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DETAILED ANALYSIS OF THE THIRD ZEUS CRITICAL EXPERIMENT WITH MCNP™*

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ABSTRACT

The Zeus experiments have been designed to test the adequacy of ^{235}U cross sections in the intermediate energy range. A detailed model of the third Zeus critical experiment for the MCNP Monte Carlo code is developed, and calculated results, based on cross sections derived from ENDF/B-V and ENDF/B-VI, are presented. A series of modeling simplifications then is described that transforms the detailed representation into a benchmark configuration, and the reactivity impact of each of those simplifications is assessed. Finally, the calculated results for this experiment are compared with those from its two predecessors.

Key Words: Critical Experiment, Benchmark, Zeus, Intermediate Spectrum, MCNP

1. INTRODUCTION

The Zeus experiments[1,2] have been designed to test the adequacy of ^{235}U cross sections in the intermediate energy range. The third experiment in the series achieved initial criticality on October 24, 2001. Its critical mass was 106.6 kg of highly enriched uranium (HEU), and the atom ratio of carbon to ^{235}U was approximately 26:1.

A detailed model of the third Zeus critical experiment has been developed for the MCNP Monte Carlo code,[3] using cross sections derived from the fifth[4] and sixth[5] editions of the Evaluated Nuclear Data File (ENDF/B-V and ENDF/B-VI, respectively). Subsequently, a series of modeling simplifications has been made to transform that detailed representation into a benchmark configuration. This paper presents results from the detailed model and assesses the reactivity impact of the simplifications. In addition, it compares these results with those for the previous two Zeus experiments.[2,6]

2. THIRD ZEUS CRITICAL EXPERIMENT

Like those of its two predecessors, the third Zeus core contained thin, circular platters of HEU separated by thicker platters of graphite. Twenty of the graphite platters and all but one of the HEU pieces had been used in one or both of the previous two experiments. The cylindrical core was reflected by copper on the top, bottom, and sides. Inner copper pieces, referred to as corner reflectors, 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

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core, and a square piece of copper rested on top of the inner pieces, slightly above the topmost graphite platter.

All three Zeus experiments were constructed on the Comet vertical assembly machine. The corner 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 in 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 cut-away schematic of the Zeus experiments is shown in Fig. 1, and a vertical slice through the third experiment is shown in Figure 2.

