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Validation of Integrated Burnup Code System SWAT2 by the Analyses of Isotopic Composition of Spent Nuclear Fuel

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This paper provides validation results of SWAT2, the revised version of SWAT, which is a code system combining point burnup code ORIGEN2 and continuous energy Monte Carlo code MVP, by the analysis of post irradiation examinations (PIEs). Some isotopes show differences of calculation results between SWAT and SWAT2. However, generally, the differences are smaller than the error of PIE analysis that was reported in previous SWAT validation activity, and improved results are obtained for several important fission product nuclides. This study also includes comparison between an assembly and a single pin cell geometry models.

KEYWORDS: SWAT2, Continuous Energy Monte Carlo Code, MVP, ORIGEN2, Burnup Calculation, Validation, Post Irradiation Examination

1. Introduction

Estimation of isotopic composition of spent nuclear fuel is crucial for taking burnup credit into account for criticality safety evaluation. The Japan Atomic Energy Research Institute (JAERI) has developed the burnup code system SWAT[**1**] for burnup credit applications and associated regulations. The code evaluates composition of approximately a thousand isotopes by using the neutron transport calculation code SRAC95 [**2**] and the point burnup calculation code ORIGEN2.1 [**3**] with data libraries based on JENDL-3.2 [**4**] and the second version of the JNDC FP library [**5**]. The experimental results of post irradiation examination, carried out at JAERI, were analyzed by using the SWAT code system. The analysis results showed good generally agreement with the experimental data, but some fission products such as samarium isotopes, had clear difference between calculation and experimental data. [**6**]

A problem of SWAT is to make generic analysis model to treat multi-dimensional geometry system for using ultra fine group resonance absorption routine. For future burnup credit analysis, burnup calculation for whole fuel assembly would be essential to evaluate k_{eff} difference by burnup and isotope distribution within the fuel assembly. To overcome the problem, SWAT2 [**7**], the improved version of SWAT, has been developed to incorporate MVP [**8**], a continuous energy Monte Carlo Code, into SWAT. By this development, SWAT2 enables us to treat complicated geometry using neutron flux evaluated by MVP, effective one group cross section data and detailed burnup chain model in ORIGEN2. Since output of ORIGEN2 can contain not only the amount of isotopes but also activities and decay heat generation information, SWAT2 has a possibility to evaluate such parameters using a function of a continuous energy Monte Carlo code. This fact may have another importance for safety evaluation purpose.

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In the previous report [**7**], the general confirmation of the function of SWAT2 was conducted by the analysis of depletion calculation benchmarks [**9**,**10**] of OECD/NEA. In this study, comparison with experimental data obtained in post irradiation examination (PIE) [**6**] will be conducted. The results using single pin-cell model in previous analyses [**6**] and using assembly model calculations are compared.

2. Calculation flow of SWAT2 [7]

The analysis flow of SWAT2 is show in **Figure 1**. Instead of SRAC95 code, MVP, a continuous energy Monte Carlo Code, is driven by SWAT2. For each burnup step, the neutron spectrum and effective multi group cross section are evaluated by MVP, then the LIBMAK routine is called to read tally file of MVP calculation. It makes the one-group cross section data file for the ORIGEN2.1. For cross section data that are not included MVP library, infinite dilution cross sections stored in the SWAT library are condensed by the neutron flux of MVP. Fission yield data of ^{233}U, ^{235}U, ^{239}Pu, and ^{241}Pu for thermal neutrons, decay constants and branching ratios for FP are taken from JNDC FP library second version. Using the library prepared by LIBMAK, a one-step burnup calculation by ORIGEN2.1 is carried out. Then, the TABMAK routine makes input files for MVP or SRAC95 and ORIGEN2.1 using the geometry data and burnup calculation results. Up to the final burnup, that procedure is repeated in every burnup step.

