Development of a One–Group Cross Section Data Base of the ORIGEN2 Computer Code for Research Reactor Applications

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ORIGEN2 전산코드를 위한 연구로용 1군 단면적 데이타베이스 개발

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Abstract

A one–group cross section data base of the ORIGEN2 computer code was developed for research reactor applications. For this, ENDF/B–IV and –V data were processed using the NJOY code system into 69–group data. The burnup–dependent weighting spectra for KMRR were calculated with the WIMS–KAERI computer code, and then the 69–group data were collapsed to one–group using the spectra. The ORIGEN2–predicted burnup–dependent actinide compositions of KMRR spent fuel using the newly developed data base show a good agreement with the results of detailed multigroup transport calculation. In addition, the burnup characteristics of KMRR spent fuel was analyzed with the new data base.

요 약

ORIGEN2 전산코드를 위한 연구로용 1군 단면적 데이타베이스를 개발하였다. 여기에는 EN-DF/B-IV와 -V가 기본 핵자료로 사용되었고 이들은 NJOY 코드시스템을 사용하여 69군으로 처리되었다. 1군 축약을 위한 가중함수는 핵연료의 연소에 따른 KMRR의 중성자 스펙트럼을 WIMS--KAERI 코드로 계산하여 사용하였다. 새로 개발된 데이타베이스는 KMRR 핵연료의 연소에 따른 악티나이드 생성량 평가를 통해 상세 다군 수송계산 결과와 잘 일치함이 입증되었다. 그리고 새로운 데이타베이스를 이용하여 KMRR의 사용후 핵연료 특성을 분석하였다.

I. Introduction

One of the most widely used point–depletion and radioactive decay computer codes to estimate the radiological contents of a spent fuel, and the resultant heat generation and radiation levels

associated with such fuel is the ORIGEN2[1]. The code was principally intended for use in predicting the characteristics of spent fuel and waste that would form the basis for the study and design of fuel reprocessing plants, spent fuel storages, shipping casks, and waste treatment and disposal facilities. The buildup and depletion of nuclides during irradiation are calculated by the ORIGEN2 code using zero–dimensional geometry and quasi–one–group cross sections developed for each fuel type/reactor model being considered. This means that the code cannot take account of spatial or resonance self–shielding effects or changes in neutron spectra other than those embodied initially. The ORIGEN2 skips the flux weighting process, and uses one–group cross sections : burnup–dependent data for important actinides and burnup–independent values for the other isotopes. These data are prveviously weighted for several standard burnup cases by external burnup program and stored on fixed data files. Due to the basic weighting procedures, the application range is restricted to the predefined burnup boundary conditions, e.g., fuel/reactor type, etc..

The ORIGEN2 code requires three different computer–readable data libraries : decay, cross section/fission–product yield, and photon. The cross section library is, therefore, dependent on reactor type, initial enrichment, and other fuel cycle parameters (e.g., specific power and both duration and number of irradiation cycles) from which it was developed. A large number of fuel/ reactor type– and operation condition–dependent data bases have been developed at Oak Ridge National Laboratory (ORNL) and released[2]-[5]. However, no data base for thermal research reactor calculations existed in the released ORIGEN2 libraries. Recently a study on actinide data base for TRIGA fuels has been attempted by I. Male et al.[6] In many cases, light water reactor models such as PWRs have been erroneously used to evaluate research reactor. In such a case, careful approach

is necessary. In order to get satisfactory results in the process of design analysis of a thermal research reactor, the reactor–dependent nuclear data base should be prepared with external computer codes using an appropriate fuel/reactor model.

The purpose of this work is to develop a new cross section data base of the ORIGEN2 code for low–enriched uranium–fueled research reactor using reasonable reactor physics computational technique. The ORIGEN2 reactor model described herein was developed to be representative of the KMRR[7] fuel behavior using a single KMRR 36–element driver fuel assembly.

The cross section processing calculations that resulted in the preparation of the master cross section library and the burnup chain model are described in Section 2. The characteristics of the burnup–dependent neutron spectrum are surveyed in Sec. 3. The methods for generating the effective and/or infinitely dilute one–group cross sections are described in Sec. 4. And in Sec. 5, the newly developed cross section data base is tested and verified.

In addition, an application of the data base to KMRR depletion was performed with the ORIGEN2 code, and the results are summarized in Appendix.

2. Preparation of Master Data and Burnup Chain

The generation of the information required for the research reactor model was begun with the processing of evaluated nuclear data files into a library of multigroup that could be used by a neutron transport code. Evaluated neutron cross sections from ENDF/B–IV[8] and –V[9] were processed into a multigroup structure of 69 neutron groups with 42 groups allowing upscattering in the thermal energy range using the NJOY code[10]. In the group averaging, a Maxwellian thermal spectrum coupled to a $1/E$ spectrum in the resonance range

which was connected to a fission spectrum in the fast region was used for weighting. The master library pepared in this work contains over 160 nuclides composing moderator, structural materials, actinides or fission–products, etc. (refer to Ref. 11 for details).