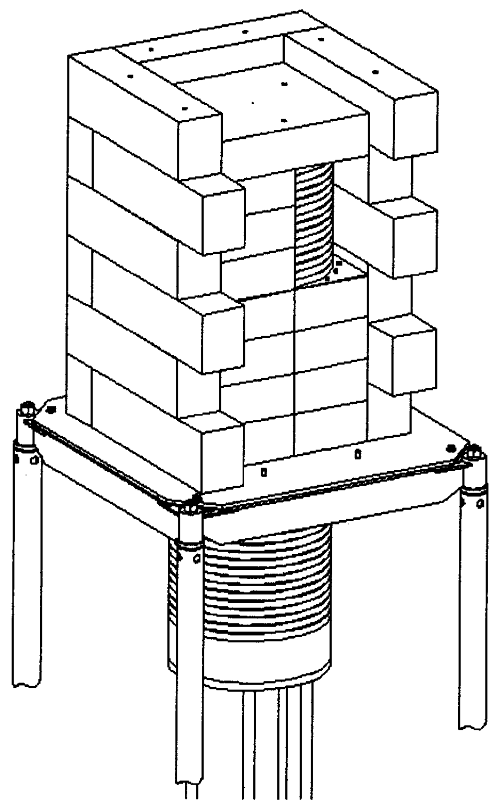
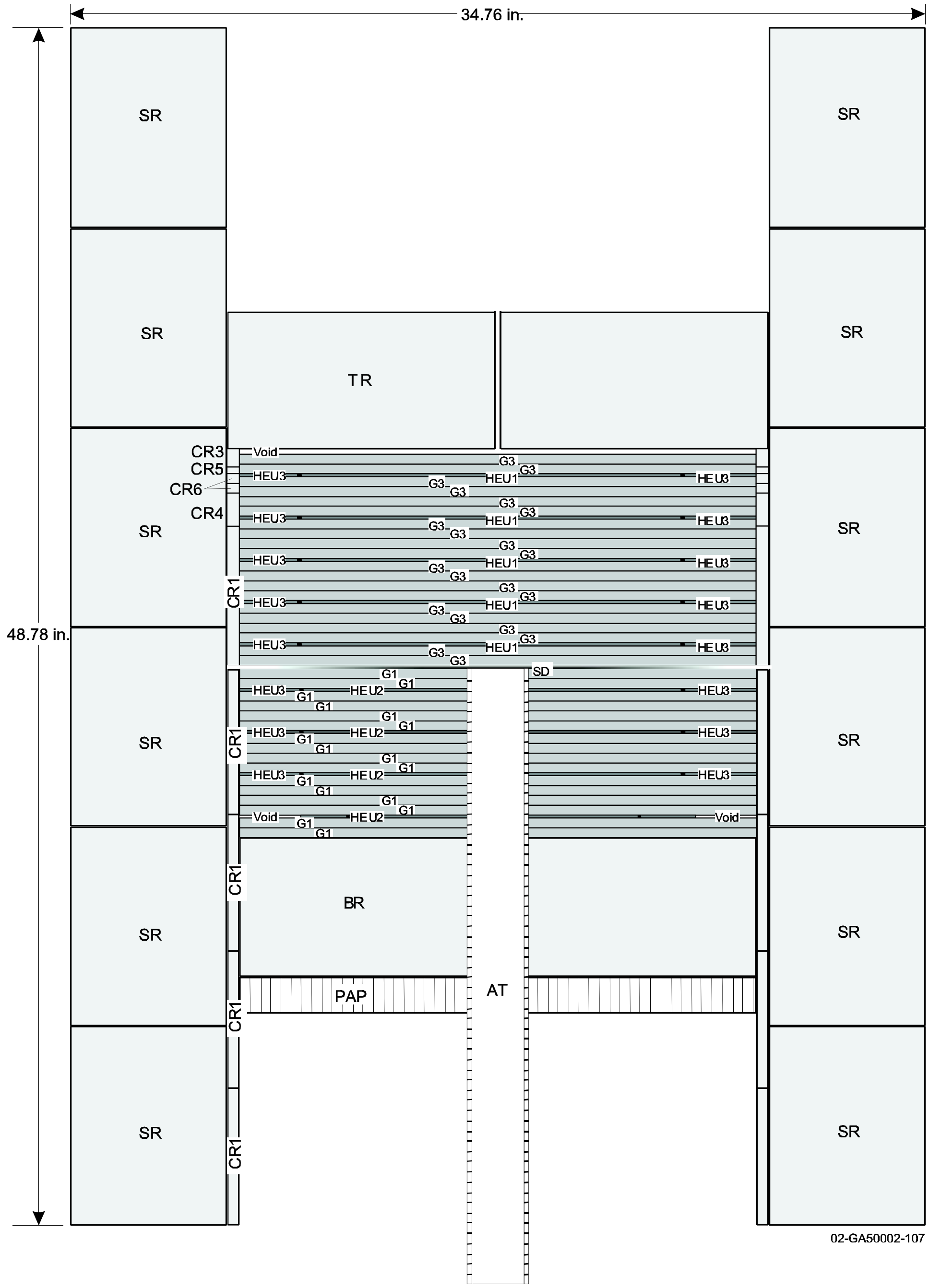


Figure 1. Schematic of the Zeus experiment on the Comet vertical assembly machine

The core for the third experiment contained nine HEU platters, each separated from its nearest neighbors by four graphite platters. The graphite plates are circular, with an outer radius of 10.5 inches (26.67 cm) and an average thickness of slightly more than 1 cm. The HEU plates also are circular, and the upper eight of them have two components, an inner disk with an outer radius of



BR = Bottom Reflector
CR = Corner Reflector
SR = Side Reflector
TR = Top Reflector

AT = Alignment Tube
G = Graphite Platter
HEU = HEU Platter
PAP = Platen
SD = Diaphragm

Figure 2. Vertical slice through the third Zeus assembly

7.5 inches (19.05 cm) and a tightly fitting outer ring with an outer radius of 10.5 inches (26.67 cm). The bottom HEU plate is simply an inner disk with no outer ring. 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 corner reflectors, another for the side reflectors, a third for the top reflector, and a fourth for the bottom reflector. It is worth noting, however, that the variation in these densities is quite small; the difference between the heaviest and the lightest is only 1.1%.

