PHYSOR 2004 -The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, Lagrange Park, IL. (2004)

Analysis of Benchmark Results for Reactor Physics of LWR Next Generation Fuels

Takanori Kitada[*1], Keisuke Okumura[2], Hironobu Unesaki[3] and Etsuro Saji[4]
[1] *Osaka University, Yamadaoka, Suita-shi, Osaka, 565-0871, Japan*
[2] *Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki, 319-1195, Japan*
[3] *Kyoto University Research Reactor Institute, Kumatori-cho, Sennan-gun, Osaka, 590-0494, Japan*
[4] *Secretariat of the Nuclear Safety Commission, Kasumigaseki 3-1-1, Chiyoda-ku, Tokyo, 100-8970, Japan*

Burnup calculation benchmark has been carried out for the LWR next generation fuels aiming at high burnup up to 70GWd/t with UO_2 and MOX. This paper summarizes the second term (FY2001-2002) activity of "Working Party on Reactor Physics for LWR Next Generation Fuels."

Based on the submitted results, the present status of calculation accuracy for the LWR next generation fuels has been confirmed, and the factors causing the calculation differences were analyzed in detail. Moreover, the future experiments and research subjects necessary to reduce the calculation differences were discussed and proposed.

KEYWORDS: High Burnup, Next Generation Fuel, LWR, Benchmark Calculation, Calculation Accuracy, Validation, Experiment Analysis, PIE

1. Introduction

In order to investigate the calculation accuracy of the nuclear characteristics of LWR next generation fuels, the Research Committee on Reactor Physics organized by Japan Atomic Energy Research Institute has proposed a suite of benchmark problem named "Reactor Physics Benchmark for LWR Next Generation Fuels".[1]

A brief review of the benchmark problem and its preliminary results was reported in Ref.[2]. Based on the preliminary results, the complete specifications of the benchmark problem were finalized and reported in Ref.[3]. The results based on the final specifications were summarized and analyzed.[4-6] Detailed comparisons and analyses of submitted results are currently being executed as the second phase of the benchmark study, aiming at the following objects;

- to identify the cause of the differences between the results in the benchmark results,
- to propose reactor physics experiments desired for clarifying the observed differences,
- to search the best solution of the benchmark based on the results of critical experiment and PIE analysis,
- to examine the demand accuracy of nuclear design parameters, and
- to extract the research topics in the future.

This paper reports what we found so far from the analysis of the benchmark results.

2. Benchmark Problem

The benchmark problems consist of UO_2 fuel and MOX fuel problems, each of which has a pin cell, PWR assembly and BWR assembly configurations. The brief benchmark calculation models are shown in Fig.1 and Ref.[6] shows the details of the benchmark problem with the submitted results of participants.

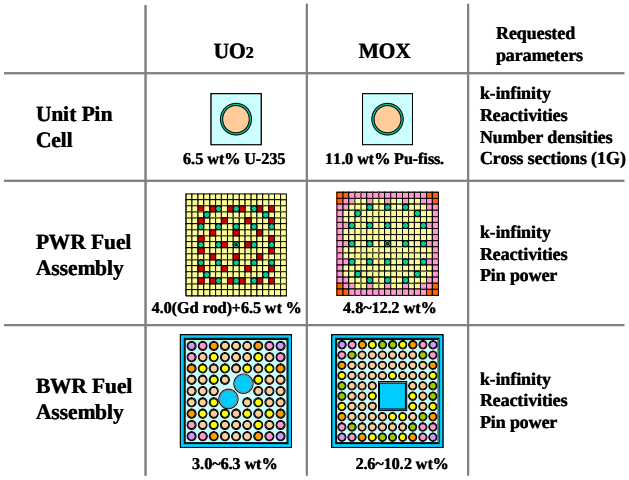


Fig.1 The brief benchmark calculation models

It should be noted that the next generation fuels aim at very high burn-up of about 70GWd/t in PWR or BWR with UO_2 or MOX fuels whose fissile enrichments may exceed the Japanese regulatory limitations for the current LWR fuels such as 5wt.% ^{235}U. Although this benchmark problem could be considered as a straightforward extension of the present LWR fuel design, hardening of neutron spectrum is caused by the higher enrichment and local variation of neutron spectrum is strengthened by the increase of UO_2-Gd_2O_3 rods. Moreover, the influence of the MA and FP becomes more significant because of the increase of burn-up.

