SANDIA REPORT

SAND2010-6830
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September 2010

Simulations of Neutron Multiplicity Measurements with MCNP-PoliMi

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Abstract

The heightened focus on nuclear safeguards and accountability has increased the need to develop and verify simulation tools for modeling these applications. The ability to accurately simulate safeguards techniques, such as neutron multiplicity counting, aids in the design and development of future systems. This work focuses on validating the ability of the Monte Carlo code MCNPX-PoliMi to reproduce measured neutron multiplicity results for a highly multiplicative sample. The benchmark experiment for this validation consists of a 4.5-kg sphere of plutonium metal that was moderated by various thicknesses of polyethylene. The detector system was the nPod, which contains a bank of 15 3He detectors. Simulations of the experiments were compared to the actual measurements and several sources of potential bias in the simulation were evaluated. The analysis included the effects of detector dead time, source-detector distance, density, and adjustments made to the value of ν-bar in the data libraries. Based on this analysis it was observed that a 1.14% decrease in the evaluated value of ν-bar for 239Pu in the ENDF-VII library substantially improved the accuracy of the simulation.

Acronyms

BeRP	Beryllium reflected plutonium
HDPE	high-density polyethylene
LANL	Los Alamos National Laboratory
nPOD	portable neutron multiplicity counter
RSICC	Radiation Safety Information Computational Center
SINBAD	Shielding Integral Benchmark Archive and Database

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1 Introduction

New applications of Monte Carlo codes must be validated against measurements before they can be used reliably to predict system performance. To improve the understanding of the ability of Monte Carlo codes to simulate neutron multiplicity measurements for highly multiplicative samples, a series of measurements were taken using a 4.5-kg sphere of alpha(α)-phase plutonium metal surrounded by a polyethylene moderator. Previous benchmarks evaluating the ability of MCNP-PoliMi to reproduce neutron multiplicity measurements have demonstrated that MCNP-PoliMi can successfully reproduce results for low multiplication samples in an Active Well Coincidence Counter (**Error! Reference source not found.**,**Error! Reference source not found.**).

2 Experimental Setup

The source for this series of experiments was the beryllium-reflected plutonium (BeRP) ball, a 4.5-kg sphere of 94% ^{239}Pu α-phase plutonium metal.[1] The sphere is clad in stainless steel 0.3 mm thick. It was measured bare and reflected by a series of nesting high-density polyethylene (HDPE) shells with total thicknesses of 1.27, 2.54, 3.81, 7.62, and 15.24 cm. In addition to altering the neutron leakage spectrum from the source, these reflectors caused the neutron multiplication to vary between 4.4 and 17.1. Figure 1 shows the plutonium source and reflectors.

Figure 1: Plutonium metal sphere and polyethylene reflectors

The source was measured with a portable neutron multiplicity counter (the nPod) designed and constructed by LANL. The nPod uses fifteen 15-inch-long, 1-inch-diameter, 10 atm, ^{3}He proportional counters embedded in an HDPE moderator block 16.6 inches tall, 16-30/32 inches wide, and 4 inches deep. The moderator is wrapped in 1/32-inch-thick cadmium to minimize the nPod's sensitivity to neutrons reflected by the floor and walls.

The nPod was positioned with its front face 50 cm from the center of the BeRP ball. The BeRP ball was aligned with the horizontal and vertical centerlines of the nPod moderator block. The BeRP ball and nPod were set on a carbon steel table with a 2.7-mm-thick shelf 1.06 m above the floor. Figure 2 illustrates the experimental setup.

[1] This plutonium source was originally constructed by Los Alamos National Laboratory (LANL) in the 1980s for criticality safety experiments with beryllium reflectors. Hence, it was dubbed the "beryllium-reflected plutonium", or BeRP ball. Beryllium reflectors were not used in the experiments described in this report.

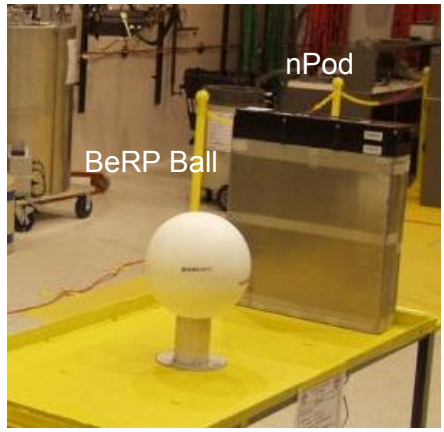

Figure 2. Polyethylene sphere and nPod detector

A more detailed description of the experimental setup is available in reference **Error! Reference source not found.**, which can be obtained from the Radiation Safety Information Computational Center (RSICC) as part of the May 2010 release of the Shielding Integral Benchmark Archive and Database (SINBAD).

In addition, the six measurements of the BeRP ball were repeated with a ^{252}Cf pellet source in place of the BeRP ball. These simpler measurements provide a basis for validating models of the reflector, of the nPod, and of the environment independent from the model of the BeRP ball.

3 Simulation

The Monte Carlo code MCNPX-PoliMi was tested against this series of experiments. MCNPX-PoliMi is a version of MCNPX v2.6.0 that has been modified to improve its ability to simulate correlated-particle measurements. Improvements have been made in the order of the physics sampling routines and to the number of neutrons and photons released from fission events (sampled from the full distributions.) MCNPX-PoliMi includes built-in energy spectra of several commonly encountered neutron sources (e.g., ^{252}Cf, ^{240}Pu, ^{238}U, Am/Li, Am/Be, ^{238}Pu(α,n), etc.) In addition MCNPX-PoliMi generates a specialized output file containing information about all events in a specified detector volume that is relevant to detector response calculation.

The experimental setup modeled in MCNPX-PoliMi included the nPod, BeRP ball, polyethylene reflectors, the table, the BeRP ball stand, air, and the floor. Figure 3 shows an image of the MCNPX-PoliMi model geometry.

