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Recent Advancements in AEGIS/SCOPE2 and Its Verifications and Validations

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Abstract – *AEGIS/SCOPE2, the next-generation in-core fuel management system, has been updated by introduction of the neutron up-scattering in the resonance energy domain within the framework of the ultra-fine energy group calculations in AEGIS to accurately estimate the Doppler effect and a new cross section model in SCOPE2 to capture the reactivity effect due to long-term fuel cooling. It is confirmed that the models are properly implemented through verifications and validations.*

I. INTRODUCTION

AEGIS/SCOPE2 has been one of the most advanced in-core fuel management system for commercial PWRs. In the development of the system, novel methods were invented and adopted to realize high-fidelity simulations[1, 2]. It was also successful from the view point of software engineering to realize fast computer program while maintaining abstract structures in the software written in the high-level system languages [3].

In 2010, the system had been well validated in combination with the ENDF/B-VII.0 library[4] and expected to be authorized by the regulatory body. Unfortunately no reviews have been initiated yet because of lack of opportunity to negotiate with the authority due to reformation of the regulatory system in Japan after the Fukushima Daiichi accident. However, continuous efforts have been made to improve accuracy of the system such as introduction of new computational models, refinement of existing models and adoption of the latest nuclear data library, JENDL-4.0u[5].

In the present paper, recent advancements on computational models in AEGIS/SCOPE2 are discussed.

II. IMPROVEMENT OF COMPUTATIONAL MODELS

1. Up-Scattering in the Resonance Calculation with the Ultra-Fine Energy Structure in AEGIS

In AEGIS, a new method for neutron up-scattering in the resonance energy domain was developed. The effect of the up-scattering is directly treated within the ultra-fine energy structure[6]. In order to reduce computation load, an efficient calculation method is implemented.

A. Computational Method and Implementation

It is reported that consideration of the neutron up-scattering in the resonance energy domain has an impact on approximately 9% increase in the negative direction on the Doppler temperature coefficients. In the conventional version of AEGIS, there was no treatment of the neutron up-scattering because it solves the slowing down equations in the ultra-fine energy structure with 32000 groups. In the previous studies it is reported that U-238 is a major contributor for this effect [7, 8]. Assuming the isotropic scattering approximation, the scattering kernel with consideration of thermal vibration of the target nucleus can be expressed as Eq. (1),

$$\sigma_{s0}^{T}(E \to E') = \frac{\beta^{5/2}}{4E}\exp(\frac{E}{kT})\int_0^\infty t\sigma_s^{tab}\left(\frac{\beta kT}{A}t^2\right)\exp(\frac{-t^2}{A})\psi_0(t)dt\,, \quad (1)$$

where

σ_s^{tab} : scattering cross section at 0 K

and

$\beta = (A+1)/A$.

In order to reduce computation time, Eq. (1) is solved 'off-line' to tabulate the kernel data for representative temperature points, i.e. every 50K between 300K and 1300K, so that AEGIS can reconstruct the kernel for arbitrary temperature conditions with simple interpolations.

In AEGIS, nuclides are categorized into 4 groups for solving the slowing-down equation: (a) H-1, (b) O-16, (c) nuclides with Z < 90 except H-1 and O-16, and (d) nuclides with Z ≥ 90. In the present method, the last group is further divided into two groups: (d-1) nuclides with Z ≥ 90 except U-238 and (d-2) U-238 in order to minimize increase of computational load which is approximately 20% due to additional nuclide groups.

Iterations are needed in solving the slowing down equation to update neutron sources considering up-

scattering from lower energy groups. The scattering matrix can be huge for the ultra-fine energy structure with a straightforward treatment, which is not feasible from the viewpoint of computational load. According to the previous study on energy breakdown of the impact on the Doppler temperature coefficient by U-238[8], the six resonance groups shown in Table I would capture most of the effect. These energy range are isolated each other, then the scattering matrix can be decomposed into sub-matrixes for each energy domain. These sub-matrixes of the scattering kernel are explicitly treated in the iterative calculation by the power method. The increase of computation time due to the iterative method is estimated 10%.

