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REALIZATION OF 3D EQUATIONS OF SURFACE HARMONICS METHOD IN SUHAM-3D CODE

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ABSTRACT

Realization of 3D equations of surface harmonics method with three transversal and two longitudinal trial matrices for each cell in SUHAM-3D code has been described. International 3D benchmark C5G7 was used for initial verification of SUHAM-3D code. The main results of this verification are the following ones: methodical error of k_{eff} is 0.12 %; maximum percent error of pin powers is 2.9 %; root mean square of the pin power percent error is 1.0 %; maximum percent error of the fuel assembly power is 0.9 %.

Key Words: Surface harmonics method, neutron transport equation, SUHAM-3D code, verification, benchmark C5G7

1. INTRODUCTION

Topic: Codes and Benchmarks.

The problem of the solving the neutron transport equation in all volume of the nuclear reactor core is hard task even on the modern computers.

In so doing, direct deterministic methods such ones as method of characteristics, S_N method and others, in principle, can cope with such a task, but, as a rule, either with highly significant computational expenditures or with additional approximations, for example, with the not enough division along the one or several variable values for obtaining the necessary accuracy.

Engineering approaches, as a rule, are based on some mechanism of spatial homogenization and subsequent solving the diffusion equation with possible use of the nodal methods. In so doing, computational expenditures are quite acceptable but computational accuracy, as a rule, is not enough. The last statement does not concern those codes, which have various semi-empirical corrections taking into account stationary experiments on the reactor assemblies, stationary reactor measurements and Monte-Carlo calculations. However, even these corrections do not guarantee the correct description of the reactor behavior far from the reference calculational points and under the accident conditions.

Side by side with above-mentioned approaches the models combining the advantages of the both deterministic and engineering methods are developed. In these approaches, neutron transport equation is solved in not great volumes (in cells, fuel assemblies (FA-s)), in so doing, the number

of such solutions (trial solutions) is appreciably more then unity and these solutions differ from one another by the boundary conditions. Total solution in each volume is presented as a linear combination of the trial solutions with the arbitrary coefficients. Then, the moments of the general solutions in these volumes are equated to each other on the adjoining sides of these volumes. As a result, the finite-difference equations for the above-mentioned arbitrary coefficients are obtained. The main point in these approaches is that the number of such trial solutions in each volume was enough one and the each trial solution was really the solution of the neutron transport equation. As example of such approach, method of response matrices and coupling currents can be listed.

Surface Harmonics Method (SHM) [1, 2] is one of the most consistent of such type methods. SHM is a mathematical model for solving the neutron transport equation in all volume of nuclear reactor core.

SUHAM code [3] is elaborated since 1995 in the beginning with connection with WIMS code [4] (code system SUHAM-W) and then with connection with UNK code [5] (code system SUHAM-U [6]). In so doing, modules of WIMS and UNK codes are used for preparation of the multigroup cross-sections of isotopes and materials. Modules of SUHAM code are used for solving the multigroup neutron transport equation in calculated object by Surface Harmonics Method.

The following 2D verification calculations have been carried out for SUHAM-2D code before:

- Benchmark calculations of VVER-1000 fuel assemblies with uranium and MOX fuel [6, 7].
- Burnup calculations of VVER-1000 fuel assemblies with uranium and MOX fuel [8].
- International benchmark for two-dimensional VVER-1000 core [9].
- International 2-D MOX benchmark C5G7 [10, 11].
- International benchmark for Doppler defect [12].
- 2D light water benchmark-experiment VENUS-2 with UO_2 and MOX fuel [13].

In this paper the first variant of SUHAM-3D code has been described. The simplest 3D SHM finite-difference equations with three transversal and two longitudinal trial matrices for each cell derived in paper [14] for square lattice and for two-stage calculations (cells – reactor core) with one calculation point per one cell and one energy group have been realized in this variant of code. International 3-D benchmark C5G7 [10] was used for initial verification of SUHAM-3D code.

