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Using MCNP6 to Estimate Fission Neutron Properties of a Reflected Plutonium Sphere

Alex Clark, Mark Nelson, Jesson Hutchinson

Abstract

The purpose of this project was to determine the fission multiplicity distribution, $p(\nu)$, for the Beryllium Reflected Plutonium (BeRP) ball and to determine whether or not it changed appreciably for various High Density Polyethylene (HDPE) reflected configurations. The motivation for this project was to determine whether or not the average number of neutrons emitted per fission, $\bar{\nu}$, changed significantly enough to reduce the discrepancy between MCNP6 and Robba, Dowdy, Atwater (RDA) point kinetic model estimates of multiplication. The energy spectrum of neutrons that induced fissions in the BeRP ball, $N_{IF}(E)$, was also computed in order to determine the average energy of neutrons inducing fissions, \bar{N}_{IF} . $p(\nu)$ was computed using the FMULT card, $N_{IF}(E)$ and \bar{N}_{IF} were computed using an F4 tally with an FM tally modifier (F4/FM) card, and the multiplication factor, k_{eff} , was computed using the KCODE card.

Although $N_{IF}(E)$ changed significantly between bare and HDPE reflected configurations of the BeRP ball, the change in $p(\nu)$, and thus the change in $\bar{\nu}$, was insignificant. This is likely due to a difference between the way that \bar{N}_{IF} is computed using the FMULT and F4/FM cards. The F4/FM card indicated that $N_{IF}(E)$ was essentially Watt-fission distributed for a bare configuration and highly thermalized for all HDPE reflected configurations, while the FMULT card returned an average energy between 1 and 2 MeV for all configurations, which would indicate that the spectrum is Watt-fission distributed, regardless of the amount of HDPE reflector. The spectrum computed with the F4/FM cards is more physically meaningful and so the discrepancy between it and the FMULT card result is being investigated. It is hoped that resolving the discrepancy between the FMULT and F4/FM card estimates of $N_{IF}(E)$ will provide better $\bar{\nu}$ estimates that will lead to RDA multiplication estimates that are in better agreement with MCNP6 simulations.

Project Overview

The purpose of this project was to determine the fission multiplicity distribution, $p(\nu)$, for the Beryllium Reflected Plutonium (BeRP) ball for various High Density Polyethylene (HDPE) reflected configurations. As the average energy of neutrons inducing fission, \bar{N}_{IF} , decreases, $p(\nu)$ tends to shift towards lower multiplicities and the average number of neutrons emitted per fission, $\bar{\nu}$, decreases. The motivation for this project was to determine whether or not this energy dependent change in $\bar{\nu}$ was significant enough to reduce the discrepancy between MCNP6 and Robba, Dowdy, Atwater (RDA) point kinetic model estimates of multiplication. The RDA model assumes that all fissions from all fission chains occur simultaneously with the source neutron emission, which works well for fast neutron systems counted by a detection system with a relatively long time constant. This assumption becomes less accurate as the neutron spectrum becomes more thermalized because the increased duration of the fission chains. It was hoped that the change in $\bar{\nu}$ could improve the accuracy of the RDA model multiplication estimate

despite the increase in the lifetime of induced fission chain reactions. In order to determine \bar{N}_{IF} , the energy spectrum of neutrons that induced fissions in the BeRP ball, $N_{IF}(E)$, was also computed.

The BeRP ball is a 4.5 kg sphere of α – phase Weapons Grade Plutonium (WGPu), which is composed primarily of ^{239}Pu (94%) and ^{240}Pu (6%) and has a neutron multiplication of about 4.5. More detailed information about the characteristics of the BeRP ball may be found in the 2007 benchmark [1]. $p(\nu)$ was computed using the FMULT card, $N_{IF}(E)$ and \bar{N}_{IF} were computed using an F4 tally with an FM tally modifier (F4/FM) card, and the multiplication factor, k_{eff} , was computed using the KCODE card [4]. The FMULT card determines $p(\nu)$ by tallying the number of times a fission results in the emission of a certain number of neutrons. Although $p(\nu)$ is tabulated for specific isotopes in the application guide [2], the FMULT card is necessary to compute an “effective” $p(\nu)$ for a material of several fissile isotopes. The FMULT card additionally returns an average energy of neutrons inducing fission. The F4/FM card tallies the number of times a neutron of a particular energy induced a fission. When normalized to the size of each bin width, the tally becomes the energy spectrum of neutrons inducing fission, from which the average energy inducing fissions may be obtained. The KCODE card estimates k_{eff} by generating neutrons in a user specified location and tallying the number of neutrons created vs lost in each generation.

