

LA-UR-10-00189

Approved for public release;  
distribution is unlimited.

<i>Title:</i>	Revisiting the "K-effective of the World" Problem
<i>Author(s):</i>	Forrest Brown
<i>Intended for:</i>	American Nuclear Society 2010 Annual Meeting 13-17 June 2010, San Diego, CA



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.

# Revisiting the “K-effective of the World” Problem

Forrest B. Brown

*Monte Carlo Codes, XCP-3, LANL  
PO Box 1663 MS A143, Los Alamos NM, USA, fbrown@lanl.gov*

## INTRODUCTION

The “K-effective of the World” problem was introduced nearly 30 years ago by G. E. Whitesides [1]. The general theme was to caution Monte Carlo code users that, despite the sophistication of the codes for representing realistic geometry and physics interactions, correct results can be obtained only if users pay attention to source convergence in the Monte Carlo iterations and to running a sufficient number of neutron histories to adequately sample all significant regions of the problem. From [1]:

The extreme example, which defines a situation in which this difficulty can exist, is the “k-effective of the World” problem. That is, if one attempts to calculate the  $k_{\text{eff}}$  of the world using a Monte Carlo calculation, what  $k_{\text{eff}}$  would be computed assuming that there are several critical assemblies located around the world? The answer would likely be the  $k_{\text{eff}}$  of the world with no critical assemblies present. The cause of the erroneous result is the fact that the volume of fissile material in the world would be so large relative to the volume of fissile material in the critical assemblies that most commonly used forms of sampling would almost never “see” the critical assemblies. Hence, this would not reflect their existence in the computed  $k_{\text{eff}}$ . . . . . The erroneous results for these types of problems are the result of the failure of the calculation to converge the source to the fundamental source mode.

For a number of years, the OECD/NEA Working Party on Nuclear Criticality Safety has sponsored the Expert Group On Source Convergence in Criticality Safety Analysis [2,3]. This Expert Group thoroughly investigated the issues in source convergence for Monte Carlo calculations and suggested improvements to Monte Carlo codes and guidance for code users [2,3,4]. In this summary, the recommended best practices from [4] are applied to the “K-effective of the World” problem. Numerical results are discussed, and causes of previously observed discrepancies identified. The general conclusion of this work is that the model problem used in [1] is not a difficult calculation today, and correct results will be obtained if currently recommended Monte Carlo criticality practices are followed.

## PROBLEM DESCRIPTION

A straightforward model problem was defined in [1] to illustrate the “K-effective of the World” problem:

. . . . . a 9 x 9 x 9 array of plutonium metal spheres with a radius of ~4 cm, spaced on 60-cm centers. The array is reflected on all sides by a thick water reflector. The  $k_{\text{eff}}$  of this system is computed to be 0.93. If the sphere in the center unit of the array is replaced by a sphere of plutonium that is exactly critical as a bare unit and the calculation repeated in the standard fashion using the Monte Carlo method, the calculation will yield a  $k_{\text{eff}}$  of 0.93, reflecting the same difficulty encountered in the “world  $k_{\text{eff}}$ ” problem.

The precise dimensions, materials, and nuclear cross-section libraries are not fundamental to the analysis. The model was constructed for MCNP5 [5,6] using ENDF/B-VII.0 nuclear data (with continuous-energy physics), and the radii of the spheres were adjusted so that the lattice of smaller spheres yielded  $k_{\text{eff}} = 0.9328 \pm .0002$  (without the larger center sphere) and the larger bare sphere had  $k_{\text{eff}} = 1.0001 \pm .0002$ . With the larger center sphere replacing the center sphere of the subcritical lattice, a lengthy benchmark calculation (following recommended best practices) gave  $k_{\text{eff}} = 1.0013 \pm .0003$ . The problem geometry, materials, and cross-section data were then held constant for all of the calculations described below. For all calculations, the initial guess for the fission distribution was chosen as a uniform distribution among the 739 spheres, at the center points of selected spheres.

## NUMERICAL RESULTS

The analysis below focuses on two concerns investigated in [2,3] and reviewed in [4]: source convergence and adequate neutron population.

### Source Convergence

Figures (1) and (2) show  $k_{\text{eff}}$  and  $H_{\text{src}}$  (the Shannon entropy of the fission distribution, a diagnostic for source distribution convergence) for each of the first 250 cycles, for calculations using different numbers of neutrons/cycle. Several observations from these plots, consistent with [2,3,4] are: (1) When fewer than 1,000 neutrons/cycle are used, there is so much statistical noise that determining convergence is problematic. (2) As noted in [4],  $k_{\text{eff}}$  converges sooner than  $H_{\text{src}}$ , about 100 cycles vs 150. (3) Convergence of  $k_{\text{eff}}$  and  $H_{\text{src}}$  depends on model geometry and physics (via the dominance ratio), and not on the number of neutrons/cycle.

