Estimation of Nuclear Test Time in Neighboring Countries using MCMC (Markov Chain Monte Carlo) based on Radioactive Xenon Isotopic Activity Ratios

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1. Introduction

The development of nuclear threat detection technologies is increasingly necessary as it is expected that the nuclear threats will be continued in neighboring countries [1]. Among various nuclear threat detection technologies, the method of using radionuclide measurement can be utilized even for a certain period of time after a nuclear test has occurred. If one detects the xenon isotopic activity ratios, it is possible to characterize the nuclear test and particularly to discriminate the nuclear test from the xenon isotopes' release from nuclear power plants [2, 3].

The objective of this work is to develop a program which can estimate the time at which nuclear test is done assuming that the type of nuclear tests has determined. This study has focused only on the estimation of the explosion time because our current study using machine learning methods can discriminate the source of the xenon isotopes' release [4]. Specifically, we choose a probabilistic method MCMC (Markov Chain Monte Carlo) with the radioactivity decay calculations using ORIGEN code. Several tests using the MCMC program were conducted to show the possibilities that the time at which nuclear test is done can be accurately estimated. For these test cases, the ORIGEN calculation results are first used as the measured data without uncertainty. Then, the tests with consideration of measurement uncertainties are additionally conducted.

2. Computational method and Model

2.1 Computational method

To generate the xenon isotopic composition at explosion time, the depletion analysis was done using the Serpent2 continuous-energy Monte Carlo reactor physics burnup calculation code which was developed by VTT [5]. The ENDF/B-VII.r0 point-wise cross section library was used for the depletion calculations. On the other hand, to obtain the xenon isotopic change after explosion, the cooling calculation was performed using ORIGEN module in SCALE 6.2, developed at Oak Ridge National Laboratory [6].

The Serpent2 code calculates the inventory of xenon isotopes with depletion assuming uranium enrichment of 90% for uranium bomb (HEU) and 93% fissile isotopes for plutonium bomb (WGPu). It is assumed that in an underground nuclear test, all fission products are held together, resulting in the production of the full cumulative yield of xenon gas [7].

Fig. 1 describes the computational flow used in this work. In MCMC Program, an ORIGEN input is generated after sampling the explosion time based on the Gaussian distribution. After the ORIGEN calculation, the xenon isotopic activity is extracted from the ORIGEN output and the xenon isotopic activity ratios are calculated. Then, the MCMC module evaluates the likelihood (see Sec. *2.2*) and samples new cooling time based on the current cooling time. We used the Metropolis algorithm for MCMC with the Gaussian distribution for the proposal or driver distribution.

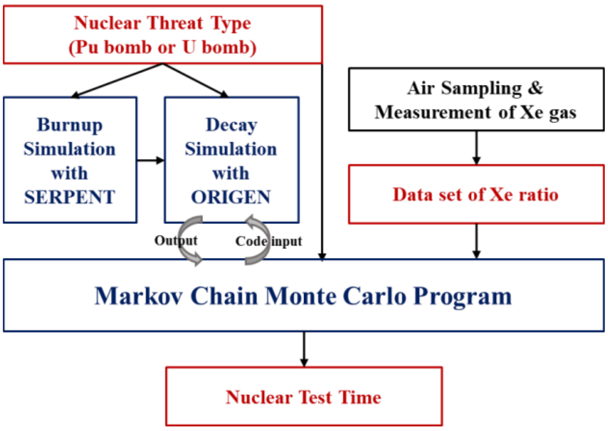


Fig. 1. Flow Chart of MCMC Program

2.2 Assumptions for MCMC Program

In this program, the following likelihood which has its maximum value when the estimated xenon isotopic activity ratios agree with the measured ones is used:

$$P(R_{53}^{mea}, R_{53m}^{mea}, R_{3m3}^{mea}|T) = exp\left[-\frac{\left(R_{53}^{mea} - \tilde{R}_{53}\right)^2}{2\sigma_{53}^2}\right] exp\left[-\frac{\left(R_{53m}^{mea} - \tilde{R}_{53m}\right)^2}{2\sigma_{53m}^2}\right] exp\left[-\frac{\left(R_{3m3}^{mea} - \tilde{R}_{3m3}\right)^2}{2\sigma_{3m3}^2}\right] \quad (1)$$

In this equation, T is the sampled explosion time, $R_{53}^{mea}, R_{53m}^{mea}, R_{3m3}^{mea}$ are measured data of the xenon isotopic activity ratios (assumed), $\tilde{R}_{53}^{mea}, \tilde{R}_{53m}^{mea}, \tilde{R}_{3m3}^{mea}$ are calculated data of the xenon isotopic activity ratios with ORIGEN module, $\sigma_{53}, \sigma_{53m}, \sigma_{3m3}$ are the standard deviations for the ratios assuming 0.1 days and

$P(R_{53}^{mea}, R_{53m}^{mea}, R_{3m3}^{mea}|T)$ is likelihood for the explosion time T.

