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ANALYSIS OF THE FOURTH ZEUS CRITICAL EXPERIMENT WITH MCNP5™

Russell D. Mosteller,* Peter J. Jaegers,† and Roger W. Brewer‡
Los Alamos National Laboratory
P. O. Box 1663, Los Alamos, NM 87545
*mosteller@lanl.gov, †pjaegers@lanl.gov, ‡rbrewer@lanl.gov

ABSTRACT

The first set of Zeus critical experiments was designed to test the adequacy of ^{235}U cross sections in the intermediate-energy range. Detailed descriptions of the first three Zeus experiments and the development of benchmark models for them have been described previously. This study focuses primarily on the fourth benchmark in the series, which has a harder spectrum than any of its predecessors. A detailed model of the experiment is developed using the MCNP5 Monte Carlo code, and calculated results for it are presented. A series of modeling simplifications then is described that transforms that detailed representation into a benchmark configuration, and the reactivity impact of each of those simplifications is assessed. Finally, calculated results for this experiment are compared with those from its three predecessors. It is shown that ENDF/B-V nuclear data produce a small but essentially constant bias in k_{eff} for the four experiments, while ENDF/B-VI and preliminary ENDF/B-VII data produce an energy-dependent bias that becomes increasingly positive as the spectrum hardens.

Key Words: Zeus, critical experiment, benchmark, MCNP5

1 INTRODUCTION

The first series of Zeus critical experiments [1,2,3] was designed to test the adequacy of ^{235}U cross sections in the intermediate-energy range. The series included four experiments, the last of which is the principal focus of this study. The fourth Zeus experiment achieved initial criticality on November 15, 2001. It had a critical mass of 106.8 kg of highly enriched uranium (HEU), and its atom ratio of carbon to ^{235}U was approximately 13.6 : 1.

Like its three predecessors, the fourth Zeus critical experiment contained thin, circular platters of HEU separated by thicker platters of graphite. All of the graphite platters and all but one of the HEU pieces had been used in one or more of the previous 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 outer surface. Heavy copper "logs" then were stacked against the outer sides of the corner reflectors to form the side reflector. A cylinder of copper provided reflection at the bottom of the core, and a square parallelepiped of copper rested on top of the corner reflectors, slightly above the topmost graphite platter.

All four Zeus experiments were carried out on the Comet vertical assembly machine at the Los Alamos Critical Experiments Facility. 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 corner reflectors to support the upper portion of the core. The bottom portion of the core rested

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MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory on the bottom reflector, which in turn was supported by the platen and platen adapter plate at the top of the machine's vertical drive. 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.

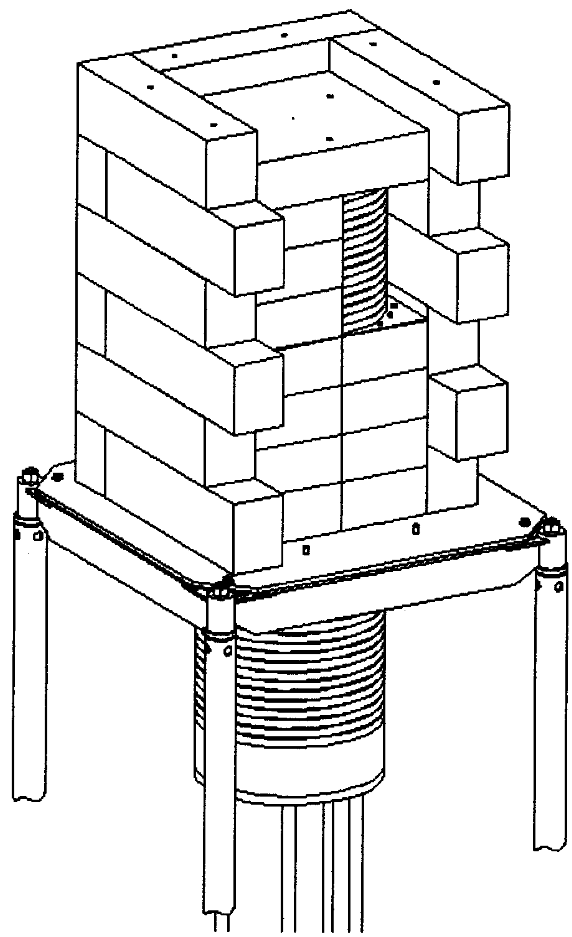


Figure 1. Schematic of a Zeus experiment on the Comet vertical assembly machine.

