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NEACRP COMPARISON OF SOURCE TERM CODES FOR THE RADIATION PROTECTION ASSESSMENT OF TRANSPORTATION PACKAGES

B. L. Broadhead
Computing Applications Division
Oak Ridge National Laboratory*
P.O. Box 2008
Oak Ridge, Tennessee USA 37831-6370

H. F. Locke and A. F. Avery
Atomic Energy Establishment Winfrith
Reactor Physics Division
Dorchester, United Kingdom

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B. L. Broadhead
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, Tennessee 37831-6370
(615)576-4476

H. F. Locke
Atomic Energy Establishment Winfrith
Reactor Physics Division
Dorchester, United Kingdom

A. F. Avery
Atomic Energy Establishment Winfrith
Reactor Physics Division
Dorchester, United Kingdom

ABSTRACT

The results for Problems 5 and 6 of the NEACRP code comparison as submitted by six participating countries are presented in summary. These problems concentrate on the prediction of the neutron and gamma-ray sources arising in fuel after a specified irradiation, the fuel being uranium oxide for problem 5 and a mixture of uranium and plutonium oxides for problem 6. In both problems the predicted neutron sources are in good agreement for all participants. For gamma rays, however, there are differences, largely due to the omission of bremsstrahlung in some calculations.

I. INTRODUCTION

The Nuclear Energy Agency Committee on Reactor Physics organized a working group in 1985 to exchange information and experience on shielding calculations for the transportation of spent reactor fuel. The group's activities consisted of an intercomparison of codes for carrying out such calculations and followed the pattern of similar exercises that had been established for criticality and heat transfer assessments of fuel transport. The proposal[1] contained six theoretical benchmark problems for which participants were invited to submit results, together with the methods of the calculation employed. The problems were divided into two groups; the first four dealt primarily with the radiation transport aspects and had sources that were defined in terms of their strength and spectra, while problems 5 and 6 involved the calculation of the sources from data provided on the fuel assemblies and their radiation histories. The goals of this paper are to summarize the results obtained for problems 5 and 6 (ref. 2), and to draw conclusions from a comparison of the source calculations.

II. PROBLEMS 5 AND 6 DESCRIPTION

The novel feature of these problems is the calculation of the neutron and gamma-ray sources arising in UO_2 and a mixed-oxide (MOX) fuel for problems 5 and 6, respectively. The fuel composition (Table 1), irradiation history of the fuel assemblies (Table 2), and all necessary operational reactor data (Table 3) were provided in a problem description. Axial variation of burnup along the active length of the fuel rods was also to be taken into account. The fuel loading for both the UO_2 and MOX cases was 513.7 kg.

III. CALCULATIONAL METHODS

Two codes were used by the participants to calculate source strengths. These were FISPIN[3] (U.K.) and ORIGEN[4-7] (U.S., Italy, Belgium, Japan, and Germany), although not always the same version of the latter.

A. FISPIN Calculations

The U.K. calculations were performed using FISPIN. This code calculates the production and removal of three groups of nuclides—the fission product group, the actinide group, and the structural material group. Modes of production and removal of a nuclide are those of decay and of neutron reactions (of any type including fission). Energies and intensities of the decaying nuclides are calculated for the various modes of decay (i.e., alpha, beta, gamma rays, and spontaneous fission).

For the U.K. calculations, the actinide cross-section data were taken from a burnup-dependent library for a pressurized-water reactor (PWR) (PWRBUG28) and

Table 1. Composition of fresh fuel for problems 5 and 6

Isotope	% by weight
Problem 5	
^{234}U	0.01
^{235}U	2.86
^{236}U	0.12
^{238}U	85.15
O	11.86
Problem 6	
^{234}U	0.01
^{235}U	0.59
^{236}U	0.1
^{238}U	83.95
^{238}Pu	0.01
^{239}Pu	2.7
^{240}Pu	0.64
^{241}Pu	0.12
^{242}Pu	0.02
O	11.86

Table 2. Irradiation history[a]

Time (days)	Specific power (MW/MTU)	Burnup (MWd/MTU)
300	32.0	9.60E+03
40	0.0	9.60E+03
300	26.0	1.74E+04
40	0.0	1.74E+04
300	38.0	2.88E+04
40	0.0	2.88E+04
300	27.3	4.00E+04

[a]Cooling time was two years.

the decay data were taken from a separate library (PWRDAT4). Fission-product data were taken from the UKFPTR4 library containing UKFPDD2 decay data and CROUCH3-I fission yields.