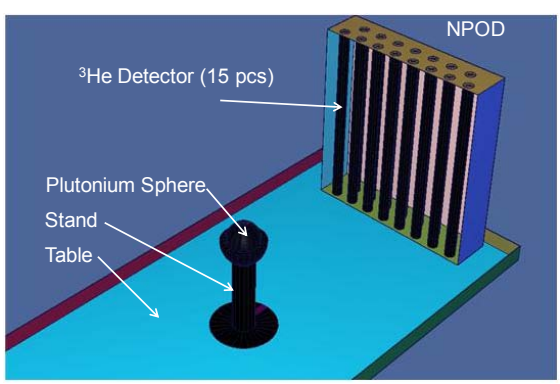

Figure 3. MCNPX-PoliMi experimental model

The detector output file produced by MCNPX-PoliMi lists detailed information about each event that occurred in each of the 15 ^{3}He detectors within the nPod. With this information it is possible to calculate the response of the nPod. A FORTRAN post-processing code was developed to perform this calculation, which requires taking into account the dead time of the individual ^{3}He detectors, an effect that cannot be simulated in MCNPX-PoliMi. The post-processor sorts all of the capture events on ^{3}He that correlate to events detected by the nPod. After the events are collected, they are sorted by time. At this point, the 4-µs dead time is applied to remove events that would not have been seen during the measurement. After the input events are cleaned, the neutron multiplicity distribution is calculated. This distribution is then used to compare the results of the simulation to the measurement.

4 Baseline Models

To establish a baseline for comparing of various alterations in the geometry or simulation parameters the experimental setup was modeled using the details recorded from the measurement without any alterations. A comparison was made between the simulated neutron multiplicity distributions and the measured neutron multiplicity distributions. To evaluate the accuracy of the simulation the percent deviations from the measured mean and variance values were calculated.

4.1 252Cf Models

The baseline ^{252}Cf results have excellent agreement with the measured data in all experimental configurations (Figure 4.) The maximum observed deviation in the mean was 2.08% and 2.75% for the variance. The excellent agreement shown by the ^{252}Cf simulations validates MCNPX-PoliMi model or the polyethylene reflectors and the nPod detector as well as the post-processing code developed to determine the multiplicity distributions.

These results are consistent with other measurements of ^{252}Cf that were taken at the Joint Research Center in Ispra, Italy (4). Figure 5 shows the neutron multiplicity distributions for a 200,000 neutron per second ^{252}Cf source.

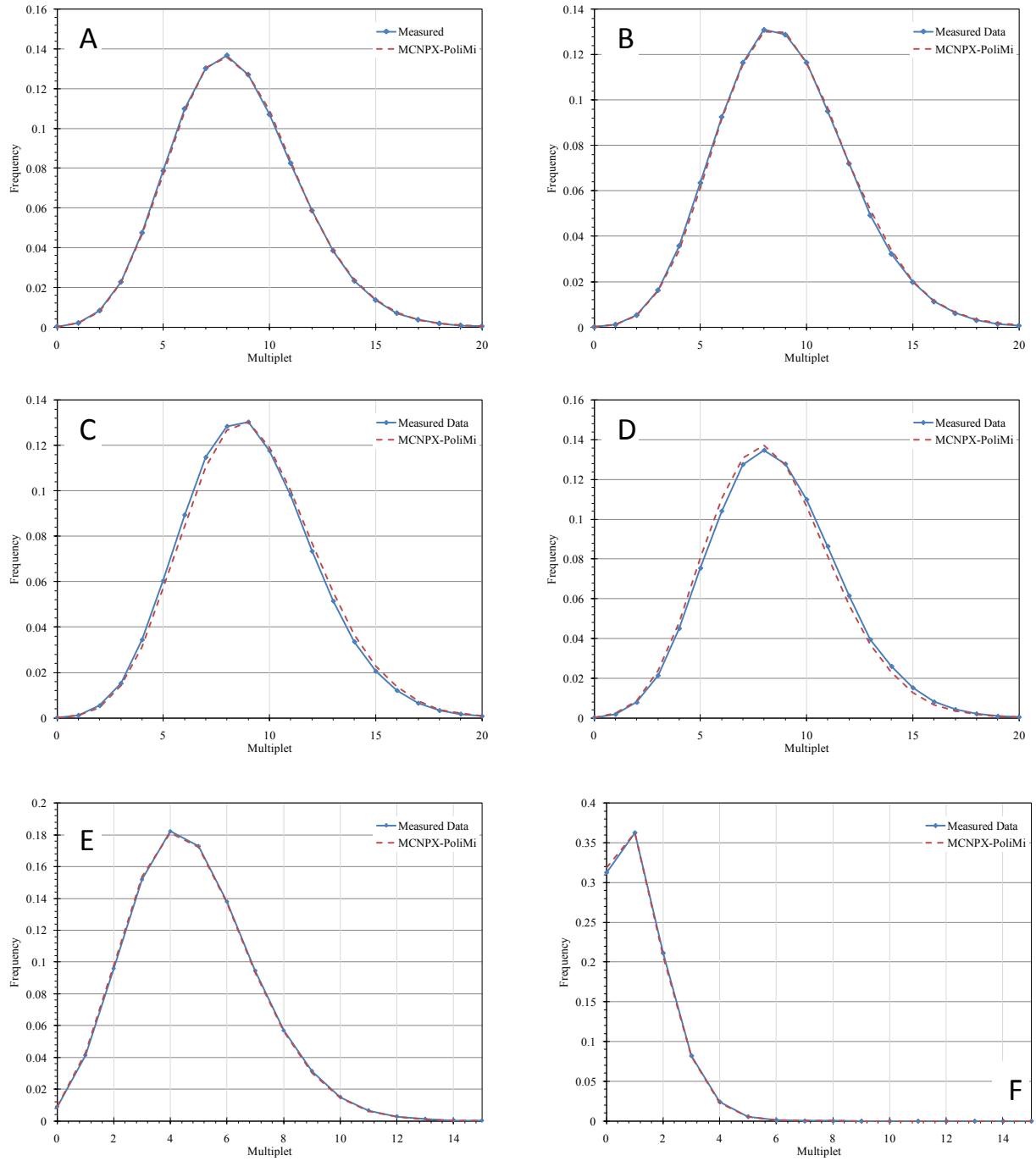

Figure 4. Comparison between measured and simulated neutron multiplicity distributions for the ^{252}Cf source A) Bare sphere, B) 0.5-inch moderated, C) 1.0-inch moderated, D) 1.5-inch moderated, E) 3.0-inch moderated, F) 6.0-inch moderated