2. 3D EQUATIONS OF SURFACE HARMONICS METHOD REALIZED IN SUHAM-3D CODE

For the first time the SHM 3D equations were obtained in [15, 16]. The simpler 3D finite-difference SHM equations with three transversal and two longitudinal trial matrices for each cell with one calculational point per one cell and one energy group were derived in [14].

$$\hat{\Lambda}^z\vec{\Phi}_k + \hat{\Lambda}^r\vec{\Phi}_k - \hat{\Sigma}_k^r\vec{\Phi}_k = 0\,, \tag{1}$$

where

$$\begin{cases} \hat{\Lambda}^z\vec{A}_k = \dfrac{1}{h_z^2}\sum\limits_{i=1}^{2}\hat{H}_{ik}^z(\vec{A}_{j_i} - \vec{A}_k) \\ \hat{\Lambda}^r\vec{A}_k = \dfrac{4}{Mh_r^2}\sum\limits_{i=1}^{M}\hat{H}_{ik}^r(\vec{A}_{j_i} - \vec{A}_k) \end{cases}, \tag{2}$$

$$\begin{cases} \hat{H}_{ik}^z = 2\hat{D}_{j_i}^z(\hat{D}_{j_i}^z + \hat{D}_k^z)^{-1}\hat{D}_k^z \\ \hat{H}_{ik}^r = 2\hat{D}_{j_i}^r(\hat{D}_{j_i}^r + \hat{D}_k^r)^{-1}\hat{D}_k^r \\ \hat{D}_k^z = \dfrac{h_z}{2}(\hat{\varphi}_k^{z,(1)})^{-1} \\ \hat{D}_k^r = \dfrac{h_r}{2}(\hat{\varphi}_k^{r,(1)})^{-1} \end{cases} \tag{3}$$

Here k – number of central cell, i – number of lateral side (i=1,2,3,4 for cell with square boundary and i=1,2,3,4,5,6 for cell with hexagonal boundary) or number of side on Z direction (i=1,2). j_i - number of cell which have common side i (lateral or in direction Z) with k-th cell. $\hat{\boldsymbol{\varphi}}_k^{z,(l)}$ and $\hat{\boldsymbol{\varphi}}_k^{r,(l)}$ are longitudinal and transversal trial matrices correspondingly. $\vec{\Phi}_k$ are unknown group vectors. $\hat{D}_k^z$ and $\hat{D}_k^r$ are longitudinal and transversal matrices of effective diffusion coefficients. More details one can see in [14, 1, 2].

Let's write operator $\hat{\Lambda}^z$ for variable pitch on Z direction.

$$\hat{\Lambda}^z\vec{A}_k = \frac{1}{h_k}\sum_{i=1}^{2}\hat{H}'^z_{ik}(\vec{A}_{j_i} - \vec{A}_k) \tag{4}$$

where

$$\hat{H}'^z_{ik} = 2\left[h_{j_i}(\hat{D}_{j_i}^z)^{-1} + h_k(\hat{D}_k^z)^{-1}\right]^{-1} \tag{5}$$

Equation (1) is the simplest 3D group finite-difference SHM equation with three transversal and two longitudinal trial matrices for each cell. It should be noted that this equation is similar to 3D finite difference diffusion equation but only on the form. Formal difference is the matrices of diffusion coefficients as transversal $\hat{D}_k^r$ as longitudinal $\hat{D}_k^z$ are nondiagonal ones. More essential difference is the unknown vectors $\vec{\Phi}_k^r$ and coefficients of equation (1) have nonstandard essence.

As a result we have essential more precise for main neutron-physical functionals. More details one can see in [14, 1, 2].

3. SUHAM-3D CODE

Considered version of SUHAM-3D code is intended for solving the 3D group neutron transport equation with square lattice in plane. Two-stage calculation (cells – reactor core) has been realized, in so doing the finite-difference SHM equation with one calculation point per one cell and one energy group is solved. 3D group finite-difference equation (1) with variable pitch on Z direction has been realized.

It should be noted that all coefficients of equation (1) depend on the unknown eigenvalue (k_{eff}) so super external iterations has been organized. Common calculational scheme of SUHAM-3D code is presented in Fig. 1.

