

LA-UR-10-06917

Approved for public release;  
distribution is unlimited.

|                      |                                                                                                    |
|----------------------|----------------------------------------------------------------------------------------------------|
| <i>Title:</i>        | An Expanded Criticality Validation Suite for MCNP and an Improved Benchmark Model for BIG TEN      |
| <i>Author(s):</i>    | Russell D. Mosteller                                                                               |
| <i>Intended for:</i> | 2010 Meeting of the Cross Section Evaluation Working Group<br>Santa Fe, NM<br>November 1 - 3, 2010 |



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

**An Expanded Criticality Validation Suite for MCNP**  
**and**  
**An Improved Benchmark Model for BIG TEN**

Russell D. Mosteller

Improvised and Foreign Design Group (XTD-4)  
Theoretical Design Division  
Los Alamos National Laboratory

To Be Presented at the 2010 CSEWG Meeting  
Santa Fe, NM                      November 1-3, 2010

An expanded criticality validation suite has been created for the MCNP Monte Carlo code. The suite includes 119 benchmarks taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. There are 119 benchmarks, which are divided into five categories of fuel –  $^{233}\text{U}$ , highly enriched uranium (HEU), intermediate enriched uranium (IEU), low enriched uranium (LEU), and plutonium. The  $^{233}\text{U}$ , HEU, IEU, and plutonium benchmarks are subdivided farther according to spectrum – fast, intermediate, or thermal. Each fast subcategory contains at least one unreflected metal case, one metal case reflected by uranium, one metal case reflected by a heavy reflector, and one metal case reflected by a light reflector. Each thermal subcategory contains at least one solution case and one lattice case. The LEU category contains only thermal cases, since LEU can reach criticality only with a thermal spectrum.

An improved benchmark for the BIG TEN experiment also will be described briefly. BIG TEN contains a cylindrical core enriched to ~ 10 wt.%, surrounded by an annulus of depleted uranium.

# An Expanded Criticality Validation Suite for MCNP and an Improved Benchmark for BIG TEN

Russell D. Mosteller

Improvised and Foreign Design Group (XTD-4)  
Theoretical Design Division  
Los Alamos National Laboratory  
mosteller@lanl.gov

Presented at the 2010 CSEWG Meeting  
Santa Fe, NM                      November 1-3, 2010



EST. 1943  
The World's Greatest Science Protecting America



# Overview of Presentation

Description of the enhanced criticality validation suite for MCNP

Selected results from the expanded suite

Succinct description of an improved benchmark for BIG TEN

# Background

For the past several years, the data team and the MCNP team at LANL have had separate criticality validation suites

The data team's suite includes only fast metal benchmarks and thermal solution benchmarks, most of them taken from CSWEG specifications or the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. It includes related benchmarks so that parameter studies (enrichment, reflector thickness, solution content, etc.) can be performed

The MCNP team's suite includes a wider variety of benchmarks, all taken from the *Handbook*, but it does not permit parameter studies

The objective for the expanded criticality benchmark suite is to consolidate the two suites, eliminate repetition and inconsistencies, and to add benchmarks that fill in gaps in nuclear data that neither suite addresses

# Expanded Criticality Validation Suite for MCNP

| Principal Fuel   | Number of Benchmarks by Spectrum |              |         |       |
|------------------|----------------------------------|--------------|---------|-------|
|                  | Fast                             | Intermediate | Thermal | Total |
| $^{233}\text{U}$ | 10                               | 1            | 7       | 18    |
| HEU              | 29                               | 5            | 6       | 40    |
| IEU              | 10                               | 1            | 6       | 17    |
| LEU              |                                  |              | 8       | 8     |
| Plutonium        | 21                               | 1            | 14      | 36    |
| Total            | 70                               | 8            | 41      | 119   |

All benchmark specifications are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

# Categorizations

## Uranium

|      |                                       |
|------|---------------------------------------|
| HEU: | Enrichment $\geq$ 60 wt.%             |
| IEU: | Enrichment between 5 wt.% and 60 wt.% |
| LEU: | Enrichment $\leq$ 5 wt.%              |