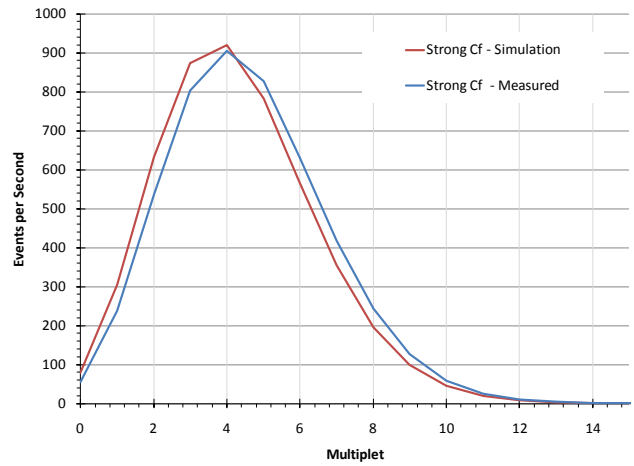

Figure 5. Comparison of simulated and measured results for a 252Cf source in Ispra, Italy (4)

4.2 Plutonium Sphere Models

When the baseline simulations are evaluated for the plutonium sphere there is a noticeable over-bias observed in all cases (shown in Figure 6). These results were generated using the full induced fission neutron distribution provided by Terrell. The results are shown in tabular form in Table 1. The maximum observed deviation in the mean is 12.93% and in 40.96% in the variance. There is a general trend of increasing deviation as the multiplication of the system increases, as shown in Figure 7.

Table 1. Summary of Results from the Baseline Simulation of the Plutonium Sphere

Reflector	k-effective	Multiplication	Percent Deviation From Experiment	
None	0.7768	4.4803	Mean	4.16
			Variance	6.37
0.5"	0.8298	5.8754	Mean	9.04
			Variance	14.11
1.0"	0.8715	7.7797	Mean	12.83
			Variance	27.82
1.5"	0.9049	10.5152	Mean	12.76
			Variance	32.68
3.0"	0.9390	16.3961	Mean	12.93
			Variance	40.96
6.0"	0.9437	17.7651	Mean	9.41
			Variance	26.84

With the validation of the MCNPX-PoliMi model and post-processing codes with the ^{252}Cf data, the over-bias in the plutonium data must come from a problem with the model of the BeRP ball or a problem in the physics simulation.

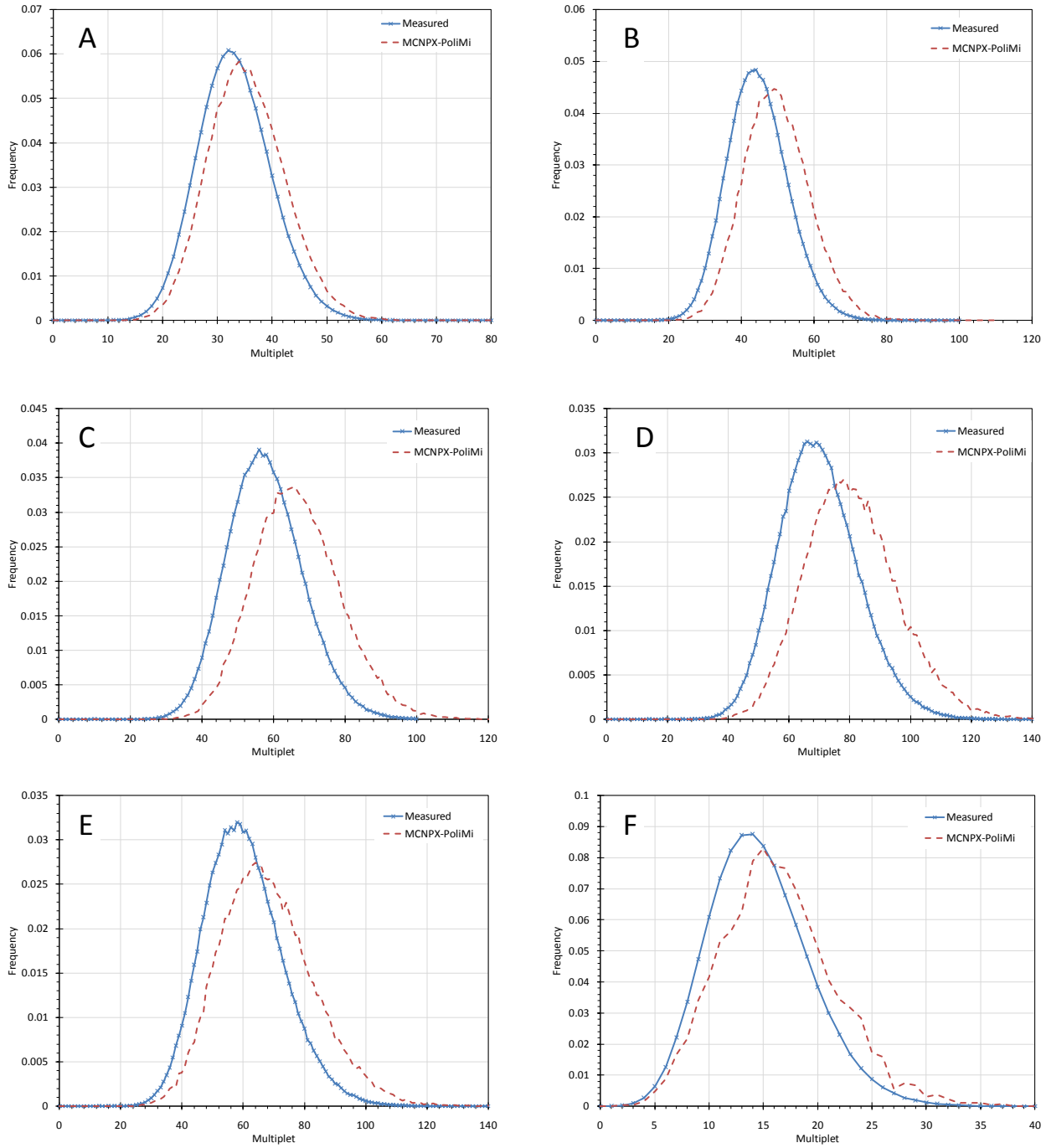

Figure 6. Comparison between simulated and measured neutron multiplicity distributions for the baseline plutonium sphere results. A) Bare sphere, B) 0.5-inch moderated, C) 1.0-inch moderated, D) 1.5-inch moderated, E) 3.0-inch moderated, F) 6.0-inch moderated

