

Practical Monte Carlo using MCNP

Assessed exercises

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Abstract

A Monte Carlo simulation was performed for 20 000 source histories, to model the light water moderated neutron fluence from a fission neutron source through the sides of a stainless steel bucket. The resulting fluence histograms were recorded, plotted against energy, and the statistical reliability of the data evaluated. One set of tally results were not found to be reliable after failing the tally fluctuation chart (TFC) Figure of Merit (FoM) slope test. The simulation was subsequently repeated for 200 000 source histories, and the corresponding statistical reliability of the data re-evaluated. It was found that simulating 200 000 source histories was sufficient for both flux tallies to pass the ten TFC tests, indicating result reliability.

A second Monte Carlo model was designed to investigate the reactivity coefficient k_{eff} of a simplified four cylinder enriched uranium reactor system. Several simulations were performed for two enrichments (20 % ^{235}U , 25 % ^{235}U) and two moderators (graphite, light water). The reactivity coefficients were found (in product order) to be 0.844 840(794), 0.932 39(74), 0.893 79(80), and 1.006 62(77), respectively.

1 Introduction

In this report, a preliminary exercise exploring process of specifying MCNP geometry was completed. Several simple geometries were defined, using the various non-macrobody primitives available. The surface tallying feature was used to obtain two energy dependent histograms describing the neutron fluence distribution incident upon surfaces within a problem geometry, and an investigation was performed into the conditions under which these tallies are invalidated. For these investigations, a neutron source was configured using the Watt Fission prompt neutron spectrum for ^{235}U , with parameters referenced from the MCNP user manual.

In a subsequent exercise, a method of estimating the reactivity coefficient of a system using the KCODE card was used to investigate the effect of varying the moderator material and fuel enrichment. The definition of a concrete floor serves a secondary purpose to shielding; to reflect a fraction of the neutrons back into the vessel. Four enriched uranium cylinders were used as fissile material for the KCODE algorithm, to serve as neutron sources for the next fission cycle. The primary neutron sites were provided as initialisation parameters for the algorithm, using the KSRC card.

2 Method

2.1 Exercise 1

An MCNP input file was written to design the simulation model (see Appendix 1). A stainless steel vessel (of density 7.92 g/cm^3) with internal base 10 cm by 20 cm, wall thickness 2 mm, and external height 20 cm was modelled as the intersection between two cuboids, centered about the z axis with the lower floor placed at $z = 0$. The moderator was defined as the intersection between the internal cuboid and an infinite planar surface of normal $(0\ 0\ -1)$ at $(0\ 0\ 19.0)$. Two void regions were then defined, one for the volume outside of the outer cuboid, and the other for the region between the moderator surface and the plane bounding the outer cuboid ceiling. All cells were defined with a neutron importance of 1, apart from the outer void region, and their materials appropriately defined in the DATA section. All cells were assigned a material with the appropriate atomic / weight composition, and assigned with the correct weight density. The moderator was assigned the light water low energy cross section library *lwtr.01[t]*.

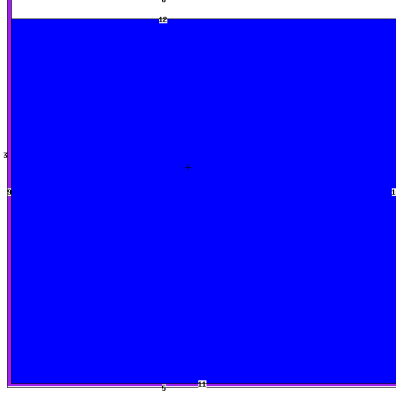


Figure 1: 2D XZ plot of Exercise 1 geometry.

Two surface neutron flux tally cards were defined, using a common set of energy bins, with upper bin edges defined along the loglinear interval between 1×10^{-9} MeV and 10 MeV. One tally recorded the flux through the two short external sides of the vessel, and the other recorded the corresponding flux through the two larger sides. A thermal neutron source with an energy distribution given by the Watt Fission spectrum for ^{235}U (see Fig 2), with parameters $a = 0.988$, $b = 2.249$, was placed at $(0 \ 0 \ 2.2)$, and the simulation performed for 20 000 neutrons (MODE N) source histories. A secondary simulation was performed with an increased number of source histories of 200 000.

