VALIDATION OF A PIN-BY-PIN HETEROGENEOUS METHOD AGAINST LWR MOX BENCHMARKS

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ABSTRACT

The 3-D pin-by-pin model based on the advanced heterogeneous reactor theory was developed in RRC "Kurchatov Institute" for analysis of consequences of reactivity accidents in LWRs. This model implemented in the BARS neutronic code and coupled with the RELAP5/MOD3.2 thermal-hydraulic code allows simulation of a wide range of transients. Previously, the BARS code package (including the UNK code used for neutron database generation) was validated against LWR UO_2 numerical and experimental benchmarks. This paper is focused on the validation for MOX-fuelled LWR systems. The UNK validation includes a number of various MOX fuel unit cells available in open literature. The multiplication factor, neutron balance, and different reactivity effects have been investigated. Comparison with calculations performed by Monte Carlo or transport codes shows a good agreement in calculation of the major neutronic parameters of MOX fuel. The spatial (pin-by-pin) power effects were analyzed for the LWR MOX experimental and numerical benchmarks. The BARS calculations were performed using 5-group neutron databases generated by UNK on the basis of ENDF/B-VI. The effective multiplication factor and pin-power distributions were compared against the measurements and other calculations. Pin-power distributions calculated by BARS agree with rather high accuracy with the experimental data or Monte Carlo or S_N calculations. The root-mean square deviations do not exceed 1.5%. The validation results show that the BARS code package can be used in calculations of LWR MOX-fuelled systems with a precision adequate for most design purposes.

1. INTRODUCTION

Large-scale use of MOX fuel in light water reactors (LWRs) will demand new approaches to confirm the LWR operational regimes in which MOX fuels comply with safety criteria. Changes in isotopic and spectral characteristics of MOX fuel compared with conventional UO_2 fuel result in lower boron and control rod worth and more negative fuel and moderator temperature coefficients. Therefore, a problem of improvements in approaches for modeling MOX cores becomes essential. Consequently, there is a need to validate calculational procedures for physics modeling of MOX-fuelled cores against the measurements and precise calculations.

The most of modern computing tools used for the LWR in-core management and safety analysis, consist in two stages. First stage includes a preparation of few-group cross-sections on the basis of the up-to-date versions of the evaluated nuclear data files, such as, JEF, ENDF/B, and JENDL. As a rule, these sets are generated as homogeneous for the whole fuel assembly using a 2-D transport code.

Second stage consists in a global 3-D calculation using assembly-by-assembly core representation. Therefore, it is necessary to validate neutronic calculational methods for both stages.

Unlike widely spread assembly-by-assembly codes, a pin-by-pin approach implemented in the BARS code, allows a detailed representation of the reactor core structure [1]. Obviously, that a neutronic database calculated for separate pin cells has a number of advantages, especially in treatment of various intra-assembly effects. Such advantages become valuable because of a modern LWR MOX fuel assembly has very complicated composition: the fuel assembly components have very different neutronic properties. There are fuel pins with different nuclide composition, burnable or control rod absorbers, water tubes, etc. Consequently, homogenized neutronic cross-section sets depend greatly on the neutron spectrum inside the assembly. As a rule, these sets are calculated using an "isolated assembly" approximation, which models the infinite array of the same fuel assemblies, i.e. at the fixed neutron spectrum. Obviously, such homogenized assembly model can not embrace all variety of intra-assembly effects, which occur during the accident, in particular, related with the neutron spectrum changes inside the assembly. Besides, "homogenized" parameters in the neutronic database of any assembly-by-assembly code, such as, for instance, fuel temperature or coolant density, are determined for the assembly as a whole and, therefore, bring additional uncertainties in calculation of the safety related parameters, such as local fuel enthalpy.

Previously, the comprehensive validation of the BARS code package has been undertaken [1-3]. This validation dealt with conventional UO_2 fuels at wide range of burnup, but did not include MOX fuel. As it was found, the approaches implemented in the BARS code package met all demands on the calculational accuracy to predict the basic neutronic parameters of LWRs: the multiplication factor, reactivity and spatial pin-power effects.

This report is focused on the validation of the BARS code package for MOX-fuelled systems. All the calculations were performed using the neutron databases generated by the UNK code [4]. In its turn UNK used a multigroup database prepared by the NJOY code on the basis of the nuclear evaluated file ENDF/B-VI. A problem with a resonance treatment for uranium and plutonium nuclides is very important. The UNK code allows a fine energy group structure for more detailed representation of the resonance regions (totally about 10,000 groups). Recently, this multigroup database was improved to extend its capabilities in calculation of MOX fuel.

Section 2 gives the features of the advanced heterogeneous method. Section 3 contains a comparison of calculations carried out by different codes using various cross-sections for LWR MOX pin cells. The pin cell is the simplest approach to calculate LWR lattice and allows to compare different neutron databases generated by using various nuclear data libraries, as well as, spectrum computing techniques, without influence of spatial effects (due to neutron leakage). The following safety related parameters were investigated: multiplication factor, neutron balance, and reactivity effects including the temperature (Doppler, void, and moderator) and poisoning (boron and Xe/Sm) effects. Section 4 focuses on spatial pin power effects within rather simple MOX-fuelled cores of LWR type. Here both the experimental and numerical benchmark cores were investigated. Five experimental benchmarks included PNL, Saxton, TCA, ESADA, KRITZ, and VENUS-2 MOX critical cores with different configurations. The effective multiplication factor and pin-power distribution inside the core were compared with the measurements and calculational results obtained by using different codes.