3 Participants

The participants and their codes are listed in Table 1. A total of 19 sets of results have been submitted by 13 organizations in the benchmark analysis with different codes and libraries including recently published JENDL-3.3[7]. Some results have been updated since it reports last time.

Table 1 List of benchmark participants and their codes

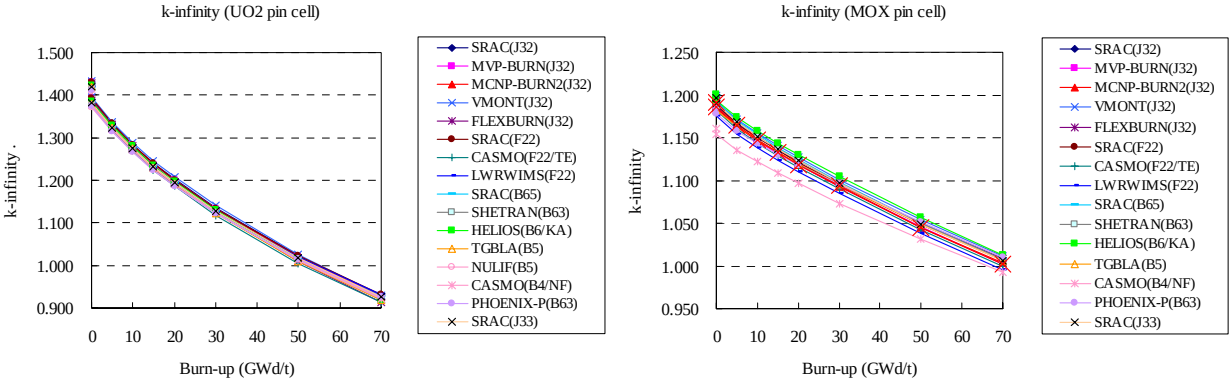
Data Index	Organization	Code	Base Library	Pin Cell		PWR Assembly		BWR Assembly	
				UO2	MOX	UO2	MOX	UO2	MOX
MVP-BURN(J32)	JAERI	MVP-BURN	JENDL-3.2	x	x				
SRAC(J32)	JAERI	SRAC	JENDL-3.2	x	x		x		
SRAC(J33)	JAERI	SRAC	JENDL-3.3	x	x				
SRAC(F22)	JAERI	SRAC	JEF-2.2	x	x				
SRAC(B65)	JAERI	SRAC	ENDF/B-VI(R5)	x	x				
MVP-BURN(J32/KU)	KURRI	MVP-BURN	JENDL-3.2			x	x		
MVP-BURN(J32/OS)	Osaka Univ.	MVP-BURN	JENDL-3.2					x	x
CASMO(F22/TE)	TEPSYS	CASMO4	JEF-2.2	x	x			x	x
CASMO(B4/NF)	NFI	CASMO4	ENDF/B-IV,V	x	x	x	x		x
NULIF(B5)	NFI	NULIF	ENDF/B-V	x					
CASMO(B4/NU)	NUPEC	CASMO4	ENDF/B-IV,V					x	x
SHETRAN(B63)	SEPCO/YONE	SHETRAN	ENDF/B-VI(R3)	x	x	x	x		
TGBLA(B5)	GNF-J	TGBLA	ENDF/B-V	x	x			x	
VMONT(J32)	GNF-J	VMONT	JENDL-3.2	x	x			x	
MCNP-BURN2(J32)	Toshiba	MCNP-BURN2	JENDL-3.2	x	x			x	
FLEXBURN(J32)	CRIEPI	FLEXBURN	JENDL-3.2	x	x	x	x		
LWRWIMS(F22)	EPDC/KCC	LWRWIMS	JEF-2.2	x	x				
PHOENIX-P(B63)	MHI	PHOENIX-P	ENDF/B-VI(R3)	x	x	x	x		
HELIOS(B6/KA)	KAERI	HELIOS	ENDF/B-VI	x	x	x	x		x

4 Analysis of Benchmark Results

The comparison of the benchmark results has been chiefly executed for the results of the pin cell problem by changing the cross section library or burn-up chain model, by using the sensitivity analysis based on the generalized perturbation theory, and by comparing one group effective cross sections.

