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Comparison of ENDF/B-VII.1, ENDF/B-VIII.0, and JEFF 3.3 Nuclear Data Libraries on Criticality Calculation Using WIMS/CITVAP Code

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ABSTRACT

This paper presents the work carried out during the first year of the research contract No. 24284 titled "accuracy evaluation of available fission yield data and updating" under the umbrella of the Coordinated Research Project (CRP): "updating fission yield data for applications" organized by the International Atomic Energy Agency (IAEA) with the main objective of updating the evaluated independent and cumulative fission yield data for U-235, U-238, and Cf-252. In this research, the latest ENDF/B-VIII.0 and JEFF3.3 data libraries that were released in 2018 and 2017, respectively, as well as the ENDF/B-VII.1 data library, were tested on the ETRR-2 using WIMS-5B/CITVAP computational codes. Since the reactor criticality calculations are very sensitive to the accuracy of the data libraries, criticality benchmarks were selected in the work for the evaluation of these libraries. The results showed that the JEFF3.3 library has better agreement with the measurements than the ENDF/B-VIII.0 library. But the ENDF/B-VIII.0 library result is within the accepted range.

INTRODUCTION

The data on fission yield is essential for the accuracy of nuclear reactor calculations and waste management. System criticality and core cycle length calculations are highly dependent on neutron poisons such as Xenon (Xe-135) and samarium (Sm-149). Calculations of delayed neutron fraction are affected by delayed neutron precursors such as bromine (Br-87), cesium (Cs-142), and iodine (I-137). Evaluation of fissile nuclides (such as residual uranium U-235 and Plutonium nuclides) and/or recovery of valuable fission nuclides (such as Molybdenum (Mo-99), Iodine (I-131), Cesium (Cs-137), etc.) is a crucial step before processing spent fuel. Evaluation of spent fuel issues such as criticality safety, decay heat output, neutron emissions, radiotoxicity, and environmental impact for transportation and storage relies heavily on fission yield statistics. As a last stage, an evaluation of the source terms of radioactivity and decay temperatures from radioactive components in spent nuclear fuels is required for the assessment of nuclear accidents.

The ENDF/B-VIII.0 [1] and JEFF 3.3 [2] evaluated nuclear data libraries were released on December 2017 and February 2018 respectively with significant updates. The accuracy of the nuclear data libraries needs to be verified and tested. Benchmarks can provide a good test of the accuracy of the unclear data and can point to deficiencies that need to be resolved.

The International Atomic Energy Agency (IAEA) has initiated a Coordinated Research Project (CRP) entitled "updating fission yield data for applications" with the primary goal of updating the evaluated independent and cumulative fission yield data for U-235, U-238, and Cf-252. One of the primary goals of this study is to evaluate the accuracy of the available fission yield statistics by simulating a series of nuclear reactor calculation benchmarks. Numerous computational operations have been conducted for this goal.

Ouadie Kabach et al, [3] conducted a comparison research using the most recently evaluated nuclear data libraries, JEFF-3.3 and ENDF/BVIII.0. The research was carried out utilizing benchmark calculations for 120 criticality problems and the TRIGA Mark II research reactor, with libraries handled using the NJOY21 Monte Carlo transport algorithm. The JEFF-3.3 and ENDF/B-VIII.0 data libraries' calculation results were determined to be extremely promising. It's worth noting that the

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performance of the JEFF-3.3 and ENDF/B-VIII.0 data libraries is satisfactory during the comparison calculation. Their impact, on the other hand, could be measured qualitatively.

LEI ZHENG et al, [4] presented the criticality benchmarking of the new versions of JEFF-3.3 and ENDF/B-VIII.0 and compared them with ENDF/B-VII.1 neutron data libraries to make a more comprehensive impact on the criticality quality of the most advanced neutron data libraries and to present a reference for the determination of the evaluated nuclear data libraries for the science and engineering applications of the RMC (Reactor Monte Carlo code). 116 benchmarks were established for the RMC criticality validation. All calculations were done utilizing a parallel version of RMC, and the standard deviations of all calculated benchmarks are lower than 30 pcm. Finally, the results display that the ENDF/B-VIII.0 data library has a good performance on average.