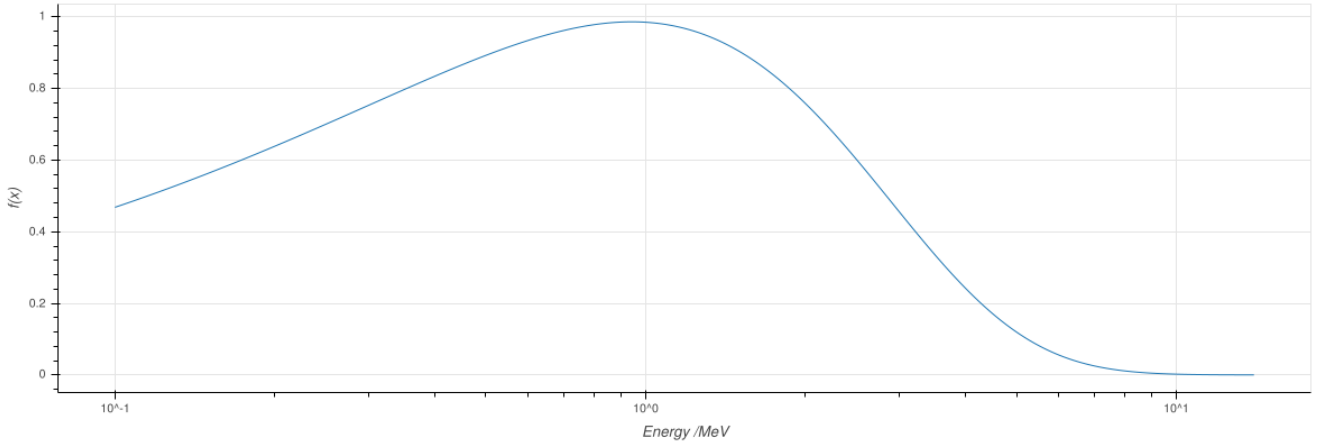


Figure 2: Watt Fission spectrum for prompt neutrons (^{235}U).

2.2 Exercise 3

The geometry described in Section 2.1 was modified such that the internal base measured 100 cm by 100 cm, with an external height of 60 cm. A concrete floor was defined, of thickness 304.8 cm, and a lateral radius of 500 cm. These two parameters were not defined in the exercise requirements; the former was taken from relevant literature, and the latter chosen to be significantly greater than the floor thickness. The moderator volume was resized to satisfy the original wall thickness constraints, and the surface moved to 2 cm from the ceiling of the vessel. For each simulation, the appropriate moderator material was defined (for graphite / water), and the corresponding low energy cross section library referenced (*lwtr.01[t]* / *grph.01[t]*) Four enriched uranium cylindrical sources, of radius 7.5 cm and height 25 cm, were placed within the moderator cell. The fuel material card was defined for a by-weight enrichment which was varied across several of the simulations. The KCODE Monte Carlo eigenvalue algorithm was used to determine the reactivity coefficient k_{eff} of the system. The KSRC card was used to distribute 1000 starting neutrons across the centroids of the uranium cylinders. The KCODE algorithm was configured for a warm up of

200 cycles, with an initial reactivity estimate of 1.0 (critical), and run for 1000 active cycles. As with Section 2.1, only the outermost void cell was given a zero neutron importance, with the remaining cell neutron importances set to unity.

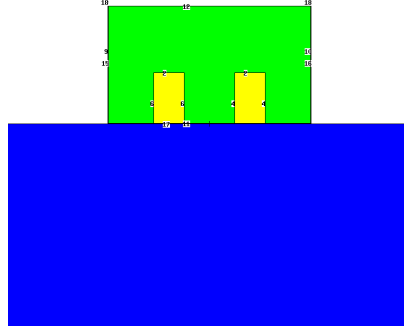


Figure 3: 2D XZ plot of Exercise 3.d. (Graphite) geometry.

