

**Detailed Analysis of the Second Zeus Critical Experiment with MCNP**

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# DETAILED ANALYSIS OF THE SECOND ZEUS CRITICAL EXPERIMENT WITH MCNP™

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## ABSTRACT

The Zeus experiments have been designed to test the adequacy of  $^{235}\text{U}$  cross sections in the intermediate energy range. The detailed modeling of the second Zeus critical experiment with the MCNP Monte Carlo code is described, and calculated results are presented. The calculations employed cross sections derived from ENDF/B-V and ENDF/B-VI, and the results have standard deviations of only 0.0003 for  $k_{\text{eff}}$ . Those results indicate that both ENDF/B-V and release 4 of ENDF/B-VI underestimate the value of  $k_{\text{eff}}$  for Zeus by approximately  $0.0015 \Delta k$ . In addition, a series of modeling simplifications is described that transforms 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  $k_{\text{eff}}$  that is only slightly different from that for the actual critical configuration.

## 1. INTRODUCTION

The Zeus experiments (Jaegers and Sanchez, 2000; Jaegers and Sanchez, 1999) have been designed to test the adequacy of  $^{235}\text{U}$  cross-sections in the intermediate energy range. This paper describes the detailed modeling of the second Zeus critical experiment with the MCNP Monte Carlo code (Briesmeister, 2000) in conjunction with cross sections derived from the fifth and sixth editions of the Evaluated Nuclear Data File, ENDF/B-V and ENDF/B-VI, respectively (Evaluated Nuclear Data File). In addition, a series of modeling simplifications is described that transforms the detailed representation into a benchmark configuration, and the reactivity impacts of those simplifications are assessed.

## 2. SECOND ZEUS CRITICAL EXPERIMENT

The second Zeus experiment reached a critical condition on October 24, 2000, with 9 platters of highly enriched uranium (HEU) and 54 platters of graphite. The first experiment, which has been analyzed previously (Mosteller and Sapir, 2000), achieved initial criticality on April 26, 1999 with 10 HEU platters and 79 platters of graphite. It had a  $C/^{235}\text{U}$  ratio of approximately 52:1 and a critical mass of 125.2 kg of uranium. The corresponding ratio for the second experiment was approximately 40:1, and its critical mass was 112.8 kg.

Like its predecessor, the second Zeus core contained thin, circular platters of highly enriched uranium (HEU) separated by similar platters of graphite. All of the graphite platters and most of the HEU platters in the second Zeus experiment also had been used in the first experiment. The cylindrical core was reflected by copper on the top, bottom, and sides. Inner copper pieces fit closely around the cylindrical core and produced a rectangular exterior surface. Heavy copper “logs” then were stacked against the outer sides of the inner copper pieces to form the side reflector. A thick cylindrical piece of copper provided reflection at the bottom of the core, and a square piece of copper rested atop the inner pieces.

Both Zeus critical experiments were constructed on the Comet vertical assembly machine. The inner and side reflectors sat on top of the platform of the machine, and a stainless steel diaphragm was inserted part way up the stack of inner copper pieces to support the upper portion of the core. The bottom portion of the core rested on the bottom reflector, which in turn was supported by the platen at the top of the machine’s vertical drive. The HEU and graphite platters that comprise the bottom portion of the core have a small central cavity with radii of 1.255 inches (3.1877 cm) and 1.25 inches (3.175 cm), respectively, through which an aluminum alignment tube was placed. Criticality was achieved by driving the bottom portion of the core up inside the reflector until it made contact with the diaphragm. A schematic of the Zeus experiments is shown in Fig. 1, and a vertical slice through the second experiment is shown in Fig. 2.

The core for the second experiment contained nine HEU plates, each separated from its nearest neighbors by six graphite plates. The graphite plates are circular, with an outer radius of 26.67 cm and an average thickness of slightly more than 1 cm. The circular HEU plates have two components, an inner disk with an outer radius of 19.05 cm and a tightly fitting outer annulus with an outer radius of 26.67 cm. The HEU plates are slightly less than 0.3 cm thick.

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 1.1%.