4.1 k-infinity

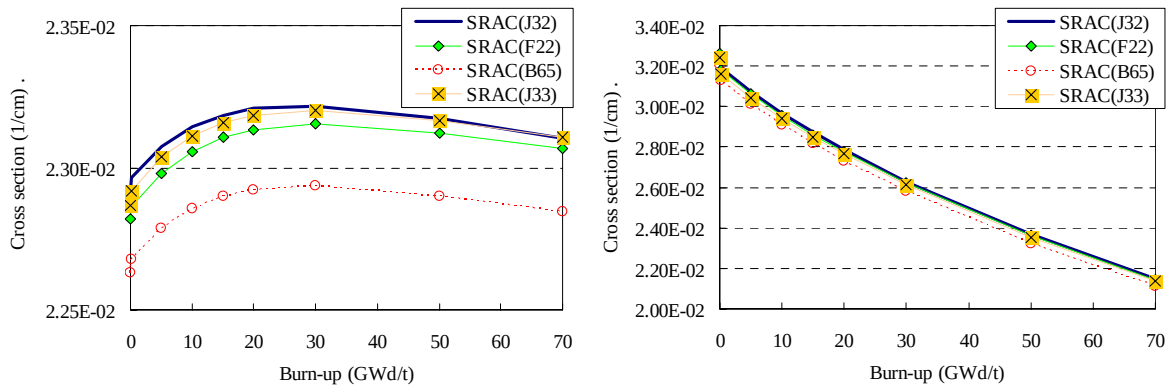
Figure 2 shows the results of k-infinities in the pin cell problems. Maximum difference of k-infinity is almost constant of about 2% during the burnup period in the UO_2 cell problem, and that is about 4% at BOL and 2% at EOL in the MOX cell problem. The maximum difference is mainly caused by the difference of the library between JENDL-3.2 and ENDF/B in the UO_2 cell problem. While the deviation of the k-infinity is small among the results of the SRAC code system with different libraries, the large difference was observed between two CASMO results with different libraries (ENDF/B, JEF-2.2) in the MOX cell problem. From a parametric survey calculation with CASMO, it was found that the difference becomes larger when Pu enrichment is high like this benchmark problem.



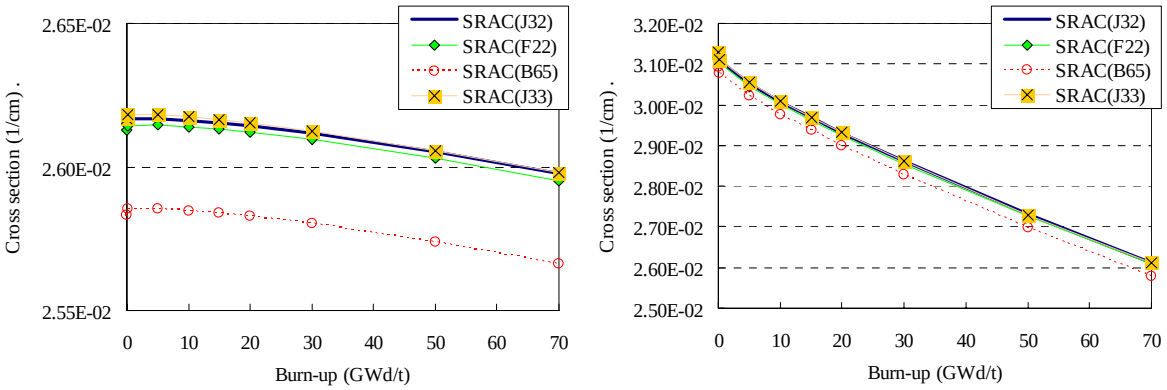
(a) UO_2 cell (b) MOX cell

Fig.2 Comparison of k-infinities in the pin cell problems

Figure 3 shows the cell-averaged one-group macroscopic cross sections calculated by the SRAC code system[8] with different four libraries (JENDL-3.2, JENDL-3.3, ENDF/B-VI(R5) and JEF2.2). ENDF/B-VI(R5) gives the smallest cross sections for all cases, and the difference among the other libraries is small. The k-infinity dependency on the libraries is almost the same degree during the burnup period, therefore the detailed analysis was performed for BOL.