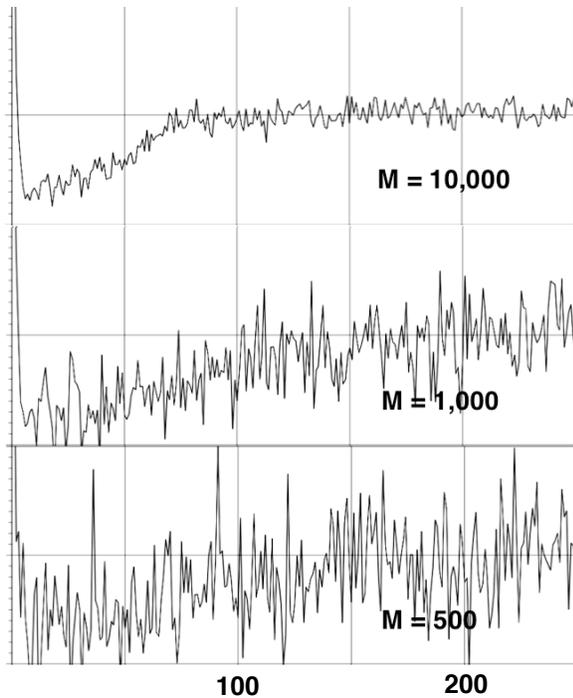


Fig. 1.  $k_{eff}$  vs cycle, for various M (M = neutrons/cycle)

For all subsequent calculations, the first 150 cycles are discarded to ensure adequate convergence of both  $k_{eff}$  and the fission distribution.

### Population Size

As discussed in [1,4], a sufficient number of neutrons/cycle must be used to ensure adequate Monte Carlo sampling of the problem. In addition, as noted in [4], using too few neutrons/cycle gives rise to a bias in  $k_{eff}$  and local tallies due to the renormalization performed at the end of each Monte Carlo cycle. The renormalization bias in  $k_{eff}$  has been shown to be proportional to  $1/M$ , where M is the neutrons/cycle.

Figure (3) shows the  $k_{eff}$  results as a function of M. For all cases shown in Fig. (3), the first 150 cycles were discarded (to ensure convergence) and enough cycles were run for each case to provide 10M total neutrons in the active cycles for each run. It is evident from Fig. (3) that using small numbers of neutrons/cycle can result in significant bias, underpredicting  $k_{eff}$ . When 5,000 or more neutrons/cycle are used, as recommended in [4], the bias in  $k_{eff}$  is negligible and smaller than the statistical noise.

### SUMMARY AND CONCLUSIONS

The results presented herein demonstrate that the model problem used to demonstrate the “K-effective of the World” problem is actually not a difficult problem to

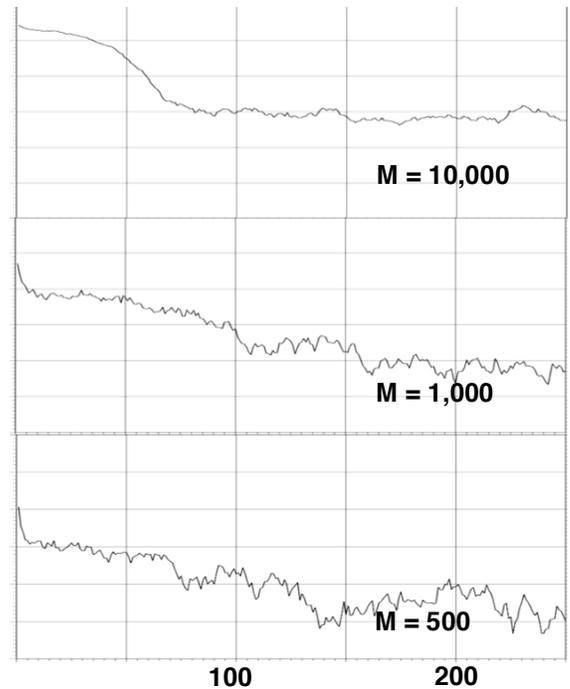


Fig. 2.  $H_{src}$  vs cycle, various M

solve, if the current recommended practices are using in performing the Monte Carlo calculations.

It should be noted that none of the results in Fig. (3) are close to  $k_{eff}=.93$ , reported in [1] when the center sphere was the larger sphere (that was critical by itself). It appears that the anomalous result for this problem noted in [1] was due largely to the severe computer limitations of 30 years ago: Due to slow computers with small memory size, the default parameters for running KENO were to use 300 neutrons/cycle, discard the first 3 cycles, and then run 100 active cycles for computing  $k_{eff}$ . As evident from Figures (1)-(3), with those default parameters for the calculations, the fission source and  $k_{eff}$  would not be converged, the 739 spheres would not be adequately sampled, and there would be a significant renormalization bias due to the small number of neutrons/cycle. From [1]:

The Monte Carlo method has opened up the path to very precise evaluations of the criticality safety of almost any situation likely to be encountered. Its use, however, should be tempered by the realization that unless the correct fission distribution is achieved, the results will most likely be nonconservative.