A close inspection of Fig. 2 reveals that the two uppermost HEU platters have the same central cavity as those in the bottom portion of the core. The final configuration contained seven HEU platters in the upper portion of the core and two in the bottom portion. However, only five inner disks without holes were available. Consequently, disks with holes were placed in the two uppermost locations, where they would have the least impact on reactivity.

This configuration was slightly supercritical, with a period of 170 seconds. That period corresponds to approximately 5¢ of excess reactivity and therefore to a value of  $k_{\text{eff}}$  very slightly greater than 1.0003. The uncertainty in reactivity due to geometric and material uncertainties is estimated to be  $\pm 0.0007 \Delta k$ , which is the same as that for the first experiment.

### 3. ANALYSIS OF THE EXPERIMENT

A detailed model of the second Zeus experiment was constructed for MCNP4C. Each graphite plate was modeled individually, with its own mass and thickness. Similarly, each inner HEU disk and each outer HEU 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.%. In addition, the detailed model includes the diaphragm, the platen, the alignment tube, each reflector piece, and the platform of the Comet assembly machine.

The MCNP4C calculations were performed with nuclear data libraries derived from both ENDF/B-V and ENDF/B-VI. The ENDF/B-VI data for the uranium isotopes were taken from an auxiliary cross-section library that was derived from release 4 of ENDF/B-VI (ENDF/B-VI.4) and given the name URES (Little and MacFarlane, 1998). Cross sections for isotopes that are not included in the URES library were taken from an earlier set named ENDF60 (Hendricks, Frankle, and Court, 1994) 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 ENDF/B-VI results can be considered consistent with release 4.

The ENDF/B-V and ENDF/B-VI.4 MCNP calculations each employed 1,250 generations with 5,000 histories per generation, and the first 50 generations were excluded from the statistics. The results therefore are based on 6,000,000 active histories. The values obtained for  $k_{\text{eff}}$  are given in Table 1, and the average flux and fission spectra within the HEU platters are shown in Fig. 3. (At the resolution of Fig. 3, the ENDF/B-V and ENDF/B-VI.4 spectra are indistinguishable.) 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 approximately  $-0.0015 \Delta k$ . The corresponding results for  $k_{\text{eff}}$  from calculations for the first Zeus experiment are  $0.9989 \pm 0.0003$  and  $0.9972 \pm 0.0003$  for ENDF/B-V and ENDF/B-VI.4, respectively (Mosteller and Jaegers, 2000). The ENDF/B-V results for the two experiments therefore are statistically indistinguishable, while there is an increase of approximately  $0.0015 \Delta k$  from the first experiment to the second for ENDF/B-VI.4. As Table 1 indicates, ENDF/B-VI.4 produces a smaller capture fraction than ENDF/B-V and a correspondingly larger leakage fraction. The lower capture

from ENDF/B-VI.4 is due primarily to copper, although the capture fraction for  $^{235}\text{U}$  also is smaller than from ENDF/B-V.

#### **4. 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, geometry simplifications and material simplifications.

The MCNP4C calculations for these simplifications were performed sequentially, so that with each new simplification the model retained all of the previous simplifications. With this approach, each result can be compared directly to any previous result, and the uncertainties in reactivity do not compound each other. All of these calculations employed the ENDF/B-VI libraries.

##### **4.1 Geometry Simplifications**

The geometry of the Zeus experiments can be made considerably less complex by removing the diaphragm, removing the platform of the assembly machine, and converting the thickness of the graphite plates to a single, average value. As shown in Table 2, these changes produce only small changes in  $k_{\text{eff}}$ , and they largely offset each other. Additional simplifications that fill in the holes in the top two HEU disks, reduce the diameter of the holes in the lower two HEU disks to match that of the adjacent graphite platters, and shift the alignment tube upward to eliminate the gap between it and the solid graphite platter above it do not produce statistically significant changes in reactivity.