(a) UO_2 cell



(b) MOX cell

Fig.3 Comparison of cell-averaged one-group macroscopic cross sections calculated by SRAC

Table 2 shows the comparison of k-infinity among four libraries (JENDL-3.2, JENDL-3.3, ENDF/B-VI(R5) and JEF2.2) calculated by the SRAC code system at BOL in the UO_2 and MOX cells. To analyze these k-infinity dependency on the libraries in detail, sensitivity analysis was performed. Table 3 shows the contribution of each nuclide and reaction to the k-infinity difference calculated as the product of the relative difference of cross sections and the sensitivity coefficient of the cross section.

Table 2 Comparison of k-infinity at BOL

	UO_2	MOX
JENDL-3.2	1.4292	1.1969
JENDL-3.3	1.4187	1.1972
JEF2.2	1.4311	1.1954
ENDF/B-VI(R5)	1.4189	1.1996

Table 3 Contribution of major isotopes and reaction to k-infinity difference from JENDL-3.2 (%dk/k)

(a) UO_2 cell

	^{235}U capture	^{235}U fission	^{238}U capture
JENDL-3.3	-0.70	-0.16	-0.05
JEF2.2	-0.08	+0.03	-0.08
ENDF/B-VI(R5)	-0.69	-0.16	-0.09

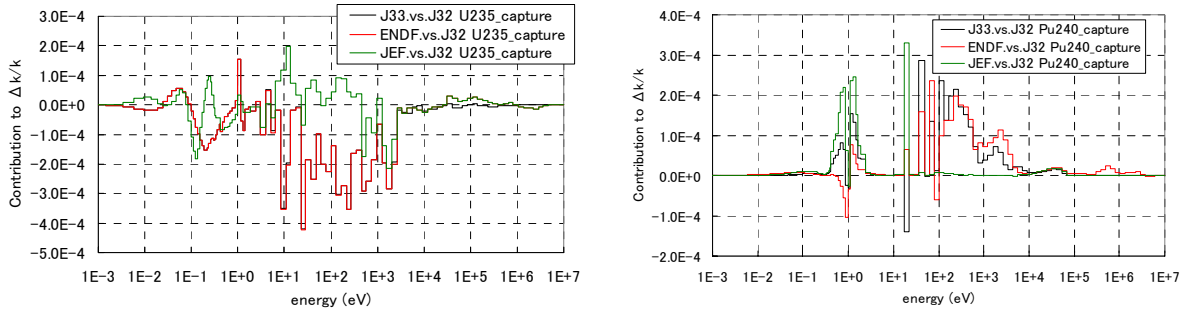
(b) MOX cell

	^{239}Pu capture	^{239}Pu fission	^{240}Pu capture	^{241}Am capture
JENDL-3.3	-0.01	-0.00	+0.30	-0.22
JEF2.2	-0.12	-0.20	+0.23	-0.18
ENDF/B-VI(R5)	+0.03	+0.00	+0.24	-0.08

From these tables, k-infinity dependency on the libraries in the UO_2 cell problem is mainly caused by ^{235}U capture cross section. On the other hand in the MOX cell problem, k-infinity dependency on the libraries is comparatively small. The contribution of individual nuclide to k-infinity difference is canceled each other for JENDL-3.3 and JEF2.2, although the positive contribution of ^{240}Pu capture cross section to k-infinity difference is not canceled for ENDF/B-VI(R5).