This configuration was slightly supercritical, with a period of 302 seconds. That period corresponds to approximately 3.7¢ of excess reactivity and therefore to a value of k_{eff} that is very slightly greater than 1.0002. The uncertainty due to geometric and material uncertainties is estimated to be ±0.0008 Δk, which is comparable to those for the first two experiments.

3. ANALYSIS OF THE EXPERIMENT

A detailed model of the third Zeus experiment was developed for the MCNP4C2 Monte Carlo code. Each graphite platter 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 density and composition. For example, the enrichment of the individual pieces ranged from 93.15 wt.% to 93.41 wt.%. In addition, the detailed model includes the diaphragm, the alignment tube, each reflector piece, and the platform and platen of the Comet assembly machine.

The MCNP4C2 calculations were performed with nuclear data libraries derived from ENDF/B-V and from ENDF/B-VI. The ENDF/B-VI calculations employed the URES library[7] and, for isotopes not present in URES, the ENDF60 library.[8] The data in the URES library are taken from release 4 (ENDF/B-VI.4), while the data in ENDF60 are taken from release 2. Aluminum is the only material present in Zeus that was updated from release 2 to release 4 but not included in URES. However, its reactivity contribution is quite small, and therefore the ENDF/B-VI results can be considered consistent with ENDF/B-VI.4.

Each of the MCNP4C2 calculations discussed herein employed 1,250 generations with 5,000 histories per generation. The first 50 generations were excluded from the statistics, and so the reported results are based on 6,000,000 active histories. The values obtained for k_{eff} are given in Table I, and the neutron balance is summarized in Table II. 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 demonstrates that Zeus achieves its design objective by producing the great majority of fissions with neutrons in the intermediate energy range.

Table I. k_{eff} for the third Zeus experiment

	Calculated	
Measured	ENDF/B-V	ENDF/B-VI.4
1.0002 ± 0.0008	0.9989 ± 0.0003	1.0006± 0.0003

Table II. Calculated neutron balance for the third Zeus experiment

Mechanism	ENDF/B-V	ENDF/B-VI.4
Fission	40.2%	40.3%
Capture	34.7%	31.4%
Leakage	25.1%	28.3%