2. BASIC FEATURES OF THE ADVANCED HETEROGENEOUS METHOD

The advanced method of the heterogeneous reactor theory, implemented in the BARS code, is based on an analytical representation of the neutron flux distribution as a superposition of Green's functions. In LWR applications this method allows directly to take into account complicated core geometry by explicit representation of fuel pins, absorber rods, water tubes, etc. Green's function is derived from a solution of few-group diffusion equations in an infinite uniform media with a singular source at the cell axis. The intensity of this singular source is determined in such a way that relationship between the neutron flux and current at the boundary of each reactor cell coincides with that obtained from the precise transport calculation for a single cell. This relationship is treated by means of a boundary condition matrix (Λ-matrix). This matrix is determined from neutron transport calculations of the cell with varying neutron currents at its boundary.

An axial distribution of the neutron flux is described by Fourier series expansion. As a result, it is derived a set of linear algebraic equations which establish a relationship between any pair of the reactor cells. It leads to unresolved computation problem in reactor calculations: only a core with few cells could be calculated by using even modern computers. To transform these equations to connect only neighboring cells, a difference approximation of Green's functions is performed. It is to be noted that the diffusion equations are used only to determine Green's function shape that weakly influences the reactor calculation accuracy; therefore, the advanced heterogeneous method does not require the validity of the diffusion approximation over the reactor.

Unlike the traditional neutron cross-sections calculated for the whole assembly, Λ-matrices take into account effects of the anisotropic diffusion, i.e. the difference in neutron migration lengths in radial and axial directions; as a result, the corresponding dipolar and axial Λ-matrix components are used. Besides, "time absorption" Λ-matrix components used in calculations of fast transients are prepared.

The anisotropic effects become essential when, for instance, local voiding occurs in the reactor core under the reactivity initiated accident conditions. Another important aspect of the problem under consideration is a correct representation of the core-reflector interface where, in general, the diffusion approach is not valid. Usually, the traditional neutron cross-sections used by modern nodal diffusion codes are corrected using the assembly discontinuity factors. These factors are derived from a comparison between the diffusion and transport solutions of a sample problem (as a rule, in 1-D geometry) and, generally, do not guarantee accurate solution near the core-reflector region [5]. On the contrary, there is no correction in the heterogeneous method.

The BARS neutron database (Λ-matrices) is prepared by the UNK code, which solves the multigroup neutron transport equation for various reactor cells using the collision probability method taking into account detailed structure of resonant cross sections. The last are treated explicitly using a fine energy mesh with optimal mesh condensing near the resonances. The UNK neutron database is generated on the basis of ENDF/B-VI by the NJOY code. The basic mesh includes 24 fast and 65 thermal groups with cut-off energy of 2.15 eV; taking into account the fine energy mesh, totally about 10,000 groups can be used. Recently, both the UNK code and the multigroup database were improved to extend their capabilities in calculation of MOX fuel. Usually, as the BARS validation results for LWR pin-by-pin calculations showed, Λ-matrix approach provides rather high accuracy using 4-5 energy groups.

3. LWR MOX FUEL CELL CALCULATIONS

3.1. LWR PIN CELL BENCHMARK INTERCOMPARISON

Calculations for LWR MOX zero-leakage fuel cell models have been performed by different codes with using different neutron databases [6,7]. Two different MOX compositions (MOX-1 and MOX-2) at two fuel temperatures of 300 K (Case 1) and 560 K (Case 2) and moderator temperature of 300 K were considered. The Doppler effect was investigated for the MOX-1 and MOX-2 cells. To compare with the UNK results, several sets of the calculational data presented in [6,7] were used; all of them were obtained using nuclear cross-sections derived from the JEF-2.2 library. A comparison of the results is presented in Table I. The Doppler effect (given in units of pcm) was determined as a difference between the multiplication factors (K_{inf}) for Cases 1 and 2. It was found that a standard deviation in K_{inf} reached its maximum of 0.25% for MOX-1 Case 2. All codes (except for MCNP-4A) estimate the Doppler effect with high accuracy: the results are within 90 pcm or 6%. Comparison of the neutron balance between the UNK and MCNP-4A results showed a very good agreement for the process rates for major nuclides: for ^{239}Pu the maximum deviation was about 0.4%.

Table I. Comparison of Calculational Results for MOX-1 and MOX-2

	MCNP-4A	APOLLO	RESMOD	MCNP-4B	KENO-VI	UNK
Multiplication Factors						
MOX-1 Case 1	1.21840	1.21817	1.2189	1.2200	1.2160	1.22199
MOX-1 Case 2	1.20048	1.20316	1.2048	1.2054	1.2010	1.20772
MOX-2 Case 1	1.26106	1.26019	1.2631	1.2621	1.2593	1.26159
MOX-2 Case 2	1.24564	1.24609	1.2498	1.2484	1.2459	1.24836
Doppler Effects (pcm)						
MOX-1	1792	1501	1410	1460	1500	1427
MOX-2	1542	1410	1330	1370	1340	1323

