Automatic Gamma Dose Rate Calculation for Radionuclides using MCNPX and ORIGEN-S

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1. Introduction

Gamma dose rate is sometimes necessary to be calculated in many applications. In the pyroprocessing activity, gamma dose rate is calculated for designing the facility with consideration of the personnel's safety. The spent fuel that is processed in the pyroprocessing facility contains a lot of radionuclides and formed in many configurations [1]. Because of that, the calculation can be messy and frail. Simple and robust method to handle the situation is needed. Herein in this paper, the difficulty is handled using the automatic processing using MCNPX and ORIGEN-S code [2, 3]. Gamma dose rate can be calculated for many configurations by using MCNPX code and many radioisotopes can be calculated by using ORIGEN-S code.

2. Method

Gamma dose rate from radionuclides is commonly calculated by using the gamma dose rate constants ($R \cdot m^2 \cdot h^{-1} \cdot C^{-1}$) for each radionuclide. Their values are usually listed in a radioisotopes handbook [4, 5, 6]. However for complicated composition and configuration, it is messy and frail to calculate the dose rate using the value from the handbook. MCNPX and ORIGEN-S code were used to get the dose rate for each radionuclide in this paper.

MCNPX code based on monte carlo method was known for its capability to calculate gamma dose rate for any configuration, including mass, density, geometry, nuclide composition, source, detector and dose function. The source definition in MCNPX can cover wide range of particles, geometry, and energy. Although MCNPX can use discrete gamma energy in the source definition, it is difficult to input all gamma energy from each radioisotopes by handmade. ORIGEN-S code was used to generate the gamma energy spectrum and source strength for each radionuclide. ORIGEN-S has the capability to apply discrete energy data and allows gamma spectra to be calculated in any energy specified group using histogram gamma energy. When the data from the library are converted to multi group yields, the gamma intensities are adjusted to conserve gamma energy release rate. The adjusted group intensity is shown in Eq. 1 [3].

$$I_g = I_a \, (E_a/E_g) \quad (1)$$

where
I_a = actual photon intensity,
E_a = actual photon energy (MeV),
E_g = mean energy of the group (MeV), and,
I_g = group photon intensity (photons per disintegration).

The method was programmed using C++ language. The program's flowchart is shown in Fig. 1. At the beginning, a radionuclide list was given to the program as an input. The list can be also taken from the depletion calculation from the ORIGEN-S. The program calls the ORIGEN-S to produce the gamma energy spectrum and source strength from the list. The spectrum and source strength are produced by a decay calculation using decay time of 10^{-9} s. The gamma spectrum is stored and used as an input for dose rate calculation by MCNPX. MCNPX can do point or volumetric source in the dose rate calculation. The dose rate was calculated using F2 tally which is the flux on a surface and was multiplied by FM card with the source strength. Flux was converted to dose rate using ICRP60 (1990) dose function.

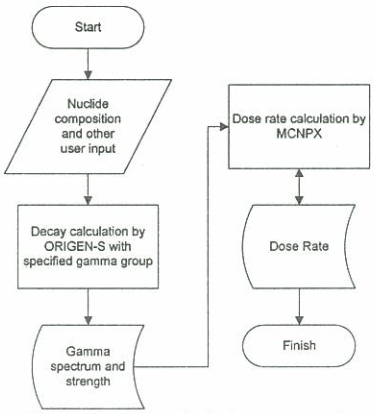

Fig. 1. Gamma dose rate calculation program flowchart

The first dose rate calculation was done for standard gamma sources which are mostly consist of two gamma discrete energy. The calculation performed to show the comparison of the MCNPX simulation with radioisotopes handbook data when the gamma discrete energy from the book was used. In the second dose rate calculation, gamma spectrum and strength calculated by ORIGEN-S were used for the standard gamma sources. The energy structures that were used are the built-in gamma ORIGEN-S gamma structures which are 18 groups SCALE and 47 groups ENDF6. The comparison with the reference is provided. The effect of energy structures that were used in ORIGEN-S to the dose rate was studied using the third dose rate calculation for some actinides. The calculation was performed to determine which group structure should be used for the dose rate calculation. For notice, all calculations were performed using point source.

3. Results

The comparison of the MCNPX simulation result and the reference for standard gamma sources is shown in Table 1. The result shows that MCNPX has a good agreement with the reference with the maximum

difference of 8.36% at Au198 case. The MCNPX calculation can be use well using the gamma discrete energy that is provided.

