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*Title:* MCNP CALCULATIONS FOR THE OECD/NEA SOURCE CONVERGENCE BENCHMARKS

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# MCNP Calculations for the OECD/NEA Source Convergence Benchmarks

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## INTRODUCTION

Improper source convergence can lead to non-conservative estimates of k-effective for various fissionable configurations, such as the "Whitesides problem", spent fuel casks, spent fuel storage pools, and fuel processing systems. To improve the robustness of criticality safety analyses with respect to source convergence the OECD/NEA established an Expert Group [1] to investigate the long-standing problem of source convergence for certain classes of nuclear criticality safety problems. Members of the Expert Group have specified and calculated a set of four source convergence benchmark problems using a variety of standard Monte Carlo computer codes. This paper describes the calculations performed at Los Alamos National Laboratory using the MCNP Monte Carlo code [2,3]. Results are presented for the four benchmark calculations, as well as for a number of additional supporting calculations performed with both Monte Carlo and deterministic codes. Illustrative results are presented in this short paper, and the complete set of calculational results is available in [4].

## MCNP BENCHMARK RESULTS

The source convergence benchmark problems are described in [1,5-8], along with a comparison of results obtained from the Expert Group participants. MCNP results obtained using MCNP4C2 and ENDF/B-VI cross-section data are included in the comparisons. We summarize here some additional calculations performed to aid in understanding the physics considerations and convergence behavior of the 4 benchmark problems: reference calculations, side studies, MCNP statistical tests, and comparison with deterministic calculations.

### Reference Calculations

For Benchmark 1, checkerboard storage of assemblies, a reference calculation was performed using MCNP4C2, ENDF/B-VI cross-section data, a uniform initial source in the fuel lattice regions, 9,055 cycles with the first 500 cycles discarded, and 10,000 particles per cycle. The total number of histories in active cycles for tallying was 85.5 million. This calculation produced a k-effective of 0.88192 ± 0.00001 and the fission distribution shown in Figure (1).

For Benchmark 4, the array of interacting spheres, a reference calculation was performed using MCNP4C2, ENDF/B-VI cross-section data, a uniform initial source in each of the 25 spheres, 6,000 cycles with the first 1,00 cycles discarded, and 10,000 particles per cycle. The total number of histories in active generations for tallying was 50 million. This calculation produced a k-effective of 1.11294 ± 0.00009 and the fission distribution is shown in Table (1).

### Side Studies

For Benchmark 1, the checkerboard storage of assemblies, we performed a number of side studies to investigate the physics properties of isolated and reflected single fuel elements (including the 15x15 array of fuel pins, the surrounding water, and iron container). These calculations included an infinite lattice of fuel elements, a single fuel element surrounded by water, a single fuel element surrounded by concrete, a single fuel element with water on 3 sides and concrete on 1 side, and a single fuel element with water on 2 sides and concrete on 2 sides. K-effective results are given in Table 2. The table results show that concrete is a more effective reflector than water for this type of fuel element, and provide insight into the causes of the highly assymetric fission distribution shown in Figure (1).

For Benchmark 4 we also performed eigenvalue calculations for isolated spheres, with radii of 10.0 cm and 8.71 cm. For these runs, all neutrons leaking from the sphere were terminated. We ran 5,000 histories per cycle, skipped 500 cycles, and calculated a total of 2,500 cycles (10 M active histories). The initial source was simply a point in the center of the sphere. For the 10.0-cm sphere, the k-eff was 1.11233 ± 0.00019, and for the 8.71-cm sphere, the k-eff was 0.99519 ± 0.00019.

### MCNP Statistical Tests

MCNP performs several statistical checks on the eigenvalue results and warns the user if the statistical checks fail in some manner. In these calculations, 3 main warning messages arose. The first is "The cycle values do not appear normally distributed at the 99% confidence level." This check is performed for each of the 3 estimators: collision, absorption, and track length. The second warning was "The first and second half values of the combined estimator appear to be different at the 99% confidence level." The third is a warning that "There appears to be an {increasing / decreasing} trend in the combined estimator over the last 10 cycles."