3.2. INTERNATIONAL BENCHMARK ON TRANSMUTATION CONCEPTS

In the framework of the international project on transmutation concepts, the MOX PWR benchmark calculations have been performed with the purpose to investigate uncertainties in the basic physics parameters: multiplication factor, the Doppler and void effects [8]. The benchmark models based on a standard or highly moderated (HM) PWR cells included two plutonium and minor actinide (MA) compositions, denoted as MOX12 and MOX22. The MA contents were 0, 1 and 2.5 % respectively. In this study, only the beginning of cycle states were used. Along with initial K_{inf}, the Doppler effect (fuel temperature change of 300 K) and the void effects for the coolant void fractures of 40, 70 and 95% were investigated. For the comparison with the UNK calculations, the SWAT, SRAC95, and KAPROS/KARBUS codes with cross-sections based on JENDL-3.2 or JEF-2.2 were chosen. Table II summarizes calculational data for K_{inf}, the Doppler and void effects (in units of pcm). The void effect results for MOX22 are also shown in Figure 1, where the average values are fitted by curves and plotted with $\pm 2\sigma$. As can be seen the void effect becomes more positive with increase in the MA content. At the same time, the higher void fraction the higher discrepancy: the largest arises at 95% void fraction, especially when the void effect is close to zero (Case MOX22 0.0% MA).

Table II. Comparison of Calculational Results for MOX12, MOX22, and MOX22 (HM)

Case Index	Code	K_{inf}	Doppler	Void 40%	Void 70%	Void 95%
MOX12 0.0% MA	UNK	1.10931	-975	-8 236	-13 801	-14 378
	SWAT	1.10399	-990	-8 100	-13 490	-15 020
	SRAC95	1.10854	-980	-8 060	-13 270	-12 860
	KAPROS	1.10694	-1 020	-8 120	-13 320	-14 580
MOX12 1.0% MA	UNK	1.08142	-871	-5 233	-5 807	1 605
	SWAT	1.07879	-860	-5 130	-5 740	330
	SRAC95	1.08437	-860	-5 130	-5 570	2 610
	KAPROS	1.08431	-920	-4 930	-5 080	1 800
MOX12 2.5% MA	UNK	1.06516	-791	-1 794	2 299	16 622
	SWAT	1.06292	-760	-1 790	1 970	14 950
	SRAC95	1.06956	-750	-1 840	2 090	17 330
	KAPROS	1.07079	-830	-1 510	2 840	16 910
MOX22 0.0% MA	UNK	1.12675	-946	-5 578	-6 887	-929
	SWAT	1.12470	-940	-5 430	-6 730	-2 150
	SRAC95	1.12957	-930	-5 420	-6 550	100
	KAPROS	1.12585	-1 000	-5 590	-6 530	-1 480
MOX22 1.0% MA	UNK	1.10505	-868	-3 541	-1 753	9 131
	SWAT	1.10426	-850	-3 460	-1 860	7 520
	SRAC95	1.10968	-840	-3 480	-1 700	9 880
	KAPROS	1.10371	-910	-3 380	-1 480	8 550
MOX22 2.5% MA	UNK	1.08682	-794	-642	4 879	21 326
	SWAT	1.08556	-750	-700	4 370	19 480
	SRAC95	1.09186	-750	-750	4 500	21 930
	KAPROS	1.08391	-820	-560	4 920	20 830
MOX22 (HM) 0.0% MA	UNK	1.18584	-870	-10 146	-21 331	-27 482
	SWAT	1.18209	-900	-10 240	-21 260	-27 950
	SRAC95	1.18597	-890	-10 180	-21 060	-25 610
	KAPROS	1.18373	-900	-10 340	-21 300	-27 540
MOX22 (HM) 1.0% MA	UNK	1.12783	-791	-9 019	-16 321	-13 165
	SWAT	1.12559	-810	-9 040	-16 220	-14 040
	SRAC95	1.13115	-800	-9 020	-16 110	-11 610
	KAPROS	1.12469	-830	-9 080	-16 080	-13 180
MOX22 (HM) 2.5% MA	UNK	1.09208	-735	-6 253	-7 838	5 577
	SWAT	1.09050	-720	-6 280	-7 910	4 080
	SRAC95	1.09784	-710	-6 330	-7 900	6 670
	KAPROS	1.08806	-770	-6 260	-7 560	5 340

Analysis of the presented results shows that the most of the K_{inf} values are within 0.5%; the Doppler effect data are agreed within ± 40 pcm (or about 5%). The void effects at 40% and 70% void fraction are predicted with a good accuracy: the mean deviations are about 100 pcm and 200 pcm respectively. At 95% void fraction the mean deviation reaches 1000 pcm and, as shown in Figure 1, it means that when the value of the void effect is expected to be less than or of order of ±2000 pcm (or about $\pm 2\sigma$) then a significant disagreement in the results occurs.