Tim Ware et al, [5] Based on the JEFF-3.3 and ENDF/B-VIII.0 evaluations, nuclear data libraries for continuous energy (BINGO) and multi-group (WIMS) have been created for the ANSWERS Monte Carlo code MONK and the deterministic code WIMS. The new BINGO and WIMS libraries were compared to current libraries based on JEFF-3.1.2 (reported at ND2013) and ENDF/B-VII.1 in calculations for a variety of MONK Monte Carlo and WIMS deterministic code validation instances. However, as the KRITZ-2 UO_2 instances show, JEFF-3.3 can provide better agreement with experiment. In the KRITZ-2 MOX fuel example, however, the change in the ^{239}Pu fission cross section results in an under prediction of k-effective at higher temperatures.

Calculations of reactor criticality are extremely sensitive to the precision of the data library. As a result, criticality benchmarks can be thought of as a type of data library acceptability testing. Thus, criticality benchmarking is required to evaluate the accuracy of newly published nuclear data libraries. In this study, the ENDF/B-VIII.0, JEFF 3.3 data libraries, and as well as the ENDF/B-VII.1 library,

were evaluated utilizing Egyptian second Research Reactor (ETRR-2) criticality benchmarks, and a computational program: WIMS-5B/CITVAP was used.

MATERIALS AND METHODS

Description of Facility

ETRR-2 is a 22 MW open-pool reactor that is light water moderated and cooled (Fig. 1). The original core contained 29 fuel elements and was loaded with three distinct types of fuel elements: Fuel element type 1 containing 146 g of U-235, Fuel element type 2 containing 209 g of U-235, and standard fuel element type containing 405 g of U-235, as well as a Co irradiation device (CID) for Co-60 production [3]. The reactor core was upgraded to 27 fuel elements in 2009 to provide two irradiation sites for irradiating LEU mini plates for the production of fission Mo-99 [6]. Fuel elements, reflectors, control plates, gadolinium injection boxes, and irradiation devices comprise the reactor core. Each fuel assembly has 19 fuel plates that are held in place by two Aluminum side plates. The fuel plates are composed of U_3O_8 powder with an enrichment of 19.7% by weight of U-235, spread in an Aluminum matrix, with an Aluminum coating.

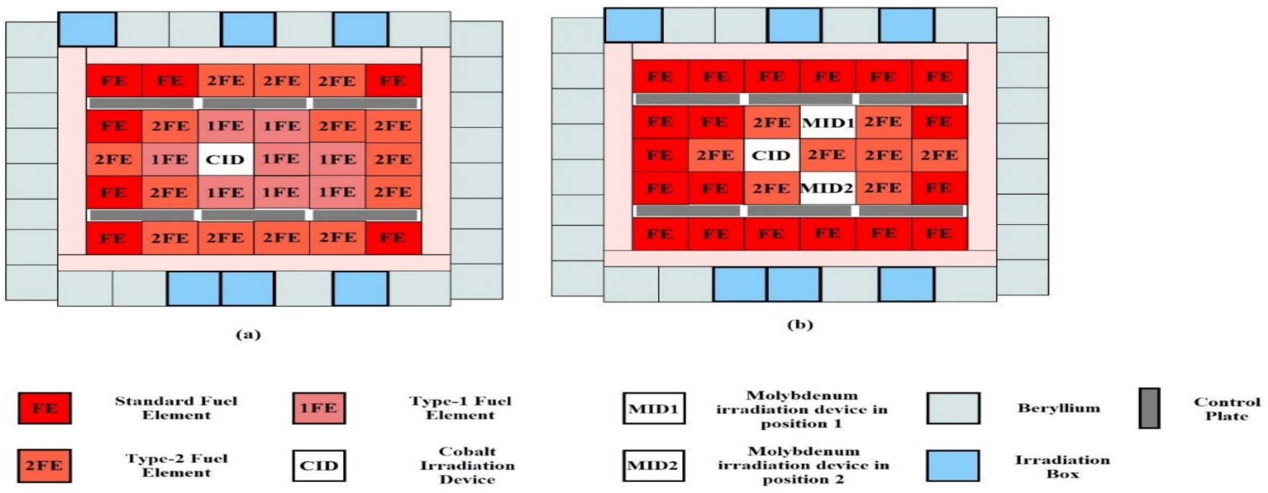


Fig. (1): Horizontal view of ETRR-2 core. (a) First 29 FE core, (b) Modified core for Molybdenum production core

