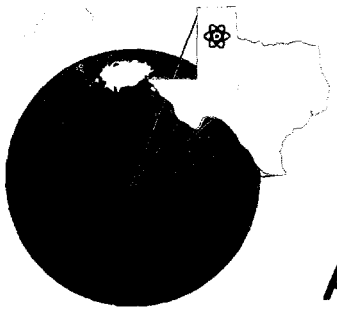

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MOX Use in Reactors: Benchmarking of Neutronic Codes--Analysis of Selected Saxton Plutonium Program Experiments Using WIMS7a

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AMARILLO NATIONAL RESOURCE CENTER FOR PLUTONIUM/
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A Report on

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Abstract

As part of the effort for the benchmarking neutronic codes for plutonium utilization, the deterministic code WIMS7a (and its associated JEF 2.2 nuclear data library) was employed to calculationally model a selected group of the SAXTON experiments. The selection of the experimental configurations to be modeled was performed based on the best experimental information available, and so as to fully exploit the neutronic variety of the SAXTON plutonium program experiments. The modular WIMS7a code can be run in many ways. For the analyses presented here, a solver strategy was implemented using WIMS7a's most evolved modules. The results showed a slightly better agreement with the experimental values for the effective neutron multiplication than the earlier results (obtained in 1997) using the codes, WIMSD4m and DIF3D. However, the calculated relative rod power distributions were not improved even though several energy group structures were tried. The simulations were carried out at Texas A&M University with access to WIMS7a being obtained via a one year lease from the AEA Technology.

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1. INTRODUCTION

The Amarillo National Resource Center for Plutonium (ANRCP) has funded a joint effort by the University of Texas at Austin (UT) and Texas A&M University (TAMU) to evaluate and calculate plutonium benchmark experiments in order to assess the capabilities and accuracy of modern neutronic codes and nuclear data libraries for analyzing MOX fuel lattices. The experimental data selected for the calculations were the taken from the Saxton Plutonium Program Experiments (Cuevas Vivas and Parish, 1998) which employed plutonium fuel with an isotopic content close to that of weapons-grade plutonium. For this group of experiments, different parameters that effect the neutronic peformance of the lattices were varied, such as the temperature and amount of the moderator, the absence or presence of control rods, the presence of both low enriched uranium (LEU) and MOX fuel rods, etc.

TAMU initiated a series of benchmark calculations based on deterministic codes to model the Saxton experimental fuel lattices in 1997. During this first step, the deterministic codes, WIMS-D4m (using a 69 group neutron cross section library derived from ENDF/B-V) and the diffusion theory code, DIF3D, were employed with various selections for pin cell and super cell modeling as discussed and reported earlier (Cuevas Vivas and Parish, 1998; 1997). The same experiments were also modeled at UT with the MCNP4B code, by Radulescu, Abdurrahman and Carron (1997), utilizing nuclear data from the ENDF/B-V and ENDF/B-VI libraries.

In 1998, TAMU has extended the Saxton neutronic benchmarking effort by applying a modern deterministic code, WIMS7a (AEA Technology, 1996). The calculations of selected Saxton experiments were carried out utilizing this modular software package while employing the latest JEF 2.2 validated nuclear data library. The criticality results were utilized to evaluate the accuracy of various calculational strategies possible through the different WIMS7a modules. The results were compared to those from the earlier calculations carried out with the WIMS-D4m and DIF3D neutronic codes.

1.1 Statement of Work

The ANRCP is interested in assessing the accuracy of predicted reactor physics parameters for MOX fuel as it might be utilized in a light water reactor. The Saxton experiments have been one of the primary, publicly available sources for information on experimental plutonium lattices. However, the first stage of the benchmarking calculations gave rise to several questions regarding certain simplifying assumptions employed, and the applicability of nuclear data library being employed. As a consequence of these questions, the proposed 1998 ANRCP activities for benchmarking of neutronic codes were described as follows:

> Sensitivity Analysis: Perform additional sensitivity analyses to identify causes of calculational biases and differences between experimentally and calculationally obtained data, starting with some of those MOX experiments that were modeled in the first year of the benchmarking effort.
>
> Use of Deterministic Lattice Physics Analysis Codes: Consider applying recently acquired (or expected to be acquired) deterministic codes, like HELIOS or LWRWIMS (WIMS7a) to the analysis of those MOX experiments that were modeled in the first year, *i.e.* Saxton.

In order to obtain results based on less stringent assumptions than those required in the WIMS-D4m/DIF3D calculational modeling of the Saxton experiments, the methodology adopted by TAMU for the second (1998) stage of the benchmarking studies included the application of the deterministic code WIMS7a to the Saxton critical experiments. WIMS7a is the most modern lattice analysis code of the WIMS family of computer programs for physics performance analysis of reactor cores. It includes all of the LWRWIMS methodology, and also has the capability to compute flux solutions closely related to those of WIMS-D4m.

2. SAXTON EXPERIMENTS

In the Saxton Plutonium Program (1965), plutonium fuel was utilized for the first time in a commercially-licensed facility (Westinghouse Reactor Evaluation Center). Both Low Enriched Uranium (LEU) fuel containing UO_2 with a uranium enrichment of 5.74 w/o U-235 and Mixed Oxide fuel with a content of 6.6% w/o PuO_2 in UO_2 were employed in square and cylindrical configurations with different values for the fuel rod pitch. The experiments included the presence of flux perturbing elements, such as water slots, aluminum plates, control rods (Ag-In-Cd), and soluble boron, as well as, changes in temperature and the amount of moderator. The Saxton reactor cores can be characterized as having high neutron leakage since the core with the maximum area had a size of only around one and a half square feet and the critical water heights did not exceed 110 cm. Given that the isotopic content of the MOX fuel was close to that of weapons-grade plutonium, the prediction of the neutron spectrum hardening in the plutonium fuel, and in the transitional areas where the plutonium fuel was neighbored by uranium fuel or water, was of primal importance. The main parameters that were used to describe the Saxton experiments are presented in Table 1.

The Saxton plutonium program experiments were classified according to three main categories. These were as follows:

(a) *Single region experiments* in which only LEU or only MOX fuel rods were employed in the cores.

(b) *Multiregion experiments* in which LEU and MOX fuel rods were both present in the cores.

(c) *Void effects plutonium experiments* in which void tubes were inserted into cores composed of only MOX fuel rods.

The first two experiment categories account for approximately 75% of the total number of experiments analyzed. They were conducted using five different fuel rod pitches. Unfortunately, there were nine cases for which the detailed x-y rod array maps were not provided in the Saxton documentation, and therefore, these nine cases were not considered for calculational modeling. The sixteen experiments in the last category (void effects plutonium experiments) were also not calculated in this study because only one lattice pitch and one type of fuel were employed in the experiments.