2 THE FOURTH ZEUS CRITICAL EXPERIMENT

The core of the fourth Zeus experiment contained nine platters of highly enriched uranium (HEU) and 18 graphite platters. The platters were arranged in a repeating pattern of "units," in which each unit contained an HEU platter sandwiched between two graphite platters. The graphite platters are circular, with an outer radius of 10.5 inches (26.67 cm) and an average thickness only very slightly more than 1 cm. The HEU platters also are circular, and eight of them have two components, an inner disk with an outer radius of 7.5 inches (19.05 cm) and a tightly fitting outer ring with an outer radius of 10.5 inches (26.67 cm). However, the bottom

HEU platter contains only an inner disk with no outer ring. The HEU platters are 0.118 inch (0.29972 cm) thick.

For the fourth Zeus experiment, there were three units in the bottom portion of the core (i.e., below the diaphragm) and six units in the upper portion. The HEU and graphite platters in the bottom portion have a small central cavity with radii of 1.255 inch (3.1877 cm) and 1.25 inch (3.175 cm), respectively, through which an aluminum alignment tube was placed. The two uppermost HEU platters in the upper portion of the core also have that cavity, because only four solid HEU inner disks were available for the experiments. A vertical slice through the center of the fourth Zeus experiment is shown in Fig. 2.

This configuration was slightly supercritical, with a period of 17.328 seconds. Based upon an assumed value of 0.0065 for β_{eff}, this period corresponds to a condition that is 29.8¢ supercritical and to a value for k_{eff} that is very slightly above 1.0019.