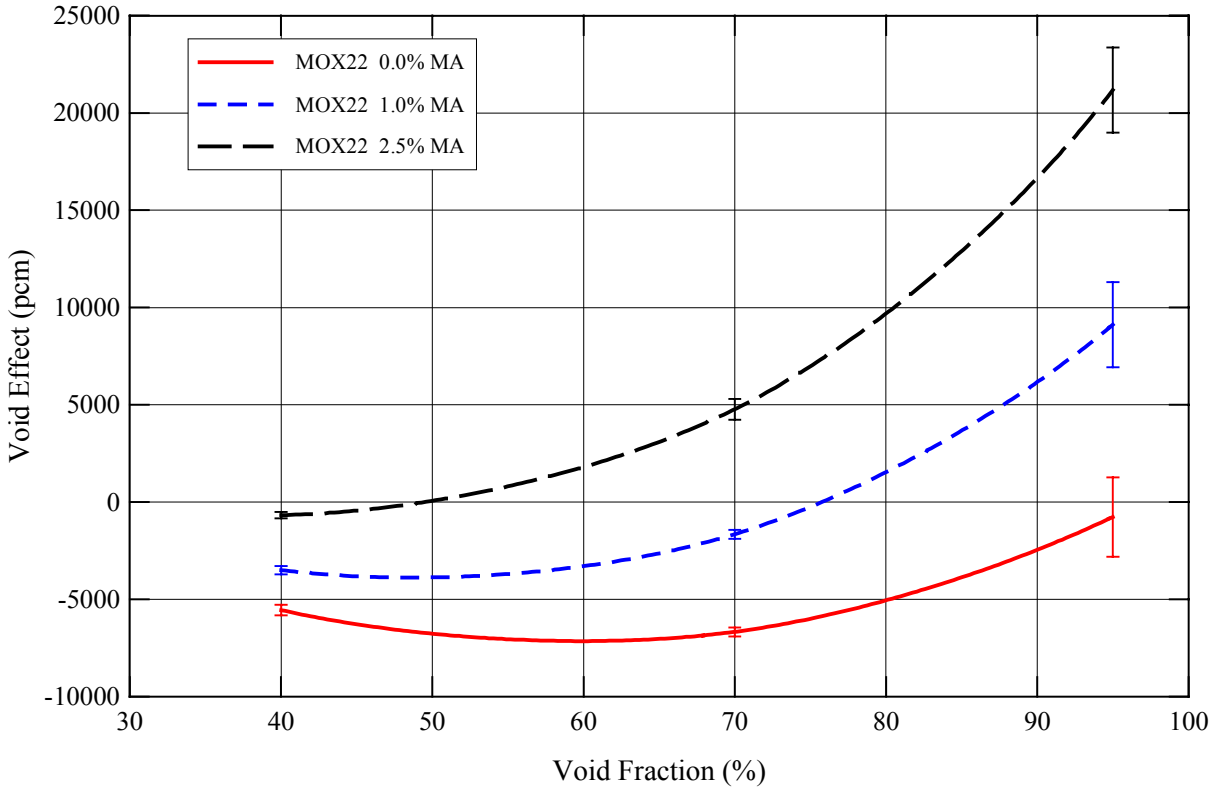

Figure 1. Void Effect vs. Void Fraction for MOX22

3.3. VVER CALCULATIONAL BENCHMARK

This calculational benchmark represents typical VVER pin cell with 1.275-cm triangular lattice pitch [9]. All cases are defined as a combination of states (denoted as S1 through S6 depending on thermal-hydraulic parameters and presence/absence of absorbers) and variants (V2, V7-10 with different fuel composition). The K_{inf} values and the following reactivity effects were investigated: the Doppler (states S5 – S4), isothermal temperature (S6 – S5), effect of presence of ^{135}Xe and ^{149}Sm in the fuel region (S4 – S1), and the boron poisoning effect (S3 – S1).

Calculational results presented in [9] were performed using the HELIOS-1.4 code with cross-sections based on ENDF/B-VI. Table III summarizes the K_{inf} values for state S1 and the reactivity effects (given in units of pcm) calculated by HELIOS-1.4 and UNK. The maximum differences in K_{inf} and the Doppler and isothermal effects are 0.9%, 6%, and 5%, respectively. Both the poisoning effects are within 1-2% uncertainty. Besides, a comparison of the neutron balance for case V2S1 was carried out. It was found an excellent agreement between the UNK and HELIOS results (the maximum deviation for uranium and plutonium nuclides is about 1%).

Table III. Comparison of Calculational Results for VVER MOX Benchmarks

Variant	Code	K_{inf} (S1)	Doppler	Isothermal	Xe/Sm	Boron
V2	HELIOS-1.4	1.2188	2000	7260	1950	2930
	UNK	1.2120	1956	7254	1974	2912
V7	HELIOS-1.4	1.3189	1720	5970	2230	3340
	UNK	1.3108	1696	5920	2244	3318
V8	HELIOS-1.4	1.1044	1880	4630	4960	5510
	UNK	1.1047	1866	4661	5009	5518
V9	HELIOS-1.4	1.5722	2050	3430	2380	3810
	UNK	1.5685	1960	3614	2373	3734
V10	HELIOS-1.4	1.1136	1860	7100	590	1340
	UNK	1.1033	1743	7128	595	1326

3.4. BENCHMARK CELL CALCULATIONS FOR UO_2-MOX CORE

This benchmark model has been proposed to compare different approaches of diffusion and transport methods as well as nuclear data sets [10]. Here only the MOX pin cell models are considered. There are three MOX cells with different plutonium enrichments (4.3%, 7.0% and 8.7%). To compare with the UNK calculations, 5 sets of calculational data presented in [10] were used. All participants used different nuclear cross-sections data derived from different libraries. Calculational results for K_{inf} are summarized in Table IV. Comparison of the neutron balance (with total absorption normalized to 100%) calculated for MOX 8.7% is shown in Table V.

Table IV. Comparison of K_{inf} for MOX Cells

	APOLLO-2	WIMS7A	HELIOS	WIMSD-4	SRAC95	UNK
MOX 4.3%	1.13710	1.13196	1.12853	1.13299	1.14152	1.13398
MOX 7.0%	1.16188	1.15749	1.15421	1.15931	1.16879	1.15751
MOX 8.7%	1.17558	1.17185	1.16908	1.17411	1.18373	1.17061

Analysis of the results presented in Table IV shows that the maximum deviation in K_{inf} reaches 1.3% between the SRAC95 and HELIOS data, which are the maximum and minimum values, respectively. The nature of such a discrepancy can be seen in Table V. About 30% of the total absorption is due to ^{239}Pu fission: the SRAC95 and HELIOS values differ by about 3%, which gives about 1% in K_{inf}.

