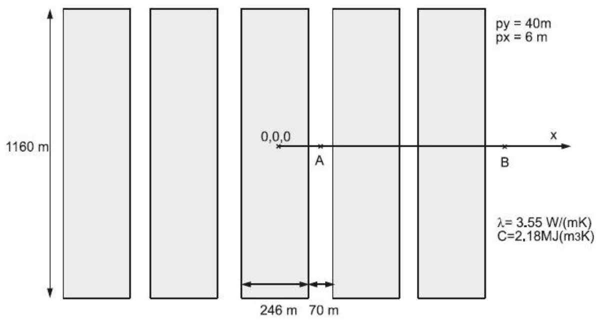

Figure 7. The top view of the layout of the repository [11].

Where line AB is the cross-section. The host rock domain was defined to be homogeneous and isotropic. The value of thermal conductivity and heat capacity of the host rock are respectively 3.55 (W/(m·K)) and 2.18 (J/m^3·K).

In the same way, the authors combined the heat decay function (4) with the analytical description for the general temperature field (2), and the calculations of the numerical process for the analytical solution were performed by executing the self-written Gaussian quadrature program in MATLAB code.

The comparisons of the data of [11] and the Gaussian quadrature program are shown in Fig. 8 and Fig. 9. The two figures show temperature increase as function of time at different points along the scan-line A on the cross section AB which is shown in Fig. 7. The legend gives the vertical distance to the repository. Similarly, the results are in a good agreement with Fig. 8 and Fig. 9. This implies that the self-written Gaussian quadrature program can deal with the analytical solution of the temperature field with different input data.

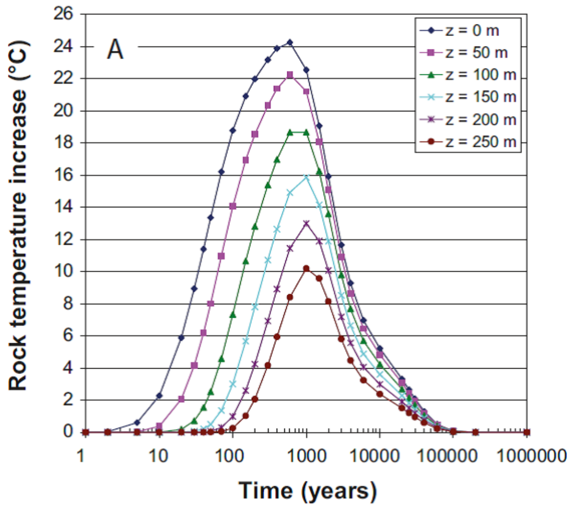

Figure 8. Temperature increase at points on scan-lines A on the cross section [11]

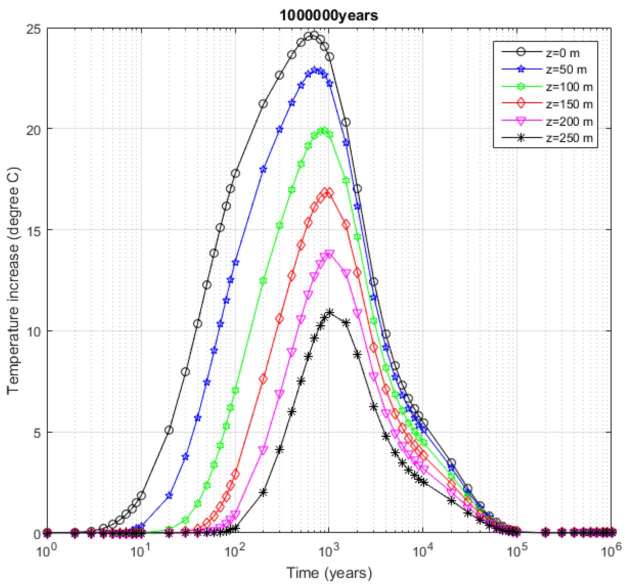

Figure 9. Temperature increase at points on scan-lines A on the cross section, made by performing the Gaussian quadrature program

The comparison of the contour of an analysis of 50 years of elapsed time is shown in Fig. 10. The comparison of the contour of an analysis of 2,000 years of elapsed time is shown in Fig. 11.