## Spectrum

|               |                                                                                    |
|---------------|------------------------------------------------------------------------------------|
| Fast:         | Majority of fissions caused by neutrons with energies $\geq$ 100 keV               |
| Intermediate: | Majority of fissions caused by neutrons with energies between 0.625 eV and 100 keV |
| Thermal:      | Majority of fissions caused by neutrons with energies $\leq$ 0.625 eV              |

# Overlap with Other Criticality Benchmark Sets

Fast benchmarks include ICSBEP specifications for 9 CSEWG fast benchmarks:

Jezebel, Jezebel-240, Jezebel-233, Godiva, BIG TEN, THOR, Flattop-Pu, Flattop-23, and Flattop-25

Thermal benchmarks include ICSBEP specifications for 19 CSEWG thermal benchmarks:

ORNL-1 through ORNL-4, ORNL-10, PNL-1, PNL-3 through PNL-6, PNL-11, PNL-12, PNL-30 through PNL-35, and HISS/HPG\*

Suite contains 35 benchmarks that were studied by Steven van der Marck in his article, "Benchmarking ENDF/B-VII.0," in the December 2006 issue of *Nuclear Data Sheets*

\* Proposed but not yet accepted; epithermal spectrum



# Fast Benchmarks

| Principal Fuel   | Number of Benchmarks by Reflector |         |       |       |       |
|------------------|-----------------------------------|---------|-------|-------|-------|
|                  | None                              | Uranium | Heavy | Light | Total |
| $^{233}\text{U}$ | 1                                 | 5       | 2     | 2     | 10    |
| HEU              | 4                                 | 9       | 5     | 11    | 29    |
| IEU              | 5                                 | 2       | 2     | 1     | 10    |
| Plutonium        | 4                                 | 5       | 5     | 7     | 21    |
| Total            | 14                                | 21      | 14    | 21    | 70    |

Uranium: HEU, normal uranium, or depleted uranium

Heavy: Aluminum, duralumin, steel, nickel, tungsten, or thorium

Light: Water, polyethylene, paraffin, beryllium, beryllium oxide, graphite, or tungsten carbide

# Thermal Benchmarks

| Principal Fuel   | Number of Benchmarks |          |       |
|------------------|----------------------|----------|-------|
|                  | Lattice              | Solution | Total |
| $^{233}\text{U}$ | 1                    | 6        | 7     |
| HEU              | 1                    | 5        | 6     |
| IEU              | 1                    | 5        | 6     |
| LEU              | 6                    | 2        | 8     |
| Plutonium        | 6                    | 8        | 14    |
| Total            | 15                   | 26       | 41    |

# Results for Metal Spheres Reflected by Tungsten or Tungsten Carbide

| Fuel             | Fuel Radius (cm) | Reflector Thickness (cm) | $k_{\text{eff}}$    |                     |                     |
|------------------|------------------|--------------------------|---------------------|---------------------|---------------------|
|                  |                  |                          | Benchmark           | ENDF/B-VII.0        | ENDF/B-VI           |
| $^{233}\text{U}$ | 5.0444           | 2.4384                   | $1.0000 \pm 0.0007$ | $1.0051 \pm 0.0003$ | $1.0017 \pm 0.0003$ |
| $^{233}\text{U}$ | 4.5999           | 5.7912                   | $1.0000 \pm 0.0008$ | $1.0051 \pm 0.0003$ | $1.0040 \pm 0.0003$ |
| HEU              | 6.6020           | 4.8260*                  | $1.0000 \pm 0.0050$ | $1.0081 \pm 0.0003$ | $1.0048 \pm 0.0003$ |
| HEU              | 6.2527           | 7.3660*                  | $1.0000 \pm 0.0050$ | $1.0095 \pm 0.0003$ | $1.0063 \pm 0.0003$ |
| HEU              | 6.0509           | 11.4300*                 | $1.0000 \pm 0.0050$ | $1.0129 \pm 0.0003$ | $1.0093 \pm 0.0003$ |
| HEU              | 6.0159           | 16.5100*                 | $1.0000 \pm 0.0050$ | $1.0166 \pm 0.0003$ | $1.0136 \pm 0.0003$ |
| Pu               | 5.0419           | 4.6990                   | $1.0000 \pm 0.0013$ | $1.0092 \pm 0.0003$ | $1.0078 \pm 0.0003$ |