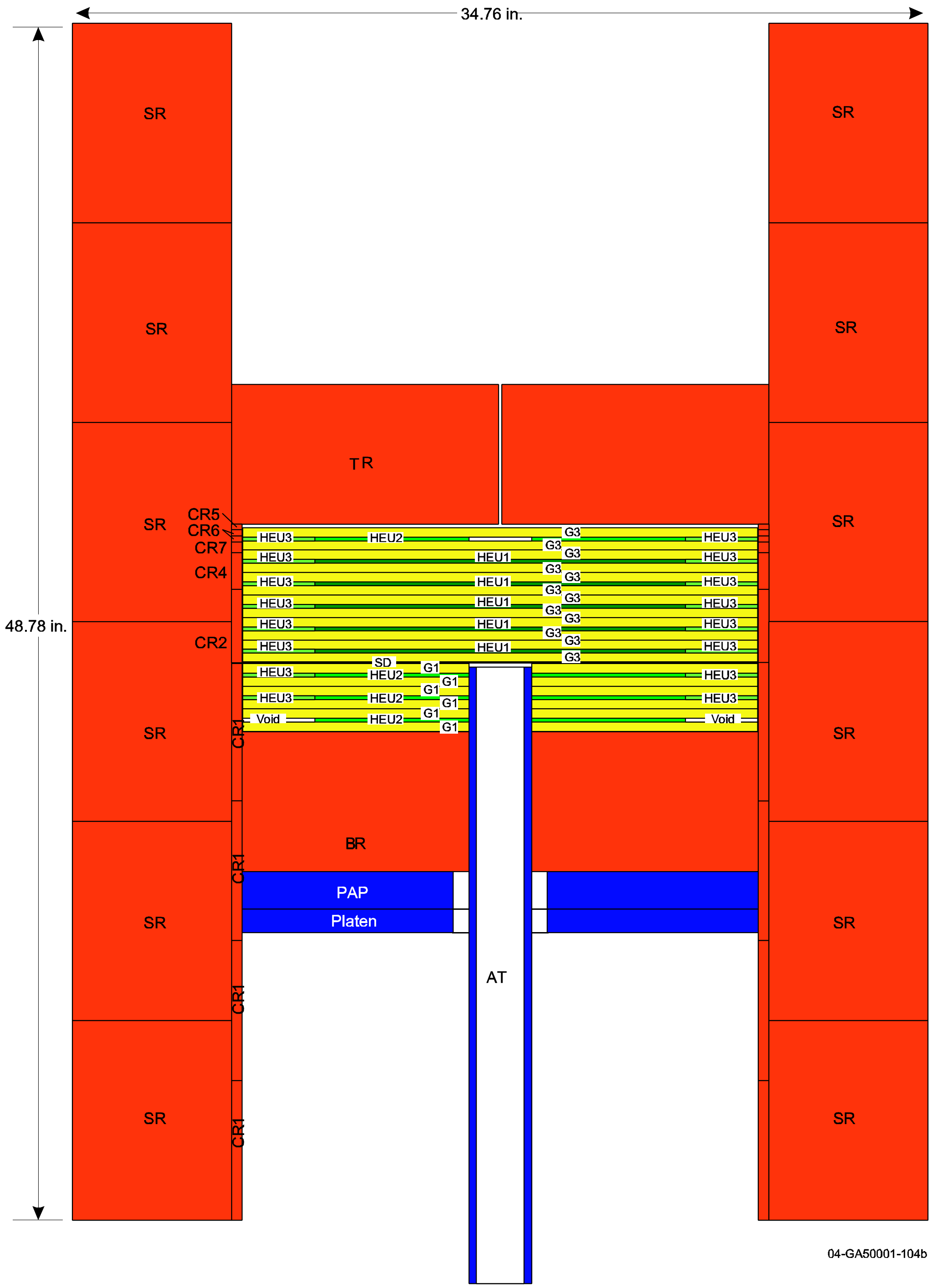
The uncertainties associated with the experiment are summarized in Table I, along with the resulting uncertainties in reactivity. The uncertainties associated with the enrichment of the HEU platters, their dimensions, and the measured period were determined to have negligible impact on reactivity, and consequently they are omitted from Table I. The experimental uncertainties produce a cumulative uncertainty of $\pm$ 0.0007 Δk in reactivity. Consequently, the experimental value for k_{eff} for the fourth Zeus experiment is 1.0019 $\pm$ 0.0007.

3 ANALYSIS OF THE EXPERIMENT

A detailed model of the fourth Zeus experiment was developed for the MCNP5 Monte Carlo code [4]. 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 of 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 individual reflector piece, and the platen, platen adapter plate, and platform of the Comet assembly machine.

The MCNP5 calculations were performed with four different continuous-energy nuclear data libraries based on ENDF/B-V, ENDF/B-VI interim release 4 (ENDF/B-VI.4), the final release of ENDF/B-VI (ENDF/B-VI.8), and a preliminary version of the initial release of ENDF/B-VII. The ENDF/B-VI.4 calculations employed a combination of the URES [5] and ENDF60 [6] libraries, while the ENDF/B-VI.8 calculations employed a combination of the ENDF66 [7] and ACTI [8] libraries. The ENDF/B-VII calculations employed data for uranium isotopes from the T16_2003 library [9,10] in conjunction with new resonance parameters [11] for ^{235}U and ^{238}U but retained ENDF66 or ACTI data for all other isotopes. Calculations to assess the reactivity worth of experimental uncertainties were performed with ENDF/B-VI.4 data to maintain consistency with corresponding calculations for the other three Zeus configurations.

