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MatMCNP: A Code for Producing Material Cards for MCNP

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Abstract

A code for generating MCNP material cards (MatMCNP) has been written and verified for naturally occurring, stable isotopes. The program allows for material specification as either atomic or weight percent (fractions). MatMCNP also permits the specification of enriched lithium, boron, and/or uranium. In addition to producing the material cards for MCNP, the code calculates the atomic (or number) density in atoms/barn-cm as well as the multiplier that should be used to convert neutron and gamma fluences into dose in the material specified.

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TABLES

1. INTRODUCTION

The use of MCNP [1] is widespread at Sandia National Laboratories for radiation transport calculations, radiation shielding calculations, reactor design calculations, and criticality safety analyses. One of the time consuming and tedious tasks in producing input files for MCNP is the proper material definitions for the different areas of calculation geometry. This is particularly true when the calculation requires neutron transport because one must define the isotopic mixture rather than the simpler elemental composition of the material. In order to reduce the effort required to produce material definitions for MCNP, the MatMCNP program was written. This report describes the technique used to create new MCNP material definitions, details the verification of the code, and provides a guide for utilizing the program for creating material cards for new applications.

1.1. Background

MatMCNP is a Fortran 90 program that takes information about a compound or mixture as input and produces a material card for MCNP for elemental mixture. The code was written by Karen C. Kajder (Saavedra) in 2004 as one of her assignments as a student intern. As originally written, MatMCNP contained data from the 2000 version of the Nuclear Wallet Cards [2]. The data extracted from the Nuclear Wallet Cards includes both the isotopic atomic abundances for the naturally occurring elements and the mass excess (Δ) for each of the naturally occurring isotopes. The code also used the ENDF/B-VI cross sections as the baseline set for the MCNP material cards that were produced.

The program has had several modifications since 2004. First, the ability to process enriched lithium, boron, and uranium material definitions was added. Second, the atomic abundances and mass excesses for all of the isotopes in the code have been updated to the current (2014) electronic version of the Nuclear Wallet Cards [3]. Finally, the baseline set for MCNP material cards have been updated to the ENDF/B-VII Release 1.0 cross sections. In addition to these changes, the code has been placed into the git configuration management tool to maintain a record of modifications of the code going forward.

1.2. Problem Solved

MatMCNP utilizes the user input information about a material mixture to calculate the atom fraction, weight fraction, and atom density for each isotope in the mixture. The program also calculates the total atom density and the MCNP tally multiplier (FM card) that can be used to convert a particle fluence tally to an estimate of the material heating or dose. The output of the MatMCNP program is a file that can be copied directly into an MCNP input deck as a material card.

1.3. Method of Solution

While MatMCNP allows the user to specify the definition of a material as either atomic percent or weight percent, the method of solution used by the code produces material cards that are provided in atomic fraction for the mixture. MatMCNP must first determine the isotopic mass and average atomic mass for each element listed by the user as input. In order to calculate the isotopic mass, MatMCNP uses this definition of the mass excess (Δ) from the Nuclear Wallet Cards. The mass excess (Δ) in MeV is calculated by Equation (1):

$$\Delta = M - A$$

$$\Delta = 0 \text{ for } {}^{12}C \text{ by definition.} \tag{1}$$

where M is the isotopic mass and A is the atomic mass number. The energy equivalent of the atomic mass unit (u) is 931.494 MeV. So, using u = 931.494 MeV, Equation (1) can be rearranged to calculate the isotopic mass (M_i) in atomic mass units:

$$M_i = A + \frac{\Delta \text{ (MeV)}}{931.494 \text{ (MeV/}u\text{)}} \tag{2}$$

As an example for isotopic mass calculations, ^{23}Na (A = 23) has a mass excess (Δ) of -9.5298 MeV:

$$M_{^{23}Na} = 23 + \frac{-9.5298 \text{ (MeV)}}{931.494 \text{ (MeV/}u\text{)}} = 22.98977\ u \tag{3}$$

The average atomic mass (M) of an element is calculated using Equation (4):

$$M = \frac{1}{100} \sum_i (\text{a/o})_i \cdot M_i \tag{4}$$

where $(\text{a/o})_i$ is the atomic abundance (in percent) for the i^{th} isotope in the element. The $(\text{a/o})_i$ values were extracted from the Nuclear Wallet Cards.

As an example of the average atomic mass calculation, boron has two natural occurring isotopes (^{10}B [Δ = 12.0507 MeV and a/o = 19.9%] and ^{11}B [Δ = 8.6679 MeV and a/o = 80.1%]):

$$M_{^{10}\mathrm{B}} = 10 + \frac{12.0507\ (\mathrm{MeV})}{931.494\ (\mathrm{MeV}/u)} = 10.01294$$

$$\mathrm{M}_{^{11}\mathrm{B}} = 11 + \frac{8.6679\ (\mathrm{MeV})}{931.494\ (\mathrm{MeV}/u)} = 11.00930 \tag{5}$$

$$M_B = \frac{1}{100}\left[(19.9)\cdot(10.01294) + (80.1)\cdot(11.00930)\right] = 10.811$$

In addition to the average atomic mass calculated in Equation (4), MatMCNP must calculate the isotopic weight percent $(\mathrm{w/o})_i$ using Equation (6):

$$\left(\mathrm{w/o}\right)_i = \frac{M_i \cdot (\mathrm{a/o})_i}{M} \tag{6}$$

Again, using boron as an example:

$$\begin{aligned}\left(\mathrm{w/o}\right)_{^{10}B} &= \frac{(10.01294)\cdot(19.9)}{10.811} = 18.43\% \\ \left(\mathrm{w/o}\right)_{^{11}B} &= \frac{(11.00930)\cdot(80.1)}{10.811} = 82.57\%\end{aligned} \tag{7}$$

The MatMCNP code also computes the total atom density of the material as well as the atom density of the individual isotopes in the material:

$$N = \frac{\rho \cdot N_A}{M}\ \ (\mathrm{atoms/cm^3\ or\ atoms/barn\text{-}cm}) \tag{8}$$

$$N_i = \frac{(\mathrm{a/o})_i}{100} \cdot \frac{\rho \cdot N_A}{M}\ \ (\mathrm{atoms/cm^3\ or\ atoms/barn\text{-}cm}) \tag{9}$$

where ρ is the physical density (g/cm^3) and N_A is Avogadro's number. [*Note: Many nuclear engineering applications are interested in using the atom density in atom/barn-cm. Thus, a value of* $N_A = 0.602214129$ *is used to get the densities in atom/barn-cm.*]

The number density for a mixture is computed according to Equation (10):

$$N_{mix} = \frac{\rho_{mix} \cdot N_A}{M_{mix}} \text{ (mixture/cm}^3\text{ or mixture/barn-cm)} \tag{10}$$

It is also possible to compute the atom density of atoms in a mixture or compound using the weight fraction:

$$N_i = \frac{(\text{w/o})_i}{100} \cdot \frac{\rho \cdot N_A}{M_i} \text{ (atoms/cm}^3\text{ or atoms/barn-cm)} \tag{11}$$

To get atom fraction of an element from a description of a material by weight fraction, use the following approach:

$$\begin{gathered} Normalization = \sum_{elem} \frac{w_{elem}}{M_{elem}} \\ (a/o)_{elem} = \frac{\left(\dfrac{w_{elem}}{M_{elem}}\right)}{Normalization} \end{gathered} \tag{12}$$

Verification of the implementation of these formulas for each of the natural occurring elements with stable isotopes and several mixtures is shown in Chapter 2. The output of MatMCNP displays the atom fraction, weight fraction, isotopic atom density, and total atom density.

2. VERIFICATION

2.1. Single Elements

Using the electronic version of the Nuclear Wallet Cards (NWC), the atomic abundance and mass excess was obtained for each element (from hydrogen to uranium) with data available. For several elements from Z = 1 – 92, there were no stable or long-lived isotopes (Tc, Pm, Po, At, Rn, Fr, Ra, Ac, and Pa). These elements do not cause a “crash” but no information is returned from the program if these elements are selected as input.

In the following sections, the extracted data will be found in the first three columns of the table while values computed using Excel complete the table columns and entries. The exception is the elemental density which was extracted from the Nuclear Wallet Cards, 8th edition [4]. The output of the MatMCNP program will be provided in the next table with comparisons of results in a third table for each element. [*NOTE: The values in the tables correspond to the precision set by both Excel and MatMCNP. The percent difference values in the verification include more digits in the calculation, so a percent difference might appear in numbers that are the same to the number of digits shown.*]

2.1.1. Hydrogen

Hydrogen (Z = 1) has two naturally occurring isotopes (^{1}H and ^{2}H) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 1. The output of MatMCNP is shown in Table 2. Finally, the verification of the implementation of hydrogen within MatMCNP is found in Table 3. With the exception of the atom density for ^{2}H, all the quantities calculated by MatMCNP are within 0.09% of the values found for the NWC or Excel calculations. The issue with ^{2}H is that the number of significant figures required to show that the atom density for ^{2}H is not zero (as shown in Table 2) would require modification to the code. This modification has not been deemed necessary because the proper atomic and weight fractions are computed. The proper atom density is calculated with an increase in the material density. This is only an issue with elemental gases with low densities and very small isotopic abundances (See Helium, specifically ^{3}He).

Table 1 – Hydrogen Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{1}H	0.999885	7.2889	1.007824956	0.999770	0.0000537
^{2}H	0.000115	13.1357	2.014101755	0.000230	0.0000000
Density (g/cm^{3}) = 8.988E-05				FM Conversion = 9.5714664E-09	
Total Atomic Density (atoms/b-cm) = 0.0000537					

Table 2 – MatMCNP Output for Elemental Hydrogen (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   H-1         0.999885           0.999770          0.0000537
C   H-2         0.000115           0.000230          0.0000000
C
C  The total compound atom density (atom/b-cm):  0.0000537
C
M1      01001.80c   0.999885
        01002.80c   0.000115
C
C  To convert a particle flux to rad[Material]
C  use FM  9.5714681E-09 1    -4  1 for neutrons
C   or FM  9.5714681E-09 1    -5 -6 for photons.
```

Table 3 – Difference between NWC and MatMCNP for Hydrogen

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{1}H	0.000%	0.000%	0.010%	-0.001%	0.000%
^{2}H	0.000%	0.088%	-100.000%		

2.1.2. Helium

Helium (Z = 2) has two naturally occurring isotopes (^{3}He and ^{4}He) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 4. The output of MatMCNP is shown in Table 5. Finally, the verification of the implementation of helium within MatMCNP is found in Table 6. It is once again clear from Table 6 that low density and low isotopic abundance causes issues with round-off. However, we again see that the atomic fraction and weight fractions are computed correctly (within the round-off of both Excel and MatMCNP). In these situations, an artificially high density (1.0 g/cm^3) will be used in Appendix A, Tables 266 through 268, to show that MatMCNP does calculate those atom density values correctly.

Table 4 – Helium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{3}He	0.00000134	14.9312	3.016029303	0.000001	0.0000000
^{4}He	0.99999866	2.4249	4.002603237	0.999999	0.0000269
Density (g/cm^3) = 1.785E-04			FM Conversion = 2.4102997E-09		
Total Atomic Density (atoms/b-cm) = 0.0000269					

Table 5 – MatMCNP Output for Elemental Helium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   He-3        0.000001           0.000001          0.0000000
C   He-4        0.999999           0.999999          0.0000269
C
C  The total compound atom density (atom/b-cm):  0.0000269
C
M2      02003.80c   0.000001
        02004.80c   0.999999
C
C  To convert a particle flux to rad[Material]
C  use FM  2.4103002E-09 2    -4  1 for neutrons
C   or FM  2.4103002E-09 2    -5 -6 for photons.
```

Table 6 – Difference between NWC and MatMCNP for Helium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{3}He	-25.373%	-0.962%	-100.000%	0.163%	0.000%
^{4}He	0.000%	0.088%	0.163%		

2.1.3. Lithium

Lithium (Z = 3) has two naturally occurring isotopes (^{6}Li and ^{7}Li) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 7. The lithium output from MatMCNP is found in Table 8. The lithium verification data for MatMCNP implementation is found in Table 9. An examination of Table 9 reveals that the MatMCNP results agree with the NWC and Excel values within 0.001% for all quantities examined.

Table 7 – Lithium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{6}Li	0.0759000	14.0868	6.015122803	0.065785	0.0035170
^{7}Li	0.9241000	14.9070	7.016003324	0.934215	0.0428202
Density (g/cm^{3}) = 0.534				FM Conversion = 1.3901181E-09	
Total Atomic Density (atoms/b-cm) = 0.0463372					

Table 8 – MatMCNP Output for Elemental Lithium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   Li-6        0.075900           0.065785         0.0035170
C   Li-7        0.924100           0.934215         0.0428203
C
C  The total compound atom density (atom/b-cm):  0.0463373
C
M3      03006.80c   0.075900
        03007.80c   0.924100
C
C  To convert a particle flux to rad[Material]
C  use FM  1.3901181E-09 3    -4  1 for neutrons
C   or FM  1.3901181E-09 3    -5 -6 for photons.
```

Table 9 – Difference between NWC and MatMCNP for Lithium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{6}Li	0.000%	0.001%	0.000%	0.000%	0.000%
^{7}Li	0.000%	0.000%	0.000%		

2.1.4. Beryllium

Beryllium (Z = 4) has just one stable isotope (^{9}Be) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 10. The beryllium output from MatMCNP is found in Table 11. The beryllium verification data for MatMCNP implementation is found in Table 12. An examination of Table 12 reveals that the MatMCNP results agree with the NWC and Excel values within the precision of the number digits shown for all quantities examined.

Table 10 – Beryllium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{9}Be	1.0000000	11.3484	9.012183009	1.0000000	0.1234874
Density (g/cm^3) = 1.848			FM Conversion = 1.0704921E-09		
Total Atomic Density (atoms/b-cm) = 0.1234874					

Table 11 – MatMCNP Output for Elemental Beryllium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   Be-9        1.000000           1.000000          0.1234875
C
C  The total compound atom density (atom/b-cm):  0.1234875
C
M4      04009.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  1.0704921E-09 4    -4  1 for neutrons
C   or FM  1.0704921E-09 4    -5 -6 for photons.
```

Table 12 – Difference between NWC and MatMCNP for Beryllium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{9}Be	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.5. Boron

Boron (Z = 5) has two naturally occurring isotopes (^{10}B and ^{11}B) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 13. The boron output from MatMCNP is found in Table 14. The verification data for MatMCNP implementation of boron is found in Table 15. An examination of Table 15 reveals that the MatMCNP results agree with the NWC and Excel values for all quantities examined.

