DETAILED ANALYSIS OF THE INITIAL ZEUS CRITICAL CONDITION

WITH MCNP™ AND ENDF/B-VI

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ABSTRACT

The Zeus experiment was designed to test the adequacy of ^{235}U cross-sections in the intermediate energy range. The detailed modeling of the initial critical configuration of Zeus with the MCNP Monte Carlo code is described, and calculated results are presented. The calculations employed cross sections derived from ENDF/B-VI, and the results have standard deviations of 0.0004 or less. Those results indicate that Release 4 of ENDF/B-VI overestimates the value of k_{eff} for Zeus by approximately 0.005 Δk. In addition, a series of modeling simplifications are described that transform the detailed representation into a benchmark configuration, and the reactivity impacts of those simplifications are assessed. The end product of these simplifications is a relatively straightforward model with a k_{eff} that is only very slightly less than that of the actual critical configuration.

1. INTRODUCTION

The Zeus experiment[1,2] was designed to test the adequacy of ^{235}U cross-sections in the intermediate energy range. This paper describes the detailed modeling of the initial critical

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configuration of Zeus with the MCNP Monte Carlo code[3] and cross sections derived from the sixth edition of the Evaluated Nuclear Data File (ENDF/B-VI).[4] In addition, a series of modeling simplifications are described that transform the detailed representation into a benchmark configuration, and the reactivity impacts of those simplifications are assessed.

2. INITIAL ZEUS CRITICAL CONFIGURATION

The Zeus experiment has been constructed on the Comet vertical assembly machine. For its initial configuration, the Zeus core contains thin, circular platters of highly enriched uranium (HEU) separated by similar platters of graphite. The cylindrical core is reflected by copper on the top, bottom, and sides. Inner copper pieces fit closely around the sides of the core to produce a parallelepiped, and a thick circular piece of copper provides reflection at the bottom of the core. A square piece of copper rests atop the inner pieces, and heavy copper “logs” are stacked against the outer sides of the inner copper pieces. A stainless steel membrane was inserted about halfway up the stack of inner copper pieces to support the upper portion of the core. The bottom portion of the core rests on the bottom reflector, which in turn is supported by the platen at the top of the vertical drive of the assembly machine. The HEU and graphite platters that comprise the bottom portion of the core have a small central cavity with a radius of 1.25 inches (3.175 cm), through which an aluminum alignment tube is placed. Criticality is achieved by driving the bottom portion of the core up inside the reflector. A schematic of the experimental configuration is shown in Figure 1, and more details are provided in a companion paper.[2]

Zeus achieved initial criticality on April 26, 1999, with 10 HEU platters and an axial loading that is almost symmetrical. Each HEU platter is 0.29972 cm thick, and all but one of 79 graphite platters are 1 cm thick. The critical, or “final,” configuration had four graphite platters above the top HEU platter, four graphite platters below the bottom HEU platter, and eight graphite platters between all but two adjacent HEU platters. The fourth and fifth HEU platters, counting from the bottom, were separated by six 1-cm-thick graphite platters, a 0.5-cm-thick graphite platter, and a platter of aluminum that is 60 mils (0.1524 cm) thick. The aluminum shim was required because Zeus currently has an operating limit of 10¢ of excess reactivity.

This configuration actually was very slightly supercritical, with a period of approximately 1100 seconds. This period corresponds to approximately 1¢ of excess reactivity and therefore to a value of k_{eff} between 1.0000 and 1.0001. Consequently, the configuration can be considered to be exactly critical for the purposes of this study.

Prior to achieving criticality, measurements had been made for two very similar but slightly subcritical configurations. The first, or “uniform,” subcritical configuration had 8 cm of graphite between all adjacent HEU platters, while the second had 7 cm between the fourth and fifth platters and 8 cm between all the others. It is estimated, based on the count rate, that the uniform configuration was approximately 30¢ subcritical. The second, or “intermediate,” subcritical configuration was only very slightly subcritical, and its count rate was measured for nearly two hours before it could be determined that the configuration was indeed subcritical.

