

SWAT2: The Improved SWAT Code System by Incorporating the Continuous Energy Monte Carlo Code MVP

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SWAT is a code system, which performs the burnup calculation by the combination of the neutronics calculation code, SRAC95 and the one group burnup calculation code, ORIGEN2.1. The SWAT code system can deal with the cell geometry in SRAC95. However, a precise treatment of resonance absorptions by the SRAC95 code using the ultra-fine group cross section library is not directly applicable to two- or three-dimensional geometry models, because of restrictions in SRAC95. To overcome this problem, SWAT2 which newly introduced the continuous energy Monte Carlo code, MVP into SWAT was developed. Thereby, the burnup calculation by the continuous energy in any geometry became possible. Moreover, using the 147 group cross section library called SWAT library, the reactions which are not dealt with by SRAC95 and MVP can be treated. OECD/NEA burnup credit criticality safety benchmark problems Phase-IB (PWR, a single pin cell model) and Phase-IIIB (BWR, fuel assembly model) were calculated as a verification of SWAT2, and the results were compared with the average values of calculation results of burnup calculation code of each organization. Through two benchmark problems, it was confirmed that SWAT2 was applicable to the burnup calculation of the complicated geometry.

KEYWORDS: SWAT2, MVP, Burnup Calculation, Burnup Credit, OECD/NEA Burnup Credit Criticality Safety Benchmark Problems

1. Introduction

With the progress of computer performance in recent years, burnup calculation using Monte Carlo method becomes possible . Japan Atomic Energy Research Institute (JAERI) developed MVP-BURN code based on the continuous energy Monte Carlo code, MVP.¹⁻²⁾ Another example of implementation is MCODE (MCNP-ORIGEN depletion program) which has been developed at Massachusetts Institute of Technology.³⁾

SWAT is a burnup calculation code system by combination of neutronics calculation code, SRAC95 and one-group depletion code, ORIGEN2.1.⁴⁻⁷⁾ SWAT performs the burnup calculation by ORIGEN2.1 using the effective one-group cross section based on the SRAC95 calculation . SWAT library is a 147 groups cross section library based on JENDL-3.2.⁸⁾ This library contains (n,γ) , (n,2n), (n,3n), (n,fission), (n,α) and (n,p) reactions.

SRAC95 is used for neutron calculation in 107 groups, using the collision probability calculation module (PIJ). For major resonant nuclides, ultra-fine group collision probability calculation by the PEACO module is available. At present, PEACO module is not directly applicable to two- or three-dimensional geometry models, because of restrictions in SRAC95. This restriction makes it difficult to prepare a calculation model for large geometry, such as a fuel assembly array. It may be overcome by introducing a procedure that makes few group cross section sets based on the single-pin cell model, using the precise treatment resonance absorption option. However, this introduces approximation due to cell model boundary condition, and it would be difficult to develop suitable models for arbitrary geometry.

Continuous energy Monte Carlo code, MVP, developed at JAERI, can treat any geometry and calculate cross section and neutron flux for arbitrary region. These features of MVP code will give advantages to SWAT from the view point not only of resonance absorption treatment in arbitrary geometry and but also of utilization of complicated geometry.

Therefore, we introduced capability to drive MVP code into SWAT. This new version, SWAT2, can perform neutronics calculations for a given geometry to obtain the neutron flux and the effective cross sections by the MVP code instead of the SRAC95. And, by the utilization of the SWAT library, it is possible to treat (n,α) , (n,p) and (n,3n) reactions can not be treated on MVP.

2. Calculation Method

SWAT2 handles ORIGEN2.1, SRAC95 and MVP as an outside module. By handling each code as an

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outside module, SWAT2 became independent from updating of each code.

Figure 1 shows the flow of analysis of SWAT2. It is possible to choose MVP or SRAC95 for the neutron spectrum calculation. According to Figure 1, burnup calculation method by SWAT2 is explained in the following.

For each burnup step, the neutron spectrum and effective multi group cross section are evaluated by either MVP or SRAC95.

After the MVP or SRAC95 calculation, the LIBMAK routine is called. It makes the one-group cross section data file for the ORIGEN2.1 using calculated neutron spectrum and cross section by MVP or SRAC95. For nuclides and reactions can not be treated in MVP or SRAC95, infinite dilution cross sections stored in the SWAT library are condensed by the neutron flux. Fission yield data of ²³³U, ²³⁵U, ²³⁹Pu, and ²⁴¹Pu for thermal neutrons, decay constants and branching ratios for FPs are taken from JNDC FP library second version.⁹⁾ 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 Flow diagram of SWAT2.