Total increase of computational time with the present method is estimated approximately 30%.

Table I. Energy groups for resonance up-scattering treatment in AEGIS.

Group	Energy Boundary [eV]		Number of groups in the UFG structure	U-238 Resonance [eV]
	Lower	Upper		
1	101.274	130.129	872	102
2	61.3762	78.9466	329	66
3	29.0179	37.2678	327	36.7
4	17.5927	22.6177	328	20.9
5	6.47888	8.32722	219	6.7

B. Verifications and Validations

The results of the scattering kernels are compared with that of the reference [7]. The neutron scattering kernels by the present method for neutrons with in-coming energy of 7.2eV at the temperature conditions of 300K and 1000K are shown in Fig. 1. Calculated results including this case agreed well with the results in the reference [7].

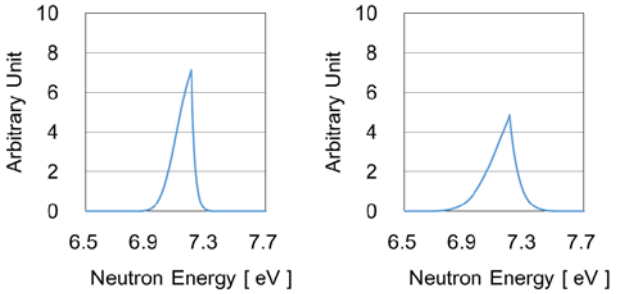


Fig. 1. Calculated Scattering kernels at each temperature

The benchmark problem on the Doppler temperature coefficient in pin cell geometry proposed by D. Mosteller [9] was solved using AEGIS with the present method in order to verify the impact on the Doppler coefficient with treatment of the neutron up-scattering in the resonance energy domain. The computational results are shown in Table II. 'ASYMP' denotes the Doppler temperature coefficient calculated with the conventional method while 'New' the present method. The impact of the present method on the Doppler temperature coefficients is approximately 9% for UO_2 and 6-7% for MOX. This trends agreed with those reported in the references [7, 10].

Validation was carried out by comparison with the empirical formula of Hellstrand et al. [11] which is widely used for validating the resonance integral. Figure 2 shows the comparison between resonance integral calculated by AEGIS and results of Hellstrand's empirical formula. Two types of S/M (fuel surface area over fuel mass) were set to 0.50 and 0.33 cm^2/g to cover the practical specification of the PWR. The calculated results by AEGIS well agreed with the results of the formula denoted as 'Measure' in Fig. 2.

Table II. Impact of the resonance scattering on the Doppler Temperature Coefficients in AEGIS

Enrichment	Asymptotic keff		δk		ρ(pcm/K) (1)	ρ_a(pcm/K) (2)	((2) - (1)) / (1)
	HZP	HFP	HZP	HFP	New	ASYMP	[%]
UO2(wt%)	UO2 FUEL						
0.71	0.66637	0.66029	-78	-134	-5.05	-4.61	-8.73
1.60	0.96225	0.95372	-116	-197	-3.40	-3.10	-8.97
2.40	1.10076	1.09127	-132	-223	-2.90	-2.63	-9.05
3.10	1.17893	1.16896	-140	-236	-2.65	-2.41	-9.08
3.90	1.24173	1.23142	-145	-244	-2.47	-2.25	-9.05
4.50	1.27725	1.26676	-148	-248	-2.37	-2.16	-8.99
5.00	1.30162	1.29104	-149	-250	-2.31	-2.10	-9.00
PuO2(wt%)	Reactor-Recycle MOX						
1.00	0.94738	0.93751	-112	-191	-4.01	-3.70	-7.71
2.00	1.02401	1.01280	-118	-201	-3.88	-3.60	-7.19
4.00	1.07992	1.06801	-117	-201	-3.70	-3.44	-6.87
6.00	1.10885	1.09681	-113	-194	-3.53	-3.30	-6.56
8.00	1.13227	1.12025	-107	-186	-3.38	-3.16	-6.41