The corresponding value for k_{eff} is less than 1.0000 but greater than 0.9999. For the purposes of this analysis, the intermediate configuration can be considered to be critical.

3. ANALYSIS OF THE EXPERIMENT

Calculations were performed with MCNP4XS, a version that is intermediate between MCNP4B and MCNP4C. The principal distinction between MCNP4B and MCNP4XS is that the latter includes a more sophisticated treatment of the unresolved resonance region. However, the Zeus spectrum is sufficiently hard that there is no significant change in reactivity when the more sophisticated treatment is employed.[5]

The nuclear data were taken primarily from a cross-section library that was derived from release 4 of ENDF/B-VI and given the name URES.[6] Cross sections for isotopes that are not included in the URES library were taken from an earlier set[7] named ENDF60 that was derived from release 2 of ENDF/B-VI. However, aluminum is the only material present in Zeus that was updated from release 2 to release 4 but was not included in the URES library, and its reactivity contribution is so small that the results can be considered consistent with release 4.

The critical experiment and its two slightly subcritical predecessors were modeled in detail with MCNP4XS. Each HEU platter, graphite platter, and copper piece were represented individually, based on measurements made by the experimenters during the construction of the experiment.

Each HEU platter has two components, an inner disk with a radius of 7.5 inches (19.05 cm) and an outer ring with an outer radius of 10.5 inches (26.67 cm). Each inner disk and each outer ring were modeled separately, because there were slight differences in mass and enrichment. For example, the enrichment of individual pieces ranges from 93.12 to 93.28 wt.%.

All of the inner reflector pieces were made from a single block of copper, and the outer copper logs were made from a separate single block. Although the experimenters weighed each copper piece individually, it is reasonable to expect that they are more realistically represented by the average density for all the pieces from that particular block than by the inferred density for each piece. Consequently, only four copper densities were used in the modeling: one for the inner pieces, another for the logs, a third for the top reflector, and a fourth for the bottom reflector. It is worth noting, however, that the variation in these four densities is quite small; the difference between the heaviest and lightest is only 0.77%.

A vertical slice through the MCNP4XS representation for the critical configuration is shown in Figure 2. Close inspection of that figure reveals that the uppermost HEU platter has the same central cavity as those in the bottom portion of the core. The final configuration contained six HEU platters in the upper portion of the core and four in the bottom portion. However, only five inner disks without holes were available. Consequently, a disk with a hole in it was placed in the uppermost location, where it would have the least impact on reactivity.

The results obtained for each of the three configurations are summarized in Table I. Each of the MCNP4XS calculations employed at least 1,050 generations with 5,000 histories per generation, and the first 50 generations were excluded from the statistics. Each of the results shown in Table I therefore is based on a minimum of 5,000,000 active histories. The average flux and fission spectra within the HEU platters are shown in Figure 3. That figure clearly indicates that Zeus achieves its design objective by producing the great majority of fissions with neutrons in the intermediate energy range.

These results are consistent with those observed experimentally, except for a bias of slightly more than 0.005 Δk. They show an increase in reactivity of approximately 0.002 Δk from the uniform configuration to the other two. Furthermore, the reactivity difference between the second subcritical configuration and the final supercritical one is statistically insignificant.

4. COMPARISON WITH PREVIOUS ANALYSIS

These results are approximately 0.005 Δk lower than the corresponding ones obtained in a preliminary analysis that used nominal densities for the core components and a uniform enrichment for all of the HEU platters.[8] The reactivity differences are consistent with modeling differences in the two analyses.

For that previous analysis, the HEU and graphite platters were taken to be spatially uniform, except for the central holes in the platters in the lower portion of the core. Furthermore, all the copper pieces had the same density, all the graphite platters had the same density, and all the HEU disks and rings had the same density and enrichment. The nominal densities and HEU enrichment assumed in the previous analysis are compared with the corresponding average densities and enrichment of the actual configuration in Table II.

The assumed densities for the graphite and uranium platters match quite closely with the actual averages. Furthermore, some compensation occurs in the density and enrichment of the HEU platters, because the assumed nominal density was slightly lower than the actual average but the assumed enrichment was slightly higher than the actual average.