3 Results

3.1 Exercise 1

3.1.1 Initial Simulation

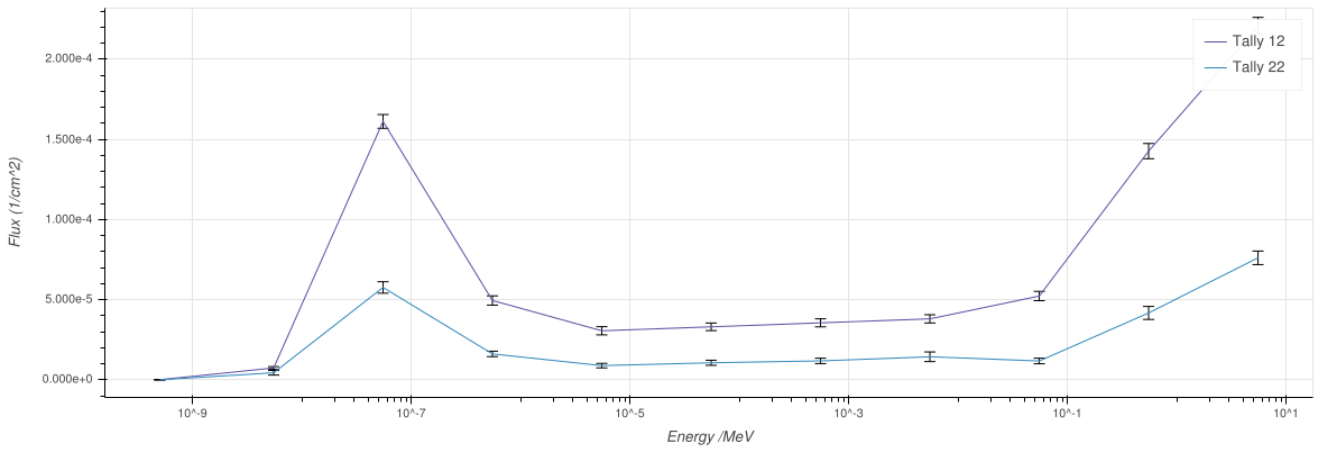


Figure 4: Fluence tallies for external surfaces of container, for 20 000 histories. Tally 12 corresponds to the fluence across the shorter sides of the container, 22 the longer sides.

The tallies are defined as follows:

- Tally 12: The short sides of characteristic length 10 cm
- Tally 22: The long sides of characteristic length 20 cm

For the tallies, MCNP reported that the tallies passed most of the 10 statistical tests for the tally fluctuation chart, which are defined as

1. Mean is randomly distributed
2. Relative error ideally less than 0.10
3. Relative error decreases over time

4. Decrease rate of relative error follows $\frac{1}{\sqrt{nps}}$
5. Variance of variance ideally less than 0.10
6. Variance of variance decreases over time
7. Decrease rate of variance of variance follows $\frac{1}{\sqrt{nps}}$
8. Figure of Merit (FoM) is roughly constant
9. FoM is randomly distributed
10. Slope of the FoM pdf is greater than 3.0

The first and last tallies passed all ten tests, whilst Tally 22 failed the final FoM slope PDF test. In addition, all tallies had at least one bin with large relative error (> 0.1).

The total fluences across each pair of surfaces were as follows

- Long sides (Tally 12): $7.708\,840(93277) \times 10^{-4} \text{ n/cm}^2$
- Short sides (Tally 34): $2.534\,000(82862) \times 10^{-4} \text{ n/cm}^2$