For Benchmark 4, the array of interacting spheres, 300 different replicas were run — 100 in each of 3 cases, skipping 0, 200, or 400 initial cycles. The percent of the replica runs for each case flagging these warning messages is indicated in the Table (3). For case 1, three of the replicas flagged the warning about "cycle values not normally distributed" for each of the three individual estimators. When this happens, MCNP draws attention to the fact by not printing "boxed" results for the final k-eff. The combined estimators for these 3 runs were 1.06226, 1.07231, and 1.07909. These are some of the worst, but certainly not the absolute worst, k-eff estimates. On the other hand, for the 15 replicas of case 1 with no MCNP eigenvalue warnings, the average k-eff is 1.10704, not great compared to the reference calculation, but much closer than the typical case 1 replica.

### Comparison with Deterministic Calculations

For Benchmark 3, the three thick 1D slabs, deterministic calculations were performed using ONEDANT, a 1D discrete-ordinates code [9] and compared to MCNP calculations. To ensure consistency between the 2 codes, the calculations were run using the same set of multigroup cross-sections with $P_0$ scattering. A high-order quadrature set was used in ONEDANT, $S_{96}$ double-Gauss. These calculations are <u>not</u> considered reference calculations, since multigroup cross-sections were used instead of the usual MCNP continuous-energy ENDF/B-VI cross-sections, but serve to verify that the MCNP calculations were converged and performed correctly. Table (4) compares k-effective for 3 symmetric cases, with the ONEDANT runs performed with fine mesh spacing of 0.25 mm, and the MCNP calculations carried out to 100 M histories. Agreement is excellent. Figure (2) shows a comparison of k-effective values for cases with the 20 cm central water region and as a function of the asymmetry, i.e., [(thickness of right slab)/(thickness of left slab) - 1] x 100%

## SUMMARY

The MCNP Team at Los Alamos was part of the OECD/NEA Expert Group on source convergence and contributed results for all of the benchmark calculations. In addition, a number of side studies were carried out to provide reference results and insight into the calculations.