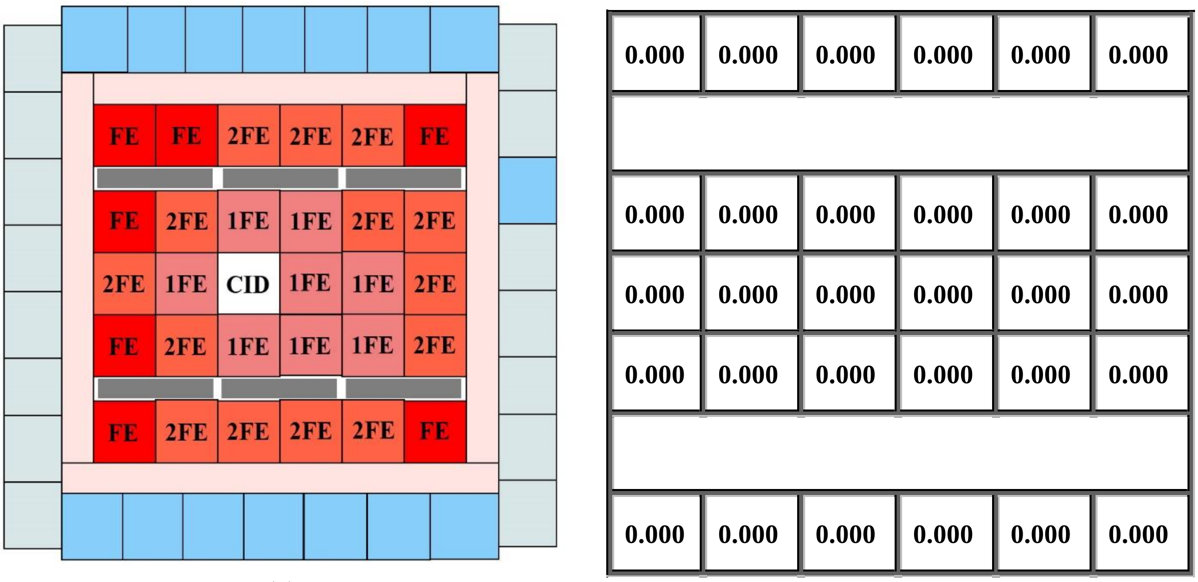
Criticality Benchmark

The benchmark is for the ETRR-2 reactor. The first critical benchmark was for a fresh core containing 29 fuel elements and one cobalt irradiation device at the center with no fission product appearing at this benchmark, the other benchmarks were for the burned core at different operation cycles after refueling of each cycle. Some of critical positions at different cycles is showing in table 1.

The Fuel elements and Beryllium blocks distribution at each cycle with the Fuel Element Burnup (in % of U^{235} consumed) at BOC is shown in figures 2 to 4 [7].

Table (1): Show some critical positions of ETRR-2 Reactors at different cycles during control rods calibration

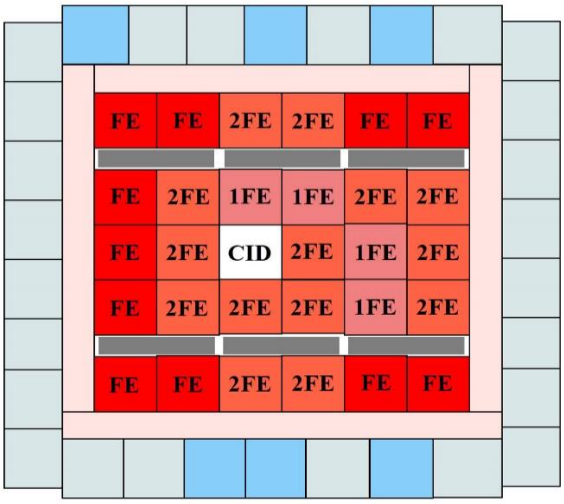
Cycle no.	Days[1]	Control rods positions percentage withdrawal					
		CR-1	CR-2	CR-3	CR-4	CR-5	CR-6
Fresh	0	0	53.5	100	100	100	0
	0	15.3	53.5	100	90.9	100	0
	0	23.4	53.5	100	82.2	100	0
	0	55.9	53.5	100	44.7	100	0
	0	72.5	53.5	100	29.1	100	0
	0	100	53.5	52.4	0	100	0
Cycle 3	23.3	100	0	100	0	100	62.1
	23.3	100	0	100	26	100	54.4
	23.3	93.5	0	100	50.1	100	0
	23.3	51	0	100	71.4	100	0
	23.3	23.6	0	100	100	100	0
Cycle 4	37.05	100	0	100	0	100	49
	37.05	75.2	0	100	0	100	63
	37.05	53.3	0	100	0	100	83.2
	37.05	30.2	0	100	26.8	100	100
	37.05	0	0	100	36	100	100