2.1 MVP Calculation Method

MVP can deal with the energy range from 20 MeV to 1.0E-5 eV, and it is possible to make neutron flux, cross section and reaction rate with arbitrary energy group structure. In order to utilize the SWAT library for burnup calculation, the output of the neutron flux and cross section by MVP has be made with 147 group energy structures same as the SWAT library.

MVP is executed at the eigenvalue calculation mode for every burnup step, and 147 groups neutron flux, microscopic cross section data are obtained. 147 groups cross section is contracted using this neutron flux, and one group cross section data are obtained.

 (n,α) , (n,p) and (n,3n) reactions which are not treated by MVP, and all reaction data of nuclides which are not treated by MVP are included in the SWAT library in the form of a 147 groups infinite dilution cross section. By condensing these cross sections with the neutron flux from MVP, effective one group cross sections of all reactions which are needed for the ORIGEN2.1 library are obtained. ORIGEN2.1 performs the burnup calculation using these one group cross section.

3. Validation of SWAT2

For the verification of SWAT2(MVP)¹, OECD/NEA burnup credit criticality safety benchmarks Phase-IB and Phase-IIIB are analyzed.

3.1 OECD/NEA Phase-IB Benchmark Problem

OECD/NEA burnup credit benchmark Phase-IB is a series of single pin-cell burnup calculation problems based on PIE data of the PWR 14 \times 14 assembly burned in Calvert Cliffs Unit 1.¹⁰⁾ The lattice geometry is shown in Figure 2. Burnup periods are 4 cycles and power densities and boron concentration of each cycle are given. For verification of SWAT2, one PIE sample of 27.35 GWd/t was selected and analyzed. For comparison with SWAT2(MVP), SWAT2(SRAC95) and MVP-BURN were used for the analysis. The neutron histories at each burnup step in SWAT2(MVP) and MVP-BURN was set to 1,000,000.



Figure 2 Lattice geometry of Phase-IB benchmark problem

The results are shown in Table 1. In the table, the ratio of SWAT2(MVP) or SWAT2(SRAC95) results to averaged value shown in Ref.10 are shown. This comparison shows that the difference of results obtained by using the MVP code or the SRAC95 code in the SWAT2 code system is small. Similar results to

¹ This means that SWAT 2 drives MVP code for neutron spectrum calculatin

MVP-BURN code were obtained by SWAT2. In the actinides, especially in Pu isotopes, SWAT2(MVP) is small rather than the average value. For some isotopes such as ¹⁵¹Sm, ¹⁵⁵Gd,the differences from the average of other codes became large. However, some of the measurement values including ¹⁵¹Sm and ¹⁵⁵Gd are not listed in Ref.10. Moreover, burnup chain model each code is different from each code. All things considered, it is impossible to make a direct discussion about difference of calculation results of ¹⁵¹Sm and ¹⁵⁵Gd.

Table 1 Comparison of calculation results of OECD/NEA/NSC Phase-IB benchmark

obtained by using 5 wA12 and WIVP-BURN								
Ratios of calculation results								
Isotope	average value in Ref.10							
	27.35 [GWd/MTU]							
	(after 1870 days cooling)							
	SW	MVP-BURN						
	MVP	SRAC95 ^{*2}	MUL BORN					
²³⁴ U	0.99	0.93	1.00					
²³⁵ U	1.01	1.01	1.01					
236U	0.95	0.98	0.96					
²³⁸ U	1.00	1.00	1.00					
²³⁸ Pu	0.89	0.96	0.90					
²³⁹ Pu	0.96	1.00	0.97					
²⁴⁰ Pu	0.95	0.98	0.95					
²⁴¹ Pu	1.02	1.01	1.00					
242Pu	1.05	1.01	1.00					
²⁴¹ Am	1.00	0.99	0.97					
²³⁷ Np	0.84	0.95	0.87					
¹⁴⁷ Sm	1.05	1.06	_* ³					
¹⁴⁹ Sm	0.85	0.87	0.89					
¹⁵⁰ Sm	0.97	0.96	0.98					
¹⁵¹ Sm	0.79	0.81	0.78					
¹⁵² Sm	0.91	1.05	0.93					
¹⁴³ Nd	0.99	0.99	0.98					
¹⁴⁵ Nd	1.01	1.01	1.00					
¹⁵³ Eu	1.04	0.94	1.02					
¹⁵⁵ Gd	0.67	0.62	0.66					

*¹ Calculation results of SWAT2 using MVP module.