\* Tungsten carbide reflector

# Results for Metal Spheres Reflected by Graphite

| Fuel | Fuel Radius (cm) | Reflector Thickness (cm) | $k_{\text{eff}}$    |                     |                     |
|------|------------------|--------------------------|---------------------|---------------------|---------------------|
|      |                  |                          | Benchmark           | ENDF/B-VII.0        | ENDF/B-VI           |
| HEU  | 9.15*            | 3.45                     | $1.0000 \pm 0.0028$ | $1.0074 \pm 0.0003$ | $1.0031 \pm 0.0003$ |
| IEU  | 14.00**          | 3.20                     | $1.0000 \pm 0.0030$ | $1.0075 \pm 0.0003$ | $1.0040 \pm 0.0003$ |
| Pu   | 6.00***          | 5.65                     | $1.0020 \pm 0.0020$ | $0.9993 \pm 0.0003$ | $0.9976 \pm 0.0003$ |

\* Inner radius 4.029 cm

\*\* Inner radius 2.788 cm

\*\*\* Inner radius 1.715 cm

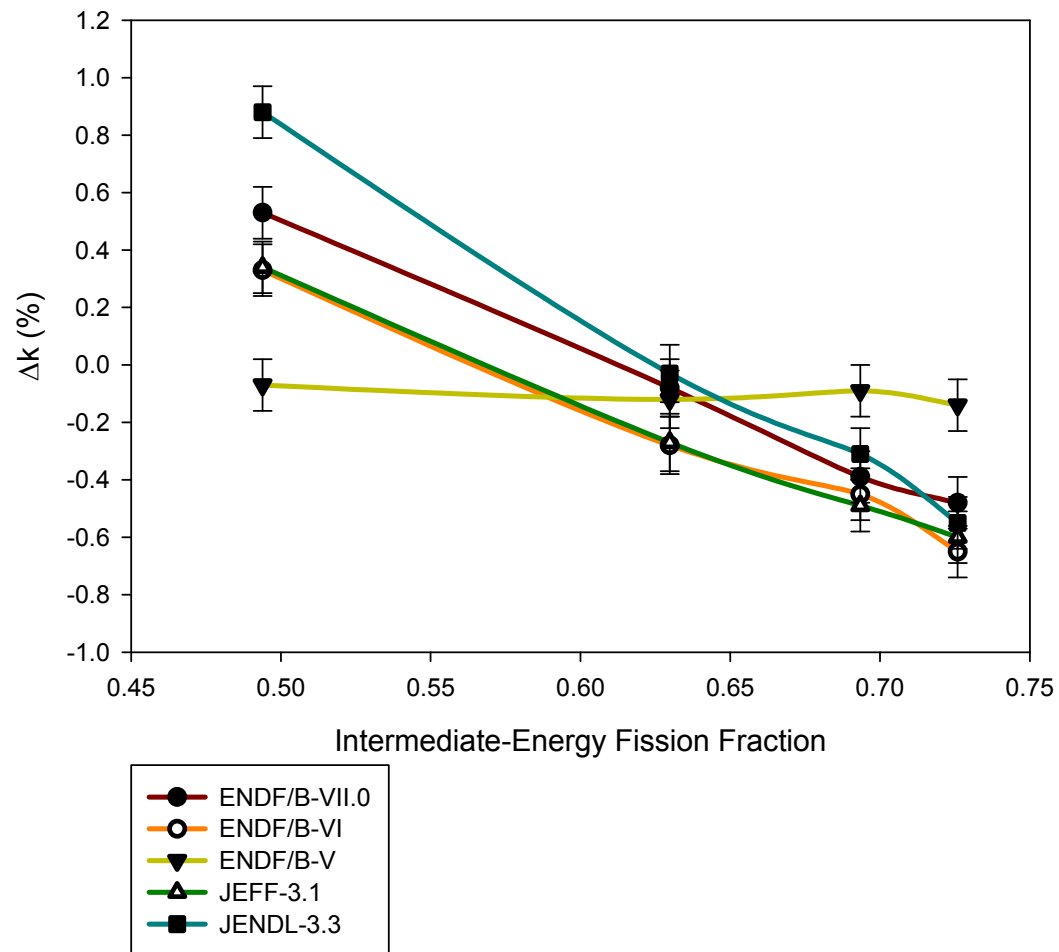
# Results for Metal Spheres Reflected by Beryllium or Beryllium Oxide