## REFERENCES


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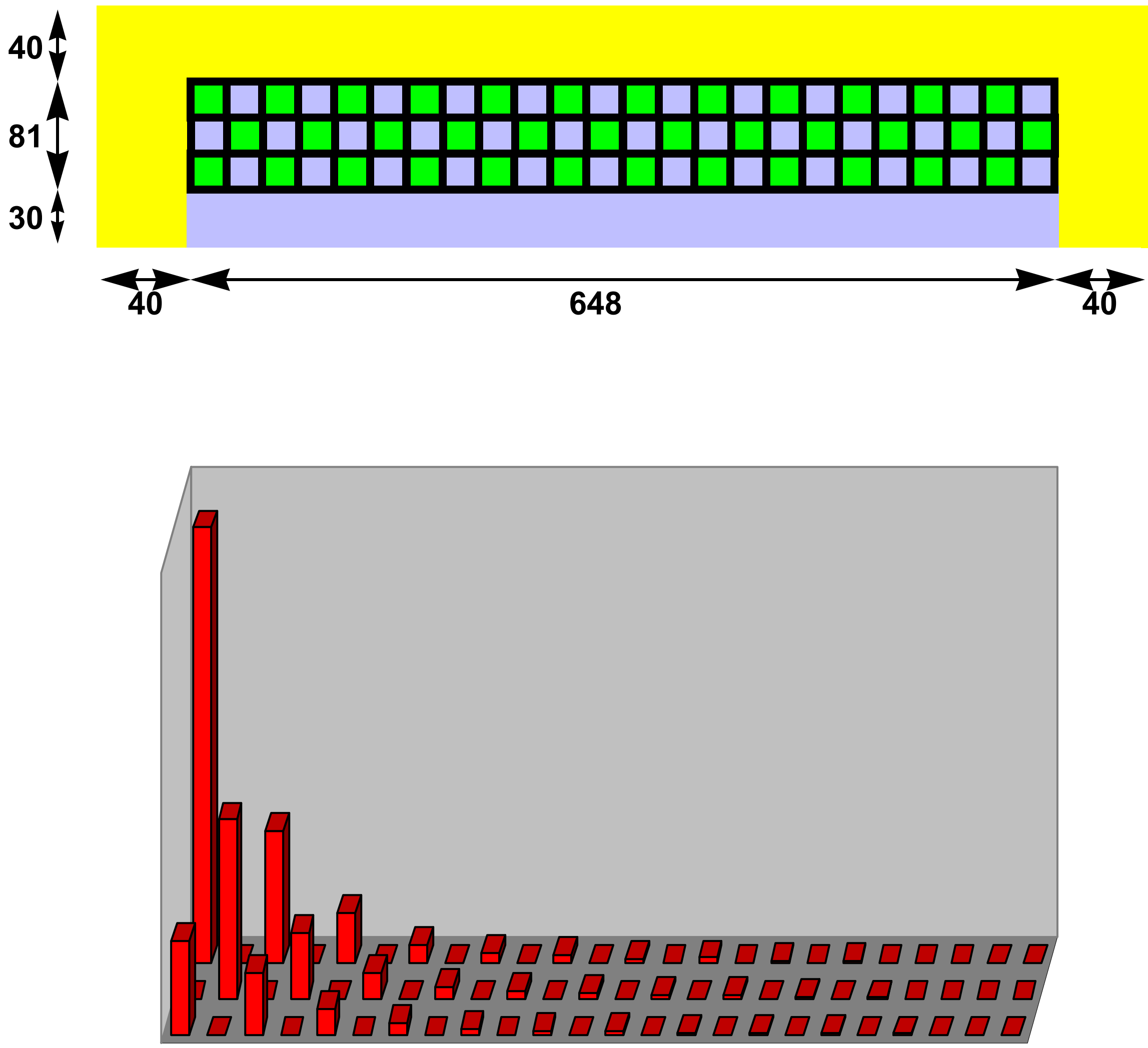


Figure 1. Fission Distribution for MCNP Reference Calculation — Benchmark 1, Checkerboard Storage of Assemblies

Table 1.Fission Distribution for MCNP Reference Calculation — Benchmark 4, Array of Interacting Spheres

| | | |
|---|---|---|
| 0.000254 | | |
| 0.002344 | 0.005783 | |
| 0.000463 | 0.11157 | 0.910624 |

Table 2. K-effective for Single-Element Side Studies — Benchmark 1, Checkerboard Storage of Assemblies

| | |
|---|---|
| Single fuel element, surrounded by water | 0.85779 ± .00034 |
| Single fuel element, water 3 sides, concrete 1 side | 0.86817 ± .00034 |
| Single fuel element, concrete 2 sides, water 2 sides | 0.88017 ± .00035 |
| Single fuel element, surrounded by concrete | 0.90390 ± .00034 |
| Infinite lattice of fuel elements | 1.11695 ± .00029 |

Table 3. MCNP Statistical Test Warnings for K-effective — Benchmark 4, Array of Interacting Spheres

| Case | Skipped Cycles | Cycle Values Not Normally Distributed | First Half / Second Half Different | Trend in Last 10 Cycles | At Least One Warning Message |
|---|---|---|---|---|---|
| 1 | 0 | 21 | 81 | 6 | 85 |
| 2 | 200 | 5 | 35 | 1 | 37 |
| 3 | 400 | 3 | 13 | 0 | 16 |