The considered range of explosion time is 0 to 10 days with 0.01 days' interval, and sampling is performed within this range. The explosion time was sampled using a Gaussian distribution which has the current explosion T as mean and 0.1 days as standard deviation. Each measured xenon isotopic activity ratios are also assumed to have Gaussian distributions and the standard deviation of the distribution related to the measurement uncertainty.

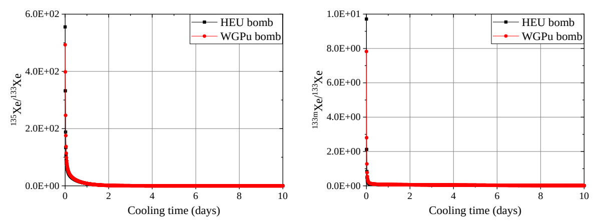
For MCMC simulation with a given initial guess of explosion time, the average of explosion time is calculated after 1000 skip cycles, considering the burn-in process. The MCMC simulation is terminated when the relative change in the average explosion time calculated with the accumulated sampled values is less than 10^{-5}. At present, the explosion time with the highest likelihood is adopted for final estimated time.

3. Results

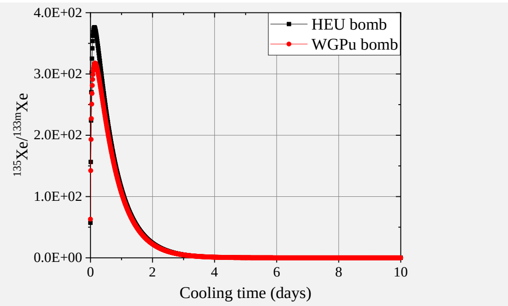
3.1 Characteristics of xenon isotopic activity ratios

Before estimating the time of explosion, we analyzed the characteristics of xenon isotopic activity ratios during nuclear tests using HEU and WGPU. In this study, only three isotopes (^{133}Xe, ^{133m}Xe, ^{135}Xe) are considered, due to difficulty in measurement of ^{131m}Xe [7].

As shown in Fig. 2, the large value in scale for a specific xenon isotopic activity ratio can result in dominant effect on likelihood calculation. Therefore, to effectively consider each of three isotopic ratios, the ratios are scaled by dividing maximum value of each one. In addition, the tendency of xenon isotopic activity ratio as the explosion time is not linear and rapidly changing, so the likelihood at a short explosion time can be very low. To use Gaussian distribution for likelihood, it is needed to correct each ratio with some scaling. Fig. 3 compares the likelihoods obtained with three different scaling methods (i.e., maximum scaling, log scaling, and maximum-log scaling). Fig. 3 shows that the likelihood with the max-log scaling has the Gaussian-like distribution as wanted.



(a) ^{135}Xe/^{133}Xe (b) ^{133m}Xe/^{133}Xe



(c) ^{135}Xe/^{133m}Xe

Fig. 2. Evolutions of Xenon isotopic activity ratios as time after explosion

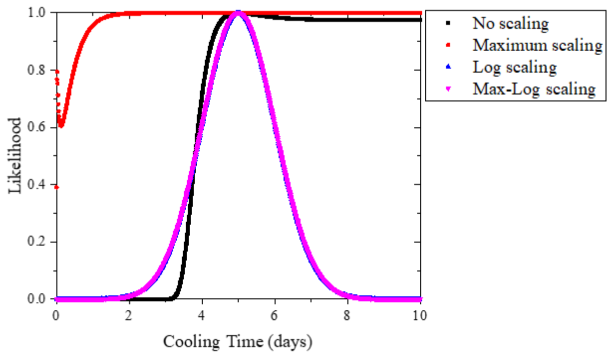


Fig. 3. Likelihood distribution with different scaling methods

3.2 Analysis without considering the measurement error

In purpose of program verification, we simulated by assuming the estimated explosion time using ORIGEN calculation is the measured value, without the measurement system error. According to Fig. 2 (c), ^{135}Xe/^{133m}Xe can have the same ratio at different points of explosion time up to 1.5 and 1.3 days, after HEU and the WGPu explosions, respectively. ^{135}Xe/^{133m}Xe has maximum value at 0.1 and 0.16 days for HEU and WGPu explosions, respectively, which is most difficult to estimate. Therefore, each time is selected as the true value on estimation.