The mean values of K_{eff} are as follows:

- MOX 4.3%: 1.1343 ± 0.0045;
- MOX 7.0%: 1.1599 ± 0.0050;
- MOX 8.7%: 1.1742 ± 0.0052.

Comparison of the neutron balance presented in Table V (note, that the original HELIOS data were properly re-normalized) shows a rather good agreement for major nuclides, except for ^{242}Pu (the maximum deviation between UNK and HELIOS is more than 15%).

Table V. Neutron Balance (%) Comparison for MOX 8.7%

		APOLLO-2	WIMS7A	HELIOS	WIMSD-4	SRAC95	UNK
^{235}U	Fission	0.813	0.816	0.804	0.814	0.832	0.812
	Absorption	1.083	1.085	1.095	1.089	1.103	1.095
^{238}U	Fission	3.269	3.157	3.189	3.121	3.079	3.128
	Absorption	22.89	22.88	22.51	22.69	22.35	22.65
^{239}Pu	Fission	29.48	29.46	29.10	29.40	29.99	29.55
	Absorption	45.27	45.15	45.51	45.04	45.77	45.41
^{240}Pu	Fission	0.412	0.407	0.392	0.373	0.370	0.374
	Absorption	15.35	15.22	15.77	15.42	15.42	15.26
^{241}Pu	Fission	6.659	6.735	6.616	6.815	6.584	6.624
	Absorption	8.742	8.868	8.634	8.926	8.728	8.645
^{242}Pu	Fission	0.067	0.066	0.065	0.062	0.061	0.063
	Absorption	1.795	1.883	1.705	1.835	1.735	2.018
^{241}Am	Fission	0.025	0.025	0.024	0.023	0.023	0.024
	Absorption	1.194	1.191	1.142	1.150	1.090	1.150

3.5. VENUS-2 MOX BENCHMARK CALCULATIONS

This benchmark exercise based on the 2-D VENUS-2 MOX core measurements was used to validate and compare the nuclear data libraries and codes used for MOX-fuelled system calculations [11]. Only the MOX pin (enriched 2.0 wt.% in ^{235}U and 2.7 wt.% in Pu) cell is considered. To compare with the UNK calculations, 5 sets of the calculational data presented in [11] were used. Calculational results for K_{inf} and the neutron balance (with total fission normalized to 100%) are given in Table VI.

Table VI. Comparison of K_{inf} and Neutron Balance (%) for MOX Cell

		SCALE-4.4	HELIOS-1.5	WIMS-D	MCNP-4B	MCU-B	UNK
K_{inf}		1.25345	1.26339	1.24858	1.25447	1.25490	1.25365
^{235}U	Fission	30.17	30.18	29.98	30.07	30.19	30.03
	Absorption	38.17	38.34	37.84	37.68	37.94	37.91
^{238}U	Fission	6.476	6.850	6.831	6.537	6.493	6.631
	Absorption	52.66	51.58	55.91	52.90	52.36	52.42
^{239}Pu	Fission	60.37	59.98	60.20	60.44	60.38	60.38
	Absorption	92.43	91.22	91.90	92.03	92.33	92.12
^{240}Pu	Fission	0.171	0.184	0.174	0.174	0.170	0.172
	Absorption	19.23	18.57	18.54	18.85	18.18	18.74
^{241}Pu	Fission	2.804	2.802	2.812	2.772	2.762	2.789
	Absorption	3.809	3.713	3.726	3.685	3.771	3.704
^{242}Pu	Fission	0.003	0.003	0.003	0.003	0.003	0.003
	Absorption	0.245	0.235	0.252	0.209	0.236	0.203

Analysis of the results presented in Table VI shows that the maximum deviation in K_{inf} reaches 1.2% between HELIOS-1.5 and WIMS-D. The mean value of K_{inf} is 1.2547 ± 0.0048. Comparison of the neutron balance shows a good agreement for major nuclides, except for ^{242}Pu.

4. LWR MOX-FUELLED CORE CALCULATIONS

4.1. PNL, SAXTON, AND TCA MOX EXPERIMENTAL BENCHMARKS

Several series of the critical experiments with MOX fuel were defined as criticality benchmarks [12]:

- PNL-30 through PNL-35 with 2.0 wt.% PuO_2 (MIX-COMP-THERM-002),
- SAXTON-1 through SAXTON-6 with 6.6 wt.% PuO_2 (MIX-COMP-THERM-003),
- TCA-1 through TCA-11 with 3.01 wt.% PuO_2 (MIX-COMP-THERM-004).

These benchmarks were analyzed by the BARS code using 5-group database calculated by the UNK code on the basis of ENDF/B-VI. The calculational results for the effective multiplication factor (K_{eff}) and root-mean-square (RMS) deviations in pin-power distribution calculated by KENO-V (using the SCALE/CENTRM sequence) [13] and BARS are presented in Table VII. The KENO-V results were obtained with average standard deviation of about 0.6-0.8%; all fuel rods were taken into account. Besides, for the PNL benchmarks, RMS deviations between the measured pin-power distribution [14] and the BARS one are also given in Table VII; number of pin-power measurements per assembly was within 19-26.