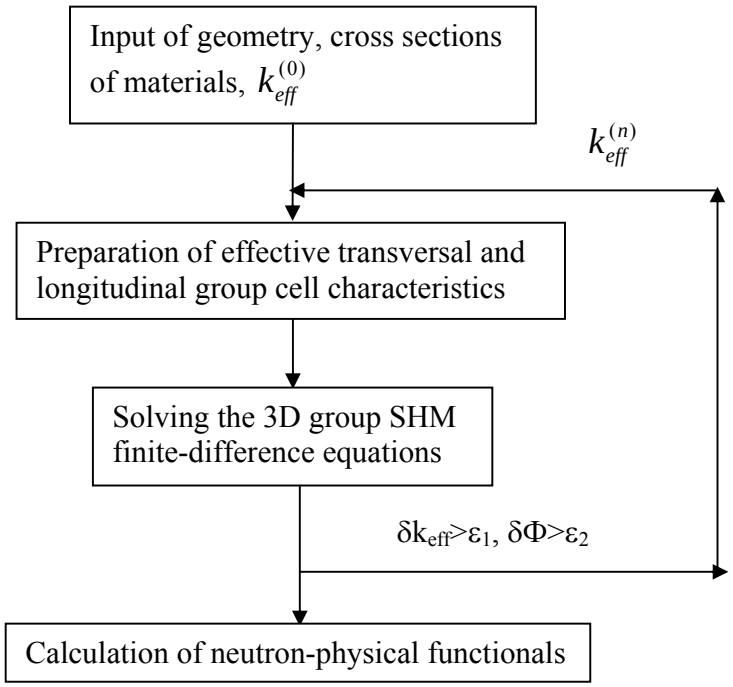

Figure 1. Calculational scheme of SUHAM-3D code.

The following quantities are the calculational results:

- Effective multiplication coefficient k_{eff} or k_∞.
- Group neutron fluxes averaged on each cell.
- Group absorption reactions in all cells.
- Group fission reactions in all cells.
- One-group neutron fluxes averaged on each cell.

- One-group absorption reactions in all cells.
- One-group fission reactions in all cells.

4. VERIFICATION OF SUHAM-3D CODE

International 3D benchmark C5G7 [10] with the predetermined values of seven-group cross sections was used for initial verification of SUHAM-3D code. Two-dimensional configuration of benchmark C5G7 (1/4 part) and scheme of fuel cells are shown in Fig. 2. Fig. 3 shows the configuration of benchmark C5G7 on Z direction. Boundary conditions are shown on these figures too.

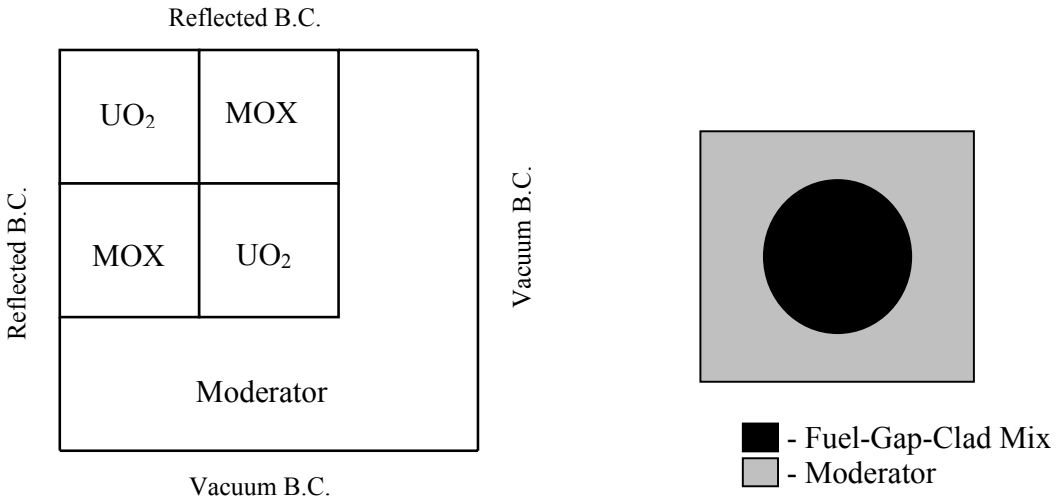

Figure 2. Two-dimensional configuration of benchmark C5G7 and scheme of fuel cell.

Fig. 4 shows two-dimensional scheme of four fuel assemblies (pin cell compositions): two fuel assemblies with uranium fuel and two ones with MOX fuel. In so doing the following designations were used: FA-UO_2-1 for left top fuel assembly with uranium fuel, FA-UO_2-2 for right bottom fuel assembly with uranium fuel and FA-MOX for fuel assembly with mixed fuel.