Actinide burnup chain which had been improved by adding most actinides from uranium to curium was selected from the WIMKAL–88 library[12], and fission–product burnup chain was taken from a model[13] which has been developed for KMRR. The model consists of 63 nuclides treated explicitly and one fissile–independent pseudo–element.

3. Burnup–dependent Reactor Spectrum

High burnup calculations are usually performed

for research reactor operation. In order to survey the spectrum characteristics of research reactor, burnup calculations of a KMRR driver fuel assembly were performed by using the WIMS–KAERI computer code[14] with the data and chain models mentioned in section 2. The WIMS–KAERI is an assembly design code which uses transport theory to calculate flux as a function of energy and position in the assembly. It first calculates spectra for a few spatial regions in the 69 energy groups, and uses them to condense the basic cross sections into appropriate few groups less than 69. A few group calculation is then carried out using a more detailed spatial representation. The resulting fluxes are then expanded using the spectra of the previous calculations, so that the reaction rates at each spatial point can be calculated in the 69–group structure. In addition to the basic
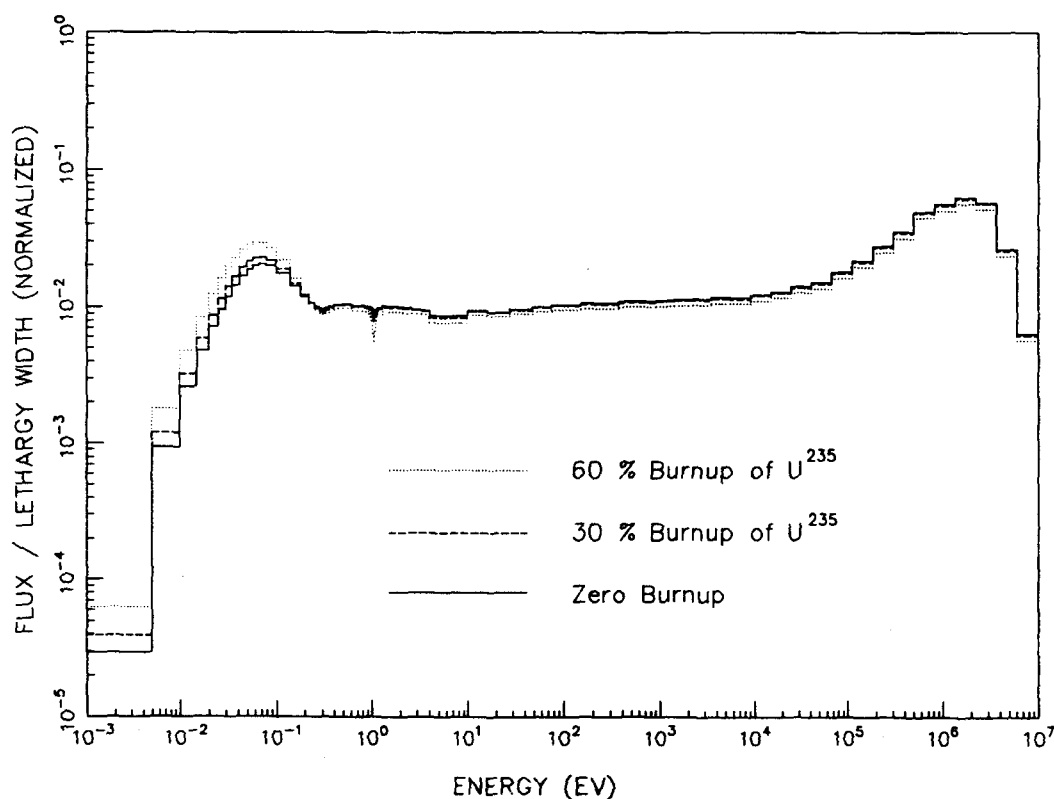

Fig. 1. Variation of Burnup–Dependent Neutron Spectra in KMRR 36–Element Fuel Assembly
36–Element

assembly calculation, the program may be used to carry out burnup calculations.

The results are given in Fig. 1. It shows variation of burnup-dependent neutron spectra in KMRR fuel assembly. The neutron spectra are softening according to the fuel depletion, and it shows a large difference between the charge and the discharge burnup.

4. Generation of One-group Data Base

4-1 Self-shielded Actinide Cross Section

One-group cross sections of the major part of actinides may be varied with burnup because of variation of burnup-dependent weighting spectrum. The cross sections near the end of irradiation are important in determining the discharge fuel composition. To reflect the burnup-dependent flux spectrum on the ORIGEN2 calculations, the effective one-group cross sections are generated for the principal actinides using the burnup -dependent weighting spectrum for KMRR.

The reactor physics computational technique employed in the preparation of the new data base for the research reactor model is the WIMS -KAERI code. WIMS-KAERI code are capable to treat consistently the resonance self-shielding of actinides, and the variation of the spectrum over time, the buildup of fission-products and transuranic nuclides. Self-shielded multigroup actinide cross sections are generated with the given nuclide concentrations for the given burnup states, with which cross sections the assembly spectrum is calculated in 69 groups.

