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#### Comparison of ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNP Criticality Validation Suite

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#### To Be Presented at the 2004 Annual Meeting of the American Nuclear Society Pittsburgh, PA June 13 - 17, 2004

An initial assessment of the reactivity impact of preliminary data proposed for ENDF/B-VII has been made using the MCNP criticality validation suite. Relative to ENDF/B-VI, the data changes primarily involve high-energy elastic and inelastic scattering in the uranium isotopes and <sup>239</sup>Pu, as well as resonance parameters for <sup>238</sup>U.

Three sets of calculations were performed for the MCNP Criticality Validation Suite using the MCNP5 Monte Carlo code. The first set employed nuclear data from ENDF/B-VI Release 8, the final release for ENDF/B-VI. The second set employed preliminary ENDF/B-VII data generated by group T-16 at Los Alamos National Laboratory for the uranium isotopes and for <sup>239</sup>Pu but retained ENDF/B-VI data for all other nuclides. The third set was the same as the second except that a new set of <sup>238</sup>U resonance parameters<sup>3</sup> generated by researchers at Oak Ridge National Laboratory (ORNL) was used in combination with the T-16 evaluation.

The preliminary ENDF/B-VII data for the uranium isotopes and <sup>239</sup>Pu produce improvements for most of the cases with fast spectra and for most of the thermal lattices and solutions. However, improvements still are needed in some areas, particularly for those cases with intermediate spectra.

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Comparison of ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNP Criticality Validation Suite

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## **OVERVIEW OF PRESENTATION**

Succinct Description of MCNP Criticality Validation Suite

Characteristics of Preliminary Nuclear Data for ENDF/B-VI

Comparison of Results from MCNP5 Using Final ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data Libraries

Conclusions



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## **MCNP Criticality Validation Suite**

Cases were selected to encompass a wide variety of

Fissile isotopes :		<sup>233</sup> U, <sup>235</sup> U, and <sup>239</sup> Pu
Spectra :	:	Fast, intermediate, and thermal
Compositions :	:	Metals, oxides, and solutions
Configurations :	:	Bare and reflected spheres and cylinders, 2-D and 3-D lattices, and infinite homogeneous and heterogeneous regions

<sup>235</sup>U Cases were subdivided into HEU, IEU, AND LEU

Input specifications for all 31 cases are taken from the International Handbook of Evaluated Criticality Safety Benchmark Experiments



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## CASES IN THE MCNP CRITICALITY VALIDATION SUITE

Spectrum	Fast			Intermed	The	rmal
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins	Solution
<sup>233</sup> U	Jezebel-233	Flattop-23	U233-MF-05	Falstaff-1*	SB-21/2	ORNL-11
HEU	Godiva Tinkertoy-2	Flattop-25	Godiver	Zeus-2 $UH_3$	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H <sup>†</sup>	IEU-CT-02	STACY-36
LEU					B&W XI-2	LEU-ST-02
Pu	Jezebel Jezebel-240 Pu Buttons	Flattop-Pu THOR	Pu-MF-11	HISS/HPG <sup>†</sup>	PNL-33	PNL-2

\* Extrapolated to critical

 $^{\dagger}$  k<sub> $\infty$ </sub> measurement





# PURPOSE AND USE OF THE MCNP CRITICALITY VALIDATION SUITE

The MCNP Criticality Validation Suite was developed to assess the reactivity impact of future improvements to MCNP as well as changes to its associated nuclear data libraries

Suite is *not* an absolute indicator of the accuracy or reliability of a given nuclear data library, nor is it intended to be

Suite can provide a general indication of the overall performance of a nuclear data library

Suite can provide an early warning of unexpected or unintended consequences resulting from changes to nuclear data



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## PRELIMINARY NUCLEAR DATA FOR ENDF/B-VII

Final version of ENDF/B-VI (Release 8) was released in October 2001

Are future nuclear data libraries likely to produce improved results?

