

Benchmark calculations for hexagonal lattices with different methods

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ABSTRACT

Necessity to increase the safety conditions of exploitation of recently designed core of modern nuclear reactors causes stronger requirements to the precision of neutron-physical analysis. To get more precise characteristics of nuclear reactor cells and assembly one can increase the accuracy of neutron-physical calculation analysis by taking account the spectral effects. This paper deals with the analysis of the ZR-6 series of experiments using some components of the KARATE code system. The goal of our investigations is the comparison of measured and calculated parameters of perturbed hexagonal lattices containing Gd_2O_3 in Al_2O_3 matrix or water holes. The quoted results include: the criticality parameters H_{cr} , dp/dh and the absorber rod efficiency: $\Delta\rho$. The experiments are based on doubling time measurements. The calculations have been compared not only to the measured data but to the Monte Carlo code results, too.

1. INTRODUCTION

Recently fuel assemblies containing Gd pins are used in VVER-440 loadings and their usage will be higher in the future. Different pin-distributions are designed and tested for VVER type reactors. In the configuration offered by BNFL there are three pins with 4 wt% gadolinium surrounding the central hole in 120 degree. In the Russian arrangements, there are six pins in an assembly, next to the corners with 3.35-4.5 wt% Gd [1]. The calculation of neutronic characteristics of such type of assemblies has special features and is more complicate in comparison with calculation of an ordinary fuel bundle. That is why the additional analyses of calculational tool accuracy applied to the systems with UO_2 -Gd fuel are necessary. The increase of the safety conditions of recently designed core of modern nuclear reactors causes stronger requirements to the precision of neutron-physical analysis.

The “adequacy” of a code system is traditionally discussed in terms of verification and validation processes. Validation, generally performed by the users, involves investigation whether the code faithfully reproduces reality for a particular range of applications of interest. The primary aim of the validation of the criticality code is to ensure that the code works properly and that it is used correctly. Moreover, the applicability of the codes and libraries are studied in order to establish their advantages and weak points. Further, errors could cancel each other out. Hence, more weight should be given to laborious studies of different type of measurements. A wide range of variants of VVER type hexagonal lattices were performed in the ZR-6 critical facility and such a way all of the parameters are provided for validating

codes, which generates few group cross sections for reactor codes. The experimental specification is written in sufficient detail to permit both 2D and 3D models to be set up. This is invaluable in benchmarking as it allows 3D Monte Carlo models to be used to check the accuracy of 2D deterministic methods. A Monte Carlo model with the use of MCNP4C2 has been developed and the effects of various uncertainties on the multiplication factor have been studied.

Currently extensive validation of nuclear libraries has been performed against these experiments with the help of the modules of the KARATE-440 code package, which is used for the calculation of VVER-440 reactor cores [2]. The system comprises units from the multigroup transport calculations up to the nodal calculations of the reactor core. In the frame of an upgrade the application of the ENDF/B-VI Release 6, nuclear data were used in all stages of the calculations instead of the former ENDF/B-IV library.

In this paper, the experimental conditions are described and the full set of experimental results is given, first. Instead of describing the experimental methods in detail, earlier works are referred, too. The analysis of the ZR-6 series of experiments using some components of the KARATE code system and MCNP4C2 code are summarized, too. The goal of our investigations is the comparison of measured and calculated parameters of perturbed hexagonal lattices containing Gd_2O_3 in Al_2O_3 matrix and/or water holes. The quoted results include the critical height H_{cr} , height reactivity coefficient dp/dh and the absorber rod efficiency $\Delta\rho$.

2. EXPERIMENTAL CONDITIONS OF REACTIVITY EFFECTS MEASUREMENTS

The experiments were carried out in the critical assembly ZR-6 at KFKI and the essential part of these results is being included in the two chapters of the NEA International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSB), so the fuel and absorber rods are specified there in detail (see [3-5]). In the investigated cases 1519 pins can be found in the core and the lattice pitch is 12.7mm. The moderator is distilled water and the temperature of the pile is 21 °C. The arrangement of fuel and absorber is an X_n type configurations. X stands for the type of absorber, namely $X=E, I, J, K, L, M$ which denotes water hole, 0, 0.2, 1.0, 2.0, 5.0, 7.5 wt% Gd content respectively. The number n indicates, that every n -th fuel rod in the lattice is changed for an absorber rod. In an other case the only one, the central pin is changed. Such configurations can be considered as composed of an infinitely large macrocell, they are denoted by X_∞ . The configuration signed by “ $X7+E_\infty$ ” stands for an $X7$ configuration, where the central absorber rod was changed for a water hole. The results of the measurements are summarized in the Table 1.