The overall dimensions of two-dimensional configuration are 64.26 × 64.26 cm, while each assembly is 21.42 × 21.42 cm. For the three-dimensional configuration, the fuel assemblies are 192.78 cm in the Z direction and an additional 21.42 cm water reflector is added axially. The overall dimensions for the three-dimensional configuration are 64.26 × 64.26 × 214.20 cm, while each assembly is 21.42 × 21.42 × 192.78 cm.

When calculating this benchmark by SUHAM-3D code, fuel assemblies and cells were divided into 3 layers on Z direction from center to upper side: 96.39 × 96.39 × 21.42 cm. In so doing when calculating the longitudinal trial matrices, pitch on Z direction was 0.9639 cm (100 points) for cells of fuel assembly and 1.071 cm (20 points) for reflector.

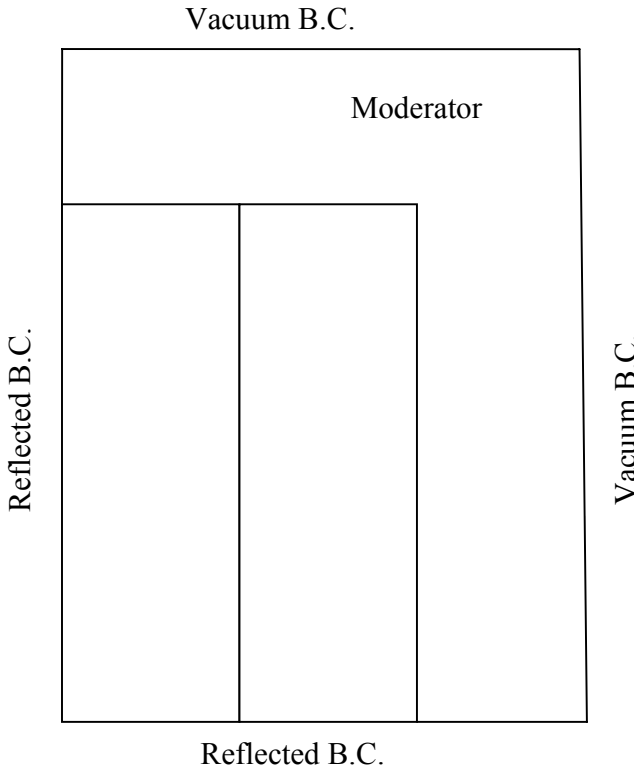

Figure 3. Configuration of benchmark C5G7 on Z direction.

Each fuel assembly is made up of a 17 × 17 lattice of square pin cells (see Fig. 4). The side length of each pin cell is 1.26 cm and all of the fuel pins and guide tubes have a 0.54 cm radius. More detail description of this benchmark see in [10].

The main feature of calculated benchmark is the seven-group cross sections of all materials are the predetermined values and so cross sections errors are absent.

Comparison was carried out with results calculated by MCNP code [10]. Value of k_{eff} calculated by MCNP code is 1.18381 (±0.008 %) and value of k_{eff} calculated by SUHAM-3D code is 1.18528. So, the methodical error of k_{eff} for SUHAM-3D code for this benchmark equals **0.12 %**.

Table I shows some integral comparisons of pin powers (fissions) calculated by SUHAM-3D and MCNP codes, in so doing AVG (average on module pin power percent distinction), RMS (root mean square of the percent distinction) and MRE (mean relative pin power percent error) were calculated by the following formulas [10].