A total of forty experiments were therefore down-selected for criticality analysis with WIMS7a based on the best information available from the Saxton experimental results. Eight of these experimental cores contained only LEU fuel, twenty contained only MOX fuel and twelve employed combinations of LEU/MOX fuel in multiregion arrays.

3. WIMS7a MODULAR CODE SYSTEM

The reactor physics code, WIMS, has been extensively applied worldwide for a number of years on many types reactors. WIMS is an acronym for Winfrith Improved Modular System. Over years of evolution, AEA Technology has produced improved advanced methods tailored to specific types of reactors; for example, LWRWIMS was designed to analyze light water reactors.

WIMS7a is the latest member of the WIMS family of codes. This code not only possesses the capabilities of its predecessors, it also makes it possible to assemble a customized calculational scheme through its collection of programs or modules organized in an open structure. This allows the nuclear engineer to design calculational strategies adapted to specific applications. To analyze a core, one builds a calculational sequence by selecting various modules which can perform well-defined operations. The WIMS7a modules communicate internally through standardized interfaces. The modules are classified according to different tasks they perform:

- Data preparation, including library reading.
- Data manipulation and linking of operations (service modules).
- Flux solution.
- Resonance shielding.
- Depletion.
- Edits, including reactivity coefficients, flux and power distributions, reaction rates, actinide and fission product inventory, etc.
- Links to codes for whole core analyses, and inventory/activity codes.

Among the latest improvements to WIMS7a is the inclusion of multi-dimensional neutron transport capabilities through the inclusion of codes, like LWRWIMS, TWOTRAN and CACTUS, as well as improvements to the geometry description and edit capabilities. The CACTUS code was the first successful implementation of the method of characteristics in a production physics code. The possible flux solution methods are extensive and include collision probabilities, characteristics, DSN, diffusion theory, Monte Carlo and hybrid techniques. A nuclear data library of sixty-nine groups (with the traditional WIMS energy structure) or one hundred and seventy-two groups can be applied in the calculations. Condensing to coarser energy group structures is also possible. Input buckling terms can be used to approximate k-effective for three-dimensional problems.

3.1 Description of WIMS7a Model for Saxton Criticals

The calculational strategy chosen for simulation of the Saxton plutonium program critical experiments used various WIMS7a modules as follows:

(1) **WHEAD** --- This is a service module in which the standard problem set up takes place. The geometry and material compositions of each cell (sub-region) are input for the particular problem and they are passed to later modules through an interface. This module also carries out the adjustment to the microscopic cross-sections of the materials with resonances due to the specified temperatures. An automatic call to the module WMIX occurs internally to calculate macroscopic cross-sections for each sub-region.

(2) **WPERSEUS** --- This module defines and calculates multicell collision probabilities based on the LWRWIMS code's methodology which was designed

for standard LWR assembly spectrum calculations. The multicell model can include conglomerates of pin cells, plates and slabs of moderator without surface contact areas and reading the geometry from the WHEAD interface.

(3) **WPIP** --- This module reads the geometry, collision probabilities and cross-sections and calculates a flux distribution and k-infinity using acceleration based on successive over-relaxation with an optimum factor for water moderation. The flux solution obtained with this module for the Saxton cores did not use the zero-flux boundary condition, as done in the earlier modeling using WIMSD4m, but did use the standard sixty-nine energy group WIMS library. By using the modules WPIP and WPERSEUS, the spectrum softening on the external rows of the fuel rods of a core, due to increased neutron moderation and leakage, is expected to be well-modeled, avoiding the need to define different subregions in the core for the supercell model as detailed in Cuevas Vivas and Parish (1998).

(4) **WCONDENSE** --- This module carries out the energy condensation of the cross section data using approximate flux distributions. Given that the space-energy flux distribution within a coarse group is, in effect, frozen by the homogenization process and that the flux spectrum is hardened by absorption in the Pu resonances, the election of an appropriate structure to condense the energy dependence and then calculate the coarse (few) group macroscopic cross-sections is important. A few group structure was taken from Stamm'ler and Abbate (1983) which has been suggested as suitable for light-water lattices with both uranium and plutonium fuel. That energy group structure is shown in Table 2 (number in parenthesis is the corresponding energy group number in the sixty-nine group WIMS library). The recommended structure has a total of eight energy groups with 4 groups below 1.3 eV. The structure differs from the one used for the WIMS-D4m calculations (see Table 3) since it gives better representations of the fast fission threshold of U-238 (a common isotope of all fuel rods) and the beginning of the fall of the hydrogen scattering cross-section. Furthermore, group five was specified so as to achieve a proper treatment of the 1.05 eV Pu-240 resonance. A twenty group structure (Table 4) was also employed for comparison purposes for those cases with flux perturbing elements, but it was not adopted for the rest of experiments in order to avoid unnecessarily slowing down the computational solution.

(5) **WCACTUS** --- This module is a two dimensional characteristic method multigroup flux solver. This program can solve the neutron transport equation by imposing zero flux boundary conditions, and in very general geometry, that is composed of shapes described with straight lines and circular arcs. This module is regarded as the major flux solution module in WIMS7 for production use. In the present implementation, up to 6 azimuthal angles were used as base tracks (directions) over which the transport equation was integrated.

(6) **WCRIT** --- This module reads the two dimensional flux solution and the macroscopic cross-sections and then modifies the flux solution and effective multiplication factor with an input

buckling term using the B1 method. The three dimensional problem is then simulated with a modified fundamental mode. For most of the Saxton criticals, the axial buckling was obtained from the reported water height. However, in some cases, the axial buckling as calculated by the experimenters was used.

4. RESULTS

The same important physical assumptions were made for the WIMS7a modeling of the Saxton experiments as were used for the Saxton simulations using the codes WIMS-D4m and DIF3D. The plutonium fuel in both cases was assumed to be homogeneous since neither set of codes was capable of modeling the effects of MOX particle size on criticality. Also, experimentally determined bucklings were not provided in the Saxton report (Taylor, 1965) for all of the criticality cases, and therefore, for the cases without reported bucklings, estimates based on the physical dimensions of the cores were utilized. Use of axial buckling values permitted the cores to be modeled as two dimensional, and significantly improved computational economy.

On the other hand, when the Saxton experiments were modeled with the WIMS-D4m and DIF3D codes, broad group, region average cross-sections were obtained with WIMS-D4m using a one-dimensional, fine group, neutron transport flux solution. The use of SUPERCELL and MULTICELL models were employed to approximate the neutron flux spectrum softening in the outermost rows of fuel rods due to increased moderation and neutron reflection. The former model permits one to define fuel rod "rings" and to accommodate a thick reflector region beyond the core boundary. The latter model may also be useful, but requires ad hoc input parameters to estimate subregion to subregion transfer probabilities. WIMS-D4m flux solution methods also posed certain limitations for modeling the Saxton experiments. For instance, the DSN solution method could only be used within SUPERCELL-based models. Similar results were obtainable only with the standard collision probability method of WIMS-D4m (PERSEUS) for MULTICELL-based models since SUPERCELL-based models demanded a larger amount of data storage than was provided in the version of WIMS-D4m that was available.