In contrast, the assumed density of the copper was approximately 2.7% higher than the actual average. Leakage from Zeus is approximately 25%, and so the lower density of the actual copper reduces k_{eff} by increasing the leakage slightly. The reactivity difference between the actual and assumed configurations was calculated to be -0.0049 ± 0.0006 Δk, and the effect of the copper by itself is -0.0041 ± 0.0006 Δk.

5. BENCHMARK SIMPLIFICATIONS

The overall design of the initial Zeus critical configuration is relatively simple, but the actual configuration is fairly complicated to model. A number of simplifications can be made that reduce the complexity substantially while having little overall impact on reactivity. These simplifications can be subdivided into two general categories, material simplifications and geometry simplifications.

5.1 MATERIAL SIMPLIFICATIONS

The most obvious material simplification is to remove the impurities. The graphite platters contain small amounts of ash, and the copper pieces contain tiny amounts of iron, chromium, and silver. The uranium disks and rings contain residual amounts of carbon, aluminum, silicon, iron, chromium, nickel, and magnesium. Calculations with MCNP4XS demonstrated that these impurities have negligible impact on reactivity and therefore can be omitted from the benchmark model.

The next step is to replace the platters and reflector pieces with corresponding platters and pieces of the same size but with average rather than individual compositions. The results of this process are summarized in Table III. In that table, “Actual” indicates that each piece of graphite or uranium has its own composition, while “Average” indicates that the composition of every piece is the same. These calculations were performed using the uniform Zeus configuration.

Replacing the individual graphite and uranium platters with platters of the average density produces almost no change in reactivity, because the effects are small, nearly equal in magnitude, and of opposite sign. Similarly, replacing the four copper compositions with a single average composition produces only a very marginal change in reactivity.

On average, the uranium disks have both a higher density and a higher enrichment than the uranium rings that surround them. Specifically, the inner disks have an average density of 18.99 g/cm^3 and an average enrichment of 93.28 wt.%, while the outer rings have an average density of 18.65 g/cm^3 and an average enrichment of 93.16 wt.%. However, the experimenters took care to alternate heavier and lighter uranium pieces. Consequently, replacing the individual disks and rings, either separately or uniformly, with average fuel has very little impact on reactivity.

The platen and the alignment tube are made of an aluminum alloy called Al 6061, which contains small amounts of magnesium, iron, copper, chromium, and a few other elements. Ideally, it would be preferable to treat the platen and tube as pure aluminum. Unfortunately, as Table III indicates, removing the other elements produces a significant increase in reactivity. Consequently, the actual Al 6061 composition will be retained in the benchmark specifications.

5.2 GEOMETRY SIMPLIFICATIONS

The first step in simplifying the Zeus geometry is to replace the final configuration with the uniform configuration. Although this transformation incurs a small reactivity penalty ($-0.0018 \pm 0.0005\ \Delta k$, as can be inferred from Table I), it produces a core of 10 identical units. Each unit has a central platter of HEU with 4 cm of graphite above and below it.

The geometry can be made considerably less complex simply by removing the diaphragm and most of the structural supports. As shown in Table IV, removal of the structural supports (but not the platen or the alignment tube) has no significant impact on reactivity, but removing the diaphragm noticeably increases the reactivity. When the diaphragm was removed, the bottom portion of the core was shifted slightly upward to retain full closure. Consequently, the distance between the fourth and fifth uranium platters is slightly smaller, and reactivity increases accordingly.

The hole in the top uranium disk and the small gap below the top reflector also were removed. As shown in Table IV, those changes have no significant impact on reactivity. The hole was filled with uranium of the average density and enrichment, which slightly increases the amount of uranium in the core. However, the importance of the top and bottom platters is much less than that of the other disks (see the 1/M plot in reference 2), and consequently the small increase in HEU mass does not produce a statistically significant change in reactivity. The top reflector was shifted downward slightly from its physical location to eliminate the gap, but its thickness and density remain unchanged. In practice, people who are validating their methodology against this benchmark can retain or omit the hole and the gap according to their individual preferences.