| Fuel             | Fuel Radius (cm) | Reflector Thickness (cm) | $k_{\text{eff}}$    |                     |                     |
|------------------|------------------|--------------------------|---------------------|---------------------|---------------------|
|                  |                  |                          | Benchmark           | ENDF/B-VII.0        | ENDF/B-VI           |
| $^{233}\text{U}$ | 5.0444           | 2.0447                   | $1.0000 \pm 0.0030$ | $0.9944 \pm 0.0003$ | $0.9950 \pm 0.0003$ |
| $^{233}\text{U}$ | 4.5999           | 4.1961                   | $1.0000 \pm 0.0030$ | $0.9925 \pm 0.0003$ | $0.9967 \pm 0.0003$ |
| HEU              | 8.3500           | 2.6500                   | $0.9992 \pm 0.0015$ | $0.9957 \pm 0.0003$ | $0.9952 \pm 0.0003$ |
| HEU              | 8.3500*          | 2.6500**                 | $0.9992 \pm 0.0015$ | $0.9955 \pm 0.0003$ | $0.9928 \pm 0.0003$ |
| Pu               | 5.0419           | 3.6881                   | $1.0000 \pm 0.0030$ | $0.9965 \pm 0.0003$ | $0.9990 \pm 0.0003$ |
| Pu               | 5.3500*          | 5.6500                   | $0.9992 \pm 0.0015$ | $0.9975 \pm 0.0003$ | $1.0011 \pm 0.0003$ |

