Criticality Benchmarks with a Continuous-Energy Monte Carlo Code MVP and JENDL-3.3

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Abstract - Criticality benchmark testing of JENDL-3.3 was performed with MVP for many critical experiments in the ICSBEP Handbook: highly enriched uranium (HEU) and low enriched uranium (LEU) fueled solutions, LEU fueled water-moderated lattices, MOX fueled water-moderated lattices and metal fueled small assemblies with hard neutron spectra. The calculations with the preliminary U235 and U238 data for ENDF/B-VII (preVII) are also made for some benchmarks to confirm their performances and to compare with the JENDL-3.3 results. The prediction accuracy of criticality with JENDL-3.3 is satisfactory, within ±0.5%Δk in most cases, except for slightly enriched uranium fueled lattices. The preVII data of U238 with lower thermal capture cross section improves the under prediction of k_{eff} for the slightly enriched lattices, while slight overestimations were observed for the LEU lattices whose U235 enrichment is more than 3wt.%. On the other hand, the preVII data gives excellent results for the metal fueled assemblies compared with JENDL-3.3.

1. INTRODUCTION

In order to clarify problems of JENDL-3.3[1] and to prepare a database for integral testing of next JENDL, an enormous number of criticality benchmark analyses are now under way by using a continuous-energy Monte Carlo code MVP[2] and its library based on JENDL-3.3. The benchmark problems are taken from the Handbook of the International Criticality Safety Benchmark Evaluation Project, so called ICSBEP Handbook[3], which covers various fuel materials (enriched ^{233}U, ^{235}U, Pu, their mixtures), fuel forms (compound, metal, solution, and their mixed ones), neutron spectra (thermal, intermediate, fast). The total number of selected benchmark cases is more than 900. For these cases, MVP calculations tracing 20 million neutrons will be finished by the end of FY2004. In addition, full sets of alternative MVP libraries based on ENDF/B-VI.8 and JEFF-3.0 have been completed[4]. In the present work, a part of the benchmark results are shown from the database.

Recently, excellent benchmark results[5] are presented by R. E. MacFarlane using preliminary evaluations for ENDF/B-VII (preVII), which are opened on the web site of LANL. It is reported that the new evaluations for U235 and U238 significantly improve prediction accuracy of criticalities for small metal fueled assemblies with hard neutron spectra (Godiva, Jezebels, Flattops, etc.), and improve under prediction of low enriched uranium fueled lattices moderated by water (TCA, TRX, etc). The under prediction is common problem not only for ENDF/B-VI.8[6] but also for JENDL-3.3 and JEFF-3.0[7].

To confirm performances of the preVII data, our benchmark results with JENDL-3.3 are compared with MacFarlane's results with MCNP5. In addition, we investigated the replacement effects of the JENDL-3.3

libraries for U235 and U238 by those based on the preVII data.

2. HIGHLY OR LOW ENRICHED URANIUM FUELED SOLUTIONS

Table 1 shows the comparison of the C/E values of k_{eff} between our JENDL-3.3 results and the preVII results[5] by MacFarlane. As far as the 27 cases of benchmark problems selected by MacFarlane are concerned, both results show very good agreement with the experimental data, and any superiority of the preVII data over JENDL-3.3 are not found, considering the uncertainties of benchmark-k_{eff} in Table 1.

Table 1 Comparison of C/E* values of k_{eff} between JENDL-3.3 and preVII results[5] for highly enriched uranium or low enriched solutions with thermal neutron spectra

Benchmark ID[a)]	Number of cases[b)]	J33 (MVP)		preVII (MCNP5)		Ave. uncertainty[c)] of benchmark-keff	Feature of problems
		Ave. C/E	Std. Dev.	Ave. C/E	Std. Dev.		
HST42	6	1.0011	0.0006	1.0006	0.0008	±0.0036	Low-leakage nitrate solutions
HST1	4	0.9989	0.0025	1.0006	0.0008	±0.0025	Mid-leakage nitrate solutions
HST9	2	1.0005	0.0005	1.0005	0.0000	±0.0057	High-leakage Fluoride solutions
LST7, LST21	8	0.9993	0.0009	0.9996	0.0008	±0.0010	Unreflected LEU solutions
LST4, LST20	7	1.0001	0.0008	1.0004	0.0009	±0.0009	Reflected LEU nitrate solutions

a) Shorthand of benchmark problem ID in ICSBEP to specify a series of experiments in a facility
(e.g. HST42 corresponds to HEU-SOL-THERM-042, LST7 corresponds to LEU-SOL-THERM-007)
b) Number of benchmark cases with different critical configurations (fuel concentrations, critical heights, etc.) selected by MacFarlane
c) Average value of evaluated uncertainties mainly caused by measurements and modeling