In contrast, the hollow alignment tube, the platen, and the gap between the uppermost graphite platter and the top reflector have been retained in the benchmark specifications. Retention of the alignment tube and the platen does not substantially increase the complexity of the benchmark configuration and, as Table 2 indicates, their removal would produce a statistically significant reduction in reactivity ( $-0.0018 \pm 0.0004 \Delta k$ ). 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. Similarly, removal of the gap between the top graphite platter and the top reflector would increase reactivity significantly ( $0.0025 \pm 0.0004 \Delta k$ ) by eliminating a streaming path that reduces the optical distance neutrons have to travel to escape from the core.

##### **4.2 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 MCNP4C demonstrated that these impurities have negligible impact on reactivity and therefore can be omitted from the benchmark model. These results from these calculations are shown in Table 3.

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 also are summarized in Table 3. In that table, “Actual” indicates that each piece of graphite or uranium has its own composition, while “Pure” indicates that all impurities have been removed. “Average” indicates that the composition of every piece is the same and that no impurities are retained.

Replacing the individual graphite and uranium platters with platters of the average density produces almost no change in reactivity. Similarly, replacing the four copper compositions with a single average composition produces only a very marginal change in reactivity.

On average, the inner 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 18.97 g/cm<sup>3</sup> and an average enrichment of 93.28 wt.%, while the outer rings have an average density of 18.70 g/cm<sup>3</sup> and an average enrichment of 93.17 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, and Table 3 indicates that removing the other elements does not produce a statistically significant change in reactivity. In contrast, such a change was statistically significant for the benchmark model of the first Zeus experiment (Mosteller and Sapir, 2000). Consequently, for the sake of consistency, the actual Al 6061 composition will be retained in these benchmark specifications as well. However, an analyst who wishes to treat the platen and alignment tube as pure aluminum can do so without significantly affecting reactivity.

### **4.3 Summary of Benchmark Simplifications**

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 inner and side reflector pieces. 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 4, 5, 6, and 7. The reactivity of the final benchmark is only marginally less than that of the actual critical configuration, as the summary in Table 8 demonstrates.

## **5 CONCLUSIONS**

The results from the detailed model indicate that ENDF/B-V and ENDF/B-VI.4 both underestimate the reactivity of the second Zeus experiment by approximately 0.0015  $\Delta k$ . They also clearly indicate that the experiment achieved its objective of producing an intermediate spectrum.

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, thickness, 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.

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Table 1. MCNP4C Results for the Detailed Model of Second Zeus Experiment

Measured $k_{\text{eff}}$	Calculated $k_{\text{eff}}$		Calculated Neutron Balance					
			ENDF/B-V			ENDF/B-VI.4		
	ENDF/B-V	ENDF/B-VI.4	Fission	Capture	Leakage	Fission	Capture	Leakage
$1.0003 \pm 0.0007$	$0.9986 \pm 0.0003$	$0.9987 \pm 0.0003$	40.3%	36.3%	23.4%	40.4%	33.1%	26.5%

Table 2. Reactivity Effects of Geometry Simplifications

Change	$k_{\text{eff}}$	$\Delta k$	
		Incremental	Cumulative
Reference	$0.9987 \pm 0.0003$	—	—
Same Thickness for all Graphite Plates	$0.9986 \pm 0.0003$	$-0.0001 \pm 0.0004$	$-0.0001 \pm 0.0004$
Remove Comet Platform	$0.9979 \pm 0.0003$	$-0.0007 \pm 0.0004$	$-0.0008 \pm 0.0004$
Remove Diaphragm	$0.9990 \pm 0.0003$	$0.0011 \pm 0.0004$	$0.0003 \pm 0.0004$
Fill Holes in Top 2 HEU Platters	$0.9992 \pm 0.0003$	$0.0002 \pm 0.0004$	$0.0005 \pm 0.0004$
Fill Hole in Top Reflector	$0.9991 \pm 0.0003$	$-0.0001 \pm 0.0004$	$0.0004 \pm 0.0004$
Remove Gap above Alignment Tube	$0.9989 \pm 0.0003$	$-0.0002 \pm 0.0004$	$0.0002 \pm 0.0004$
Remove Gap below Top Reflector	$1.0014 \pm 0.0003$	$0.0025 \pm 0.0004$	$0.0027 \pm 0.0004$
Remove Alignment Tube and Platen	$0.9971 \pm 0.0003$	$-0.0018 \pm 0.0004$	$-0.0016 \pm 0.0004$