The energy dependency of the contribution to k-infinity difference caused by the difference of ^{235}U and ^{240}Pu capture cross sections is shown in Fig.4. JENDL-3.3 and ENDF/B-VI(R5) shows similar energy dependency for both nuclides. In the UO_2 cell problem, ^{235}U capture cross section at the energy range from 10eV to 1keV has a large contribution to k-infinity difference. In the MOX cell problem, the

contribution of ^{240}Pu capture cross section to k-infinity difference is large at the energy range from 30eV to 4keV for JENDL-3.3 and ENDF/B-VI(R5), and at around 1eV and 20eV for JEF2.2.

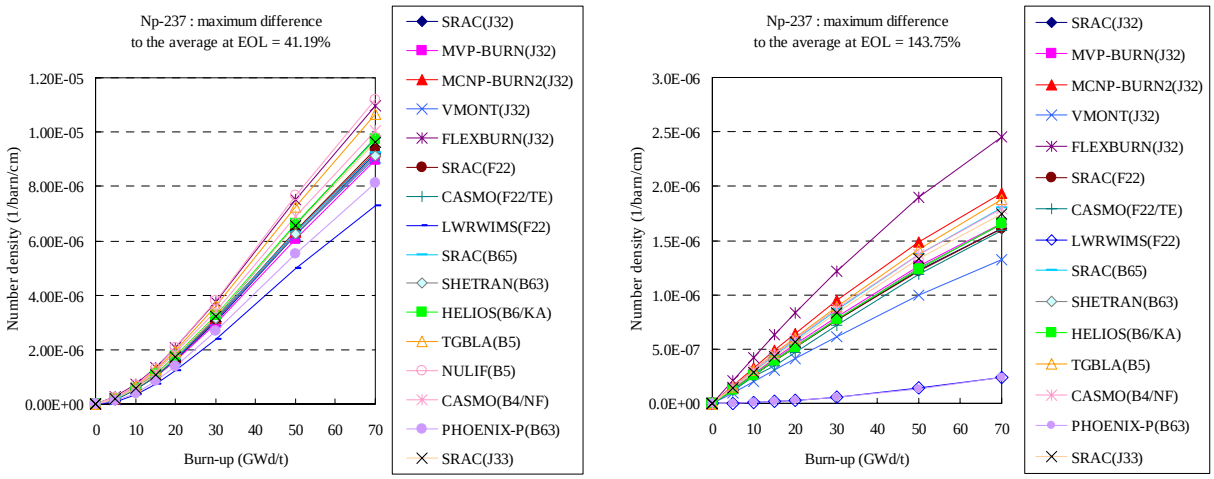


(a) ^{235}U capture cross section (UO_2 cell) (b) ^{240}Pu capture cross section (MOX cell)

Fig.4 Energy dependency of contribution to dk/k caused by the difference among the libraries

4.2 Isotopic Composition

There is a difference more than 20% at 70GWd/t for atomic number density of ^{237}Np, ^{242}Am, Sm etc. The dependency on the libraries is not observed except ^{155}Gd. Therefore it is expected that the burnup chain model and the accuracy of the cross section are the main causes of the difference for atomic number density at EOL.