With today’s faster computers and Monte Carlo codes with tools for diagnosing convergence, it is not difficult to resolve the issues of convergence and population size for the model problem. As far as the real “K-effective of the World” problem is concerned, however, a 1 km spherical shell covering the earth’s

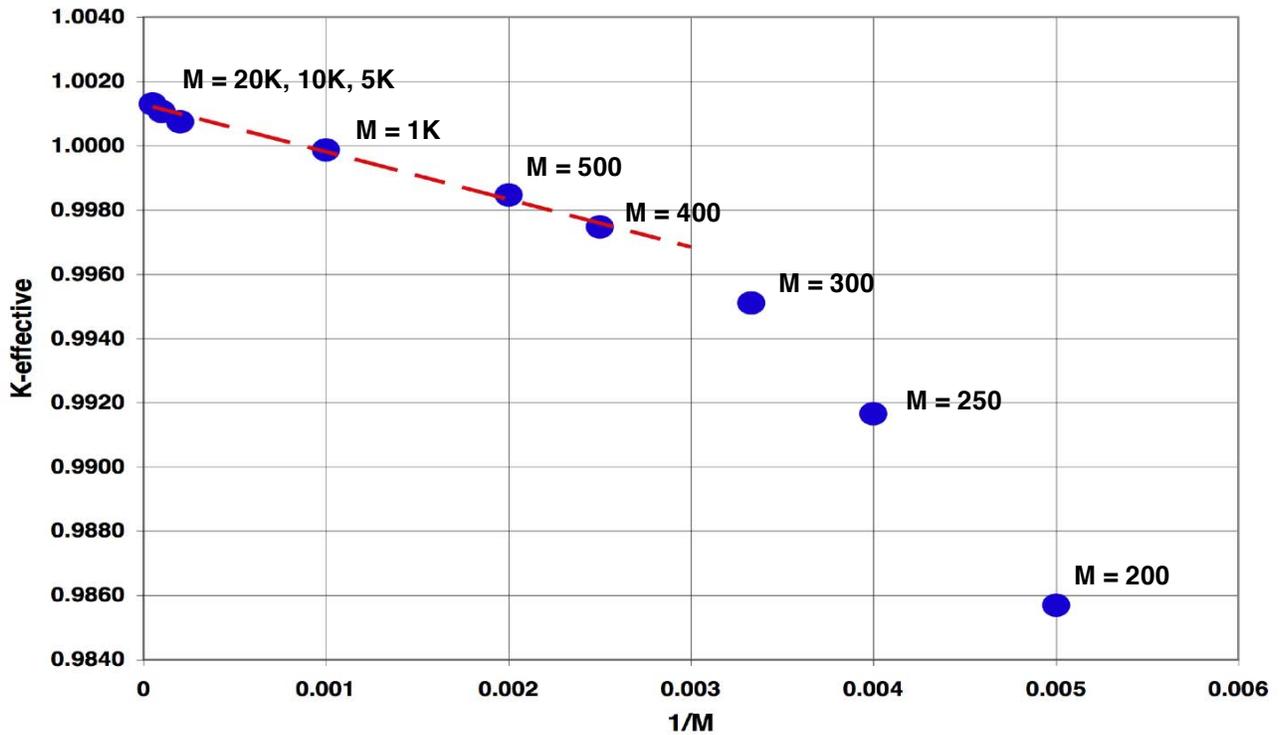


Fig. 3.  $k_{eff}$  vs  $1/M$ , where  $M$  = neutrons/cycle

surface has a volume roughly  $10^{15}$  times that of the model problem; computing  $k_{eff}$  for the entire earth will require beyond-exaflop computers, and may well be 30 more years away.

## REFERENCES

1. G.E. WHITESIDES, "A Difficulty in Computing the  $k$ -effective of the World," *Trans. Am. Nucl. Soc.*, **14**, No. 2, 680 (1971).
2. R.N. BLOMQUIST, ET AL., "Source Convergence in Criticality Safety Analysis, Phase I: Results of Four Test Problems", OECD Nuclear Energy Agency, OECD NEA No. 5431 (2006).
3. R.N. BLOMQUIST, ET AL., "NEA Expert Group on Source Convergence Phase II: Guidance for Criticality Calculations", 8<sup>th</sup> International International Conference on Criticality Safety, St. Petersburg, Russia, May 28 – June 1, 2007 (May 2007).
4. F.B. BROWN, "A Review of Best Practices for Monte Carlo Criticality Calculations", ANS NCS-2009, Richland, WA, Sept 13-17 (2009).
5. X-5 MONTE CARLO TEAM, "MCNP – A General N-Particle Transport Code, Version 5 – Volume I:

Overview and Theory", LA-UR-03-1987, Los Alamos National Laboratory (April, 2003).

6. F.B. BROWN, ET AL. "MCNP5-1.51 Release Notes", LA-UR-09-00384, Los Alamos National Laboratory (2009).