Preparing model for the experiments two problems are outlined, namely the dry part of the pins, above the water level and the effect of the grid plate (see Figure 1).

The dry part can be simulated by 3D calculation (e.g. Monte Carlo), or an axial buckling can be introduced, according to the results of the experiments:

$$B_z^2 = \left(\frac{\pi}{H_{cr} + \lambda_z} \right)^2 \quad \text{where } \lambda_z = 13.27 \pm 0.09 \text{ cm} \quad (1)$$

This assumption is based on two aspects of ZR-6 cores:

- axial cosine shape fundamental mode exists in all the cores studied,
- the axial extrapolation length λ_z only depends on the lattice pitch [3,5].

Table 1: Results of the criticality measurements

Lattice Type	Core Ident.	H_{cr} [mm]	$\partial\rho/\partial H$ [¢/mm]	\overline{H} [mm]	B_z^2 [m ⁻²]	β_{eff} [%]
E7	138/138	314.0 ±0.01	8.63±0.06	314.0	49.60	0.774
E∞	293/293	318.72 ±0.02	9.42±0.11	318.7	48.44	0.7735
L∞	294/294	322.90 ±0.02	9.29±0.10	322.9	47.55	0.7735
L7+E∞	295/295	373.24 ±0.02	6.61±0.07	373.2	38.56	0.766
L7	296/296	379.51 ±0.01	6.40±0.03	379.5	37.62	0.766
I7+E∞	297/297	320.88 ±0.01	9.25±0.10	320.9	47.97	0.774
I7	298/298	321.27 ±0.03	8.69±0.15	321.3	47.88	0.774
I∞	299/299	319.48 ±0.06	9.26±0.30	319.5	48.27	0.7735
K∞	302/302	320.16 ±0.02	8.45±0.09	320.1	48.14	0.7735
K7	303/303	368.90 ±0.01	6.37±0.02	368.9	39.23	0.767
K7+E∞	304/304	366.23±0.05	6.27±0.17	366.3	39.65	0.767
M∞	305/305	323.48±0.01	7.77±0.09	323.5	47.42	0.7735
M7+E∞	306/306	384.56±0.06	6.11±0.09	384.6	36.88	0.7645
M7	307/307	391.97±0.08	5.79±0.17	392.0	35.85	0.7645
N∞	308/308	323.70±0.07	7.88±0.30	323.7	47.38	0.7735
N7+E∞	309/309	388.71±0.03	5.68±0.64	388.7	36.30	0.764
N7	310/310	396.77±0.01	5.26±0.32	396.8	35.20	0.764
J∞	311/311	320.72±0.07	8.04±0.30	320.8	47.99	0.7735
J7	312/312	347.60±0.01	7.28±0.04	347.6	42.78	0.7695
J7+E∞	313/313	345.05±0.02	7.22 ±0.06	345.05	43.23	0.7695

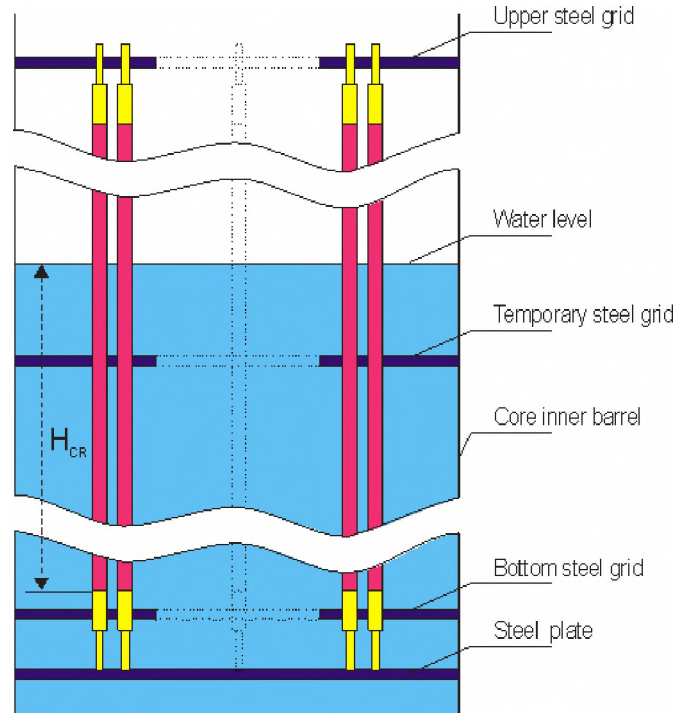


Figure 1 The axial cross section of the cylindrical ZR-6 core

A grid plate positioned in the core for safety reason causes the other problems for the simulation. It has a strong effect on the reactivity if the plate is below the moderator level and the following perturbation formula was developed for it [5]:

$$\Delta\rho(H_g, H_{cr}) = \eta \frac{\cos^2(B_z z_g)}{\frac{H_{cr}}{2} \left(1 + \frac{\sin(B_z H_{cr})}{B_z H_{cr}} \right)} \quad (2)$$

where:

- $z_g = H_g - H_{cr}/2$ is the distance between the grid plate and the middle of the core,
- η is a coefficient depending on the thickness and material of the grid plate (see [5]).

The effect of the plate has no roll in the recently investigated set of experiment as in these cases the critical water level was about 200 mm below the grid plate, but some other experiments referred later on need the correction (see Table 3).

The rod worth for rod type “X” in configuration “K” was not measured directly it was determined by combining the directly measured data, according to the formula:

$$\rho_K^X = \int_{\bar{H}_0^K}^{\bar{H}_X^K} \frac{\partial \rho}{\partial H} dH = \left| \frac{\partial \rho}{\partial B_z^2} \right|_0^K \left[\frac{\pi^2}{(\bar{H}_0^K + \lambda_z)^2} - \frac{\pi^2}{(\bar{H}_X^K + \lambda_z)^2} \right] \quad (3)$$

Here, \bar{H}_0^K is the critical water level measured in a critical state with water hole in place of the absorber, \bar{H}_X^K is the critical water level measured in the presence of the absorber rod. The λ_z is the axial extrapolation length, which is known from axial reaction rate distributions (measured in a larger class of lattices, see [5]). The factor $\partial \rho / \partial B_z^2$ depends only slightly on the configuration if C_B , the temperature, and the lattice pitch do not change. Principally, there are two possibilities for determining the absorber rods' reactivity worth. The first one is to use $\partial \rho / \partial B_z^2$ from independent measurements performed for similar lattices, the other one is to determine $\partial \rho / \partial B_z^2$ based on the following relation:

$$\frac{\partial \rho}{\partial H} = - \frac{\partial \rho}{\partial B_z^2} \frac{2\pi^2}{(H_{cr} + \lambda_z)^3} \quad (4)$$

by substituting, the data measured for the lattice at hand. The difference is not significant. The following value was used: $\left| \partial \rho / \partial B_z^2 \right| = 32.0 \pm 0.3 \text{ cm}^2$ for the reactivity worth presented in Table 2, where, three different rod worths are given.

The values in the second column are related to a single absorber rod inserted in the central lattice position of a regular lattice. In this case, the subscript “0” in Equation 3 corresponds to the E_∞ lattice while the subscript “X” to the X_∞ lattice.

The values given in the third column are related to the rod in the central lattice position of the X7-type core. In this case, the subscript “0” in Equation 3 corresponds to the X7+ E_∞ core, while the subscript “X” indicates the usual X7 lattice.

The values given in the fourth column are the reactivity worth averaged for the 31 absorber rods. In this case, the subscript “0” in Equation 3 corresponds to the E7 lattice while the subscript “X” corresponds to the X7 lattice, and the resulting total reactivity worth is divided by 31. Thus, the rod worth given in this column of Table 2 are also related to one absorber rod.

Table 2: Effective Reactivity Worth of Gd-Bearing Rods

Rod Type (X)	In X_{∞} Configuration	In $X7-E_{\infty}$ Configuration	In $X7$ Configuration
I	$6.83 \pm 0.63 \text{ } \phi$	$3.38 \pm 0.32 \text{ } \phi$	$2.10 \pm 0.30 \text{ } \phi$
J	$17.6 \pm 0.83 \text{ } \phi$	$18.9 \pm 0.37 \text{ } \phi$	$8.90 \pm 0.32 \text{ } \phi$
K	$12.7 \pm 0.38 \text{ } \phi$	$17.4 \pm 0.51 \text{ } \phi$	$13.6 \pm 0.26 \text{ } \phi$
L	$36.6 \pm 0.66 \text{ } \phi$	$38.8 \pm 0.60 \text{ } \phi$	$15.8 \pm 0.29 \text{ } \phi$
M	$41.6 \pm 0.68 \text{ } \phi$	$42.7 \pm 1.06 \text{ } \phi$	$18.1 \pm 0.66 \text{ } \phi$
N	$42.6 \pm 1.07 \text{ } \phi$	$45.4 \pm 0.69 \text{ } \phi$	$19.0 \pm 0.33 \text{ } \phi$