(a) UO_2 cell (b) MOX cell

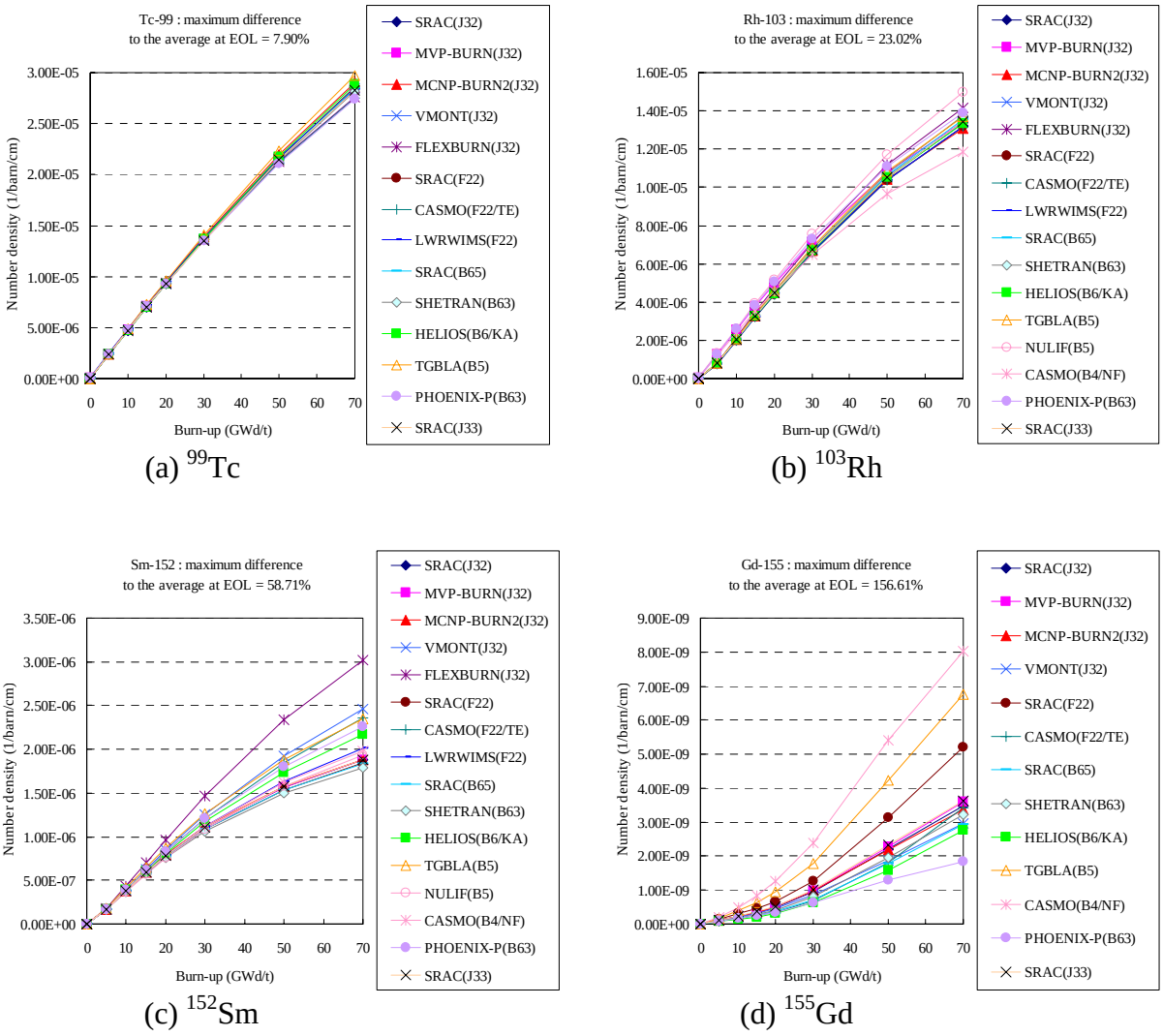
Fig. 5 Results of atomic number density of ^{237}Np

For ^{237}Np, the difference of the number density is larger in the MOX cell problem than the UO_2 cell problem as shown in Fig.5. To clarify the fact, it is necessary to consider that there are two producing routes of ^{235}U-^{236}U-^{237}U-^{237}Np and ^{238}U-^{237}U-^{237}Np and the second route is predominant in the MOX cell problem. It is thought there is a large ambiguity in the cross section of ^{238}U (n,2n) reaction included in the second route. Because many codes disregard the reaction above 10MeV, statistical uncertainty of (n,2n) reaction is large in Monte Carlo calculation and there is a little verification of (n,2n) cross section having a low importance to the neutronic properties. The lowest two results in Fig.5 can be almost reproduced by the SRAC calculation when the second route from ^{238}U (n,2n) reaction is ignored in the burnup chain model.

The atomic number density of Sm isotopes shows relatively large difference at EOL among FP isotopes as shown in Fig.6(c). This result comes from the facts: complexity of burnup chain model including Sm isotopes, existence of the isotopes with resonance absorption and difference of the isomeric ratio of ^{147}Pm capture reaction. Especially to suppress the large difference of ^{152}Sm, it was found from the verification results of the SRAC code system that the self-shielding effect of the resonance around 8.0eV has an important role.