Preliminary changes to <sup>233</sup>U, <sup>235</sup>U, <sup>238</sup>U, and <sup>239</sup>Pu for ENDF/B-VII offer encouragement

Data changes primarily involve high-energy elastic and inelastic scattering in the uranium isotopes and <sup>239</sup>Pu (LANL group T-16), as well as resonance parameters for <sup>238</sup>U (ORNL)



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# MCNP5 CALCULATIONS FOR CRITICALITY VALIDATION SUITE

Each calculation employed 550 generations with 10,000 neutrons per generation (SB-5 and Zebra-8H employed 350 generations)

Results from first 50 generations were excluded from the statistics

Results therefore are based on 5,000,000 active histories for each case (3,000,000 for SB-5 and Zebra-8H)



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# **RESULTS FOR <sup>233</sup>U BENCHMARKS**

	Benchmark	Calculated k <sub>eff</sub>		
Case	k <sub>eff</sub>	ENDF/B-VII	ENDF/B-VI	
Jezebel-233	1.0000 ± 0.0010	0.9984 ± 0.0003	0.9931 ± 0.0003	
Flattop-23	1.0000 ± 0.0014	0.9988 ± 0.0003	1.0003 ± 0.0003	
U233-MF-05	1.0000 ± 0.0030	0.9964 ± 0.0003	0.9976 ± 0.0003	
Falstaff-1	1.0000 ± 0.0083	0.9876 ± 0.0005	0.9894 ± 0.0005	
SB-21/2	1.0000 ± 0.0024	0.9946 ± 0.0005	0.9967 ± 0.0005	
ORNL-11	1.0006 ± 0.0029	1.0002 ± 0.0002	0.9968 ± 0.0002	

 $|\Delta \mathbf{k}| \leq \sigma$ 

 $\sigma < |\Delta \mathbf{k}| \le 2\sigma$ 

 $k_{eff}$  for Jezebel-233 improves dramatically, and reactivity swing from Jezebel-233 to Flattop-23 is eliminated

 $k_{\text{eff}}$  for ORNL-11 improves substantially, although results deteriorate for U233-MF-05 and SB-21/2





### **RESULTS FOR HEU BENCHMARKS**

· · · · · · · ·	Benchmark	Calculated k <sub>eff</sub>		
Case	k <sub>eff</sub>	ENDF/B-VII	ENDF/B-VI	
Godiva	1.0000 ± 0.0010	0.9992 ± 0.0003	0.9962 ± 0.0003	
Tinkertoy-2	1.0000 ± 0.0038	1.0001 ± 0.0003	0.9972 ± 0.0003	
Flattop-25	1.0000 ± 0.0030	1.0025 ± 0.0003	1.0024 ± 0.0003	
Godiver	0.9985 ± 0.0011	0.9978 ± 0.0004	0.9948 ± 0.0003	
UH <sub>3</sub>	1.0000 ± 0.0047	0.9926 ± 0.0003	0.9914 ± 0.0003	
Zeus-2	0.9997 ± 0.0008	0.9948 ± 0.0003	0.9942 ± 0.0003	
SB-5	1.0015 ± 0.0028	0.9943 ± 0.0005	0.9963 ± 0.0005	
ORNL-10	1.0015 ± 0.0026	0.9994 ± 0.0002	0.9992 ± 0.0002	

 $k_{\mbox{\tiny eff}}$  improves substantially for Godiva and Godiver but deteriorates for SB-5

Reactivity swing from Godiva to Flattop-25 is reduced significantly



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### **RESULTS FOR IEU BENCHMARKS**

	Benchmark	Calculated k <sub>eff</sub>	
Case	k <sub>eff</sub>	ENDF/B-VII	ENDF/B-VI
IEU-MF-03	1.0000 ± 0.0017	1.0026 ± 0.0003	0.9987 ± 0.0003
BIG TEN	0.9948 ± 0.0013	0.9950 ± 0.0003	1.0071 ± 0.0002
IEU-MF-04	1.0000 ± 0.0030	1.0077 ± 0.0003	1.0038 ± 0.0003
Zebra-8H	1.0300 ± 0.0025	1.0190 ± 0.0002	1.0405 ± 0.0002
IEU-CT-02	1.0017 ± 0.0044	1.0005 ± 0.0003	1.0007 ± 0.0003
STACY-36	0.9988 ± 0.0013	0.9983 ± 0.0003	0.9988 ± 0.0003

k<sub>eff</sub> improves dramatically for BIG TEN

 $k_{\mbox{\scriptsize eff}}$  is worse for IEU-MF-03 and IEU-MF-04 and drops substantially for Zebra-8H