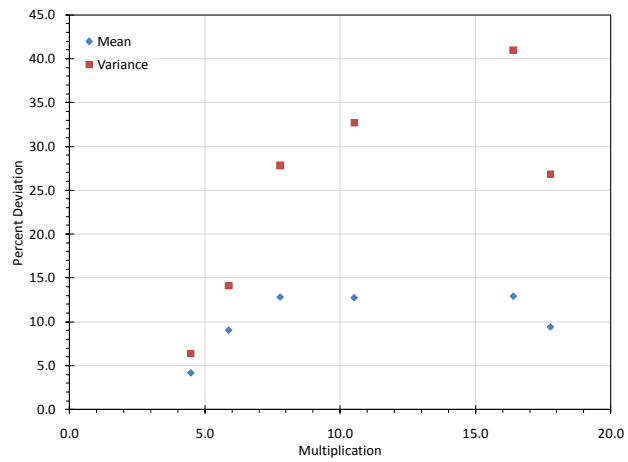

Figure 7. Deviation in the Mean and Variance as a Function of Multiplication

5 Sensitivity Analysis

To identify the cause of the over-bias, the following parameters were investigated:

- Source/Detector Distance
- Dead time effects
- Count rate dependent effects
- Volume of the plutonium sphere
- Density of the plutonium sphere
- ν-bar value for ^{239}Pu

Ideally, one change in one of these parameters will provide a significantly improved result for all of the plutonium cases.

5.1 Source/Detector Distance

Increasing the distance between the nPod detector and the plutonium sphere will result in a decrease in the mean of the neutron multiplicity distribution. The accuracy of the distance measurements during the actual experiment was estimated to be approximately ± 1 cm. By determining the magnitude of the distance needed to correct the over-prediction, the feasibility of distance as the cause for the discrepancy can be evaluated.

In Figure 8, the change in distance needed to correct the distribution for the bare sphere is approximately a 1-cm increase in the source/detector distance, which is reasonable. However, the amount of distance needed to adjust the 1.5-inch moderated sphere will be between 3 and 4 cm. This shift is much greater than the position uncertainty in the measurement. Similar large distance shifts were needed for the other moderated cases. Due to this large shift needed for the moderated cases, a measurement error in the source/detector distance is unlikely to be the cause for the observed over-bias.

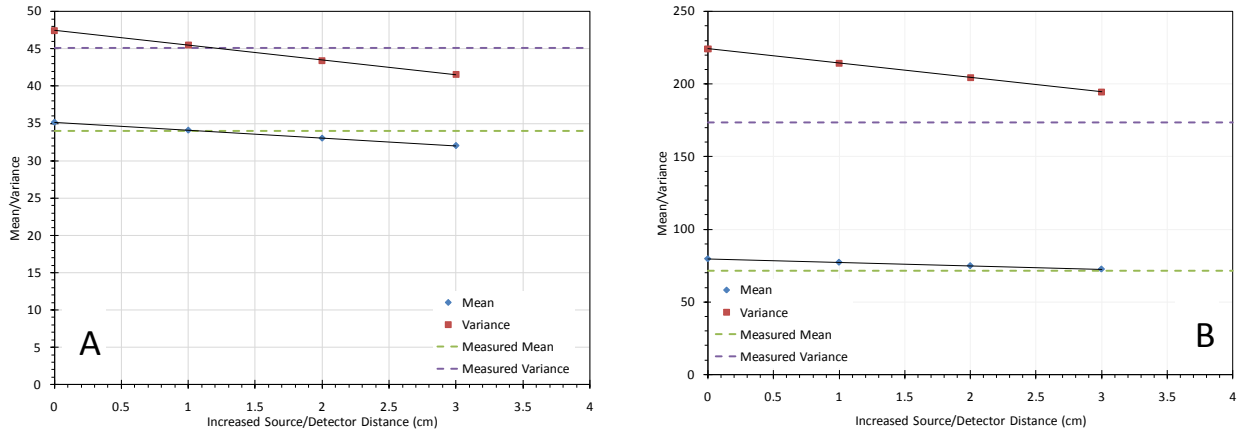

Figure 8. A) Effect of Distance on the Bare Sphere B) Effect of Distance on the 1.5-inch Moderated Sphere

5.2 Dead time

The dead time of the nPod detector ^{3}He tubes could also account for the over-prediction that was observed in the plutonium sphere results. If the dead time was increased, then it would result in the distribution shifting in the correct direction. The simulated dead time was 4 µs. To evaluate the accuracy of that number, the autocorrelation functions for the nPod detector tubes were determined. Several cases with varying count rates are shown in Figure 9.