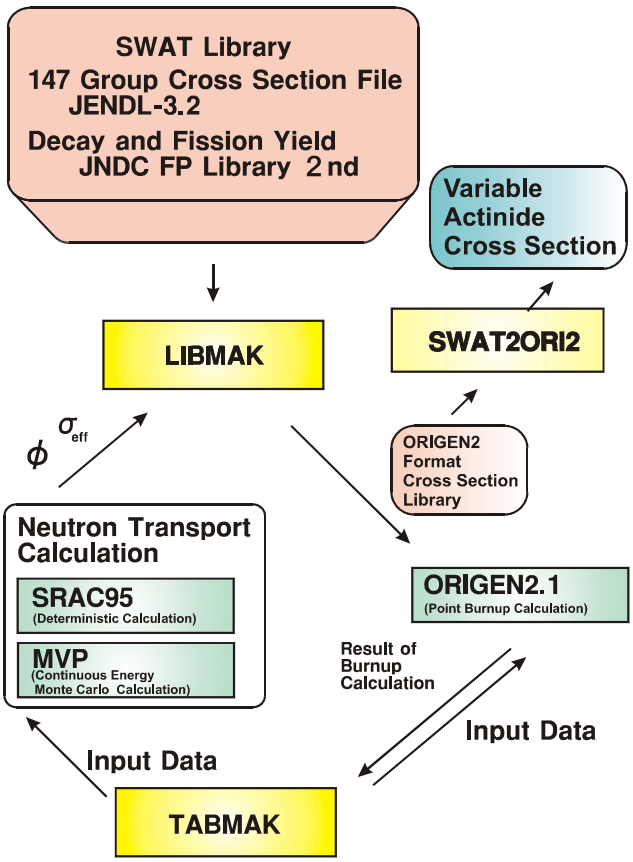

Figure 1 Calculation Flow of SWAT2 [**7**]

3. PIE Analyses

3.1 Single Pin-cell Model

For comparison, we selected three PIE data of PWR measured at JAERI and conducted analysis using the same geometrical description based on the single pin-cell model used in previous analysis with SWAT. [**6**] In **Table 1**, specifications of selected PIE samples from Takahama-3 PWR are shown. These samples were selected because they had highest burnup values in each sample series, SF95, SF96 and SF97. The geometry model data are shown in **Table 2** and **Table 3**. The temperatures of fuel and clad regions were 900K and 600K, respectively. The temperature of coolant region was estimated based on the idea that the increment in the coolant temperature was in proportion to the integral power at the sample position from the bottom of the active fuel region. The power history and boric acid concentration was compiled and shown in the reference. [**1**] In this analysis, neutron history for MVP calculation was 1,000,000 neutrons (5,000 neutrons for one batch, total batch number was 250 and initial 50 batches were discarded). Total calculation time was 25 hours for the case of SF95-4, which had 20 burnup steps using HP j6700 server (2 CPUs of PA-8700; 750 MHz; no parallel calculation) under HP-UX11i operating system.

Table 1 Specifications of selected PIE samples from Takahama-3 PWR [**6**]

Sample Name	SF95-4	SF96-4	SF97-5
Assembly Name	NT3G23	NT3G23	NT3G24
^{235}U Enrichment (%)	4.1	2.6%*	4.1
Burnup (GWd/t)	36.69	28.91	47.25
Sampling position (mm) from bottom of active length	1646	1671	881
Coolant temperature (K)	570.40	570.82	559.14

* 2.6%UO_2-6%Gd_2O_3

Table 2 Cell Geometry Data for SF95-4 and SF97-5 Analyses [**6**]

Region	**Radius (cm)**
Fuel (UO_2)	0.4025
Clad	0.475
Coolant	0.739716

Table 3 Cell Geometry Data for SF96-4 Analysis [**6**]

Region	**Radius (cm)**
Fuel (UO_2 -Gd_2O_3)	0.4025
Clad	0.475
Coolant	0.739716
Coolant	1.339091
Clad	1.421260
Fuel (UO_2)	1.729745
Clad	1.794111
Coolant	2.122887
Coolant	2.597006
Clad	2.682922
Fuel (UO_2)	3.128925
Clad	3.200594
Coolant	3.532930
Coolant	4.000900
Clad	4.085052
Fuel (UO_2)	4.500199
Clad	4.575176
Coolant	4.945487

In **Table 4**, the results of analysis using SWAT and SWAT2 are compared. SWAT2 calculation results are comparable with the SWAT calculation results. Generally, plutonium calculation results of SWAT2 are smaller than those of SWAT. However, the differences between the results of SWAT and SWAT2 are less than five percents, which were reported errors for PWR PIE data analysis [**1**]. For curium isotopes, SWAT2 results are larger than SWAT. This may result from the increased amount of ^{243}Am in the SWAT2 analysis

For fission products, generally, almost same or improved results are obtained. Especially, results of ^{149,150,152}Sm are improved.

