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VALIDATION SUITES FOR MCNP™

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SUMMARY

Two validation suites, one for criticality and another for radiation shielding, have been defined and tested for the MCNP Monte Carlo code. All of the cases in the validation suites are based on experiments so that calculated and measured results can be compared in a meaningful way. The cases in the validation suites are described, and results from those cases are discussed.

I. INTRODUCTION

For several years, the distribution package for the MCNP Monte Carlo code[1] has included an installation test suite to verify that MCNP has been installed correctly. However, the cases in that suite have been constructed primarily to test options within the code and to execute quickly. Consequently, they do not produce well-converged answers, and many of them are physically unrealistic.

To remedy these deficiencies, sets of validation suites are being defined and tested for specific types of applications. All of the cases in the validation suites are based on benchmark experiments. Consequently, the results from the measurements are reliable and quantifiable, and calculated results can be compared with them in a meaningful way. Currently, validation suites exist for criticality and radiation-shielding applications.

II. CRITICALITY VALIDATION SUITE

The primary objective for the criticality validation suite is to assess the reactivity impact of future improvements to the MCNP methodology and changes to its associated nuclear data libraries. Agreement between the measured and calculated results therefore is a secondary, although important, criterion for the selection of cases in the suite.

Accordingly, the components of the criticality validation suite were chosen to include a wide variety of fissile materials and spectra. More specifically, they include the three major fissile isotopes — ^{233}U, ^{235}U, and ^{239}Pu — in configurations that produce fast, intermediate, and thermal spectra. Furthermore, the ^{235}U cases were chosen so that they include highly enriched uranium (HEU), intermediate-enriched uranium (IEU), and low-enriched uranium (LEU) fuels.

The cases also were chosen to include, where possible, a variety of configurations. The fast-spectrum cases include bare spheres, cores reflected by a heavy material (normal U), and cores reflected by a light material (Be or water). The thermal-spectrum cases include lattices of fuel pins as well as homogeneous solutions. The number of experiments with intermediate spectra is much more limited, and those cases were chosen primarily for availability rather than specific attributes.

The specifications for all 26 cases in the criticality validation suite are taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*.[2] The cases are summarized in Table 1, and calculated results are presented in Table 2. All of the cases are at room temperature and pressure.

The calculations were performed with MCNP4C2 and its associated ENDF/B-VI data libraries. The cross sections for the actinides and tungsten are taken from the URES library,[3] which is based on release 4 of ENDF/B-VI. Cross sections for the remaining isotopes, which are not present in the URES library, are taken from the ENDF60 library,[4] which is based on release 2. All calculations were performed with 250 generations of 5,000 neutrons each, and the results from the first 50 generations were discarded. Consequently, the results for each case are based on 1,000,000 active neutron histories.

Execution of the criticality validation suite takes a significant amount of computer resources. The results reported in Table 2 were obtained from a Silicon Graphics Origin 2000 supercomputer with a clock speed of 250 MHz, running in sequential (single-processor) mode. The total run time, as shown in Table 2, is nearly 19 CPU hours. When run on a Pentium III PC with 256 MB of RAM, a clock speed of 800 MHz, and the Windows 2000 operating system, the suite consumed approximately 11 CPU hours.