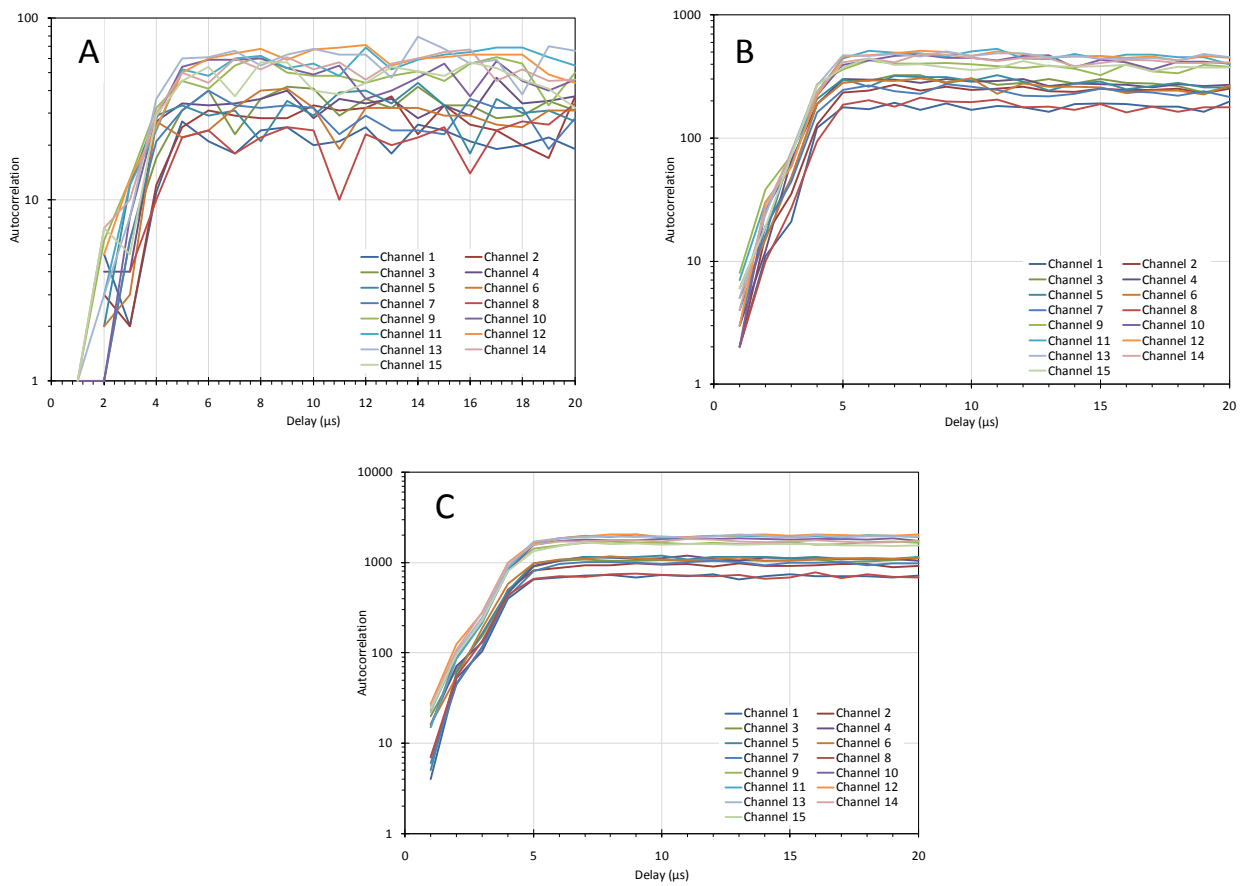

Figure 9. A) Autocorrelation function for the bare Cf source (2004 counts per second) B) Autocorrelation function for the 1.5-inch moderated Pu sphere (17527 counts per second) C) Autocorrelation function for a strong AmBe source (11933 counts per second)

As shown in Figure 9, the dead time is consistently 4-5 µs regardless of the count rate. The dead time is shown as the time until the plateau region is reached. This clearly shows that the dead time was correctly modeled and that there were no count-rate-dependent effects altering the dead time.

With the correct dead time known an investigation to determine the effect of small perturbations was performed to determine the sensitivity of the system to changes in dead time and to determine the increase in dead time required to correct the plutonium results.

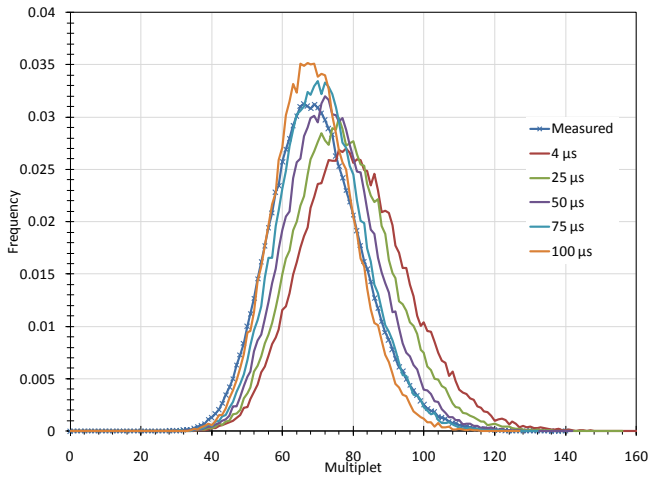

Figure 10. Effect of Dead time on the 1.5-inch moderated Pu sphere

As shown in Figure 10 the dead time needed to adjust the 1.5-inch moderated plutonium case is approximately 50 to 75 µs, a change that is much too large to be reasonable. Based on this analysis, it can be concluded that the dead time is modeled correctly and that a small shift in the dead time is not responsible for the observed over bias.

5.3 Volume

Due to the fabrication process for the BeRP ball, there is some uncertainty in the exact dimensions in the radius of the sphere. It is believed that the sphere is completely α-phase plutonium with a density of 19.60 g/cm^3. However, the plutonium sphere is encased in a stainless steel shell that is slightly larger than the outer radius of the plutonium. Therefore, it is possible that the plutonium sphere is slightly larger than predicted and the density is slightly less than the predicted value. The effect of increasing the radius of the sphere while maintaining the mass of the plutonium was investigated.

The minimum density that the sphere could have while preserving the mass and still fitting inside the known dimensions of the stainless steel shell is 19.08 g/cm^3. Figure 11 shows the trends in the values of the mean and the variance for the bare and 1-inch moderated cases. The bare case reaches a best match with the measured data with a density of approximately 19.1 g/cm^3. However, the1-inch moderated case would need a volume increase that would exceed the dimensions of the stainless steel shell. This same result was seen for the other moderated cases as well. Also as shown in Figure 11, there is no single change in density for the sphere that can correct all of the over-bias observed in the plutonium cases.

Based on this analysis, the authors concluded that the density of the plutonium sphere is not responsible for the large observed over-bias.

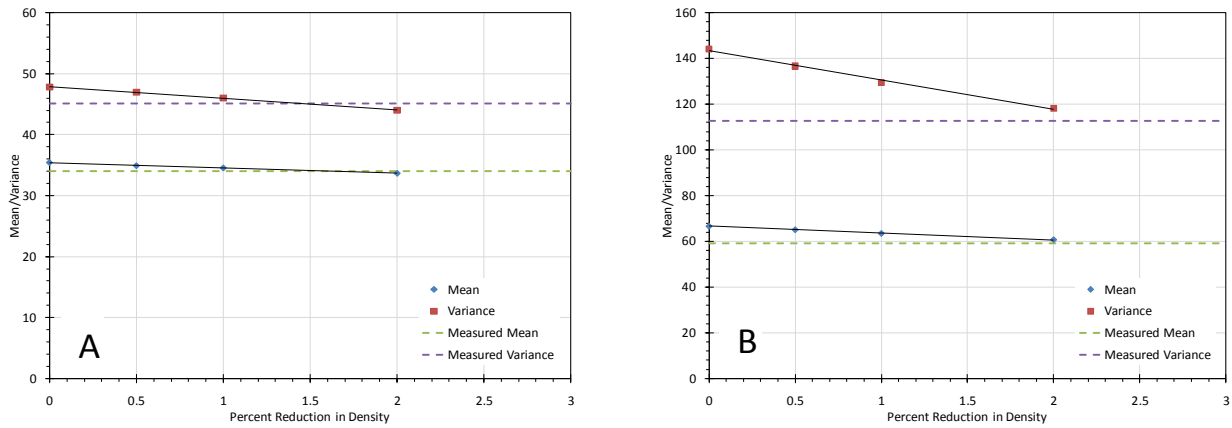

Figure 11. A) Effect of Density on the Bare Pu Sphere B) Effect of Density on the 1-inch Moderated Pu sphere

5.4 Density/Mass

The mass of the plutonium sphere is well known. However, a net change in the mass can be used to simulate a net change in the reaction cross sections for ^{239}Pu. To test this effect, the density of the plutonium was reduced without adjusting the radius, effectively reducing the mass of the sphere.