*² Calculation results of SWAT2 using SRAC95 module.
*³ Not obtained due to the limitation of the applicable nuclides.

3.2 OECD/NEA Phase-IIIB Benchmark Problem

The calculation model of OECD/NEA burnup credit criticality safety benchmark Phase-IIIB is BWR 8×8 assembly which have arranged one water rod at the center.¹¹⁾ In this assembly, five types of fuel rods having different initial uranium enrichments are allocated. Only one type of fuel rods is with 3.0 wt% of Gd₂O₃. The lattice geometry is shown in Figure 3. The channel box is surrounded by 8.5-mm-thick water, and the reflective boundary condition is imposed outside the 15.24 cm-square fuel assembly cell. Fuel rods are classified into nine kinds of fuel rods shown in Figure 4 from the difference among burnup conditions. From difference of void fraction (0%, 40% and 70%) and difference of cooling time (no-cooling and 5-year cooling), there are 6 kinds of calculation cases (See Table 2). The neutron histories at each burnup step in SWAT2(MVP) was set to 600,000.

The calculation results of k-infinity to each void fraction are shown in Figure 5. In these figures, average values over all participating calculation codes in Ref.11 are also described. The SWAT2 calculation results agree well i with the average value.

Comparison of burnup distribution in the assembly is shown in Table 3. The burnup distribution of SWAT2(MVP) agrees comparatively well, though there is a difference a little for the average value. The burnup of a fuel rod with Gd_2O_3 is decreasing as the void fraction rises in the in-channel. The burnup of fuel rods beside the water rod such as #7 and #9, are larger than 40 GWd/tHM of assembly average value, contrary to the fuel rod around Gd_2O_3 fuel. Calculation results of nuclide compositions are shown in Table4.

Table 2 Benchmark cases of Phase-IIIB

Case	Void Fraction[%]	Cooling Time[year]
1	0	0
2	0	5
3	40	0
4	40	5
5	70	0
6	70	5



Figure 3 Lattice geometry of Phase-IIIB benchmark problem



Figure 4 Position number of fuel rods for lattice geometry of Phase-IIIB benchmark problem

4. Conclusion

We revised SWAT code system to develop SWAT2, the new version of SWAT, by incorporating the continuous energy Monte Carlo code, MVP. It enables us to conduct detailed burnup calculation using ORIGEN2.1 code with latest nuclear data and precise treatment of neutron absorption in arbitrary geometry. For the verification of SWAT2, the burnup calculation was carried out on OECD/NEA burnup credit criticality safety benchmark problems Phase-IB and Phase-IIIB, and the calculation results were compared with the average value of calculation results of burnup calculation code of each organization. In Phase-IB calculation calculation. Pu238 result by SWAT2(MVP) became about 10% low compared with the average value of Ref.10. This trend was similar to the tendency to MVP-BURN. Moreover, it became 10% or more lower than the average value for ²³⁷Np in SWAT2(MVP) and MVP-BURN calculation results. In the Phase-IIIB calculation, k-infinity and the burnup distribution showed the almost same tendency as the average values of Ref.11. The nuclide composition calculation results have lowered more than the average value for ²³⁸Pu, ²³⁷Np, and ²⁴³Am as well as Phase-IB. It is necessary to perform the verification by comparison with the post irradiation examination data, and to understand the characteristics of a nuclear data file.

The following two improvements are in scope:

- (1) building the SWAT library based on the JENDL-3.3.¹²⁾
- (2) introduction of the predictor-corrector method in preparation of cross section data required for burnup calculation.



Figure 5 Comparison of k-infinity in Phase-IIIB benchmark result of SWAT2

Position No.	0% void			40% void			70% void		
	SWAT2		Augro 93	SWAT2		Average	SWAT2		Average
	MVP*1	SRAC95 ^{*2}	Average	MVP	SRAC95	Average	MVP*1	SRAC95 ^{*2}	Average
#1	37.8	35.4	36.9	39.6	37.3	38.5	41.4	39.3	40.1
#2	38.7	38.3	39.0	39.5	39.4	39.9	40.1	40.5	40.6
#3	42.2	41.2	41.2	42.8	41.9	41.6	43.4	42.5	41.8
#4	40.3	40.9	40.4	40.6	41.4	40.6	40.7	41.9	40.7
#5	38.9	39.1	39.0	39.0	39.0	39.0	39.0	38.8	38.9
#6	31.0	31.0	31.7	30.7	30.6	31.6	30.5	30.1	31.4
#7	43.6	44.7	43.6	42.9	43.6	42.7	42.1	42.4	41.9
#8	42.3	44.0	43.1	41.3	42.7	42.1	40.7	41.4	41.4
#9	44.2	45.4	44.5	43.0	44.2	43.6	42.2	43.0	43.0
Average	39.9	40.1	40.0	39.9	40.1	40.0	39.9	40.0	40.0