Each of the MCNP5 calculations discussed herein employed 650 generations with 10,000 neutron 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 II, and the corresponding fission fractions are shown in Table III. The ENDF/B-VI and ENDF/B-VII results indicate that the fissions are split almost evenly between



AT	=	Alignment Tube	BR	=	Bottom Reflector
CR	=	Corner reflector	G	=	Graphite platter
HEU	=	HEU platter	PAP	=	Platen adapter plate
SD	=	Steel diaphragm	SR	=	Side reflector
TR	=	Top reflector			

Figure 2. Vertical slice through the fourth Zeus experiment.

Table I. Experimental uncertainties for the fourth Zeus experiment

Source	Uncertainty	Δk
HEU Mass	0.021 %	± 0.0001
Graphite Mass	0.035 %	± 0.0001
Copper Mass	0.4 %	± 0.0006
Graphite Thickness	± 0.0034 in	± 0.0002

the fast and intermediate regions (above and below 100 keV, respectively). This behavior clearly demonstrates that the fourth Zeus experiment has met its design objective by producing a soft-fast / hard-intermediate spectrum.

Table II. k_{eff} for the fourth Zeus experiment

Measured	ENDF/B-VII	ENDF/B-VI.8	ENDF/B-VI.4	ENDF/B-V
1.0019 ± 0.0008	1.0085 ± 0.0003	1.0053 ± 0.0003	1.0067 ± 0.0003	1.0009 ± 0.0003

Table III. Calculated fission fractions for the fourth Zeus experiment

Mesh	ENDF/B-VII	ENDF/B-VI.8	ENDF/B-VI.4	ENDF/B-V
Fast	0.5037	0.5041	0.5043	0.5220
Intermediate	0.4963	0.4959	0.4967	0.4780
Thermal	0.0	0.0	0.0	0.0

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 introduced 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 MCNP5 calculations for each of the simplifications were performed sequentially, so that each new simplification 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 were performed with ENDF/B-VI.4 data to maintain consistency with the corresponding calculations for the previous three Zeus configurations. Furthermore, as Tables II and III demonstrate, the reactivity and spectrum produced by ENDF/B-VI.4 are very similar to those from ENDF/B-VI.8, the final release of ENDF/B-VI.

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 IV, these modifications produce only small changes in k_{eff}.

Table IV. Reactivity effect of geometry simplifications

Change	Δk	
	Incremental	**Cumulative**
Same thickness for all graphite platters	0.0 ± 0.0004	0.0 ± 0.0004
Remove Comet platform	0.0006 ± 0.0004	0.0006 ± 0.0004
Remove diaphragm	0.0011 ± 0.0004	0.0017 ± 0.0004
Change inner radius of HEU disks to 1.25 inches	0.0001 ± 0.0004	0.0018 ± 0.0004
Fill holes in top HEU plates	0.0 ± 0.0004	0.0018 ± 0.0004
Fill hole in top reflector	0.0001 ± 0.0004	0.0019 ± 0.0004
Remove gap above alignment tube	-0.0008 ± 0.0004	0.0011 ± 0.0004

The possibility of removing the platen, platen adapter plate, and alignment tube also was investigated. However, their removal was found to produce a reactivity change of -0.0075 ± 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, platen, and platen adapter plate partially offset this effect by reflecting some of the neutrons that would otherwise escape from the system.

4.2 Material Simplifications

Material simplifications include the removal of minor impurities from all compositions, the replacement of individual platters by platters with a single, average density and composition, and the homogenization of the copper reflector pieces so that they all have the same density. The reactivity effects of those changes are shown in Table V.