First, for the HEU simulation, the six initial guesses of the explosion time were considered to be 0.05, 0.15, 0.5, 1.0, 5.0, and 10.0 days and the estimated explosion times were compared. As shown in Table. 1, regardless of the initial value, all the cases have the same estimated value as the true value and the likelihoods showed 1.0 at this time. The average values of the sampled values occur around 0.1 days, regardless of the initial value, and the standard deviations are smaller than 0.1 days.

Fig. 4 shows the tendency of the sampled explosion time as sampling proceeds for different the initial values in the HEU scenario. As the iterations, the sampled values approach the true value. The sampled value decreases quickly at the beginning and then, fluctuates around the true value. For all the cases, the estimated one reached to the true value within 300 iterations (i.g., samplings).

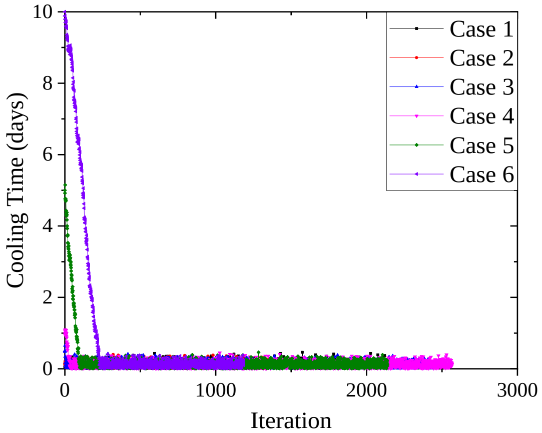


Fig. 4. The tendency of the sampled explosion time as iteration with different initial values in HEU scenario

Fig. 5 is the relative frequency distribution of the sampled explosion times in the HEU scenario, and the interval was divided by 0.1 days. We compared the Cases 1 and 6, which have the largest difference in the initial values. It is noted from Fig. 5 that the explosion times are sampled only within 0~0.5 days for Case 1 but over the entire range for Case 6. However, most of the iterations were sampled near the true value, regardless of the initial value.

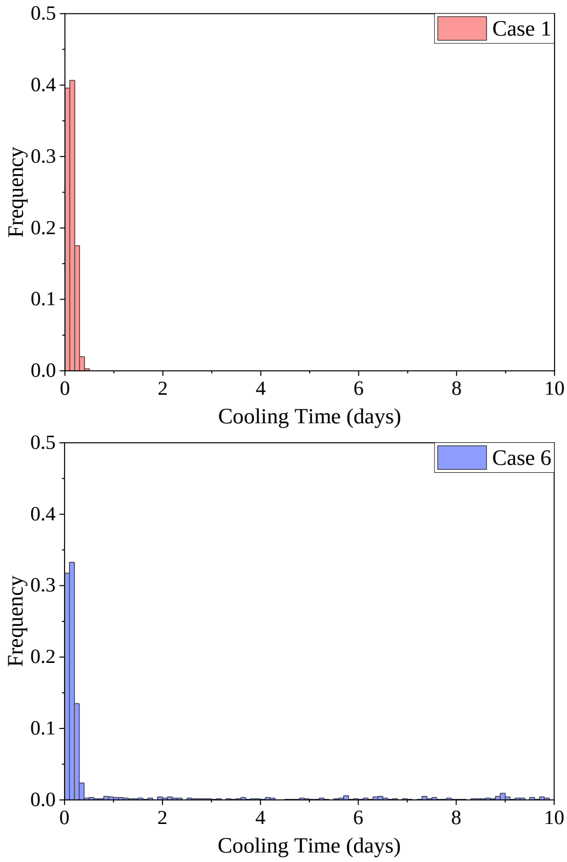


Fig. 5. The relative frequency distribution with different initial values on HEU scenario

Next, the initial explosion times was set to be 0.05, 0.15, 0.5, 1.0, 5.0, 10.0 days for the WGPu explosion and the results of estimation were compared in Table 2. Regardless of the initial value, the estimated values were same as the true values, with the likelihoods of 1.0. The average values were around 0.16 days for all the cases and the standard deviation was less than 0.1 days.