The analysis of the density determined that the optimal change in density that would reduce the error on both the mean and the variance for all of the plutonium cases was a 1.76% decrease in the density. With the new density of 19.25 g/cm^3, the mass of the sphere would be 4403.9g. This is a loss of 79.9g of plutonium or a 1.76% decrease in the total macroscopic cross section. With this optimal adjustment in the amount of mass in the sphere, the maximum deviation in the mean was 9.12% and 7.86% in the variance across all six measurements.

However, a net decrease in the cross section is unlikely to be the cause of the discrepancy that was observed in the baseline BeRP ball simulations. Measurements taken with the nPod detector of MOX fuel samples in Ispra, Italy, have shown that MCNP-PoliMi is able to accurately predict the neutron multiplicity distribution as shown in Figure 12 (4). This demonstrates that the cross sections should be accurate and that the observed discrepancy in the baseline case is a function of the high level of multiplication in the system.

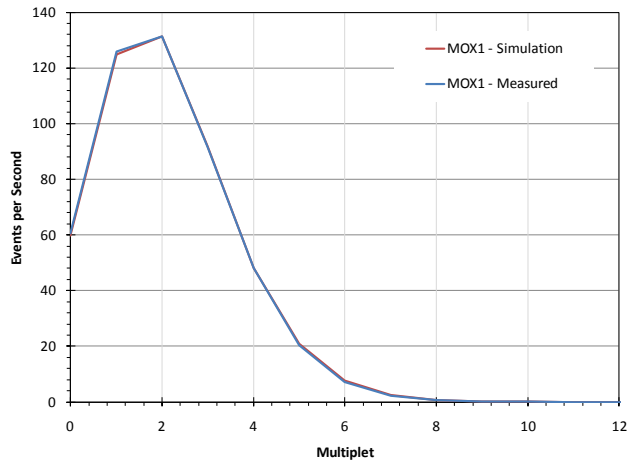

Figure 12. Comparison of the measured and simulated neutron multiplicity distribution for a MOX sample (4).

5.5 ν-Bar

It is common practice when establishing the nuclear data libraries to adjust the values of ν-bar to ensure that the results to certain benchmark criticality experiments are correctly simulated. The deviation of the value of ν-bar set in the data libraries can be clearly seen at energies below 2 MeV in Figure 13.

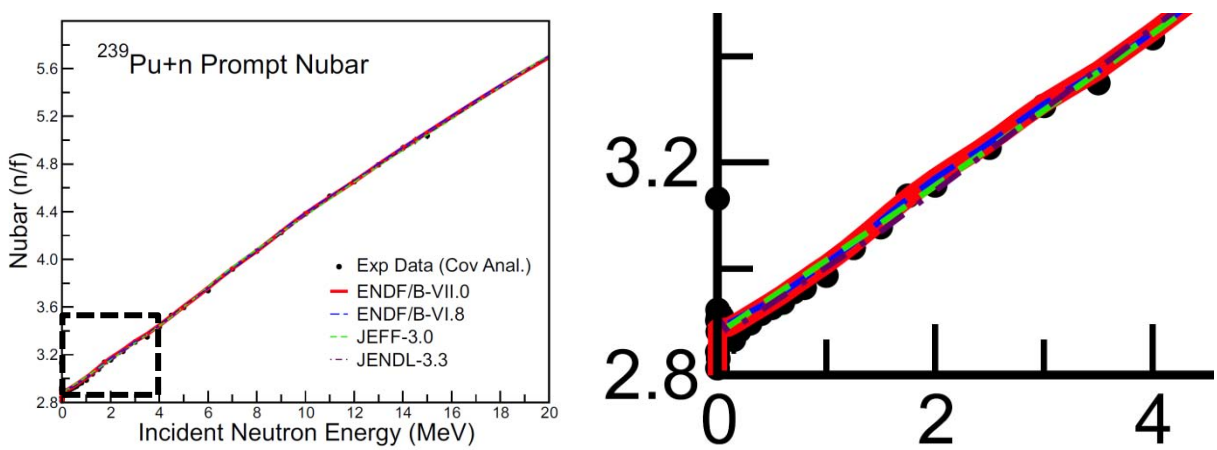

Figure 13. Prompt Fission neutron multiplicity ν-Bar compared to experimental data, with the boxed section enlarged on the right ()

This deviation between experiment and the values included in the data libraries are acknowledged in the ENDF/B-VII paper:

> *The most serious departure from the covariance data occurs below 1.5 MeV, where the evaluation lies about two standard deviations above the experimental data. This difference, however, was influenced strongly by the desire to match the integral data results for the JEZEBEL fast critical experiment.*

To determine if the adjustment made in the value of ν-bar was responsible for the observed over-bias in the plutonium results, it was lowered in the sampling subroutines. An optimal value of ν-bar was

determined by determining a best fit line for the mean and variance of each case, then using these fits to find the ν-bar value that would minimize the error in all simulated plutonium cases. The optimal change in ν-bar was a 1.14% decrease in the nominal value. A change of -1.14% seems reasonable when comparing the measured values of ν-bar to the experiment in Figure 13. The adjusted distributions for all plutonium cases are shown in Figure 14.