Python was used to process the MCNP6 output files and generate the plots of $p(\nu)$ and multiplication comparisons. Fission multiplicity, tally, and k_{eff} information were extracted from the MCNP6 output files and used to compute fission multiplicity distribution moments, $N_{IF}(E)$ and \bar{N}_{IF} , and neutron multiplication. The RDA point kinetic model of the Feynman Y curve was fitted to BeRP ball list mode data obtained from the nPod neutron multiplicity counter measurements of the BeRP ball to estimate neutron multiplication using the MCNP6 generated values of $\bar{\nu}$ and the Levenberg-Marquardt (LM) algorithm. A description of the experiment and LM fitting may be found in [3]. The MCNP6 and RDA estimates of neutron multiplication were plotted against one another for comparison.

Methods

The MCNP6 model was adapted from the detailed benchmark input deck given in [1]. Included in the model were the BeRP ball, the stainless steel cladding, and a thickness of a HDPE shell. Other entries of the benchmark input deck, such as the aluminum stand and table, were not included. Table 1 summarizes the HDPE thicknesses used. Figure 1 is a cross sectional plot of the MCNP model and Figure 2 is the same plot zoomed in for greater detail.

Table 1 – Thickness of High Density Polyethylene (HDPE) used in the MCNP model of the BeRP ball.

Configuration ID	00	05	10	15	30	60
Thickness (in)	0	0.5	1	1.5	3	6

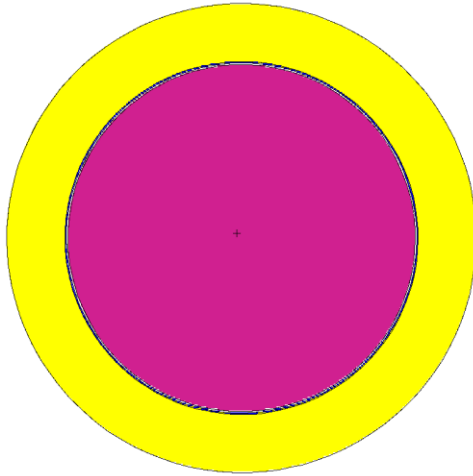


Figure 1 – Cross sectional plot of BeRP ball MCNP model. The BeRP ball is magenta, the stainless steel cladding is blue, and the HDPE reflector is yellow.

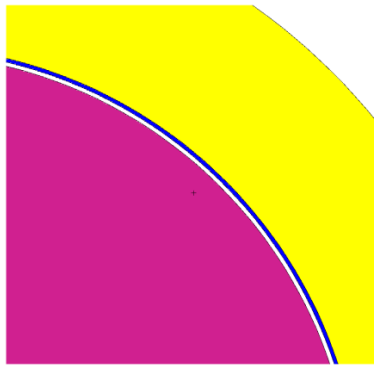


Figure 2 – Cross sectional plot of BeRP ball MCNP model. The BeRP ball is magenta, the stainless steel cladding is blue, and the HDPE reflector is yellow. Zoomed in to show greater detail.

Although only the BeRP ball, cladding, and reflector were modeled, the material and isotopic composition from the detailed benchmark model was used. The flange on the cladding was not modeled. The neutron source was modeled as a ^{240}Pu Watt-fission source. The specified options for the FMULT, F4/FM, and KCODE cards may be found in Table 6 through Table 8 in Appendix A. A sample input deck using the FMULT and F4/FM cards may be found in Appendix B and a sample deck using the KCODE and F4/FM cards may be found in appendix C. More detailed information about the cards may be found in the MCNP6 user's manual [4] and more information about the fission multiplicity distribution may be found in Lestone's 2014 work [5].