(a) (b)

Fig (2): (a) the Core configuration and Be blocks distribution of the Fresh Core, and (b) the fuel element burn up (in % of U^{235} consumed) distribution at the BOC

[1] Total operation time in days

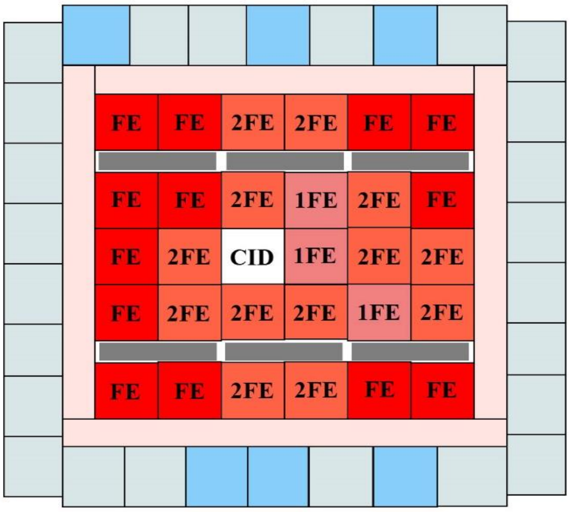


(a)

5.959	6.387	9.130	9.383	6.783	4.845
6.982	10.201	12.827	12.882	10.737	10.411
6.950	9.825	CID	12.098	13.538	10.938
6.023	9.345	10.239	10.840	12.372	9.971
0.000	0.000	8.472	8.932	6.284	4.428

(b)

Fig. (3). (a) the Core configuration and Be block distribution of cycle no. 3 and (b) the fuel element burn up (in % of U^{235} consumed) distribution at the BOC of cycle no. 3.



(a)

0.000	9.803	13.898	14.074	10.106	8.013
9.202	10.812	15.749	19.294	16.289	0.000
11.057	16.058	CID	20.054	16.200	15.393
10.060	15.113	16.495	16.786	18.486	14.861
4.209	4.345	13.861	13.858	9.562	7.458

(b)

Fig. (4): (a) the Core configuration and Be block distribution of cycle no. 4 and (b) the fuel element burn up (in % of U^{235} consumed) distribution at the BOC of cycle no. 4.

Computational Code

The calculation of a nuclear reactor was done in several steps using deterministic codes WIMS5B/CITVAP. A deterministic code leads to a solution that doesn't take into account how random the processes are and instead predicts a single end state. If you run the code more than once without changing it, you will always get the same result. For a nuclear code to be deterministic, it must make several assumptions and simplify the transport equation [8].

The calculation was done in two steps: In the first step called “cell calculation”, we prepared the cross sections data for different cells of the reactor by using WIMS5B code [9]. In the second step called “core model”, we modeled the full reactor core 3D by CITVAP (improved version of CITATION code by INVAP) [10].

The WIMS5B code selects five energy groups for the three different libraries (ENDF/B-VII.1, ENDF/B-VIII.0, and JEFF 3.3) and condensates it to the three groups to perform core calculations with The CITVAP diffusion code in three dimensions and with an energy discretization of three groups as [11]:

• Group 1: 10 MeV → 0.821 MeV

• Group 2: 0.821 Mev → 0.625 eV

• Group 3: 0.625 eV → 0.000 eV

WIMS-69 group library code

The WIMS standard library has a list of nuclides, a tabulation of resonance, and a matrix for thermal scattering. It also has a burnup library with information about how fuel and fission products are burned up, how many fission products are made, and how much energy is released. It also has the fission spectrum for the 69-group library, the absorption cross-section at 2200 m/s, and the resonance absorption integral (0.55 eV–2 MeV) for each nuclide in the library[12].

Nuclear fission in the core fuel of a nuclear reactor leads to the accumulation of fission products. Some of these products have a substantial effect on the nuclear characteristics of the core and must be carefully addressed. Others, although individually minor, have a cumulative effect that cannot be ignored; often, they are grouped together into pseudo-fission products.

The pseudo-fission product for the selected libraries is also shown in table 2 [13].