Table 3 Pinwise burnup results for Phase-IIIB benchmark problem

¹ Result from SWAT2 using MVP module. ^{*2} Result from SWAT2 using SRAC95 module. ^{*3} The average value of the calculation result shown in Ref.11.

Table 4 Results of calculation for Phase-IIIB benchmark problem (5 year cooling)

		0% void		40% void			70% void			
Nuclide	MVP/	SRAC95/	MVP/	MVP/	SRAC95/	MVP/	MVP/	SRAC95/	MVP/	
	Average*1	Average ^{*2}	SRAC95*3	Average	Average	SRAC95	Average	Average	SRAC95	
²³⁴ U	0.99	1.04	0.95	0.99	1.05	0.94	0.99	1.06	0.94	
²³⁵ U	1.00	1.04	0.97	1.00	1.03	0.97	0.98	1.02	0.96	
²³⁶ U	0.98	0.98	1.00	0.98	0.98	1.00	0.98	0.98	0.99	
²³⁸ U	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
²³⁸ Pu	0.89	0.95	0.94	0.88	0.94	0.94	0.86	0.91	0.95	
²³⁹ Pu	1.04 -	1.00	1.04	1.03	1.00	1.03	0.99	0.98	1.01	
²⁴⁰ Pu	1.11	1.05	1.06	1.11	1.05	1.06	1.11	1.04	1.06	
²⁴¹ Pu	0.95	1.05	0.90	0.93	1.04	0.90	0.90	1.01	0.89	
²⁴² Pu	0.95	1.04	0.91	0.95	1.04	0.92	0.96	1.04	0.93	
²⁴¹ Am	0.96	1.06	0.90	0.94	1.05	0.90	0.91	1.02	0.89	
²⁴³ Am	0.80	1.03	0.78	0.79	1.02	0.77	0.79	1.02	0.77	
²³⁷ Np	0.98	0.97	1.01	0.97	0.96	1.01	0.95	0.94	1.01	
⁹⁵ Mo	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
⁹⁹ Tc	1.03	1.01	1.02	1.04	1.02	1.02 `	1.04	1.02	1.02	
¹⁰¹ Ru	0.99	0.99	1.00	0.99	0.99	1.00	0.99	0.99	1.00	
¹⁰³ Rh	1.02	1.03	1.00	1.03	1.03	1.00	1.03	1.03	1.00	
¹⁰⁹ Ag	1.09	1.14	0.96	1.09	1.14	0.96	1.10	1.14	0.97	
¹³³ Cs	1.01	1.02	0.98	1.01	1.03	0.98	1.01	1.03	0.98	
¹⁴⁷ Sm	1.02	1.03	0.99	1.03	1.03	0.99	1.04	1.04	1.00	
¹⁴⁹ Sm	0.96	0.92	1.04	0.94	0.92	1.02	0.89	0.89	1.00	
¹⁵⁰ Sm	1.01	0.94	1.07	1.01	0.94	1.08	1.01	0.93	1.08	
¹⁵¹ Sm	0.90	1.04	0.87	0.88	1.03	0.85	0.82	0.99	0.83	
¹⁵² Sm	0.92	1.10	0.83	0.90	1.12	0.80	0.88	1.15	0.76	
¹⁴³ Nd	0.98	1.01	0.97	0.98	1.01	0.97	0.98	1.01	0.98	
¹⁴⁵ Nd	1.00	1.01	0.99	1.01	1.01	1.00	1.01	1.01	1.00	
¹⁵³ Eu	1.01	0.94	1.07	1.01	0.94	1.08	1.01	0.93	1.09	
¹⁵⁵ Eu	1.00	0.93	1.07	0.94	0.86	1.09	0.87	0.79	1.10	
¹⁵⁵ Gd	1.40	1.23	1.14	1.31	1.15	1.14	1.21	1.06	1.15	
156Gd	1.40	1.40	1.01	1.39	1.39	1.00	1.39	1.39	1.00	
157Gd	1.37	1.55	0.88	1.42	1.58	0.90	1.42	1.58	: 0.90	
¹⁵⁸ Gd	1.41	1.41	1.00	1.41	1.41	1.00	1.41	1.41	1.00	
¹³¹ Xe	0.99	1.03	0.96	0.99	1.03	0.96	1.00	1.05	0.96	

^{*1} Ratios of SWAT2 calculations result using MVP module to average value in Ref.11. ^{*2} Ratios of SWAT2 calculations results using SRAC95 module to average value in Ref.11. ^{*3} Ratios of SWAT2(MVP) calculations results to SWAT2(SRAC95) calculations results.