Table 13 – Boron Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{10}B	0.1990000	12.0507	10.01293696	0.184309	0.0259390
^{11}B	0.8010000	8.6679	11.00930537	0.815691	0.1044076
Density (g/cm^3) = 2.34			FM Conversion = 8.9237307E-10		
Total Atomic Density (atoms/b-cm) = 0.1303465					

Table 14 – MatMCNP Output for Elemental Boron (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   B-10        0.199000           0.184309          0.0259390
C   B-11        0.801000           0.815691          0.1044077
C
C  The total compound atom density (atom/b-cm):  0.1303466
C
M5       05010.80c   0.199000
         05011.80c   0.801000
C
C  To convert a particle flux to rad[Material]
C  use FM  8.9237312E-10 5    -4  1 for neutrons
C   or FM  8.9237312E-10 5    -5 -6 for photons.
```

Table 15 – Difference between NWC and MatMCNP for Boron

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{10}B	0.000%	0.000%	0.000%	0.000%	0.000%
^{11}B	0.000%	0.000%	0.000%		

2.1.6. Carbon

Carbon (Z = 6) has two naturally occurring isotopes (^{12}C and ^{13}C) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 16. The carbon output from MatMCNP is found in Table 17. The verification data for MatMCNP implementation of carbon is found in Table 18. An examination of Table 18 reveals that the MatMCNP results agree with the NWC and Excel values within 0.003% for all quantities examined. [*NOTE: The carbon implementation within MatMCNP uses the elemental cross section (06000.80c) rather than an isotopic description.*]

Table 16 – Carbon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{12}C	0.9893000	0.0000	12	0.988416	0.1041666
^{13}C	0.0107000	3.1250	13.00335483	0.011584	0.0011266
Density (g/cm^3) = 2.1				FM Conversion = 8.0323724E-10	
Total Atomic Density (atoms/b-cm) = 0.1052932					

Table 17 – MatMCNP Output for Elemental Carbon (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   C-12        0.989300           0.988416          0.1041666
C   C-13        0.010700           0.011584          0.0011266
C
C  The total compound atom density (atom/b-cm):  0.1052933
C
M6       06000.80c   1.000000
C
C  Caution: The natural zaid is used for Carbon.
C
C  To convert a particle flux to rad[Material]
C  use FM  8.0323725E-10 6    -4  1 for neutrons
C   or FM  8.0323725E-10 6    -5 -6 for photons.
```

Table 18 – Difference between NWC and MatMCNP for Carbon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{12}C	0.000%	0.000%	0.000%	0.000%	0.000%
^{13}C	0.000%	-0.003%	-0.003%		

2.1.7. Nitrogen

Nitrogen (Z = 7) has two naturally occurring isotopes (^{14}N and ^{15}N) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 19. The output of MatMCNP for nitrogen is shown in Table 20. Finally, the verification of the implementation of nitrogen within MatMCNP is found in Table 21. It is once again clear from Table 21 that low density and low isotopic abundance causes issues with round-off (See Appendix A, Tables 269 through 271 for high density verification).

Table 19 – Nitrogen Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{14}N	0.9963600	2.8634	14.00307399	0.996102	0.0000536
^{15}N	0.0036400	0.1014	15.00010886	0.003898	0.0000002
Density (g/cm^3) = 0.0012506				FM Conversion = 6.8877524E-10	
Total Atomic Density (atoms/b-cm) = 0.0000538					

Table 20 – MatMCNP Output for Elemental Nitrogen (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   N-14        0.996360           0.996102           0.0000536
C   N-15        0.003640           0.003898           0.0000002
C
C  The total compound atom density (atom/b-cm):  0.0000538
C
M7      07014.80c   0.996360
        07015.80c   0.003640
C
C  To convert a particle flux to rad[Material]
C  use FM  6.8877531E-10 7    -4  1 for neutrons
C   or FM  6.8877531E-10 7    -5 -6 for photons.
```

Table 21 – Difference between NWC and MatMCNP for Nitrogen

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{14}N	0.000%	0.000%	0.050%	0.057%	0.000%
^{15}N	0.000%	-0.004%	2.187%		

2.1.8. Oxygen

Oxygen (Z = 8) has three naturally occurring isotopes (^{16}O, ^{17}O, and ^{18}O) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 22. The output of MatMCNP for oxygen is shown in Table 23. Finally, the verification of the implementation of oxygen within MatMCNP is found in Table 24. It is once again clear from Table 24 that low density and low isotopic abundance causes issues with round-off (See Appendix A, Tables 272 through 274 for high density verification). [*NOTE: The oxygen implementation within MatMCNP uses the ^{16}O cross section for the ^{18}O atoms because a cross section for ^{18}O is not available.*]

Table 22 – Oxygen Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{16}O	0.9975700	-4.7370	15.99491462	0.997290	0.0000491
^{17}O	0.0003800	-0.8087	16.99913182	0.000404	0.0000000
^{18}O	0.0020500	-0.7828	17.99915963	0.002306	0.0000001
Density (g/cm^3) = 0.001308				FM Conversion = 6.0298932E-10	
Total Atomic Density (atoms/b-cm) = 0.0000492					

Table 23 – MatMCNP Output for Elemental Oxygen (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   O-16        0.997570           0.997290          0.0000491
C   O-17        0.000380           0.000404          0.0000000
C   O-18        0.002050           0.002306          0.0000001
C
C  The total compound atom density (atom/b-cm):  0.0000492
C
M8      08016.80c   0.997570
        08017.80c   0.000380
        08016.80c   0.002050
C
C  Caution: The O-18 has been set to O-16.
C
C  To convert a particle flux to rad[Material]
C  use FM  6.0298933E-10 8    -4  1 for neutrons
C   or FM  6.0298933E-10 8    -5 -6 for photons.
```

Table 24 – Difference between NWC and MatMCNP for Oxygen

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{16}O	0.000%	0.000%	-0.027%	-0.067%	0.000%
^{17}O	0.000%	0.063%	-100.000%		
^{18}O	0.000%	-0.010%	-0.919%		

2.1.9. Fluorine

Fluorine (Z = 9) has just one stable isotope (^{19}F) listed in the NWC. The mass defect and Excel computed quantities are found in Table 25. The fluorine output from MatMCNP is found in Table 26. The fluorine verification data for MatMCNP implementation is found in Table 27. An examination of Table 27 reveals that the MatMCNP results agree with the NWC and Excel values within 0.074% for all quantities examined.

Table 25 – Fluorine Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{19}F	1.0000000	-1.4874	18.99840321	1.0000000	0.0000538
Density (g/cm^3) = 0.001696			FM Conversion = 5.0780427E-10		
Total Atomic Density (atoms/b-cm) = 0.0000538					

Table 26 – MatMCNP Output for Elemental Fluorine (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   F-19        1.000000          1.000000          0.0000538
C
C  The total compound atom density (atom/b-cm):  0.0000538
C
M9      09019.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  5.0780424E-10 9    -4  1 for neutrons
C   or FM  5.0780424E-10 9    -5 -6 for photons.
```

Table 27 – Difference between NWC and MatMCNP for Fluorine

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{19}F	0.000%	0.000%	0.074%	0.074%	0.000%

2.1.10. Neon

Neon (Z = 10) has three naturally occurring isotopes (^{20}Ne, ^{21}Ne, and ^{22}Ne) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 28. The output of MatMCNP for neon is shown in Table 29. Finally, the verification of the implementation of neon within MatMCNP is found in Table 30. Examining Table 30, it is apparent that low density and low isotopic abundance causes issues with round-off (See Appendix A, Tables 275 through 277 for high density verification). In addition, the FM value for converting fluence to dose is not computed by MatMCNP for neon. [*NOTE: The neon implementation within MatMCNP does not result in a material card because there are no suitable cross sections available for neon.*]

Table 28 – Neon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{20}Ne	0.9048000	-7.0419	19.99244021	0.896388	0.0000243
^{21}Ne	0.0027000	-5.7317	20.99384677	0.002809	0.0000001
^{22}Ne	0.0925000	-8.0247	21.99138513	0.100803	0.0000025
Density (g/cm^3) = 8.999E-04			FM Conversion = 4.7806978E-10		
Total Atomic Density (atoms/b-cm) = 0.0000269					

Table 29 – MatMCNP Output for Elemental Neon (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ne-20        0.904800           0.896388          0.0000243
C  Ne-21        0.002700           0.002809          0.0000001
C  Ne-22        0.092500           0.100803          0.0000025
C
C  The total compound atom density (atom/b-cm):  0.0000269
C
C  One or more of the elements in the compound does not have a cross-section
C  and therefore the MCNP Card will not be created.
```

Table 30 – Difference between NWC and MatMCNP for Neon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{20}Ne	0.000%	0.000%	0.007%	0.168%	Not computed by MatMCNP
^{21}Ne	0.000%	0.004%	37.916%		
^{22}Ne	0.000%	0.000%	0.641%		

2.1.11. Sodium

Sodium (Z = 11) has one naturally occurring isotope (^{23}Na) listed in the NWC. The mass defect and Excel computed quantities are found in Table 31. The sodium output from MatMCNP is found in Table 32. The sodium verification data for MatMCNP implementation is found in Table 33. An examination of Table 33 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 31 – Sodium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{23}Na	1.0000000	-9.5298	22.98976934	1.0000000	0.0254352
Density (g/cm^3) = 0.971				FM Conversion = 4.1964189E-10	
Total Atomic Density (atoms/b-cm) = 0.0254352					

Table 32 – MatMCNP Output for Elemental Sodium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Na-23        1.000000           1.000000          0.0254352
C
C  The total compound atom density (atom/b-cm):  0.0254352
C
M11     11023.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  4.1964190E-10 11   -4  1 for neutrons
C   or FM  4.1964190E-10 11   -5 -6 for photons.
```

Table 33 – Difference between NWC and MatMCNP for Sodium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{23}Na	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.12. Magnesium

Magnesium (Z = 12) has three naturally occurring isotopes (^{24}Mg, ^{25}Mg, and ^{26}Mg) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 34. The output for magnesium from MatMCNP is shown in Table 35. Finally, the verification of the implementation of magnesium within MatMCNP is found in Table 36. Table 36 shows that the implementation of magnesium within MatMCNP has been performed correctly.

Table 34 – Magnesium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{24}Mg	0.7899000	-13.9335	23.98504177	0.779500	0.0340154
^{25}Mg	0.1000000	-13.1927	24.98583705	0.102801	0.0043063
^{26}Mg	0.1101000	-16.2145	25.98259302	0.117699	0.0047412
Density (g/cm^3) = 1.738			FM Conversion = 3.9693272E-10		
Total Atomic Density (atoms/b-cm) = 0.0430630					

Table 35 – MatMCNP Output for Elemental Magnesium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Mg-24        0.789900           0.779500          0.0340155
C  Mg-25        0.100000           0.102801          0.0043063
C  Mg-26        0.110100           0.117699          0.0047412
C
C  The total compound atom density (atom/b-cm):  0.0430630
C
M12     12024.80c   0.789900
        12025.80c   0.100000
        12026.80c   0.110100
C
C  To convert a particle flux to rad[Material]
C  use FM  3.9693276E-10 12   -4  1 for neutrons
C   or FM  3.9693276E-10 12   -5 -6 for photons.
```

Table 36 – Difference between NWC and MatMCNP for Magnesium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{24}Mg	0.000%	0.000%	0.000%	0.000%	0.000%
^{25}Mg	0.000%	0.000%	0.000%		
^{26}Mg	0.000%	0.000%	-0.001%		

2.1.13. Aluminum

Aluminum (Z = 13) has just one naturally occurring isotope (^{27}Al) listed in the NWC. The mass defect and Excel computed quantities are found in Table 37. The aluminum output from MatMCNP is found in Table 38. The aluminum verification data for MatMCNP implementation is found in Table 39. An examination of Table 39 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 37 – Aluminum Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{27}Al	1.0000000	-17.1967	26.98153858	1.0000000	0.0602380
Density (g/cm^3) = 2.6989			FM Conversion = 3.5755820E-10		
Total Atomic Density (atoms/b-cm) = 0.0602380					