Results

Figure 3 is a plot of $p(v)$ for the BeRP ball configurations given in Table 1, while Table 2 summarizes several moments and other statistical quantities of $p(v)$ and Table 3 defines the terms given in Table 2. $p(v)$ does not shift as HDPE reflection is added and its the statistical uncertainty is smaller than the data points. The quantities given in Table 2 do not vary significantly with HDPE reflection thickness.

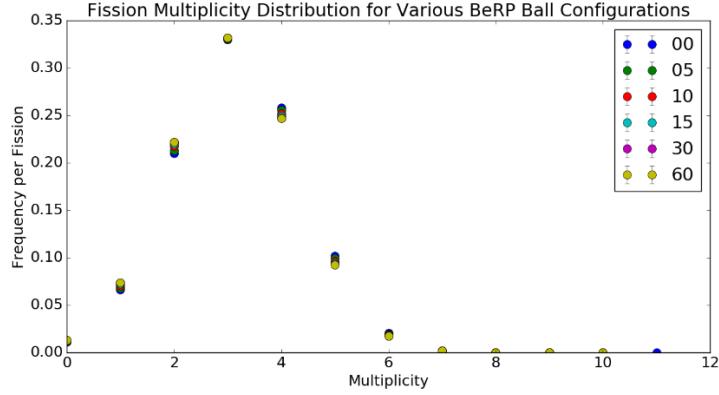


Figure 3 – Plot of $p(v)$ for various BeRP ball configurations given in Table 1.

Table 2 – Various moments and statistics of $p(v)$ for various configurations of the BeRP given in Table 1.

Configuration	00	05	10	15	30	60
\bar{v}	3.16	3.14	3.11	3.10	3.09	3.08
σ^2	1.44	1.44	1.44	1.43	1.43	1.43
\bar{v}_2	8.24	8.14	8.02	7.94	7.87	7.86
\bar{v}_3	17.20	16.87	16.49	16.24	16.02	16.01
\bar{v}_{2R}	4.12	4.07	4.01	3.97	3.94	3.93
\bar{v}_{3R}	2.87	2.81	2.75	2.71	2.67	2.67
H	1.91	1.90	1.90	1.89	1.89	1.89
D	2.61	2.59	2.57	2.56	2.55	2.55
$RMSE/\bar{v}$	6.29e-03	5.71e-03	5.70e-03	6.11e-03	6.71e-03	6.77e-03

Table 3 – Definitions of the various moments and statistics given in Table 2.

Quantity	Definition
\bar{v}	$\sum_{v=0}^{v_{max}} vp(v)$
σ^2	$\sum_{v=0}^{v_{max}} (v - \bar{v})^2 p(v)$
\bar{v}_2	$\frac{v(v-1)}{v(v-1)(v-2)}$
\bar{v}_3	$\frac{v(v-1)(v-2)}{v(v-1)/2}$
\bar{v}_{2R}	$\frac{v(v-1)(v-2)/6}{\bar{v}_{2R}/(\bar{v}-1)}$
\bar{v}_{3R}	\bar{v}_2/\bar{v}
H	
D	
$RMSE/\bar{v}$	$\sqrt{\sum_{v=0}^{v_{max}} (p(v) - p_{Pu239}^{2 MeV}(v))^2 / \bar{v}}$
$p_{Pu239}^{2 MeV}(v)$	Fission multiplicity distribution for ^{239}Pu at 2 MeV incident neutron energy

Figure 4 is a plot of several of the quantities given in Table 2 as a function of BeRP ball configuration. As in Table 2, these quantities do not vary appreciably with HDPE reflector thickness.