Table 1. Summary of MCNP Criticality Validation Suite

Name	Spectrum	*Handbook* ID	Description
Jezebel-233	Fast	U233-MET-FAST-001	Bare sphere of ^{233}U
Flattop-23	Fast	U233-MET-FAST-006	Sphere of ^{233}U reflected by normal U
U233-MF-005 (2)	Fast	U233-MET-FAST-005, case 2	Sphere of ^{233}U reflected by beryllium
Falstaff (1)	Intermediate	U233-SOL-INTER-001, case 1	Sphere of uranyl fluoride solution enriched in ^{233}U
ORNL-11	Thermal	U233-SOL-THERM-008	Large sphere of uranyl nitrate solution enriched in ^{233}U
Godiva	Fast	HEU-MET-FAST-001	Bare HEU sphere
Flattop-25	Fast	HEU-MET-FAST-028	HEU sphere reflected by normal U
"Godiver"	Fast	HEU-MET-FAST-004	HEU sphere reflected by water
HISS/HUG	Intermediate	HEU-COMP-INTER-004	Infinite, homogeneous mixture of HEU, hydrogen, and graphite
ZEUS (2)	Intermediate	HEU-MET-INTER-006, case2	HEU platters moderated by graphite and reflected by copper
HEU-MT-003 (4)	Thermal	HEU-MET-THERM-003, case 4	Three-dimensional lattice of HEU cubes reflected by water
ORNL-10	Thermal	HEU-SOL-THERM-032	Large sphere of HEU nitrate solution
IEU-MF-003	Fast	IEU-MET-FAST-003	Bare sphere of IEU (36 wt.%)
BIG TEN	Fast	IEU-MET-FAST-007	Cylinder of IEU (10 wt.%) reflected by normal U
IEU-MF-004	Fast	IEU-MET-FAST-004	Sphere of IEU (36 wt.%) reflected by graphite
IEU-CT-002 (3)	Thermal	IEU-COMP-THERM-002, case 3	Lattice of IEU (17 wt.%) fuel rods in water
BAW XI (2)	Thermal	LEU-COMP-THERM-008, case 2	Large lattice of PWR fuel pins in borated water
SHEBA-2	Thermal	LEU-SOL-THERM-001	Annular cylinder of LEU (5 wt.%) fluoride solution
Jezebel	Fast	PU-MET-FAST-001	Bare sphere of Pu
Jezebel-240	Fast	PU-MET-FAST-002	Bare sphere of Pu (20.1 at.% ^{240}Pu)
Flattop-Pu	Fast	PU-MET-FAST-006	Pu Sphere reflected by normal U
PU-MF-011	Fast	PU-MET-FAST-011	Pu Sphere reflected by water
Pu Buttons	Fast	PU-MET-FAST-003, case 3	3 x 3 x 3 array of small cylinders of Pu
HISS/HPG	Intermediate	PU-COMP-INTER-001	Infinite, homogeneous mixture of Pu, hydrogen, and graphite
PNL-33	Thermal	MIX-COMP-THERM-002, case 4	Lattice of mixed-oxide fuel pins in borated water
PNL-2	Thermal	PU-SOL-THERM-021, case 3	Sphere of plutonium nitrate solution