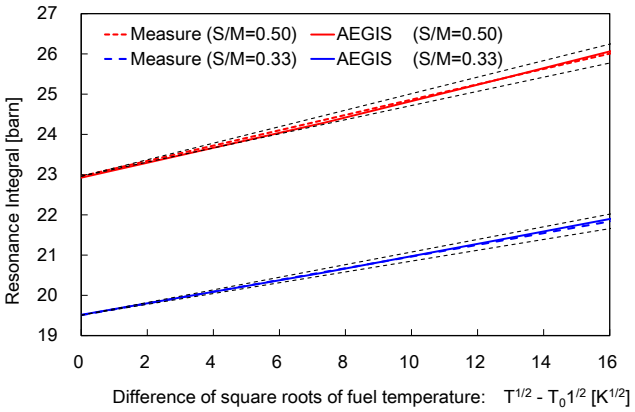


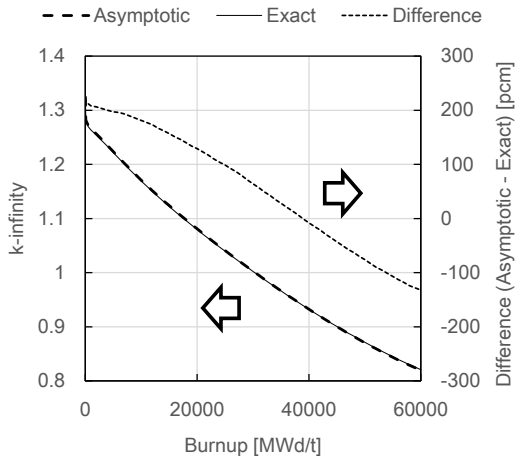
Fig. 2. Comparison of resonance integral between calculated results by AEGIS and the Hellstrand's empirical formula.

Impact on depletion characteristics by the neutron up-scattering is also studied. The k-infinity values through depletion calculations are compared between the cases with the conventional method (denoted as 'asymptotic') and that with the present method (denoted as 'exact) for typical Westinghouse-type 17x17 UO2, Gd and MOX fuel assemblies. Results are shown in the Fig. 3.

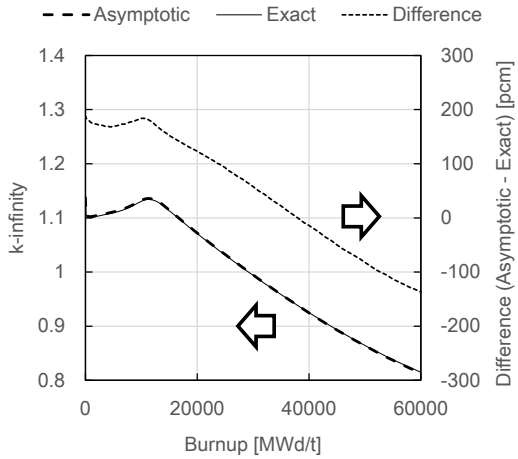
Verification for core calculation with SCOPE2 was also conducted; cross section libraries for SCOPE2 were prepared with AEGIS. Core calculations are performed for typical reload cores with UO_2 fuel assemblies. The calculation results of the Doppler temperature coefficients with the conventional and the present methods are shown in Table III. The results are consistent with those in Table II. Therefore it was confirmed that the impact of neutron up-scattering in the resonance energy domain to the Doppler temperature coefficient is properly reflected to the results of SCOPE2.

Table III. Impact of the resonance scattering on the Doppler Temperature Coefficients in SCOPE2.