In the ICSBEP Handbook (Ed.2003), 432 and 90 cases of benchmark problems are stored in the HEU-SOL-THERM (HST) and LEU-SOL-THERM (LST) categories, respectively. Among them, we selected 52 and 76 cases for our database, from the viewpoints of appropriateness to benchmark testing of nuclear data, that is to say, uniformity of fuel, variety of changed physics parameters, simplicity of core configuration, easy convergence of Monte Carlo eigenvalue calculation (single unit assembly), and so on.

Figures 1 and 2 show the obtained C/E values with JENDL-3.3 plotted versus H/U235 atom ratio. The prediction accuracy of JENDL-3.3 is satisfactory (within about ±0.5%Δk) for both LEU and HEU fueled solutions. However, a slight trend of C/E values are observed in the LST cases (LST16-19: STACY 28cm-thick slab experiments), when U235 concentration, and simultaneously leakage in most cases, becomes larger. Future benchmark testing of next JENDL for solution systems should be carried out with a focus on this trend.

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* In the present work, a C/E value is defined as calculated k_{eff} over benchmark-k_{eff} evaluated in ICSBEP which may includes small bias due to benchmark modeling. The error bar in all figures means uncertainty of benchmark-k_{eff} evaluated in ICSBEP. In the error bar, statistical error of Monte Carlo calculation is not included, because it is smaller or comparable, compared with size of marker in figures.

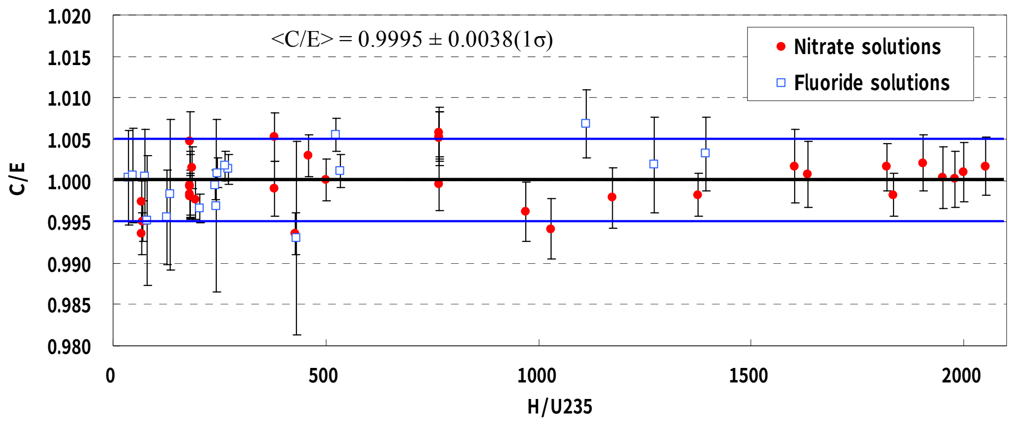

Fig.1 C/E values of k_{eff} with JENDL-3.3 for highly enriched uranium fueled solutions (all configurations in HEU-SOL-THERM-1,4,9,10,11,12,13,32,35,42,43)