4.3 Summary of Benchmark Specifications

These simplifications produce a core with platters of uranium and graphite that have uniform compositions, densities, and dimensions. Reactivity comparisons for the detailed and benchmark models are shown in Table VI, and a more comprehensive comparison based on ENDF/B-VI.4 results is given in Table VII. All four libraries produce reactivity differences

Table V. Reactivity effect of material simplifications

Change	Δk Incremental	Δk Cumulative
Change density of all graphite platters to average	0.0002 ± 0.0004	0.0002 ± 0.0004
Remove impurities from copper pieces	0.0 ± 0.0004	0.0002 ± 0.0004
Change density of all copper pieces to average	-0.0011 ± 0.0004	-0.0009 ± 0.0004
Remove impurites from fuel	0.0002 ± 0.0004	-0.0007 ± 0.0004
Change density and enrichment of all HEU platters to average	-0.0002 ± 0.0004	-0.0009 ± 0.0004

between the benchmark and detailed models that are statistically consistent with impact of the simplifications shown in Tables IV and V (i.e., a net difference of 0.0002 ± 0.0004 Δk). Based on the experimental value for k_{eff} and the ENDF/B-VI.4 bias in Table VI, the value for k_{eff} for the benchmark model is 1.0016 ± 0.0008. A complete set of benchmark specifications is provided in the Appendix.

Table VI. Calculated values of k_{eff} for the fourth Zeus experiment

Model	ENDF/B-VII	ENDF/B-VI.8	ENDF/B-VI.4	ENDF/B-V
Detailed	1.0085 ± 0.0003	1.0053 ± 0.0003	1.0067 ± 0.0003	1.0009 ± 0.0003
Benchmark	1.0085 ± 0.0003	1.0049 ± 0.0003	1.0064 ± 0.0003	1.0009 ± 0.0003
Difference	0.0 ± 0.0004	-0.0004 ± 0.0004	-0.0003 ± 0.0004	0.0 ± 0.0004

5 COMPARISONS WITH ANALYSES OF PREVIOUS ZEUS EXPERIMENTS

All four 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 fourth Zeus experiment reached initial criticality on November 15, 2001. The same side-reflector logs were used in all four experiments, and many of the corner reflectors were the same as well. The differences among the four cores are summarized in Table VIII. The successive decreases in the C : ^{235}U atom ratio, which were achieved principally 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 four Zeus experiments are shown in Table IX, and the differences between the measured and calculated values are plotted in Fig. 3. As Fig. 3 clearly illustrates, ENDF/B-V produces a small, essentially constant bias relative to the experimental values of k_{eff}. In contrast, the ENDF/B-VI and preliminary ENDF/B-VII data produce biases that become increasingly positive as the spectra harden. Furthermore, the swing in those biases, from most negative to most positive, is quite sizeable, approaching or even

Table VII. Comparison of results from detailed and benchmark models

Parameter		Model: Detailed	Model: Benchmark
k_{eff}		1.0067 ± 0.0003	1.0064 ± 0.0003
Fission Distribution, by Energy	Fast	0.5041	0.5061
	Intermediate	0.4959	0.4939
	Thermal	0	0
Fission Distribution, by Isotope	^{234}U	0.0037	0.0038
	^{235}U	0.9924	0.9923
	^{236}U	0.0004	0.0004
	^{238}U	0.0035	0.0035
Average Number of Neutrons Produced per Fission		2.495	2.495

Table VIII. Summary of Zeus experiments

Experiment	HEU Platters	Graphite Platters	Critical Mass (kg U)	C : ^{235}U (atom ratio)
1	10	79.5†	126.5	51.2 : 1
2	9	54	112.8	38.6 : 1
3	9*	36	106.6	27.4 : 1
4	9*	18	106.8	13.6 : 1

* Bottom platter had outer diameter of 15 inches rather than 21 inches

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

exceeding 0.01 Δk. This behavior suggests an energy-dependent bias in the ENDF/B-VI and preliminary ENDF/B-VII data in the upper portion of the intermediate energy range.