For ^{125}Sb and ^{106}Ru, the large differences of calculation from experimental values result from a problem in the destructive experiment, such as sample dissolution in HNO_3. [**11**] Similarly, ^{142}Nd calculation results have large differences from experimental results. For this isotope, the problem of reliability of the experimental data was informed. [**12**]

^{152}Sm and ^{154}Eu show relatively large differences between SWAT and SWAT2 calculations. It was reported that the differences in calculation result of these isotopes were based on the mutual shielding effect between ^{152}Sm and ^{238}U. [**13**] For ^{148}Sm, SWAT2 and SWAT have large difference of more than 10%. **Table 5** compares the one-grouped capture cross sections related to ^{148}Sm generation. It is understood that the increase in ^{148}Sm, ^{148}Pm and ^{148m}Pm capture cross sections and the decrease in the capture cross sections of ^{147}Pm results in the difference of ^{148}Sm calculation results, instead of the increase in ^{147}Sm capture cross section. However, since the capture cross section of ^{148}Sm is small and the result of ^{149}Sm that has large capture cross section was improved, the difference of ^{148}Sm would not be

so important from the viewpoint of practical burnup credit application.

Table 4 C/E values for SF95-4, SF96-4 and SF97-5 samples by the analysis using SWAT and SWAT2 based on Single Pin Cell Model

	SF95-4			SF96-4			SF97-5		
	SWAT	SWAT2	Difference (%)	SWAT	SWAT2	Difference (%)	SWAT	SWAT2	Difference (%)
& ^{234}U	1.181	1.182	0.10	1.039	1.053	1.36	1.002	1.002	-0.04
& ^{235}U	1.015	1.001	-1.34	1.014	1.032	1.75	1.002	0.976	-2.62
^{236}U	0.950	0.956	0.64	0.948	0.951	0.36	0.949	0.957	0.86
& ^{238}U	1.000	1.001	0.07	1.001	1.001	0.03	1.001	1.002	0.08
^{237}Np	No Data	No Data	No Data	1.478	1.337	-9.52	0.938	0.884	-5.74
& ^{238}Pu	0.877	0.848	-3.36	0.814	0.745	-8.53	0.798	0.772	-3.25
& ^{239}Pu	1.009	0.980	-2.83	0.982	0.954	-2.89	1.007	0.975	-3.17
& ^{240}Pu	1.014	0.985	-2.90	0.971	0.992	2.19	1.027	0.997	-2.94
& ^{241}Pu	0.966	0.956	-1.07	0.968	0.957	-1.17	0.964	0.946	-1.87
& ^{242}Pu	0.936	0.941	0.50	0.943	0.971	2.99	0.940	0.941	0.09
& ^{241}Am	1.559	1.530	-1.86	1.057	1.072	1.46	1.087	1.052	-3.19
^{242m}Am	0.744	0.777	4.41	0.701	0.733	4.59	0.712	0.731	2.65
^{243}Am	0.918	0.941	2.49	0.917	0.923	0.67	0.877	0.898	2.36
^{242}Cm	0.532	0.536	0.77	0.769	0.789	2.59	1.190	1.188	-0.18
^{243}Cm	0.629	0.633	0.69	No Data	No Data	No Data	0.655	0.650	-0.79
^{244}Cm	0.761	0.816	7.27	0.778	0.777	-0.17	0.732	0.782	6.87
^{245}Cm	0.787	0.869	10.48	No Data	No Data	No Data	0.754	0.824	9.28
^{246}Cm	0.685	0.777	13.43	No Data	No Data	No Data	0.629	0.712	13.24
^{247}Cm	No Data	No Data	No Data	No Data	No Data	No Data	0.592	0.663	12.04
* ^{142}Nd	0.834	0.795	-4.69	No Data	No Data	No Data	No Data	No Data	No Data
# ^{143}Nd	0.974	0.970	-0.43	0.962	0.958	-0.46	0.990	0.981	-0.89
^{144}Nd	0.955	0.961	0.60	0.900	0.899	-0.07	0.952	0.959	0.76
# ^{145}Nd	1.006	1.007	0.15	0.999	1.001	0.23	1.019	1.020	0.14
^{146}Nd	0.989	0.989	-0.05	0.970	0.963	-0.68	0.982	0.982	-0.01
^{148}Nd	0.997	0.997	0.03	0.991	0.989	-0.21	1.008	1.009	0.06
^{150}Nd	0.975	0.973	-0.25	0.977	0.977	0.04	1.001	0.999	-0.22
^{137}Cs	0.978	0.978	0.03	1.033	1.034	0.06	0.989	0.989	0.03
^{134}Cs	0.887	0.893	0.68	0.949	0.897	-5.44	0.896	0.908	1.29
^{154}Eu	0.764	0.849	11.19	1.241	1.271	2.41	0.779	0.856	9.85
^{144}Ce	1.044	1.047	0.32	1.142	1.143	0.07	1.075	1.078	0.26
* ^{125}Sb	2.548	2.536	-0.47	1.631	1.641	0.59	1.304	1.299	-0.42
* ^{106}Ru	1.260	1.257	-0.28	1.450	1.460	0.70	1.795	1.796	0.03
# ^{147}Sm	No Data	No Data	No Data	No Data	No Data	No Data	1.023	1.034	1.06
^{148}Sm	No Data	No Data	No Data	No Data	No Data	No Data	1.032	0.907	-12.08
# ^{149}Sm	No Data	No Data	No Data	No Data	No Data	No Data	0.960	1.007	4.93
# ^{150}Sm	No Data	No Data	No Data	No Data	No Data	No Data	0.955	1.004	5.18
^{151}Sm	No Data	No Data	No Data	No Data	No Data	No Data	0.933	0.923	-1.10
# ^{152}Sm	No Data	No Data	No Data	No Data	No Data	No Data	1.265	1.075	-14.98
^{154}Sm	No Data	No Data	No Data	No Data	No Data	No Data	0.971	0.970	-0.13