Table 2. MCNP4C2 Results for Cases in Criticality Validation Suite

Case	Benchmark k_{eff}	Calculated k_{eff} (ENDF/B-VI)	Δk	Time (CPU Minutes)
Jezebel-233	1.0000 ± 0.0010	0.9924 ± 0.0006	-0.0076 ± 0.0012	2.09
Flattop-23	1.0000 ± 0.0014	0.9993 ± 0.0007	-0.0007 ± 0.0016	16.05
U-233-MF-005, case 2	1.0000 ± 0.0030	0.9979 ± 0.0006	-0.0021 ± 0.0031	3.47
Falstaff (1)	1.0000 ± 0.0083	0.9904 ± 0.0011	-0.0096 ± 0.0084	14.54
ORNL-11	1.0006 ± 0.0029	0.9960 ± 0.0004	-0.0046 ± 0.0029	107.04
Godiva	1.0000 ± 0.0010	0.9973 ± 0.0006	-0.0027 ± 0.0012	2.91
Flattop-25	1.0000 ± 0.0030	0.9979 ± 0.0006	-0.0021 ± 0.0031	17.57
Godiver	0.9985 ± 0.0011	0.9954 ± 0.0008	-0.0031 ± 0.0014	53.89
HISS/HUG	1.0000 ± 0.0040	1.0129 ± 0.0005	0.0129 ± 0.0040	111.91
Zeus (2)	0.9997 ± 0.0008	0.9975 ± 0.0007	-0.0022 ± 0.0011	31.29
HEU-MT-003 (4)	0.9876 ± 0.0040	0.9814 ± 0.0009	-0.0062 ± 0.0041	82.29
ORNL-10	1.0015 ± 0.0026	0.9987 ± 0.0004	-0.0028 ± 0.0026	99.47
IEU-MF-003	1.0000 ± 0.0017	1.0005 ± 0.0006	0.0005 ± 0.0018	20.27
BIG TEN	0.9948 ± 0.0013	1.0099 ± 0.0005	0.0151 ± 0.0014	41.69
IEU-MF-004	1.0000 ± 0.0030	1.0038 ± 0.0006	0.0038 ± 0.0031	14.73
IEU-CT-002 (3)	1.0017 ± 0.0044	1.0002 ± 0.0007	-0.0015 ± 0.0045	79.74
BAW XI (2)	1.0007 ± 0.0012	0.9984 ± 0.0006	-0.0023 ± 0.0013	58.37
Sheba-2	0.9991 ± 0.0029	1.0106 ± 0.0008	0.0115 ± 0.0030	32.89
Jezebel	1.0000 ± 0.0020	0.9969 ± 0.0006	-0.0031 ± 0.0021	1.98
Jezebel-240	1.0000 ± 0.0020	0.9988 ± 0.0006	-0.0012 ± 0.0021	2.36
Flattop-Pu	1.0000 ± 0.0030	1.0014 ± 0.0007	0.0014 ± 0.0031	20.79
Pu-MF-011	1.0000 ± 0.0010	0.9974 ± 0.0008	-0.0026 ± 0.0013	58.88
Pu Buttons	1.0000 ± 0.0030	0.9958 ± 0.0007	-0.0042 ± 0.0031	6.24
HISS/HPG	1.0000 ± 0.0110	1.0113 ± 0.0006	0.0113 ± 0.0110	103.20
PNL-33	1.0024 ± 0.0021	1.0058 ± 0.0008	0.0034 ± 0.0022	118.39
PNL-2	1.0000 ± 0.0065	1.0003 ± 0.0010	0.0003 ± 0.0066	13.74

Total time: 1115.79 CPU minutes (Silicon Graphics Origin 2000 supercomputer, 250 MHz)

III. RADIATION SHIELDING VALIDATION SUITE

The primary objective for the radiation shielding validation suite is to assess the impact on dose rates and attenuation factors of future improvements to the MCNP methodology and its neutron and photon data libraries. There are three subcategories within the suite: time-of-flight spectra for neutrons, neutron and photon spectra at shield walls within a simulated fusion reactor, and photon dose rates. Two of the cases are coupled neutron-photon calculations, while the others are exclusively neutron or exclusively photon calculations. All of the cases are taken from existing neutron[5] and photon[6] benchmark suites for MCNP.

A. Time-of-Flight Spectra

Pulsed-sphere experiments were begun at Lawrence Livermore National Laboratory in the late 1960s and continued into the 1980s.[7-15] The objective of these experiments was to measure the neutron emission spectrum from a variety of materials bombarded by 14 MeV neutrons. The spectra were measured using time-of-flight techniques.

A thin disk of titanium tritide was placed at the center of spheres of a variety of materials using a small hole from the outside to the center of the sphere. A beam of deuterons from an accelerator was directed at the disk to produce a nearly isotropic source of 14 MeV neutrons from a $t(d,n)^4He$ reaction. Depending upon the material of interest, the sphere could be bare, clad in stainless steel, or contained within a stainless steel dewar. The thicknesses of the spheres ranged from 0.5 to 5.0 mean free paths (mfp) for 14 MeV neutrons, and the flight paths to the detectors ranged from 750 to 975 cm. The materials that were studied included isotopes, elements, and compounds such as water, polyethylene, and concrete.

The measurements were made over the energy range from 2 to 16 MeV, using either a Pilot B or an NE213 detector placed at an angle of 30° with respect to the incident deuteron beam. The lone exception was the measurement for concrete, where the detector was placed at an angle of 120°. Eight of these cases have been chosen for inclusion in the radiation shielding validation suite, as shown in Table 3. These cases include individual isotopes, elements, and compounds. They include both types of detectors and both angles of measurement. They include both light (lithium and beryllium) and heavy (lead) targets, and the spheres range in size from 0.8 to 3.1 mfp. The input for these eight cases has been updated to use the ENDF60 library,[4] and each case has been standardized to use 1,000,000 neutron histories.