Table 3. Reactivity Effects of Material Simplifications

Aluminum	Fuel		Copper	Graphite	$k_{\text{eff}}$	$\Delta k$	
	Inner	Outer				Incremental	Cumulative
Al 6061	Actual	Actual	Actual	Actual	$0.9989 \pm 0.0003$	—	—
Al 6061	Actual	Actual	Actual	Average	$0.9986 \pm 0.0003$	$-0.0003 \pm 0.0004$	$-0.0003 \pm 0.0004$
Al6061	Actual	Actual	Pure	Average	$0.9986 \pm 0.0003$	$0.0 \pm 0.0004$	$-0.0003 \pm 0.0004$
Al 6061	Actual	Actual	Average	Average	$0.9981 \pm 0.0003$	$-0.0005 \pm 0.0004$	$-0.0008 \pm 0.0004$
Al6061	Pure Inner	Pure Outer	Average	Average	$0.9984 \pm 0.0003$	$0.0003 \pm 0.0004$	$-0.0005 \pm 0.0004$
Al 6061	Avg Inner	Avg Outer	Average	Average	$0.9982 \pm 0.0003$	$-0.0002 \pm 0.0004$	$-0.0007 \pm 0.0004$
Al 6061	Average	Average	Average	Average	$0.9982 \pm 0.0003$	$0.0 \pm 0.0004$	$-0.0007 \pm 0.0004$
Pure Al	Average	Average	Average	Average	$0.9980 \pm 0.0003$	$-0.0002 \pm 0.0004$	$-0.0009 \pm 0.0004$

Table 4. Material Specifications for Benchmark

Material	Density (g/cm <sup>3</sup> )	Composition	
		Component	wt.%
Al 6061	2.7000	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	8.7351	Cu	100.000
Graphite	1.7117	C	100.000
HEU	18.8156	<sup>234</sup> U	1.024
		<sup>235</sup> U	93.224
		<sup>236</sup> U	0.332
		<sup>238</sup> U	5.420

Table 5. Dimensions for Fuel/Moderator Unit in Benchmark

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Outer Radium (cm)
Upper Graphite	3.32180	6.34388	3.175*	26.670
HEU	3.02208	3.32180	3.175*	26.670
Lower Graphite	0.0	3.02208	3.175*	26.670

\*Bottom 2 Units only

Table 6. Dimensions for Central Column in Benchmark

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Outer Radius (cm)
Unit 9	95.77208	102.11596	—	26.6700
Unit 8	89.42820	95.77208	—	26.6700
Unit 7	83.08432	89.42820	—	26.6700
Unit 6	76.74044	83.08432	—	26.6700
Unit 5	70.39656	76.74044	—	26.6700
Unit 4	64.05268	70.39656	—	26.6700
Unit 3	57.70880	64.05268	—	26.6700
Unit 2	51.36492	57.70880	3.1750	26.6700
Unit 1	45.02104	51.36492	3.1750	26.6700
Bottom Reflector	30.59384	45.02104	3.1750	26.6700
Platen	26.78384	30.59384	—	26.6700
Alignment Tube	-5.79120	57.70880	—	26.6700

Table 7. 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	123.9012	—	55.8800	88.2904
Inner Reflector	0.0	102.8954	26.7970	—	55.8800
Top Reflector	102.89540	117.3226	—	—	55.8800

Table 8. Comparisons of MCNP4C Results for Detailed and Benchmark Models

Library	$k_{\text{eff}}$		$\Delta k$
	Detailed Model	Benchmark Model	
ENDF/B-V	$0.9986 \pm 0.0003$	$0.9985 \pm 0.0003$	$-0.0001 \pm 0.0004$
ENDF/B-VI.4	$0.9987 \pm 0.0003$	$0.9981 \pm 0.0003$	$-0.0006 \pm 0.0004$