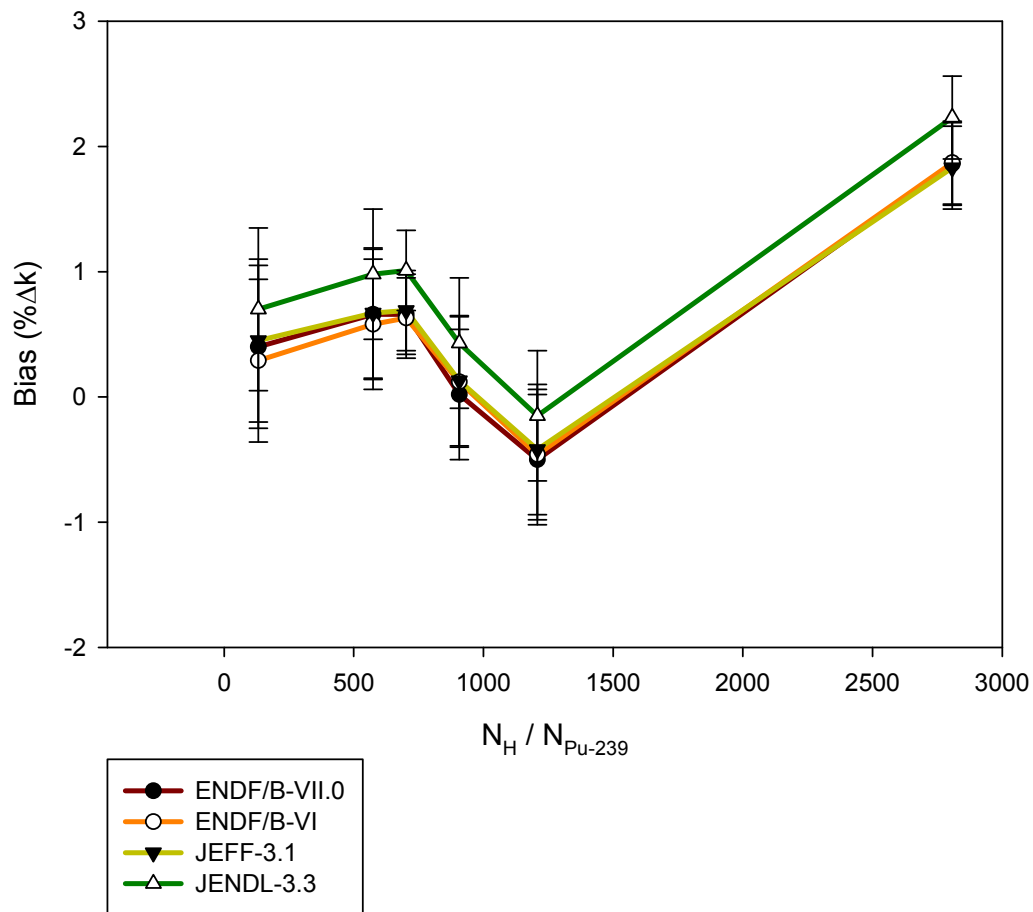
\* Inner radius 1.4 cm

\*\* Beryllium oxide reflector

# Results for the Zeus Graphite Benchmarks



# Reactivity Biases for Plutonium Solution Benchmarks



# BIG TEN Critical Experiment

The BIG TEN critical assembly was constructed and operated at the Los Critical Experiments Facility at LANL in the 1970s

It was designed to allow measurements of nuclear data in a spectrum reasonably representative of a liquid-metal fast breeder reactor

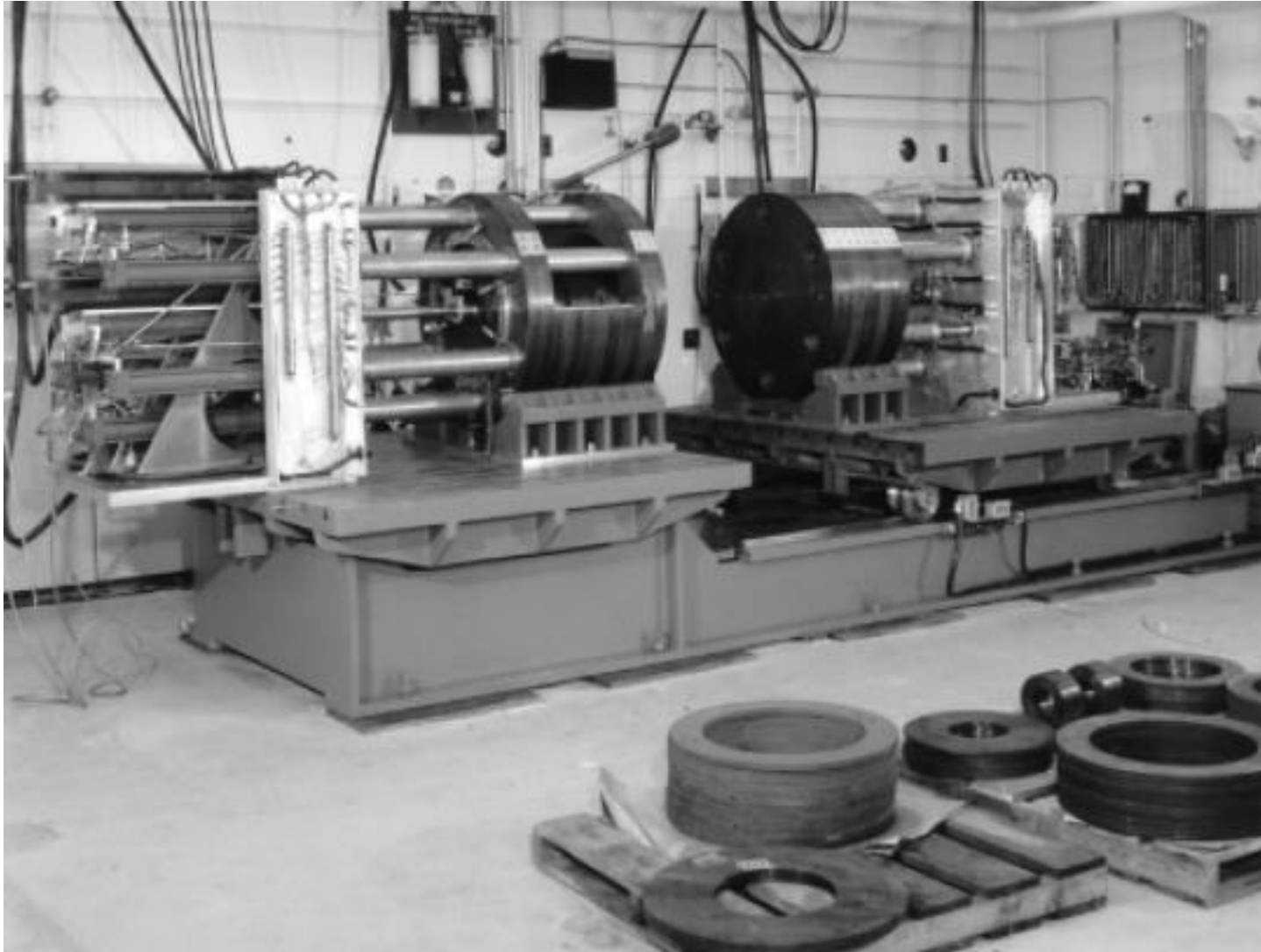
BIG TEN was so named both because it was massive (~ 10 metric tons) and because its core contained an average enrichment of ~ 10 wt.%

