

ISSN(Online): 2319-8753 ISSN (Print): 2347-6710

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization) Vol. 5, Issue 1, Januray 2016

MCNPX Evaluation of the Integral Parameters and Power Distribution for PWR Lattice Benchmark Problem

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ABSTRACT: Confidence in the neutronic analysis results can be obtained by comparing calculated results with measured data. For this purpose benchmark problems were formulated for various reactor types. In the present paper, infinite multiplication factor, the integral parameters and pin power distribution of a typical PWR assembly are calculated using the current version of MCNPX 2.7 code. The data used are based on experimental PWR benchmark performed by BABCOCK andWILOX, which was formulated by the American Nuclear Society. Also, the effective multiplication factor and the power density distribution are determined for thecores, which include fuel pins, water holes and perturbing (absorbing) pins. The goal of the presentwork is to assess the accuracy of the cross section libraries and the processing methodology that areused. The results show good agreement with those obtained experimentally for core calculations andby other research organizations for assembly calculations.

KEYWORDS: Integral parameters, Power distribution, PWR and MCNPX code.

I. INTRODUCTION

The neutronic analysis of a nuclear reactor includes multiple steps; nuclear data generation, fuel and fuel assembly modeling, lattice parameter generation, and reactor system modeling and analysis. If there is any imperfectness in any of these steps, this will lead to uncertainties in simulation results. It is essential that the computational tools and methods should predict the nuclear reactor system accurately so that the nuclear reactor operates safely and economically as designed, many benchmark problems were formulated to achieve this purpose. One of these benchmarks is based upon light water reactor (LWR) assembly experiments performed by Babcock and Wilcox in the early 1970's which were formulated as a benchmark[1]. Three assembly configurations are given, first one consists of only fuel pins (assembly type A), the second assembly consists of fuel pins and water holes(assembly type B), the third assembly consists of fuel pins, water holes and perturbing (absorber) pins (assembly type c). These problems are well suited for analysis by assembly codes as well as Monte Carlo codes.

The experiments were performed inside a large aluminum tank containing borated water, UO_2 fuel pins, and a number of perturbing pins. The fuel pins contained low-enriched uranium (LEU) and were clad in aluminum. The water contained soluble boron in the form of dissolved boric acid (H₃BO₃). The water height was exactly 145 cm. The central region of the core closely resembled 3x3 array of pressurized water reactor (PWR) fuel assemblies with fuel pins arranged in a 15x15 lattice. The nine assemblies were surrounded by a driver region of LEU fuel pins identical to those in the assemblies. The driver region had an irregular boundary, as shown in figure 1. The region between the driver boundary and the inner wall of the tank contained only water. The vertical dimension of the core is shown in figure2.

Many research studies were performed for the specified benchmark using different methodologies with different codes and nuclear data libraries [2]. Some of them use the deterministic method and others use the probabilistic method (Monte Carlo). The methodology of the code that will be used in this paper is the Monte Carlo method so the results will be compared with those using the same methodology. In the following paragraphs some of these studies are mentioned.

Russell D.Mosteller in the LOS Alamos National Laboratory has performed the calculations using the MCNP Monte Carlo code (Version 4A). Three set of libraries were used, ENDF/B-V, ENDF/B-VI.2 and ENDF/B-VI.3. The results of the three sets were compared with each other.



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Roger N.Blomquist in the Argonne National Laboratory has performed the calculations using VIM code. The libraries used are based on ENDF/B-V, except for the thermal scattering data, which were taken from ENDF/B-III.

Yi-Kang Lee in the CEA (Commissariat à l'énergieatomiqueet aux énergies alternatives) has performed the calculations using TRIPOLI-4 code. The library used is based on JEF2.2.

V.I. Bryzgalov, M.S. Yudkevich in the Russian Research Center, has performed the calculations using MCU-RFFI code. The libraries used are part of the DLC/MCUDAT-1.0 data collection of the MCU project.

In this paper the calculations for a typical PWR assembly in the specified benchmark are performed. The calculations include the infinite multiplication factor, the integral parameters and pin power distribution of the three assembly configurations (A, B, C). The calculations also include the power density distribution at the core mid-plane for the central assembly for cores with assembly types B and C. All the calculations are done using the MCNPX code version (2.7) [3]. The libraries used are the pre ENDF/B-VII evaluation library (T16_2003)[4]for the uranium isotopes and the ENDF66 [5] for the other isotopes. The calculations are also performed using the ENDF71x library[6]. All the results for the assembly calculations are compared with the average of those obtained by the various research organizations that worked on this benchmark using the Monte Carlo techniques, while the results for the core calculations are compared with the average with the available experimental measurements.