In this study, the sensitivity of the calculated k-effective values to the available solution methods and nuclear data available in WIMS7a were addressed. Several different types of pin cell calculations were performed since these are free of assumptions about leakage, and can be directly compared to the one-dimensional transport solutions from WIMS-D4m. Calculations for the Saxton cores were also performed using several of the solution methods available in WIMS7a, and these were compared to the results obtained from WIMSD4m and DIF3D. Therefore, the Saxton calculations performed with WIMS7a can be classified as follows:

(1) Pin cell calculations, and
(2) K-effective calculations for Saxton cores.

The k-effective calculations for the Saxton cores were also used to obtain relative rod power values for comparison to measured values.

4.1 Pin Cell Calculations

The data for each of the Saxton fuel types were employed to obtain calculated k-infinities for the pin cells. Pin cell results were obtained using the three different flux solution methods (and the ENDF/B-V based fine group library) available in WIMS-D4m. Results were also calculated using the standard solution method of CASMO-3 (with its associated nuclear data library). Finally, a reference solution was obtained using the WIMS7a module, WCACTUS (method of characteristics) with the calculational strategy described earlier in Section 3.1). The WIMS-D4m and WIMS7a calculations used the fine group nuclear cross-section libraries derived from ENDF/B-V and JEF 2.2, respectively. The CASMO-3 nuclear data library contained

seventy fine groups (CASMO-3 User's Manual, 1992).

The one dimensional, transport solution methods applied in WIMSD4m were (1) the DSN method with S4 (default) and S32 angular discretizations, (2) the PERSEUS (collision probability) method that is recommended for use in most problems by the WIMS-D4m user's manual (Dean, Woodruff, Costescu, 1995) and (3) the PIJ-PERSEUS (collision probability) method. The CASMO-3 neutron transport solution is also based on the collision probability method.

Figures 3 and 4 present the k-infinity values obtained for the Saxton LEU and MOX fuel rod types, respectively. Figures 5 and 6 depict the percentage differences for each method relative to the references values obtained from WIMS7a. The results are shown in each figure as a function of the ratio of the lattice pitch to pellet diameter ratio (Table 5). Recall from Table 1 that the diameters of the LEU and MOX fuel rods were 0.9067 cm and 0.8569 cm, respectively. The k-infinity of the LEU fuel lattices (see Figure 3) showed that experimental lattice pitch 3 (pitch to pellet diameter ratio of 2.05) is close to the optimum moderator to fuel ratio, i.e., it achieves the highest value of k-infinity. The pin cell at the largest pitch studied experimentally is clearly over-moderated. The MOX pin cell calculations (see Figure 4) showed that the optimum pitch to pellet diameter ratio is between 2.178 and 2.347 (experimental lattice pitches 3 and 4). Experimental lattice pitches 1 and 5 for the MOX fuel are clearly under-moderated and over-moderated, respectively. Both experimental lattice pitches 3 and 4 are close to optimum moderation. The optimally moderated pitch to pellet diameter ratio is greater for MOX fuel (~2.3) than for LEU fuel (~1.9). This is caused by the harder spectrum of the MOX pin cells relative to the LEU pin cells at the same pitch to pellet diameter ratio. Furthermore, the typical pitch to pellet diameter ratio used in LEU fueled LWRs is ~1.3. Therefore, all of the lattices investigated in the Saxton experiments for both LEU and MOX fuel had somewhat more moderation than in typical light water reactors. It is also worth noting that for these pin cell calculations all of the methods employed tended to show their best agreement in the most under-moderated lattices and differences were greatest and were increasing for the most over-moderated lattices. Moderation effects are also an important factor when considering the influence of neutron leakage on the k-effective of the small Saxton cores.

The pin cell k-infinity results obtained using the assembly analysis code CASMO-3 were in most cases quite close (within 0.5%) to the reference values from the WIMS7a calculations for the MOX lattices. Also, the PIJ-PERSEUS method generally provided similar results to the reference values for the LEU lattices. Both of these methods and WIMS7a using WCACTUS are based on the collision probability technique to solve the neutron transport equation. Therefore, the agreement was not totally unexpected. Differences are most likely due to the cross-section libraries employed. However, the DSN and standard PERSEUS methods recommended for use in the WIMS-D4m manual showed the relative differences of up to 4% from the reference calculations even when a very fine angular discretization was used with the DSN method. These methods predicted lower k-infinities than the reference calculations at large lattice pitches for both types of fuel. The large discrepancy demonstrated by the DSN and PERSEUS for the LEU fuel at the largest rod pitch can be explained by the large over-moderation of this lattice relative to the MOX pin cell for the same rod pitch. It is also worth noting that the k-infinities from WIMS7a were slightly larger

than those calculated by the other methods for all of the LEU lattices, but in general, were lower for the MOX lattices except at the largest pitch to pellet diameter ratio considered.

4.2 Calculated K-effectives of the Selected Saxton Experiments

The forty selected experiments were all modeled with WIMS7a. This code provided a more user-friendly way to model the Saxton experiments as compared to the application of the different cell models and homogenization schemes that were necessary for the WIMS-D4m and DIF3D calculations. Physical descriptions of the selected cores and the calculated effective neutron multiplication factors are presented in Tables 6 and 7. The values of k-effective were calculated using a modified spatial flux solution including an input axial buckling. The average value of k-effective and its standard deviation considering all of the Saxton cores calculated were slightly improved when compared to the corresponding results obtained with WIMSD4m and DIF3D (see Table 8).

Criticality calculations for the Saxton selected cores were reported earlier by TAMU using the deterministic codes, WIMS-D4m and DIF3D (Cuevas Vivas and Parish, 1998; 1997) and by UT (Radulescu, Abdurrahman and Carron) using the Monte Carlo code, MCNP4B (1997). It was reported that the calculated k-effectives for the cores loaded with MOX fuel changed slightly and increased to values larger than 1.0 as the lattice pitch was increased in the Saxton experiments. For the calculations based on WIMSD4m-DIF3D, the delta k-effective (calculated minus measured) for the MOX cores increased to a value of ~2% at a pitch of 2.64 cm. For the corresponding Monte Carlo results, the delta k-effective only increased to a value of 1.0%. Fitting of the calculated k-effective values for the Saxton MOX cores to a straight line (see Figure 7), the slope for the WIMS7A results is -0.009 delta k_{eff} per cm of lattice pitch as compared to +0.022 delta k_{eff} per cm of lattice pitch for the values calculated using WIMS-D4m and DIF3D. The fact that the results from the DIF3D (diffusion theory method) and MCNP4B (Monte Carlo method) codes agreed with one another better than either agreed with the results from WIMS7a, suggests that the greatest source of discrepancy between the earlier and WIMS7a results may be due to the different nuclear data libraries used, i.e., ENDF/B-V and VI versus JEF2.2.