BIG TEN was reflected by an annulus of depleted uranium

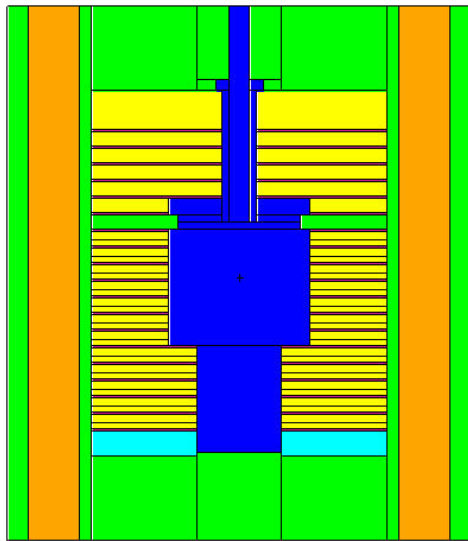
Criticality was achieved by bringing the two subassemblies into contact (one of the subassemblies was mounted on rails)



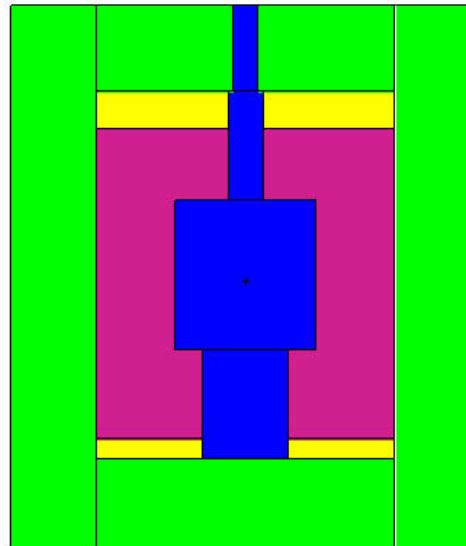
# BIG TEN Assembly



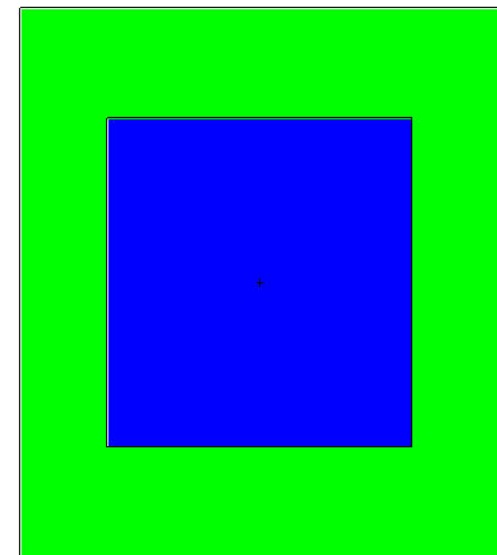
# Comparison of BIG TEN Benchmark Models



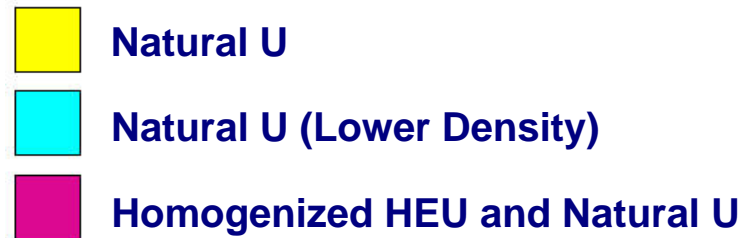
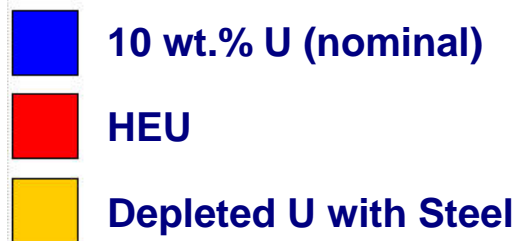
“Simplified”



