Comparison and Evaluation of Calculation Codes Used for Shielding Analysis of Spent-Fuel Packages

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INTRODUCTION

Transport package shielding calculations are performed to predict external dose rates from gamma rays and neutrons. In Japan, for gamma ray shielding calculations, the QAD-CGGP2 code (Cain 1977) has generally been used, and for neutron shielding calculations ANISN (Engle 1967) or DOT (Rhoades 1973) codes have been used in many cases. However, when those codes are used there are many limiting calculation conditions. QAD is a three-dimensional code which uses the point-kernel method. It is easy to treat the complex geometry problems, and the computing time is short, but it is only possible to use one build-up factor for one shielding model. ANISN is a one-dimensional code following transport theory using the discrete ordinate (Sn) method. The calculations, which include the effect of the direct ray and scattering are performed exactly but the computing time is longer and, of course, it is only available to treat one-dimensional problems. The DOT code is the same as the ANISN code except that it is a two-dimensional code.

In this study, the MARMER (Kloosterman 1990)and MCNP (Briesmeister 1991) codes, which were recently developed in The Netherlands and the United States were investigated and examined to see whether they could be used instead of the QAD and ANISN codes. The MARMER code is three-dimensional code which employs the point-kernel method. The MCNP code is a three-dimensional code using Monte Carlo methods, and it can treat any complex geometry, although the computing time is the longest of all the four previously mentioned codes.

In this paper, the calculation results obtained by using those four codes on a benchmark problem are compared with measured values from experiments. Those results are then compared and evaluated on a simulated actual multilayer packaging body wall problem.

BENCHMARK PROBLEM

Experiment

Figure 1 shows the geometrical arrangement of this experiment (Bishop et al.

1972) using a ¹³⁷Cs point source. Table 1 describes the experimental conditions, measurement method, and equipment. This experiment was performed to measure the gamma ray build-up factor on the aluminium and lead multilayer slab wall. Table 2 shows the measured build-up factors in the 21 experimental cases.

Calculation

Calculations were performed using the QAD, MARMER, ANISN, and MCNP codes on the above experimental problem using the following calculation conditions:

(1) Fine geometrical detail in QAD-CGGP2 and MARMER is modeled using the threedimensional combination geometry(CG) method.

(2) Geometry detail in ANISN is modeled as a one-dimensional slab plate.

(3) Geometry detail in MCNP is modeled in the spherical geometry.

(4) The build-up factor in QAD-CGGP2 can be chosen from the 26 materials in the user's manual. In this case the material (aluminium or lead) on the outer-most region was chosen.
(5) The build-up factor in MARMER can be chosen from three methods. One is a method to choose the material build-up factor from the material composition. Another one is a method using a revised build-up factor by the Kitazume formula (Kitazume 1965). The final method uses a revised build-up factor by the Broder formula. (Broder et al. 1962).

(6) The nuclear data library in ANISN was used for DLC-23E/CASK (ORNL-RSIC 1973) library which has 22 neutron and 18 gamma ray energy groups.

(7) The nuclear data library in MCNP is available to use the continuous energy method (for example ENDF/B VI) because of using the Monte Carlo method.

The gamma radiation dose rates were calculated at the surface on the center of the slab plate that is at the same point as an experimental measurement point. Table 3 shows the calculated build-up factors using the above four codes compared with the measured values. Figures 2, 3, and 4 compare and evaluate results for the above-mentioned four codes in 21 multilayer aluminium-lead slabs.

Discussion

The following comments can be made with regard to the above calculation results.

(1) Using the QAD code, there are cases of both under-and over-estimates compared with the measured values. The ratio of the calculated to the measured values (expressed as a percentage) is from -30% to +120%.

(2) For the MARMER code, the results using the formula of Kitazume are closest to the measured values. The results using the formula of Broder are conservative in all cases.

(3) When using the ANISN code, the results are closest to the measured values and conservative in all cases. The calculated/measured ratio is from +7% to +29%.

(4) When using the MCNP code, the results are slightly under the measurement value. The C/E range is from -22% to +6%.

ACTUAL PACKAGING PROBLEM

In this section the calculation results on a simulated actual packaging body wall problem

calculated using the above four codes are compared.

Calculation model

Figure 5 shows a one dimensional calculation model for a simulated side shielding for a packaging composed of lead and neutron shielding material.

Calculation

The gamma radiation dose rates were calculated at the surface, at 1 m and 2 m distances from the packaging mid-height using the QAD, MARMER, ANIAN and MCNP codes. Table 4 shows the gamma source conditions (source energy and strength) that simulated the gamma ray spectra from PWR spent fuel calculated by ORIGEN2 (Croff 1980) codes. Table 5 shows the atomic concentration in each material region. A one-dimensional cylinder model was used in all calculation codes. The other calculation conditions are the same as the previous experimental conditions. Figure 6 shows the results obtained by the above calculation codes.