The MCNP input files employ a variety of techniques to reduce the run time and to improve the statistics. An energy cut-off was imposed at 1.6 MeV to prevent the code from tracking particles whose energies had dropped below the sensitivity threshold of the detectors. In addition, because the model is symmetric about the incident deuteron beam, ring detectors are employed to calculate the flux at the appropriate distance and polar angle. Finally, the figure of merit is improved for some of the cases with larger spheres by subdividing the sphere into concentric shells, with the importance increasing with the distance from the center of the sphere.

The dose and the uncollided flux are edited by time interval. As was the case with the criticality validation suite, however, the principal objective of the radiation shielding validation suite is to assess the impact of future improvements to the MCNP methodology and changes to the nuclear data libraries. Consequently, the results edited from these cases will be used as a baseline from which to judge future changes. A more detailed study of the pulsed-sphere experiments was performed with MCNP a few years ago,[16] and the interested reader is referred to that article.

B. Fusion Shielding

The second subset of cases in the radiation shielding validation suite is based on an experiment that was performed at Oak Ridge National Laboratory in 1980. This experiment has been accepted as a benchmark by the Cross Section Evaluation Working Group.[17]

The objective of the experiment was to simulate the deuterium-tritium neutron spectrum that would exist at the first wall of a fusion reactor as well as the spectrum of secondary photons that would be produced from neutron interactions within that wall.[18] As with the pulsed-sphere experiments, a

Table 3. Summary of MCNP Radiation Shielding Validation Suite: Pulsed Spheres

Target Material	Target Configuration	Target Thickness (mfp)	Detector Type	Angle
Beryllium	Bare Sphere	0.8	Pilot B	30°
Carbon	Bare Sphere	2.9	NE 213	30°
Concrete	Bare Sphere	2.0	NE 213	120°
Iron	Bare Sphere	0.9	NE 213	30°
Lead	Clad Sphere	1.4	NE 213	30°
^6Li	Dewar	1.6	NE 213	30°
Nitrogen	Dewar	3.1	Pilot B	30°
Water	Dewar	1.9	Pilot B	30°

deuteron beam from an accelerator was directed to a titanium tritide disk to produce a nearly isotropic source of 14 MeV neutrons from a $t(d,n)^4He$ reaction. The target disk was placed at one end of a cylindrical iron duct that was imbedded in a concrete block. The other end of the duct opened to the air outside the concrete block. Neutron and gamma detectors were arranged in a variety of configurations and alignments outside the concrete beyond the open end of the duct.

The original MCNP neutron benchmark suite contains nine cases from three different experimental configurations, numbered 1, 3, and 7. The principal distinction among the three configurations is the material at the end of the duct. In configuration 1, the end of the duct was completely open. In configuration 3, a block of stainless steel 304 that was 30.48 cm (12 inches) thick was placed at the end of the duct. In configuration 7, a 35.56-cm (14-inch) block of stainless steel was placed at the end of the duct, and two sets of alternating blocks of borated polyethylene and stainless steel were appended to it. Each of the latter blocks was 5.08 cm (2 inches) thick.

Detectors were either aligned with (“on”) the axis of the duct or displaced to the side (“off”). The “on” detectors were 154.5 cm from the source, while the location of the “off” detectors varied from one configuration to another. The “off” detectors for configuration 3 were displaced from the “on” detector by slightly more than 100 cm, while the “off” detectors for configuration 7 were displaced by 46 cm.

Five of those nine cases have been selected for inclusion in the radiation shielding validation suite, as shown in Table 4. These cases include the on-axis calculation for configuration 1 and both an on-axis and an off-axis calculation for configurations 3 and 7. Configuration 1 included no intermediate material (other than air) between the target and the detector. Consequently, only an “on” measurement for that neutron spectrum was modeled.

Table 4. Summary of MCNP Radiation Shielding Validation Suite: Fusion Shielding

Configuration	Tally Type	On / Off Axis
1	neutron	On
3	neutron	Off
3	photon	On
7	neutron	On
7	photon	Off

Two of the cases are coupled neutron-photon problems with photon detectors. Consequently, these cases test the capability of MCNP to replicate responses from both neutron and photon detectors.