B. ORIGEN Calculations

1. SAS2H/ORIGEN-S. The basic computational tool used by the U.S. delegation for these problems was Shielding Analysis Sequence 2H (SAS2H) of the SCALE-4.0 code system.[4] This

Table 3. Characteristics of Model Fuel Assembly

Dimensions (in cm)	
Total assembly length	445.0
Width over flats	23.0
Total rod length	393.0
Length of active zone	342.0
Length of lower rod plug	1.8
Length of bottom expansion space	31.4
Length of top expansion space	16.0
Length of upper rod plug	1.8
Height of bottom fitting	23.0
Height of top fitting	27.0
Void between bottom fitting and rod	1.0
Void between top fitting and rod	1.0
Pitch (square lattice)	1.53
Pellet outer diameter	0.969
Cladding inner diameter	1.00
Cladding outer diameter	1.15
Guide tube inner diameter	1.25
Guide tube inner diameter	1.40
Number of rod positions	225
fuel rods	210
control rods	15

sequence uses the point-depletion code ORIGEN-S to calculate burnup and decay and to produce the radiation source strengths and spectra. The SAS2H procedure uses two-part spectrum calculations (part 1 is a pin-cell model, part 2 is an assembly model) at selected times in the irradiation history to generate burnup-dependent cross sections. The burnup-dependent cross sections are then used in an ORIGEN-S calculation to predict the nuclide isotopics and radiation source strengths for a given assembly burnup and decay time.

2. ORIGEN2. The U.S. delegation also applied ORIGEN2 to problem 5 for comparison with ORIGEN-S. The ORIGEN2 and ORIGEN-S (used in SAS2H) codes use the same basic matrix exponential expansion method and numerical scheme as the original ORIGEN code.[5] The primary differences between ORIGEN-S and ORIGEN2 are the cross-section and fission-product yield data used by the two codes. At the time of these calculations, both codes

used essentially identical decay data (half-lives, branching ratios, etc.) and photon data (energies and intensities of gamma-ray and X-ray spectra). ORIGEN-S has since been updated to include ENDF/B-VI decay data.

ORIGEN2 uses burnup-dependent cross-section and fission-product yield libraries developed by performing multigroup reactor physics and depletion calculations for selected reactor models instead of carrying out such calculations for the problem-specific assembly and reactor design. These ORIGEN2 libraries include a uranium-fueled PWR using a once-through fuel cycle at a typical burnup (33 GWd/MTU) and at an extended burnup (50 GWd/MTU).[6] The average burnup for problems 5 and 6 was given as 40 GWd/MTU. The library used for problem 5 is the PWR library with extended burnup, as there is no provision for reactor problems where the burnup exceeds the library maximum. The 33-GWd/MTU burnup was also used to illustrate the differences that can be expected as a result of improper cross-section data.

ORIGEN2 calculations were also performed by the Belgium and Japanese delegates using the standard data library provided with the code for a PWR fueled with ^{235}U-enriched UO_2 and a burnup of 33 GWd/MTU. For problem 6, the ORIGEN2 cross-section library for a PWR fueled with Pu-enriched UO_2 in a self-generating Pu recycle reactor was used.

3. SAS2. Burnup calculations were also performed by the Italian delegates using ORIGEN-S in the SAS2 automatic sequence of the SCALE-3 modular system. The SAS2 sequence is an earlier version of the SAS2H sequence described above. The primary difference between SAS2 and SAS2H is the addition of the part 2 assembly model for SAS2H. SAS2 only allows for a single pin cell model in the spectrum calculations used to generate burnup-dependent cross-section libraries for use by ORIGEN-S.