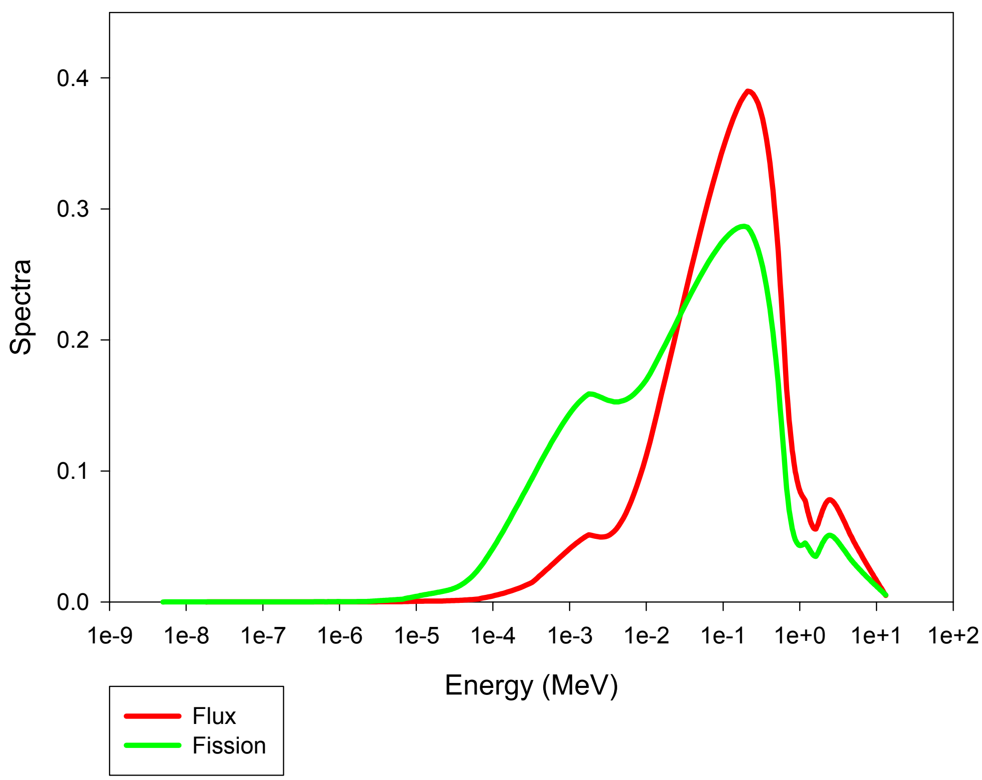


Figure 3. Flux and fission spectra in Zeus fuel platters

As Table II indicates, ENDF/B-VI.4 produces a smaller capture fraction than ENDF/B-V and a correspondingly larger leakage fraction. The lower capture with ENDF/B-VI.4 is due primarily to copper, although the capture fraction for ^{235}U also is smaller than that with ENDF/B-V.

4. BENCHMARK SIMPLIFICATIONS

The overall design of the Zeus experiments is relatively simple, but the actual configurations are fairly complicated to model in detail. 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 and material compositions.

The MCNP4C2 calculations for each of the simplifications were performed sequentially, so that with each new simplification the model retained all of the previous ones. 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 ENDF/B-VI cross sections.

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 thicknesses of the graphite plates to a single average value. Further simplifications can be made to remove small void regions. As shown in Table III, these modifications produce only small changes in k_{eff}.

Table III. Reactivity effects of geometry simplifications

Change	Δk Incremental	Δk Cumulative
Same thickness for all graphite plates	0.0010 ± 0.0004	0.0010 ± 0.0004
Change inner radius of HEU disks to 1.25 inches	-0.0002 ± 0.0004	0.0008 ± 0.0004
Remove Comet platform	-0.0005 ± 0.0004	0.0003 ± 0.0004
Remove diaphragm	0.0012 ± 0.0004	0.0015 ± 0.0004
Fill hole in top reflector	0.0003 ± 0.0004	0.0018 ± 0.0004
Remove gap above alignment tube	0 ± 0.0004	0.0018 ± 0.0004
Remove gap below top reflector	0.0008 ± 0.0004	0.0026 ± 0.0004

The possibility of removing the alignment tube and the platen also was investigated. However, their retention does not substantially increase the complexity of the benchmark configuration, and their removal produces a reactivity change of -0.0037 ± 0.0004 Δk, which was deemed too large to accept. 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 otherwise would escape from the system.

4.2 Material Simplifications

The obvious material simplifications are to remove the minor impurities from the various components, replace individual platters by platters of a single, average composition, and to homogenize the copper pieces so that they all have the same density. The reactivity effects of these changes are shown in Table IV.

Table IV. Reactivity effects of material simplifications

Change	Δk Incremental	Δk Cumulative
Change density of all graphite platters to average	-0.0004 ± 0.0004	-0.0004 ± 0.0004
Remove impurities from copper pieces	0.0001 ± 0.0004	-0.0003 ± 0.0004
Change density of all copper pieces to average	0.0008 ± 0.0004	0.0005 ± 0.0004
Remove impurities from fuel	-0.0012 ± 0.0004	-0.0007 ± 0.0004
Change density and enrichment of all HEU platters to average	-0.0011 ± 0.0004	-0.0018 ± 0.0004

The changes to the HEU platters produce more substantial reactivity changes than do those to the graphite platters and the copper reflector. At first thought, it might seem that removing the impurities from the fuel should increase reactivity, because absorbing materials are being removed. However, at these energies, those impurities act more like moderators than absorbers, and therefore their removal slightly decreases reactivity.