Table 38 – MatMCNP Output for Elemental Aluminum (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Al-27        1.000000          1.000000          0.0602381
C
C  The total compound atom density (atom/b-cm):  0.0602381
C
M13     13027.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  3.5755818E-10 13   -4  1 for neutrons
C   or FM  3.5755818E-10 13   -5 -6 for photons.
```

Table 39 – Difference between NWC and MatMCNP for Aluminum

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{27}Al	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.14. Silicon

Silicon (Z = 14) has three naturally occurring isotopes (^{28}Si, ^{29}Si, and ^{30}Si) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 40. The output for silicon from MatMCNP is shown in Table 41. Finally, the verification of the implementation of silicon within MatMCNP is found in Table 42. Table 42 shows that the implementation of silicon within MatMCNP has been performed correctly.

Table 40 – Silicon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{28}Si	0.9222300	-21.4927	27.97692664	0.918665	0.0460748
^{29}Si	0.0468500	-21.8950	28.97649475	0.048336	0.0023406
^{30}Si	0.0309200	-24.4329	29.97377020	0.032999	0.0015448
Density (g/cm^3) = 2.330			FM Conversion = 3.4350361E-10		
Total Atomic Density (atoms/b-cm) = 0.0499602					

Table 41 – MatMCNP Output for Elemental Silicon (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Si-28        0.922230           0.918665          0.0460749
C  Si-29        0.046850           0.048336          0.0023406
C  Si-30        0.030920           0.032999          0.0015448
C
C  The total compound atom density (atom/b-cm):  0.0499603
M14     14028.80c   0.922230
        14029.80c   0.046850
        14030.80c   0.030920
C
C  To convert a particle flux to rad[Material]
C  use FM  3.4350364E-10 14   -4  1 for neutrons
C   or FM  3.4350364E-10 14   -5 -6 for photons.
```

Table 42 – Difference between NWC and MatMCNP for Silicon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{28}Si	0.000%	0.000%	0.000%	0.000%	0.000%
^{29}Si	0.000%	-0.001%	-0.002%		
^{30}Si	0.000%	0.000%	0.002%		

2.1.15. Phosphorus

Phosphorus (Z = 15) has one stable isotope (^{31}P) listed in the NWC. The mass defect and Excel computed quantities are found in Table 43. The phosphorus output from MatMCNP is found in Table 44. The phosphorus verification data for MatMCNP implementation is found in Table 45. An examination of Table 45 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 43 – Phosphorus Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{31}P	1.0000000	-24.4405	30.97376204	1.0000000	0.0353857
Density (g/cm^3) = 1.82			FM Conversion = 3.1147235E-10		
Total Atomic Density (atoms/b-cm) = 0.0353857					

Table 44 – MatMCNP Output for Elemental Phosphorus (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   P-31        1.000000           1.000000          0.0353857
C
C  The total compound atom density (atom/b-cm):  0.0353857
C
M15     15031.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  3.1147235E-10 15   -4  1 for neutrons
C   or FM  3.1147235E-10 15   -5 -6 for photons.
```

Table 45 – Difference between NWC and MatMCNP for Phosphorus

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{31}P	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.16. Sulfur

Sulfur (Z = 16) has four naturally occurring isotopes (^{32}S, ^{33}S, ^{34}S, and ^{36}S) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 46. The output for sulfur from MatMCNP is shown in Table 47. Finally, the verification of the implementation of sulfur within MatMCNP is found in Table 48 Table 48 shows that the implementation of sulfur within MatMCNP has been performed correctly.

Table 46 – Sulfur Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{32}S	0.9499000	-26.0155	31.97207121	0.947153	0.0369292
^{33}S	0.0075000	-26.5858	32.97145897	0.007712	0.0002916
^{34}S	0.0425000	-29.9316	33.96786710	0.045022	0.0016523
^{36}S	0.0001000	-30.6641	35.96708073	0.000112	0.0000039
Density (g/cm^3) = 2.070				FM Conversion = 3.0087430E-10	
Total Atomic Density (atoms/b-cm) = 0.0388770					

Table 47 – MatMCNP Output for Elemental Sulfur (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   S-32        0.949900           0.947153          0.0369293
C   S-33        0.007500           0.007712          0.0002916
C   S-34        0.042500           0.045022          0.0016523
C   S-36        0.000100           0.000112          0.0000039
C
C  The total compound atom density (atom/b-cm):  0.0388770
C
M16      16032.80c   0.949900
         16033.80c   0.007500
         16034.80c   0.042500
         16036.80c   0.000100
C
C  To convert a particle flux to rad[Material]
C  use FM  3.0087433E-10 16   -4  1 for neutrons
C   or FM  3.0087433E-10 16   -5 -6 for photons.
```

Table 48 – Difference between NWC and MatMCNP for Sulfur

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{32}S	0.000%	0.000%	0.000%	0.000%	0.000%
^{33}S	0.000%	-0.001%	0.008%		
^{34}S	0.000%	-0.001%	0.002%		
^{36}S	0.000%	-0.152%	0.316%		

2.1.17. Chlorine

Chlorine (Z = 17) has two naturally occurring isotopes (^{35}Cl and ^{37}Cl) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 49. The output of MatMCNP for chlorine is shown in Table 50. Finally, the verification of the implementation of chlorine within MatMCNP is found in Table 51. Table 51 shows that the implementation of chlorine within MatMCNP has been performed correctly.

Table 49 – Chlorine Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{35}Cl	0.7576000	-29.0135	34.96885272	0.747256	0.0000414
^{37}Cl	0.2424000	-31.7615	36.96590263	0.252744	0.0000132
Density (g/cm^3) = 0.003214			FM Conversion = 2.7212048E-10		
Total Atomic Density (atoms/b-cm) = 0.0000546					

Table 50 – MatMCNP Output for Elemental Chlorine (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Cl-35        0.757600           0.747255          0.0000414
C  Cl-37        0.242400           0.252744          0.0000132
C
C  The total compound atom density (atom/b-cm):  0.0000546
C
M17     17035.80c   0.757600
        17037.80c   0.242400
C
C  To convert a particle flux to rad[Material]
C  use FM  2.7212047E-10 17   -4  1 for neutrons
C   or FM  2.7212047E-10 17   -5 -6 for photons.
```

Table 51 – Difference between NWC and MatMCNP for Chlorine

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{35}Cl	0.000%	0.000%	0.096%	0.011%	0.000%
^{37}Cl	0.000%	0.000%	-0.254%		

2.1.18. Argon

Argon (Z = 18) has three naturally occurring isotopes (^{36}Ar, ^{38}Ar, and ^{40}Ar) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 52. The output for argon from MatMCNP is shown in Table 53. Finally, the verification of the implementation of argon within MatMCNP is found in Table 54. Examining Table 54, it is apparent that low density and low isotopic abundance causes issues with round-off (See Appendix A, Tables 278 through 280 for high density verification).

Table 52 – Argon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{36}Ar	0.0033360	-30.2315	35.96754515	0.003004	0.0000001
^{38}Ar	0.0006290	-34.7147	37.96273223	0.000598	0.0000000
^{40}Ar	0.9960350	-35.0398	39.96238323	0.996399	0.0000268
Density (g/cm^3) = 0.0017837			FM Conversion = 2.4150193E-10		
Total Atomic Density (atoms/b-cm) = 0.0000269					

Table 53 – MatMCNP Output for Elemental Argon (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ar-36        0.003336           0.003004          0.0000001
C  Ar-38        0.000629           0.000598          0.0000000
C  Ar-40        0.996035           0.996399          0.0000268
C
C  The total compound atom density (atom/b-cm):  0.0000269
C
M18     18036.80c   0.003336
        18038.80c   0.000629
        18040.80c   0.996035
C
C  To convert a particle flux to rad[Material]
C  use FM  2.4150193E-10 18   -4  1 for neutrons
C   or FM  2.4150193E-10 18   -5 -6 for photons.
```

Table 54 – Difference between NWC and MatMCNP for Argon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{36}Ar	0.000%	0.013%	11.479%	0.040%	0.000%
^{38}Ar	0.000%	0.043%	-100.000%		
^{40}Ar	0.000%	0.000%	0.065%		

2.1.19. Potassium

Potassium (Z = 19) has three naturally occurring isotopes (^{39}K, ^{40}K, and ^{41}K) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 55. The output for potassium from MatMCNP is shown in Table 56. Finally, the verification of the implementation of potassium within MatMCNP is found in Table 57. Table 57 shows that the implementation of potassium within MatMCNP has been performed correctly.

Table 55 – Potassium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{39}K	0.9325810	-33.8071	38.96370658	0.929371	0.0127841
^{40}K	0.0001170	-33.5354	39.96399827	0.000120	0.0000016
^{41}K	0.0673020	-35.5595	40.96182530	0.070510	0.0009226
Density (g/cm^3) = 0.89				FM Conversion = 2.4674909E-10	
Total Atomic Density (atoms/b-cm) = 0.0137083					

Table 56 – MatMCNP Output for Elemental Potassium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   K-39        0.932581           0.929371          0.0127841
C   K-40        0.000117           0.000120          0.0000016
C   K-41        0.067302           0.070510          0.0009226
C
C  The total compound atom density (atom/b-cm):  0.0137083
C
M19     19039.80c   0.932581
        19040.80c   0.000117
        19041.80c   0.067302
C  To convert a particle flux to rad[Material]
C  use FM  2.4674909E-10 19   -4  1 for neutrons
C   or FM  2.4674909E-10 19   -5 -6 for photons.
```

Table 57 – Difference between NWC and MatMCNP for Potassium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{39}K	0.000%	0.000%	0.000%	0.000%	0.000%
^{40}K	0.000%	0.342%	-0.241%		
^{41}K	0.000%	0.000%	0.001%		

2.1.20. Calcium

Calcium (Z = 20) has six naturally occurring isotopes (^{40}Ca, ^{42}Ca, ^{43}Ca, ^{44}Ca, ^{46}Ca, and ^{48}Ca) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 58. The output for calcium from MatMCNP is shown in Table 59. Finally, the verification of the implementation of calcium within MatMCNP is found in Table 60. Table 60 shows that the implementation of calcium within MatMCNP has been performed correctly. In order to assess this for calcium, we examine the values in Table 58 and Table 59. The values in both tables are the same within round off, but the percent differences calculated by Excel include extra digits. (*NOTE: The NWC atomic abundances sum to 100.003. The numbers below and within MatMCNP take that into account.*)

Table 58 – Calcium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{40}Ca	0.9693709	-34.8463	39.96259096	0.966575	0.0224312
^{42}Ca	0.0064698	-38.5472	41.95861788	0.006773	0.0001497
^{43}Ca	0.0013500	-38.4089	42.95876635	0.001447	0.0000312
^{44}Ca	0.0208994	-41.4688	43.95548141	0.022921	0.0004836
^{46}Ca	0.0000400	-43.1399	45.95368741	0.000046	0.0000009
^{48}Ca	0.0018699	-44.2234	47.95252422	0.002237	0.0000433
Density (g/cm^3) = 1.54				FM Conversion = 2.4071629E-10	
Total Atomic Density (atoms/b-cm) = 0.0231400					

Table 59 – MatMCNP Output for Elemental Calcium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ca-40        0.969371           0.966575          0.0224313
C  Ca-42        0.006470           0.006773          0.0001497
C  Ca-43        0.001350           0.001447          0.0000312
C  Ca-44        0.020899           0.022921          0.0004836
C  Ca-46        0.000040           0.000046          0.0000009
C  Ca-48        0.001870           0.002237          0.0000433
C
C  The total compound atom density (atom/b-cm):  0.0231400
C
M20      20040.80c   0.969371
         20042.80c   0.006470
         20043.80c   0.001350
         20044.80c   0.020899
         20046.80c   0.000040
         20048.80c   0.001870
C
C  To convert a particle flux to rad[Material]
C  use FM  2.4071631E-10 20   -4  1 for neutrons
C   or FM  2.4071631E-10 20   -5 -6 for photons.
```

Table 60 – Difference between NWC and MatMCNP for Calcium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{40}Ca	0.000%	0.000%	0.000%	0.000%	0.000%
^{42}Ca	0.003%	-0.005%	-0.008%		
^{43}Ca	0.003%	0.001%	-0.122%		
^{44}Ca	-0.002%	-0.001%	-0.002%		
^{46}Ca	0.003%	0.299%	-2.763%		
^{48}Ca	0.003%	-0.015%	0.068%		

2.1.21. Scandium

Scandium (Z = 21) has only one stable isotope (^{45}Sc) listed in the NWC. The mass defect and Excel computed quantities are found in Table 61. The scandium output from MatMCNP is found in Table 62. The scandium verification data for MatMCNP implementation is found in Table 63. An examination of Table 63 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 61 – Scandium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{45}Sc	1.0000000	-41.0703	44.95590922	1.0000000	0.0400396
Density (g/cm^3) = 2.989			FM Conversion = 2.1459849E-10		
Total Atomic Density (atoms/b-cm) = 0.0400396					

Table 62 – MatMCNP Output for Elemental Scandium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Sc-45        1.000000           1.000000          0.0400396
C
C  The total compound atom density (atom/b-cm):  0.0400396
C
M21     21045.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  2.1459849E-10 21   -4  1 for neutrons
C   or FM  2.1459849E-10 21   -5 -6 for photons.
```

Table 63 – Difference between NWC and MatMCNP for Scandium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{45}Sc	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.22. Titanium

Titanium (Z = 22) has five naturally occurring isotopes (^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, and ^{50}Ti) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 64. The output for titanium from MatMCNP is shown in Table 65. Finally, the verification of the implementation of titanium within MatMCNP is found in Table 66. Table 66 shows that the implementation of titanium within MatMCNP has been performed correctly.

Table 64 – Titanium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{46}Ti	0.0825000	-44.1270	45.95262771	0.079201	0.0046811
^{47}Ti	0.0744000	-44.9364	46.95175879	0.072978	0.0042215
^{48}Ti	0.7372000	-48.4917	47.94794202	0.738451	0.0418291
^{49}Ti	0.0541000	-48.5628	48.94786569	0.055322	0.0030697
^{50}Ti	0.0518000	-51.4307	49.94478687	0.054049	0.0029392
Density (g/cm^3) = 4.51				FM Conversion = 2.0154849E-10	
Total Atomic Density (atoms/b-cm) = 0.0567405					

Table 65 – MatMCNP Output for Elemental Titanium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ti-46        0.082500           0.079201          0.0046811
C  Ti-47        0.074400           0.072978          0.0042215
C  Ti-48        0.737200           0.738451          0.0418291
C  Ti-49        0.054100           0.055322          0.0030697
C  Ti-50        0.051800           0.054049          0.0029392
C
C  The total compound atom density (atom/b-cm):  0.0567406
C
M22      22046.80c   0.082500
         22047.80c   0.074400
         22048.80c   0.737200
         22049.80c   0.054100
         22050.80c   0.051800
C
C  To convert a particle flux to rad[Material]
C  use FM  2.0154851E-10 22   -4  1 for neutrons
C   or FM  2.0154851E-10 22   -5 -6 for photons.
```

Table 66 – Difference between NWC and MatMCNP for Titanium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{46}Ti	0.000%	0.000%	0.000%	0.000%	0.000%
^{47}Ti	0.000%	0.000%	0.000%		
^{48}Ti	0.000%	0.000%	0.000%		
^{49}Ti	0.000%	0.000%	0.001%		
^{50}Ti	0.000%	0.000%	0.001%		

2.1.23. Vanadium

Vanadium (Z = 23) has two naturally occurring isotopes (^{50}V and ^{51}V) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 67. The output of MatMCNP for vanadium is shown in Table 68. Finally, the verification of the implementation of vanadium within MatMCNP is found in Table 69. Table 69 shows that the implementation of vanadium within MatMCNP has been performed correctly.