In contrast, the hollow alignment tube and the platen have been retained in the benchmark specifications. Their retention does not substantially increase the complexity of the benchmark configuration and, as Table IV indicates, their removal would produce a statistically significant reduction in reactivity ($-0.0014 \pm 0.0006\ \Delta k$). The central cavity inside the alignment tube constitutes a streaming path for neutrons, but the tube and the platen partially offset this effect by reflecting some of the neutrons that would otherwise escape from the system.

5.3 SUMMARY OF BENCHMARK SIMPLIFICATONS

The simplifications that have been made produce a core with alternating platters of uranium and graphite that have uniform densities and isotopic compositions. Similarly, the copper reflector regions all have the same density and composition, and there is no need to retain the identity of the individual corner and side reflector pieces. The alignment tube and the platen beneath it have been retained because they act, in a limited but significant capacity, as reflectors. In addition, the compositions of the principal components have been simplified by omitting any impurities.

Detailed specifications for the benchmark geometry and materials are given in Tables V, VI, VII, and VIII. The reactivity of the final benchmark is only marginally less than that of the actual critical configuration, as the summary in Table IX demonstrates.

6. CONCLUSIONS

The results from the detailed model indicate that release 4 of ENDF/B-VI overestimates the critical condition of Zeus by approximately $0.005\ \Delta k$. Although this bias is acceptable for many applications, it indicates that further refinement of the cross sections for ^{235}U in the intermediate energy range is desirable.

A number of simplifications have been made to transform the actual Zeus configuration into a more straightforward benchmark. These simplifications include removing the impurities from the principal components, replacing the individual uranium and graphite platters with corresponding platters that have the average mass and (for uranium) enrichment, replacing the copper reflector pieces with a single composition that has the average density, and removing all of the structural components except the platen and the alignment tube. These changes produce only minor changes in reactivity. Consequently, the reactivity of the resulting benchmark configuration is only very slightly less than that of the actual critical configuration.

This study has not addressed the reactivity uncertainties that result from uncertainties associated with measurements or the physical components of the experiment. Consequently, no definitive uncertainty can be assigned to the k_{eff} for the benchmark at this point. However, that work will be undertaken in the near future, and this benchmark will be submitted for inclusion in a future edition of the International Handbook of Evaluated Criticality Safety Benchmark Experiments.[9]

In addition, spectral measurements are planned for this configuration of Zeus. When they are completed, comparisons of the measured and calculated spectra may provide further insight into the discrepancy between the measured and calculated reactivity.

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Table I. MCNP4XS Results for Zeus Configurations

Configuration	k_{eff}
Uniform	1.0036 ± 0.0003
Intermediate	1.0059 ± 0.0004
Final	1.0054 ± 0.0004

Table II. Comparison between Nominal Values and Actual Averages

Item	Nominal Value	Actual Average
Copper Density (g/cm^3)	8.960	8.734
Graphite Density (g/cm^3)	1.750	1.745
Uranium Density (g/cm^3)	18.730	18.804
Uranium Enrichment (wt.%)	93.261	93.224

Table III. Reactivity Effects of Material Simplifications

Aluminum	Copper	Fuel		Graphite	k_{eff}	Δk	
		Inner	Outer			Incremental	Cumulative
Al 6061	Actual	Actual	Actual	Actual	1.0036 ± 0.0003		
Al 6061	Actual	Actual	Actual	Average	1.0046 ± 0.0003	0.0010 ± 0.0004	0.0010 ± 0.0004
Al 6061	Actual	Avg Inner	Avg Outer	Average	1.0043 ± 0.0003	-0.0003 ± 0.0004	0.0007 ± 0.0004
Al 6061	Actual	Average	Average	Average	1.0038 ± 0.0003	-0.0005 ± 0.0004	0.0002 ± 0.0004
Al 6061	Average	Average	Average	Average	1.0029 ± 0.0003	-0.0009 ± 0.0004	-0.0007 ± 0.0004
Pure Al	Average	Average	Average	Average	1.0048 ± 0.0003	0.0019 ± 0.0004	0.0012 ± 0.0004