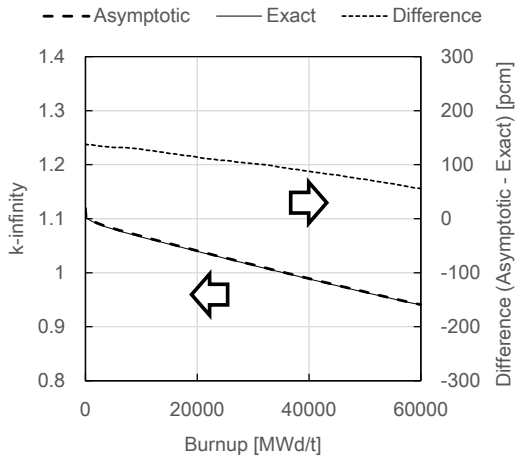
Core	Core Average Exposure [GWd/t]	Doppler Temp. Coef.(pcm/K)		Difference
		Asymptotic (1)	New (2)	((1)-(2))/(2)*100 [%]
A	14.5	-2.89	-3.15	-8.22
B	14.3	-2.97	-3.24	-8.19
C	16.3	-3.07	-3.33	-7.93



(a) UO_2 Assembly



(b) Gd Assembly



(c) MOX Assembly

Fig. 3. Impact on k-infinity in depletion by the neutron up-scattering in the resonance energy domain.

Finally, impact on prediction accuracy was studied as a part of validation of the present method. Core depletion calculations for a Westinghouse-type 3-loop PWR are performed. Most of the fuel assemblies are UO2 and some are Gd. Bias on critical boron concentration were compared between the conventional method (denoted as 'old') and the present method ('new'). The results are shown in Fig. 4. The bias on critical boron concentration shifted to the positive direction because the present method gives lower reactivity due to more resonance capture, which leads to lower critical boron concentration and larger bias. The standard deviations of the bias curves were almost at the same level between the two methods, however the present method tends to give flatter curve since the bias at the BOC shifted slightly to the positive direction.

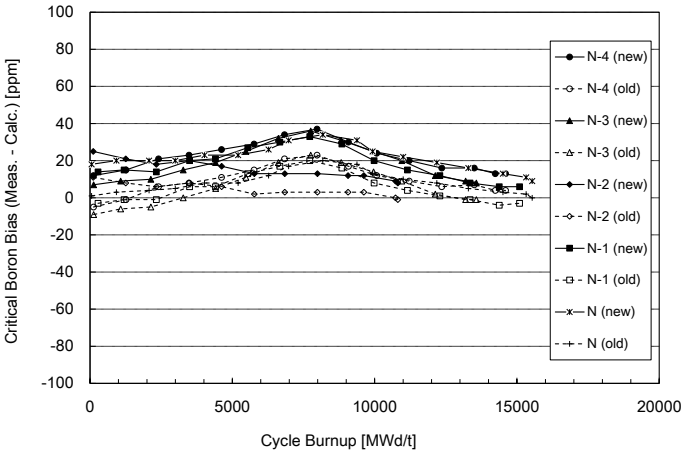


Fig. 4. Impact on critical boron concentration by the up-scattering in the resonance energy domain

2. **New Cross Section Modeling in SCOPE2 for Long Cooling Time**

Under the situation with long suspension of NPPs in Japan, some fuel assemblies experience very long cooling time from the last irradiation, for example 15 years. In such a case, reactivity of fuel assembly drastically changes as time passes. Fig. 5 illustrates degradation of reactivity of typical UO2 and MOX fuel assemblies whose average burnup is 45GWd/t in cooling up to 20 years.

In-core fuel management system is well validated against typical operational conditions such as the base load operation at the full power rate followed by shutdown of a few months for inspections. One of the most extreme but possible cases is the very short operation of reload core with fuel assemblies which have been cooled long time. A similar operational condition was observed in Japan after the Fukushima Daiichi accident. In order to maintain prediction accuracy even for such extreme cases, in-core fuel management system should be robust for all possible conditions.