4.3 Relative Rod Power Distributions

Calculated rod powers from three MOX single region experiments with flux perturbing elements and two multi-region experiments were selected for comparisons to the Saxton measurements. All of the calculations employed in the rod power calculations were performed with few group structures of both eight and twenty energy groups. The fission rates calculated with the WIMS7a module, WCACTUS, were used to obtain the relative rod power distributions. The comparisons with the experimental values were not as good as expected, possibly indicating that the nuclear data and modeling methods require further improvement. One improvement in the WIMS7a modeling would be to increase to ten the number of discretized angles employed in the method of characteristics (3, 5 and 6 angles were employed here). In addition, the use of twenty groups yielded a small improvement both in the k-effectives and in the rod power distributions. Provided convergence difficulties do not arise, it may be possible recompute the rod power cases using up to sixty-nine groups. Figures 8 and 9 show the relative differences between the calculated and experimental rod power values for the MOX single region and multi-region cores,

respectively. Differences of up to 19% were observed for some plutonium rods in the multi-region problems near the core outer boundary (see Figure 9). Using twenty energy groups, the fractional relative rod power standard deviations (square roots of the calculated and experimental relative rod power variance) of the MOX single region cores were approximately 4.99% for the core with a central water slot, 5.17% for the core with a central aluminum plate, 3.93% for the core with centrally localized control rods. Similarly for the multi-region cores, the standard deviations for each type of fuel in each core were (1) 6.08% for the LEU rods and 1.5% for the MOX rods of the external LEU rod core and (2) 1.28% for LEU rods and 7.4% for the MOX rods of the external MOX rod core (see Table 9).

The DIF3D calculations, performed with the macroscopic cross-sections calculated with WIMS-D4m, provided better results than WIMS7a when compared with the experimental rod power measurements. These results indicate that the supercell method in which the reactor core is divided into zones of different moderation such as the external ring of rods and rods facing the perturbing elements in combination with diffusion theory, fortuitously provided a better localized estimation of the experimental rod powers.

5. CONCLUSIONS

The LWRWIMS and CACTUS methodology implemented in the modular code WIMS7a was tested on the Saxton criticality experiments with mixed results. While the calculated k-effectives in most cases matched and in some cases were slightly improved relative to the values obtained with WIMSD4m-DIF3D, the calculated relative rod power distributions were not better. This suggests that further tuning is needed in the calculational strategy applied in modeling the Saxton experiments using WIMS7A. From the results obtained, it can be inferred that the criticality results will probably not be improved further by employing a finer few group structure. Successful improved simulation of the Saxton experiments will likely require modified nuclear cross -ection data as well as better modeling methods. The input parameters of the method of characteristics such as the angle discretization and convergence tolerance may be capable of improving the results. Also, the agreement in the rod power distribution may be further improved if the axial leakage effect is imposed rather than using only the output of the method of characteristics solution.

Finally, the one hundred seventy-two group JEF2.2 library of WIMS7a should be tested and the results compared with those obtained using the sixty-nine group library. WIMS7 has the capability to use either sixty-nine or one hundred seventy-two group libraries based on JEF2.2. However, the sixty-nine group library was the default library on the computer workstations at TAMU.

On the other hand, the application of WIMS7a to the Saxton experiments has provided useful information about the accuracy of the sixty-nine group JEF 2.2 data and the two dimensional method of characteristics. In addition, the effects of various flux solution methods and nuclear data libraries on pin cell parameters were studied. The pin cell calculations showed that a reasonable level of confidence can be given to WIMS7a's method of characteristics, given its agreement with the pin cell results obtained from the CASMO-3 code and the PIJ-PERSEUS method of the WIMS-D4m code. However, these results showed also that there is a significant discrepancy in the pin cell results obtained with the standard WIMS-D4m solution methods, PERSEUS and DSN, especially for strongly over-moderated pin cells.

One particular bias observed in the earlier calculations using WIMSD4m-DIF3D and MCNP4B was not seen in the WIMS7a calculations, i.e., the reported over prediction of k-effective for the Saxton MOX cores as a function of the rod pitch was not confirmed by WIMS7a. The WIMS7a results showed an under prediction of k-effective as a function of fuel rod pitch as compared to the WIMS-D4m-DIF3D and MCNP4B results. It has been supposed that the bias in k-effective with lattice pitch may be attributable to the reactivity effects due to Pu particle self-shielding that are neglected in the present calculational modeling.. However, if this is true, the use of different nuclear data libraries may mask the reactivity bias due to the MOX fuel in homogeneity.

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Table 1: Fuel Type Characteristics

Fuel Type	Enrichment	Density	Geometry	Clad Material
Uranium Dioxide	5.74 w/o U-235 in UO_2	Theoretical: 10.96 g/cm^3 (93% of Theoretical Density)	Pellet Diameter = 0.9067 cm	304 SS
			Clad I.D. = 0.91694 cm	
			Clad O. D. = 0.99314 cm	
			Rod Length = 92.964 cm	
MOX	6.6 w/o PuO_2 in UO_2 Pu components: Pu-239 (90.49%) Pu-240 (8.57 %) Pu-241 (0.89 %) Pu-242 (0.04 %)	Theoretical: 11.46 g/cm^3 (94% of Theoretical Density)	Pellet Diameter = 0.8569 cm	Zircaloy 4
			Clad I.D. = 0.87503 cm	
			Clad O. D. = 0.99314 cm	
			Rod Length = 92.964 cm	

Table 2: Eight Energy Group Structure for WIMS7a

Group	Energy Bounds (eV)
1	10^7 - 500,000 (7)
2	500,000 – 9118.0 (15)
3	9118.0 - 148.73 (22)
4	148.73 - 1.30 (33)
5	1.30 - 0.625 (46)
6	0.625 - 0.180 (55)
7	0.180 - 0.08 (58)
8	0.08 - 0.005 (69)

Table 3: Seven Energy Group Structure for WIMS-D4m

Group	Energy Bounds (eV)
1	10^7 - 9118.0 (15)
2	9118.0 - 4.00 (28)
3	4.00 - 1.071 (37)
4	1.071 - 0.78 (45)
5	0.78 - 0.18 (55)
6	0.18 - 0.058 (60)
7	0.058 - 0.005 (69)