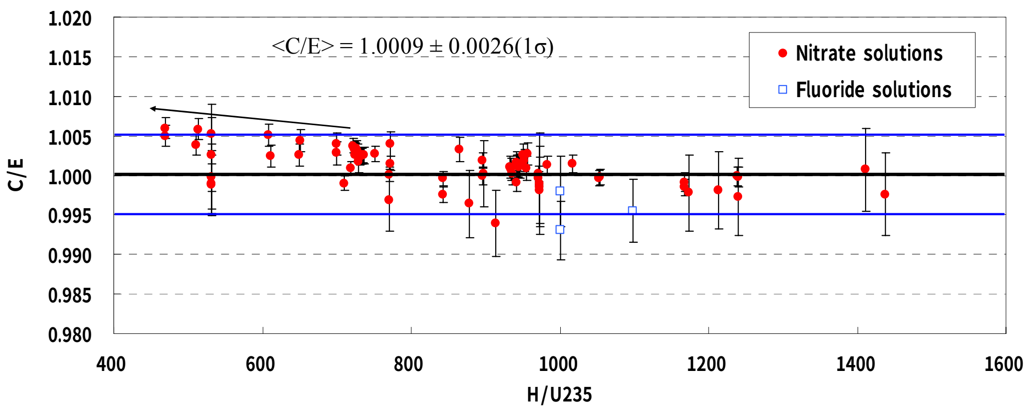

Fig.2 C/E values of k_{eff} with JENDL-3.3 for low enriched uranium fueled solutions (all configurations in LEU-SOL-THERM-2, 3, 4, 5, 6, 7, 8, 9, 10, 16, 17, 18, 19, 20, 21)

3. LOW ENRICHED URANIUM FUELED LATTICES MODERATED BY WATER

Under prediction of k_{eff} for LEU fueled assemblies moderated by water is a common problem of recent nuclear data files. As shown in Fig.3, the under prediction becomes more serious when U235 enrichment becomes lower. Therefore, it is important to select experimental data which cover wide range of U235 enrichments especially for lower ones. From this point, several benchmarks out of the ICSBEP handbook are added here, they are TRX-1&2[8], KRITZ2-1&13[9]. The MVP result for MISTRAL-1[10] by NUPEC is also added. All of the assemblies selected here are uniform lattices consist of a kind of cylindrical fuel rods, whose material forms are UO_2 except for TRX cores using metal-U.

Figure 4 shows the comparison among the following four sets of results: 1) all nuclide data are based on JENDL-3.3 (specified as J33), 2) U235 and U238 are based on the preVII data and others are based on JENDL-3.3 (U5U8preVII+J33), 3) only U238 is based on the preVII data (U8preVII+J33), 4) the preVII results[5] presented by MacFarlane with MCNP5.

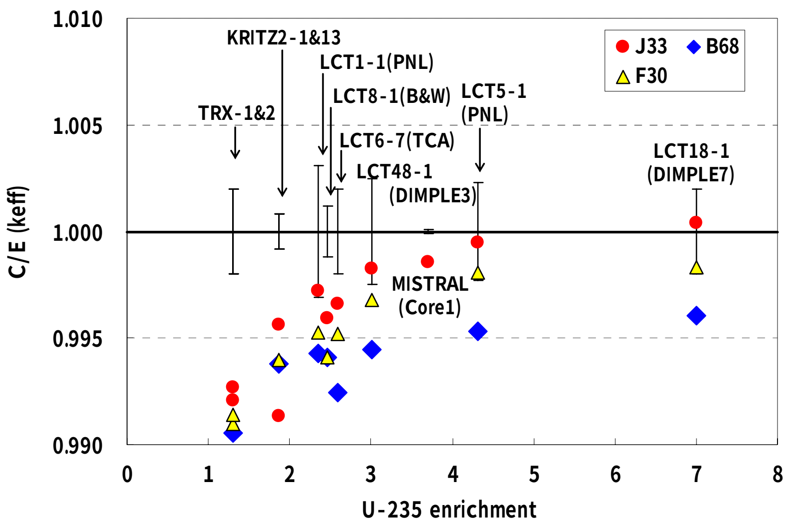

Fig.3 Dependence of C/E on U235 enrichment in LEU fueld water-moderated lattices (J33:JENDL-3.3, B68:ENDF/B-VI.8, F30:JEFF-3.0)*