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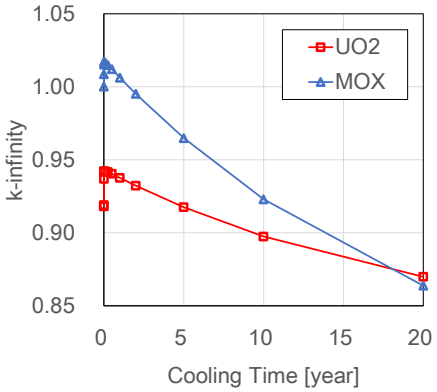
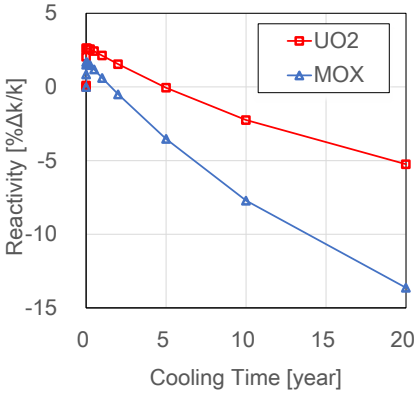


(a) Change of k-infinity



(b) Change of reactivity

Fig. 5. Change of k-infinity and reactivity of fuel assembly at 45GWd/t as functions of cooling time.

After a new burnup solver based on the Krylov subspace method in SCOPE2 is developed [12], use of the microscopic-correction model [13] became a default option because of its robustness. It was expected that this model could precisely treat reactivity change during cooling between operations. However when we verify the validity of the cross section model in SCOPE2 in comparison with AEGIS, it was found that SCOPE2 tends to overestimate the k-infinity after very long cooling time. The cause of the issue was a change of the microscopic cross sections during cooling which have major impacts on reactivity. Fig. 6 shows the change of microscopic cross section of Pu-239 during cooling. This is because the change of self-shielding effect due to that of the background cross section. However the conventional model in SCOPE2 did not treat this effect and assumed constant microscopic cross sections over cooling. Therefore a new cross section model was developed.

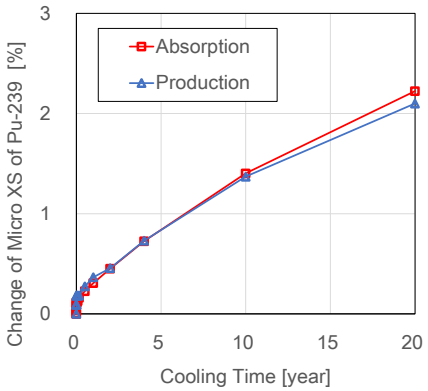


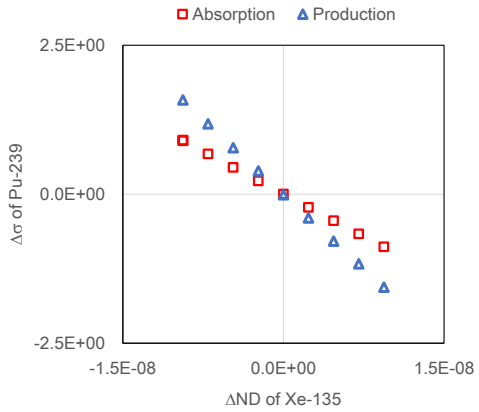
Fig. 6. Example of change of microscopic cross section during cooling.

A. Computational Method and Implementation

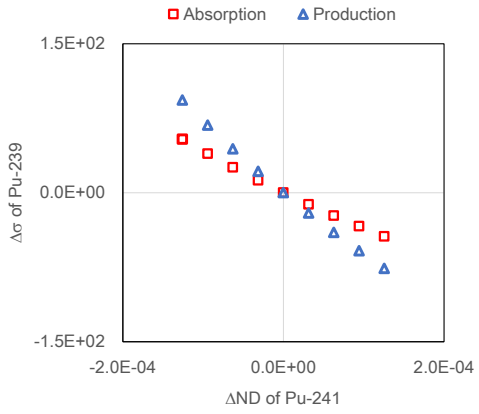
Theoretically, microscopic cross sections of all the nuclides will change during cooling. From the viewpoint of background cross section change, three major nuclides (hereafter referred as initiators) are chosen in the modeling, i.e. ^{135}Xe, ^{241}Pu, ^{241}Am. Change of number density of the initiators affects microscopic cross sections of the others through the background cross sections. It was found that cross section change for 6 major nuclides (^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{241}Am) should be considered in this model in order to capture the effect. The change of the cross section is correlated to that of number density of initiators. Fig 7 shows examples of the correlation; the change of micro XS of Pu-239 can be expressed as linear functions of the change of number densities of Xe-135, Pu-241 and Am-241 from the reference condition.