The input files for each of these cases have been updated to use the ENDF60 library. In addition, they have been standardized to use 1,000,000 neutron histories.

For the coupled neutron-photon calculations, the ENDF60 neutron data from ENDF/B-VI is augmented with photon data form the MCPLIB02 photon data library.[19] MCPLIB02 is part of the ENDF60 library release, but it is not based on ENDF/B-VI. Instead, it is an extension of the original MCPLIB photon library that has been used with MCNP for more than 20 years. Specifically, it extends the range of data for photon interactions up to 100 GeV, based on the Lawrence Livermore National Laboratory Evaluated Photon Data Library.[20]

The MCNP4C2 calculations produce reasonably good agreement with the measurements. For example, Figure 1 compares the measured and predicted results for the first case.

C. Photon Dose Rates

The cases in the last subset of the radiation shielding validation suite are based on experimental measurements of photon dose rates. The first case is based on a 1980 measurement of air-scattered photon radiation far from the source (“skyshine”).[21] The second case is an idealization of a number of measurements of the radiation environment in an open field covered by fallout.[22] The remaining four cases model some of the Hupmobile thermoluminescent dosimeter (TLD) experiments performed at Lawrence Berkeley Laboratory between 1967 and 1969.[23,24] The six cases are summarized in Table 5.

Table 5. Summary of MCNP Radiation Shielding Validation Suite: Photon Dose Rates

Case	Source	Principal Media
Skyshine	^{60}Co	Air and Soil
Air over Ground	^{60}Co	Air and Soil
^{60}Co through Air	^{60}Co	Air
^{60}Co through Teflon	^{60}Co	Teflon
Sm K_α through Air	Sm K_α	Air
Sm K_α through Teflon	Sm K_α	Teflon

All of the MCNP calculations for these cases use the MCPLIB02 photon data library[19] for all nuclides, and all of them employ 1 million photon histories. As noted previously, MCPLIB02 is part of the ENDF60 library release, but it is not based on ENDF/B-VI. Instead, it is an extension of the original MCPLIB photon library that has been used with MCNP for more than 20 years. Speci-fically, it extends the range of data for photon interactions up to 100 GeV, based on the Law-rence Livermore National Laboratory Evaluated Photon Data Library.[20]

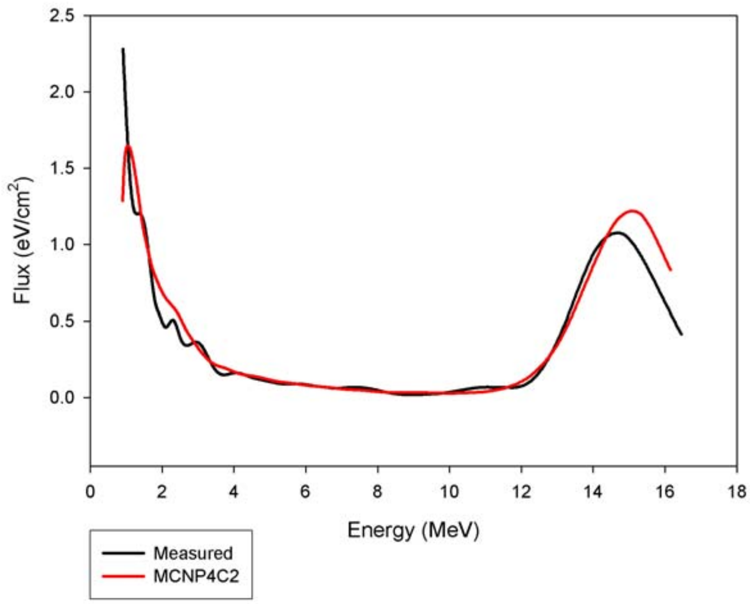

Figure 1. Neutron spectra for fusion shielding configuration 1.

In the skyshine experiment, a collimated gamma-ray source was placed at ground level in an open field. The resulting dose rates and differential flux densities then were measured by detectors on the ground out to 700 m from the source, in intervals of 100 m.