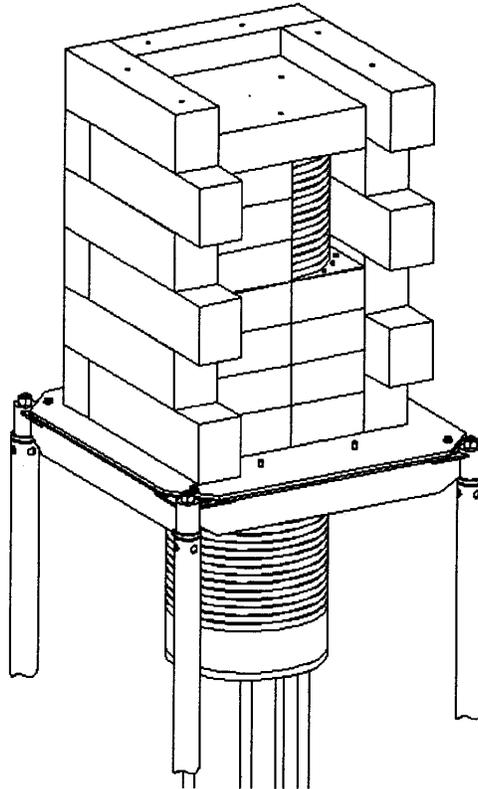


Figure 1. Schematic of the Zeus Experiment on the Comet Vertical Assembly Machine.