Fig.1Core configuration



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Fig.2The Vertical dimensions of the core

II. PWR ASSEMBLY DESCRIPTION

The assemblies consist of a 15x15 array of fuel pins, water holes and perturbing pins. All of the loadings are laid out on a square pitch of 1.63576 cm. Assembly type A contains fuel rods in all locations, assembly type B contains 17 water holes, while assembly type C contains 16 Pyrex rods (perturbing pins) inserted in the positions of the water holes except the central hole.

The geometrical characteristics of the Uo_2 fuel pins, clad and the perturbing pins are given in table.1 while the materials compositions are given in table2. Table.3 shows the Boron isotopic concentrations in water , specified for each of the three configurations. The temperature at which the calculations are performed is taken to be 20 °C for all the materials.



Fig.3 The Assembly configurations (B) and (C)



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Material	PARAMETERS	VALUES
	Pellet diameter (cm)	1.029716
	Active length (cm)	153.3398
Fuel pins	Mass per fuel pin (g)	1305.5
	Pellet density (g/cm ³)	10.24
	Outer diameter (cm)	1.205992
	Thickness (cm)	0.081280
Clad (AI-6001)	Length (cm)	156.4386
	Density (g/cm^3)	2.7
	Diameter (cm)	1.17
Pyrex Perturbing rods	Length (cm)	188
	Mass(g)	453.6

Table1The geometrical characteristics of the materials

Table2 The materials compositions

Material	Isotope	Number Density(a/b-cm)
	U-234	4.5689x10 ⁻⁶
	U-235	5.6868 x10 ⁻⁴
Fuel pins	U-238	2.2268 x10 ⁻²
_	O-16	4.5683 x10 ⁻²
	B-10	2.6055 x10 ⁻⁷
Watan	H-1	6.6737 x10 ⁻²
Water	O-16	3.3369 x10 ⁻²
	Mg (Nat.)	$6.2072 \text{ x}10^{-4}$
	Al-27	5.3985x10 ⁻²
	Si(Nat.)	3.2230×10^{-4}
Clad(A) (0(1)	Ti (Nat.)	4.7263 x10 ⁻⁵
Clau (Al-0001)	Cr (Nat.)	5.8029 x10 ⁻⁵
	Mn-55	4.1191x10 ⁻⁵
	Fe (Nat.)	$1.8910 \text{ x} 10^{-4}$
	Cu (Nat.)	5.9353 x10 ⁻⁵
	B-10	9.7491 x10 ⁻⁴
	B-11	$3.9241 \text{ x} 10^{-3}$
Dynay Dontunbing rods	O-16	$4.4829 \text{ x}10^{-2}$
r yrex r erturbing roas	Na-23	$1.7444 \text{ x}10^{-3}$
	Al-27	$1.0018 \text{ x} 10^{-3}$
	Si(Nat.)	1.8306 x10 ⁻²



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Configuration	Critical Soluble Boron	Number Density (a/b-cm)			
Configuration	Concentration (PPM)	B-10	B-11		
А	1511	1.6769 x10 ⁻⁵	6.7497 x10 ⁻⁵		
В	1335.5	1.4821 x10 ⁻⁵	5.9657x10 ⁻⁵		
С	794	8.8117 x10 ⁻⁶	3.5468x10 ⁻⁵		

Table3. Boron Isotopic Concentrations in Water

III. LIBRARIES AND CODE USED

MCNPX is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori. Pointwise cross-section data are used.

In this paper the MCNPX code [3] is used to simulate the assembly for the three configurations (A, B, C), with two sets of cross section libraries. In the first set (Set I) the cross section data for the uranium isotopes are taken from the pre ENDF/B-VII evaluation library (T16_2003), while the cross section data for the other isotopes are taken from the ENDF/B-VI (ENDF66). Thermal neutrons are described by both the free gas and S (α , β) models.

The continuous-energy MCNP neutron library T16_2003 has been created for 15 isotopes, the library is based upon recent Los Alamos GroupT-16 evaluations. Data are provided for ³H, ²³²U, ²³³U, ²³⁴U, ²³⁵U, ²³⁶U, ²³⁷U, ²³⁸U, ²³⁹U, ²⁴⁰U, ²⁴¹U, ²³⁷Np, ²³⁹Pu, ²⁴¹Am, and ²⁴³Am. The majority of the evaluations represented on T16_2003 are intended to be tested as candidates for ENDF/B-VII[4].