Table 67 – Vanadium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{50}V	0.0025000	-49.2240	49.94715586	0.002451	0.0001773
^{51}V	0.9975000	-52.2039	50.94395680	0.997549	0.0707528
Density (g/cm^3) = 6.0			FM Conversion = 1.8938345E-10		
Total Atomic Density (atoms/b-cm) = 0.0709301					

Table 68 – MatMCNP Output for Elemental Vanadium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   V-50        0.002500           0.002451          0.0001773
C   V-51        0.997500           0.997549          0.0707528
C
C  The total compound atom density (atom/b-cm):  0.0709301
C
M23     23050.80c   0.002500
        23051.80c   0.997500
C  To convert a particle flux to rad[Material]
C  use FM  1.8938345E-10 23   -4  1 for neutrons
C   or FM  1.8938345E-10 23   -5 -6 for photons.
```

Table 69 – Difference between NWC and MatMCNP for Vanadium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{50}V	0.000%	-0.008%	-0.014%	0.000%	0.000%
^{51}V	0.000%	0.000%	0.000%		

2.1.24. Chromium

Chromium (Z = 24) has four naturally occurring isotopes (^{50}Cr, ^{52}Cr, ^{53}Cr, and ^{54}Cr) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 70. The output for chromium from MatMCNP is shown in Table 71. Finally, the verification of the implementation of chromium within MatMCNP is found in Table 72. Table 72 shows that the implementation of chromium within MatMCNP has been performed correctly.

Table 70 – Chromium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{50}Cr	0.0434500	-50.2619	49.94604163	0.041737	0.0035981
^{52}Cr	0.8378900	-55.4180	51.94050633	0.836994	0.0693861
^{53}Cr	0.0950100	-55.2858	52.94064825	0.096736	0.0078678
^{54}Cr	0.0236500	-56.9336	53.93887926	0.024534	0.0019585
Density (g/cm^3) = 7.15			FM Conversion = 1.8554208E-10		
Total Atomic Density (atoms/b-cm) = 0.0828105					

Table 71 – MatMCNP Output for Elemental Chromium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Cr-50        0.043450           0.041737          0.0035981
C  Cr-52        0.837890           0.836994          0.0693862
C  Cr-53        0.095010           0.096736          0.0078678
C  Cr-54        0.023650           0.024534          0.0019585
C
C  The total compound atom density (atom/b-cm):  0.0828106
C
M24      24050.80c   0.043450
         24052.80c   0.837890
         24053.80c   0.095010
         24054.80c   0.023650
C  To convert a particle flux to rad[Material]
C  use FM  1.8554210E-10 24   -4  1 for neutrons
C   or FM  1.8554210E-10 24   -5 -6 for photons.
```

Table 72 – Difference between NWC and MatMCNP for Chromium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{50}Cr	0.000%	0.000%	0.000%	0.000%	0.000%
^{52}Cr	0.000%	0.000%	0.000%		
^{53}Cr	0.000%	0.000%	0.000%		
^{54}Cr	0.000%	0.001%	0.002%		

2.1.25. Manganese

Manganese (Z = 25) has just one stable isotope (^{55}Mn) listed in the NWC. The mass defect and Excel computed quantities are found in Table 73. The MatMCNP for manganese is found in Table 74. The manganese verification data for MatMCNP implementation is found in Table 75. An examination of Table 75 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 73 – Manganese Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{55}Mn	1.0000000	-57.7117	54.93804394	1.0000000	0.0802944
Density (g/cm^3) = 7.325			FM Conversion = 1.7560637E-10		
Total Atomic Density (atoms/b-cm) = 0.0802944					

Table 74 – MatMCNP Output for Elemental Manganese (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Mn-55        1.000000           1.000000          0.0802944
C
C  The total compound atom density (atom/b-cm):  0.0802944
C
M25      25055.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  1.7560638E-10 25   -4  1 for neutrons
C   or FM  1.7560638E-10 25   -5 -6 for photons.
```

Table 75 – Difference between NWC and MatMCNP for Manganese

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{55}Mn	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.26. Iron

Iron (Z = 26) has four naturally occurring isotopes (^{54}Fe, ^{56}Fe, ^{57}Fe, and ^{58}Fe) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 76. The output from MatMCNP for iron is shown in Table 77. Finally, the iron verification data for MatMCNP implementation is found in Table 78. An examination of Table 78 shows that the implementation of iron within MatMCNP has been performed correctly.

Table 76 – Iron Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{54}Fe	0.0584500	-56.2538	53.93960906	0.056456	0.0049630
^{56}Fe	0.9175400	-60.6063	55.93493646	0.919015	0.0779086
^{57}Fe	0.0211900	-60.1811	56.93539293	0.021604	0.0017993
^{58}Fe	0.0028200	-62.1544	57.93327450	0.002925	0.0002394
Density (g/cm^3) = 7.874				FM Conversion = 1.7275397E-10	
Total Atomic Density (atoms/b-cm) = 0.0849103					

Table 77 – MatMCNP Output for Elemental Iron (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Fe-54        0.058450           0.056456          0.0049630
C  Fe-56        0.917540           0.919015          0.0779087
C  Fe-57        0.021190           0.021604          0.0017993
C  Fe-58        0.002820           0.002925          0.0002394
C
C  The total compound atom density (atom/b-cm):  0.0849104
C
M26      26054.80c   0.058450
         26056.80c   0.917540
         26057.80c   0.021190
         26058.80c   0.002820
C
C  To convert a particle flux to rad[Material]
C  use FM  1.7275398E-10 26   -4  1 for neutrons
C   or FM  1.7275398E-10 26   -5 -6 for photons.
```

Table 78 – Difference between NWC and MatMCNP for Iron

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{54}Fe	0.000%	0.001%	0.000%	0.000%	0.000%
^{56}Fe	0.000%	0.000%	0.000%		
^{57}Fe	0.000%	0.001%	0.003%		
^{58}Fe	0.000%	-0.015%	-0.020%		

2.1.27. Cobalt

Cobalt ($Z = 27$) has one stable isotope (^{59}Co) listed in the NWC. The mass defect and Excel computed quantities are found in Table 79. The MatMCNP for cobalt is found in Table 80. The cobalt verification data for MatMCNP implementation is found in Table 81. An examination of Table 81 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 79 – Cobalt Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{59}Co	1.0000000	-62.2290	58.93319442	1.0000000	0.0909454
Density (g/cm^3) = 8.90			FM Conversion = 1.6370181E-10		
Total Atomic Density (atoms/b-cm) = 0.0909454					

Table 80 – MatMCNP Output for Elemental Cobalt (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Co-59        1.000000           1.000000          0.0909455
C
C  The total compound atom density (atom/b-cm):  0.0909455
C
M27     27059.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  1.6370182E-10 27   -4  1 for neutrons
C   or FM  1.6370182E-10 27   -5 -6 for photons.
```

Table 81 – Difference between NWC and MatMCNP for Cobalt

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{59}Co	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.28. Nickel

Nickel ($Z = 28$) has five naturally occurring isotopes (^{58}Ni, ^{60}Ni, ^{61}Ni, ^{62}Ni, and ^{64}Ni) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 82. The output for nickel from MatMCNP is shown in Table 83. Finally, the verification of the implementation of nickel within MatMCNP is found in Table 84. Table 84 shows that the implementation of nickel within MatMCNP has been performed correctly.

Table 82 – Nickel Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{58}Ni	0.6807700	-60.2281	57.93534247	0.671978	0.0621799
^{60}Ni	0.2622300	-64.4725	59.93078592	0.267759	0.0239514
^{61}Ni	0.0113990	-64.2212	60.93105570	0.011834	0.0010412
^{62}Ni	0.0363460	-66.7458	61.92834543	0.038349	0.0033198
^{64}Ni	0.0092550	-67.0984	63.92796690	0.010080	0.0008453
Density (g/cm^3) = 8.902			FM Conversion = 1.6437076E-10		
Total Atomic Density (atoms/b-cm) = 0.0913375					

Table 83 – MatMCNP Output for Elemental Nickel (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ni-58        0.680770           0.671978          0.0621799
C  Ni-60        0.262230           0.267759          0.0239515
C  Ni-61        0.011399           0.011834          0.0010412
C  Ni-62        0.036346           0.038349          0.0033198
C  Ni-64        0.009255           0.010080          0.0008453
C
C  The total compound atom density (atom/b-cm):  0.0913376
C
M28     28058.80c   0.680770
        28060.80c   0.262230
        28061.80c   0.011399
        28062.80c   0.036346
        28064.80c   0.009255
C  To convert a particle flux to rad[Material]
C  use FM  1.6437075E-10 28   -4  1 for neutrons
C   or FM  1.6437075E-10 28   -5 -6 for photons.
```

Table 84 – Difference between NWC and MatMCNP for Nickel

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{58}Ni	0.000%	0.000%	0.000%	0.000%	0.000%
^{60}Ni	0.000%	0.000%	0.000%		
^{61}Ni	0.000%	0.003%	0.004%		
^{62}Ni	0.000%	-0.001%	0.001%		
^{64}Ni	0.000%	-0.004%	-0.003%		

2.1.29. Copper

Copper (Z = 29) has two naturally occurring isotopes (^{63}Cu and ^{65}Cu) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 85. The output of MatMCNP for copper is shown in Table 86. Finally, the verification of the implementation of copper within MatMCNP is found in Table 87. An examination of Table 87 shows that the implementation of copper within MatMCNP has been performed correctly.

Table 85 – Copper Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{63}Cu	0.6915000	-65.5792	62.92959783	0.684792	0.0587168
^{65}Cu	0.3085000	-67.2633	64.92778987	0.315208	0.0261954
Density (g/cm^3) = 8.96			FM Conversion = 1.5181859E-10		
Total Atomic Density (atoms/b-cm) = 0.0849122					

Table 86 – MatMCNP Output for Elemental Copper (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Cu-63        0.691500           0.684792          0.0587168
C  Cu-65        0.308500           0.315208          0.0261954
C
C  The total compound atom density (atom/b-cm):  0.0849123
C
M29     29063.80c   0.691500
        29065.80c   0.308500
C
C  To convert a particle flux to rad[Material]
C  use FM  1.5181861E-10 29   -4  1 for neutrons
C   or FM  1.5181861E-10 29   -5 -6 for photons.
```

Table 87 – Difference between NWC and MatMCNP for Copper

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{63}Cu	0.000%	0.000%	0.000%	0.000%	0.000%
^{65}Cu	0.000%	0.000%	0.000%		

2.1.30. Zinc

Zinc (Z = 30) has five naturally occurring isotopes (^{64}Zn, ^{66}Zn, ^{67}Zn, ^{68}Zn, and ^{70}Zn) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 88. The output for zinc from MatMCNP is shown in Table 89. Finally, the verification of the implementation of zinc within MatMCNP is found in Table 90. Table 90 shows that the implementation of zinc within MatMCNP has been performed correctly.

Table 88 – Zinc Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{64}Zn	0.4917000	-66.0036	63.92914222	0.480805	0.0323112
^{66}Zn	0.2773000	-68.8990	65.92603388	0.279625	0.0182223
^{67}Zn	0.0404000	-67.8800	66.92712782	0.041357	0.0026548
^{68}Zn	0.1845000	-70.0068	67.92484460	0.191688	0.0121241
^{70}Zn	0.0061000	-69.5646	69.92531933	0.006524	0.0004009
Density (g/cm^3) = 7.134				FM Conversion = 1.4756497E-10	
Total Atomic Density (atoms/b-cm) = 0.0657133					

Table 89 – MatMCNP Output for Elemental Zinc (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Zn-64        0.491700           0.480805          0.0323113
C  Zn-66        0.277300           0.279625          0.0182223
C  Zn-67        0.040400           0.041357          0.0026548
C  Zn-68        0.184500           0.191688          0.0121241
C  Zn-70        0.006100           0.006524          0.0004009
C
C  The total compound atom density (atom/b-cm):  0.0657134
C
M30     30064.80c   0.491700
        30066.80c   0.277300
        30067.80c   0.040400
        30068.80c   0.184500
        30070.80c   0.006100
C
C  To convert a particle flux to rad[Material]
C  use FM  1.4756497E-10 30   -4  1 for neutrons
C   or FM  1.4756497E-10 30   -5 -6 for photons.
```

Table 90 – Difference between NWC and MatMCNP for Zinc

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{64}Zn	0.000%	0.000%	0.000%	0.000%	0.000%
^{66}Zn	0.000%	0.000%	0.000%		
^{67}Zn	0.000%	-0.001%	-0.001%		
^{68}Zn	0.000%	0.000%	0.000%		
^{70}Zn	0.000%	-0.005%	0.012%		

2.1.31. Gallium

Gallium (Z = 31) has two naturally occurring isotopes (^{69}Ga and ^{71}Ga) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 91. The output of MatMCNP for gallium is shown in Table 92. Finally, the verification of the implementation of gallium within MatMCNP is found in Table 93. An examination of Table 93 shows that the implementation of gallium within MatMCNP has been performed correctly.