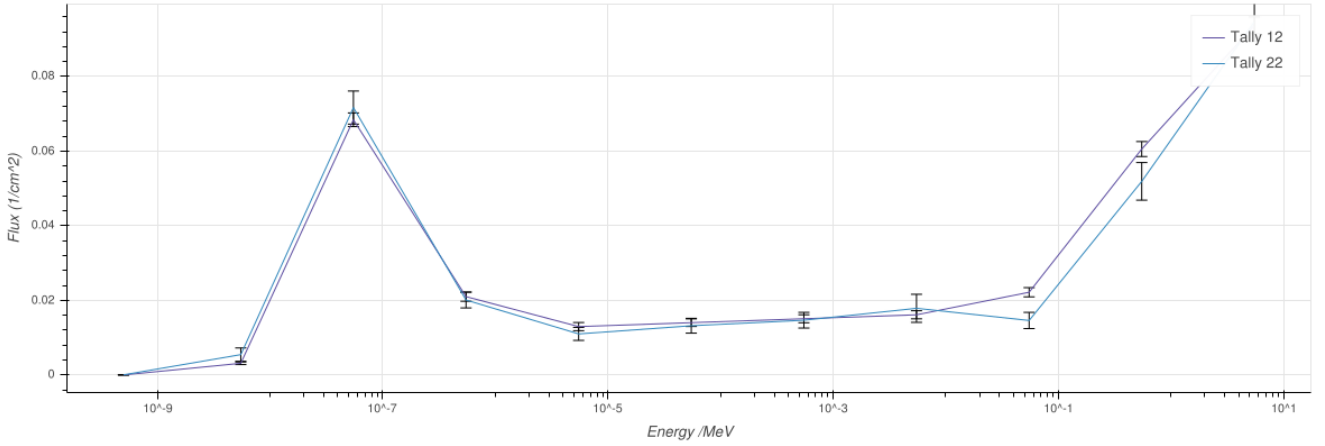


Figure 5: Area normalised fluence tallies for external surfaces of container, for 20 000 histories. Tally 12 corresponds to the fluence across the shorter sides of the container, 22 the longer sides.

3.1.2 Flux

For a source of 10^{10} neutrons per second, the corresponding fluxes would be $7.708\,840(93277) \times 10^6 \text{ n/cm}^2/\text{s}$ and $2.534\,000(82862) \times 10^6 \text{ n/cm}^2/\text{s}$ respectively.

3.1.3 Increasing Number of Histories

By increasing the particle histories limit to 200000, the standard uncertainty upon the tally amplitudes diminishes, approximately $\frac{1}{2}$ as expected. The bin amplitude for Tally 22 corresponding to $(1 \times 10^{-8} < x < 1 \times 10^{-9})$ did not lie within the uncertainty permitted by its previous value. However, this tally did not pass all statistical tests for 20000 to allow such a constraint in the first place, and so was to be expected. By increasing the number of particle histories to the new limit, all statistical tests were subsequently passed. Furthermore, the difference in neutron energy distribution between the two tallies became more apparent; in particular, in the higher energy regime the two distributions diverged most significantly, with the narrower surfaces (further from the source) showing greater attenuation at higher energies. The recorded fluences were as follows:

- Long sides (Tally 12): $7.655\,310(29856) \times 10^{-4} \text{ n/cm}^2$
- Short sides (Tally 34): $2.515\,000(25402) \times 10^{-4} \text{ n/cm}^2$

Table 1: Reactivity coefficient for various simulated scenarios.

Moderator	Enrichment	k_{eff}
Light water	20 %	0.844 840(794)
Graphite	20 %	0.932 39(74)
Light water	25 %	0.893 79(80)
Graphite	25 %	1.006 62(77)

3.2 Exercise 3

4 Analysis

4.1 Exercise 1

The final FoM slope test evaluates whether the central limit theorem has been satisfied; that is, both the first and second moments of the PDF exist (and are therefore finite). The second moment $\int_{-\infty}^{\infty} x^2 f(x) dx$ is observed to exist when $f(x)$ decreases faster than $\frac{1}{x^3}$, and hence the final test evaluates this condition. Consequently, in failing this test for the initial simulation, it cannot be concluded that Tally 22 is reliable.

The significant difference between the total fluences for the two tallies can be explained by both the variation in solid angle between the two surfaces (each surface is sufficiently large relative to the distance to the source, that the incident flux varies along the surface), and the difference in neutron absorption along the axes of the detector. The neutron absorption probability through a medium is given by the Beer Lambert law, and is exponential in the distance travelled. The normalised (by area) neutron energy distributions are approximately equal, and what variation there exists between the two tallies lies predominantly within the uncertainty on the recorded values. However, there are several points, particularly in the higher energy regime whose standard errors do not account for the observed deviation. In these cases, the nonlinear attenuation function, which depends upon neutron energy, leads to a distortion of the tallied energy spectrum.