The ENDF66 library contains data for 173 nuclides based on ENDF/B-VI evaluations of the cross Section Evaluation Working Group (CSEWG) and was processed with the NJOY99 code. Updated evaluations for uranium, plutonium, tungsten, and iron isotopes have been performed[5].

In the second set (Set II) the cross section data for all of the isotopes are taken from the ENDF71x library and the thermal neutrons are described by both the free gas and S (α , β) models. The ENDF71x library is a thoroughly tested set of ACE-format data tables released by the Nuclear Data Team at Los Alamos National Laboratory (LANL). It is based on ENDF/B-VII. 1, the most recently released set of evaluated nuclear data files produced by the US Cross Section Evaluation Working Group (CSEWG). A variety of techniques were used to test and verify the ENDF71x library before its public release. A comparison of ENDF71x with its predecessor ACE library, ENDF70, showed that dramatic changes have been made in the neutron cross section data for a number of isotopes between ENDF/B-VII.0 and ENDF/B-VII.1. Based on the results of the verification tests and the validation tests performed by Kahler, et al., the ENDF71x library is recommended for use in all Monte Carlo applications[6].

IV. INTEGRAL PARAMETERS

The integral parameters are a number of quantities which are useful in a comparison of different analysis techniques and basic data. Therefore, the following quantities for an infinite lattice should be computed[1]:

- Infinite multiplication factor (K_{∞})

- δ^{25} , that is the ratio of epithermal-to-thermal ²³⁵U fissions δ^{28} , that is the ratio of ²³⁸U fissions to ²³⁵U fissions
- $\begin{array}{l} -\rho^{25}, \mbox{ that is the ratio of epithermal-to-thermal capture in ^{235}U \\ -\rho^{28}, \mbox{ that is the ratio of epithermal-to-thermal ^{238}U capture \\ CR , \mbox{ that is the ratio of ^{238}U captures / ^{235}U absorptions \\ \end{array}$



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V. CALCULATION RESULTS AND DISCUSSION

1- Lattice calculation results

Tables4, 5, 6 and 7 show the values of infinite multiplication factors and integral parameters for assembly types A, B and C respectively. The calculations are performed using MCNPX (2.7) code and the nuclear data libraries Set I and Set II. The results are compared with the averaged from Monte Carlo results that are mentioned in reference 7.

Table4Comparison of the infinite multiplication factors

Assembly type	Set I	Set II	Avg. MC
Α	1.05692	1.06059	1.05607
В	1.04782	1.05131	1.04697
С	0.98662	0.98888	0.98558

Table5 Results of integral parameters for assembly type A

Parameters	SetI	SetII	Avg. MC
δ^{25}	0.145	0.1446	0.1301
δ^{28}	0.0642	0.0635	0.06478
ρ ²⁵	0.3718	0.3714	0.34234
ρ ²⁸	2.2879	2.304	2.26459
CR	0.464	0.4608	0.46676

Table6 Results of integral parameters for assembly type B

Parameters	SetI	SetII	Avg. MC
δ^{25}	0.1290	0.1285	0.11534
δ^{28}	0.0596	0.0589	0.06011
ρ ²⁵	0.3302	0.3301	0.30377
ρ ²⁸	2.0352	2.049	2.0210
CR	0.4353	0.432	0.43701

Table7 Results of integral parameters for assembly type C

Parameters	Set I	Set II	Avg. MC
δ^{25}	0.1428	0.1424	0.12862
δ ²⁸	0.0651	0.06448	0.06592
ρ ²⁵	0.375	0.367	0.33900
ρ ²⁸	2.273	2.289	2.25849
CR	0.463	0.459	0.46451

Figures 4 and 6 show the results of the pin power distribution for assembly types B and C respectively. The results obtained using the nuclear data libraries Set I and Set II are compared with the averaged Monte Carlo results. The errors for the results of the nuclear data libraries Set I and Set II with respect to the Average Monte Carlo results are shown in Figures 5 and 7.