Discussion

The calculation results show the same trends for the above benchmark problem. The following are the considerations for the above calculation results:

(1) The dose rate calculated the QAD code using the lead build-up factor is lower than the value using the iron build-up factor.

(2) The dose rate calculated by the ANISN code is lower than the value by QAD using the iron build-up factor.

(3) When using the MARMER code, the results are different between the value using outermost material build-up factor and the formulas of Kitazume and Broder. The results the formula of Broder were relatively underestimated compared with other calculation results.

(4) Using the MCNP code, the results may show the most nearly true dose rate because of the above results of the benchmark problem calculation.

CONCLUSION

This study compared the calculated gamma ray build-up factors using four shielding calculation codes (QAD, MARMER, ANISN, and MCNP) with experimental measurements. The calculated results using MARMER and MCNP were also compared with measurements. When applied to a simulated actual packaging problem, it was found that the results using MCNP agreed with the results using ANISN, and the results using QAD and MARMER were underestimated according to the build-up factor used. This work clears the application of these codes for gamma shielding calculations as well as the calculation conditions for those codes. Further studies are needed to confirm the various calculation codes for neutron shielding calculations.

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AI-Pb multilayer (51 cm x 51 cm)

Figure 1. Geometrical configuration used in measurements of dose build-up factor.



Figure 2. The comparison of relative build-up factor (C/E) with shielding thickness. (Shielding material is a single aluminium plate.) Key: (\bigcirc) QAD, (\square) MARMER. (\blacksquare) MARMER (Kitazume), (\diamondsuit) MARMER (Broder). (\blacktriangle) ANISN, (\bigtriangleup) MCNP.



Figure 3. The comparison of relative build-up factor (C/E) with shielding thickness. (Shielding material is of complex composition. The outermost material is aluminium.) Key: (○) QAD,
 (□) MARMER. (■) MARMER (Kitazume), (◇) MARMER (Broder), (▲) ANISN, (△) MCNP.



Figure 4. The comparison of relative build-up factor (C/E) with shielding thickness value. (Shielding material is of complex composition. The outermost material is lead.) Key: (○) QAD,
 (□) MARMER. (■) MARMER (Kitazume). (◇) MARMER (Broder). (▲) ANISN. (△) MCNP.

Fue	1	Void	Carbon	Lead	Carbon	Neutron shielding	Air	Carbon	Air	Air
70.2	T	1.3	3.2	12.7	6	18.5	1.0	1.5	10.5	100
70.2	t	1.3	3.2	12.7	6	18.5	1.0	1.5		10.5

Figure 5. One-dimensional calculation model using a simulated packaging shielding side body composition.



Figure 6. The comparative dose rate for results using the MCNP code on an actual packaging problem. Key: (O) QAD (Lead). (•) QAD (Iron) (□) MARMER. (•) MARMER (Kitazume). (◊) MARMER (Broder). (▲) ANISN. (△) MCNP.

Table I. Experimental conditions and measurement method.

Experimental type	Slab gamma ray penetration
Source	4 Ci ¹³⁷ Cs 662 keV gamma ray source
Material	Aluminium-lead (51 cm × 51 cm)
Geometry	Slab (one-dimension)
Instrument	LiF TLD (TLD-700, Harshaw)

Table 2. Transmission, dose build-up factors for normally incident 662 keV gamma on multi-layer Al-Pb slabs.

Case	Multi-layer combination	Dose build-up factor	
1	1.040 mfn (Al)	1.86	
2	2 080 mfn (Al)	2.97	
3	3.120 mfp (Al)	3.78	
4	1.040 mfp (Al)-1.028 mfp (Pb)	1.81	
5	1.040 mfp (Al)=2.056 mfp (Pb)	1.72	
6	1.040 mfp (A1) - 3.084 mfp (Pb)	2.16	
7	1.028 mfp (Pb)-1.040 mfp (Al)	2.34	
8	1.028 mfp (Pb)-2.080 mfp (Al)	3.40	
9	1.028 mfp (Pb)-3.120 mfp (Al)	4.62	
10	2.080 mfp (Al)-1.028 mfp (Pb)	2.30	
11	2.080 mfp (Al)-2.056 mfp (Pb)	2.19	
12	2.056 mfp (Pb)-1.040 mfp (Al)	2.77	
13	2.056 mfp (Pb)-2.080 mfp (Al)	3.82	
14	3.120 mfp (Al)-1.028 mfp (Pb)	2.60	
15	3.084 mfp (Pb)-1.040 mfp (Al)	2.84	
16	1.040 mfp (Al)-1.028 mfp (Pb)-1.040 mfp (Al)	2.80	
17	2.080 mfp (Pb)-1.040 mfp (Al)-1.028 mfp (Pb)	1.97	
18	1.028 mfp (Pb)-1.040 mfp (A1)-1.028 mfp (Pb)-1.040 mfp (A1)	3.44	
19	1.040 mfp (Al)-1.028 mfp (Pb)-1.040 mfp (Al)-1.028 mfp (Pb)	2.50	
20	1.040 mfp (Al)-2.056 mfp (Pb)-1.040 mfp (Al)	2.94	
21	1.028 mfp (Pb)-2.080 mfp (Al)-1.028 mfp (Pb)	2.56	