4.2 Exercise 3

4.2.1 Graphite Moderator

When replacing the moderator material with graphite, the effective criticality of the system was observed to increase. The criticality of a reactor depends upon the number of neutrons which are thermalised (by the moderator) and lead to thermal fission in the fuel. In transitioning the moderator material from light water to graphite, the mean logarithmic energy decrement of the moderator ξ decreases (lesser energy loss per collision), such that the average number of collisions required to thermalise a fast neutron increases by a factor $\frac{\xi_{H_2O}}{\xi_C} = 5.8$. However, the scattering to capture ratio of graphite is far higher than that of light water (1500 vs 77.17), and thus its effective "moderating ratio" $\frac{\xi \sigma_s}{\sigma_a}$ is greater. This result was observed in the predicted reactivity coefficients for the two systems. In the case of the graphite moderator, the reactivity coefficient was greater (closer to criticality) than that of the light water. For both moderators, the application of the Shapiro–Wilke (W) test for normality indicated that the results are normally distributed with a 95 % confidence interval for all of the reactivity estimators.

4.2.2 Increasing Enrichment

After increasing the enrichment of the uranium cylinders, the reactivity coefficient of both modelled systems was observed to increase. Similarly to the previous configuration, the predicted coefficient for the graphite moderator remained greater than that of the light water. As for the previous scenario, the application of the Shapiro–Wilke (W) test for normality indicated that the results are normally distributed with a 95 % confidence interval for all of the reactivity estimators.

The observed increase in reactivity derives from the increased effective fission cross section of the fuel that follows fuel enrichment (see 6). ^{235}U has a greater fission cross section than ^{238}U , and thus increasing the ratio of ^{235}U to ^{238}U in the fuel serves to increase the fission probability, moving the system towards criticality (see *Fig*).

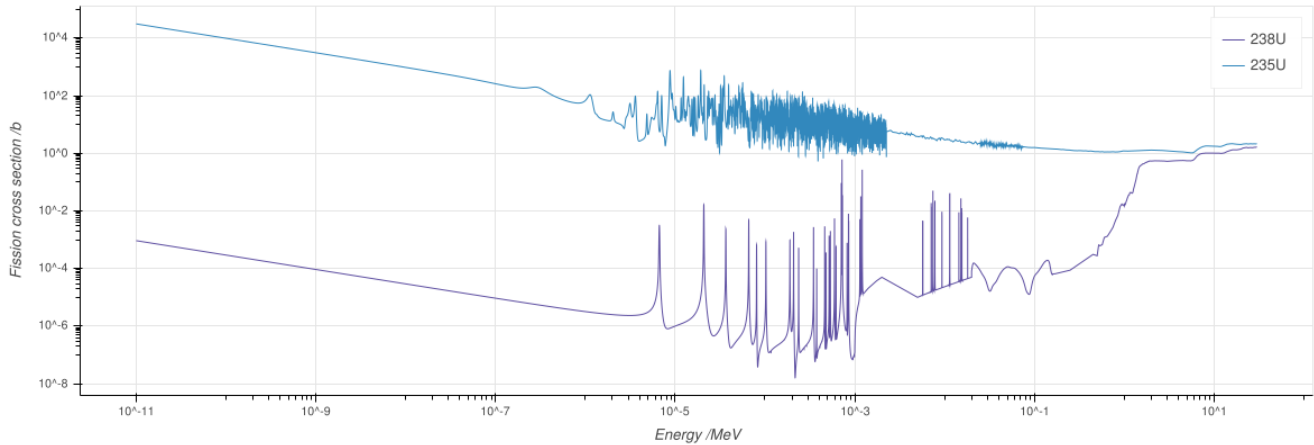


Figure 6: Fission cross sections of ^{238}U and ^{235}U

5 Conclusions

In completing the two exercises, several important observations were made concerning the various MCNP features which may be used to ensure valid results, and identify problematic cases (such as undersampled paths). The final exercise shows explicitly the importance of selecting the correct fuel enrichment, and moderator material, to avoid a reactor becoming supercritical on prompt neutrons alone.