Table (2): Fission product Nuclides lumped into a pseudo-fission product

No.	Nuclide	No.	Nuclide	No.	Nuclide	No.	Nuclide
1	32-Ge-72	**21**	38-Sr-88	**41**	48-Cd-114	**61**	54-Xe-132
2	32-Ge-73	**22**	39-Y-89	**42**	48-Cd-116	**62**	56-Ba-134
3	32-Ge-74	**23**	40-Zr-90	**43**	49-In-113	**63**	56-Ba-135
4	32-Ge-76	**24**	40-Zr-91	**44**	50-Sn-115	**64**	56-Ba-136
5	33-As-75	**25**	40-Zr-92	**45**	50-Sn-117	**65**	56-Ba-137
6	34-Se-76	**26**	40-Zr-93	**46**	50-Sn-118	**66**	56-Ba-138
7	34-Se-77	**27**	40-Zr-94	**47**	50-Sn-119	**67**	58-Ce-140
8	34-Se-78	**28**	40-Zr-96	**48**	50-Sn-126	**68**	58-Ce-142
9	34-Se-88	**29**	41-Nb-94	**49**	51-Sb-121	**69**	59-Pr-141
10	34-Se-82	**30**	42-Mo-96	**50**	51-Sb-123	**70**	60-Nd-142
11	35-Br-79	**31**	42-Mo-97	**51**	52-Te-122	**71**	60-Nd-144
12	35-Br-81	**32**	44-Ru-99	**52**	52-Te-123	**72**	60-Nd-146
13	36-Kr-80	**33**	44-Ru-100	**53**	52-Te-124	**73**	60-Nd-148
14	36-Kr-82	**34**	44-Ru-102	**54**	52-Te-125	**74**	60-Nd-150
15	36-Kr-84	**35**	44-Ru-104	**55**	52-Te-126	**75**	62-Sm-154
16	36-Kr-86	**36**	46-Pd-104	**56**	52-Te-128	**76**	64-Gd-152
17	37-Rb-85	**37**	46-Pd-106	**57**	52-Te-130	**77**	64-Gd-160
18	37-Rb-87	**38**	46-Pd-110	**58**	53-I-129	**78**	65-Tb-159
19	38-Sb-86	**39**	48-Cd-111	**59**	54-Xe-128	**79**	65-Tb-160
20	38-Sb-87	**40**	48-Cd-112	**60**	54-Xe-130	**80**	-------------

WIMS code update library process

The process of updating the WIMS5B library used have several step, the first step involves downloading the existing WIMS5B library in an open format (.lib). This library contains essential neutron cross-section data that are crucial for performing neutronic calculations in nuclear reactor physics. Once the library is acquired, the WIMS5B Library Update Project provides a dedicated tool known as WELLI. WELLI serves as the means to convert the open-format library (.lib) into a binary format (. bib) compatible with the WIMS5B code. This binary format is specifically designed to be read by the WIMS5B code, ensuring seamless integration into the reactor physics simulation framework. The conversion process undertaken by WELLI is a critical preparatory step before generating a new WIMS5B library [14]. After successfully creating new libraries, the subsequent phase entails running the WIMS (Winfrith Improved Multigroup Scheme) input files specific to the ETRR-2 fuel elements. This critical step is essential for calculating the Macroscopic cross section parameter as function of burnup.

RESULTS AND DISCUSSION

During the commissioning of the first core of ETRR-2 (29 fuel elements), the control rod calibration experiments were done and the critical positions were recorded. This case represents a fresh core (there are no fission products were generated with considerable amounts). WIMS-B5/CITVAP codes with the different three data libraries of interest (ENDF/B-VII.1, ENDF/B-VIII.0, and JEFF 3.3) were simulated in the reactor at the different criticality positions. JEFF 3.3 data library resulted in a more accurate estimation of the criticality than ENDF/B-VII.1 and ENDF/B-VIII.0 in the same computational codes, i.e. as shown in Fig.5. The average discrepancies between the WIMS-B5/CITVAP codes calculations and measurements are around 100, 300 and 400 PCM for JEFF 3.3, ENDF/B-VIII.0, ENDF/B-VII.1, respectively.

It should be noted that, besides the uncertainties in the nuclear data libraries, discrepancies between the calculations and measurements can result from the approximations in the simulation model and the uncertainties in the measured control rod positions and cross sections. The accuracy of cross sections can be evaluated using multi-cycles core calculations.