$$AVG = \frac{1}{N}\sum_{n=1}^{N}|e_n| \tag{6}$$

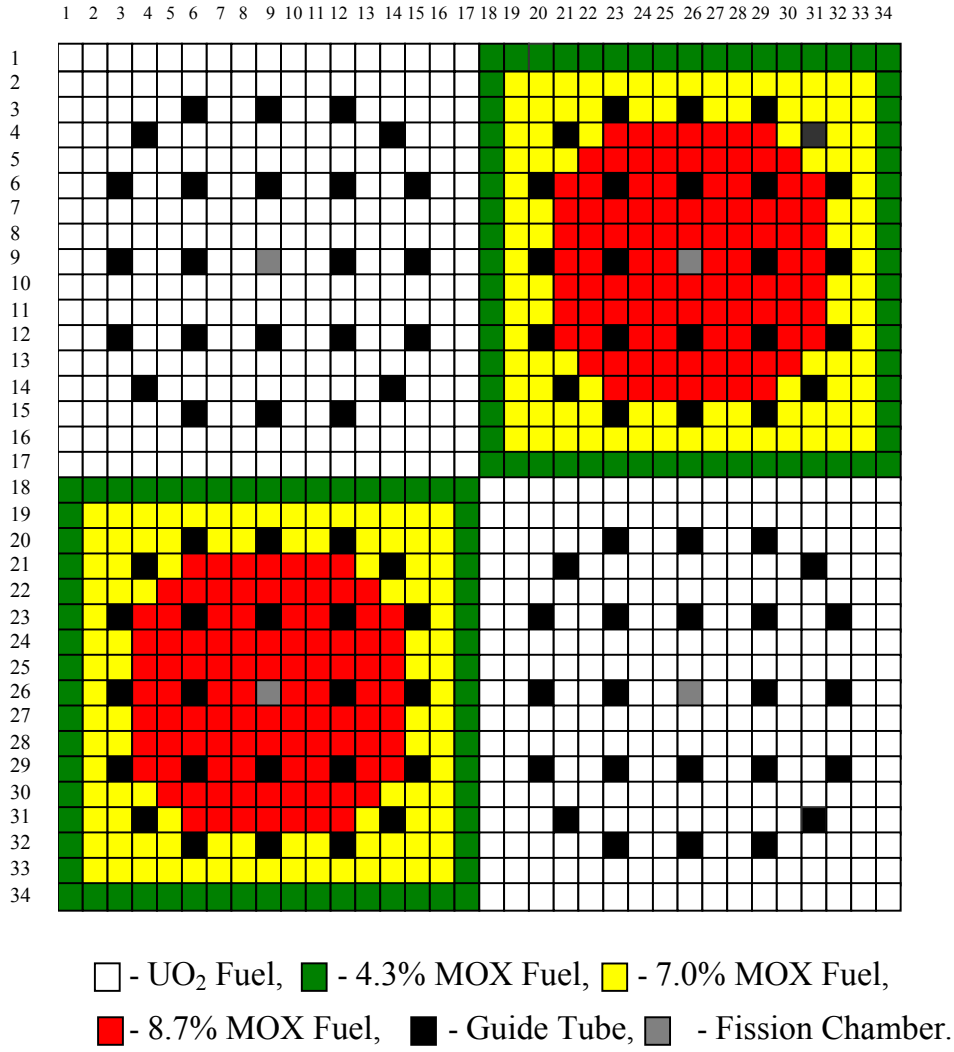

Figure 4. Two-dimensional scheme of four fuel assemblies.

$$RMS = \frac{1}{\sqrt{N}} \sqrt{\sum_{n=1}^{N} e_n^2} \tag{7}$$

$$MRE = \frac{\sum_{n=1}^{N} |e_n| p_n}{N p_{avg}} \tag{8}$$

Here N is the number of fuel pins and e_n is the calculated percent error for the n-th pin power p_n.

Table II shows the comparison of fuel assembly powers calculated by SUHAM-3D and MCNP codes. Powers in Table II and the assemblies in Fig. 2 are shown in the same order.

Table I. Integral comparisons of local powers (fissions), calculated by SUHAM-3D and MCNP codes

Quantity	MCNP	SUHAM-3D	Distinction from MCNP, %
Average pin power	1.000	1.000	–
Maximum pin power	2.500(±0.16%)	2.515	0.62
Minimum pin power	0.231(±0.58%)	0.226	-2.09
Maximum percent error	–	2.92	–
AVG, %	0.32	0.77	–
RMS, %	0.34	0.97	–
MRE, %	0.27	0.65	–
Number of pins within reference confidence interval of MCNP (0.999δ)	–	316	
Total number of pins	1056	1056	
Average pin power in FA-UO_2-1	1.867	1.878	0.58
Average pin power in FA-MOX	0.802	0.799	-0.37
Average pin power in FA--UO_2-2	0.529	0.524	-0.90

Table II. Comparison of fuel assembly powers calculated by SUHAM-3D and MCNP codes

MCNP		SUHAM-3D		Distinction from MCNP, %	
492.9(±0.10%)	211.7(±0.18%)	495.7	211.0	0.58	-0.37
211.7(±0.18%)	139.6(±0.20%)	211.0	138.4	-0.37	-0.90

Tables III - V show the percent distinctions of pin powers in each fuel assemblies FA-UO_2-1, FA-UO_2-1 and FA-MOX correspondingly calculated by SUHAM-3D code from values calculated by MCNP code.