Table IV. Reactivity Effects of Geometry Simplifications

Platen	Alignment Tube	Gap below Top Reflector	Hole in Top Platter	Diaphragm	Structural Supports	k_{eff}	Δk	
							Incremental	Cumulative
Present	Present	Present	Present	Present	Present	1.0029 ± 0.0003		
Present	Present	Present	Present	Present	Absent	1.0028 ± 0.0004	-0.0001 ± 0.0005	-0.0001 ± 0.0005
Present	Present	Present	Present	Absent	Absent	1.0045 ± 0.0004	0.0017 ± 0.0006	0.0016 ± 0.0005
Present	Present	Present	Absent	Absent	Absent	1.0047 ± 0.0003	0.0002 ± 0.0005	0.0018 ± 0.0004
Present	Present	Absent	Absent	Absent	Absent	1.0044 ± 0.0004	-0.0003 ± 0.0005	0.0015 ± 0.0005
Present	Absent	Absent	Present	Absent	Absent	1.0038 ± 0.0004	-0.0006 ± 0.0006	0.0009 ± 0.0005
Absent	Absent	Absent	Present	Absent	Absent	1.0030 ± 0.0004	-0.0008 ± 0.0006	0.0001 ± 0.0005

Table V. Material Specifications for Benchmark

Material	Density (g/cm^3)	Composition	
		Component	wt.%
Al 6061	2.700	Mg	1.000
		Al	97.175
		Si	0.600
		Ti	0.075
		Cr	0.250
		Mn	0.075
		Fe	0.350
		Cu	0.275
		Zn	0.125
Copper	8.734	Cu	100.000
Graphite	1.745	C	100.000
HEU	18.804	^{234}U	1.021
		^{235}U	93.224
		^{236}U	0.332
		^{238}U	5.423

Table VI. Dimensions for Fuel/Moderator Unit in Benchmark

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Outer Radium (cm)
Upper Graphite	4.29972	8.29972	3.175*	26.670
HEU	4.00000	4.29972	3.175*	26.670
Lower Graphite	0.0	4.00000	3.175*	26.670

*Units 1 through 4 only

Table VII. Dimensions for Central Column in Benchmark

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Outer Radius (cm)
Unit 10	99.47156	107.77128	—	26.6700
Unit 9	91.17184	99.47156	—	26.6700
Unit 8	82.87212	91.17184	—	26.6700
Unit 7	74.57240	82.87212	—	26.6700
Unit 6	66.27268	74.57240	—	26.6700
Unit 5	57.97296	66.27268	—	26.6700
Unit 4	49.67324	57.97296	3.1750	26.6700
Unit 3	41.37352	49.67324	3.1750	26.6700
Unit 2	33.07380	41.37352	3.1750	26.6700
Unit 1	24.77408	33.07380	3.1750	26.6700
Bottom Reflector	10.34688	24.77408	3.1750	26.6700
Alignment Tube	10.34688	57.97296	2.5400	3.1496
Platen	7.80688	10.34688	—	26.6700
Gap	0.0	7.80688	—	26.6700

Table VIII. Dimensions for Side and Top Reflectors in Benchmark

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Inner Distance, Side-to-Side (cm)	Outer Distance, Side-to-Side (cm)
Outer Reflector	0.0	123.90120	—	55.8800	88.2904
Inner Reflector	0.0	107.77128	26.7970	—	55.8800
Top Reflector	107.77128	122.19848	—	—	55.8800

Table IX. Reactivity Effects of Modeling Simplifications

Simplification	Δk	
	Incremental	Cumulative
Material Simplifications	-0.0007 ± 0.0004	-0.0007 ± 0.0004
Final to Uniform Geometry	-0.0018 ± 0.0005	-0.0025 ± 0.0005
Other Geometry Simplifications	0.0015 ± 0.0005	-0.0010 ± 0.0006