Table VII. Calculational Results for LWR MOX Benchmarks

Benchmark index →	PNL-30	PNL-31	PNL-32	PNL-33	PNL-34	PNL-35
Multiplication factor	1.00023	1.00228	1.00706	1.00750	1.01065	1.00648
RMS (%) – KENO-V	0.58	0.67	0.96	1.08	0.45	0.98
RMS (%) – measured	1.40	0.91	0.87	1.55	1.01	1.37

Benchmark index →	SAXTON-1	SAXTON-2	SAXTON-3	SAXTON-4	SAXTON-5	SAXTON-6
Multiplication factor	1.00321	1.00663	1.00688	1.00918	1.00980	1.01129
RMS (%) – KENO-V	1.74	0.76	0.82	0.57	0.35	0.46

Benchmark index →	TCA-1	TCA-2	TCA-3	TCA-4	TCA-5	TCA-6
Multiplication factor	0.99476	0.99628	0.99699	0.99737	0.99906	1.00038
RMS (%) – KENO-V	0.92	0.78	0.68	0.76	0.77	0.79

Benchmark index →	TCA-7	TCA-8	TCA-9	TCA-10	TCA-11
Multiplication factor	1.00058	1.00149	1.00241	1.00184	1.00209
RMS (%) – KENO-V	0.60	0.75	0.78	0.86	0.62

The mean values of K_{eff} are as follows:

- PNL cores: 1.0057 ± 0.0038;
- SAXTON cores: 1.0078 ± 0.0029;
- TCA cores: 0.9994 ± 0.0026.

As shown in Table VII, average RMS deviations of the BARS results from the KENO-V data do not exceed 0.8%; the maximum value is 1.74%. The average RMS deviation from the PNL experimental data is less than 1.2%; Figure 2 gives a comparison between the measured and calculated pin-power distributions in four PNL assemblies.

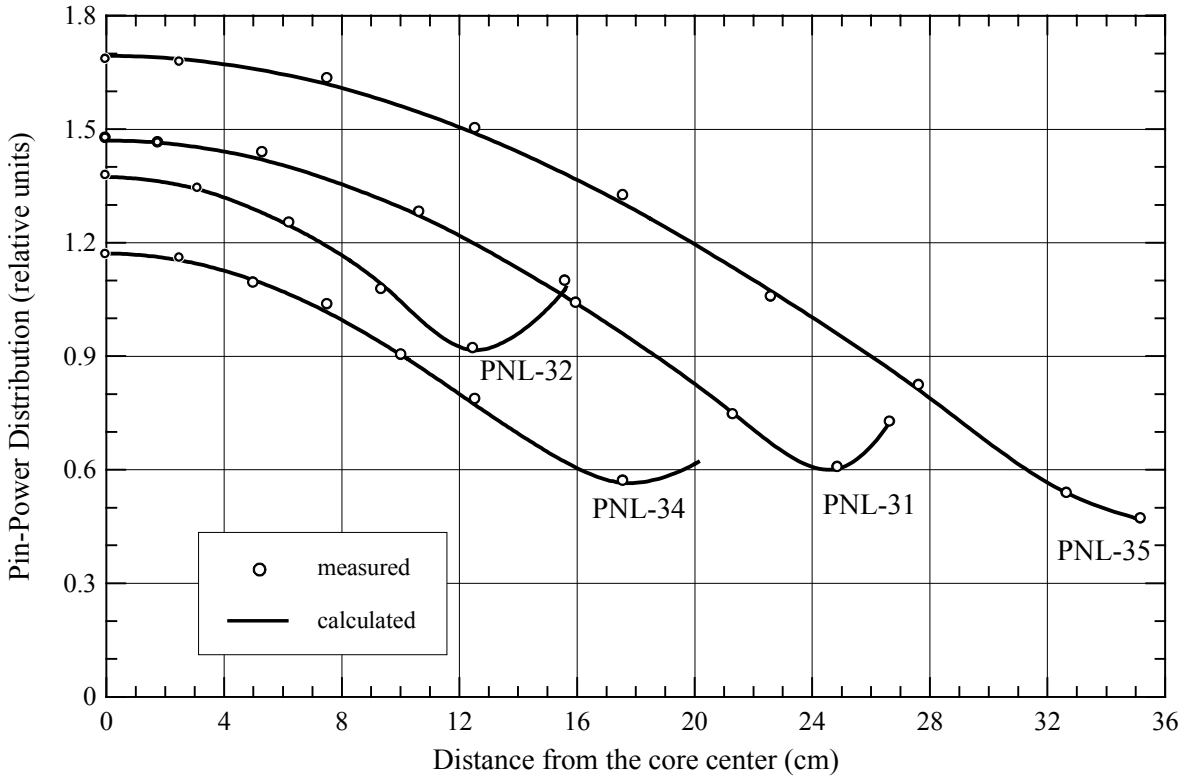

Figure 2. Pin-Power Distributions for PNL Assemblies

4.2. ESADA MOX EXPERIMENTS

A series of the ESADA critical experiments with mixed-oxide and UO_2 fuels in various configurations were performed in 1967 [15]. The MOX fuel contained 2-wt.% PuO_2 in natural UO_2 with 8-wt.% or 24-wt.% ^{240}Pu content. The experiments were carried out at different critical core configurations (with various lattice pitches) including both single-region and multi-region ones. The last were concentric-region configurations, salt-and-pepper configurations, and a third configuration that can be generally described as two rectangular slabs loaded with UO_2, sandwiching a center region loaded with MOX fuel. Concentric-region configurations used two different fuels in the inner and outer regions of the core with various combinations of the available fuel pins. Salt-and-pepper core configurations had a checkerboard pattern for loading two different fuels. This study deals mainly with concentric-region and salt-and-pepper core configurations.