Table 4: Twenty Energy Group Structure for WIMS7a

Group	Energy Bounds (eV)	Group	Energy Bounds (eV)
1	10^7 - 8.21×10^6 (6)	11	1.071 - 1.02 (39)
2	8.21×10^6 - 1.83×10^6 (9)	12	1.02 - 0.996 (40)
3	1.83×10^6 - 9118.0 (15)	13	0.996 - 0.95 (42)
4	9118.0 - 1425.1 (19)	14	0.95 - 0.78 (45)
5	1425.1 - 48.052 (24)	15	0.78 - 0.4 (48)
6	48.052 - 4.0 (28)	16	0.4 - 0.3 (51)
7	4.0 - 2.6 (30)	17	0.3 - 0.18 (55)
8	2.6 - 1.3 (33)	18	0.18 - 0.1 (57)
9	1.3 - 1.123 (35)	19	0.1 - 0.058 (60)
10	1.123 - 1.071 (37)	20	0.058 - 0.005 (69)

Table 5: Saxton Pitch Parameters for the Two Fuel Rod Types

#	Saxton lattice pitch (cm)	Pitch/Diameter Ratio	
		LEU	MOX
1	1.3208	1.456	1.541
2	1.4224	1.568	1.659
3	1.8669	2.058	2.178
4	2.0117	2.218	2.347
5	2.6416	2.913	3.082

Table 6: Saxton Critical Experiments (Single Region Cases)

Fuel	**Lattice pitch** (cm)	**Temp.** (°K)	**Core config.**	**Critical height** (cm)	**Features**	**K_eff** WIMS-D4m/ DIF3D	**K_eff** WIMS7A
LEU	1.4224	291.15	19x19	83.710		0.999193	1.004230
	2.0117	290.45	13x14	88.960		1.001271	0.995729
MOX	1.3208	298.95	22x23	84.560		1.008095	1.004430
	1.4224	290.15	19x19	80.800		1.001792	1.000700
	1.4224	288.90	19x19	83.450		1.002489	1.001660
	1.4224	291.15	21x21	88.700	Boron: 337 ppm	1.010336	0.998948
	1.8669	297.25	13x13	70.110		1.019590	0.991419
	2.0117	289.25	12x12	78.430		1.018905	0.994246
	2.6416	293.05	11x11	81.170		1.023851	0.991813
LEU	1.4224	291.55	19x19	80.00	Water Slot (Center)	0.991759	1.001880
	1.4224	291.55		83.60	(Unperturbed)	0.990267	1.000090
	1.4224	291.15	19x19	87.38	Al Plate (Center)	0.986826	0.999758
	1.4224	291.55		83.60	(Unperturbed)	0.992231	1.000090
	1.4224	291.15	21x21	89.02	Ag-In-Cd (Center)	0.978745	1.001190
	1.4224	289.25		52.66	(Unperturbed)	0.976889	1.005660
MOX	1.4224	288.55	19x19	75.90	Water Slot (Center)	1.002480	0.997424
	1.4224	290.15		82.41	(Unperturbed)	1.001603	0.990665
	1.4224	289.15	19x19	83.02	Al Plate (Center)	0.997141	1.002300
	1.4224	290.15		82.41	(Unperturbed)	1.003802	0.990665
	1.4224	288.55	21x21	79.01	Ag-In-Cd (Center)	0.989780	1.005800
	1.4224	288.55		52.04	(Unperturbed)	0.983940	0.991821
					Borated Water		
MOX	1.4224	290.05	19x19	83.000	0 ppm	0.994295	0.991315
	1.4224	290.05	19x19	89.410	25 ppm	0.995188	0.993134
	1.4224	290.05	19x19	99.440	50 ppm	0.997279	0.996900
					Borated Water		
	1.4224	288.55	21x21	52.130	0 ppm	0.984555	0.992093
	1.4224	291.15	21x21	72.470	228 ppm	0.998995	0.999654
	1.4224	291.15	21x21	84.660	309 ppm	1.002856	1.001360
	1.4224	291.15	21x21	89.700	337 ppm	1.003685	1.001580

Table 7: Saxton Critical Experiments (Multiregion Cases)

External fuel config.	**Internal fuel config.**	**Lattice Pitch** (cm)	**Temp.** (°K)	**Critical height** (cm)	**Additional feature**	**Boron conc.** (ppm)	**K_eff** WIMS-D4m/ DIF3D	**K_eff** WIMS7A
LEU 19x19	MOX 11x11	1.4224	289.35	91.070		0	0.993475	1.005670
LEU 27x27	MOX 19x19	1.4224	291.35	93.350		1453	0.998208	1.001240
LEU 27x27	MOX 19x19	1.4224	291.65	89.140	3x3 LEU rods at center	1425	0.996087	1.000350
MOX 19x19	LEU 11x11	1.4224	288.75	76.111		0	0.995835	0.999496
MOX 27x27	LEU 19x19	1.4224	293.15	86.65		1252	0.991768	0.998981
LEU 19x19	MOX 3x3	1.4224	294.35	83.77		0	0.992139	0.999936
MOX 19x19	LEU 3x3	1.4224	287.85	81.56		0	1.003014	1.003050
LEU 27x27	MOX 19x19	1.4224	291.65	92.190	L-shaped LEU rods	1425	0.997889	1.001360
LEU 19x19	MOX 11x11	1.4224	288.15	92.070	w/ Al Plate off center	0	0.992159	1.002060
LEU 21x21	MOX 11x11	1.4224	288.65	73.550	w/ control rods off center	0	0.986240	1.009820
LEU 27x27	MOX 19x19	1.4224	291.15	99.800	w/ Water Slot off center	1453	0.999570	1.002400
LEU 27x27	MOX 19x19	1.4224	290.95	106.35	w/ Al Plate	1453	1.001523	1.003580

Table 8: Statistical Parameters for WIMS-D4m/DIF3D and WIMS7a

Cases	**WIMSD4m / DIF3D** Average K-eff (Standard Deviation)	**WIMS7a** Average K-eff (Standard Deviation)
LEU	0.99185 (0.0066)	1.0010 (0.0033)
MOX	1.0024 (0.010)	0.99689 (0.0055)
Multiregion	0.99565 (0.0045)	1.00232 (0.0041)

Table 9: Standard Deviation of the Relative Rod Power Error

	Using 8 group energy structure	Using 20 group energy structure
MOX core with a water slot at the center	5.14 %	4.99 %
MOX core with an aluminum plate at the center	5.34 %	5.17 %
MOX core with control rods at the center	3.96 %	3.93 %
Multiregion core with LEU rods in the interior	1.3 % for LEU rods 7.41 % for MOX rods	1.28 % for LEU rods 7.4 % for MOX rods
Multiregion core with MOX rods in the interior	6.14 % for LEU rods 1.7 % for MOX rods	6.08 % for LEU rods 1.51 % for MOX rods