In the ETRR-2 fuel management, the highest two fuel element burnup are replaced by fresh ones with core shuffling. Figs 6 and 7 show the criticality calculation results of cycles, No.3 and No.4 of ETRR-2 after reactor operation of 23.3 Full Power Days (FPDs) and 37.05 FPDs, respectively.

As demonstrated, the highest average inaccuracy in the critical position when employing CITVAP with ENDF/B-VII.0 was around 500 PCM due to the value of cross sections. The disparity across libraries resulted from variations in microscopic cross sections and the number of fission products generated by some libraries.

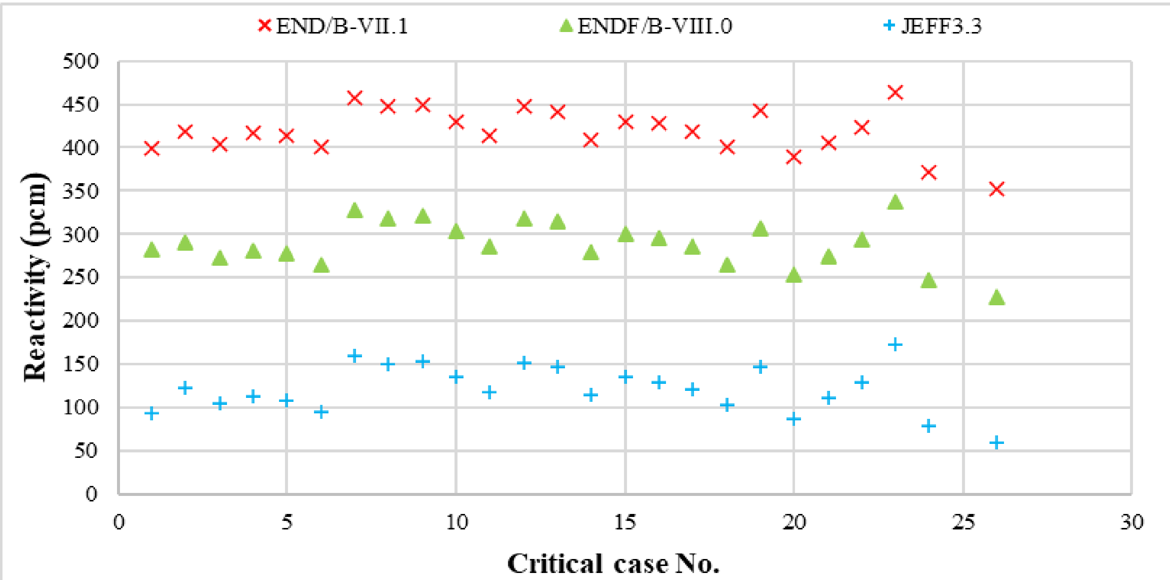


Fig. (5): Calculation results of criticality positions using WIMS/CITVAP for the first (fresh fuel) ETRR-2 cycle.