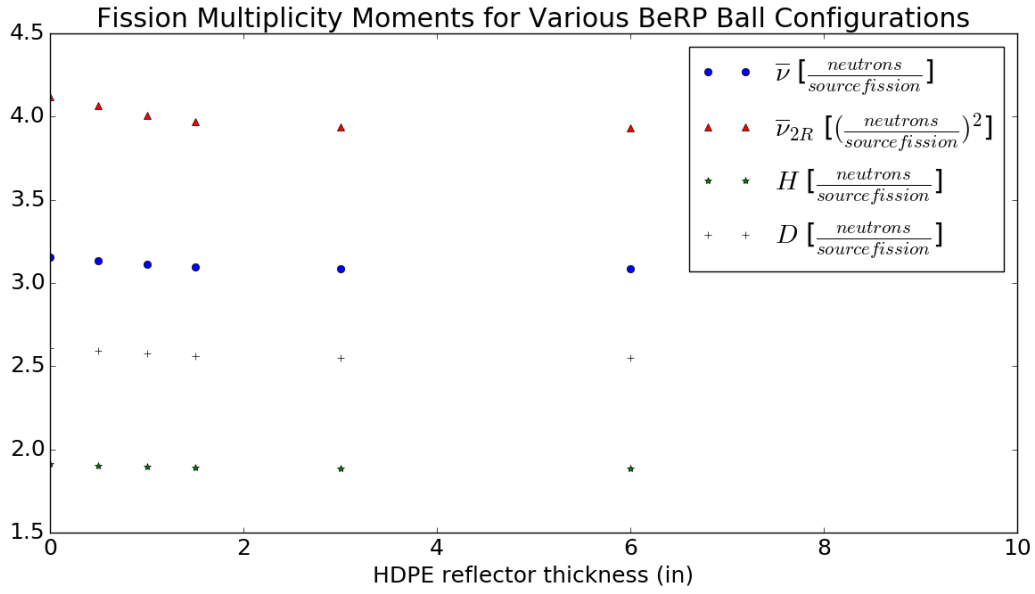


Figure 4 – Plot of select quantities from Table 5 as a function of BeRP ball configuration.

Figure 5 is a plot of the $N_{IF}(E)$ for the BeRP ball configurations given in Table 1, while Table 7 compares \bar{N}_{IF} computed by the FMULT card and F4/FM card. The spectrums in Figure 5 closely resembles a ^{239}Pu Watt-fission spectrum for the bare case and is highly thermalized in all HDPE reflected cases. The average energies given in Table 4 are significantly different with respect to configuration.

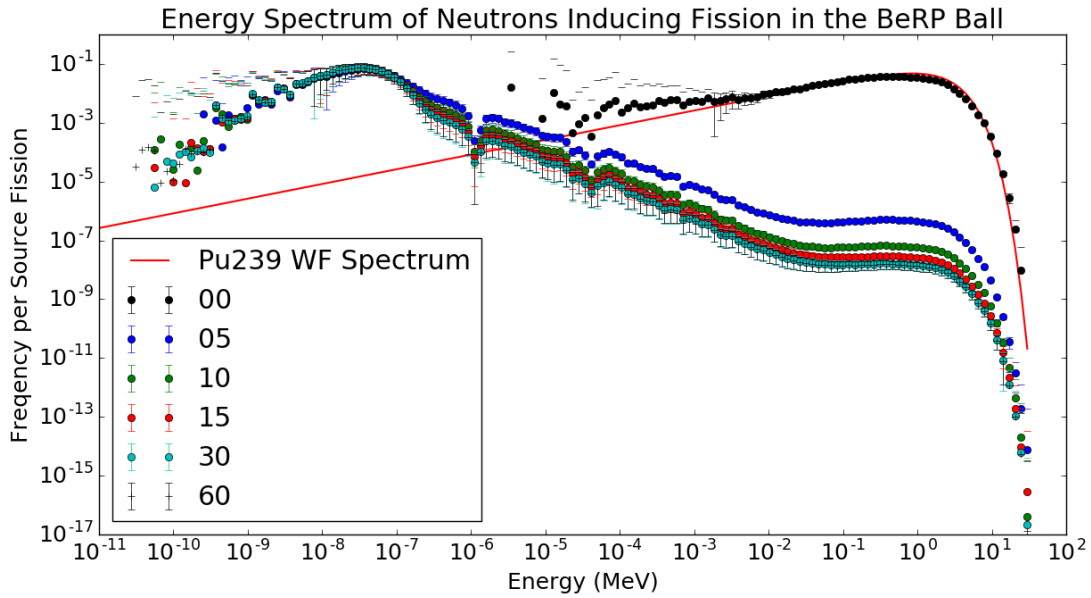


Figure 5 – Plot of $N_{IF}(E)$ for the BeRP ball configurations given in Table 1.