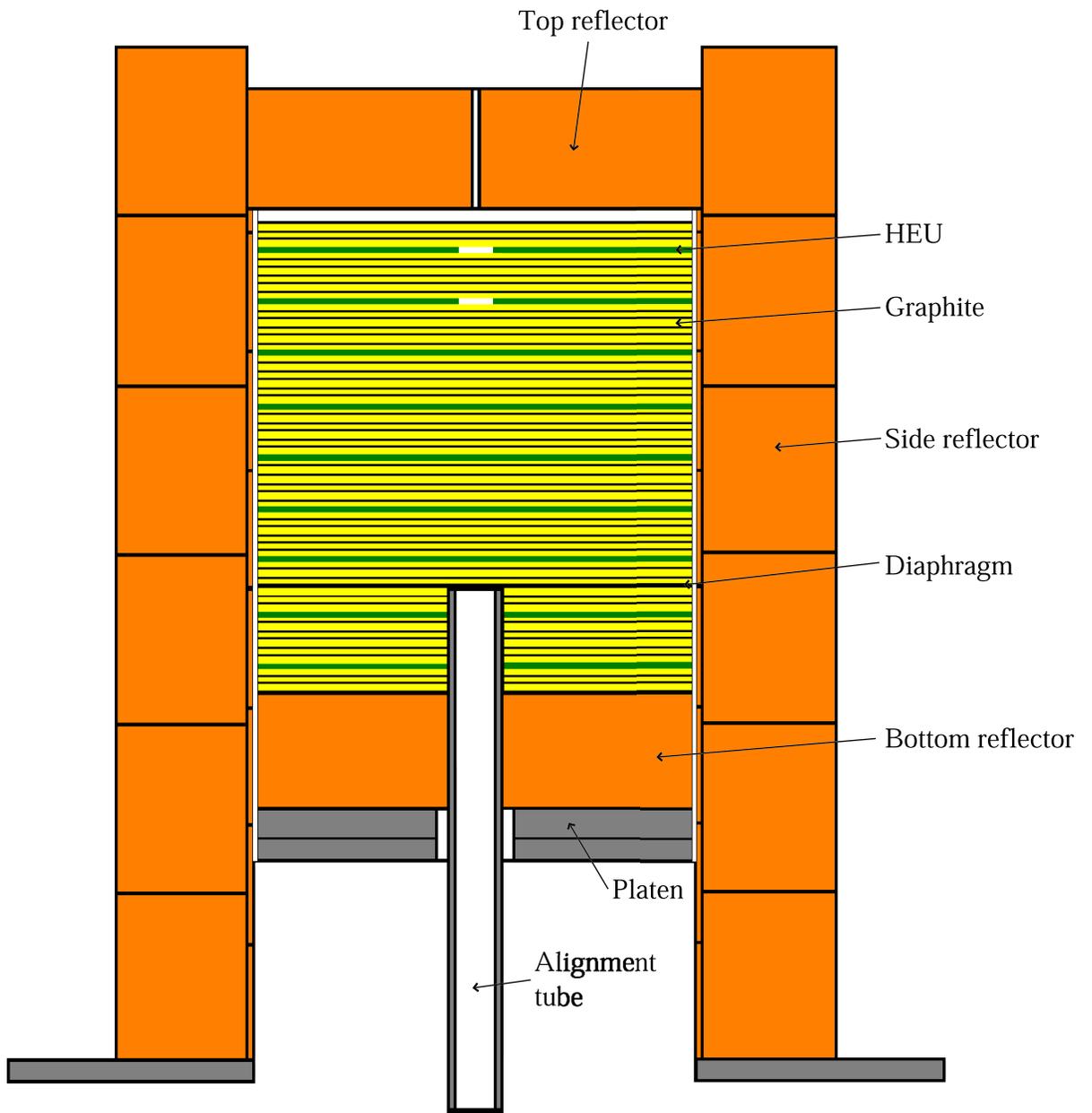


Figure 2. Vertical slice through the second Zeus experiment.

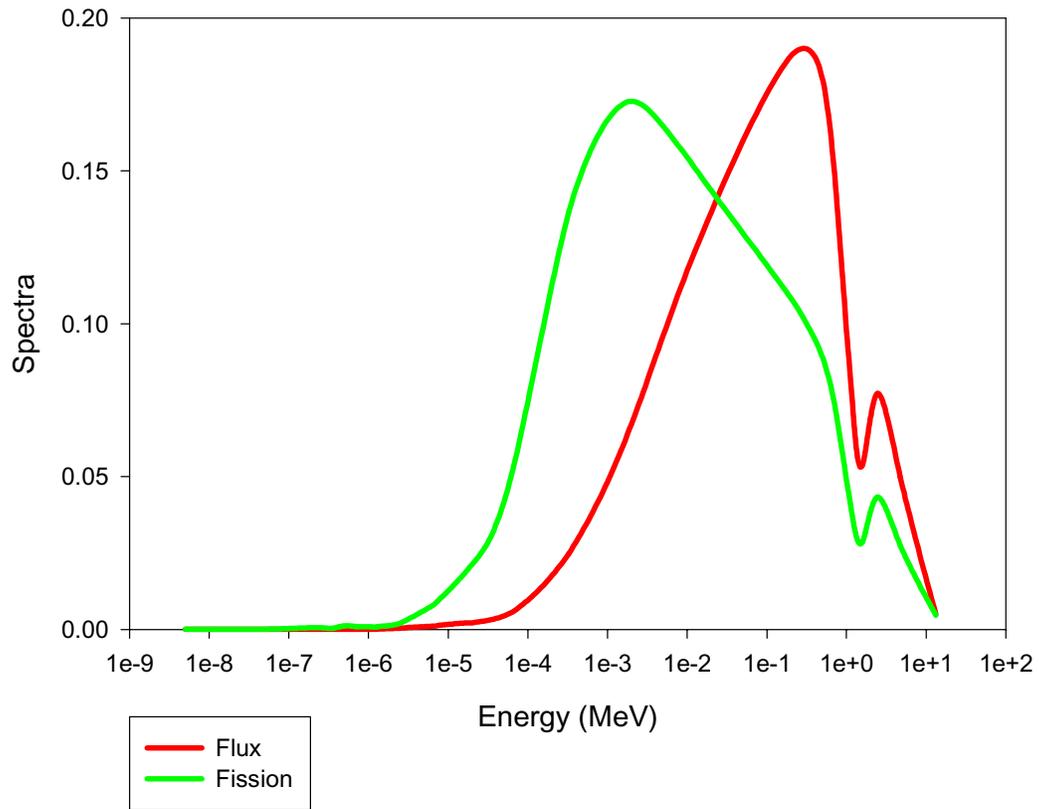


Figure 3. Flux and Fission Spectra in ZEUS Fuel Platters.