On average, the inner HEU disks have both a higher density and a higher enrichment than the HEU rings that surround them. Specifically, the inner disks have an average density of 18.94 g/cm^3 and an average enrichment of 93.30 wt.%, while the outer rings have an average density of 18.70 g/cm^3 and an average enrichment of 93.17 wt.%. Consequently, the net effect of homogenizing the uranium disks and rings is to move both mass and ^{235}U content outward. Not surprisingly, this movement produces a small but statistically significant decrease in reactivity.

The platen and 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 tube and platen as pure aluminum. Furthermore, calculations with MCNP4C2 indicate that removing those 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,[2] and therefore, 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 the reactivity of the model.

4.3 Summary of Benchmark Simplifications

These simplifications produce a core with platters of uranium and graphite that have uniform densities and isotopic compositions. Consequently, there is no need to retain a distinction between adjacent graphite platters. Similarly, the copper reflector regions all have the same density and composition, and so there is no need to retain the identity of the individual corner and side reflector pieces. Furthermore, the composition of the principal components have been simplified by omitting all impurities.

A vertical slice through the center of the benchmark is presented in Fig. 4, and 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 greater than that of the actual critical configuration, as the summary in Table IX demonstrates.

5. COMPARISON WITH ANALYSES OF PREVIOUS ZEUS EXPERIMENTS

All three Zeus experiments were performed on the Comet vertical assembly machine, over a period of about 2½ years. The first Zeus experiment achieved initial criticality on April 26, 1999, and the second achieved initial criticality on October 24, 2000. The third achieved initial criticality exactly one year later, on October 24, 2001. The same side reflector pieces were used in all three experiments, and most of the corner reflector pieces were the same as well. The differences between the cores of the three experiments are summarized in Table X. The successive decreases in the atom ratio of C:^{235}U, which were achieved by reducing the number of graphite platters in the core, produce an increasingly harder neutron spectrum.

The calculated values for k_{eff} for the detailed models of the three experiments are shown in Table XI. Both ENDF/B-V and ENDF/B-VI.4 produce an average bias of about -0.0015 Δk. However, as Table XII indicates, the bias from ENDF/B-V is reasonably constant, whereas the ENDF/B-VI.4 bias shows a consistent trend as the spectra of the experiments hardens. This behavior suggests a small energy-dependent bias in the ENDF/B-VI.4 cross sections.

The successive hardening of the spectra for the three experiments is illustrated in Table XIII. The fission fraction remains almost constant (as it should, since it is simply the inverse of the average number of neutrons per fission). However, the spectrum hardens as the core becomes physically smaller and the amount of moderator decreases. Accordingly, the leakage fraction increases from experiment to experiment, while the capture fraction decreases.

Table XIII also shows that ENDF/B-VI.4 consistently produces a smaller capture fraction and a correspondingly larger leakage fraction than ENDF/B-V. As noted previously in Section 3, the lower capture with ENDF/B-VI.4 is due primarily to copper, although the capture fraction for ^{235}U also is smaller than with ENDF/B-V.