Table IX. k_{eff} for the Zeus experiments

No	Measured	ENDF/B-VII	ENDF/B-VI.8	ENDF/B-VI.4	ENDF/B-V
1	1.0001 ± 0.0007	0.9948 ± 0.0003	0.9941 ± 0.0003	0.9968 ± 0.0003	0.9989 ± 0.0003
2	1.0003 ± 0.0007	0.9953 ± 0.0003	0.9949 ± 0.0003	0.9987 ± 0.0003	0.9986± 0.0003
3	1.0002 ± 0.0008	0.9977 ± 0.0003	0.9981 ± 0.0003	1.0006 ± 0.0003	0.9989 ± 0.0003
4	1.0019 ± 0.0007	1.0085 ± 0.0003	1.0053 ± 0.0003	1.0067 ± 0.0003	1.0009 ± 0.0003

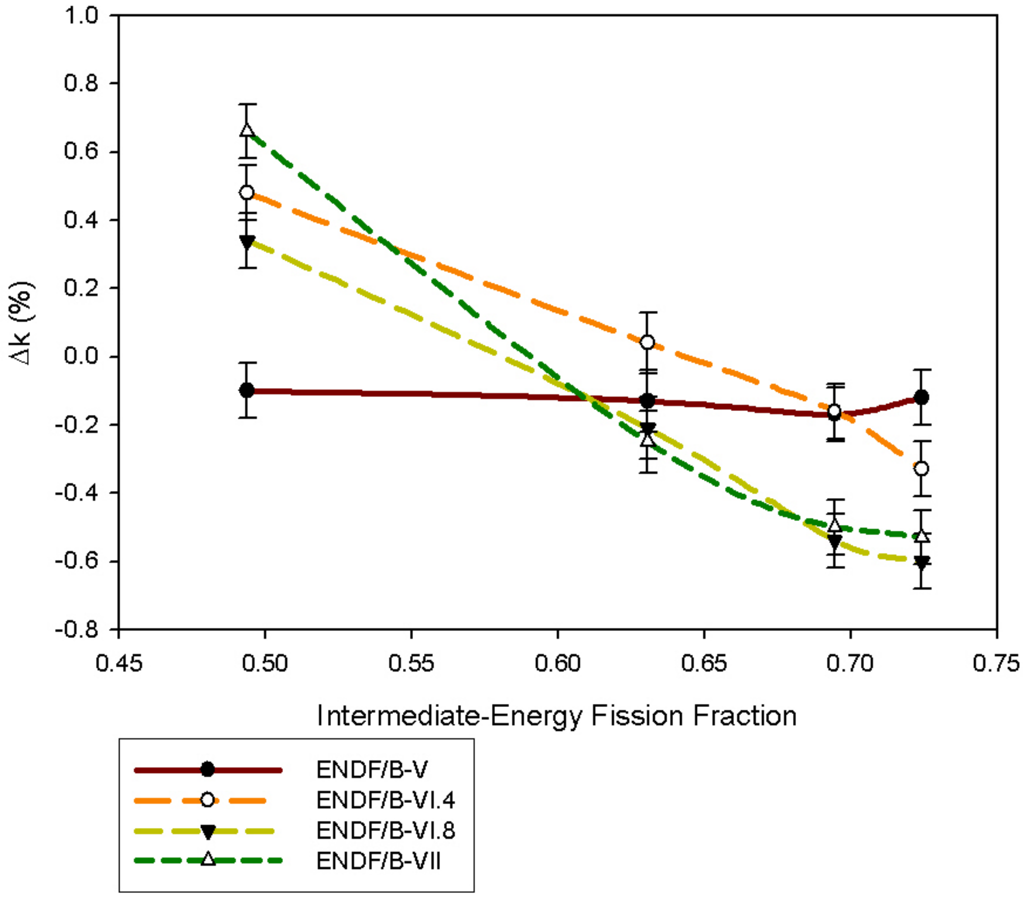


Figure 3. Reactivity biases for the Zeus experiments.