The spectrum is used to collapse the 69-group (n, γ) and (n, f) reaction cross sections that take into account of spatial and energy self-shielding effects were generated for principal actinides at 28 burnup steps ranging from zero to 120 GWD/MTIHM. Fig. 2 shows the assembly geometry selected for this reactor model. In the WIMS-KAERI calculation, the assembly is mod-

eled to one-dimensional concentric zones, such as averaged inner, middle and outer fuel zone divided by fuel meat, cladding and moderator.
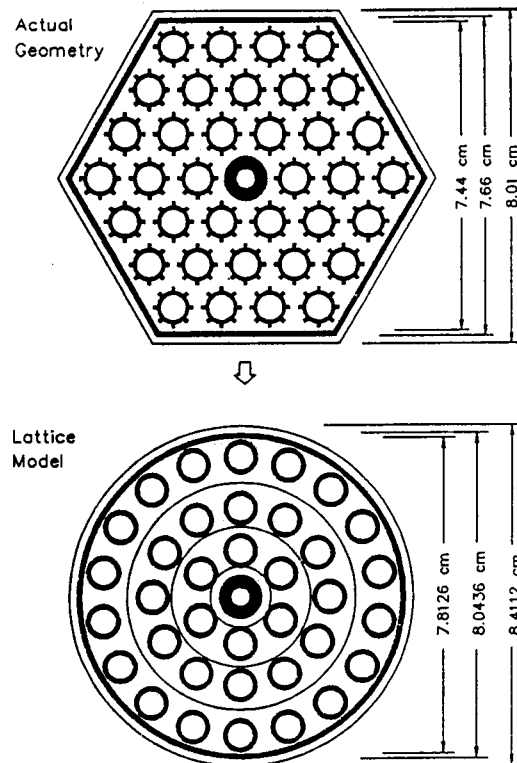
Fig. 2. 36-Element Fuel Assembly Model of KMRR

Actinide reactions of burnup-dependent one-group cross sections generated in this work are

U-234(n, γ), U-235(n, γ), U-235(n, f),
U-236(n, γ), U-238(n, γ), Np-237(n, γ)
Np-238(n, f), Np-239(n, γ), Pu-238(n, γ),
Pu-239(n, γ), Pu-239(n, f), Pu-240(n, γ),
Pu-241(n, γ), Pu-241(n, f), Pu-242(n, γ),
Pu-241(n, γ), Am-242m(n, γ),
Am-242m(n, f), Am-243(n, γ)
and Cm-244(n, γ).

The principal data having significant variation with burnup are shown in Fig. 3(a) and 3(b). These figures show large differences of one-group data between the charge and discharge burnup

step. Fission cross sections of fissile nuclides, such as U–235, Pu–239 and Pu–241 are increased over 50%, while (n, γ) reaction cross section of Pu–240 is decreased to 80% of initial value. All data show large variation at the range over the discharge burnup (33 GWD/MTIHM) of power reactors.
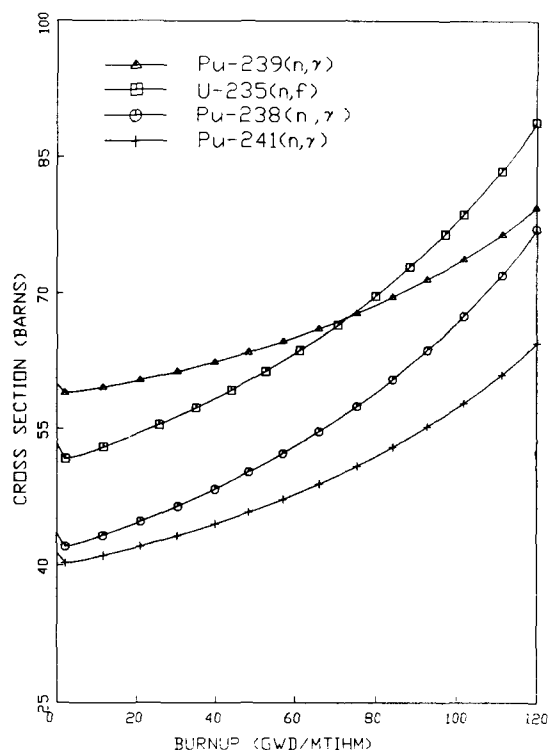

Fig. 3(a). Burnup–Dependent One–Group Cross Sections of Actinides

4–2 Infinitely Dilute Cross Section

The nuclides contained in the ORIGEN2 data bases have been divided into three segments : 130 actinides, 850 fission–products, and 720 activation products (a total of 1700 nuclides).