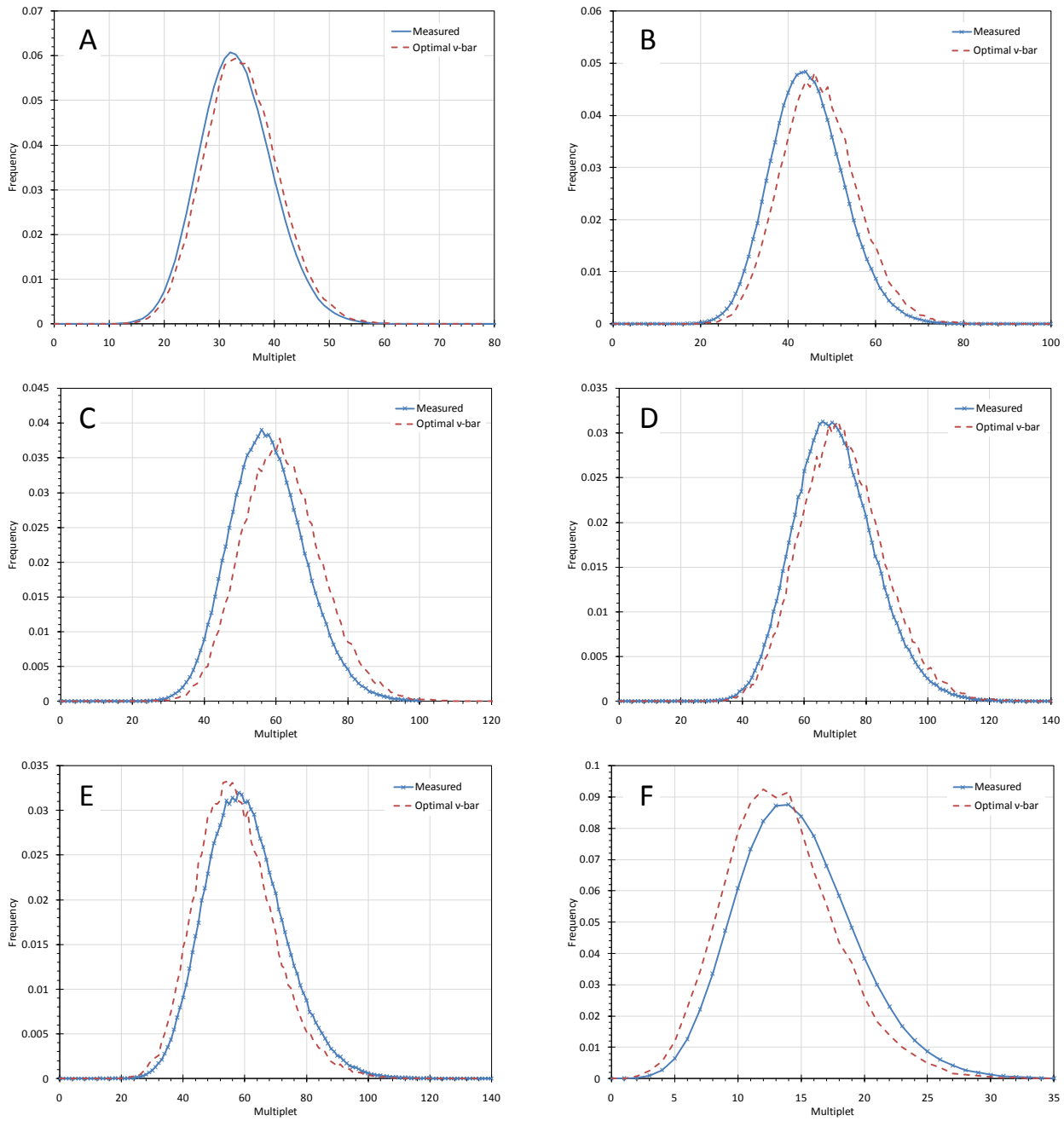

Figure 14. Comparison between the simulated and measured neutron multiplicity distributions for the -1.14% adjustment to ν-bar A) Bare sphere, B) 0.5-inch moderated, C) 1.0-inch moderated, D) 1.5-inch moderated, E) 3.0-inch moderated, F) 6.0-inch moderated

Figure 14 shows a clear improvement over the baseline cases shown in Figure 6. The maximum deviation in the mean is now 10.36% and the maximum deviation in the variance is 11.57%, both in the 6-inch moderated case. These numbers are slightly higher than the improvement observed with the changes made in the density of the sphere; however, an adjustment to the value of ν-bar, which is known to be increased, makes this a better correction over changing the magnitude of the cross sections. A summary of the results for the plutonium runs using the optimized data is shown in Table 2.

Table 2. Comparison of Results between the Baseline and Adjusted ν-bar Simulation of the Plutonium Sphere

Reflector		Percent Deviation from Experiment (ENDF VII ν-bar)	Percent Deviation from Experiment (Adjusted ν-bar)
None	Mean	4.16	0.31
	Variance	6.37	-0.08
0.5”	Mean	9.04	3.36
	Variance	14.11	4.35
1.0”	Mean	12.83	4.44
	Variance	27.82	9.39
1.5”	Mean	12.76	1.27
	Variance	32.68	3.79
3.0”	Mean	12.93	-5.37
	Variance	40.96	-5.74
6.0”	Mean	9.41	-10.36
	Variance	26.84	-11.57

The improvement observed with the adjusted ν-bar values is dramatic. There is improvement in all cases, except the mean on the 6-inch case. However, the optimal ν-bar was selected to reduce the combined error on all cases. ν-bar is an energy-dependent value and it is possible that an energy-dependent correction to ν-bar would alleviate the somewhat large bias still present in the 6-inch case.

5.6 Distance adjustment applied to optimal ν-bar

As shown, a single, uniform reduction to the value of ν-bar given in the nuclear data libraries offers dramatic improvement to all of the plutonium cases. With this optimal ν-bar in place the effect of varying the source/detector distance was revisited. With the added correction of the adjusted ν-bar the amount of distance required to improve the simulation is considerably smaller. The optimal distance adjustments needed for the adjusted ν-bar plutonium cases are shown in Table 3.

Table 3. Optimum Changes in source/detector distance with a modified ν-bar

Reflector	Optimum Change in Distance (cm)
None	-0.04
0.5”	-0.21
1.0”	-1.57
1.5”	-0.59
3.0”	1.16
6.0”	0.52

The required distance needed to further improve the results is considerably less than without the correction on ν-bar. The largest correction needed is 1.57 cm, which is pushing the upper limits on the measurement error, yet these distance corrections appear more feasible. It is also likely that with an energy-dependent correction of ν-bar these values would be even smaller.

5.7 Case-dependent optimal ν-bar

In addition to determining the adjusted value of ν-bar that would reduce the error in all cases simultaneously, the optimal value of ν-bar was also determined for each individual case. Table 4 shows the mean and the variance for each individually optimized case.