* Results for reference purpose because of the problem of experimental data.

& Selected actinides that are included for the criticality safety evaluation in a guide introducing burnup credit, preliminary version [**14**]

One of the fission products that could be included for the criticality safety evaluation in a guide introducing burnup credit, preliminary version [**14**]

Table 5 Comparison of one-grouped Capture Cross Section (barn) Concerning to ^{148}Sm Generation (SF97-5, final burnup step)

	SWAT	SWAT2	SWAT2/SWAT
^{147}Pm	4.98E1	4.78E1	0.96
^{148}Pm	1.80E2	1.89E2	1.05
^{148m}Pm	2.26E3	2.36E2	1.04
^{147}Sm	2.30E1	2.51E1	1.09
^{148}Sm	1.57	1.63	1.04

3.2 Assembly Model

By introducing MVP control option into the SWAT2 code, analysis of PIE data became possible using a detail geometry description. We analyzed SF95-4 samples data using assembly geometry. **Figure 2** shows the geometry description for MVP calculation. In this analysis, the neutron history for MVP calculation was 600,000 neutrons (6,000 neutrons for one batch, total batch number was 120 and initial 20 batches were discarded). Total calculation time is 64 hours for the case of SF95-4, which has 38 burnup steps using HP j6700 server (2 CPUs of PA-8700; 750 MHz; no parallel calculation) under HP-UX11i operating system.

Figure 3 is a view graph of neutron multiplication factor against averaged burnup of the fuel assembly. We plotted error bars of 3σ in the figure but they are hidden in the bullets. **Table 6** shows the C/E values for analyses of SWAT2 single pin cell and assembly models. Since the amounts of fissile isotopes have larger differences, it is understood that the neutron spectrum is different from the case of the single pin-cell model. However, the differences among the geometry models are around five percent for many uranium and plutonium isotopes. The C/E values of curium isotopes of assembly model are improved than those by single pin cell model. It results from the difference of parent isotopes such as ^{242}Pu and ^{243}Am because of the change of the neutron spectrum field during the irradiation, mentioned above.