The BARS calculations were carried out for a 2-D core model with uniform axial representation using 5-group library calculated by the UNK code. The calculated K_{eff} values are given in Table VIII. Case notation is given using two numbers: first - according to numbering in [15] and second one - according to numbering in [16].

The mean values of K_{eff} are as follows:

- Concentric-region cores: 1.0042 ± 0.0046;
- Salt-and-pepper cores: 1.0078 ± 0.0062.

Table VIII. K_{eff} Calculational Results for ESADA Assemblies

Concentric-Region Configurations								
Core	15-10	16-12	17-14	18-11	19-13	20-15	21-16	22-17
K_{eff}	0.99935	1.00628	1.00126	0.99893	1.00668	1.00196	1.00688	1.01253

Salt-and-Pepper Configurations						
Core	23-04	24-05	25-06	26-07	27-08	28-09
K_{eff}	1.00235	0.99767	1.01186	1.01166	1.01058	1.01260

4.3. KRITZ REACTOR SERIES

The KRITZ reactor experiments on regular light water lattices with 25×24 MOX fuel rods with 1.5 wt.% PuO_2 and 91.5% ^{239}Pu (Core 2:19) were carried out at two temperatures: 21 and 236°C [17]. Fission rate distributions from gamma scanning measurements on irradiated fuel rods were provided. The BARS calculations were performed using a 2-D model and 5-group database calculated by UNK. The K_{eff} values calculated by BARS and RMS deviations in pin-power distribution are presented in Table IX.

Table IX. Calculational Results for KRITZ Cores

Core index	2:19 (T = 21°C)	2:19 (T = 236°C)
K_{eff}	1.00667	1.00510
RMS (%) – measured	1.31	1.34

4.4. VENUS-2 MOX CORE MEASUREMENTS

The objective of this benchmark exercise was to validate and compare the nuclear data sets and codes used for MOX-fuelled system calculation [11]. The VENUS-2 facility is a zero power critical reactor containing UO_2 in the central part of the core and MOX fuel at the core periphery. Besides, the reactor contains the central water hole, inner and outer baffles, and core barrel. This configuration is a good example to analyze uncertainties in reactor modeling near the core/baffle/reflector interface. Pin-by-pin measurements of the gamma activity of irradiated fuel pins (totally 121) were used as benchmark data to validate the BARS code. Besides, comparisons with the calculations performed by other codes (for 325 fuel pins) were also provided.

Calculational results for the K_{eff} values and RMS deviations in pin-power distribution relative to the measured data are shown in Table X. The mean value of K_{eff} is as follows: 0.9978 ± 0.0044. Analysis of the pin-power distributions shows that most of the Monte Carlo and transport calculations agreed with the measurements within 4.5%; the diffusion results show the largest discrepancy: more than 5%. Comparison of the BARS calculation for pin-power distribution with some other codes is given in Table XI. It was found a very good agreement in the results between BARS and other codes: MCU-B, HELIOS-1.4, and MCNP-4B.

Table X. Comparison of the VENUS-2 Calculational Results

Calculational Method	Code Name (Participant)	K_{eff}	RMS (%)
Transport	DORT (NEA)	0.99452	4.02
	DORT (SCK•CEN)	0.99233	3.86
	HELIOS-1.5 (KAERI)	0.99817	3.39
	HELIOS-1.4 (ORNL)	0.99870	2.45
	BOXER (PSI)	1.00378	4.69
Monte Carlo	MCNP-4B (NEA+KAERI)	1.00213	1.83
	MCU-B (RRC KI)	0.99652	2.31
	MCNP-4B (KFKI)	1.00050	4.26
	MCNP-4B (GRS)	1.00430	2.46
	MCNP-4B (IJS)	0.99570	4.50
Diffusion nodal	GNOMER/B-VI (IJS)	0.99450	5.27
	GNOMER/JEF-2.2 (IJS)	0.98977	5.15
Heterogeneous	BARS-UNK (RRC KI)	0.99973	2.14

Table XI. BARS RMS Deviations (%) in Pin-Power Distribution for VENUS-2

Code Name (Participant)	DORT (SCK•CEN)	HELIOS-1.5 (KAERI)	HELIOS-1.4 (ORNL)	MCNP-4B (GRS)	MCNP-4B (NEA+KAERI)	MCU-B (RRC KI)
RMS (%)	2.49	1.92	1.30	1.38	1.35	1.37

Based on the previous calculational data for 40 experimental benchmark assemblies (PNL, SAXTON, TCA, ESADA, KRITZ, and VENUS-2), the following mean value of K_{eff} calculated by the BARS code can be derived:

$$K_{eff} = 1.0042 \pm 0.0049.$$

4.5. UO_2-MOX CORE CALCULATIONAL BENCHMARK

This core benchmark model has been designed to compare different techniques used for pin-by-pin flux prediction [10]. Geometry of the benchmark core consists of a 17×17 MOX assembly surrounded by eight 17×17 UO_2 assemblies with 21.42-cm water reflector. The MOX assembly contains fuel pins of different Pu enrichments.

To compare with the BARS calculation, 15 sets of calculational data, obtained by various codes [10], were used; among them Monte-Carlo, transport or diffusion nodal codes which used different nuclear cross-sections data derived from different libraries. Calculational results for the K_{eff} values and RMS deviations in pin-power distribution relative to the APOLLO-2 (CEA) results are shown in Table XI. The last column gives the maximum deviation. The mean value of K_{eff} is as follows: 1.0698 ± 0.0060. Analysis of the calculated pin-power distributions shows that most of the Monte Carlo and transport calculations agreed within a few percent; on the contrary, the diffusion results, even with the flux reconstruction methods, gave a very large discrepancy except for the SILWER results. Comparison of the BARS calculation for pin-power distribution with some other codes is given in Table XII.