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SetI		1.049	0.998	0.979	0.968	0.981	0.959	0.951
Set II	Water	1.061	1.002	0.975	0.976	0.985	0.960	0.940
Avg.MC.		1.058	0.998	0.972	0.973	0.975	0.959	0.948
		1.024	1.055	1.002	1.005	1.040	0.978	0.951
		1.022	1.060	0.995	1.000	1.045	0.982	0.948
		1.028	1.055	1.001	1.000	1.041	0.982	0.951
				1.076	1.070		1.030	0.962
			Water	1.071	1.069	Water	1.032	0.959
				1.070	1.077		1.037	0.961
				1.053	1.091	1.077	0.989	0.952
				1.046	1.096	1.084	0.985	0.950
				1.047	1.087	1.081	0.993	0.955
			-			1.060	0.972	0.943
					Water	1.060	0.970	0.940
						1.060	0.970	0.946
						0.989	0.952	0.940
						0.990	0.949	0.939
						0.988	0.950	0.941
							0.936	0.931
							0.938	0.934
							0.939	0.937
								0.939
								0.941
								0.930

Fig.4 Pin power distribution for assembly type B

Watan	0.008	0.000	0.007	0.005	0.006	0.000	0.003
w ater	0.004	0.004	0.003	0.004	0.010	0.001	0.009
	0.003	0.000	0.001	0.006	0.001	0.004	0.000
	0.006	0.005	0.006	0.000	0.004	0.001	0.003
·		XV-t	0.006	0.006	XX - 4	0.007	0.000
		w ater	0.001	0.007	w ater	0.004	0.002
	-		0.006	0.003	0.004	0.004	0.003
			0.001	0.008	0.002	0.008	0.005
				Watan	0.001	0.002	0.003
				vv ater	0.000	0.000	0.006
					0.002	0.002	0.001
					0.002	0.001	0.002
				·		0.002	0.006
						0.000	0.003
							0.009
							0.011
	Water	Water 0.008 0.004 0.003 0.003 0.006	Water 0.008 0.004 0.000 0.004 0.003 0.000 0.005 0.005 Water Water	Water 0.008 0.004 0.000 0.004 0.007 0.003 0.003 0.000 0.001 0.006 0.005 0.006 Water 0.006 0.001 0.003 0.001 0.005 0.006 0.001 0.006	Water 0.008 0.000 0.007 0.005 0.004 0.004 0.003 0.004 0.003 0.000 0.001 0.006 0.006 0.005 0.006 0.006 0.006 0.005 0.006 0.006 0.006 0.007 0.006 0.006 0.001 0.006 0.007 0.006 0.001 0.006 0.001 0.007 0.006 0.001 0.007 0.006 0.001 0.003 0.001 0.008	Water 0.008 0.000 0.007 0.005 0.006 0.004 0.004 0.003 0.004 0.010 0.003 0.000 0.001 0.006 0.001 0.006 0.005 0.006 0.000 0.001 0.006 0.005 0.006 0.000 0.004 0.006 0.005 0.006 0.000 0.004 0.006 0.005 0.006 0.000 0.004 0.006 0.005 0.006 0.000 0.004 0.001 0.002 0.002 0.002 0.002 0.002 0.002 0.002 0.002 0.002	Water 0.008 0.000 0.007 0.005 0.006 0.000 0.004 0.004 0.003 0.004 0.001 0.001 0.001 0.001 0.003 0.000 0.001 0.006 0.001 0.004 0.001 0.006 0.005 0.006 0.000 0.004 0.001 0.006 0.005 0.006 0.000 0.004 0.001 0.006 0.005 0.006 0.000 0.004 0.001 0.006 0.006 0.000 0.004 0.004 0.004 0.001 0.006 0.003 0.004 0.004 0.001 0.002 0.002 0.002 0.002 0.002 0.002 0.002 0.002 0.002 0.002 0.000 0.000 0.000 0.000 0.000 0.002 0.002

Fig.5 Errors of Pin power distribution for assembly type B



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Fig.6Pin power distribution for assembly type C



Fig.7Errors of Pin power distribution for assembly type C

It is shown from the above tables and figures that the results obtained for assembly types A, B and C are in good agreement with the Average Monte Carlo results mentioned in reference 7.

2- Core calculation results:

Table 8 shows the values of effective multiplication factors obtained using MCNPX (2.7) code and the nuclear data libraries Set Iand Set IIfor core configurations with assembly type A, B and C. The results are compared withboth the experimental values and the average calculations with Monte Carlo.