Table 1. First dose rate calculation

Source	Half Life	Gamma Energy (Mev)	R·m²·h⁻¹·C⁻¹		
			Reference	MCNPX	% Difference
Au198	2.696 d	0.412 - 96% 0.676 - 1.1% 1.088 - 0.23%	0.24000	0.22148	-8.36
Ba137m	2.551 m	0.662 - 90%	0.34000	0.33875	-0.37
Co60	5.271 y	1.173 - 100% 1.332 - 100%	1.29500	1.26470	-2.40
Na22	2.602 y	1.275 - 100% 0.511 - 180%	1.19000	1.13890	-4.49
Cl38	37.3 m	1.642 - 33% 2.168 - 44%	0.68000	0.67261	-1.10
Na24	15.02 h	1.369 - 100% 2.754 - 100%	1.83000	1.79260	-2.09

In the second dose rate calculation, shown in Table 2, the built-in gamma spectrums from ORIGEN-S were used and Table 2 shows that it can be use well in the dose rate calculation by MCNPX. The maximum difference is 18.89% for 18group SCALE and 24.90% for 47 groups ENDF6. The result shows that the specified group matters for the dose rate calculation of each nuclide. For some nuclides, the energy structure is suitable and not for the other. For this reason, we study the effect using the third dose rate calculation.

Table 2. Second dose rate calculation

Source	R·m²·h⁻¹·C⁻¹				
	Reference	18GrpSCALE		47GrpENDF6	
		Value	% Difference	Value	% Difference
Au198	0.24000	0.24374	1.53	0.26546	9.59
Ba137m	0.34000	0.34192	0.56	0.33572	-1.27
Co60	1.29500	1.26740	-2.18	1.28160	-1.05
Na22	1.19000	1.21060	1.70	1.21450	2.02
Cl38	0.68000	0.83836	18.89	0.90542	24.90
Na24	1.83000	1.81690	-0.72	1.85900	1.56

The dose rate value of each radionuclide is converged to a certain value when the number of group is increased. This is because the mean gamma energy within group comes closer to the true gamma discrete energy of the radionuclides. The built-in gamma spectrum from the ORIGEN-S uses a log scale so that the higher energy has wider energy range within group. This is suitable for many radionuclides that have many discrete energy at low energy and little discrete energy at higher energy. The energy group in ORIGEN-S was modified with higher number of group with linear division from 10 keV to 10 MeV. The result is shown in Fig. 2. The graph shows that using 10000 groups, which is equal 1 keV width/group, is enough to get the accuracy that is needed.

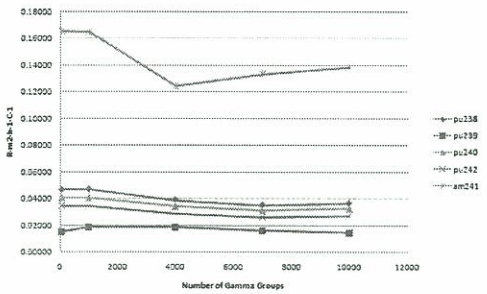

Fig. 2. Dose rate convergence from the third calculation.

4. Conclusions

Gamma dose rate calculation using MCNPX and ORIGEN code was performed and studied. The result shows good agreement with the reference. The calculation was done using point source and can be extended to volumetric source with self shielding effect. 10000 groups linear energy structure is used and shows good accuracy for any radionuclides because it equally divides the gamma energy range into groups.

5. ACKNOWLEDGEMENT

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6. REFERENCES

[1] S. D. Herrmann and S. X. Li, Separation and Recovery of Uranium Metal from Spent Light Water Reactor Fuel via Electrolytic Reduction and Electrorefining, Nuclear technology, Vol. 171, pg. 247-265, 2010.
[2] B. P. Denise, MCNPXTM User's Manual Version 2.5.0, LA-CP-05-0369, 2005.
[3] L. C. Gauld, O. W. Hermann, R. M. Westfall, ORIGEN-S: Scale System Module to Calculate Fuel Depletion ..., Oak Ridge National Laboratory, 2009.
[4] C. M. Lederer and V. S Shierly, Table of Isotopes, 7th ed. J. Willey & Son, Inc., New York (1978)
[5] NCRP report No. 58 (1978).