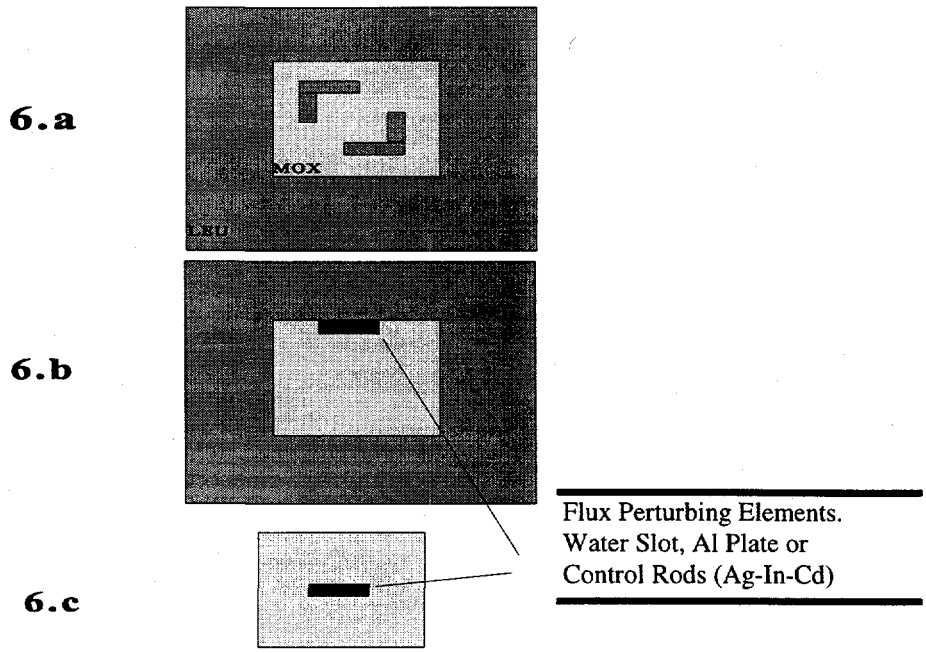


Figure 1: Typical Configurations from the Saxton Plutonium Program Experiments (6.a) Multiregion Core with an L-shaped Array of LEU Fuel Rods Immersed in an Internal Square Array of MOX Fuel Rods. (6.b) Multiregion Core Showing the Off-Set Location of Flux Perturbing Elements. (6c). Single Region Core with a Centered Location of Flux Perturbing Elements.