The difference of ^{99}Tc is small and the number density is proportional to burnup period. This shows that the number density of ^{99}Tc is dominant to the fission yield and has a little dependency on the cross section and burnup chain model. On the other hand, it was found that the difference of ^{103}Rh comes from the different treatment of the burnup chain with or without considering the decay of ^{103}Ru($T_{1/2}$=39d).

The large difference of ^{155}Gd in Fig.6(d) is mainly attributed to the differences of thermal capture cross sections of ^{154}Eu, ^{155}Eu and ^{154}Gd. Especially, the results based on JEF-2.2, ENDF/B-IV and ENDF/B-V, whose thermal capture cross sections of ^{154}Eu are common, gives larger atomic number density of ^{155}Gd compared with the JENDL-3.2/-3.3 and ENDF/B-VI results.



(a) ^{99}Tc (b) ^{103}Rh

(c) ^{152}Sm (d) ^{155}Gd

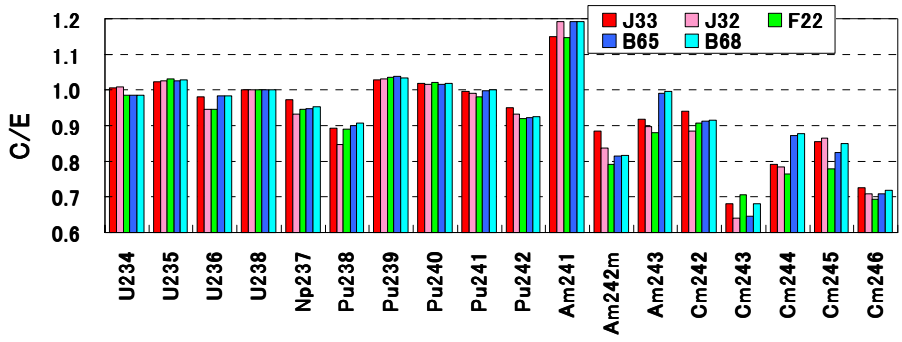
Fig. 6 Results of atomic number density in UO_2 cell problem

4.3 Best Solution of Benchmark Results

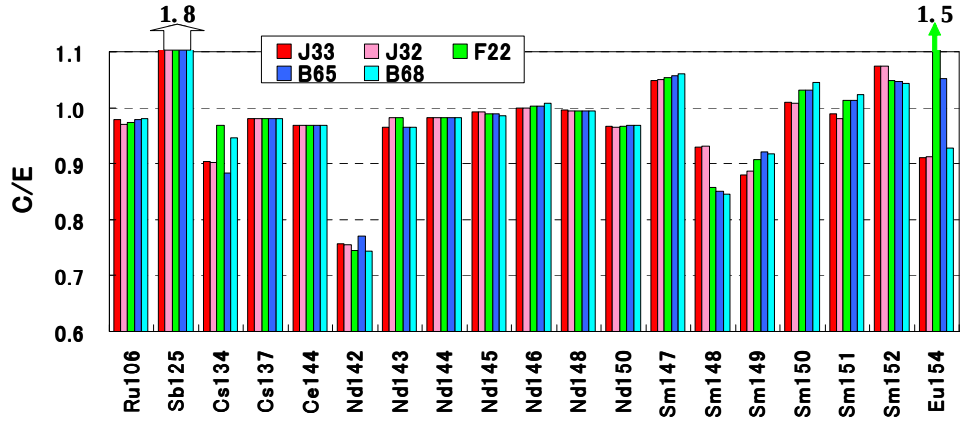
We tried to guess the best solution of the benchmark results through the comparison of the results by the SRAC code system between the benchmark problem and PIE data for irradiated UO_2 fuel rods. It is noticed that the enrichment of ^{235}U is different between the benchmark problem (6.5wt%) and the PIE data (4.1wt%). Figure 7 shows the averaged C/E values of heavy isotopes and FP isotopes for the sample fuels irradiated in the range from 14 to 47GWd/t in a commercial PWR. Here, ^{237}Np and ^{152}Sm are selected as examples, because of the small standard deviation of the measured data and the large standard deviation of the calculation results for these isotopes.