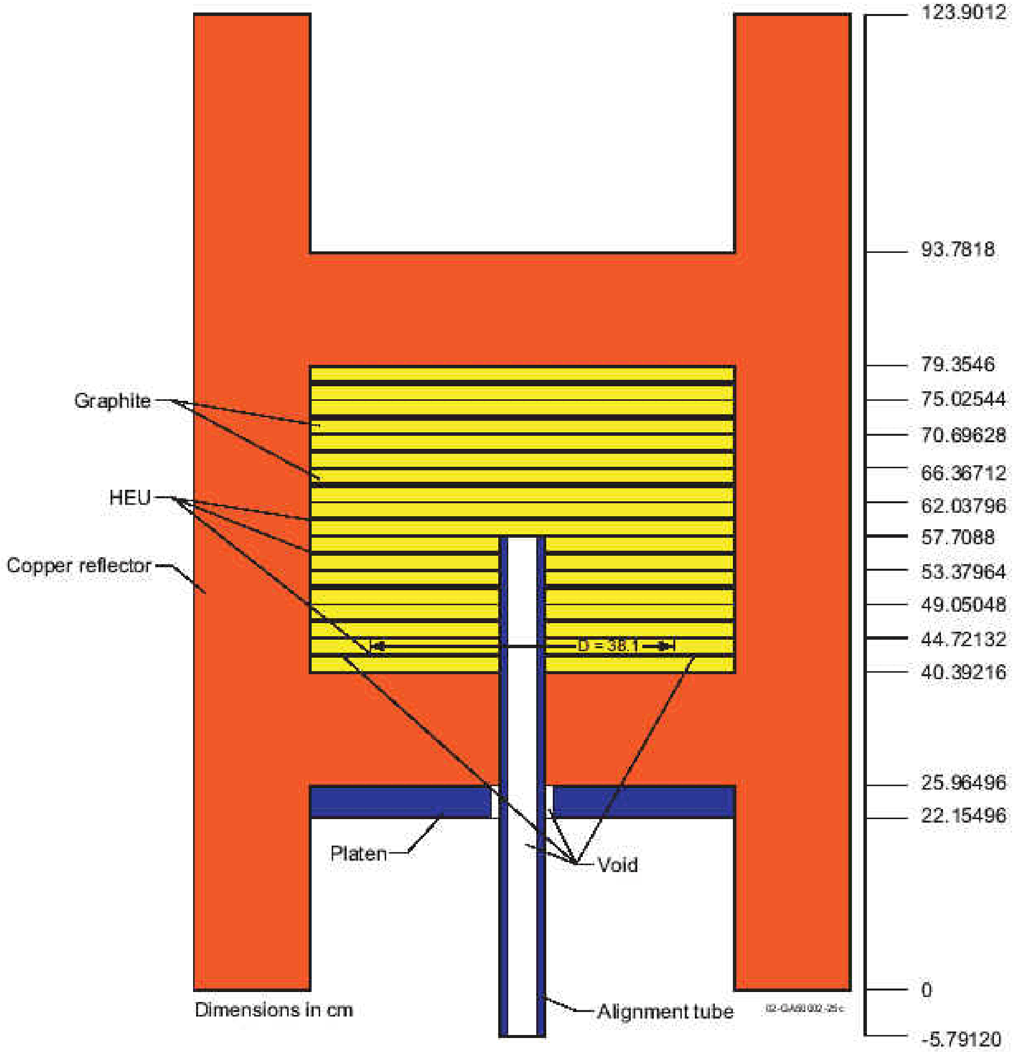


Figure 4. Vertical slice through the benchmark model of the third Zeus assembly

6. SUMMARY AND CONCLUSIONS

The results from the detailed model of the third Zeus experiments clearly indicate that, like its predecessors, it achieved its design objective of producing an intermediate spectrum. In addition, both ENDF/-V and ENDF/B-VI.4 produce values for k_{eff} that agree qute closely with the measured value.

A number of simplifications have been made to transform that detailed model into a more straightforward benchmark model. The net reactivity effect of these changes is relatively minor (0.0008 ± 0.0004), and consequently the reactivity of the benchmark configuration is only

Table V. Material specifications for benchmark model

Material	Density (g/cm^3)	Composition Component	wt.%
		Mg	1.000
		Al	97.175
		Si	0.600
		Ti	0.075
Al 6061	2.7000	Cr	0.250
		Mn	0.075
		Fe	0.350
		Cu	0.275
		Zn	0.125
Copper	8.7351	Cu	100.000
Graphite	1.7239	C	100.000
		^{234}U	1.024
HEU	18.8086	^{235}U	93.237
		^{236}U	0.326
		^{238}U	5.413

slightly higher than that of the actual critical configuration. In addition, both ENDF/-V and ENDF/B-VI.4 produce values for k_{eff} that agree quite closely with the measured value.

The results obtained from the detailed model for the third Zeus experiment were compared with the corresponding results from its two predecessors. Both ENDF/B-V and ENDF/B-VI.4 produce an average bias of about -0.0015 Δk for the three experiments, but the trends are not the same. Specifically, the bias from ENDF/B-V is reasonably constant, whereas the ENDF/B-VI.4 bias shows a consistent upward trend as the spectra of the experiments harden. This behavior suggests a small energy-dependent bias in the ENDF/B-VI.4 cross sections.