4. OREST. Calculations of the source strengths were performed by the German delegates, using OREST[7] which contains the HAMMER code for fuel lattice cell simulation to derive the cross sections, and the ORIGEN code for the calculation of the inventories of actinides and fission products. OREST thus generates problem-dependent neutron fluxes during the burnup simulation. The ORIGEN code used in OREST is an enlarged version of ORIGEN-73 (ref. 5), the predecessor to both ORIGEN2 and ORIGEN-S.

IV. CALCULATIONAL RESULTS

A. Problem 5

Table 4 shows the total neutron and gamma-ray source strengths for five subassemblies. This total includes the separate contributions from spontaneous fission and α-n reactions for neutrons, and from actinides and decay fission products for gamma rays. The agreement for the neutron source is good for spontaneous fission, which provides ~98% of the total, and also for α-n reactions, except for the OREST value which is higher by a factor of ~2. This factor of 2 overprediction of α,n neutrons from actinides is a known problem with early versions of the ORIGEN and ORIGEN-S codes. The original version of ORIGEN used an analytical function to predict the neutrons produced per α decay which was shown to overpredict measured values by a factor of 2. Comparison of the individual nuclide decay rates in Table 5 shows general agreement, except for ^{243}Cm, ^{248}Cm, and ^{252}Cf which have negligible contributions to the source. These differences should be primarily due to data differences. The individual source contributions (n/decay) agree for the dominant isotope ^{244}Cm and, in general, for the other isotopes, although the OREST results have much higher values for ^{238}Pu, ^{239}Pu, ^{241}Am, ^{243}Am, and ^{243}Cm. Again, the factor of 2 overprediction is clearly seen between the FISPIN, SAS2, and SAS2H results, which used the newer measured α,n data, versus the OREST results, which use the older analytical function for α,n production.

The agreement for the total gamma-ray source is not as good, with factors as large as 2.2 between the total source strengths (in gammas/s). The results fall into two groups: the first comprised of results from SAS2, ORIGEN2-82, ORIGEN2(U.S.), and SAS2H; and the second consisting of the remaining results. The SAS2 result is ~20% lower than the others in their group due to the tabulation of photons into a different group structure. The values in Table 4 cover the entire gamma-ray energy range. Comparison over a reduced energy range of 0.4–3.0 MeV yields good agreement and suggests that the inclusion of bremsstrahlung in some libraries, which yields gamma rays with energies predominantly below 0.4 MeV, may explain the overall differences. Gamma rays with these low energies do not contribute to dose rates outside the flask. The bremsstrahlung contributions to actual dose rates were investigated, but conclusions were hampered by the lack of common group structure and lack of consistency in reported dose rates. The bremsstrahlung contribution arises from the radiative interactions in

Table 4. Problem 5: Total neutron and gamma-ray sources for five subassemblies

NEUTRONS		Spontaneous fission	α,n	Total
Country	Code	n/s	n/s	n/s
Belgium	ORIGEN2	1.38E+09	3.42E+07	1.41E+09
Italy	SAS2	1.40E+09	3.23E+07	1.43E+09
U.K.	FISPIN	1.38E+09	2.86E+07	1.41E+09
Japan	ORIGEN2-82	1.37E+09	3.27E+07	1.41E+09
U.S.	SAS2H	1.32E+09	3.07E+07	1.35E+09
U.S.	ORIGEN2[a]	1.50E+09	3.65E+07	1.54E+09
U.S.	ORIGEN2[b]	1.37E+09	3.36E+07	1.41E+09
Germany	OREST	1.35E+09	6.63E+07	1.42E+09

GAMMA RAYS		Actinides	Decay fission products	Total
Country	Code	gamma/s	gamma/s	gamma/s
Belgium	ORIGEN2	2.15E+14	5.03E+16	5.05E+16
Italy	SAS2	1.80E+14	8.15E+16	8.17E+16
U.K.	FISPIN	1.61E+15	4.76E+16	4.92E+16
Japan	ORIGEN2-82	2.18E+14	1.07E+17	1.08E+17
U.S.	SAS2H	2.16E+14	1.03E+17	1.05E+17
U.S.	ORIGEN2[a]	2.39E+14	1.09E+17	1.10E+17
U.S.	ORIGEN2[b]	2.17E+14	1.07E+17	1.07E+17
Germany	OREST	8.15E+13	5.07E+16	5.08E+16

[a]PWR-U library (33 GWd/ton).
[b]PUD50 library (50 GWd/ton).

the fuel due to energetic electrons emitted in beta decay.