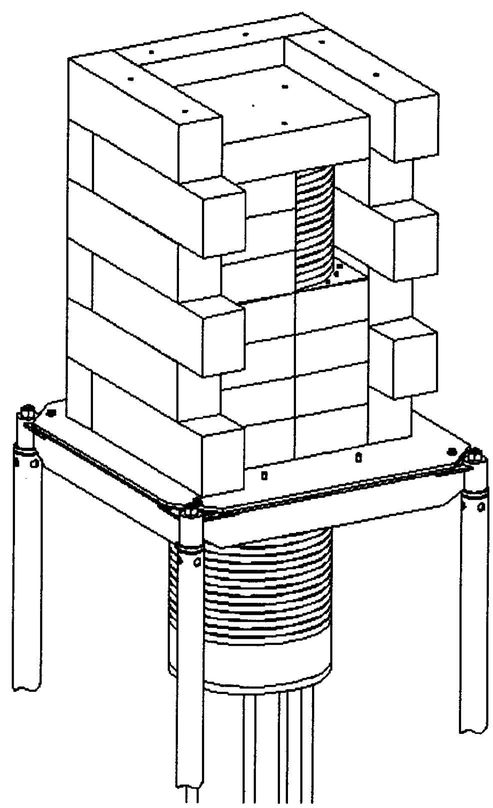

Figure 1. Schematic of the Zeus Experiment on the Comet Vertical Assembly Machine.

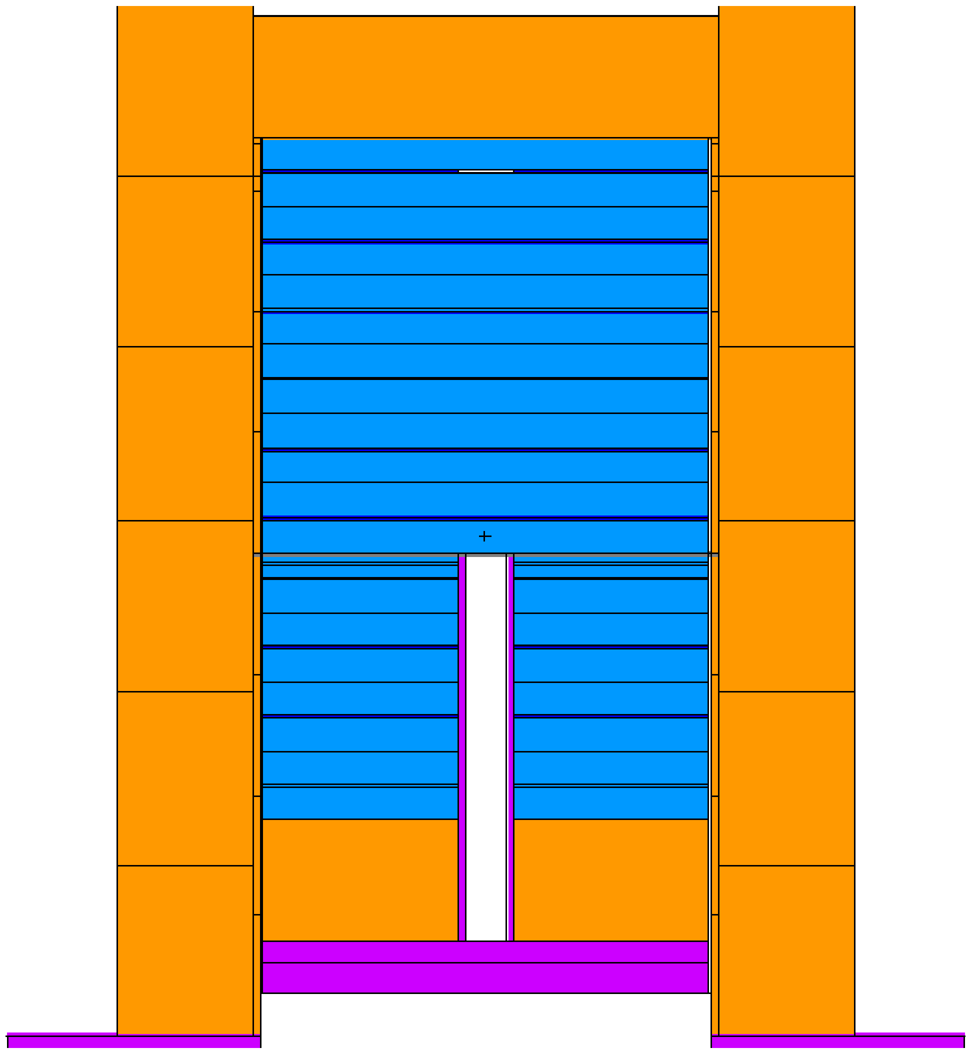

Figure 2. Vertical Slice through Zeus in Its Initial Critical Configuration.