Table 91 – Gallium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{69}Ga	0.6010800	-69.3277	68.92557365	0.594205	0.0306516
^{71}Ga	0.3989200	-70.1390	70.92470268	0.405795	0.0203426
Density (g/cm^3) = 5.904				FM Conversion = 1.3836842E-10	
Total Atomic Density (atoms/b-cm) = 0.0509942					

Table 92 – MatMCNP Output for Elemental Gallium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ga-69        0.601080           0.594205          0.0306516
C  Ga-71        0.398920           0.405795          0.0203426
C
C  The total compound atom density (atom/b-cm):  0.0509942
C
M31     31069.80c   0.601080
        31071.80c   0.398920
C
C  To convert a particle flux to rad[Material]
C  use FM  1.3836841E-10 31   -4  1 for neutrons
C   or FM  1.3836841E-10 31   -5 -6 for photons.
```

Table 93 – Difference between NWC and MatMCNP for Gallium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{69}Ga	0.000%	0.000%	0.000%	0.000%	0.000%
^{71}Ga	0.000%	0.000%	0.000%		

2.1.32. Germanium

Germanium (Z = 32) has five naturally occurring isotopes (^{70}Ge, ^{72}Ge, ^{73}Ge, ^{74}Ge, and ^{76}Ge) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 94. The output for germanium from MatMCNP is shown in Table 95. Finally, the verification of the implementation of germanium within MatMCNP is found in Table 96. Table 96 shows that the implementation of germanium within MatMCNP has been performed correctly.

Table 94 – Germanium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{70}Ge	0.2057000	-70.5618	69.92424879	0.198044	0.0090790
^{72}Ge	0.2745000	-72.5856	71.92207615	0.271834	0.0121157
^{73}Ge	0.0775000	-71.2972	72.92345930	0.077816	0.0034206
^{74}Ge	0.3650000	-73.4221	73.92117813	0.371501	0.0161101
^{76}Ge	0.0773000	-73.2128	75.92140282	0.080806	0.0034118
Density (g/cm^3) = 5.323			FM Conversion = 1.3283486E-10		
Total Atomic Density (atoms/b-cm) = 0.0441373					

Table 95 – MatMCNP Output for Elemental Germanium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ge-70        0.205700           0.198044          0.0090790
C  Ge-72        0.274500           0.271834          0.0121157
C  Ge-73        0.077500           0.077816          0.0034206
C  Ge-74        0.365000           0.371501          0.0161101
C  Ge-76        0.077300           0.080806          0.0034118
C
C  The total compound atom density (atom/b-cm):  0.0441373
C
M32     32070.80c   0.205700
        32072.80c   0.274500
        32073.80c   0.077500
        32074.80c   0.365000
        32076.80c   0.077300
C
C  To convert a particle flux to rad[Material]
C  use FM  1.3283488E-10 32   -4  1 for neutrons
C   or FM  1.3283488E-10 32   -5 -6 for photons.
```

Table 96 – Difference between NWC and MatMCNP for Germanium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{70}Ge	0.000%	0.000%	0.000%	0.000%	0.000%
^{72}Ge	0.000%	0.000%	0.000%		
^{73}Ge	0.000%	0.000%	-0.001%		
^{74}Ge	0.000%	0.000%	0.000%		
^{76}Ge	0.000%	0.000%	0.000%		

2.1.33. Arsenic

Arsenic (Z = 33) has just one stable isotope (^{75}As) listed in the NWC. The mass defect and Excel computed quantities are found in Table 97. The MatMCNP output for arsenic is found in Table 98. The arsenic verification data for MatMCNP implementation is found in Table 99. An examination of Table 99 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 97 – Arsenic Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{75}As	1.0000000	-73.0337	74.92159509	1.0000000	0.0462180
Density (g/cm^3) = 5.75				FM Conversion = 1.2876755E-10	
Total Atomic Density (atoms/b-cm) = 0.0462180					

Table 98 – MatMCNP Output for Elemental Arsenic (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  As-75        1.000000           1.000000          0.0462181
C
C  The total compound atom density (atom/b-cm):  0.0462181
C
M33     33075.80c   1.000000
C  To convert a particle flux to rad[Material]
C  use FM  1.2876755E-10 33   -4  1 for neutrons
C   or FM  1.2876755E-10 33   -5 -6 for photons.
```

Table 99 – Difference between NWC and MatMCNP for Arsenic

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{75}As	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.34. Selenium

Selenium (Z = 34) has six naturally occurring isotopes (^{74}Se, ^{76}Se, ^{77}Se, ^{78}Se, ^{80}Se and ^{82}Se) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 100. The output for selenium from MatMCNP is shown in Table 101. Finally, the verification of the implementation of selenium within MatMCNP is found in Table 102. Table 102 shows that the implementation of selenium within MatMCNP has been performed correctly.

Table 100 – Selenium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{74}Se	0.0089000	-72.2127	73.92247647	0.008332	0.0003251
^{76}Se	0.0937000	-75.2518	75.91921387	0.090092	0.0034231
^{77}Se	0.0763000	-74.5993	76.91991435	0.074329	0.0027874
^{78}Se	0.2377000	-77.0258	77.91730940	0.234563	0.0086838
^{80}Se	0.4961000	-77.7598	79.91652142	0.502114	0.0181239
^{82}Se	0.0873000	-77.5940	81.91669941	0.090570	0.0031893
Density (g/cm^3) = 4.79				FM Conversion = 1.2218269E-10	
Total Atomic Density (atoms/b-cm) = 0.0365327					

Table 101 – MatMCNP Output for Elemental Selenium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Se-74        0.008900          0.008332          0.0003251
C  Se-76        0.093700          0.090092          0.0034231
C  Se-77        0.076300          0.074329          0.0027875
C  Se-78        0.237700          0.234563          0.0086838
C  Se-80        0.496100          0.502114          0.0181239
C  Se-82        0.087300          0.090570          0.0031893
C
C  The total compound atom density (atom/b-cm):  0.0365328
C
M34      34074.80c   0.008900
         34076.80c   0.093700
         34077.80c   0.076300
         34078.80c   0.237700
         34080.80c   0.496100
         34082.80c   0.087300
C
C  To convert a particle flux to rad[Material]
C  use FM  1.2218269E-10 34   -4  1 for neutrons
C   or FM  1.2218269E-10 34   -5 -6 for photons.
```

Table 102 – Difference between NWC and MatMCNP for Selenium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{74}Se	0.000%	-0.003%	-0.013%	0.000%	0.000%
^{76}Se	0.000%	0.000%	-0.001%		
^{77}Se	0.000%	0.000%	0.002%		
^{78}Se	0.000%	0.000%	0.000%		
^{80}Se	0.000%	0.000%	0.000%		
^{82}Se	0.000%	0.000%	0.000%		

2.1.35. Bromine

Bromine (Z = 35) has two naturally occurring isotopes (^{79}Br and ^{81}Br) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 103. The output of MatMCNP for bromine is shown in Table 104. Finally, the verification of the implementation of bromine within MatMCNP is found in Table 105. An examination of Table 105 shows that the implementation of bromine within MatMCNP has been performed correctly.

Table 103 – Bromine Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{79}Br	0.5069000	-76.0684	78.91833721	0.500650	0.0119196
^{81}Br	0.4931000	-77.9755	80.91628985	0.499350	0.0115951
Density (g/cm^3) = 3.12				FM Conversion = 1.2073898E-10	
Total Atomic Density (atoms/b-cm) = 0.0235147					

Table 104 – MatMCNP Output for Elemental Bromine (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Br-79        0.506900           0.500650          0.0119196
C  Br-81        0.493100           0.499350          0.0115951
C
C  The total compound atom density (atom/b-cm):  0.0235147
C
M35     35079.80c   0.506900
        35081.80c   0.493100
C
C  To convert a particle flux to rad[Material]
C  use FM  1.2073899E-10 35   -4  1 for neutrons
C   or FM  1.2073899E-10 35   -5 -6 for photons.
```

Table 105 – Difference between NWC and MatMCNP for Bromine

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{79}Br	0.000%	0.000%	0.000%	0.000%	0.000%
^{81}Br	0.000%	0.000%	0.000%		

2.1.36. Krypton

Krypton (Z = 36) has six naturally occurring isotopes (^{78}Kr, ^{80}Kr, ^{82}Kr, ^{83}Kr, ^{84}Kr and ^{86}Kr) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 106. The output for krypton from MatMCNP is shown in Table 107. Finally, the verification of the implementation of krypton within MatMCNP is found in Table 108. Examining Table 108, it is apparent that low density and low isotopic abundance causes issues with round-off (See Appendix A, Tables 281 through 283 for high density verification).

Table 106 – Krypton Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{78}Kr	0.0035500	-74.1795	77.92036503	0.003301	0.0000001
^{80}Kr	0.0228600	-77.8925	79.91637896	0.021801	0.0000006
^{82}Kr	0.1159300	-80.5902	81.91348286	0.113323	0.0000031
^{83}Kr	0.1150000	-79.9900	82.91412720	0.113787	0.0000031
^{84}Kr	0.5698700	-82.4393	83.91149777	0.570642	0.0000153
^{86}Kr	0.1727900	-83.2656	85.91061070	0.177146	0.0000046
Density (g/cm^3) = 0.003733				FM Conversion = 1.1512769E-10	
Total Atomic Density (atoms/b-cm) = 0.0000268					

Table 107 – MatMCNP Output for Elemental Krypton (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Kr-78        0.003550           0.003301          0.0000001
C  Kr-80        0.022860           0.021801          0.0000006
C  Kr-82        0.115930           0.113323          0.0000031
C  Kr-83        0.115000           0.113787          0.0000031
C  Kr-84        0.569870           0.570642          0.0000153
C  Kr-86        0.172790           0.177146          0.0000046
C
C  The total compound atom density (atom/b-cm):  0.0000268
C
M36     36078.80c   0.003550
        36080.80c   0.022860
        36082.80c   0.115930
        36083.80c   0.115000
        36084.80c   0.569870
        36086.80c   0.172790
C
C  To convert a particle flux to rad[Material]
C  use FM  1.1512769E-10 36   -4  1 for neutrons
C   or FM  1.1512769E-10 36   -5 -6 for photons.
```

Table 108 – Difference between NWC and MatMCNP for Krypton

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{78}Kr	0.000%	0.000%	5.002%	-0.101%	0.000%
^{80}Kr	0.000%	0.000%	-2.164%		
^{82}Kr	0.000%	0.000%	-0.324%		
^{83}Kr	0.000%	0.000%	0.482%		
^{84}Kr	0.000%	0.000%	0.078%		
^{86}Kr	0.000%	0.000%	-0.765%		

2.1.37. Rubidium

Rubidium (Z = 37) has two naturally occurring isotopes (^{85}Rb and ^{87}Rb) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 109. The output of MatMCNP for rubidium is shown in Table 110. Finally, the verification of the implementation of rubidium within MatMCNP is found in Table 111. An examination of Table 111 shows that the implementation of rubidium within MatMCNP has been performed correctly.