Table 4 – Comparison of \bar{N}_{IF} for the BeRP ball configurations given in Table 1 between the FMULT (\bar{N}_{IF}^{FMULT}) and the F4/FM card ($\bar{N}_{IF}^{F4/FM}$).

Configuration	\bar{N}_{IF}^{FMULT} (MeV)	$\bar{N}_{IF}^{F4/FM}$ (MeV)
00	1.93E+00	5.76E-01
05	1.83E+00	8.00E-06
10	1.71E+00	1.12E-06
15	1.62E+00	5.33E-07
30	1.52E+00	3.12E-07
60	1.50E+00	2.95E-07

Figure 6 is a plot of the neutron multiplication estimated with nonlinear regression of the RDA point kinetic model for the Feynman Y statistic using the $\bar{\nu}$ given in Table 2, as detailed in Okowita's work in [3], vs neutron multiplication estimated via MCNP6, while Table 5 summarizes the data sets plotted in Figure 6. The solid red line in Figure 6 indicates where the two data sets would be equal and is used to compare them. As HDPE reflection is added, the difference between MCNP6 and RDA estimates increases.

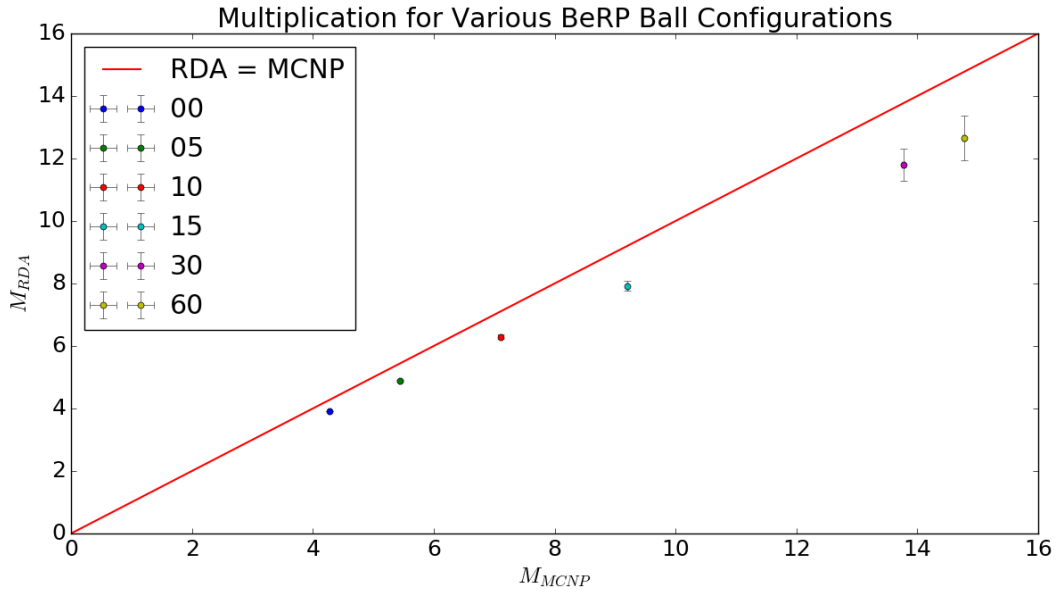


Figure 6 – Plot of neutron multiplication estimated via nonlinear regression of RDA point kinetic model (RDA) vs MCNP6 (MCNP). The solid red line indicates where the two data sets would be equal.

Table 5 – Neutron multiplication estimated via RDA point kinetic models and MCNP6 various configurations of the BeRP given in Table 1.

Configuration	00	05	10	15	30	60
M_{MCNP6}	4.28	5.44	7.11	9.20	13.77	14.77
σ_{MCNP6}	0.01	0.03	0.06	0.16	0.52	0.71
M_{RDA}	3.76	4.69	6.05	7.62	11.35	12.18
σ_{RDA}	0.01	0.01	0.02	0.02	0.02	0.02
Fractional difference	0.12	0.14	0.15	0.17	0.18	0.18