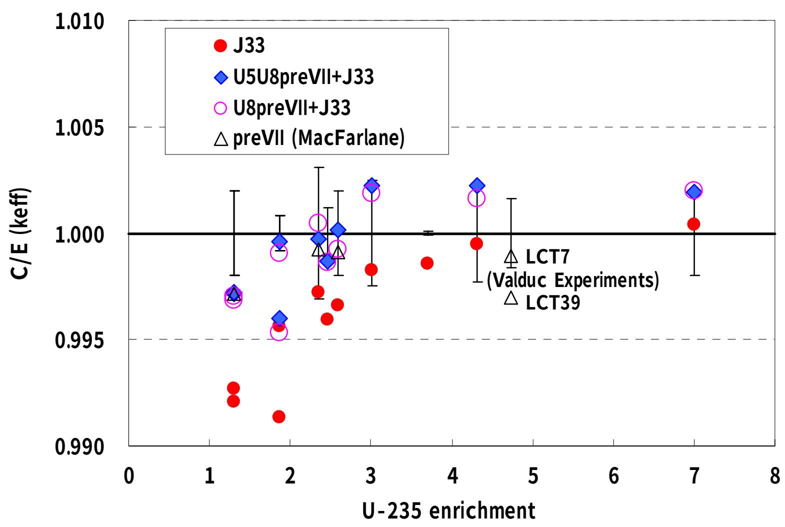

Fig.4 Comparison of C/E results by using the preVII data of U235 and U238

The dependence of the C/E on U235 enrichment is mitigated by using the preVII data of U238, while slight over predictions by about 0.25%Δk are observed for our benchmark problems (LCT48, LCT5, LCT18) where U235 enrichments are more than 3 wt.%. Benchmark data with MVP have not prepared yet for the Valduc experiments (LCT2 and LCT39), for which relatively lower C/E values are presented by MacFarlane using the preVII data.

The improvement in the preVII results is thought to be mainly due to the lower U238 thermal capture cross section (2.680 barn at 2200m/sec), compared with other evaluations (e.g. 2.717 barn in JENDL-3.3).

* For all B68 and F30 calculations in the present work, isotope-wise nuclear data library were used for the impurities or structure materials with natural compositions, where the JENDL-3.3 libraries were used only for the isotopes not evaluated in ENDF/B-VI.8 or JEFF-3.0 (isotopes of Mg, S, Cl, K, Ca, Ti, Ga).

The U238 thermal capture cross section is sensitive to dependence of k_{eff} on U235 enrichment especially when the enrichment becomes lower than 3 wt.%. This can be explained by the following relation between macroscopic thermal η–value and U235 enrichment w^{235}.

$$\eta = \frac{N^{235}\nu\sigma_f^{235}}{N^{235}\sigma_a^{235} + N^{238}\sigma_a^{238}} \approx \left\{\frac{\nu\sigma_f^{235}}{\sigma_a^{235}}\right\} \cdot \left\{\frac{1}{1+(\frac{N^{238}}{N^{235}})(\frac{\sigma_c^{238}}{\sigma_f^{235}})}\right\} \equiv \eta^{235} \cdot F(w^{235}), \qquad \text{(Eq.1)}$$

where, σ and N denote condensed microscopic cross sections in thermal energy range and atomic number densities, respectively. The function $F(w^{235})$ has the shape like shown in Fig. 5, where 2200 m/s values of JENDL-3.3 are assumed for the condensed thermal cross sections of U235 for convenience. Thus the systematic under prediction of k_{eff} observed in Fig.3 has strong correlation with thermal η–value and it is sensitive to thermal U238 capture cross section. On the other hand, other three factors (p, ε, f) of k-infinity have not strong correlations on U235 enrichments. This fact was confirmed by calculating four factors of k-infinities with MVP for the infinite unit cells of the benchmark problems here.

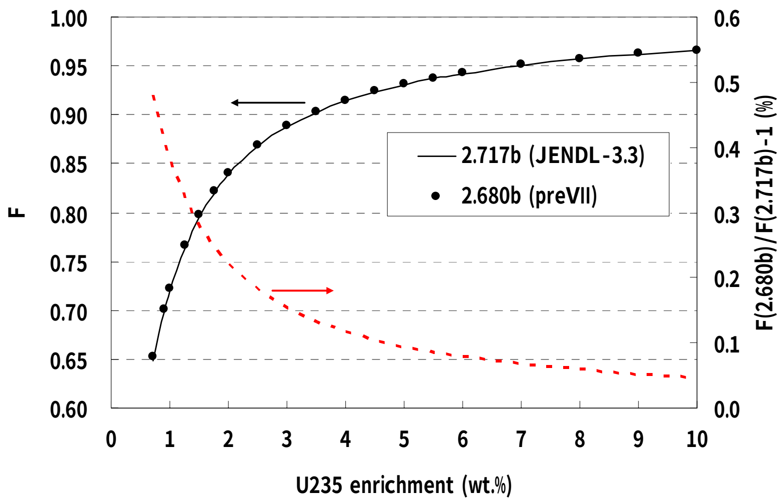

Fig.5 Dependence of function F on U235 enrichment and U238 thermal capture cross section

Further and more detailed benchmark testing including spectral indices are necessary. In addition, well-evaluated experimental data are expected for the water-moderated uranium fueled lattices whose U235 enrichment is less than 2.0 wt.%.