A new case matrix was implemented in AEGIS to do branch calculations where the number density of the initiator are virtually changed. With the results in the branch cases at all the depletion points, the cross section change of 6 major nuclides due to the change of number densities of 3 initiators can be estimated. Since correlations between difference of number density of the initiators and that of the micro cross sections of the major nuclides is linear as shown in Fig. 7, only coefficients of the correlation calculated with an one branch case at each depletion point should be stored in the tabulation library for SCOPE2.

In burnup/cooling calculations by SCOPE2, number densities of 87 nuclides are explicitly tracked. As the number densities of the initiators are changed, the differences of the microscopic cross sections of 6 major nuclides can be computed with the coefficients of the correlation obtained at the stage of cross section compile. Then the microscopic cross sections can be corrected properly for arbitrary cooling conditions.

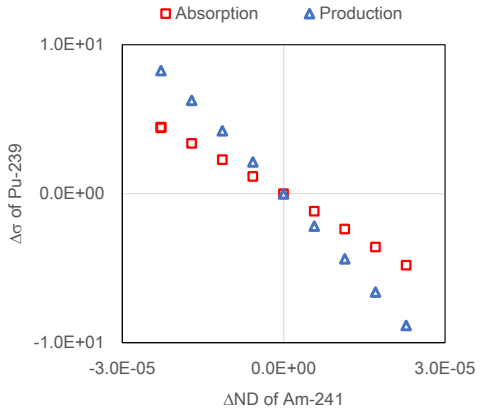


(a) Δσ of Pu-239 vs ΔND of Xe-135



(b) Δσ of Pu-239 vs ΔND of Pu-241

Fig. 7. Examples of the correlation in changes of micro cross sections and number densities of initiators



(c) Δσ of Pu-239 vs ΔND of Am-241

Fig. 7. Examples of the correlation in changes of micro cross sections and number densities of initiators (continued)

B. Computational Method and Implementation

Comparisons of the cooling effects between AEGIS and SCOPE2 were done for a 4.1wt% UO_2 assembly and a typical MOX assembly[14] under the following condition:

Burn up to 30 GWd/t → 20-year cooling → burn up to 45 GWd/t.

Difference of k-infinity values between SCOPE2 and AEGIS during the cooling are summarized in Table IV and V for the UO2 and the MOX assemblies, respectively. There was a slight bias in the conventional method for the UO2 case while it is small enough as shown in Table IV. With the present method, SCOPE2 can almost reproduce the result by AEGIS. As for the MOX case, SCOPE2 overestimate k-infinity values under the long cooling condition as shown in Table V and Fig 8. This is a modeling error in the conventional method as discussed earlier. With the present method, consistency between AEGIS and SCOPE2 has been much improved.

Table IV. Difference of k-infinity during cooling (UO2)

Cooling Time	Difference of k-infinity from AEGIS [%Δk/k]	
	Conventional	New
0 days	-0.021	-0.020
10 days	-0.066	0.010
3 months	-0.102	-0.026
1 year	-0.104	-0.025
2 years	-0.109	-0.025
5 years	-0.118	-0.023
10 years	-0.126	-0.013
20 years	-0.126	0.017

Table V. Difference of k-infinity during cooling (MOX)

Cooling Time	Difference of k-infinity [%Δk/k]	
	Conventional	New
0 days	-0.009	-0.009
10 days	-0.038	0.031
3 months	-0.076	0.005
1 year	-0.127	-0.006
2 years	-0.195	-0.018
5 years	-0.407	-0.056
10 years	-0.745	-0.105
20 years	-1.290	-0.163

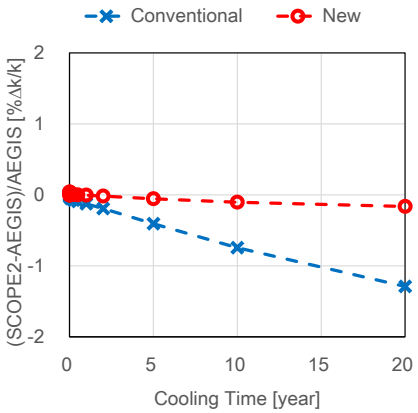


Fig. 8. Discrepancy between AEGIS and SCOPE2 in reactivity during cooling (MOX).