Table 6 compares the contributions to the gamma-ray source from important nuclides by presenting both decay rates and source strengths in MeV per decay. The decay rates show reasonable agreement for the important isotopes ^{90}Y, ^{106}Rh, ^{134}Cs, ^{137m}Ba, ^{144}Pr, and ^{154}Eu. However, the MeV per decay values for ^{90}Y, ^{106}Rh, and ^{144}Pr show large differences. These differences have been shown to be due to bremsstrahlung. The SAS2H and SAS2 codes treat bremsstrahlung while the FISPIN code does not.

All the above results correspond to a uniform distribution of burnup along the length of the fuel assemblies. Complete results in Ref. 2 give the axial distribution of neutron and gamma-ray sources (for five subassemblies) for the entire range of burnups covering the axial variations. As above, the neutron sources from the various countries are in good agreement and show the same axial variation. The gamma-ray source strengths are again different due to the low energy contributions, but the relative strengths agree. The relative gamma source strength [i.e., the ratio of source strength to the source at mean burnup (axial peaking = 1.0)] is similar to the peaking factor for the burnup itself; however, for neutrons there is a marked difference (e.g., for a peaking factor of 1.33 the relative source is 3.37, and for 0.31 it is 0.01). This means that the axial variation of burnup cannot be treated by a linear multiplication factor to determine the variation of the neutron source.

B. Problem 6

Tables 7-8 give the source strengths and relative decay rates and yields for neutrons calculated for problem 6. The neutron source strength for MOX fuel is greater than that for UO_2 by almost a factor of 4. As for problem 5, the calculated neutron sources are in agreement, but with a ~20% variation, and the contributions from spontaneous fission and α,n reaction also agree except for the OREST result for the latter, which is again a factor of 2 higher. The decay rates and source strengths for the important nuclides show some variation apart from the dominant isotope ^{244}Cm (see Table 8).

Table 5. Relative decay rates and yields for nuclides contributing to the neutron source in UO_2

Nuclide	Mean decay rate (Bq)	U.K. FISPIN	U.S. SAS2H	Italy SAS2	Germany OREST	Japan ORIGEN2-82	U.K. FISPIN	U.S. SAS2H	Italy SAS2	Germany OREST
		Ratio of decay rate to the mean[a]					Neutron source per decay			
^{238}Pu	3.97E+14	0.97	1.04	1.10	0.88		2.60E-08	2.79E-08	2.78E-08	6.07E-08
^{239}Pu	2.84E+13	0.99	1.02	1.09	0.90		1.73E-08	1.83E-08	1.83E-08	4.21E-08
^{240}Pu	4.26E+13	1.20	1.10	1.10	0.60		1.40E-07	1.24E-07	1.26E-07	3.48E-07
^{242}Pu	2.51E+11	1.05	0.90	0.91	1.14		1.18E-05	1.19E-05	1.18E-05	1.43E-05
^{241}Am	5.10E+13	0.99	1.05	1.11	0.85		2.17E-08	2.34E-08	2.32E-08	5.40E-08
^{243}Am	2.66E+12	0.99	1.05	1.10	0.86		1.93E-08	2.07E-08	2.04E-08	5.28E-08
^{242}Cm	2.52E+14	0.96	0.96	1.05	0.92	1.11	2.05E-07	2.18E-07	2.10E-07	2.54E-07
^{243}Cm	1.35E+12	1.26	0.55	0.56	1.60		2.69E-08	3.03E-08	2.97E-08	7.60E-08
^{244}Cm	3.59E+14	1.02	0.93	1.00	0.94	1.12	3.65E-06	3.78E-06	3.73E-06	3.89E-06
^{246}Cm	9.99E+09	1.03	0.98	1.03	0.96		7.72E-04	7.61E-04	7.83E-04	8.05E-04
^{248}Cm	1.82E+05	1.01		1.53	0.45		2.62E-01		2.60E-01	2.76E-01
^{252}Cf	1.19E+07	0.45		2.10	0.45		1.16E-01		1.16E-01	1.19E-01

[a]The ratios are given relative to the mean of all calculated values for each isotope.