It should be mentioned that the difference of ^{148}Nd calculation result between two models is larger than one percent, even thought it is within the estimated error of the burnup measurement by ^{148}Nd method. [**15**] One of the reasons of this difference is a change in the effective fission yield of ^{148}Nd because the burnup value of the sample was estimated using the effective fission yield considering fission ratio of ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu for single pin cell model. [**6**]

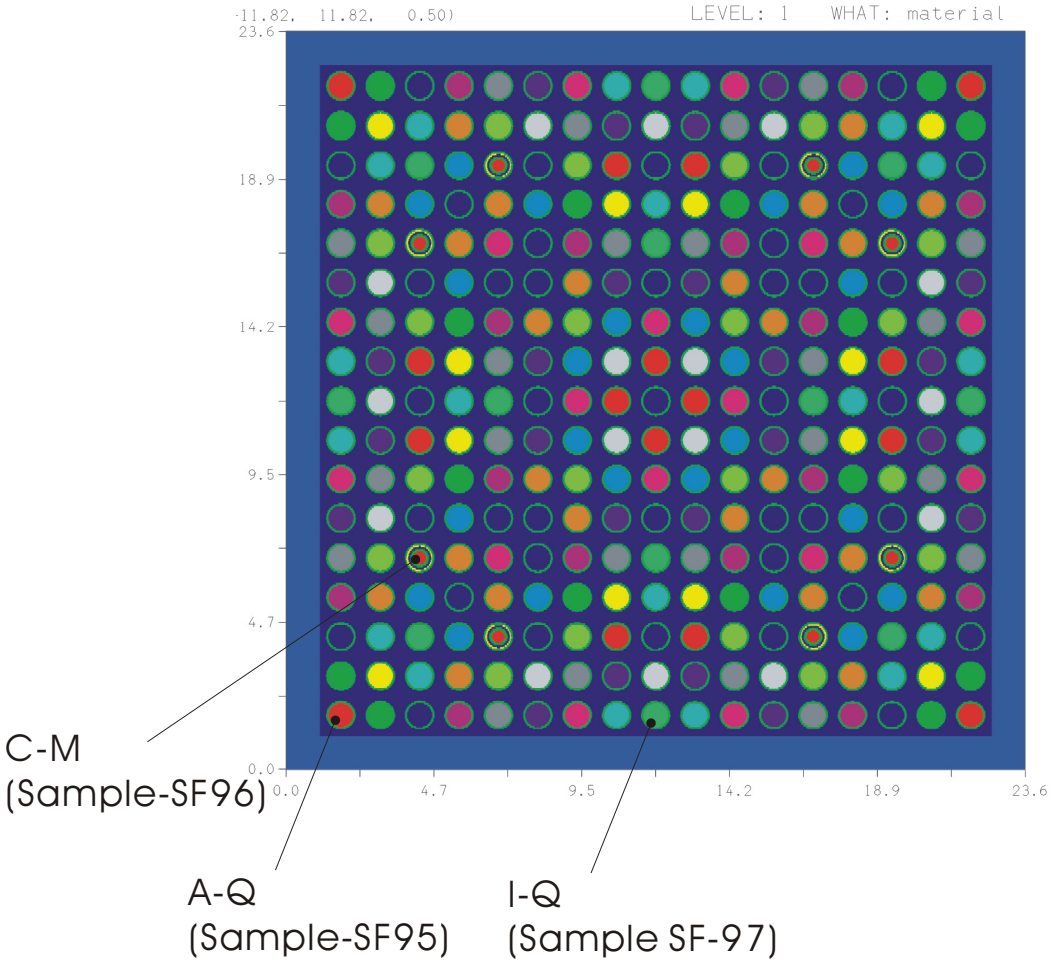

Figure 2 Fuel Assembly Model of MVP calculation for SF95

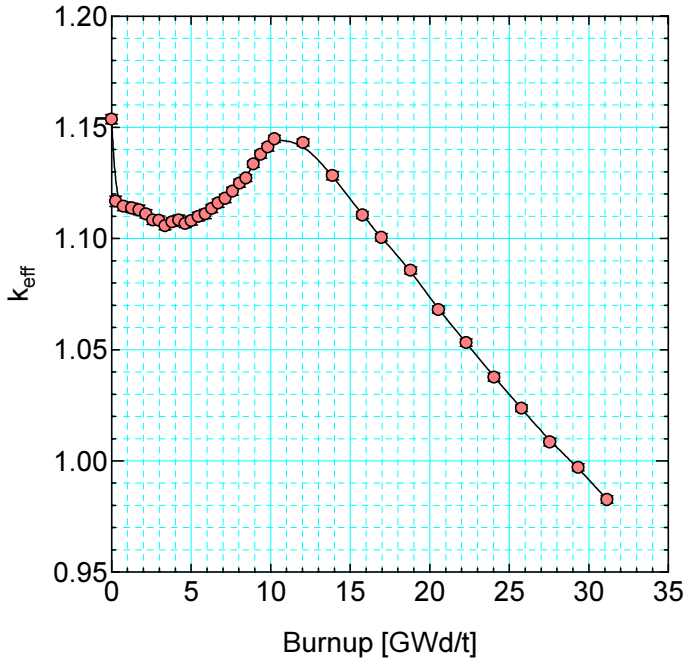

Figure 3 Neutron Multiplication Factor against NG3G23 Assembly Averaged Burnup

Table 6 Comparison of C/E values for SF95-4 sample by the analysis Using SWAT2 Single Pin Cell and Assembly Models.

	Pin Cell	Assembly	Difference (%)
^{234}U	1.182	1.182	-0.05
^{235}U	1.001	1.059	5.76
^{236}U	0.956	0.946	-1.05
^{238}U	1.001	1.000	-0.07
^{238}Pu	0.848	0.876	3.34
^{239}Pu	0.980	1.041	6.18
^{240}Pu	0.985	1.001	1.66
^{241}Pu	0.956	1.006	5.28
^{242}Pu	0.941	0.920	-2.15
^{241}Am	1.530	1.653	8.03
^{242m}Am	0.777	0.857	10.27
^{243}Am	0.941	0.943	0.21
^{242}Cm	0.536	0.546	1.76
^{243}Cm	0.633	0.646	1.99
^{244}Cm	0.816	0.813	-0.43
^{245}Cm	0.869	0.912	4.86
^{246}Cm	0.777	0.738	-4.99
^{137}Cs	0.978	0.965	-1.31
^{134}Cs	0.893	0.897	0.46
^{154}Eu	0.849	0.875	3.06
^{144}Ce	1.047	1.030	-1.66