For IEU-CT-02 and STACY-36, changes to <sup>238</sup>U resonance parameters offset reactivity effects of scattering changes for uranium isotopes





### **RESULTS FOR LEU BENCHMARKS**

	Benchmark	Calculated k <sub>eff</sub>	
Case	k <sub>eff</sub>	ENDF/B-VII	ENDF/B-VI
B&W XI-2	1.0007 ± 0.0012	0.9997 ± 0.0003	0.9968 ± 0.0003
LEU-ST-02	1.0024 ± 0.0037	0.9957 ± 0.0003	0.9957 ± 0.0003

k<sub>eff</sub> improves substantially for B&W XI-2, which eliminates need for *ad hoc* adjustment to <sup>238</sup>U resonance integral (used in many nuclear data libraries since early 1970s)

For LEU-ST-02, changes to <sup>238</sup>U resonance parameters offset reactivity effects of scattering changes for uranium isotopes





## **RESULTS FOR PU BENCHMARKS**

	Benchmark	Calculated k <sub>eff</sub>		
Case	k <sub>eff</sub>	ENDF/B-VII	ENDF/B-VI	
Jezebel	1.0000 ± 0.0020	1.0004 ± 0.0003	$0.9975 \pm 0.0003$	
Jezebel-240	1.0000 ± 0.0020	1.0001 ± 0.0003	0.9979 ± 0.0003	
Pu Buttons	1.0000 ± 0.0030	0.9986 ± 0.0003	0.9962 ± 0.0003	
Flattop-Pu	1.0000 ± 0.0030	1.0006 ± 0.0003	1.0019 ± 0.0003	
THOR	1.0000 ± 0.0006	1.0081 ± 0.0003	1.0062 ± 0.0003	
Pu-MF-11	1.0000 ± 0.0010	0.9986 ± 0.0003	0.9970 ± 0.0003	
HISS/HPG	1.0000 ± 0.0110	1.0111 ± 0.0003	1.0105 ± 0.0003	
PNL-33	1.0024 ± 0.0021	1.0057 ± 0.0003	1.0029 ± 0.0003	
PNL-2	1.0000 ± 0.0065	1.0039 ± 0.0005	1.0033 ± 0.0005	

Striking improvement in  $k_{eff}$  for fast cases except THOR, and reactivity swing from Jezebel to Flattop-Pu is eliminated



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# SUMMARY OF RESULTS FOR MCNP CRITICALITY VALIDATION SUITE

Range	Pre-ENDF/B-	ENDF/B-VI
$ \Delta \mathbf{k}  \leq \sigma$	17	13
$\sigma <  \Delta \mathbf{k}  \le$	8	9
∆k  > 2σ	6	9

Substantial improvements for bare metal spheres (Jezebel-233, Godiva, and Jezebel), BIG TEN, HEU and Pu metal spheres in water (Godiver and Pu-MF-011, respectively), and LEU lattice (B&W XI-2)

ORNL resonance parameters improve results for Godiver, ORNL-10, IEU-CT-03, STACY-36, B&W XI-2, and LEU-ST-02





#### CONCLUSIONS

Overall, Pre-ENDF/B-VII produces major reactivity improvements relative to ENDF/B-VI

Reactivity swings from bare spheres to similar systems reflected by normal uranium are eliminated or substantially reduced

Need for *ad hoc* adjustment to <sup>238</sup>U resonance integral may be eliminated

Improvements still are needed, particularly for cases with intermediate spectra or with thorium