Table VI. Dimensions for HEU/graphite unit in benchmark model

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Outer Radius (cm)
Upper Graphite	2.31444	4.32916	3.175*	26.670
HEU	2.01472	2.31444	3.175*	26.670
Lower Graphite	0.0	2.01742	3.175*	26.670

*Bottom 4 Units only

Table VII. Dimensions for central column in benchmark model

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Outer Radius (cm)
Unit 9	75.02544	79.35460	—	26.6700
Unit 8	70.69628	75.02544	—	26.6700
Unit 7	66.36712	70.69628	—	26.6700
Unit 6	62.03796	66.36712	—	26.6700
Unit 5	57.70880	62.03796	—	26.6700
Unit 4	53.37964	57.70880	3.1750	26.6700
Unit 3	49.05048	53.37964	3.1750	26.6700
Unit 2	44.72132	49.05048	3.1750	26.6700
Unit 1	40.39216	44.72132	3.1750	26.6700
Bottom Reflector	25.96496	40.39216	3.1750	26.6700
Platen	22.15496	25.96496	—	26.6700
Alignment Tube	-5.79120	57.70880	—	26.6700

It was also found that ENDF/B-VI.4 produces a smaller capture fraction and a correspondingly larger leakage fraction than ENDF/B-V. This pattern occurs primarily because copper captures fewer neutrons with ENDF/B-VI.4, although the capture fraction for ^{235}U also is smaller than that with ENDF/B-V.

Table VIII. Dimensions for inner, outer and top reflectors in benchmark model

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	79.3546	26.7970	—	55.8800
Top Reflector	79.3546	93.7818	—	—	55.8800

Table IX. Comparisons of MCNP4C2 results for detailed and benchmark models

Library	k_{eff}		
	Detailed Model	**Benchmark Model**	**Δk**
ENDF/B-V	0.9989 ± 0.0003	1.0004 ± 0.0003	0.0015 ± 0.0004
ENDF/B-VI.4	1.0006 ± 0.0003	1.0016 ± 0.0003	0.0010 ± 0.0004

Table X. Summary of Zeus experiments

Experiment	HEU Platters*	Graphite Platters	Critical Mass (kg U)	$C:^{235}U$
1	10	79.5**	125.6	52 : 1
2	9	54	112.8	40 : 1
3	9	36	106.6	26 : 1

*HEU platters contain both an inner disk and an outer ring, except for the lowermost platter in the third experiment, which was only an inner disk

**Core contained 79 full-height graphite platters, as well as a half-height graphite platter and a very thin stainless-steel platter that acted as a shim

Table XI. k_{eff} for Zeus experiments

Experiment	Measured k_{eff}	Calculated k_{eff} ENDF/B-V	ENDF/B-VI.4
1	1.0001 ± 0.0007	0.9989 ± 0.0003	0.9967 ± 0.0003
2	1.0003 ± 0.0007	0.9986 ± 0.0003	0.9987 ± 0.0003
3	1.0002 ± 0.0008	0.9989 ± 0.0003	1.0006± 0.0003

Table XII. Bias for Zeus experiments

Experiment	Measured k_{eff}	Δ k_{eff}, Calculated - Measured ENDF/B-V	ENDF/B-VI.4
1	1.0001 ± 0.0007	-0.0012 ± 0.0008	-0.0034 ± 0.0008
2	1.0003 ± 0.0007	-00017 ± 0.0008	-0.0016 ± 0.0008
3	1.0002 ± 0.0008	-0.0013 ± 0.0009	0.0004 ± 0.0009

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Table XIII. Calculated neutron balance for the three Zeus experiments

Experiment	Mechanism	ENDF/B-V	ENDF/B-VI.4
1	**Fission**	40.4%	40.4%
	Capture	37.6%	34.5%
	Leakage	22.0%	25.1%
2	**Fission**	40.2%	40.3%
	Capture	36.3%	32.9%
	Leakage	23.5%	26.8%
3	**Fission**	40.2%	40.3%
	Capture	34.7%	31.4%
	Leakage	25.1%	28.3%

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