Fig. 6 shows the tendency of the sampled explosion time as iteration for the different initial values in the WGPu scenario. WGPu simulations have a similar tendency as HEU ones. The estimated value reached near the true value within 300 times, with a rapid decrease in the sampled values in the early stages.

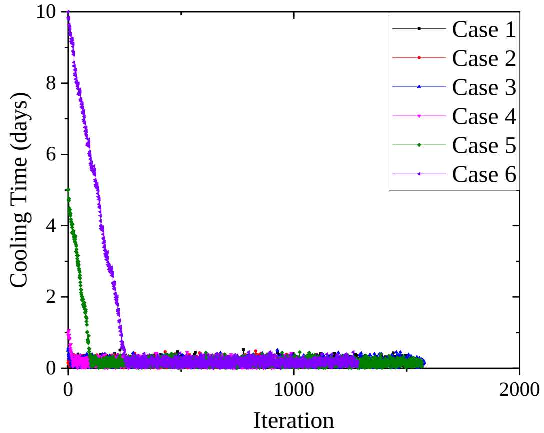
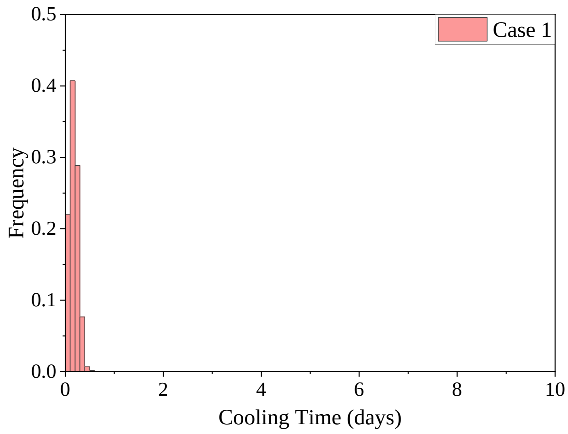


Fig. 6. The tendency of the estimated explosion time as iteration with different initial values in WGPu scenario

Fig. 7 is the relative frequency distribution of the sampled explosion times in the WGPu scenario. The distribution is divided into time interval by 0.1 days. The highest relative frequency occurred in the range of 0.1~0.2 d, including the true values.



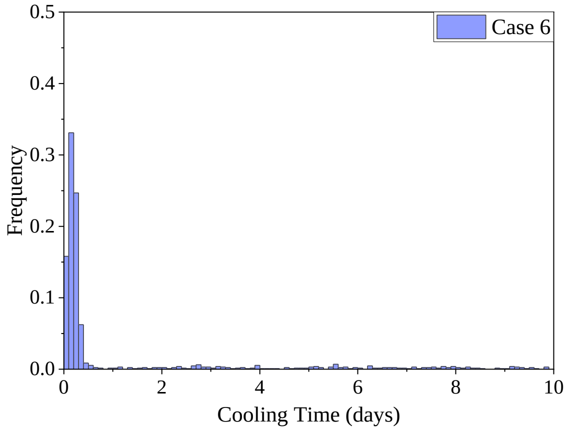


Fig. 7. The relative frequency distribution with different initial values on WGPu scenario

3.3 Analysis with considering the measurement error

Due to a measurement error occurring when collecting xenon gas, we considered the error in the true value, which is the result of ORIGEN cooling calculation, as the measured data. The simulation was performed by assuming the error following a Gaussian distribution with a standard deviation of 20%. The error was sampled at the beginning of the simulation. As in Sec. *3.2*, 0.1 and 0.16 days for HEU and WGPu scenarios were selected as true values of the explosion time. For the both HEU and WGPu scenarios, we simulated 100 times with sampling the different errors for each xenon isotropic activity ratio with 10.0 days as the initial value.

The relative frequency distribution of the sampled explosion time on the HEU simulation considering the measurement error is shown in Fig. 8. The estimated value observed around the true value and the estimation probability increases as the estimated value gets closer to the true value. The estimated value ranges between 0.06~0.14 days, with a likelihood higher than 0.96. The probability that the estimated value is the same as the true value is highest at 21%, and the probability of estimating the true value within an error range of 0.01 days (14.4 min) is 56%. The average of the estimated explosion times for HEU scenario is 0.1019 days.