Table 4. Values for Individually Optimized ν-bar Values

Reflector	Average Energy Inducing Fission (MeV)	Percent Change in Nominal ν-bar Value	Percent Deviation from Mean	Percent Deviation from Variance
None	1.9836	-1.15	0.24	0.68
0.5”	1.8409	-1.75	0.71	1.42
1.0”	1.7020	-1.91	-0.06	-1.21
1.5”	1.6005	-1.37	-3.42	-2.10
3.0”	1.5018	-0.95	-3.01	0.11
6.0”	1.4969	-0.56	-3.96	-3.17

As shown in Table 4, if individual ν-bar values are applied, the mean values can be further reduced. This helps demonstrate the effect of an energy-dependent correction to ν-bar because the energy spectrum of neutrons incident on the nPod changes with moderator thickness. Our previous combined optimal value of ν-bar was very close to the best fit value for the bare case. Choosing an optimal ν-bar that fits the higher energy bare case helps explain the large deviation that occurs in the lower energy cases in

Table 2. The case-dependent optimal fits also offer considerable improvement on the appearance of the distributions as well. Figure 15 shows the optimal distributions. All cases show good agreement.

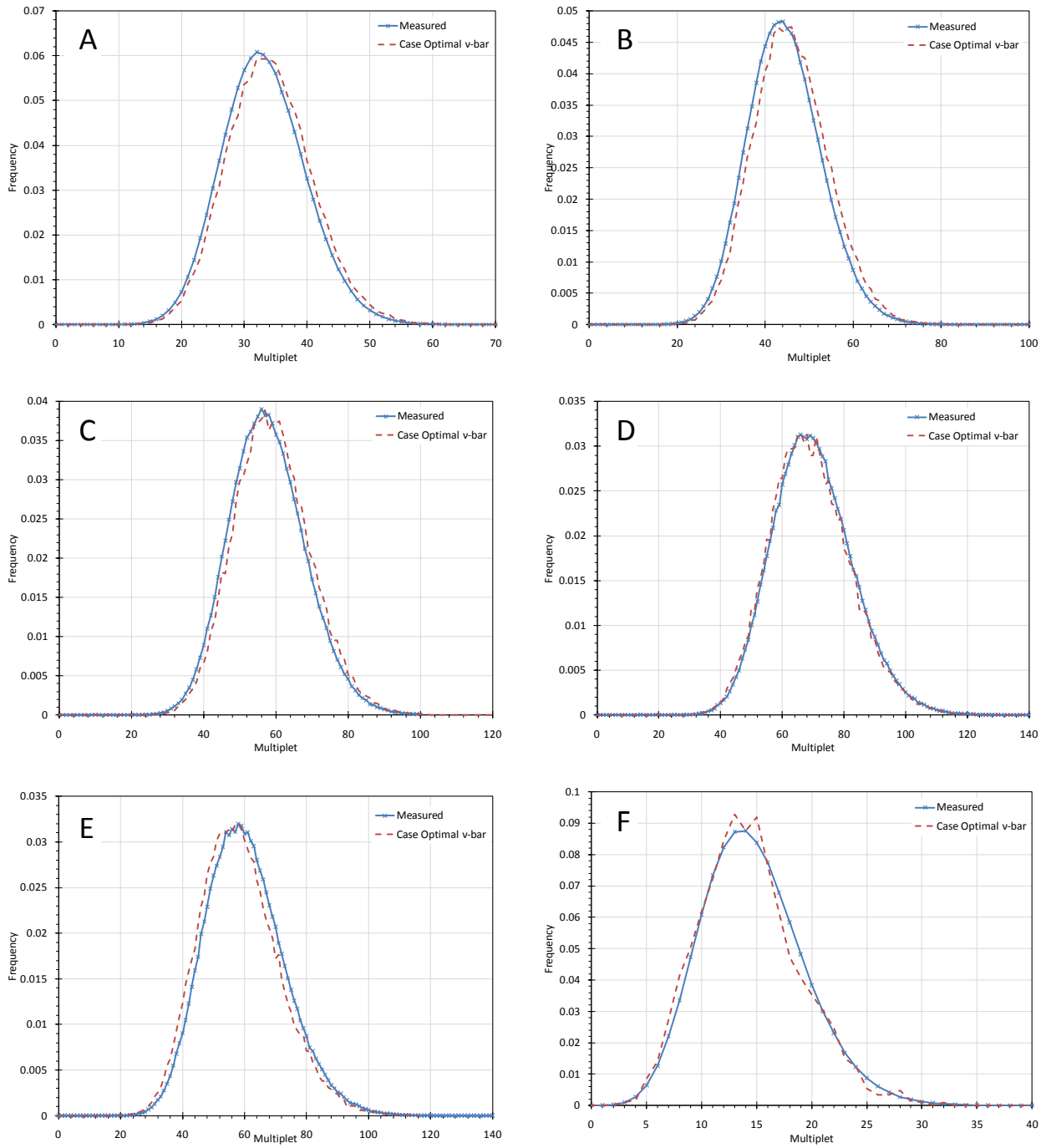

Figure 15. Comparison of the measured and simulated neutron multiplicity distributions for the case dependent optimal ν-bar A) Bare sphere, B) 0.5-inch moderated, C) 1.0-inch moderated, D) 1.5-inch moderated, E) 3.0-inch moderated, F) 6.0-inch moderated

6 Summary

Excellent agreement was observed in the mean and the variance in all cases when compared to the ^{252}Cf experiments. The maximum deviation in the mean was 2.08% and 2.75% in the variance. When the plutonium sphere measurements were modeled, there was significant overestimation of the mean and variance in all of the cases, with a maximum deviation in the mean of 12.93% and 40.96% in the variance.

To determine the cause of the overestimation, several factors were investigated. The authors concluded that factors such as source/detector distance, volume, and density of the plutonium could not adequately account for the observed shift. However, a small change (-1.14%) in the value of ν-bar resulted in a dramatic improvement in all cases.

Despite the significant improvement that resulted from a small change in the evaluated value of ν-bar, there is still room for improvement. The source/detector distance analysis was repeated using the adjusted ν-bar value and the maximum distance needed to adjust the distribution was 1.57cm. Though smaller than the distance corrections required without adjusting the evaluated value of v-bar, this is still larger than the experimental uncertainty in the source/detector distance.

The case-dependent corrections to ν-bar offered additional improvement over the single optimized correction. The largest deviation in the mean was 3.96% and 3.17% for the variance. These values are comparable to the values that were seen for the ^{252}Cf data.

In the future, we will repeat this analysis using original measured values for ν-bar.

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