Table 109 – Rubidium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{85}Rb	0.7217000	-82.1673	84.91178977	0.717006	0.0077905
^{87}Rb	0.2783000	-84.5977	86.90918063	0.282994	0.0030041
Density (g/cm^3) = 1.532			FM Conversion = 1.1287860E-10		
Total Atomic Density (atoms/b-cm) = 0.0107946					

Table 110 – MatMCNP Output for Elemental Rubidium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Rb-85        0.721700           0.717006          0.0077905
C  Rb-87        0.278300           0.282994          0.0030041
C
C  The total compound atom density (atom/b-cm):  0.0107946
C
M37     37085.80c   0.721700
        37087.80c   0.278300
C
C  To convert a particle flux to rad[Material]
C  use FM  1.1287861E-10 37   -4  1 for neutrons
C   or FM  1.1287861E-10 37   -5 -6 for photons.
```

Table 111 – Difference between NWC and MatMCNP for Rubidium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{85}Rb	0.000%	0.000%	0.000%	0.000%	0.000%
^{87}Rb	0.000%	0.000%	-0.001%		

2.1.38. Strontium

Strontium (Z = 38) has four naturally occurring isotopes (^{84}Sr, ^{86}Sr, ^{87}Sr, and ^{88}Sr) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 112. The output for strontium from MatMCNP is shown in Table 113. Finally, the verification of the implementation of strontium within MatMCNP is found in Table 114. Table 114 shows that the implementation of strontium within MatMCNP has been performed correctly.

Table 112 – Strontium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{84}Sr	0.0056000	-80.6493	83.91341941	0.005363	0.0001016
^{86}Sr	0.0986000	-84.5232	85.90926061	0.096679	0.0017891
^{87}Sr	0.0700000	-84.8800	86.90887757	0.069435	0.0012702
^{88}Sr	0.8258000	-87.9213	87.90561260	0.828524	0.0149845
Density (g/cm^3) = 2.64			FM Conversion = 1.1011002E-10		
Total Atomic Density (atoms/b-cm) = 0.0181455					

Table 113 – MatMCNP Output for Elemental Strontium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Sr-84        0.005600           0.005363          0.0001016
C  Sr-86        0.098600           0.096679          0.0017891
C  Sr-87        0.070000           0.069435          0.0012702
C  Sr-88        0.825800           0.828524          0.0149845
C
C  The total compound atom density (atom/b-cm):  0.0181455
C
M38      38084.80c   0.005600
         38086.80c   0.098600
         38087.80c   0.070000
         38088.80c   0.825800
C  To convert a particle flux to rad[Material]
C  use FM  1.1011003E-10 38   -4  1 for neutrons
C   or FM  1.1011003E-10 38   -5 -6 for photons.
```

Table 114 – Difference between NWC and MatMCNP for Strontium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{84}Sr	0.000%	-0.006%	-0.014%	0.000%	0.000%
^{86}Sr	0.000%	0.000%	-0.002%		
^{87}Sr	0.000%	0.001%	0.001%		
^{88}Sr	0.000%	0.000%	0.000%		

2.1.39. Yttrium

Yttrium (Z = 39) has one stable isotope (^{89}Y) listed in the NWC. The mass defect and Excel computed quantities are found in Table 115. The MatMCNP output for yttrium is found in Table 116. The yttrium verification data for MatMCNP implementation is found in Table 117. An examination of Table 117 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 115 – Yttrium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{89}Y	1.0000000	-87.7096	88.90583987	1.000000	0.0302713
Density (g/cm^3) = 4.469			FM Conversion = 1.0851335E-10		
Total Atomic Density (atoms/b-cm) = 0.0302713					

Table 116 – MatMCNP Output for Elemental Yttrium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   Y-89        1.000000           1.000000          0.0302713
C
C  The total compound atom density (atom/b-cm):  0.0302713
C
M39      39089.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  1.0851335E-10 39   -4  1 for neutrons
C   or FM  1.0851335E-10 39   -5 -6 for photons.
```

Table 117 – Difference between NWC and MatMCNP for Yttrium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{89}Y	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.40. Zirconium

Zirconium (Z = 40) has five naturally occurring isotopes (^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr, and ^{96}Zr) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 118. The output for zirconium from MatMCNP is shown in Table 119. Finally, the verification of the implementation of zirconium within MatMCNP is found in Table 120. Table 120shows that the implementation of zirconium within MatMCNP has been performed correctly.

Table 118 – Zirconium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{90}Zr	0.5145000	-88.7742	89.90469697	0.507061	0.0221450
^{91}Zr	0.1122000	-87.8973	90.90563836	0.111809	0.0048293
^{92}Zr	0.1715000	-88.4607	91.90503353	0.172781	0.0073817
^{94}Zr	0.1738000	-87.2725	93.90630911	0.178911	0.0074807
^{96}Zr	0.0280000	-85.4477	95.90826812	0.029438	0.0012052
Density (g/cm^3) = 6.52				FM Conversion = 1.0575625E-10	
Total Atomic Density (atoms/b-cm) = 0.0430418					

Table 119 – MatMCNP Output for Elemental Zirconium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Zr-90        0.514500           0.507061          0.0221450
C  Zr-91        0.112200           0.111809          0.0048293
C  Zr-92        0.171500           0.172781          0.0073817
C  Zr-94        0.173800           0.178911          0.0074807
C  Zr-96        0.028000           0.029438          0.0012052
C
C  The total compound atom density (atom/b-cm):  0.0430419
C
C
C  This material contains an isotope that is often modified by
C  an S(alpha,beta). Check MCNP Manual Appendix G to see if an
C  S(alpha,beta) card (i.e., an MTn card) is required.
C
M40     40090.80c   0.514500
        40091.80c   0.112200
        40092.80c   0.171500
        40094.80c   0.173800
        40096.80c   0.028000
C
C  To convert a particle flux to rad[Material]
C  use FM  1.0575626E-10 40   -4  1 for neutrons
C   or FM  1.0575626E-10 40   -5 -6 for photons.
```

Table 120 – Difference between NWC and MatMCNP for Zirconium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{90}Zr	0.000%	0.000%	0.000%	0.000%	0.000%
^{91}Zr	0.000%	0.000%	0.000%		
^{92}Zr	0.000%	0.000%	0.000%		
^{94}Zr	0.000%	0.000%	0.000%		
^{96}Zr	0.000%	0.000%	0.002%		

2.1.41. Niobium

Niobium (Z = 41) has only one stable isotope (^{93}Nb) listed in the NWC. The mass defect and Excel computed quantities are found in Table 121. The MatMCNP output for niobium is found in Table 122. The niobium verification data for MatMCNP implementation is found in Table 123. An examination of Table 123 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 121 – Niobium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{93}Nb	1.0000000	-87.2142	92.9063717	1.000000	0.0555502
Density (g/cm^3) = 8.57			FM Conversion = 1.0384078E-10		
Total Atomic Density (atoms/b-cm) = 0.0555502					

Table 122 – MatMCNP Output for Elemental Niobium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Nb-93        1.000000           1.000000          0.0555503
C
C  The total compound atom density (atom/b-cm):  0.0555503
C
M41     41093.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  1.0384080E-10 41   -4  1 for neutrons
C   or FM  1.0384080E-10 41   -5 -6 for photons.
```

Table 123 – Difference between NWC and MatMCNP for Niobium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{93}Nb	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.42. Molybdenum

Molybdenum (Z = 42) has seven naturally occurring isotopes (^{92}Mo, ^{94}Mo, ^{95}Mo, ^{96}Mo, ^{97}Mo, ^{98}Mo, and ^{100}Mo) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 124. The output for molybdenum from MatMCNP is shown in Table 125. Finally, the verification of the implementation of molybdenum within MatMCNP is found in Table 126. An examination of Table 126 shows that the implementation of molybdenum within MatMCNP has been performed correctly.

Table 124 – Molybdenum Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{92}Mo	0.1453000	-86.8093	91.90680638	0.139163	0.0093192
^{94}Mo	0.0915000	-88.4141	93.90508355	0.089541	0.0058686
^{95}Mo	0.1584000	-87.7119	94.90583740	0.156660	0.0101594
^{96}Mo	0.1667000	-88.7949	95.90467475	0.166604	0.0106917
^{97}Mo	0.0960000	-87.5448	96.90601679	0.096947	0.0061572
^{98}Mo	0.2439000	-88.1161	97.90540347	0.248845	0.0156431
^{100}Mo	0.0982000	-86.1878	99.90747359	0.102240	0.0062983
Density (g/cm^3) = 10.22				FM Conversion = 1.0053660E-10	
Total Atomic Density (atoms/b-cm) = 0.0641375					

Table 125 – MatMCNP Output for Elemental Molybdenum (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Mo-92        0.145300          0.139163          0.0093192
C  Mo-94        0.091500          0.089541          0.0058686
C  Mo-95        0.158400          0.156660          0.0101594
C  Mo-96        0.166700          0.166604          0.0106917
C  Mo-97        0.096000          0.096947          0.0061572
C  Mo-98        0.243900          0.248845          0.0156432
C  Mo-100       0.098200          0.102240          0.0062983
C
C  The total compound atom density (atom/b-cm):  0.0641376
C
M42     42092.80c   0.145300
        42094.80c   0.091500
        42095.80c   0.158400
        42096.80c   0.166700
        42097.80c   0.096000
        42098.80c   0.243900
        42100.80c   0.098200
C
C  To convert a particle flux to rad[Material]
C  use FM  1.0053659E-10 42   -4  1 for neutrons
C   or FM  1.0053659E-10 42   -5 -6 for photons.
```

Table 126 – Difference between NWC and MatMCNP for Molybdenum

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{92}Mo	0.000%	0.000%	0.000%	0.000%	0.000%
^{94}Mo	0.000%	0.000%	0.000%		
^{95}Mo	0.000%	0.000%	0.000%		
^{96}Mo	0.000%	0.000%	0.000%		
^{97}Mo	0.000%	0.000%	0.000%		
^{98}Mo	0.000%	0.000%	0.000%		
^{100}Mo	0.000%	0.000%	0.000%		

2.1.43. Technetium

Technetium (Z = 43) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains technetium, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing technetium.

2.1.44. Ruthenium

Ruthenium (Z = 44) has seven naturally occurring isotopes (^{96}Ru, ^{98}Ru, ^{99}Ru, ^{100}Ru, ^{101}Ru, ^{102}Ru, and ^{104}Ru) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 127. The output for ruthenium from MatMCNP is shown in Table 128. Finally, the verification of the implementation of ruthenium within MatMCNP is found in Table 129. An examination of Table 129 shows that the implementation of ruthenium within MatMCNP has been performed correctly.

Table 127 – Ruthenium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{96}Ru	0.0554000	-86.0804	95.90758888	0.052573	0.0039943
^{98}Ru	0.0187000	-88.2248	97.90528678	0.018115	0.0013483
^{99}Ru	0.1276000	-87.6202	98.90593584	0.124874	0.0092000
^{100}Ru	0.1260000	-89.2222	99.90421602	0.124553	0.0090846
^{101}Ru	0.1706000	-87.9529	100.9055787	0.170331	0.0123003
^{102}Ru	0.3155000	-89.1012	101.9043459	0.318120	0.0227476
^{104}Ru	0.1862000	-88.0923	103.9054290	0.191433	0.0134250
Density (g/cm^3) = 12.1				FM Conversion = 9.5458130E-11	
Total Atomic Density (atoms/b-cm) = 0.0721000					

Table 128 – MatMCNP Output for Elemental Ruthenium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ru-96        0.055400          0.052573          0.0039943
C  Ru-98        0.018700          0.018115          0.0013483
C  Ru-99        0.127600          0.124874          0.0092000
C  Ru-100       0.126000          0.124553          0.0090846
C  Ru-101       0.170600          0.170331          0.0123003
C  Ru-102       0.315500          0.318120          0.0227476
C  Ru-104       0.186200          0.191433          0.0134250
C
C  The total compound atom density (atom/b-cm):  0.0721001
C
M44      44096.80c   0.055400
         44098.80c   0.018700
         44099.80c   0.127600
         44100.80c   0.126000
         44101.80c   0.170600
         44102.80c   0.315500
         44104.80c   0.186200
C
C  To convert a particle flux to rad[Material]
C  use FM  9.5458141E-11 44   -4  1 for neutrons
C   or FM  9.5458141E-11 44   -5 -6 for photons.
```

Table 129 – Difference between NWC and MatMCNP for Ruthenium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{96}Ru	0.000%	0.000%	-0.001%	0.000%	0.000%
^{98}Ru	0.000%	-0.002%	0.002%		
^{99}Ru	0.000%	0.000%	0.000%		
^{100}Ru	0.000%	0.000%	0.000%		
^{101}Ru	0.000%	0.000%	0.000%		
^{102}Ru	0.000%	0.000%	0.000%		
^{104}Ru	0.000%	0.000%	0.000%		

2.1.45. Rhodium

Rhodium (Z = 45) has only one stable isotope (^{103}Rh) listed in the NWC. The mass defect and Excel computed quantities are found in Table 130. The MatMCNP output for rhodium is found in Table 131. The rhodium verification data for MatMCNP implementation is found in Table 132. An examination of Table 132 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 130 – Rhodium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{103}Rh	1.0000000	-88.0256	102.9055006	1.000000	0.0726246
Density (g/cm^3) = 12.41			FM Conversion = 9.3750774E-11		
Total Atomic Density (atoms/b-cm) = 0.0726246					

Table 131 – MatMCNP Output for Elemental Rhodium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Rh-103       1.000000           1.000000          0.0726247
C
C  The total compound atom density (atom/b-cm):  0.0726247
C
M45     45103.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  9.3750771E-11 45   -4  1 for neutrons
C   or FM  9.3750771E-11 45   -5 -6 for photons.
```

Table 132 – Difference between NWC and MatMCNP for Rhodium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{103}Rh	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.46. Palladium

Palladium (Z = 46) has six naturally occurring isotopes (^{102}Pd, ^{104}Pd, ^{105}Pd, ^{106}Pd, ^{108}Pd and ^{110}Pd) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 133. The output for palladium from MatMCNP is shown in Table 134. Finally, the verification of the implementation of palladium within MatMCNP is found in Table 135. An examination of Table 135 shows that the implementation of palladium within MatMCNP has been performed correctly.