5. CONCLUSIONS

In this paper the first variant of SUHAM-3D code has been described. The simplest 3D finite-difference equations of Surface Harmonics method with three transversal and two longitudinal trial matrices for each cell derived for square lattice and for two-stage calculation with one calculation point per one cell and one energy group have been realized in this variant of code. International benchmark C5G7 was used for initial verification of SUHAM-3D code. Comparison was carried out with results calculated by MCNP code. The main results of this verification are the following ones:

- The methodical error of k_{eff} is **0.12 %**.
- Maximum percent error of pin powers is 2.9 %.
- Average on module of the pin power percent error is 0.8 %.
- Root mean square of the pin power percent error is 1.0 %.

- Maximum percent error of the fuel assembly power is 0.9 %.
- Maximum error of both pin and fuel assembly power is observed for FA-UO_2-2, which is in the most heterogeneous environment.

Results of verification show that SUHAM-3D code calculates the benchmark C5G7 with enough high accuracy and with not large computational expenditures – 1 hour and 15 minutes on PC 3.2 MHz. It is assumed that subsequent development of SUHAM-3D will be directed at the objects with triangular lattices including three-stage 3D calculation of VVER-1000 core.

Table III. Percent distinctions of pin powers in FA-UO_2-1 calculated by SUHAM-3D code from values calculated by MCNP code

UO2-1	Percent Errors																	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
1	0.47	0.52	0.44	0.42	0.70	0.59	0.47	0.64	0.61	0.44	0.70	0.70	0.62	0.41	0.43	0.27	0.18	1
2		0.55	0.66	0.68	0.64	0.62	0.50	0.67	0.70	0.55	0.57	0.75	0.61	0.63	0.56	0.43	0.10	2
3			0.39	0.78	0.65		0.73	0.68		0.88	0.91		0.88	0.73	0.55	0.40	0.06	3
4					0.62	0.87	0.57	0.48	0.67	0.64	0.64	0.92	0.63		0.66	0.55	0.18	4
5					0.45	0.87	0.58	0.53	0.72	0.55	0.67	0.84	0.67	0.60	0.62	0.31	0.24	5
6							0.75	0.67		0.96	0.84		0.85	0.86		0.41	0.14	6
7							0.53	0.57	0.83	0.51	0.48	0.75	0.68	0.63	0.66	0.32	0.23	7
8								0.46	0.69	0.51	0.60	0.73	0.59	0.41	0.65	0.35	0.05	8
9										0.86	0.83		0.82	0.70		0.54	0.19	9
10										0.66	0.58	0.70	0.48	0.26	0.64	0.15	0.09	10
11											0.62	0.69	0.59	0.52	0.61	0.22	-0.02	11
12													0.83	0.72		0.39	0.17	12
13													0.51	0.62	0.47	0.37	0.16	13
14															0.53	0.41	0.25	14
15															0.05	0.34	0.18	15
16																-0.16	-0.38	16
17																	-0.52	17

Table IV. Percent distinctions of pin powers in FA-UO_2-2 calculated by SUHAM-3D code from values calculated by MCNP code

UO2-2 / Percent Errors	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	
18	-0.93	-0.86	-0.69	-0.42	-0.16	-0.33	-0.73	-0.88	-0.77	-0.94	-1.15	-1.08	-1.59	-1.73	-1.82	-1.42	-0.64	18
19		-0.61	-0.51	-0.20	-0.33	-0.46	-0.43	-0.53	-0.56	-0.90	-0.83	-1.34	-1.44	-1.48	-1.58	-1.29	-0.33	19
20			-0.16	-0.11	-0.06		-0.21	-0.31		-0.25	-0.39		-0.78	-1.32	-1.37	-0.79	0.00	20
21					-0.09	-0.07	-0.33	-0.24	-0.49	-0.74	-1.01	-0.82	-1.29		-0.97	-0.93	-0.17	21
22					-0.34	0.00	-0.24	-0.41	-0.49	-0.80	-0.88	-0.77	-1.23	-1.33	-1.23	-1.06	0.29	22
23							-0.29	-0.55		-0.53	-0.86		-1.34	-1.27		-1.13	-0.13	23
24							-0.61	-0.52	-0.42	-0.83	-1.21	-1.10	-1.48	-1.96	-1.64	-1.34	-0.28	24
25								-0.62	-0.71	-1.10	-1.01	-0.96	-1.35	-1.96	-1.53	-1.48	-0.40	25
26										-0.72	-1.18		-1.32	-1.67		-1.42	-0.37	26
27										-1.10	-1.75	-1.56	-1.69	-2.08	-2.05	-1.78	-0.73	27
28											-1.64	-1.94	-2.19	-2.15	-2.18	-2.03	-0.92	28
29													-1.99	-2.38		-2.08	-1.23	29
30													-2.51	-2.92	-2.80	-2.45	-1.23	30
31															-2.82	-1.98	-1.61	31
32															-2.79	-2.57	-1.71	32
33																-2.09	-1.94	33
34																	-1.43	34