Figure 2 compares the MCNP4C2 results with the measured data. Agreement is reasonably good, although MCNP slightly overpredicts the dose rate at the larger distances.

In the model of the air-over-ground case, a ^{60}Co gamma-ray source was distributed uniformly over a flat, infinitely wide and deep medium of soil covered by an infinitely wide and high medium of air. The buildup factor in air three feet above the ground was calculated, as was the angular kerma rate.

MCNP4C2 produces a buildup factor of 1.20. This value falls within the range of experimental measurements (1.15 to 1.38).[25]

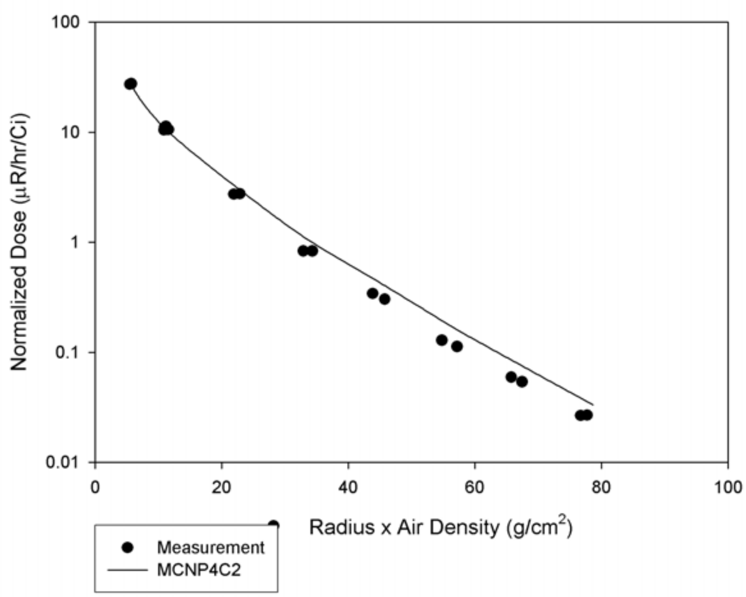

Figure 2. Normalized dose rates for skyshine case.

The Hupmobile TLD experiments employed a 1-foot-long teflon cylinder with TLDs imbedded in it along its axis. A point source of gamma rays or x-rays then was placed 1 m from one end of the cylinder, directly across from that end. An additional TLD, used for normalization, was placed 1 m on the other side of the source. Six different sources were studied, and the most energetic (^{60}Co, which emits 1.33 and 1.17 MeV gamma rays) and the least energetic (Sm K_α X-rays, emitted at 39.9 KeV) were selected for inclusion in the validation suite. For the sake of computational efficiency, the calculations for the normalization TLDs are performed separately from those for the TLDs in the teflon cylinder. Consequently, four separate calculations are included in the suite.

The dose rates from MCNP4C2 for the TLDs embedded in the teflon cylinder, relative to the dose from the normalization TLD, are shown in Figure 3. The agreement with the measured values is generally quite good, except for the bump in the dose at approximately 3.5 cm into the teflon for the case with the ^{60}Co source. This anomaly also was observed in the results presented in the previous report.[26]

D. Computer Resource Requirements
Execution of the radiation shielding validation suite requires a significant expenditure of computer resources. The results reported in Table 6 were obtained from a Silicon Graphics Origin 2000 supercomputer with a clock speed of 250 MHz, running in sequential (single-processor) mode.

Table 6. Computer Resource Requirements for Radiation Shielding Validation Suite

Case	CPU Time (Minutes)
Pulsed Spheres: Beryllium	3.23
Pulsed Spheres: Carbon	4.24
Pulsed Spheres: Concrete	5.44
Pulsed Spheres: Iron	3.63
Pulsed Spheres: Lead	8.23
Pulsed Spheres: ^{6}Li	12.37
Pulsed Spheres: Nitrogen	10.09
Pulsed Spheres: Water	7.04
Fusion Shielding: 1, Neutron, On	12.48
Fusion Shielding: 3, Neutron, Off	13.02
Fusion Shielding: 3, Photon, On	131.21
Fusion Shielding: 7, Neutron, On	13.38
Fusion Shielding: 7, Photon, Off	135.16
Photon Dose: Skyshine	18.14
Photon Dose: Air over Ground	15.94
Photon Dose: ^{60}Co through Air	0.83
Photon Dose: ^{60}Co through Teflon	43.38
Photon Dose: Sm K_α through Air	0.65
Photon Dose: Sm K_α through Teflon	197.93
Total	636.39