Table VI and VII summarize the difference of k-infinity values during burnup after cooling. In the conventional method the discrepancy become smaller as the burnup increase, however, the initial difference is quite large for the MOX case. With the present method, the discrepancy was decreased for the initial step at 30GWd/t and through the last step at 45GWd/t. Figure 9 illustrate the improvement with the present method.

Table VI. Difference of k-infinity during burnup after cooling (UO2)

Assembly Bunrup [GWd/t]	Difference of k-infinity from AEGIS [%Δk/k]	
	Conventional	New
30.0	-0.109	0.029
30.1	-0.126	-0.068
30.5	-0.097	-0.045
31.0	-0.088	-0.039
33.0	-0.075	-0.043
35.0	-0.067	-0.046
40.0	-0.043	-0.039
45.0	-0.026	-0.029

Table VII. Difference of k-infinity during burnup after cooling (MOX)

Assembly Bunrup [GWd/t]	Difference of k-infinity [%Δk/k]	
	Conventional	New
30.0	-1.303	-0.183
30.1	-1.260	-0.210
30.5	-1.215	-0.217
31.0	-1.172	-0.231
33.0	-1.000	-0.242
35.0	-0.847	-0.234
40.0	-0.540	-0.194
45.0	-0.312	-0.147

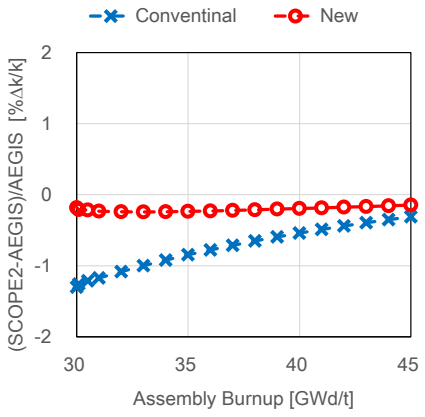


Fig. 9. Discrepancy between AEGIS and SCOPE2 in reactivity during depletion after cooling (MOX).

Verification in core geometry is also conducted. Critical boron concentrations were calculated with the both methods and compared. The present method predicts higher critical boron concentration because negative error on reactivity discussed above was fixed. The average increase of critical boron concentration is approximately 9 ppm and the standard deviation is 2 ppm at 1σ as configurations of fuel cooling vary each cycle.

In principle, the present model is more robust over the conventional methods and expects to give more accurate prediction. However, in practice, there are no sufficient data to discuss the superiority of the present method. It is expected to show validity of the present method through analysis of reload cores of restarting plants after long shutdown.

IV. CONCLUSIONS

A straightforward method for the treatment of neutron up-scattering in the resonance energy domain was implemented in AEGIS. The Doppler temperature coefficient calculated by AEGIS agreed with the results in the references. Addition of total calculation time is approximately 30% due to increase of nuclide groups to be treated and introduction of the explicit treatment of the neutron up-scattering in the ultra-fine group calculations in the resonance energy domain. It is confirmed that the effect by the neutron up-scattering is also reflected to the core calculation by SCOPE2 in combination with the cross section library generated by the improved AEGIS.

A new cross section model is introduced in SCOPE2 to address the issue of inconsistency with the results by AEGIS for the case with long cooling time. Correlations between microscopic cross sections and number densities of nuclides during cooling are considered in generation of tabulation library for SCOPE2. The coefficients of the correlations are utilized in the reconstruction of the microscopic cross sections in SCOPE2 during burnup calculation. Consistency between AEGIS and SCOPE2 in cooling calculation was greatly improved for the MOX case.

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