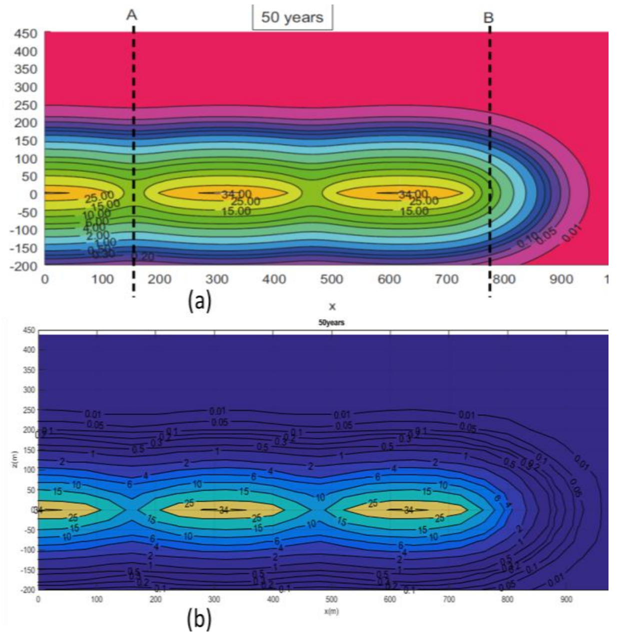

Figure 10: (a) Analytical solution of temperature for 50 years [11]. (b) Analytical solution by self-written MATLAB program.

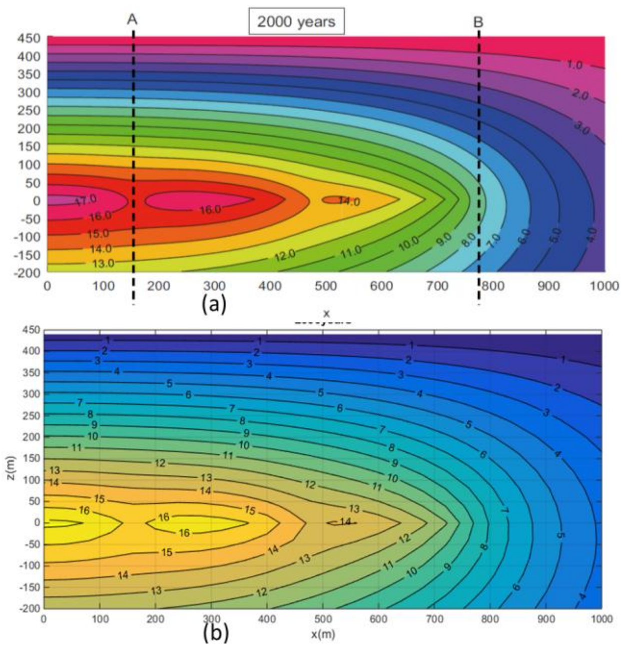

Figure 11. (a) Analytical solution of temperature for 2,000 years [11]. (b) Analytical solution by self-written MATLAB program.

IV. Conclusion

In this paper, the authors have reproduced the analytical solution which is presented by [13] through the Gaussian numerical integration process. The Gaussian quadrature program was compiled in MATLAB code. The numerical model has been built in FLAC^{3D} as well. Importantly, the data comparisons are in a good agreement with the results which are displayed in Fig. 3, Fig. 4, Fig. 8, and Fig. 9. The results confirm that the applicability of the self-developed Gaussian quadrature program for the analytical solution of the global temperature field. It should be noted that this study has been primarily concerned with the early stage of decay function (3) rather the new one (4), so the temperature increases again after 200 years for another 200 years in Fig. 4. In other words, the fluctuations of the temperature increases are controlled by the given decay function.

In the view of [11], the analytical solution is to obtain the preliminary spacing of canisters and tunnels. Overall, with the self-developed Gaussian quadrature program for the analytical solution, the relations of the tunnel spacing, the canister spacing, the thermal conductivity of the rock wall, and other parameters can be established. And having this program, the authors hope that this research can be a reference for the design of repositories and contribute to the construction of a deep geological repository in Taiwan.

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