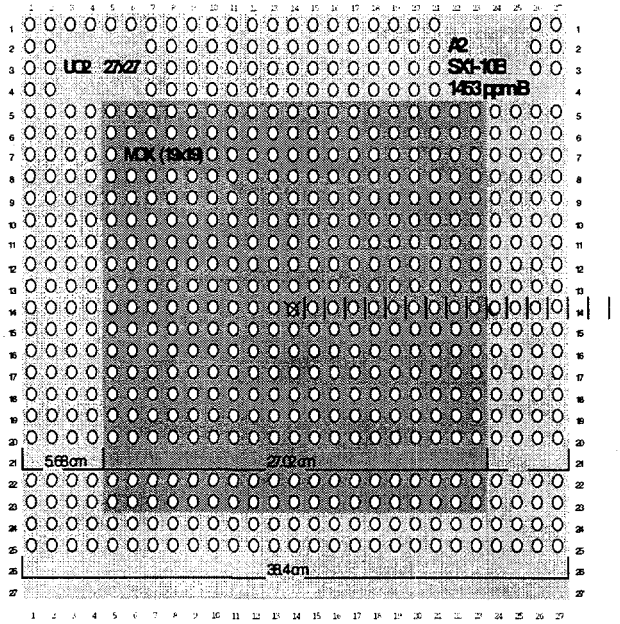


Figure 2: Example of a Typical Multiregion Square Fuel Rod Array

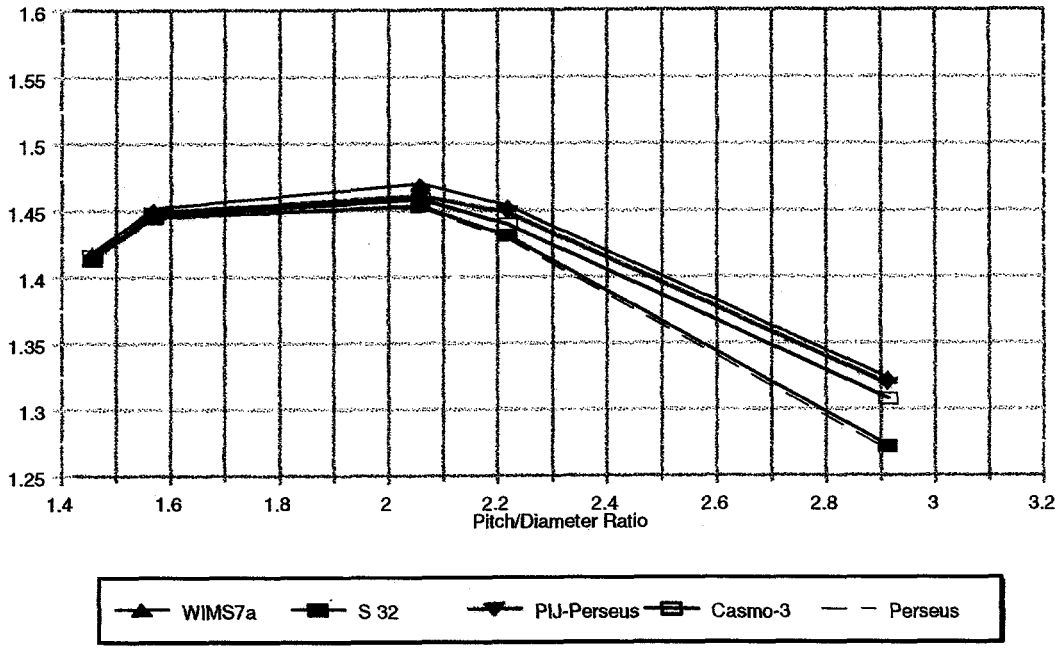


Figure 3: LEU Pin cells: K-inf vs Fuel Rod Pitch/Diameter Ratio

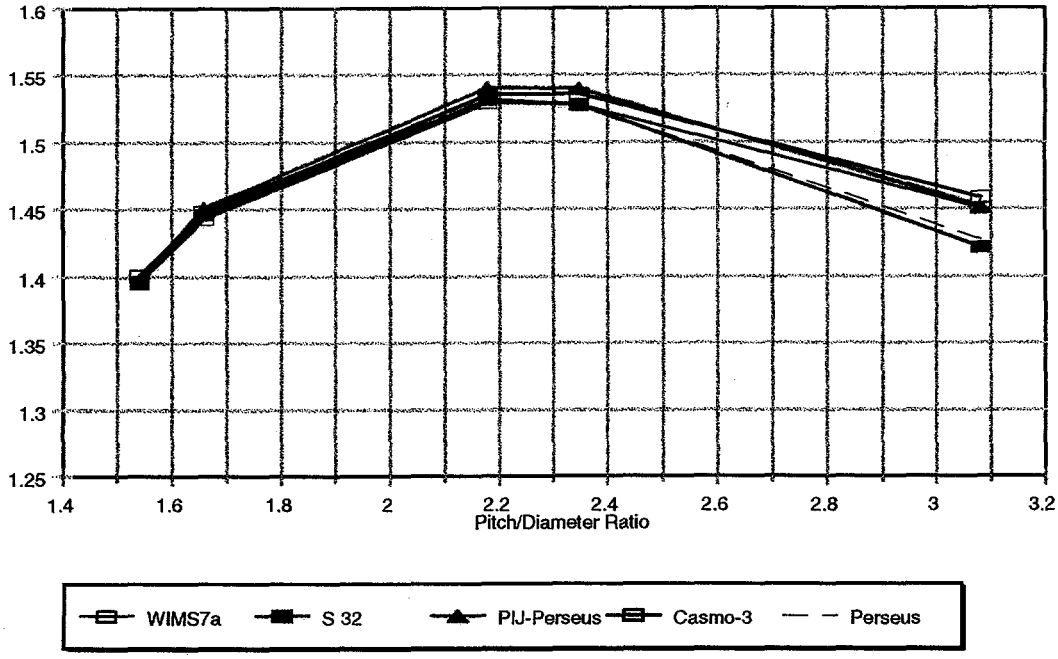


Figure 4: MOX Pin cell: K-inf vs Fuel Rod Pitch/Diameter Ratio

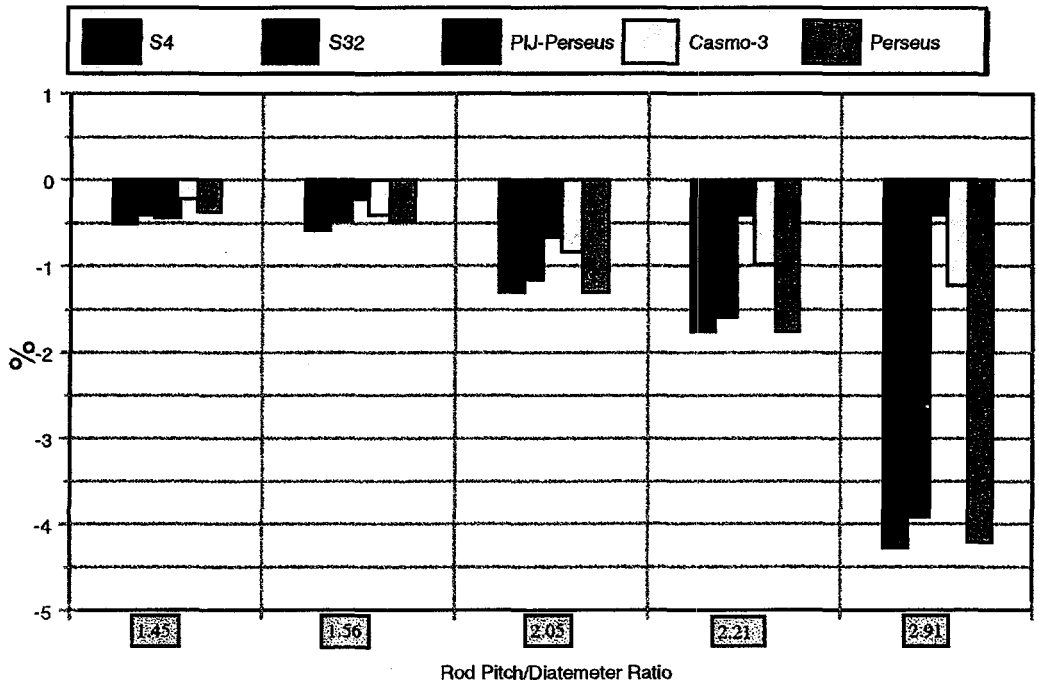


Figure 5: LEU Pin cells: K-inf Relative Differences (%) Using WIMS7a Values as References

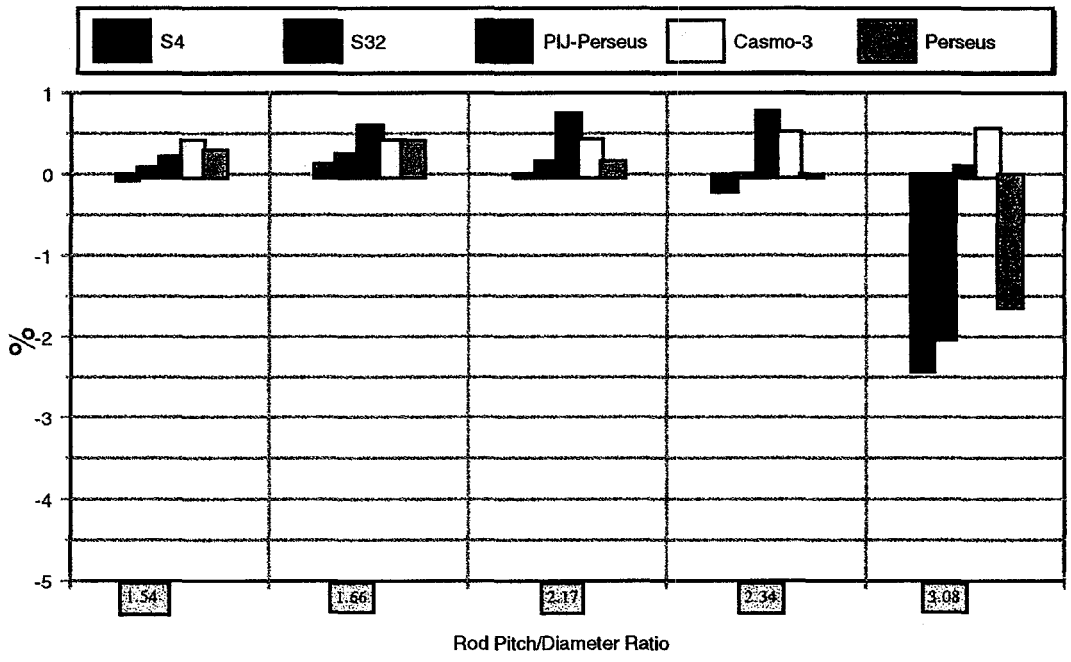


Figure 6: MOX Pin cells: K-inf Relative Differences (%) Using WIMS7a Values as References