Improved



“Two-Zone”



# Comparison of Benchmark Models for BIG TEN

| Parameter                              |                  | Benchmark Model      |                      |                      |
|----------------------------------------|------------------|----------------------|----------------------|----------------------|
|                                        |                  | “Simplified”         | Improved             | “Two-Zone”           |
| Benchmark $k_{\text{eff}}$             |                  | $1.0045 \pm 0.0007$  | $1.0049 \pm 0.0008$  | $0.9948 \pm 0.0013$  |
| Bias in benchmark $k_{\text{eff}}$     |                  | $-0.0017 \pm 0.0005$ | $-0.0013 \pm 0.0006$ | $-0.0114 \pm 0.0012$ |
| Neutron leakage (%)                    |                  | 10.82                | 10.75                | 10.84                |
| Fission, by Energy (%)                 | Fast             | 80.18                | 79.88                | 79.81                |
|                                        | Intermediate     | 19.82                | 20.12                | 20.19                |
|                                        | Thermal          | 0                    | 0                    | 0                    |
| Fission, by Isotope (%)                | $^{234}\text{U}$ | 0.22                 | 0.20                 | 0.21                 |
|                                        | $^{235}\text{U}$ | 74.39                | 73.90                | 73.60                |
|                                        | $^{236}\text{U}$ | 0.03                 | 0.02                 | 0.02                 |
|                                        | $^{238}\text{U}$ | 25.36                | 25.88                | 26.17                |
| Average Number of Neutrons per Fission |                  | 2.567                | 2.565                | 2.566                |

# MCNP Calculations

Calculations were performed for the the three benchmark models with the MCNP5 Monte Carlo code, using ENDF/B-VII.0, ENDF/B-VI, JEFF-3.1, and JENDL-3.3 nuclear data libraries

Each calculation employed 550 generations of 10,000 neutrons each

Results from the first 50 generations were excluded from the statistics

⇒ Results for each case are based on 5,000,000 active neutron histories

# MCNP5 Results for BIG TEN Benchmark Models

| Model                       |              | “Simplified”        | Improved            | Two-Zone            |
|-----------------------------|--------------|---------------------|---------------------|---------------------|
| Benchmark $k_{\text{eff}}$  |              | $1.0045 \pm 0.0007$ | $1.0049 \pm 0.0008$ | $0.9948 \pm 0.0013$ |
| Calculated $k_{\text{eff}}$ | ENDF/B-VII.0 | $1.0044 \pm 0.0002$ | $1.0048 \pm 0.0002$ | $0.9948 \pm 0.0002$ |
|                             | ENDF/B-VI    | $1.0165 \pm 0.0002$ | $1.0166 \pm 0.0002$ | $1.0071 \pm 0.0002$ |
|                             | JEFF-3.1     | $0.9980 \pm 0.0002$ | $0.9979 \pm 0.0002$ | $0.9876 \pm 0.0002$ |
|                             | JENDL-3.3    | $0.9952 \pm 0.0002$ | $0.9949 \pm 0.0002$ | $0.9851 \pm 0.0002$ |

$$0.005 < |\Delta k| \leq 0.010$$

$$|\Delta k| > 0.010$$

ENDF/B-VII.0 produces very close agreement with the benchmark value of  $k_{\text{eff}}$  for all three models

JEFF-3.1 and JENDL-3.3 underpredict the benchmark value of  $k_{\text{eff}}$  by 0.5% to 1%, and ENDF/B-VI overpredicts it by more 1%

# Summary and Conclusions

An expanded criticality validation suite has been created for MCNP

The 119 benchmarks in the expanded suite cover a broad range of fuels, spectra, and configurations

The expanded suite includes several sets of related benchmarks so that parameter studies can be conducted

One of the benchmarks in that suite is an improved benchmark model for the BIG TEN critical assembly, which will be submitted for approval by the ICSBEP at its meeting in May