The analysis results of PIE data by the SRAC code system for the number density of ^{237}Np show the underestimation of about 5% regardless of the library used as shown in Fig.7(a). On the other hand, the number density of ^{237}Np obtained by the SRAC code system in the benchmark results shows a little low value in the spread omitting the lowest two results shown in Fig.5(a). From these considerations, the best solution for ^{237}Np is expected to be around the middle point in the spread of the benchmark results omitting the lowest two results.

The analysis results of PIE data show the overestimation of about 5% for the number density of ^{152}Sm as shown in Fig.7(b), and the benchmark results shows a little low value in the spread of benchmark results shown in Fig.6(c). From these considerations, the best solution for ^{152}Sm is expected to be lower end of the spread of the benchmark results.



(a) Heavy isotopes



(b) FP isotopes

Fig. 7 C/E value of number density from PIE Analysis with SRAC for a current PWR

Although ^{155}Gd is not measured in PIE, it is found that JEF-2.2 significantly overestimates atomic number density of ^{154}Eu. Thus it is recommended to use more recent nuclear data for Eu isotopes to obtain the best solution for ^{155}Gd.

4.4 Research Topics in Future

There are some proposals to reduce the large variance of the calculation results and to estimate the best solution among them: calculation of "reference" results of the benchmark problems for verification of the analysis method and acquisition of experimental data with high reliability for verification of the libraries.

The burnup results of two different continuous-energy Monte Carlo codes based on JENDL-3.2 show good agreements in most cases. Therefore, the Monte Carlo codes can be used to obtain "reference" results from the view point of the analysis method. It should be noted that the results are dependent on the library used.

The followings are required to find the true solution of the benchmark problem.

- Critical experiments as a function of enrichment of ^{235}U or Pu and Pu vector covered the benchmark problem
- Development of the method to measure accurately a Doppler reactivity in the thermal neutron field
- Accurate PIE data of ^{103}Rh, ^{155}Gd etc. which have large difference in the benchmark results

Acknowledgements

The authors wish to thank all participants of this benchmark activity for four years. Thanks are also due to all members of the Working Party on LWR Next Generation Fuels organized in the Research Committee of Reactor Physics, for their continuous effort on finalizing and analyzing the benchmark problems and for their valuable discussions and comments.

References

1) Research Committee on Reactor Physics, "Proposal and Analysis of the Benchmark Problem Suite for Reactor Physics Study of LWR Next Generation Fuels," JAERI-Research 2001-046 (2001) [in Japanese].
2) E. Saji, "Proposal and Analysis of the Benchmark Problem Suite for Reactor Physics Study of LWR Next Generation Fuels," Trans. Am. Nucl. Soc. **86**, 330 (2002).
3) A. Yamamoto, T. Ikehara, T. Ito and E. Saji, "Benchmark Problem Suite for Reactor Physics Study of LWR Next Generation Fuels," J. Nucl. Sci. Technol., **39**[8], 900 (2002).
4) K. Okumura, H. Unesaki, T. Kitada and E. Saji, "Benchmark Results of Burn-up Calculations for LWR Next Generation Fuels," Proc. Int'l. Conf. On the New Frontiers of Nuclear technology: Reactor Physics, Safety and High-Performance Computing (PHYSOR2002), 9A-03 (2002).
5) H. Unesaki, K. Okumura, T. Kitada and E. Saji, "Update Status of Benchmark Activity for Reactor Physics Study of LWR Next Generation Fuels", Trans. Am. Nucl. Soc. **88**, 436 (2003).
6) http://hachi.tokai.jaeri.go.jp/Committee/LWR-benchmark/
7) K.Shibata, T. Kawano et al., "Japanese Evaluated Nuclear Data Library Version 3 Revision-3 : JENDL-3.3," J. Nucl. Sci. Technol., **39**[11], 1125 (2002).
8) K. Okumura, K. Kaneko and K. Tsuchihashi, "SRAC95: General Purpose Neutronics Code System," JAERI-Data/Code 96-015 (1996) [in Japanese].