It follows from the above explanations that the reactivity values given in the individual columns of Table 2 may not be compared with one another since they mean different things. In all three columns, the rod worth increases with increasing Gd content. There is only one exception: the first two values (i.e. for the X_{∞} and $X7+E_{\infty}$ configurations) obtained for the J and/or K-type rods seem to be outliers to this picture. The insertion of a wrong absorber rod in the core center can not be excluded.

3. MONTE CARLO CALCULATIONS

Since MCNP has been widely validated for different reactor configurations, here it was used to investigate the role of 3D effects and the influence of some uncertainties. The version MCNP4C2 [6] and ENDF/B-VI data libraries were used. The geometry and material composition of the set-up is described in the ICSB report [5] in a very detailed manner. According to this specification, a simplified and a full 3D core calculation models were constructed. A 30 degree symmetry sector was described in the models. The detailed model describes the experimental geometry as precisely as possible, as it includes lower filling plate, reactor support, bottom, temporary/movable intermediate and upper grids, top and bottom construction units. Special attention was paid for the description of the dry lattice, which characterizes the water level controlled critical facilities. On the other hand, in the simplified model axially only three parts were taken into account (the water layer below the pins, pins with moderators and the dry parts). The grid was taken into account by water level correction. All Monte Carlo calculations were performed using at least 50 passive and 600 active cycles with 25000 or more neutrons per cycle. To show the good functioning of the detailed model, a set of criticality calculation were performed. Some of these data can be seen in the Table 3.

Table 3: Measured buckling and k_{eff} for lattices calculated by MULTICELL and MCNP codes

Lattice type	B^2 measured [m ⁻²]	k_{eff} calc.using ENDF/B-VI.	k_{eff} calc. using ENDF/B-IV.[5]	k_{eff} calc.by MCNP ENDF/B-VI.
11.0/3.6/0.0	66.01 ± 0.55	0.9975	0.9940	0.98973
11.0/3.6/1.0	62.14 ± 0.62	1.0020	0.9981	0.98726
12.7/3.6/0.0	100.40 ± 0.41	1.0087	1.0082	0.99415
12.7/3.6/5.8	64.95 ± 0.26	1.0079	1.0054	0.99430
15.0/3.6/0.0	120.36 ± 0.65	1.0087	1.0112	0.99463
15.0/3.6/4.0	70.25 ± 0.81	1.0137	1.0134	1.00039
15.0/4.4/0.0	136.80 ± 0.64	1.0033	1.0054	0.99266

A non trivial perturbation in these experiments is the movable grid plate which has an effect on the reactivity especially if it is below the moderator level (see Figure 2). By means of 3D diffusion calculations it was shown that the effect can be described by the first order perturbation formula, which depends on the axial position of the grid plate and its material and geometrical characteristic (Eq. 2).

This can be applicable for Al and Plexiglas plate, because Δp is small for them. However, its applicability is questionable for stainless steel grid plates, which were mostly used in these experiments. In Table 4 some preliminary results can be seen for given measured states. Here σ_t means the square root of the squared sum of the standard deviations of the two calculations. In case of the direct measured water level the detailed model was used, while the corrected one was used in the simplified calculation. Only a limited number of data can be compared. This preliminary result suggests that the correction method suggested in [5] can be used in general, but its usage needs further studies.

Table 4: Comparison of k_{eff} values computed by MCNP4C2 using accurate 3D geometry and calculated by water level correction at 400°K

Lattice type	Δk_{eff}	σ_t
246/154	-4.0e-04	2.75e-04
163/161	1.4e-03	2.82e-04
188/188	1.0e-04	2.68e-04

Another source of inaccuracy is the influence of the grid plate if it is above the critical water level. The distance between the critical water level and the grid decreases as the temperature increases or content of Gd is changed and such a way the “dry part” of the core, which was characterized by a given reflector savings, was perturbed. In these cases the grid plate has two effects.