Conclusions

Figure 3, Table 2, and Figure 4 indicates that $p(\nu)$ and its moments do not vary appreciably with changing BeRP ball configuration. The $RMSE/\bar{\nu}$ values given in Table 2 indicate that $p(\nu)$ is very similar to $p(\nu)$ for ^{239}Pu at 2 MeV incident neutron energy. The behavior of $p(\nu)$ is consistent with \bar{N}_{IF} given in Table 4 for the FMULT card. The average energy reported is between 1 and 2 MeV, regardless of BeRP ball configuration. These results are at odds with those given by Figure 5 and the average energy given in Table 4 for the F4/FM card. $N_{IF}(E)$ for the bare BeRP ball is essentially Watt-fission distributed while all HDPE reflected configurations have a highly thermalized energy spectrum. These latter results are more physically meaningful for an HDPE-reflected system and suggests a discrepancy in the way that the FMULT and F4/FM cards determine the neutron energies, which is being investigated.

Figure 6 and Table 5 indicate that the difference between multiplication estimated via MCNP6 and the RDA point kinetic model increases as more HDPE reflection is added. The point kinetic model assumption that all fissions occur simultaneously with the source neutron emission is valid for an unreflected system but becomes increasingly inaccurate for more thermalized systems. It is hoped that resolving the discrepancy between the FMULT and F4/FM card estimates of $N_{IF}(E)$ and \bar{N}_{IF} will provide better $\bar{\nu}$ estimates that will lead to RDA multiplication estimates that are in better agreement with MCNP6 simulations.

References

- [1] Hutchinson, Jesson, et al. (2007). Plutonium Sphere Reflected by Beryllium. *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (PU-MET-FAST-038). Nuclear Energy Agency.
- [2] Ensslin, N., et al. (1998). "Application Guide to Neutron Multiplicity Counting". Los Alamos National Laboratory. Nov. 1998
- [3] A. Okowita, J. Mattingly. 2012. "Analysis of the Feynman variance to mean ratio using nonlinear regression". INMM 53rd Annual Meeting, Orlando, Florida, USA.
- [4] Pelowitz, Denise B., et al. "MCNP6™ User's Manual". Los Alamos National Laboratory. Version 1.0. May 2013
- [5] Lestone, John Paul. "Energy and Isotope Dependence of Neutron Multiplicity Distributions (LA-UR-05-0288). Los Alamos National Laboratory, submitted to Nuclear Science and Engineering of Sep. 17th, 2014.

Appendix A

Table 6 – Specified options for the FMULT card.

Option	Value	Description
method	0	MCNP5 sin/cos sampling method
data	1	Use Lestone re-evaluated Gaussian width by isotope for multiplicities
shift	0	MCNP5 integer number of neutrons emitted per fission

Table 7 – Specified options for the F4/FM card.

Option	Value	Description
multiplicative constant	-1	Multiplies the microscopic cross section by the atom density of the material
reaction list	-6	Total fission microscopic cross section
energy bin	1e-11 150ilog 3e1	152 energy bins with logarithmic spacing ranging from 1e-11 to 3e+01 MeV

Table 8 – Specified options for the KCODE card.

Option	Value	Description
nsrck	1e+04	Number of source histories per cycle
ikz	50	Number of cycles to be skipped before beginning tally accumulation
kct	1250	Total number of cycles to be done

Appendix B

BeRP Ball, 0.5 inch HDPE, fmult and f4/fm cards

```

c
c ~~~~~ BERP ball ~~~~~
c
1 100 4.91571E-02 -10    imp:n=1
c
c ~~~~~ space between ball and cladding ~~~~~
c
2 0      +10 -20  imp:n=1
c
c ~~~~~ Cladding ~~~~~
c
3 200 8.29740E-02 +20 -30  imp:n=1
c
c ~~~~~ HDPE shell ~~~~~
c
4 300 1.198E-01  +30 -40  imp:n=1
c
c ~~~~~ gap between shell and boundary ~~~~~
c
5 0      +40 -999  imp:n=1
c
c ~~~~~ Outside the system ~~~~~
c
99 0      +999    imp:n=0

c ~~~~~ BERP ball ~~~~~
c
10 so 3.7938    $ Plutonium sphere OR
20 so 3.82778   $ SS clad IR
30 so 3.85826   $ SS clad OR
c
c ~~~~~ HDPE shell ~~~~~
c
40 so 5.12826   $ 0.5 inch thick
c
c ~~~~~ Outside universe ~~~~~
c
999 so 21

c ~~~~~ energy binned fission reaction tally on the BeRP ball ~~~~~
c
f4:n 1 $ flux tally on the BeRP ball.
fm4 (-1 100 (-6))          $ total fission reaction rate tally modifier
                           $ "-1" - multiply by atomic density of material
                           $ "100" - material 100
                           $ "-6" total fission cross section

e4 1e-11 150ilog 3e1      $ energy bins for the tally.
c
c ~~~~~ source energy specification ~~~~~
c
sdef pos = 0 0 0 erg = d1    $ Pu-240 watt fission spectrum
sp1 -3 0.794930 4.68927
fmult method = 0 data = 1 shift = 0
print
c
c ~~~~~ Material 1: Alpha phase Plutonium ~~~~~
c
m100      94238.66c 9.87090E-06
          94239.66c 4.60684E-02
          94240.66c 2.91208E-03
          94241.66c 9.77932E-05
          94242.66c 1.35904E-05
          95241.66c 5.53502E-05