Table V. Percent distinctions of pin powers in FA-MOX calculated by SUHAM-3D code from values calculated by MCNP code

MOX	Percent Errors																	
	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	
1	0.30	-0.05	0.03	-0.05	-0.16	0.34	-0.16	-0.50	-0.09	-0.57	-0.68	-0.35	-1.22	-1.40	-1.45	-1.18	0.38	1
2	0.28	0.19	0.15	0.43	-0.72	-0.02	-0.79	-0.52	-0.06	-0.92	-0.97	-0.78	-1.55	-0.80	-1.16	-0.87	0.32	2
3	0.28	0.28	-0.32	0.46	-0.44		0.70	0.51		0.25	0.15		-1.14	-0.30	-1.53	-1.22	0.32	3
4	0.25	0.34	0.69		-0.38	1.06	-0.87	-0.90	0.46	-0.94	-1.00	0.40	-1.17		-0.79	-0.60	0.59	4
5	0.31	-0.21	-0.10	-0.48	-1.33	0.35	-0.96	-0.90	0.51	-1.17	-1.12	0.31	-2.31	-1.41	-1.54	-1.32	0.64	5
6	0.56	-0.03		0.84	0.52		0.42	0.26		0.50	0.00		-0.11	-0.10		-0.78	0.61	6
7	0.22	-0.51	0.46	-1.02	-0.76	0.64	-1.18	-1.35	0.37	-1.35	-1.40	0.12	-1.88	-1.54	-0.45	-1.60	-0.06	7
8	0.14	-0.48	0.53	-0.89	-1.10	0.37	-1.22	-1.10	0.67	-1.47	-1.44	-0.02	-1.96	-1.87	-0.97	-1.46	0.29	8
9	0.40	-0.14		0.31	0.66		0.40	0.22		0.31	-0.15		-0.23	-0.64		-0.89	0.44	9
10	-0.03	-0.76	0.69	-0.81	-0.98	0.43	-1.35	-1.60	0.18	-1.59	-1.66	-0.20	-2.24	-1.97	-0.58	-1.94	0.10	10
11	0.20	-0.43	0.50	-0.80	-1.10	0.24	-1.10	-0.94	0.20	-1.30	-1.52	-0.34	-2.00	-1.87	-0.95	-2.30	0.14	11
12	0.51	0.02		0.82	0.25		0.29	0.18		0.08	-0.15		-0.51	-0.16		-1.14	0.04	12
13	0.16	-0.56	-0.41	-0.74	-1.32	0.39	-1.21	-1.48	0.02	-1.59	-1.79	-0.24	-2.27	-1.78	-1.62	-1.80	0.07	13
14	0.09	0.07	0.25		-0.66	0.59	-1.03	-1.20	0.23	-1.74	-1.48	-0.24	-1.90		-1.05	-1.09	0.32	14
15	0.22	-0.03	-0.56	0.39	-0.68		0.08	0.11		-0.30	-0.37		-1.37	-1.00	-2.18	-1.54	-0.01	15
16	-0.11	-0.02	-0.11	0.08	-0.95	-0.25	-0.98	-1.11	-0.46	-1.56	-1.70	-1.16	-1.75	-1.26	-1.80	-1.05	-0.30	16
17	-0.30	-0.11	-0.12	-0.29	-0.17	0.12	-0.32	-0.49	-0.22	-1.07	-1.32	-0.76	-1.23	-1.46	-1.23	-1.15	0.27	17

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