 $\begin{array}{l} 1.0 \mbox{ mfp (Al)} = 4.975 \mbox{ cm } (\mu = 0.201 \mbox{ cm }^{\rm 1}) \\ 1.0 \mbox{ mfp (Pb)} = 0.840 \mbox{ cm } (\mu = 1.191 \mbox{ cm}^{\rm -1}) \end{array}$

Case	Measurement value	QAD-CGGP2 code	MARMER code			ANISN	MCNP	Composition
			15	2**	3***	code	cour	numbers
1	1.86	1,19	1.14	1.14	1.14	1.09	1.05	1
2	2.97	1.30	1.23	1.23	1.23	1.08	0.95	1
3	3.78	1.56	1.43	1.43	1.43	1.22	0.99	1
4	1.81	0.84	0.76	0.93	1.29	1.04	0.91	2
5	1.72	0.99	0.91	0.95	1.43	1.24	0.96	2
6	2.16	0.86	0.80	0.81	1.22	1.11	0.93	2
7	2.34	1.63	1.56	1.16	1.20	1.11	0.97	2
8	3,40	1.72	1.59	1.29	1.34	1.17	0.91	2
-	4.62	1,79	1.69	1.46	1.51	1.21	0.87	2
0	2.30	0.74	0.68	0.97	1.66	1.07	0.86	2
11	2.19	0.85	0.78	0.87	1.80	1.19	0.91	2
12	2.77	2.11	1.94	1.09	1.16	1.11	0.92	2
13	3.82	2.17	2.04	1.38	1.48	1.21	0.90	2
14	2.60	0.72	0.66	1.09	2.14	1.18	0.88	2
15	2.84	2.89	2.76	1.32	1.44	1.25	1.06	2
16	2,80	2.09	1.93	1.93	1.46	1.21	0.94	3
17	1.97	0.86	0.80	0.80	1.50	1.15	0.87	3
18	3.44	2.39	2.29	1.21	1.58	1.17	0.81	4
19	2.50	0.69	0.69	0.90	1.71	1.12	0.89	4
20	2.94	2.81	2.65	1.29	1.67	1.29	0.92	3
21	2.56	0.73	0.68	1.00	1.85	1.13	0.78	3

Table 3. The calculated build-up factors (C/E) for a benchmark problem.

* Using the outermost region build-up factor. **Using the formula of Kitazume. **Using the formula of Broder.

Table 4. The gamma ray source strength of multi-energy groups calculated by the ORIGEN2 code.

Average energy (MeV)	Source strength (photons.s ⁻¹ per package)		
0.375	5.750 × 10 ¹⁶		
0.575	9.501 × 1016		
0.85	3.310×10^{16}		
1.25	5.316×10^{15}		
1.75	2.766×10^{14}		
2.25	3.179×10^{14}		
2.75	7.305×10^{12}		
3.5	9.234×10^{11}		
Total	1.398×10^{17}		

Table 5. The atomic concentrations in each region.

	Fuel region	Stainless steel	Carbon steel	Lead	Neutron shielding material region
11	4.07×10^{-2}		1.1.1	Sec. State	4.71 × 10 ⁻²
B10	9.02 × 10 *				3.94×10^{-4}
C					8.67 × 10 ¹
0	2.72×10^{-2}				1.60×10^{-2}
Al					3.86 × 10 *
Si					4.05 × 10 '
TI					5.94 × 10 '
Cr	1.73 × 10 '	1.65×10^{-2}			
Fe	6.45×10^{-1}	6.30×10^{-2}	8.46×10^{-2}		
Ni	7.84×10^{-4}	6.49 × 10 ⁺			
Cu					4,91 × 10 ⁻²
7.1	2.23×10^{-1}				
Pb				3.28×10^{-2}	
U	3.49×10^{-1}	1 N. + 1 1			