```

26054.66c 1.23559E-07
 26056.66c 1.93962E-06
 26057.66c 4.47942E-08
 26058.66c 5.96128E-09
 31000.66c 5.67230E-05
 4009.66c 6.54982E-07
 13027.66c 1.09387E-06
 28058.66c 3.42347E-07
 28060.66c 1.31871E-07
 28061.66c 5.73286E-09
 28062.66c 1.82747E-08
 28064.66c 4.65669E-09
 42000.66c 1.10747E-06
 82206.66c 3.48162E-08
 82207.66c 3.19268E-08
 82208.66c 7.56999E-08
 5010.66c 1.08108E-07
 5011.66c 4.37894E-07
 14028.66c 9.69216E-07
 14029.66c 4.92122E-08
 14030.66c 3.24403E-08
 29063.66c 6.42525E-08
 29065.66c 2.86382E-08
 47107.66c 2.83677E-08
 47109.66c 2.63550E-08
 83209.66c 2.82459E-08
 11023.66c 1.28379E-05
 20000.66c 8.83702E-07
 30000.42c 4.51356E-07
 48106.66c 6.56395E-09
 48108.66c 4.67353E-09
 48110.66c 6.55870E-08
 48111.66c 6.72149E-08
 48112.66c 1.26711E-07
 48113.66c 6.41692E-08
 48114.66c 1.50866E-07
 48116.66c 3.93312E-08
 12000.66c 2.42865E-07
 24050.66c 2.46632E-08
 24052.66c 4.75606E-07
 24053.66c 5.39299E-08
 24054.66c 1.34243E-08
 40000.66c 6.47070E-06
 50000.42c 2.48624E-07
 6000.66c 2.26068E-04

c
 c ~~~~~ Material 2: 304 SS Cladding ~~~~~
 c

m200 24050.66c 7.40303E-04
 24052.66c 1.42760E-02
 24053.66c 1.61878E-03
 24054.66c 4.02949E-04
 26054.66c 3.42442E-03
 26056.66c 5.37561E-02
 26057.66c 1.24146E-03
 26058.66c 1.65216E-04
 28058.66c 5.00281E-03
 28060.66c 1.92706E-03
 28061.66c 8.37757E-05
 28062.66c 2.67054E-04
 28064.66c 6.80494E-05
 6000.66c 1.55280E-04
 25055.66c 8.48717E-04
 14028.66c 7.65589E-04
 14029.66c 3.88730E-05
 14030.66c 2.56248E-05

```

15031.66c 3.38707E-05
16000.66c 2.18086E-05
c
c ~~~~~ Material 3: HDPE ~~~~~
c
m300    1001.66c 6.66662E-01
        6000.66c 3.33338E-01
mt300    poly.60t
c
c ~~~~~ problem parameters ~~~~~
c
mode n
nps 1e+04