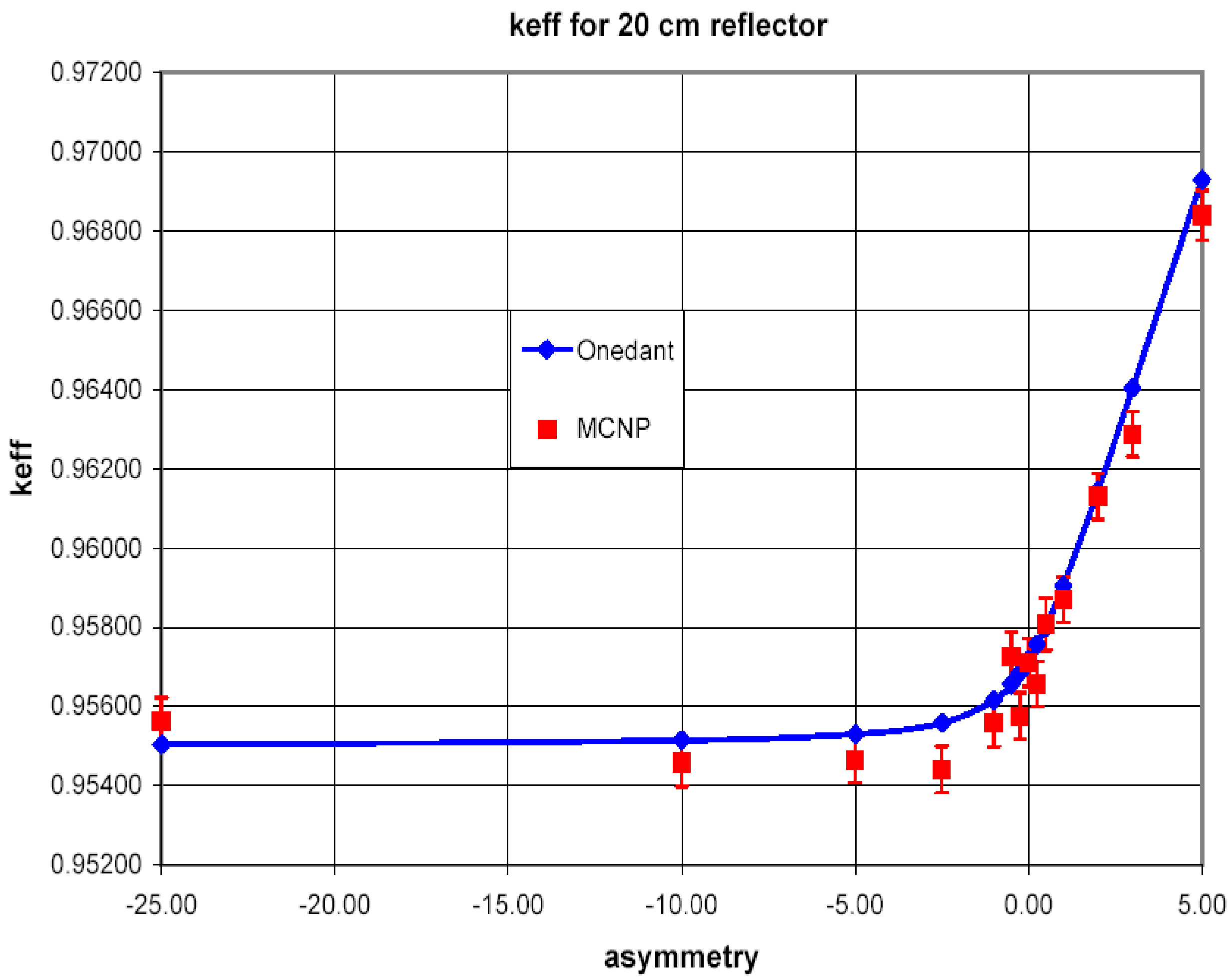


Figure 2. K-effective from ONEDANT and MCNP — Benchmark 3, Thick 1D Slabs, 20 cm Central Water Region