Table 133 – Palladium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{102}Pd	0.0102000	-87.9286	101.9056048	0.009768	0.0006938
^{104}Pd	0.1114000	-89.3932	103.9040324	0.108771	0.0075777
^{105}Pd	0.2233000	-88.4160	104.9050815	0.220131	0.0151894
^{106}Pd	0.2733000	-89.9056	105.9034824	0.271985	0.0185905
^{108}Pd	0.2646000	-89.5211	107.9038951	0.268301	0.0179987
^{110}Pd	0.1172000	-88.3484	109.9051541	0.121044	0.0079722
Density (g/cm^3) = 12.02				FM Conversion = 9.0658654E-11	
Total Atomic Density (atoms/b-cm) = 0.0680222					

Table 134 – MatMCNP Output for Elemental Palladium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Pd-102       0.010200           0.009768          0.0006938
C  Pd-104       0.111400           0.108771          0.0075777
C  Pd-105       0.223300           0.220131          0.0151894
C  Pd-106       0.273300           0.271985          0.0185905
C  Pd-108       0.264600           0.268301          0.0179987
C  Pd-110       0.117200           0.121044          0.0079722
C
C  The total compound atom density (atom/b-cm):  0.0680223
C
M46     46102.80c   0.010200
        46104.80c   0.111400
        46105.80c   0.223300
        46106.80c   0.273300
        46108.80c   0.264600
        46110.80c   0.117200
C
C  To convert a particle flux to rad[Material]
C  use FM  9.0658661E-11 46   -4  1 for neutrons
C   or FM  9.0658661E-11 46   -5 -6 for photons.
```

Table 135 – Difference between NWC and MatMCNP for Palladium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{102}Pd	0.000%	0.003%	-0.004%	0.000%	0.000%
^{104}Pd	0.000%	0.000%	0.000%		
^{105}Pd	0.000%	0.000%	0.000%		
^{106}Pd	0.000%	0.000%	0.000%		
^{108}Pd	0.000%	0.000%	0.000%		
^{110}Pd	0.000%	0.000%	0.000%		

2.1.47. Silver

Silver (Z = 47) has two naturally occurring isotopes (^{107}Ag and ^{109}Ag) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 136. The output of MatMCNP for silver is shown in Table 137. Finally, the verification of the implementation of silver within MatMCNP is found in Table 138. An examination of Table 138 shows that the implementation of silver within MatMCNP has been performed correctly.

Table 136 – Silver Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{107}Ag	0.5183900	-88.4055	106.9050928	0.513762	0.0303881
^{109}Ag	0.4816100	-88.7195	108.9047557	0.486238	0.0282320
Density (g/cm^3) = 10.50			FM Conversion = 8.9437617E-11		
Total Atomic Density (atoms/b-cm) = 0.0586201					

Table 137 – MatMCNP Output for Elemental Silver (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ag-107       0.518390           0.513762          0.0303881
C  Ag-109       0.481610           0.486238          0.0282321
C
C  The total compound atom density (atom/b-cm):  0.0586202
C
M47     47107.80c   0.518390
        47109.80c   0.481610
C
C  To convert a particle flux to rad[Material]
C  use FM  8.9437617E-11 47   -4  1 for neutrons
C   or FM  8.9437617E-11 47   -5 -6 for photons.
```

Table 138 – Difference between NWC and MatMCNP for Silver

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{107}Ag	0.000%	0.000%	0.000%	0.000%	0.000%
^{109}Ag	0.000%	0.000%	0.000%		

2.1.48. Cadmium

Cadmium (Z = 48) has eight naturally occurring isotopes (^{106}Cd, ^{108}Cd, ^{110}Cd, ^{111}Cd, ^{112}Cd, ^{113}Cd, ^{114}Cd, and ^{116}Cd) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 139. The output for cadmium from MatMCNP is shown in Table 140. Finally, the verification of the implementation of cadmium within MatMCNP is found in Table 141. An examination of Table 141 shows that the implementation of cadmium within MatMCNP has been performed correctly.

Table 139 – Cadmium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{106}Cd	0.0125000	-87.1304	105.9064617	0.011777	0.0005819
^{108}Cd	0.0089000	-89.2524	107.9041836	0.008543	0.0004143
^{110}Cd	0.1249000	-90.3503	109.903005	0.122113	0.0058146
^{111}Cd	0.1280000	-89.2547	110.9041811	0.126284	0.0059589
^{112}Cd	0.2413000	-90.5777	111.9027608	0.240208	0.0112335
^{113}Cd	0.1222000	-89.0464	112.9044048	0.122736	0.0056889
^{114}Cd	0.2873000	-90.0180	113.9033617	0.291113	0.0133750
^{116}Cd	0.0749000	-88.7164	115.9047590	0.077228	0.0034869
Density (g/cm^3) = 8.69			FM Conversion = 8.5822764E-11		
Total Atomic Density (atoms/b-cm) = 0.0465543					

Table 140 – MatMCNP Output for Elemental Cadmium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Cd-106       0.012500          0.011777          0.0005819
C  Cd-108       0.008900          0.008543          0.0004143
C  Cd-110       0.124900          0.122113          0.0058146
C  Cd-111       0.128000          0.126284          0.0059589
C  Cd-112       0.241300          0.240208          0.0112336
C  Cd-113       0.122200          0.122736          0.0056889
C  Cd-114       0.287300          0.291113          0.0133750
C  Cd-116       0.074900          0.077228          0.0034869
C
C  The total compound atom density (atom/b-cm):  0.0465543
C
M48     48106.80c   0.012500
        48108.80c   0.008900
        48110.80c   0.124900
        48111.80c   0.128000
        48112.80c   0.241300
        48113.80c   0.122200
        48114.80c   0.287300
        48116.80c   0.074900
C
C  To convert a particle flux to rad[Material]
C  use FM  8.5822766E-11 48   -4  1 for neutrons
C   or FM  8.5822766E-11 48   -5 -6 for photons.
```

Table 141 – Difference between NWC and MatMCNP for Cadmium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{106}Cd	0.000%	0.003%	-0.005%	0.000%	0.000%
^{108}Cd	0.000%	-0.002%	-0.008%		
^{110}Cd	0.000%	0.000%	0.000%		
^{111}Cd	0.000%	0.000%	-0.001%		
^{112}Cd	0.000%	0.000%	0.001%		
^{113}Cd	0.000%	0.000%	-0.001%		
^{114}Cd	0.000%	0.000%	0.000%		
^{116}Cd	0.000%	0.001%	0.000%		

2.1.49. Indium

Indium (Z = 49) has two naturally occurring isotopes (^{113}In and ^{115}In) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 142. The output of MatMCNP for indium is shown in Table 143. Finally, the verification of the implementation of indium within MatMCNP is found in Table 144. Table 144 shows that the implementation of indium within MatMCNP has been performed correctly.

Table 142 – Indium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{113}In	0.0429000	-89.3683	112.9040592	0.042185	0.0016448
^{115}In	0.9571000	-89.5363	114.9038788	0.957815	0.0366957
Density (g/cm^3) = 7.31				FM Conversion = 8.4023960E-11	
Total Atomic Density (atoms/b-cm) = 0.0383405					

Table 143 – MatMCNP Output for Elemental Indium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  In-113       0.042900           0.042185          0.0016448
C  In-115       0.957100           0.957815          0.0366957
C
C  The total compound atom density (atom/b-cm):  0.0383405
C
M49     49113.80c   0.042900
        49115.80c   0.957100
C
C  To convert a particle flux to rad[Material]
C  use FM  8.4023968E-11 49   -4  1 for neutrons
C   or FM  8.4023968E-11 49   -5 -6 for photons.
```

Table 144 – Difference between NWC and MatMCNP for Indium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{113}In	0.000%	0.000%	0.000%	0.000%	0.000%
^{115}In	0.000%	0.000%	0.000%		

2.1.50. Tin

Tin (Z = 50) has ten naturally occurring isotopes (^{112}Sn, ^{114}Sn, ^{115}Sn, ^{116}Sn, ^{117}Sn, ^{118}Sn, ^{119}Sn, ^{120}Sn, ^{122}Sn, and ^{124}Sn) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 145. The output for tin from MatMCNP is shown in Table 146. Finally, the verification of the implementation of tin within MatMCNP is found in Table 147. An examination of Table 147 shows that the implementation of tin within MatMCNP has been performed correctly.

Table 145 – Tin Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{112}Sn	0.0097000	-88.6579	111.9048218	0.009144	0.0002839
^{114}Sn	0.0066000	-90.5594	113.9027805	0.006333	0.0001932
^{115}Sn	0.0034000	-90.0338	114.9033447	0.003291	0.0000995
^{116}Sn	0.1454000	-91.5259	115.9017429	0.141960	0.0042560
^{117}Sn	0.0768000	-90.3977	116.9029541	0.075631	0.0022480
^{118}Sn	0.2422000	-91.6528	117.9016067	0.240550	0.0070895
^{119}Sn	0.0859000	-90.0650	118.9033112	0.086040	0.0025144
^{120}Sn	0.3258000	-91.0982	119.9022021	0.329072	0.0095365
^{122}Sn	0.0463000	-89.9426	121.9034426	0.047545	0.0013553
^{124}Sn	0.0579000	-88.2370	123.9052737	0.060434	0.0016948
Density (g/cm^3) = 5.77				FM Conversion = 8.1269153E-11	
Total Atomic Density (atoms/b-cm) = 0.0292711					

Table 146 – MatMCNP Output for Elemental Tin (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Sn-112       0.009700           0.009144          0.0002839
C  Sn-114       0.006600           0.006333          0.0001932
C  Sn-115       0.003400           0.003291          0.0000995
C  Sn-116       0.145400           0.141960          0.0042560
C  Sn-117       0.076800           0.075631          0.0022480
C  Sn-118       0.242200           0.240550          0.0070895
C  Sn-119       0.085900           0.086040          0.0025144
C  Sn-120       0.325800           0.329072          0.0095365
C  Sn-122       0.046300           0.047545          0.0013553
C  Sn-124       0.057900           0.060434          0.0016948
C
C  The total compound atom density (atom/b-cm):  0.0292711
C
M50     50112.80c   0.009700
        50114.80c   0.006600
        50115.80c   0.003400
        50116.80c   0.145400
        50117.80c   0.076800
        50118.80c   0.242200
        50119.80c   0.085900
        50120.80c   0.325800
        50122.80c   0.046300
        50124.80c   0.057900
C
C  To convert a particle flux to rad[Material]
C  use FM  8.1269165E-11 50   -4  1 for neutrons
C   or FM  8.1269165E-11 50   -5 -6 for photons.
```

Table 147 – Difference between NWC and MatMCNP for Tin

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{112}Sn	0.000%	0.001%	-0.010%	0.000%	0.000%
^{114}Sn	0.000%	0.004%	0.006%		
^{115}Sn	0.000%	0.001%	-0.022%		
^{116}Sn	0.000%	0.000%	0.000%		
^{117}Sn	0.000%	0.000%	-0.001%		
^{118}Sn	0.000%	0.000%	0.001%		
^{119}Sn	0.000%	0.000%	0.001%		
^{120}Sn	0.000%	0.000%	0.000%		
^{122}Sn	0.000%	-0.001%	0.004%		
^{124}Sn	0.000%	0.000%	0.000%		

2.1.51. Antimony

Antimony (Z = 51) has two naturally occurring isotopes (^{121}Sb and ^{123}Sb) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 148. The output of MatMCNP for antimony is shown in Table 149. Finally, the verification of the implementation of antimony within MatMCNP is found in Table 150. Table 150 shows that the implementation of antimony within MatMCNP has been performed correctly.

Table 148 – Antimony Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{121}Sb	0.5721000	-89.5998	120.9038107	0.568078	0.0189015
^{123}Sb	0.4279000	-89.2261	122.9042118	0.431922	0.0141373
Density (g/cm^3) = 6.68			FM Conversion = 7.9233637E-11		
Total Atomic Density (atoms/b-cm) = 0.0330387					

Table 149 – MatMCNP Output for Elemental Antimony (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Sb-121       0.572100           0.568078          0.0189015
C  Sb-123       0.427900           0.431922          0.0141373
C
C  The total compound atom density (atom/b-cm):  0.0330387
C
M51     51121.80c   0.572100
        51123.80c   0.427900
C
C  To convert a particle flux to rad[Material]
C  use FM  7.9233640E-11 51   -4  1 for neutrons
C   or FM  7.9233640E-11 51   -5 -6 for photons.
```

Table 150 – Difference between NWC and MatMCNP for Antimony

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{121}Sb	0.000%	0.000%	0.000%	0.000%	0.000%
^{123}Sb	0.000%	0.000%	0.000%		

2.1.52. Tellurium

Tellurium (Z = 52) has eight naturally occurring isotopes (^{120}Te, ^{122}Te, ^{123}Te, ^{124}Te, ^{125}Te, ^{126}Te, ^{128}Te, and ^{130}Te) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 151. The output for tellurium from MatMCNP is shown in Table 152. Finally, the verification of the implementation of tellurium within MatMCNP is found in Table 153. An examination of Table 153 shows that the implementation of tellurium within MatMCNP has been performed correctly.