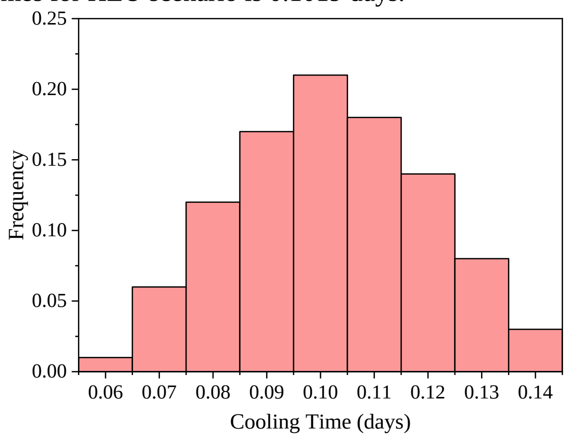


Fig. 8. The relative frequency distribution of the sampled explosion time considering the measurement error on HEU scenario

Fig. 9 shows the relative frequency distribution of the sampled explosion time on the WGPu scenario considering the measurement error. Similarly, the estimated value observed near the true value and the higher estimated probability observed closer to true value. However, it shows a wider range of the estimated explosion time, compared to the HEU case, ranging from 0.11~0.21 days. The likelihood is higher than 0.93, which indicates a high level of confidence in the estimated values. The probability of the estimated value being the same as the true value is at 16%, and the probability of estimating the true value within an error range of 0.01 days (14.4 min) and 0.02 days (28.8 min) are 43% and 66%, respectively. The average of the estimated explosion times is 0.1593 days.

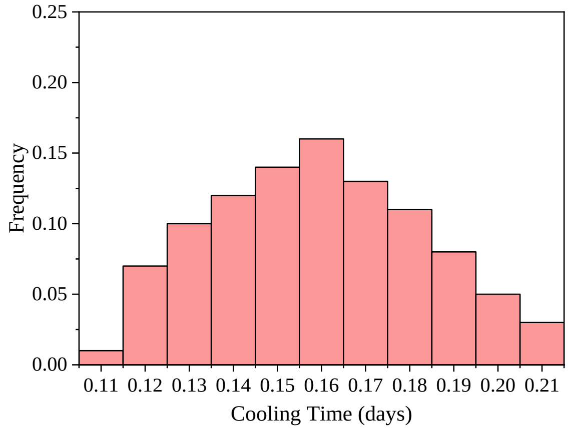


Fig. 9. The relative frequency distribution of the sampled explosion time considering the measurement error on WGPu scenario

4. Conclusions

In this work, we developed MCMC program using xenon isotopic activity ratios to estimate the time at which nuclear test is done. During every iteration with MCMC, ORIGEN calculation was performed to estimate the xenon isotopic activity ratio with the sampled explosion time. The convergence of MCMC simulation was checked based on the convergence in the average of sampled explosion times. The final result of estimated value was determined as the time giving the maximum value of the likelihood function.

First, we tested the program without considering the measurement error, for the purpose of program verification. For both HEU and WGPu bombs, the program accurately estimated the explosion time, and it was confirmed that the estimated value gradually approaches the true value as sampling proceeds regardless of the initial guess.

With consideration of 20% measurement uncertainty, we performed 100 independent simulations with sampled measured values for the both HEU and WGPu scenarios, respectively. From these simulations, it was shown that the explosion time can be estimated within 0.08 and 0.1 days for HEU and WGPu explosion, respectively.

5. Acknowledgement

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Table I. Estimated explosion times with different initial guesses (HEU)

Parameters	***Case 1***	***Case 2***	***Case 3***	***Case 4***	***Case 5***	***Case 6***
Initial guess	0.05	0.15	0.5	1.0	5.0	10.0
Number of iterations	2124	1372	2446	2567	2139	1187
Estimated value	0.1	0.1	0.1	0.1	0.1	0.1
Likelihood	1	1	1	1	1	1
Average	0.1286	0.1297	0.1217	0.1280	0.1286	0.1299
Standard deviation	0.0766	0.0756	0.0736	0.0798	0.0763	0.0817

Table II. Estimated explosion times with different initial guesses (WGPu)

Parameters	***Case 1***	***Case 2***	***Case 3***	***Case 4***	***Case 5***	***Case 6***
Initial guess	0.05	0.15	0.5	1.0	5.0	10.0
Number of iterations	1502	1125	1577	1111	1568	1284
Estimated value	0.16	0.16	0.16	0.16	0.16	0.16
Likelihood	1	1	1	1	1	1
Average	0.1706	0.1698	0.1701	0.1701	0.1608	0.1702
Standard deviation	0.0883	0.0836	0.0873	0.0779	0.0834	0.0797