Table 5: Influence of the spacer grid on k_{eff} as function of grid position above the water level

H (mm)	K_{eff}	Σ	Δk_{eff}
1	0.99307	7.0e-05	7.0e-04
7	0.99307	7.0e-05	7.0e-04
13	0.99302	7.0e-05	6.5e-04
20	0.99294	7.0e-05	5.7e-04
30	0.99306	7.0e-05	6.9e-04
40	0.99294	7.0e-05	5.7e-04
54	0.99280	7.0e-05	4.3e-04
70	0.99279	7.0e-05	4.2e-04
No grid	0.99237	7.0e-05	

It shields the dry core and reflects the neutrons. To investigate this effect in some cases the realistic distance between the grid and the critical water level was changed. In these calculations the detailed model was used. On table 5, the quantity Δk_{eff} as function of the position is shown. Δk_{eff} is the difference of the multiplication factor calculated at a particular grid position and calculated without the grid. It can be seen, that as the grid approaches the water level, the multiplication factor increases however this effect is rather small.

4. BRIEF DESCRIPTION OF THE CALCULATIONS

The critical water level and the reactivity changes introduced by the insertion of the absorber rod were simulated by the KARATE-440 program system, in two steps. First, the few group constants were generated by lattice calculation code, then the COREMICRO 2D fine diffusion code was used for the measurements [1].

The aim of the multigroup calculations is the generation of the few-group fine-mesh diffusion-type constants for each type of the lattice cells of the further fine-mesh assembly calculations. The epithermal-to thermal flux ratio (Spectral Index) is a parameter, which accounts for the non-asymptotic behaviour of the neutron spectrum. The calculations are performed using 35 epithermal and 35 thermal energy groups on the basis of the ENDF/B-VI (version 6.) nuclear data library. The thermal scattering is described by the Nelkin-model. The cross sections of the three resonance isotopes (U^{235} , U^{238} , Pu^{239}) and the Bell-factors are tabulated as a function of the dilution cross section of a homogeneous material and the temperature. The equivalence theory is used for the calculation of the shielded multigroup cross sections for the heterogeneous case, where the Dancoff factor is determined from the first flight collision probabilities. The following modules can be used for calculating the cell averaged few-group constants:

- the BETTYC code is applied for the fuel cells,
- the COLA code is applied for the cells containing absorber or water hole surrounded by fuel cells,
- The MULTICEL program can be used close to the complicated heterogeneities, for example near the edge of the fuel assemblies or the reflector,

The fuel assembly characteristics are calculated by the COREMICRO code solving the few (2 or 4)-group fine-mesh diffusion equation in hexagonal geometry for the given assembly or for the assembly and its surroundings. The irregularity between the assemblies is also taken into account in the difference scheme. The group constants depend on the parameters listed above, and the feedback via the Spectral Index accounts for the non-asymptotic spectrum. The boundary condition can be the traditional white boundary condition on the edge of the fuel assembly, or it can be a given flux distribution on the boundary of the calculation.

The simplest way to characterize criticality with 2D code is to calculate the k_{eff} values of the investigated lattices using the measured axial buckling (eq. 1) and to compare it to $k_{eff}=1$, which is considered as measured value. The k_{eff} calculated by COREMICRO using different few group libraries and by the MCNP code using ENDFB-6 library their averages and variances are also shown in table 6. The criticality calculations became slightly closer to the unity by the applied spectral index correction in 2 group, but there is no practical effect in 4 groups.

The MCNP underestimates the criticality, which is our general practice in connection of the MCNP4C2 code and its ENDFB-6(ver. 2) library. This effect was investigated in [7] in detail. The measured rod efficiencies were calculated by the COREMICRO code, too (Tab. 7–9).

Only the last series of measurements (average worth of 31 pins) can be accepted. In table 9 one can see that the COREMICRO slightly overestimates the rod worth, especially in case of spectral correction. Because of hidden experimental problems the other two series of measurements can not be fully accepted. The calculated figures could be in good agreement with our former results [8].