6 CONCLUSIONS

The results for the fourth Zeus experiment clearly indicate that it achieved its design objective by producing a soft-fast / hard-intermediate energy spectrum. Although calculations with nuclear data based on ENDF/B-V produce good agreement with measurement, calculations with nuclear data based on ENDF/B-VI and preliminary ENDF/B-VII nuclear data overestimate k_{eff} by approximately 0.0035 to 0.0065 Δk.

A benchmark model for the fourth Zeus experiment has been constructed that preserves all of its important neutronic behavior while simplifying both its geometry and material compositions. The overall reactivity difference between a very detailed model and the benchmark model has been shown to be negligible. A complete set of specifications for the benchmark model is provided in the Appendix.

Comparisons of the results for the fourth Zeus experiment and those from its predecessors produce consistent trends. Calculations based on ENDF/B-V nuclear data produce a small, essentially constant bias relative to the experimental values of k_{eff}. In contrast, calculations that employ ENDF/B-VI and preliminary ENDF/B-VII data produce biases that become increasingly positive as the spectra harden. Furthermore, the swing in those biases, from most negative to most positive, is quite sizeable, approaching or even exceeding 0.01 Δk. This behavior suggests an energy-dependent bias in the ENDF/B-VI and preliminary ENDF/B-VII data in the upper portion of the intermediate energy range.

7 ACKNOWLEDGMENTS

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APPENDIX
BENCHMARK SPECIFICATIONS FOR THE FOURTH ZEUS EXPERIMENT

A vertical slice through the center of the benchmark configuration is presented in Fig. A-1. Detailed specifications for the benchmark geometry are given in Tables A-I through A-III, and the material specifications are shown in Table A-IV.