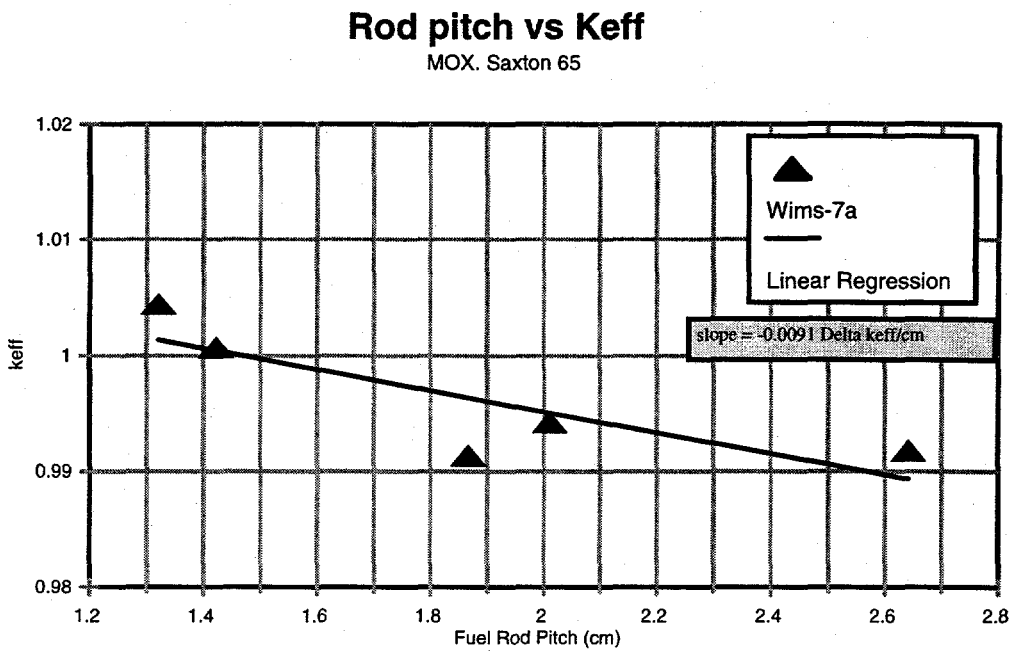
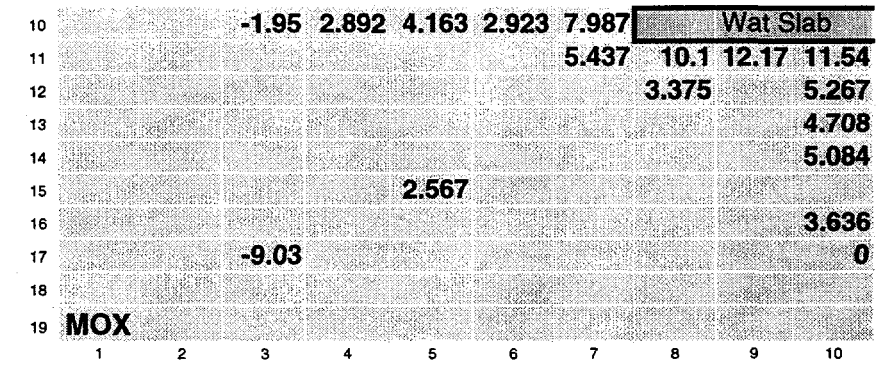
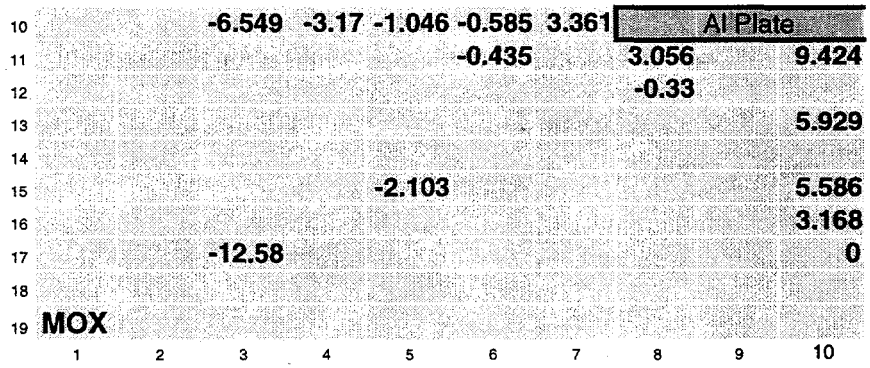


Figure 7: Effective Multiplication Factor Trend with Increasing Fuel Rod Pitch





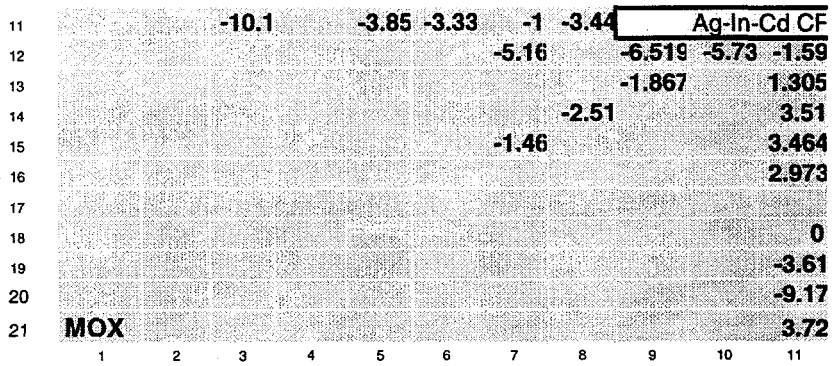


Figure 8: Relative Error (%) in Rod Powers for Experiments with Flux Perturbing Elements at the Center of a Square Fuel Rod Array (only a quarter core is shown)

10	11	12	13	14	15	16	17	18	19	
1.455			2.362		-0.53				-2.23	1
-5.231		-6.836		-8.4		-11.3		-19.1		2
-1.161							-11.04			3
0		0.133				-3.32				4
-2.868			-1.53		-3.08					5
-2.757		-3.057		-4.66						6
0.184	-0.38		-1.18							7
-1.081		-2.02								8
-0.28	-0.93									9
0			MOX		-3.97	-0.01		LEU		10

10	11	12	13	14	15	16	17	18	19	
-4.65			-5.19		-4.52				-6.7	1
-15.3		-13.3		-14.6		-21.1		-27.4		2
-8.42			-9.31		-8.75		-16.8			3
0		-0.73		-2.57		-7.84				4
-1.4			-2.15		-4.47					5
-1.1		-0.74		0.14						6
0.101	-0.32		0.511							7
0.544		0.188								8
-0.37	-0.77									9
0		0.513		LEU				MOX		10

Figure 9: Relative Error (%) in Rod Powers for Experiments with MOX and LEU Fuel Rods in 19x19 Fuel Rod Arrays (Only a Quarter Core is Shown)