The infinitely dilute cross sections for all nuclides and (n, 2n) cross sections for actinides in the master multigroup data library were collapsed to one–group cross sections using a neutron spec-
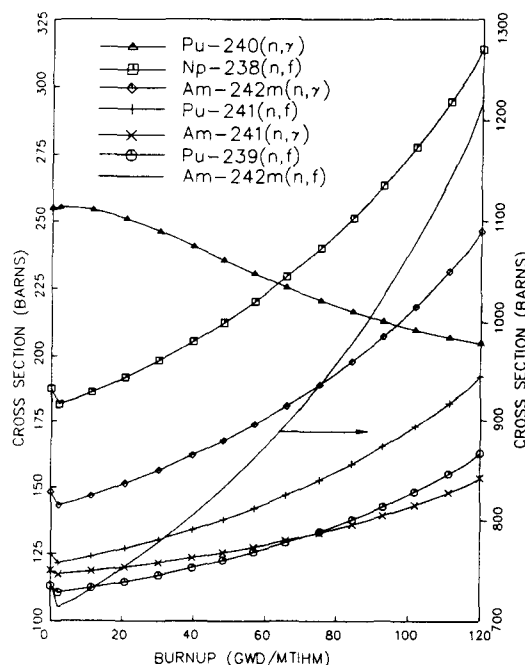
Fig. 3(b). Burnup–Dependent One–Group Cross Sections of Actinides

trum at zero burnup state. The approximately 100 fission–prduct nuclides important to reactor burnup calculations are processed in this case. Cross section data of the remaining nuclides which are not included in the master library, the fission–product yield values for the principal actinides and the energy release values were taken from the PWR model data base maintained at ORNL, without corrections. In this case the PWR model based on the burnup of 50 GWD/MTIHM and 3.2 wt % enriched UO$_2$ fuel was used.

A schematic flow diagram for the processing of the basic evaluated neutron data into 69–group master library and then the master cross sections into the burnup–dependent effective or burnup –independent infinitely dilute one–group cross sections using an auxiliary code PONECX[11] is outlined in Fig. 4.

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        (     Evaluated  Nuclear  Data  Library )
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              (   69-group Cross-Section   )
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          ( Burnup-dependent  )  (  Self-shielded    )
          ( Neutron Spectrum  )  (  Cross-Sections   )
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      (   Zero Burnup       )  (  Burnup-dependent   )
      (  Spectrum-weighted  )  (  Spectrum-weighted  )
      ( One-group Cross-Sections) ( One-group Cross-Sections)
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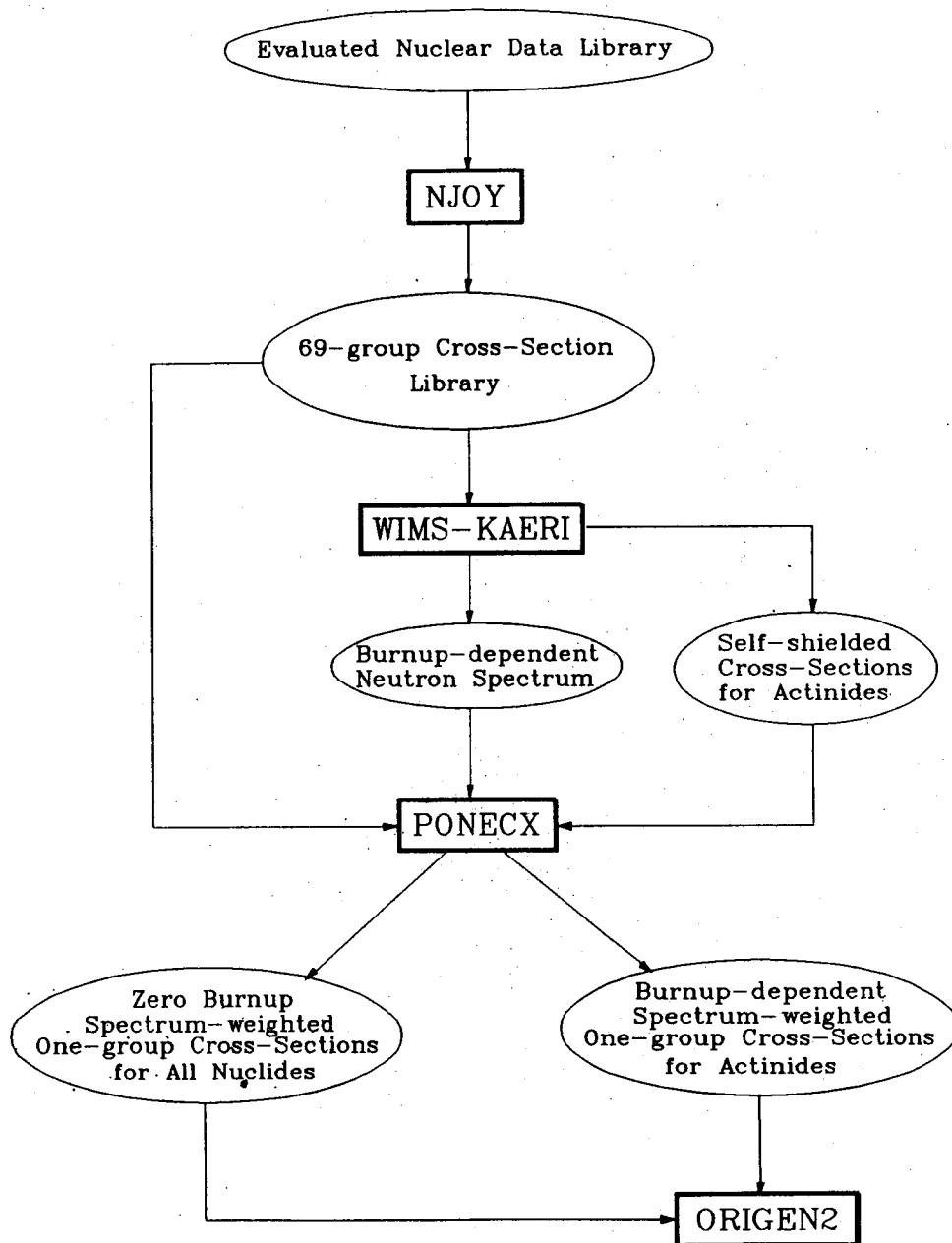
Fig. 4. Procedure for Processing ENDF/B–Formatted Libraries into ORIGEN2 Cross Section Data Base