Table XI. Comparison of Calculational Results for UO_2-MOX Core

Calculational Method	Code Name (Participant)	K_{eff}	RMS (%)	σ_{max} (%)
Transport	APOLLO-2 (CEA)	1.07441	-	-
	APOLLO-2 (EDF)	1.07132	1.03	-4.8
	TWOTRAN (NRG)	1.06279	3.20	-9.8
	DORT (Delft)	1.06980	0.39	-1.1
	DORT (SCK•CEN)	1.09231	1.74	5.3
	TWODANT (IPPE)	1.08220	2.02	10.2
	ICM2-D (IKE)	1.07390	0.85	-4.2
Diffusion	SILWER (PSI)	1.06996	0.65	-2.3
	MASTER (KAERI)	1.06103	5.39	-21.8
	NRMPO (SCK•CEN)	1.07724	7.31	-25.3
	MOSRA (JAERI)	1.06459	5.09	-26.1
	PROMETHEUS (Delft)	1.06430	4.03	17.2
	TWODANT (IPPE)	1.06570	8.83	33.9
Monte Carlo	KENO-Va (Delft)	1.07240	1.20	-4.4
	MVP (JAERI)	1.06050	2.34	9.2
Heterogeneous	BARS-UNK (RRC KI)	1.06700	1.55	-7.1

Table XII. BARS RMS Deviations (%) in Pin-Power Distribution for UO_2-MOX Core

Code Name (Participant)	APOLLO-2 (EDF)	DORT (Delft)	DORT (SCK•CEN)	ICM2-D (IKE)	KENO-Va (Delft)	MVP (JAERI)
RMS (%)	1.29	1.46	1.65	0.90	1.19	2.68

Analysis of the calculated pin-power distributions showed that the maximum deviations (σ_{max} in the last column of Table XI) were observed at the corner part of the core, especially for two or three last rows of UO_2 pins near the core-reflector interface. These deviations are both positive and negative: ±10% for the transport and Monte Carlo calculations and about ±30% for the diffusion results. Consequently, RMS deviations vary from 0.9 to 3.2% for the transport and Monte Carlo results and from 4.0 to 8.8% for the diffusion results (except for the SILWER diffusion calculation).

CONCLUSIONS

Growing interest in large-scale use of MOX fuel in LWRs, engenders a need to improve calculational tools used for the in-core management and safety analysis of nuclear reactors with convenient UO_2 fuel. So, it is necessary to improve approaches for modeling MOX cores and corresponding validation procedures. This report is focused on the BARS code package validation for MOX-fuelled systems.

The pin cell models were used to validate a procedure to generate neutron database by the UNK code. A number of different MOX fuel cells with various compositions and geometries were considered. The following important parameters were investigated: the multiplication factor, neutron balance, and the reactivity effects. The last effects include the fuel temperature (Doppler), void and moderator temperature, and boron poisoning ones. Comparisons were carried out using the calculational results obtained by modern codes (based on Monte Carlo or transport methods) with most advanced nuclear

libraries, such as ENDF/B-V, ENDF/B-VI, JEF-2.2, and JENDL-3.2. It was found that uncertainties in the MOX cell parameters are, as a rule, higher compared with those for UO_2 cells. It is necessary to use advanced methods for plutonium resonance treatment with increased number of energy groups. Besides, it turned out that the Monte Carlo calculation did not guarantee a better result.

The validation results show that the UNK code provides very good agreement in calculations of the multiplication factor, neutron balance, and the reactivity effects in the MOX fuel cells. The Doppler, moderator temperature, and boron poisoning effects are calculated within 5% uncertainty. The void effect up to 70% void fraction is predicted with 5-10% uncertainty. Besides, the UNK results are very close to the mean values when compared with other codes.

The spatial pin-power effects were investigated within rather simple LWR type MOX-fuelled cores. Both the experimental and numerical benchmarks were used. The effective multiplication factor and pin-power distribution inside the core were compared with the measurements and calculational results obtained by using different codes. It was found that the BARS-UNK calculations were in very good agreement with both the measured data and calculational results obtained by precise Monte Carlo or transport methods. The root-mean square deviations do not exceed 1.5%. This deviation is of the same order as it was found during the previous validation for UO_2-systems [1-3].

It should be mentioned that unlike S_N or, especially, Monte Carlo methods, a heterogeneous method implemented in BARS is fast-running one. This advantage allows successfully to use the BARS code for LWR full-scale calculations including modeling of various transients in LWRs. Nodal diffusion codes used for most LWR design purposes and widely spread all around, need a special adjustment procedure for the cross-sections. Otherwise, as it was reported in [10], the diffusion methods gave a large discrepancy in pin-power distribution, especially near the core-reflector region (more than 30%) in comparison with precise calculations. In contrast to diffusion codes, there is no correction of the BARS neutron database.

It seems reasonable to conclude from above validation results that the BARS code package can be used in calculations of MOX-fuelled LWR with a precision adequate for most design purposes. The BARS code package allows predicting all basic safety-related parameters of MOX fuel. The BARS validation results demonstrate very good accuracy in prediction of the pin-power effects in the cores containing both UO_2 and MOX fuels.

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