References

- T. Mori, M. Nakagawa and M. Sasaki, "Vectorization of Continuous Energy Monte Carlo Method for Neutron Transport Calculation," *J. Nucl. Sci. Technol.*, Vol. 29, No.4, p.325 (1992).
- 2) K. Okumura, T. Mori, M. Nakagawa and K. Kaneko, "Validation of a Continuous-Energy Monte Carlo Burn-up Code MVP-BURN and Its Application to Analysis of Post Irradiation Experiment," J. Nucl. Sci. Technol., Vol. 37, No. 2, pp.128-138 (2000).
- 3) Zhiwen Xu, Pavel Hejzlar, Michael J. Driscoll, and S. Kazimi, "An Improved MCNP-ORIGEN Depletion Program (MCODE) and Its Verification for High-Burnup Applications," Proc. PHYSOR 2002 Int. Conf. on New Frontiers of Nuclear Technology: Reactor Physics, Safety and High-Performance Computing, Seoul, Korea, Oct. 7-10, 2002, 2A-04 (2002).
- 4) K. Suyama, H. Mochizuki and T. Kiyosumi, "Revised Burnup Code System SWAT: Description and Validation Using Postirradiation Examination Data," *Nuclear Technology*, Vol 138, No.2, pp 97-110 (May 2002).
- K. Okumura, K. Kaneko and K. Tsuchihashi, "SRAC95; General Purpose Neutronics Code System," JAERI-Data/Code 96-015, Japan Atomic Energy Research Institute (1996) [in Japanese].
- 6) Allen G. Croff, "A User's Manual for the ORIGEN2 Computer Code," ORNL/TM-7175, Oak Ridge National Laboratory (July 1980).
- 7) K.J.Notz, "ORIGEN2, Version 2.1 Release Notes," CCC-371, pp 200-208 (August 1991).

- 8) T. Nakagawa, K. Shibata, S. Chiba, T. Fukahori, Y. Nakajima, Y. Kikuchi, T. Kawano, Y. Kanda, T. Ohsawa, H. Matsunobu, M. Kawai, A. Zukeran, T. Watanabe, S. Igarashi, K. Kosako, and T. Asami, "Japanese Evaluated Nuclear Data Library Version 3 Revison-2: JENDL-3.2," J.Nucl. Sci. Technol., 32, 1259 (1995).
- 9) K. Tasaka, J. Katakura, H. Ihara, T. Yoshida, S. Iijima, R. Nakashima, T. Nakagawa, and H. Takano, "JNDC Nuclear Data Library of Fission Products - Second Version," JAERI-1320, Japan Atomic Energy Research Institute (1990).
- M.D.DeHart, M.C.Brady, and C.V.Parks, "OECD/NEA Burnup Credit Calculational Criticality Benchmark Phase-I-B Results," ORNL-6901, Oak Ridge National Laboratory (1996).
- 11) H. Okuno, Y. Naito and K. Suyama, "OECD/NEA Burnup Credit Criticality Benchmarks Phase IIIB: Burnup Calculations of BWR Fuel Assemblies for Storage and Transport," JAERI-Research 2001-01, NEA/NSC/DOC(2002)2 (2002).
- 12) K. Shibata, T. Kawano, T. Nakagawa, O. Iwamoto, J. Katakura, T. Fukahori, S. Chiba, A. Hasegawa, T. Murata, H. Matsunobu, T. Ohsawa, Y. Nakajima, T. Yoshida, A. Zukeran, M. Kawai, M. Baba, M. Ishikawa, T. Asami, T. Watanabe, Y. Watanabe, M. Igashira, N. Yamamuro, H. Kitazawa, N. Yamano and H. Takano: "Japanese Evaluated Nuclear Data Library Version 3 Revision-3: JENDL-3.3," J. Nucl. Sci. Technol., 39, 1125 (2002).