5. Verification of New Data Base

As a test of the newly developed data base, the ORIGEN2 calculations with both the PWR and the new data bases were performed, respectively, to simulate the burnup of the KMRR fuel. The specific power in the fuel was assumed to be 428.05 MW/MTIHM and the maximum fuel burnup was taken to be 120 GWD/MITHM. The results of

these calculations were then compared with those of the detailed multigroup WIMS–KAERI code used as a reference.

The variation of actinide inventories as a function of burnup were summarized in Table 1. The PWR data base in KMRR burnup treatment gives poor estimation as expected. It is important to note that previous use of the PWR model for high burnup research reactor calculations may severely

Table 1. Comparison of ORIGEN2 Results Using Two Different Data Bases(Composition of Actinides vs. Burnup)   (Unit:Grams)

Burnup, GWD/MTIHM	Reference	Data Base used		Reference	Data Base used	
		PWR50**	NEW		PWR50	NEW
	U–235				U–236	
20	1.742+5*	−0.4***	~0.2	4.582+3	8.1	1.1
40	1.517+5	−0.9	−0.4	8.482+3	8.3	1.1
60	1.268+5	−1.6	−0.7	1.268+4	8.4	1.1
80	1.057+5	−2.6	−1.2	1.614+4	8.2	1.2
100	8.199+5	−4.3	−2.1	1.988+4	7.4	1.3
120	6.255+5	−6.1	−3.4	2.281+4	6.2	1.3
	U–237				U–238	
20	1.537+1	30.4	1.6	7.974+5	0.0	−0.0
40	2.740+1	42.2	2.0	7.949+5	0.1	−0.0
60	4.035+1	58.7	2.1	7.918+5	0.1	−0.0
80	5.233+1	82.0	2.5	7.889+5	0.1	−0.0
100	6.764+1	112.3	2.4	7.852+5	0.0	−0.0
120	8.216+1	144.5	3.5	7.818+5	−0.1	−0.1
	Np–237				Np–238	
20	3.589+1	28.2	1.3	1.681−1	33.5	2.6
40	1.266+2	34.9	1.9	6.778−1	43.2	3.4
60	2.795+2	43.0	1.9	1.678+0	57.6	3.6
80	4.521+2	53.8	2.0	3.005+0	79.8	4.1
100	6.909+2	69.1	2.0	5.278+0	111.8	4.4
120	9.236+2	83.6	1.7	8.173+0	144.9	5.9
	Np-239				Pu-238	
20	1.792+2	−15.9	0.8	7.864−1	33.5	3.4
40	1.881+2	−11.7	0.9	6.176+0	40.2	3.9
60	2.008+2	−5.2	0.8	2.305+1	49.7	3.9
80	2.144+2	3.3	1.0	5.143+1	63.4	4.1
100	2.362+2	15.4	0.7	1.052+2	85.7	4.1
120	2.632+2	27.8	2.3	1.735+2	110.9	4.2

Table 1. (continued)

	Pu–239			Pu–240		
20	1.986+3	−20.2	0.5	1.112+2	7.2	2.4
40	3.386+3	−20.1	0.4	3.465+2	10.9	1.9
60	4.454+3	−18.6	0.1	6.797+2	16.6	1.6
80	5.010+3	−16.8	−0.3	9.883+2	21.8	1.5
100	5.283+3	−13.7	−1.0	1.336+3	25.6	1.6
120	5.252+3	−9.7	−1.9	1.608+3	26.8	1.7
	Pu–241			Pu–242		
20	1.885+1	−17.3	4.9	4.179−1	−1.2	8.1
40	1.095+2	−27.2	4.1	5.259−0	−13.5	7.6
60	3.095+2	−29.4	2.9	2.666+1	−20.1	7.0
80	5.426+2	−22.5	2.1	7.041+1	−17.7	6.9
100	8.278+2	−10.5	0.7	1.643+2	−10.1	7.0
120	1.043+3	1.7	−0.4	2.941+2	−1.9	7.3
	Am–241			Am–243		
20	2.813−2	−11.8	7.5	6.750−1	12.9	2.5
40	3.157−1	−22.5	5.5	1.711−1	−2.6	0.8
60	1.374+0	−28.7	3.0	1.416+0	−11.3	−2.1
80	3.110+0	−28.4	0.8	5.143+0	−7.8	−4.4
100	5.842+0	−24.6	−1.9	1.616+1	4.2	−7.3
120	8.299+0	−20.5	−4.7	3.602+1	19.6	−9.4