6 Appendix

Listing 1: Exercise 1. MCNP input file.

MESSAGE:

```
Practical Monte Carlo part 1. Angus Hollands
C
C Cells
1 1 -7.92 1 -2 3 -4 5 -6 (-7:8:-9:10:-11) $ Walls
2 0 (-1:2:-3:4:-5:6) $ Void
3 2 -1.0 7 -8 9 -10 11 -12 $ Water
4 0 7 -8 9 -10 12 -6 $ Air gap (void)

C Surfaces
C Define outer walls
1 PX -5.20
2 PX 5.20
3 PY -10.20
4 PY 10.20
5 PZ 0.0
6 PZ 20.0
C Define XY wall surfaces
7 PX -5.00
8 PX 5.00
9 PY -10.0
10 PY 10.0
C Define Z wall / water surfaces
11 PZ 0.20
```

12 PZ 19.0

C Cell importance MAP

IMP:N 1 0 1 1 \$ s

M1 26000.42c -0.74 24000.42c -0.18 28000.42c -0.08 \$ Stainless steel

M2 1001.42c 2.0 8016.42c 1.0 \$ Pure water

MT2 lwtr.01

C Tallying energy fluence (nX where X is type (2) and n an ID: {1, 2, ...})

F12:N (1 2)

F22:N (3 4)

C F32:N (1 2 3 4)

C Tally energy bins for all tallies (log 10 space)

E0 1E-9 1E-8 1E-7 1E-6 1E-5 1E-4 1E-3 1E-2 1E-1 1 10

C MC type

MODE N

C Thermal neutron induced fission of 235U at (0,0,22mm)

SDEF POS=0.0 0.0 2.2 ERG=D1

SP1 -3 0.988 2.249

C NUMBER OF PARTICLE HISTORIES TO RUN

NPS 200000

PRDMP 0 0 1 1 0

Listing 2: Exercise 3.d. (Graphite) MCNP input file.

MESSAGE:

C Cells

1 4 -19.2 -3 -2 11 \$ Uranium source 1

2 4 -19.2 -4 -2 11 \$ Uranium source 2

3 4 -19.2 -5 -2 11 \$ Uranium source 3

4 4 -19.2 -6 -2 11 \$ Uranium source 4

5 3 -1.7 13 -14 15 -16 11 -12 #1 #2 #3 #4 \$ Moderator

6 1 -7.92 7 -8 9 -10 17 -18 (-13:14:-15:16:-11) \$ Wall

7 2 -2.3 -17 19 -20 \$ Concrete floor

8 0 #1 #2 #3 #4 #5 #6 #7 \$ VOID

C Source surfaces

2 PZ 25.2

3 C/Z -20 0 7.5

4 C/Z 0 20 7.5

5 C/Z 20 0 7.5

6 C/Z 0 -20 7.5

C Internal surfaces

7 PX -50.2

8 PX 50.2

9 PY -50.2

10 PY 50.2

11 PZ 0.2

12 PZ 58.0

C Internal surfaces

13 PX -50

14 PX 50

15 PY -50

16 PY 50

17 PZ 0
18 PZ 60
C Concrete floor lower surface
19 PZ -304.8
20 CZ 500

MODE N
KCODE 1000 1.0 200 1000
KSRC 20 0 12.7 -20 0 12.7 0 20 12.7 0 -20 12.7
M1 26000.42c -0.74 24000.42c -0.18 28000.42c -0.08 \$ Stainless steel
M2 8016.42c -0.53 14000.42c -0.34 20000.42c -0.10 1001.42c -0.03 \$ Concrete
M3 6012.42c 1.0 \$ Graphite
MT3 GRPH.01
M4 92238.42c -0.75 92235.42c -0.25 \$ 80% 238U, 20% 235U
IMP:N 1 1 1 1 1 1 1 0