4. MOX FUELED LATTICES MODERATED BY WATER

MVP calculations with JENDL-3.3 have been carried out for 63 cases of MOX fueled water-moderated lattices selected from the ICSBEP benchmarks categorized in MIX-COMP-THERM (MCT). The selected benchmark problems and the ranges of typical physics parameters are shown in Table 2. The obtained C/E values were plotted on a graph for each of physics parameters like leakage, thermal fission rate, and so on, besides the parameters specified in Table 2. Typical graphs are shown in Fig.6(a)-(c).

Table 2 Ranges of physics parameters of thermal MOX fuel benchmarks

Physics parameters	Range of parameter	Selected benchmark problems MIX-COM-THERM (MCT)
Pu/(U+Pu)	1.5~6.6 and 22.5 [%]	MCT1 (1~4), MCT2 (1~6), MCT3 (1~6), MCT4 (1~11), MCT5 (1~7), MCT6 (1~6), MCT7 (1~5), MCT8 (1~6), MCT9 (1~6)
Pu239/Pu	68~92 [%]	
Pu240/Pu	8~24 [%]	
Am241/Pu	590~12540 [ppm]	
H/H.M.	3.5~53.4	

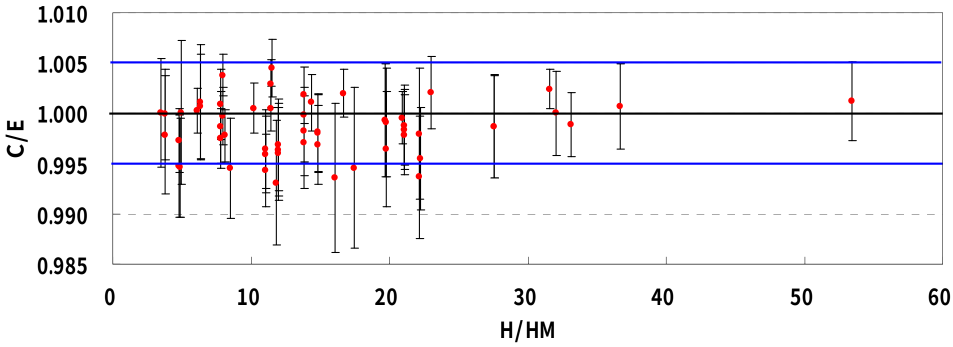

Fig. 6 (a) C/E (k_{eff} with JENDL-3.3) vs H over Heavy Metal atom ratio in MCT benchmarks