```

Appendix C

BeRP Ball, 0.5 inch HDPE, f4/fm and kcode cards

```

c
c ~~~~~ BERP ball ~~~~~
c
1 100 4.91571E-02 -10    imp:n=1
c
c ~~~~~ space between ball and cladding ~~~~~
c
2 0      +10 -20  imp:n=1
c
c ~~~~~ Cladding ~~~~~
c
3 200 8.29740E-02 +20 -30  imp:n=1
c
c ~~~~~ HDPE shell ~~~~~
c
4 300 1.198E-01  +30 -40  imp:n=1
c
c ~~~~~ gap between shell and boundary ~~~~~
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c
c ~~~~~ Outside the system ~~~~~
c
99 0      +999    imp:n=0

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30 so 3.85826   $ SS clad OR
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40 so 5.12826   $ 0.5 inch thick
c
c ~~~~~ Outside universe ~~~~~
c
999 so 21

c ~~~~~ energy binned fission reaction tally on the BeRP ball ~~~~~
c
f4:n 1 $ flux tally on the BeRP ball.
fm4 (-1 100 -6) $ total fission reaction rate tally modifier
      $ "-1" - multiply by atomic density of material
      $ "100" - material 100
                  $ "-6" total fission cross section
e4 1e-11 150ilog 3e1 $ energy bins for the tally.
c
c ~~~~~ ksrc and kcode options ~~~~~
c
ksrc 0 0 0
kcode 1e+04 1 50 1250
print
c
c ~~~~~ Material 1: Alpha phase Plutonium ~~~~~
c
m100      94238.66c 9.87090E-06
          94239.66c 4.60684E-02
          94240.66c 2.91208E-03
          94241.66c 9.77932E-05
          94242.66c 1.35904E-05
          95241.66c 5.53502E-05
          26054.66c 1.23559E-07

```

26056.66c 1.93962E-06
 26057.66c 4.47942E-08
 26058.66c 5.96128E-09
 31000.66c 5.67230E-05
 4009.66c 6.54982E-07
 13027.66c 1.09387E-06
 28058.66c 3.42347E-07
 28060.66c 1.31871E-07
 28061.66c 5.73286E-09
 28062.66c 1.82747E-08
 28064.66c 4.65669E-09
 42000.66c 1.10747E-06
 82206.66c 3.48162E-08
 82207.66c 3.19268E-08
 82208.66c 7.56999E-08
 5010.66c 1.08108E-07
 5011.66c 4.37894E-07
 14028.66c 9.69216E-07
 14029.66c 4.92122E-08
 14030.66c 3.24403E-08
 29063.66c 6.42525E-08
 29065.66c 2.86382E-08
 47107.66c 2.83677E-08
 47109.66c 2.63550E-08
 83209.66c 2.82459E-08
 11023.66c 1.28379E-05
 20000.66c 8.83702E-07
 30000.42c 4.51356E-07
 48106.66c 6.56395E-09
 48108.66c 4.67353E-09
 48110.66c 6.55870E-08
 48111.66c 6.72149E-08
 48112.66c 1.26711E-07
 48113.66c 6.41692E-08
 48114.66c 1.50866E-07
 48116.66c 3.93312E-08
 12000.66c 2.42865E-07
 24050.66c 2.46632E-08
 24052.66c 4.75606E-07
 24053.66c 5.39299E-08
 24054.66c 1.34243E-08
 40000.66c 6.47070E-06
 50000.42c 2.48624E-07
 6000.66c 2.26068E-04

c

c ~~~~~ Material 2: 304 SS Cladding ~~~~~

c

m200 24050.66c 7.40303E-04
 24052.66c 1.42760E-02
 24053.66c 1.61878E-03
 24054.66c 4.02949E-04
 26054.66c 3.42442E-03
 26056.66c 5.37561E-02
 26057.66c 1.24146E-03
 26058.66c 1.65216E-04
 28058.66c 5.00281E-03
 28060.66c 1.92706E-03
 28061.66c 8.37757E-05
 28062.66c 2.67054E-04
 28064.66c 6.80494E-05
 6000.66c 1.55280E-04
 25055.66c 8.48717E-04
 14028.66c 7.65589E-04
 14029.66c 3.88730E-05
 14030.66c 2.56248E-05
 15031.66c 3.38707E-05


```

16000.66c 2.18086E-05
c
c ~~~~~ Material 3: HDPE ~~~~~
c
m300    1001.66c 6.66662E-01
        6000.66c 3.33338E-01
mt300   poly.60t
c
c ~~~~~ problem parameters ~~~~~
c
mode n

```