*   Read as 1.742×10^5

**   Data base for PWR model using 3.2 wt % enriched UO_2 and 50 GWD/MTIHM burnup

***   Percent difference relative to the reference

underestimate the fissile plutonium (Pu–239, Pu–241) composition and overestimate the fertile plutonium (Pu–238, Pu–240) composition of the spent fuel. However, the differences resulting from the use of the newly developed data base are in a few percent. In all actinide inventories an agreement with reference ranged from satisfactory to excellent.

Table 2 shows the intercomparison of some source terms calculated using two different data bases. The source terms are radioactivity, radioactive decay heat, neutron emission rate and photon release rate. The data in Table 2 are those

of KMRR spent fuel after a five–year decay period. The discharge burnup of spent fuel is approximately 60% depletion of U–235.

The total radioactivity for spent fuel assemblies agrees within 1%. It is important to note the over-estimation of radioactive decay heat in PWR model since the design and optimization of shipping casks or storage facilities require these data. It is also notable that the (α, n) reaction in the neutron source strength increased, while the decrease in the spontaneous neutron fission value reduced the total neutron emission rate by about 4%.

Table 2. Intercomparison of Source Terms of KMRR Spent Fuel after a Five–Year Decay Period Calculated Using both PWR and New Data Bases

	PWR50**	NEW	DIFF(%)***
Radioactivity, Ci/MTIHM			
Actinides	6.492+4*	7.097+4	-8.5
Fission–Products	1.672+6	1.681+6	-0.5
Total	1.737+6	1.752+6	-0.9
Radioactive Decay Heat, Watts/MTIHM			
Actinides	1.624+2	1.150+2	41.2
Fission–Products	5.411+3	5.128+3	5.5
Total	5.573+3	5.243+3	6.3
Neutron Emission Rate, neutrons/sec/MTIHM			
(α, n)	4.541+6	3.179+6	42.8
Spontaneous Fission	2.977+7	3.241+7	-8.2
Total	3.431+7	3.559+7	-3.6
Photon release Rate, photons/sec/MTIHM			
Actinides	3.820+13	3.092+13	23.5
Fission–Products	4.486+16	4.231+16	6.0
Total	4.490+16	4.234+16	6.1

*   Read as 6.492×10^4.

**   Data base for PWR using 3.2 wt % enriched UO_2, 50 GWD/MTIHM burnup and 5 cycle model

*** DIFF=(PWR50/NEW −1)×100

6. Conclusion

A new one–group cross section data base of the ORIGEN2 computer code for a research reactor model operating on low–enriched uranium fuels has been developed.

The specific types of information are as follows :

1) 69–group neutron spectra at multiple burnups,

2) One–group, effective cross sections of principal actinides as a function of burnup and

3) One–group, infinitely dilute absorption or

(n, 2n) cross section for over 160 nuclides including the actinides at zero burnup.

By the evaluation of actinide compositions of KMRR spent fuel, it was verified that the results using the newly developed data base show good agreements with the reference values. However, further comparisons with experimental data are necessary to confirm the accuracy of new data base for research reactor calculations.

As an application of the data base, the burnup characteristics of KMRR fuel was studied and the results are summarized in Appendix.

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Appendix : Application of New Data Base to KMRR Depletion

The newly developed one-group data base with the ORIGEN2 code was applied to analyze the burnup characteristics of KMRR spent fuel. Some selected results are provided in this appendix :

1) Variation of burnup-dependent principal actinide inventories (Fig. A1(a), (b) and (c))

2) Actinide compositions of the spent fuel at discharge and after a five-year decay period (Table A1)

3) Principal fission-product radioativities of the spent fuel after a five-year decay period (Table A1)

4) Variation of decay-time-dependent radioactivity (Fig. A2) and radioactive decay heat (Fig. A3) for the spent fuel.

In general, since the data for spent fuel of power reactor are well known to us, the same kinds of PWR data as those of KMRR are added in the tables and figures for intercomparison purpose only.