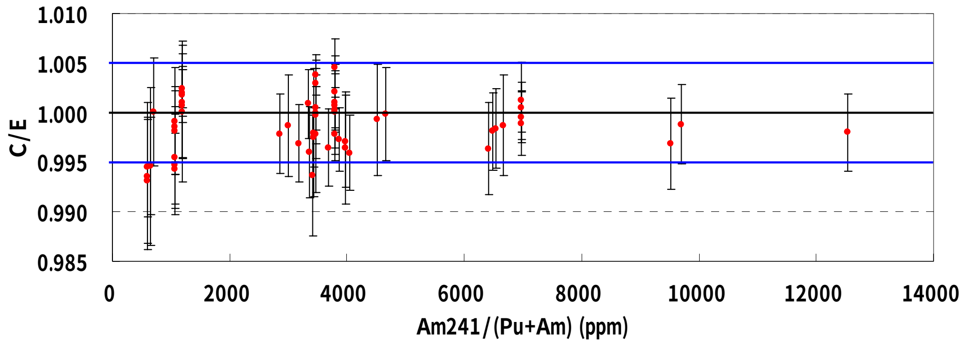

Fig. 6 (b) C/E (k_{eff} with JENDL-3.3) vs Am contents in MCT benchmarks

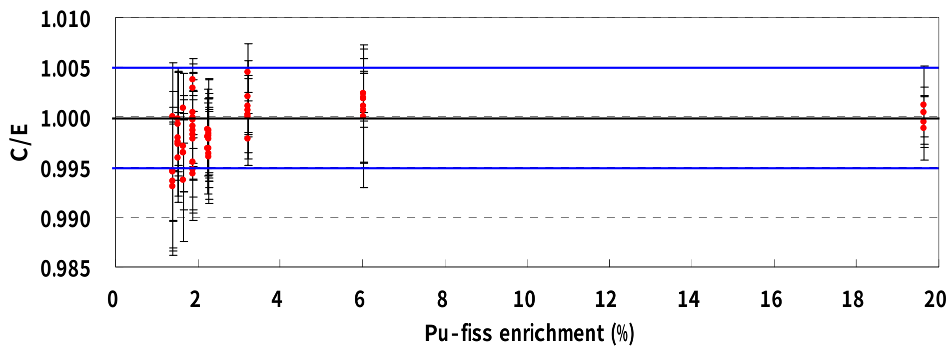

Fig. 6 (c) C/E (k_{eff} with JENDL-3.3) vs fissile Pu enrichment in MCT benchmarks

The average C/E value and its standard deviation are 0.9985 and 0.0027, respectively. Although significant trends were not observed on the considered physics parameters, a slight dependence on fissile plutonium enrichment appears in lower enriched cases. If this dependence is due to the same reason concerning to the U238 thermal capture cross sections at the LEU fueled lattices, it may be eliminated by using the preVII data. The effect of the preVII data has not investigated for the MOX-thermal problems.

5. METAL FUELED SMALL ASSEMBLIES

At the last, benchmark results with JENDL-3.3 for metal fueled small assemblies with hard neutron spectra (See Table 3) are shown in comparison with the results obtained by using the preVII data of U235 and U238. The problems are well known fast reactor benchmarks by CSEWG[8], but benchmark-k_{eff} (E-value) and calculation models are taken from the ICSBEP Handbook.

All calculated results are shown in Figure 7, where the meanings of the captions in the figure are the same as described in Chapter 1.

Table 3 Benchmark problems for metal fueled small assemblies

Assembly names	Fuel of Core (wt.%)	Reflector	Assembly names	Fuel of Core (wt.%)	Reflector
Godiva	U235(94)	No	Flattop-Pu	Pu239(95)	Nat.U
Flattop-25	U235(93)	Nat.U	PMF11(ICSBEP)	Pu239(94)	Water
Bigten	U235(10)	Nat.&Dep.U	Thor	Pu239(95)	Th-232
HMF4(ICSBEP)	U235(96)	Water	Jezebel-233	U233(98)	No
Jezebel	Pu239(95)	No	Flattop-233	U233(98)	Nat.U
Jezebel-240	Pu239(76)	No			

HMF4 (HEU-METAL-FAST-004) and PMF11(PU-MET-FAST-011) are problems selected by MacFarlane[5]