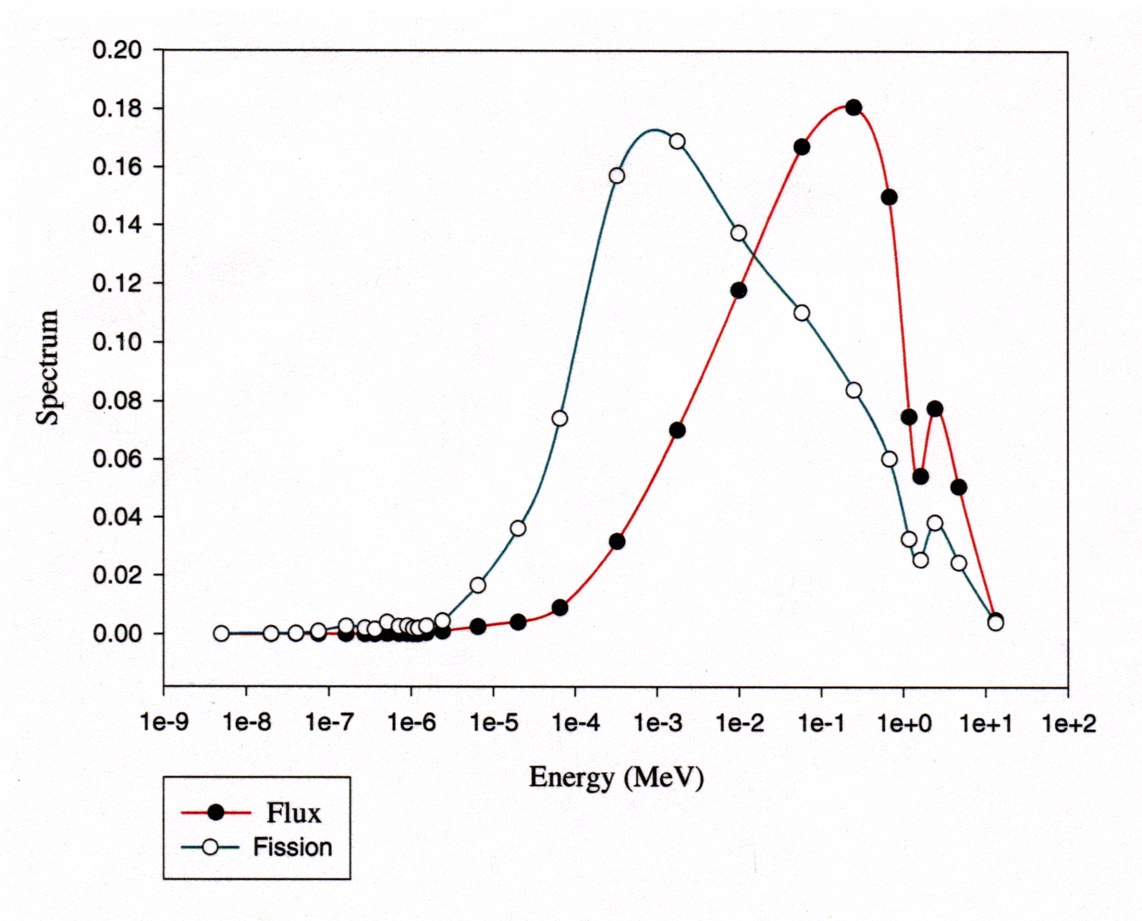

Figure 3. Flux and Fission Spectra in ZEUS Fuel Platters.