Predicted values for a 36-element assembly of KMRR spent fuel (initial heavy metal : 2.474kg) after a five-year decay period are as follows :

O Fissile plutonium (g) : 15

O Fissile conservation ratio : 0.43

O Total heavy metal (g) : 2.212×10^3

O Radioactivity (Ci) : 4.334×10^3

O Radioactive decay heat (Watts) : 13

O Neutron emission rate (neutron/sec) : 8.805×10^4

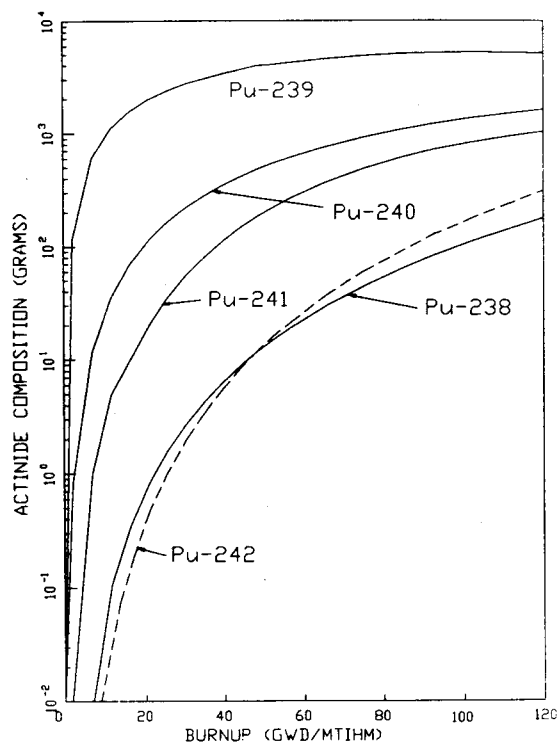O Photon release rate (photons/sec) : 1.047×10^{14}

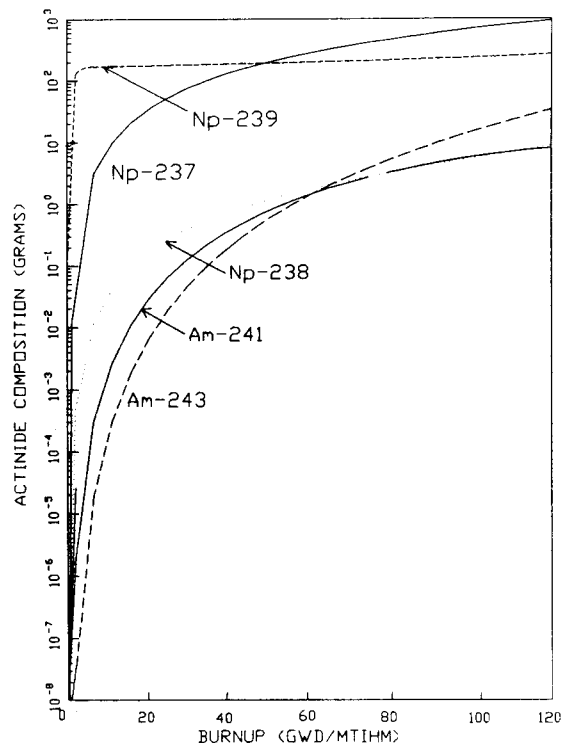**Fgi. A1(a).** Variation of Actinide Compositions vs. Burnup

Fgi. A1(b). Variation of Actinide Compositions vs. Burnup
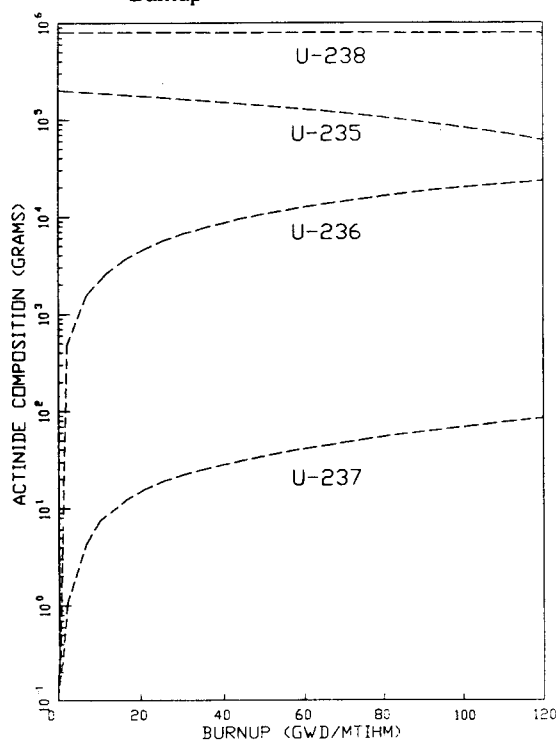

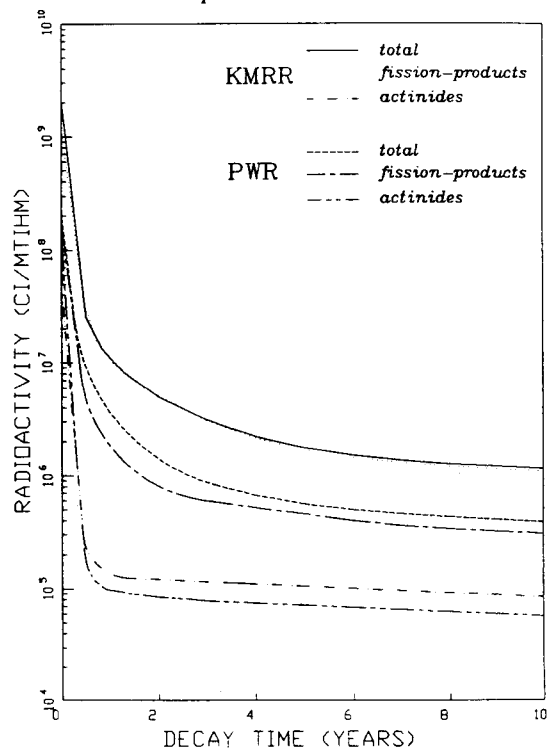**Fgi. A1(c).** Variation of Actinide Compositions vs. Burnup