(Silicon Graphics Origin 2000 supercomputer, 250 MHz)

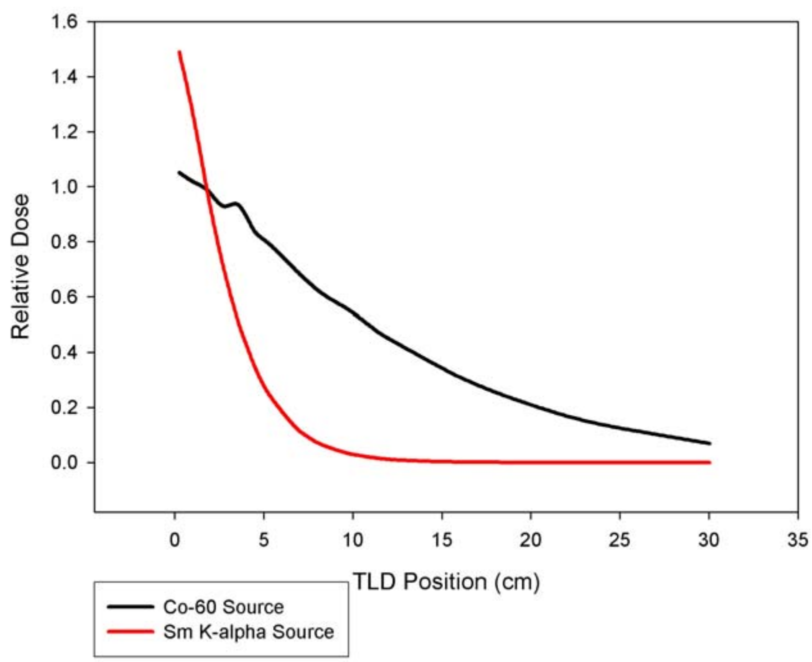

Figure 3. Normalized dose rates for Hupmobile TLD cases.

The overall time is approximately 10½ CPU hours. On a PC running Windows 2000 with 256 MB of RAM and a clock speed of 800 MHz, the suite takes approximately 6 CPU hours.

Nearly ⅓ of the CPU time is consumed by a single case, Sm K_α transmission through teflon. This case takes more than 4 times as long as the corresponding case with a ^{60}Co source because the photon energy is lower and therefore the mean free path is shorter.

The bulk of the remaining time is consumed by the two coupled neutron-photon cases. The reason that these two cases take so much longer than the neutron-only cases is that an energy cut-off can be applied at the lower end of the detector range (0.85 MeV) for the latter cases. However, no such cut-off for neutron energies can be employed for the coupled neutron-photon cases, because low-energy neutrons can produce photons with energies that exceed the sensitivity threshold of the photon detector (0.75 MeV).

IV. CONCLUSIONS

Two validation suites, one for criticality and the other for radiation shielding, have been assembled for the MCNP Monte Carlo code. The suites provide an indication of the accuracy of MCNP and its associated libraries. More importantly, the suites provide a basis to assess the impact of future improvements to the MCNP methodology and changes to its associated nuclear data libraries.

Execution of the validation suites requires a significant expenditure of computer resources. The criticality validation suite consumes nearly 19 CPU hours on a Silicon Graphics Origin 2000 supercomputer with a clock speed of 250 MHz, running in sequential (single-processor) mode. The radiation shielding validation suite requires approximately 10½ CPU hours on the same computer. A Pentium III PC with 256 MB of RAM and a clock speed of 800 MHz running the Windows 2000 operating system is somewhat faster. It requires approximately 11 CPU hours for the criticality suite and approximately 6 CPU hours for the radiation-shielding suite.

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