Table 6. Relative decay rates and yields for nuclides contributing to the gamma-ray source

	Mean decay rate (Bq)	U.K. FISPIN	Italy SAS2	U.S. SAS2H	Germany OREST	Japan ORIGEN2-82	U.K. FISPIN	Italy SAS2	U.S. SAS2H
		Ratio of decay to mean[a]					Gamma-ray source (MeV) per decay		
^{85}Kr	7.83E+14	0.99	1.00	1.00	1.00		0.06	0.01	0.00
^{90}Sr	5.79E+15	0.52	1.18	1.15	1.15			0.01	0.00
^{90}Y	6.73E+15	1.00	1.02	0.99	0.99		0.00	0.07	0.07
^{95}Zr	5.13E+13	1.14	0.96	0.95	0.95		0.73	0.74	0.74
^{95}Nb	1.14E+14	1.11	0.96	0.96	0.98		0.76	0.77	0.76
^{106}Rh	1.41E+16	0.99	0.95	0.94	0.98	1.14	0.21	0.35	0.35
^{110m}Ag	6.74E+13	1.00	1.00	0.97	1.03		2.75	2.74	2.76
^{125}Sb	5.55E+14	0.97	1.08	1.07	0.87		0.43	0.43	0.43
^{125m}Te	1.05E+14	0.55	1.40	1.38	0.66		0.01	0.03	0.04
^{134}Cs	1.16E+16	1.09	0.79	0.75	0.76	0.89	1.56	1.55	1.56
^{137}Cs	8.64E+15	0.51	1.19	1.15	1.14			0.00	0.00
^{137m}Ba	9.50E+15	1.00	1.02	0.99	0.99		0.59	0.60	0.60
^{144}Ce	1.67E+16	1.01	1.00	1.00	1.00		0.02	0.02	0.02
^{144}Pr	1.71E+16	0.98	0.97	0.97	0.98	1.09	0.03	0.15	0.14
^{144m}Pr	1.82E+14	0.62	1.09	1.10	1.19		0.00	0.01	0.01
^{154}Eu	1.11E+15	0.98	1.24	0.95	0.79	1.05	1.21	1.23	1.23
^{155}Eu	5.06E+14	1.42	0.48	1.17	0.92		0.06	0.06	0.06

[a]Ratios are given relative to the mean of all the calculated decay rates for each isotope.

Table 7. Problem 6: Total neutron and gamma-ray sources (for five subassemblies)

NEUTRONS Contributor	Code	Spontaneous fission neutrons/s	α-n neutrons/s	Total neutrons/s
Belgium	ORIGEN2	4.04E+09	9.57E+07	4.14E+09
Italy	SAS2	5.17E+09	1.02E+08	5.27E+09
U.K.	FISPIN	5.17E+09	1.01E+08	5.27E+09
Japan	ORIGEN2-82	4.65E+09	1.08E+08	4.75E+09
U.S.	SAS2H	4.86E+09	9.63E+07	4.95E+09
Germany	OREST	5.05E+09	2.24E+08	5.28E+09

GAMMA RAYS Contributor	Code	Actinides gammas/s	Decay fission products gammas/s	Total gammas/s
Belgium	ORIGEN2	6.28E+14	5.31E+16	5.37E+16
Italy	SAS2	5.60E+14	8.55E+16	8.60E+16
U.K.	FISPIN	4.45E+15	4.37E+16	4.82E+16
Japan	ORIGEN2-82	6.42E+14	1.16E+17	1.17E+17
U.S.	SAS2H	6.80E+14	1.08E+17	1.09E+17
Germany	OREST	2.87E+14	5.34E+16	5.37E+16

Table 8. Relative decay rates and yields for nuclides contributing to the neutron source in the MOX fuel