Tables Comparison of the effective multiplication factors								
Core type	Set I	Set II	Avg. MC	Exp.				
Α	0.99631	0.99932	0.99754	1.0007				
В	0.99645	0.99994	0.99729	1.0007				
С	0.99603	0.99920	0.99611	1.0007				

Table8	Com	parison	of the	effective	multi	plicatior	factors
1 abieo	Com	parison	or the		munu	pheation	1 Iactors



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Figures8 and 10 show the results of the pin power distribution at the core mid-plane for the central assembly of core configurations with assembly types B and C respectively. The results obtained using the nuclear data libraries Set I and Set II are compared with the experimental results. The errors for the results of the nuclear data libraries Set I and Set II with respect to the experimental results are shown in Figures 9 and 11.

Set I		1.104	1.048	1.011	1.003	0.988	0.991	0.953
Set II	Water	1.111	1.045	1.040	1.013	1.034	1.003	0.970
Exp.		1.107	1.026	1.000	1.025	1.026	0.980	0.983
		1.067	1.117	1.051	1.036	1.068	1.007	0.946
		1.105	1.105	1.066	1.060	1.065	1.015	0.980
		1.068	1.075	1.036	1.047	1.098	1.026	1.003
	-			1.148	1.142		1.061	0.972
			Water	1.119	1.113	Water	1.054	0.967
				1.116	1.118		1.070	0.961
				1.095	1.150	1.145	1.051	0.948
				1.073	1.161	1.142	1.018	0.987
				1.091	1.145	1.133	1.032	0.924
						1.093	1.004	0.978
					Water	1.078	0.983	0.943
						1.109	1.007	0.974
						1.023	0.948	0.947
						1.016	0.993	0.912
						1.015	0.973	0.971
							0.960	0.955
							0.948	0.913
							0.970	0.950
								0.949
								0.930
								0.920

Set I	Water	0.003	0.022	0.011	0.022	0.037	0.011	0.030
Set II		0.004	0.018	0.040	0.012	0.008	0.023	0.013
		0.001	0.039	0.015	0.010	0.027	0.019	0.057
		0.035	0.028	0.029	0.012	0.030	0.010	0.023
			Watan	0.028	0.022	Watan	0.009	0.011
			water	0.003	0.005	vv ater	0.015	0.006
				0.004	0.004	0.011	0.019	0.026
				0.016	0.014	0.008	0.014	0.068
			-		XX-+	0.014	0.003	0.004
					vv ater	0.028	0.023	0.032
						0.008	0.026	0.024
						0.001	0.021	0.061
							0.010	0.006
							0.023	0.039
								0.031
								0.011

Fig.8Core power distribution for assembly type B

Fig.9 Errors of core power distribution for assembly type B



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Fig.10Core power distribution for assembly type C

S et I	Water	0.004	0.029	0.015	0.049	0.019	0.016	0.019
S et II		0.023	0.026	0.029	0.041	0.014	0.037	0.001
		0.042	0.004	0.002	0.024	0.036	0.012	0.008
		0.034	0.009	0.040	0.001	0.011	0.007	0.007
	-		n	0.039	0.003	n	0.008	0.012
			Pyrex	0.029	0.020	Fyrex	0.023	0.036
				0.047	0.033	0.026	0.007	0.044
				0.036	0.023	0.019	0.008	0.026
							0.024	0.024
				ryrex	0.021	0.013	0.032	
						0.035	0.014	0.005
						0.023	0.013	0.042
							0.027	0.040
							0.009	0.001
								0.011
								0.023

Fig.11Errors of core power distribution for assembly type C

It is shown from the above tables and figures that the results obtained for core configurations with assembly types A, B and C are in good agreement with the experimental results mentioned in reference 7.

VI. CONCLUSION

The multiplication factors, the integral parameters and power distribution of a typical PWR assembly and core are calculated using the current version of MCNPX (2.7) and the nuclear data libraries (T16_2003, ENDF66) and the ENDF71x. The results obtained are compared with the experimental results for core calculations and the Average Monte Carlo results obtained by other research organizations for assembly calculations. It was found that the results showed good agreement for all studied cases. It was concluded that the current version of MCNPX (2.7) and the cross section nuclear data libraries used, can be applied to accurately calculate the integral parameters and power distribution for a typical PWR lattice.



ISSN(Online): 2319-8753 ISSN (Print): 2347-6710

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization)

Vol. 5, Issue 1, Januray 2016

ACKNOWLEDGMENT

The Authors would like to express their deep appreciation and thanks to **Prof. Dr. E. H. Amin** (Safety Engineering Department, ENRRA, Cairo, Egypt) for her valuable scientific guidance, support and encouragement during this work.

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