Fgi. A2. Variation of Radioactivity during Decay Time

Table A1. Composition of Actinides of KMRR Spent Fuel at Discharge and after a Five-Year Decay Period

(Unit : g/MTIHM)

Actinides	At Discharge		After a 5-year Decay	
U-235	8.031+4*	(7.969+3)**	8.031+4	(7.969+3)
236	2.013+4	(3.959+3)	2.013+4	(3.961+3)
237	6.922+1	(1.110+1)	2.029-5	(2.966+5)
238	7.849+5	(9.441+5)	7.849-5	(9.41+5)
Np-237	7.045+2	(4.313+2)	7.745+2	(4.437+2)
239	2.378+2	(9.512+1)	1.295-5	(7.321-5)
Pu-238	1.094+2	(1.315+2)	1.123+2	(1.418+2)
239	5.231+3	(4.938+3)	5.469+3	(5.033+3)
240	1.357+3	(2.308+3)	1.357+3	(2.311+3)
241	8.335+2	(1.219+3)	6.552+2	(9.580+2)
242	1.757+2	(4.511+2)	1.757+2	(4.511+2)
Am-241	5.730+0	(3.255+1)	1.832+2	(2.919+2)
243	1.497+1	(8.509+1)	1.507+1	(8.519+1)
Cm-242	1.866+0	(1.475+1)	1.009-3	(8.116-2)
244	3.296+0	(2.376+1)	2.747+0	(1.963+1)

* Read as 8.031×10^4

** PWR spent fuel data using 3.2 wt% enriched UO_2 fuel, 33 GWD/MTIHM burnup and 3 cycle model for intercomparison purpose only

Table A2. Principal Fission-Product Radioactivities of KMRR Spent Fuel after a Five-Year Decay Period

(Unit : Ci/MTIHM)

Fission Product	Radioactivity		Fission Product	Radioactivity	
H-3	1.116+3*	(4.120+2)**	Cs-134	6.456+4	(2.805+4)
Kr-85	2.793+4	(6.708+3)	Cs-137	2.915+5	(9.220+4)
Sr-90	2.676+5	(6.439+4)	Ba-137m	2.758+5	(8.722+4)
Y-90	2.676+5	(6.441+4)	Ce-144	9.702+2	(1.278+4)
Tc-99	4.370+1	(1.306+1)	Pr-144	9.702+4	(1.278+4)
Ru-106	2.884+4	(1.714+4)	Pr-144m	1.164+3	(1.534+2)
Rh-106	2.884+4	(1.714+4)	Pm-147	2.091+5	(3.554+4)
Cd-113m	4.942+1	(4.408+1)	Sm-151	1.037+3	(3.130+2)
Sb-125	7.852+3	(4.062+3)	Eu-154	8.792+3	(6.920+3)
Te-125m	1.916+3	(9.911+2)	Eu-155	4.614+3	(3.186+3)
			Total	1.681+6	(4.545+5)

* Read as 1.116×10^3

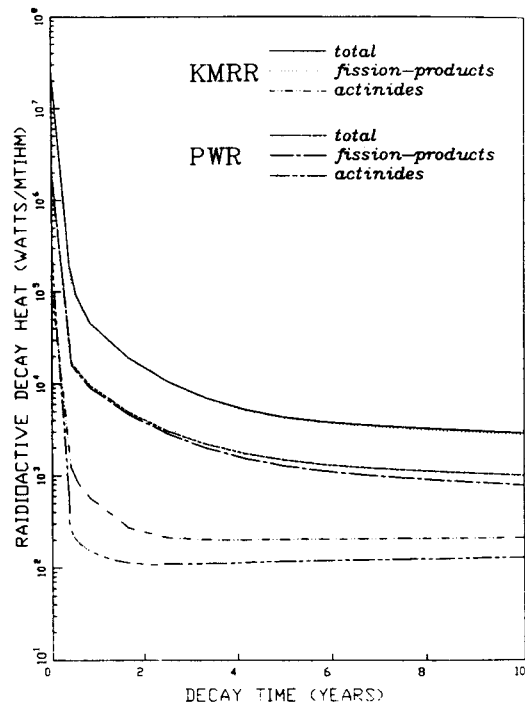** PWR spent fuel data using 3.2 wt % enriched UO_2 fuel, 33 GWD/MTIHM burnup and 3 cycle model for intercomparison purpose only

Fig. A3. Variation of Radioactive Decay Heat during
Cooling Time