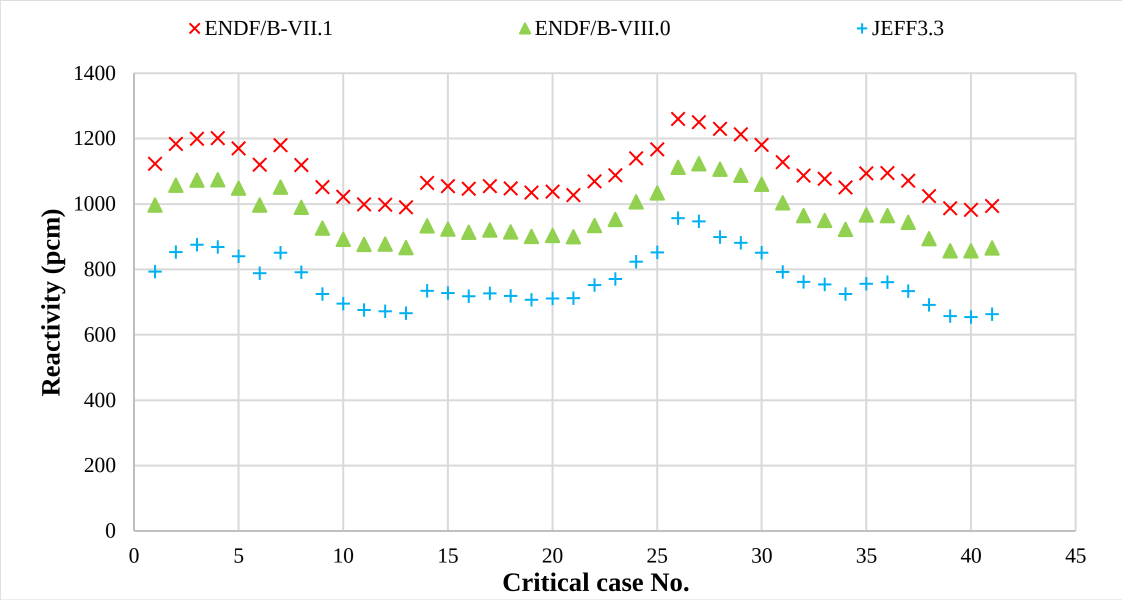


Fig. (6): Calculation results of criticality positions using WIMS/CITVAP for the 3rd ETRR-2 cycle.

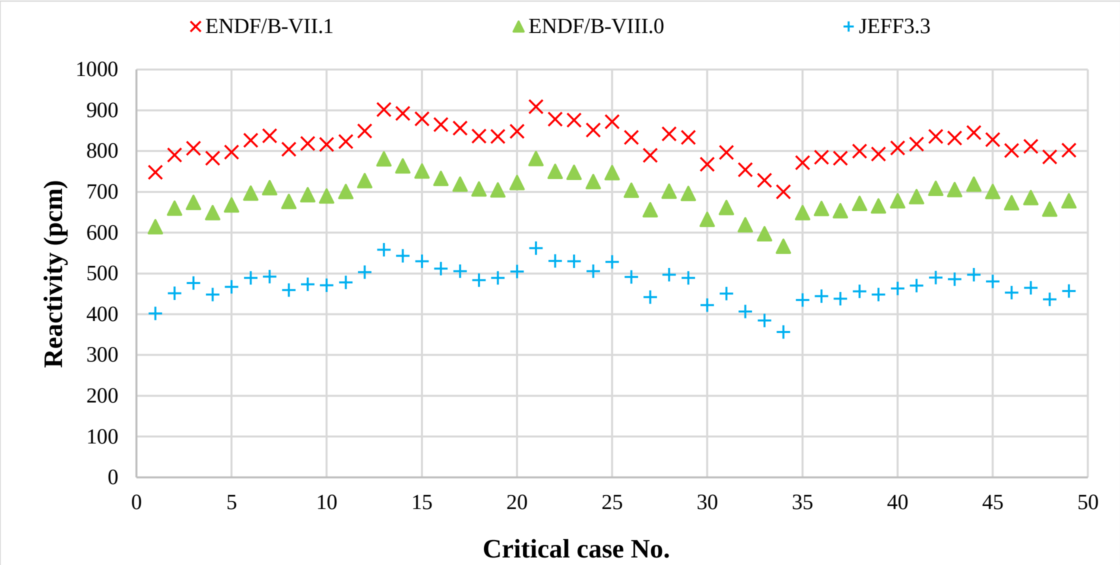


Fig. (7): Calculation results of criticality positions using WIMS/CITVAP of 4th ETRR-2 cycle.

The source of error for burned core compared to the fresh core maybe come from [14]:

- Error is caused by the calibration of the three fission counters used to calculate the criticality of a nuclear reactor (device error),
- Error due to the contribution of neutrons from (γ, n) reactions with the beryllium reflector, which affects the determination of the criticality state.
- Error resulting from control plate position sensors' inability to detect minute variations in the motion of control mechanism motors (device error),
- Personnel error of the operators for examination of the plotted graphs of the response of the fission counters displayed on the control panel's screen; Errors caused by the short number of bits in the analog-digital converter.
- Error resulting from the precision of the reactor operating data (burnup data) from the reactor sources (CIC, Thermal power, N16).

CONCLUSION

WIMS-B5/CITVAP computational codes were utilized in the ETRR-2 criticality benchmark, and the findings for fresh fuel core calculations showed good agreement. When the same computational codes were used in multi-cycle calculations (where the fission products were built-up) of the same benchmark, large discrepancies were observed between the WIMS-B5/CITVAP code and measurements. These discrepancies can be attributed to devise error, human error, and cross section uncertainty. When using WIMS/CITVAP code, the JEFF 3.3 library instead of other libraries provides an accurate result.

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