Table 6: Results of the criticality measurements done during absorber pin measurements

Lattice Type	Calculated 2-G	Calculated 2-G sp. corr.	Calculated 4-G	Calculated 4-G sp. corr.	MCNP
E7	1.0066	1.0052	1.0021	1.0031	0.98843
E ∞	1.0057	1.0042	1.0014	1.0017	0.99328
L ∞	1.0055	1.0039	1.0012	1.0014	0.99361
L7+E ∞	1.0015	1.0001	0.9993	0.9996	0.99175
L7	1.0013	0.99979	0.99917	0.99933	0.99148
I7+E ∞	1.0057	1.0043	1.0023	1.0030	0.99358
I7	1.0055	1.0041	1.0022	1.0029	0.99287
I ∞	1.0058	1.0042	1.0015	1.0018	0.99241
K ∞	1.0041	1.0025	0.99972	0.99989	0.99080
K7	1.0005	0.99915	0.99826	0.99859	0.99020
K7+E ∞	1.0020	1.00070	0.99972	1.0001	0.99249
M ∞	1.00560	1.00400	1.00130	1.0015	0.99268
M7+E ∞	1.0027	1.0012	1.0006	1.0007	0.99239
M7	1.0025	1.0008	1.0004	1.0004	0.99303
N ∞	1.0056	1.0040	1.0013	1.0015	0.99262
N7+E ∞	1.0029	1.0013	1.0007	1.0007	0.99319
N7	1.0027	1.0010	1.0006	1.0005	0.99209
J ∞	1.0055	1.0039	1.0012	1.0014	0.99236
J7	1.0038	1.0025	1.0011	1.0018	0.99399
J7+E ∞	1.0041	1.0029	1.0014	1.0021	0.99354
Average	1.00398	1.00249	1.00077	1.0011	0.99234
St. dev.	0.00184	0.00183	0.00108	0.00124	0.00129

Table 7: Effective Reactivity Worth of Gd-Bearing Rods in X ∞ Configuration

Rod (X)	Measured [ρ]	Calculated 2-G	Calculated 2-G sp. corr.	Calculated 4-G	Calculated 4-G sp. corr.
I	6.83 \pm 0.63	5.11	6.41	5.16	5.17
J	17.6 \pm 0.83	20.48	20.55	20.66	21.94
K	12.7 \pm 0.38	32.00	33.42	33.61	35.40
L	36.6 \pm 0.66	35.90	37.30	37.50	39.40
M	41.6 \pm 0.68	39.75	41.16	41.51	43.57
N	42.6 \pm 1.07	41.03	42.45	43.30	45.38

Table 8: Effective Reactivity Worth of Gd-Bearing Rods in X7-E ∞ Configuration

Rod (X)	Measured [ρ]	Calculated 2-G	Calculated 2-G sp. corr.	Calculated 4-G	Calculated 4-G sp. corr.
I	3.38 \pm 0.32	6.39	6.40	5.15	5.14
J	18.9 \pm 0.37	21.95	22.00	22.20	22.04
K	17.4 \pm 0.51	35.55	36.56	36.10	37.00
L	38.8 \pm 0.60	39.30	40.98	40.51	42.21
M	42.7 \pm 1.06	43.47	45.83	44.97	46.90
N	45.4 \pm 0.69	45.84	47.43	46.57	48.28

Table 9: Effective Reactivity Worth of Gd-Bearing Rods in X7 Configuration

Rod (X)	Measured [ϵ]	Calculated 2-G	Calculated 2-G sp. corr.	Calculated 4-G	Calculated 4-G sp. corr.
I	2.10 ± 0.30	2.52	2.54	2.13	2.27
J	8.90 ± 0.32	9.60	9.56	9.29	9.48
K	13.6 ± 0.26	15.56	15.59	15.30	15.67
L	15.8 ± 0.29	17.34	17.42	17.10	17.58
M	18.1 ± 0.66	19.17	19.32	19.02	19.60
N	19.0 ± 0.33	19.93	20.10	19.85	20.46

5. CONCLUSIONS

In the present work, we have performed the analysis of ZR-6 measurements by using the modules of the KARATE-440 code system with the new nuclear data libraries based on ENDF/B-VI.

The criticality calculations on the several pin-cell and perturbed lattices show good agreement with the measurements. In that case Monte Carlo calculations were performed to investigate the effect of the movable grid plate. Preliminary results indicated that the corrected critical water level can be used without modification, however further investigation is required for the grid plate. Moreover, the applicability of the COREMICRO code and its libraries were studied in order to reveal their advantages and weak points. The validation was extended to the efficiency of absorber pins containing different quantity of Gd in different basic sets. The results concerning the calculations are partially fruitful as some errors of the chosen set of measurement may be hypothesized.

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