*^{125}Sb	2.536	2.528	-0.32
*^{106}Ru	1.257	1.255	-0.11
*^{142}Nd	0.795	0.763	-4.02
^{143}Nd	0.970	0.971	0.13
^{144}Nd	0.961	0.929	-3.26
^{145}Nd	1.007	0.992	-1.49
^{146}Nd	0.989	0.974	-1.45
^{148}Nd	0.997	0.984	-1.31
^{150}Nd	0.973	0.965	-0.79

* Results for reference purpose because of a problem in experimental data.

4. Conclusion

In this study, the verification of a new revision of code system, SWAT2, was carried out by the analysis of PIE data taken from Japanese PWR. Generally, the differences between PIE analysis with single pin cell model of SWAT and SWAT2 were not so large than expected, and results for some important fission product nuclides were improved from those of SWAT.

Also, SWAT2 assembly model showed consistent results with single pin cell model even though several percent differences were indicated. CPU time was found not extremely long when we used current engineering workstation.

By combining the MVP and ORIGEN2, users can carry out the burnup calculation of approximately a thousand isotopes using a detailed geometry model with a precise treatment of resonance absorption. It might be necessary to conduct further PIE data analysis and benchmark calculations in order to compare with other code system for further verification of SWAT2. And also, the dependency of calculation results on the neutron history and the effect of geometry modeling should be studied.

Acknowledgements

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