Nuclide	Mean decay rate (Bq)	U.K. FISPIN	U.S. SAS2H	Italy SAS2	Germany OREST	U.K. FISPIN	U.S. SAS2H	Italy SAS2	Germany OREST
		Ratio of decay rate to the mean[a]				Neutron source per decay			
^{238}Pu	5.92E+14	0.96	1.02	1.07	0.94	2.59E-08	2.76E-08	2.77E-08	6.09E-08
^{239}Pu	5.46E+13	0.63	1.14	1.26	0.97	1.73E-08	1.85E-08	1.85E-08	4.22E-08
^{240}Pu	1.51E+14	0.68	1.08	1.08	1.16	1.40E-07	1.28E-07	1.27E-07	1.60E-07
^{242}Pu	7.47E+11	1.38	0.78	0.75	1.10	1.18E-05	1.18E-05	1.18E-05	1.43E-05
^{241}Am	2.01E+14	0.89	1.06	1.12	0.92	2.16E-07	2.34E-08	2.32E-08	5.41E-08
^{243}Am	8.78E+12	1.22	0.98	0.98	0.82	1.92E-08	2.03E-08	2.05E-08	4.83E-08
^{242}Cm	1.20E+15	1.18	0.92	0.95	0.95	2.04E-07	2.10E-07	2.10E-07	2.55E-07
^{243}Cm	6.74E+12	1.53	0.28	0.26	1.93	2.69E-08	2.98E-08	2.96E-08	7.61E-08
^{244}Cm	1.29E+15	1.05	0.96	1.02	0.96	3.66E-06	3.73E-06	3.75E-06	3.92E-06
^{246}Cm	3.94E+10	0.72	1.04	1.15	1.09	7.71E-04	7.90E-04	7.82E-04	8.05E-04
^{248}Cm	1.14E+06	0.27	1.44	1.84	0.44	2.61E-01	2.67E-01	2.55E-01	2.77E-01
^{250}Cf	7.49E+07	0.22	1.40	1.74	0.64	2.71E-03	2.71E-03	2.73E-03	-
^{252}Cf	8.90E+07	0.04	1.61	2.02	0.33	1.16E-01	1.17E-01	1.19E-01	1.19E-01

[a]The ratios are given relative to the mean of the calculated decay rates for each isotope.

The gamma-ray sources are similar to those in problem 5 and fall into the same two groups according to whether bremsstrahlung is included. (The SAS2 result is again ~20% lower than those from SAS2H due to the group structure.) A comparison of the gamma-ray spectrum shows good agreement, for all participants, for the total source above 0.4 MeV.

VI. CONCLUSIONS

Contributions to problems 5 and 6 have been provided by six participants, and these involve the use of two codes to calculate source strengths, FISPIN and ORIGEN. Several versions of ORIGEN were used which involved different data libraries and group structures.

Calculations of total neutron source were in good agreement; however, there is some variation in the contributions from individual actinides except for the dominant isotope ^{244}Cm. This implies that there are some differences in the data used in the calculation of the buildup of actinides. The neutron sources per decay as used in FISPIN and ORIGEN-S are in general agreement for the actinides, although those for α,n events in OREST show marked differences due to known problems in the ORIGEN code. The differences in actinide production may be more significant when calculating neutron sources in fuel with irradiation and decay periods where isotopes other than ^{244}Cm are important.

Calculations of the gamma-ray source fall into two categories, those with and without bremsstrahlung. This makes a factor of 2 difference to the total source in photons/s; but if energy is considered, there is better agreement. Further comparison showed agreement between photon source strengths for the energy range 0.4 to 3.0 MeV where bremsstrahlung is not significant. Photons with energies below this threshold would not contribute to dose rates outside the flask, and, therefore, are not significant for shielding calculations; however, they could be important for energy deposition within the basket and radiolysis in water for wet flasks. There was also a 20% difference in source strength (gamma rays/s) when differing group structures were utilized. Further comparisons of the spectra from the various contributors were attempted but were hampered by the use of differing group structures.

There are small differences between results for the contributions to the gamma-ray source which cannot be explained entirely by the effect of bremsstrahlung. In general, the decay rates are similar so that the discrepancies are attributed to differences in gamma-ray yield data from the various libraries.

There are no significant differences, other than those already mentioned, in the calculated source strengths from the two methods of calculation [i.e, those which carry out detailed cell calculations to provide cross sections (ORIGEN-S and OREST) or those which use a standard library (FISPIN and ORIGEN2)].

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