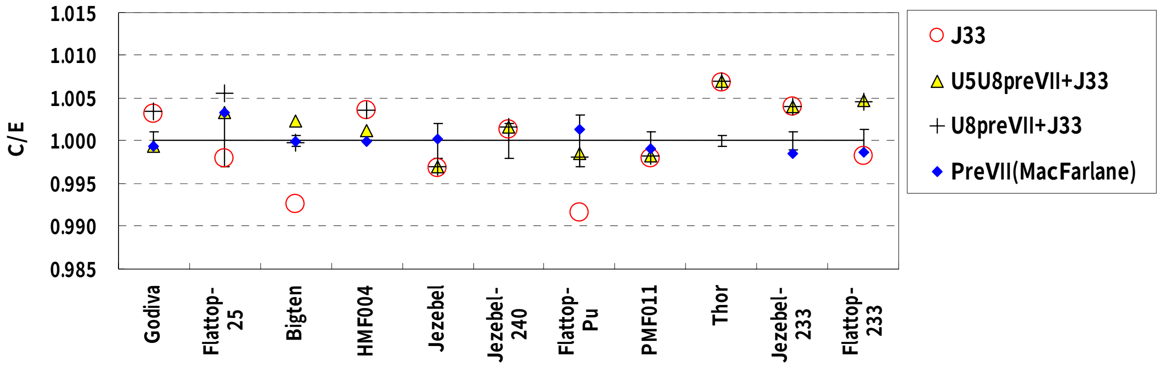

Fig.7 Benchmark results for metal fueled small assemblies

In comparison with the pure JENDL-3.3 results (J33), the U235 data of preVII has an effect to decrease k_{eff} by about 0.2-0.4%Δk for the HEU fueled bare assemblies: Godiva, Flattop-25 and HFM4. On the other hand, the U238 data of preVII has an effect to increase k_{eff} by about 0.7%Δk for the assemblies which have natural or depleted uranium reflectors: Flattop-25, Bigten, Flattop-Pu and Flattop-233. Consequently, the preVII data of U235 and U238 give more excellent results than JENDL-3.3 for uranium or plutonium fueled assemblies except for Thor whose reflector is pure Th-232. Although the C/E value for Flattop-233 deviates from unity when the preVII data of U238 is used with JENDL-3.3, it seems consistent with the jezebel-233 result. It may be interesting to investigate effects of the preVII data for U233 and Th232.

6. CONCLUSIONS

Criticality benchmark testing of JENDL-3.3 was performed with MVP for many critical experiments in the ICSBEP Handbook: HEU and LEU fueled solutions, LEU fueled water-moderated lattices, MOX fueled water-moderated lattices and metal fueled small assemblies with hard neutron spectra. The calculations using the preliminary U235 and U238 data for ENDF/B-VII (preVII) are also made for comparisons.

The prediction accuracy of criticality with JENDL-3.3 is satisfactory, that is within ±0.5%Δk in most cases, except for slightly enriched uranium fueled lattices. The preVII data of U238 with lower thermal capture cross section improves the under prediction of k_{eff} for the slightly enriched lattices, while slight overestimations were observed for the LEU lattices whose U235 enrichment is more than 3wt.%. On the other hand, the preVII data give excellent results for the metal fueled assemblies with hard neutron spectra compared with JENDL-3.3.

REFERENCES

[1] K. Shibata, *et al.*: "Japanese Evaluated Nuclear Data Library Version 3 Revision-3: JENDL-3.3," J. Nucl. Sci. Technol. 39, 1125, (2002).

[2] Y. Nagaya, T. Mori, K. Okumura and Y. Nakagawa: "MVP/GMVP: General Purpose Monte Carlo Codes for Neutron and Photon Transport Calculations based on Continuous Energy and Multigroup Methods Version 2," to be published in JAERI report (2005).

[3] NEA Nuclear Science Committee: "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NSC/DOC(95)03, Sep. 2003 Edition.

[4] T. Mori, Y. Nagaya, K. Okumura and K. Kaneko: "Production of MVP Neutron Cross Section Libraries Based on the Latest Evaluated Nuclear Data Files," JAERI-Data/Code 2004-011 (2004) [in Japanes].

[5] R. E. MacFarlane: "Testing New Actinide Cross Sections Proposed for ENDF/B-VII," Proc. of Int. Conf. on Nuclear Data for Science and Technology (ND2004), Santa Fe, Sep.26-Oct.1, (2004).

[6] (Comp. and Ed.) P.F. Rose: "ENDF-201, ENDF/B-VI Summary Documentation, " BNL-NCS-17541, 4th Edition (1991). See also WWW page of Cross Section Evaluation Working Group (CSEWG), http://www.nndc.bnl.gov/csewg/, National Nuclear Data Center, BNL.

[7] R.Jacqmin, R.Forrest, J.Rowlands, A.Nouri and M.Kellett: "Status of the JEFF-3 Project," J. Nucl. Sci. Technol., Suppl. 2, Vol.1, 54 (2002).

[8] "ENDF-202, Cross Section Evaluation Working Group Benchmark Specifications," BNL 19302 (ENDF-202), (1974).

[9] I. Remec, *et al.*: "OECD/NEA KRITZ-2 UO_2 and MOX Benchmark," Proc. of Int. Conf. PHYSOR2002, 11B-03, Seoul, Korea, 7-10 October, (2002).

[10] A. Zukeran: "JENDL Reactor Constant and its Application," Proc. of the 2003 symposium on Nuclear Data, pp.103-110, Nov. 27-28, 2003, Tokai, Japan, JAERI-Conf 2004-005 (2004).