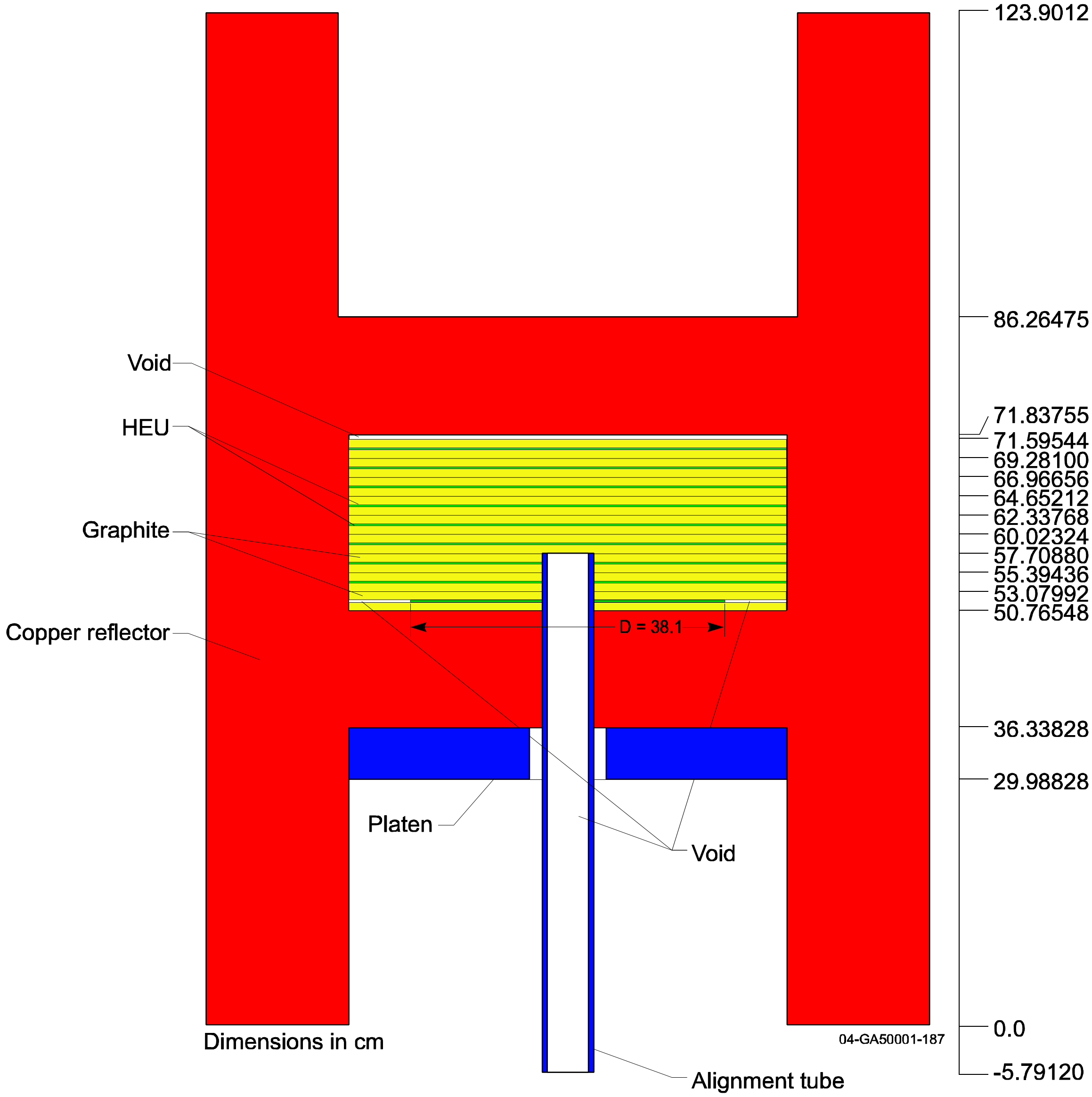

Figure A-1. Vertical dimensions for the benchmark model of the fourth Zeus experiment.

Table A-I. Dimensions for various reflector regions in benchmark model

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Inner Width Side to Side (cm)	Outer Width Side to Side (cm)
Outer reflector	0.0	123.90120	—	55.88	88.2904
Inner reflector	0.0	71.83755	26.797	—	55.88
Upper reflector	71.83755	86.26475	—	—	55.88

Table A-II. Dimensions for HEU/graphite unit in benchmark model

Region	Bottom (cm)	Top (cm)	Inner Radius* (cm)	Outer Radius (cm)
Upper graphite	1.30708	2.31444	3.175	26.67
HEU	1.00736	1.30708	3.175	26.67†
Lower graphite	0.0	1.00736	3.175	26.67

* Bottom three units only

† Outer radius of bottom HEU platter is 19.05 cm

Table A-III. Dimensions for central column in benchmark model

Region	Bottom (cm)	Top (cm)	Inner Radius (cm)	Outer Radius (cm)
Unit 9	69.28100	71.59544	—	26.67
Unit 8	66.96656	69.28100	—	26.67
Unit 7	64.65212	66.96656	—	26.67
Unit 6	62.33768	64.65212	—	26.67
Unit 5	60.02324	62.33768	—	26.67
Unit 4	58.70880	60.02324	—	26.67
Unit 3	55.39436	57.70880	3.175	26.67
Unit 2	53.07992	55.39436	3.175	26.67
Unit 1	50.76548	53.07992	3.175	26.67
Bottom reflector	36.33828	50.76548	3.175	26.67
Platen	29.98828	36.33828	4.7625	26.67
Alignment tube	-5.79120	57.70880	2.54	3.1496

Table A-IV. Material specifications for benchmark model

Material	Density (g/cm^3)	Component	wt.%
Al 6061*	2.6657	Al	97.175
		Mg	1.000
		Si	0.600
		Fe	0.350
		Cu	0.275
		Cr	0.250
		Zn	0.125
		Ti	0.075
		Mn	0.075
Copper	8.7351	Cu	100.000
Graphite	1.7263	C	100.000
HEU	18.8170	^{234}U	1.024
		^{235}U	93.234
		^{236}U	0.326
		^{238}U	5.416

* 0.075 wt.% of other components is ignored