Table 151 – Tellurium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{120}Te	0.0009000	-89.3697	119.9040577	0.000846	0.0000265
^{122}Te	0.0255000	-90.3158	121.9030420	0.024361	0.0007498
^{123}Te	0.0089000	-89.1735	122.9042683	0.008572	0.0002617
^{124}Te	0.0474000	-90.5266	123.9028157	0.046025	0.0013937
^{125}Te	0.0707000	-89.0243	124.9044285	0.069205	0.0020787
^{126}Te	0.1884000	-90.0666	125.9033095	0.185890	0.0055393
^{128}Te	0.3174000	-88.9937	127.9044613	0.318150	0.0093322
^{130}Te	0.3408000	-87.3529	129.9062228	0.346951	0.0100202
Density (g/cm^3) = 6.23			FM Conversion = 7.5605282E-11		
Total Atomic Density (atoms/b-cm) = 0.0294020					

Table 152 – MatMCNP Output for Elemental Tellurium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Te-120       0.000900           0.000846          0.0000265
C  Te-122       0.025500           0.024361          0.0007498
C  Te-123       0.008900           0.008572          0.0002617
C  Te-124       0.047400           0.046025          0.0013937
C  Te-125       0.070700           0.069205          0.0020787
C  Te-126       0.188400           0.185890          0.0055393
C  Te-128       0.317400           0.318150          0.0093322
C  Te-130       0.340800           0.346951          0.0100202
C
C  The total compound atom density (atom/b-cm):  0.0294021
C
M52     52120.80c   0.000900
        52122.80c   0.025500
        52123.80c   0.008900
        52124.80c   0.047400
        52125.80c   0.070700
        52126.80c   0.188400
        52128.80c   0.317400
        52130.80c   0.340800
C
C  To convert a particle flux to rad[Material]
C  use FM  7.5605286E-11 52   -4  1 for neutrons
C   or FM  7.5605286E-11 52   -5 -6 for photons.
```

Table 153 – Difference between NWC and MatMCNP for Tellurium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{120}Te	0.000%	0.036%	0.144%	0.000%	0.000%
^{122}Te	0.000%	0.000%	0.006%		
^{123}Te	0.000%	-0.003%	0.008%		
^{124}Te	0.000%	-0.001%	0.003%		
^{125}Te	0.000%	0.000%	-0.001%		
^{126}Te	0.000%	0.000%	-0.001%		
^{128}Te	0.000%	0.000%	0.000%		
^{130}Te	0.000%	0.000%	0.000%		

2.1.53. Iodine

Iodine (Z =53) has only one stable isotope (^{127}I) listed in the NWC. The mass defect and Excel computed quantities are found in Table 154. The MatMCNP output for iodine is found in Table 155. The iodine verification data for MatMCNP implementation is found in Table 156. An examination of Table 156 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 154 – Iodine Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{127}I	1.0000000	-88.9847	126.904471	1.000000	0.0233949
Density (g/cm^3) = 4.93				FM Conversion = 7.6021517E-11	
Total Atomic Density (atoms/b-cm) = 0.0233949					

Table 155 – MatMCNP Output for Elemental Iodine (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   I-127       1.000000           1.000000          0.0233949
C
C  The total compound atom density (atom/b-cm):  0.0233949
C
M53     53127.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  7.6021522E-11 53   -4  1 for neutrons
C   or FM  7.6021522E-11 53   -5 -6 for photons.
```

Table 156 – Difference between NWC and MatMCNP for Iodine

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{127}I	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.54. Xenon

Xenon (Z = 54) has nine naturally occurring isotopes (^{124}Xe, ^{126}Xe, ^{128}Xe, ^{129}Xe, ^{130}Xe, ^{131}Xe, ^{132}Xe, ^{134}Xe, and ^{136}Xe) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 157. The output for xenon from MatMCNP is shown in Table 158. Finally, the verification of the implementation of xenon within MatMCNP is found in Table 159. Examining Table 159, it is apparent that low density and low isotopic abundance causes issues with round-off (See Appendix A, Tables 284 through 286 for high density verification).

Table 157 – Xenon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{124}Xe	0.0009520	-87.6612	123.9058918	0.000898	0.0000000
^{126}Xe	0.0008900	-89.1462	125.9042976	0.000853	0.0000000
^{128}Xe	0.0191021	-89.8602	127.9035311	0.018609	0.0000005
^{129}Xe	0.2640071	-88.6960	128.9047809	0.259205	0.0000071
^{130}Xe	0.0407102	-89.8804	129.9035094	0.040279	0.0000011
^{131}Xe	0.2123208	-88.4136	130.9050841	0.211694	0.0000057
^{132}Xe	0.2690871	-89.2789	131.9041552	0.270340	0.0000073
^{134}Xe	0.1043574	-88.1245	133.9053945	0.106434	0.0000028
^{136}Xe	0.0885734	-86.4291	135.9072145	0.091686	0.0000024
Density (g/cm^3) = 0.005887			FM Conversion = 7.3480595E-11		
Total Atomic Density (atoms/b-cm) = 0.0000270					

Table 158 – MatMCNP Output for Elemental Xenon (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Xe-124       0.000952           0.000898          0.0000000
C  Xe-126       0.000890           0.000853          0.0000000
C  Xe-128       0.019102           0.018609          0.0000005
C  Xe-129       0.264007           0.259205          0.0000071
C  Xe-130       0.040710           0.040279          0.0000011
C  Xe-131       0.212321           0.211694          0.0000057
C  Xe-132       0.269087           0.270340          0.0000073
C  Xe-134       0.104357           0.106434          0.0000028
C  Xe-136       0.088573           0.091686          0.0000024
C
C  The total compound atom density (atom/b-cm):  0.0000270
C
M54      54124.80c   0.000952
         54126.80c   0.000890
         54128.80c   0.019102
         54129.80c   0.264007
         54130.80c   0.040710
         54131.80c   0.212321
         54132.80c   0.269087
         54134.80c   0.104357
         54136.80c   0.088573
C
C  To convert a particle flux to rad[Material]
C  use FM  7.3480604E-11 54   -4  1 for neutrons
C   or FM  7.3480604E-11 54   -5 -6 for photons.
```

Table 159 – Difference between NWC and MatMCNP for Xenon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{124}Xe	0.000%	-0.049%	-100.000%	-0.009%	0.000%
^{126}Xe	0.000%	-0.056%	-100.000%		
^{128}Xe	0.000%	0.000%	-3.064%		
^{129}Xe	0.000%	0.000%	-0.405%		
^{130}Xe	0.000%	-0.001%	0.066%		
^{131}Xe	0.000%	0.000%	-0.579%		
^{132}Xe	0.000%	0.000%	0.468%		
^{134}Xe	0.000%	0.000%	-0.636%		
^{136}Xe	0.000%	0.000%	0.347%		

2.1.55. Cesium

Cesium (Z =55) has only one stable isotope (^{133}Cs) listed in the NWC. The mass defect and Excel computed quantities are found in Table 160. The MatMCNP output for cesium is found in Table 161. The cesium verification data for MatMCNP implementation is found in Table 162. An examination of Table 162 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 160 – Cesium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{133}Cs	1.0000000	-88.0709	132.905452	1.000000	0.0084868
Density (g/cm^3) = 1.873			FM Conversion = 7.2588974E-11		
Total Atomic Density (atoms/b-cm) = 0.0084868					

Table 161 – MatMCNP Output for Elemental Cesium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ce-133       1.000000           1.000000          0.0084868
C
C  The total compound atom density (atom/b-cm):  0.0084868
C
M55     55133.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  7.2588976E-11 55   -4  1 for neutrons
C   or FM  7.2588976E-11 55   -5 -6 for photons.
```

Table 162 – Difference between NWC and MatMCNP for Cesium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{133}Cs	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.56. Barium

Barium (Z = 56) has seven naturally occurring isotopes (^{130}Ba, ^{132}Ba, ^{134}Ba, ^{135}Ba, ^{136}Ba, ^{137}Ba, and ^{138}Ba) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 163. The output for barium from MatMCNP is shown in Table 164. Finally, the verification of the implementation of barium within MatMCNP is found in Table 165. An examination of Table 165 shows that the implementation of barium within MatMCNP has been performed correctly.

Table 163 – Barium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{130}Ba	0.0010600	-87.2618	129.9063206	0.001003	0.0000168
^{132}Ba	0.0010100	-88.4349	131.9050612	0.000970	0.0000160
^{134}Ba	0.0241700	-88.9501	133.9045081	0.023568	0.0003837
^{135}Ba	0.0659200	-87.8508	134.9056883	0.064758	0.0010465
^{136}Ba	0.0785400	-88.8872	135.9045757	0.077727	0.0012468
^{137}Ba	0.1123200	-87.7215	136.9058271	0.111976	0.0017830
^{138}Ba	0.7169800	-88.2619	137.9052469	0.720000	0.0113818
Density (g/cm^3) = 3.63				FM Conversion = 7.0251866E-11	
Total Atomic Density (atoms/b-cm) = 0.0158746					

Table 164 – MatMCNP Output for Elemental Barium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ba-130       0.001060           0.001003          0.0000168
C  Ba-132       0.001010           0.000970          0.0000160
C  Ba-134       0.024170           0.023568          0.0003837
C  Ba-135       0.065920           0.064758          0.0010465
C  Ba-136       0.078540           0.077727          0.0012468
C  Ba-137       0.112320           0.111976          0.0017830
C  Ba-138       0.716980           0.720000          0.0113818
C
C  The total compound atom density (atom/b-cm):  0.0158746
C
M56     56130.80c   0.001060
        56132.80c   0.001010
        56134.80c   0.024170
        56135.80c   0.065920
        56136.80c   0.078540
        56137.80c   0.112320
        56138.80c   0.716980
C
C  To convert a particle flux to rad[Material]
C  use FM  7.0251867E-11 56   -4  1 for neutrons
C   or FM  7.0251867E-11 56   -5 -6 for photons.
```

Table 165 – Difference between NWC and MatMCNP for Barium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{130}Ba	0.000%	0.028%	-0.161%	0.000%	0.000%
^{132}Ba	0.000%	-0.013%	-0.208%		
^{134}Ba	0.000%	0.001%	0.003%		
^{135}Ba	0.000%	0.000%	0.004%		
^{136}Ba	0.000%	0.001%	0.001%		
^{137}Ba	0.000%	0.000%	-0.002%		
^{138}Ba	0.000%	0.000%	0.000%		

2.1.57. Lanthanum

Lanthanum (Z = 57) has two naturally occurring isotopes (^{138}La and ^{139}La) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 166. The output of MatMCNP for lanthanum is shown in Table 167. Finally, the verification of the implementation of lanthanum within MatMCNP is found in Table 168. Table 168 shows that the implementation of lanthanum within MatMCNP has been performed correctly. (*NOTE: The NWC atomic abundances sum to 100.00071. The numbers below and within MatMCNP take that into account.*)

Table 166 – Lanthanum Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{138}La	0.0008881	-86.5215	137.9071153	0.000882	0.0000237
^{139}La	0.9991119	-87.2282	138.9063567	0.999118	0.0266175
Density (g/cm^3) = 6.145				FM Conversion = 6.9453495E-11	
Total Atomic Density (atoms/b-cm) = 0.0266412					

Table 167 – MatMCNP Output for Elemental Lanthanum (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  La-138       0.000888           0.000882          0.0000237
C  La-139       0.999112           0.999118          0.0266175
C
C  The total compound atom density (atom/b-cm):  0.0266412
C
M57     57138.80c   0.000888
        57139.80c   0.999112
C  To convert a particle flux to rad[Material]
C  use FM  6.9453505E-11 57   -4  1 for neutrons
C   or FM  6.9453505E-11 57   -5 -6 for photons.
```

Table 168 – Difference between NWC and MatMCNP for Lanthanum

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{138}La	-0.011%	0.033%	0.170%	0.000%	0.000%
^{139}La	0.000%	0.000%	0.000%		

2.1.58. Cerium

Cerium (Z = 58) has four naturally occurring isotopes (^{136}Ce, ^{138}Ce, ^{140}Ce, and ^{142}Ce) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 169. The output for cerium from MatMCNP is shown in Table 170. Finally, the verification of the implementation of cerium within MatMCNP is found in Table 171. An examination of Table 171 shows that the implementation of cerium within MatMCNP has been performed correctly.

Table 169 – Cerium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{136}Ce	0.0018500	-86.4736	135.9071668	0.001794	0.0000538
^{138}Ce	0.0025100	-87.5643	137.9059959	0.002470	0.0000730
^{140}Ce	0.8845000	-88.0786	139.9054437	0.883173	0.0257365
^{142}Ce	0.1111400	-84.5320	141.9092512	0.112563	0.0032339
Density (g/cm^3) = 6.77				FM Conversion = 6.8853584E-11	
Total Atomic Density (atoms/b-cm) = 0.0290973					

Table 170 – MatMCNP Output for Elemental Cerium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ce-136       0.001850           0.001794          0.0000538
C  Ce-138       0.002510           0.002470          0.0000730
C  Ce-140       0.884500           0.883172          0.0257366
C  Ce-142       0.111140           0.112563          0.0032339
C
C  The total compound atom density (atom/b-cm):  0.0290973
C
M58     58136.80c   0.001850
        58138.80c   0.002510
        58140.80c   0.884500
        58142.80c   0.111140
C  To convert a particle flux to rad[Material]
C  use FM  6.8853589E-11 58   -4  1 for neutrons
C   or FM  6.8853589E-11 58   -5 -6 for photons.
```

Table 171 – Difference between NWC and MatMCNP for Cerium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{136}Ce	0.000%	-0.024%	-0.056%	0.000%	0.000%
^{138}Ce	0.000%	-0.017%	-0.047%		
^{140}Ce	0.000%	0.000%	0.000%		
^{142}Ce	0.000%	0.000%	0.001%		

2.1.59. Praseodymium

Praseodymium (Z =59) has only one stable isotope (^{141}Pr) listed in the NWC. The mass defect and Excel computed quantities are found in Table 172. The MatMCNP output for praseodymium is found in Table 173. The praseodymium verification data for MatMCNP implementation is found in Table 174. An examination of Table 174 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 172 – Praseodymium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{141}Pr	1.0000000	-86.0158	140.9076582	1.000000	0.0289466
Density (g/cm^3) = 6.773			FM Conversion = 6.8466615E-11		
Total Atomic Density (atoms/b-cm) = 0.0289466					

Table 173 – MatMCNP Output for Elemental Praseodymium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Pr-141       1.000000          1.000000          0.0289466
C
C  The total compound atom density (atom/b-cm):  0.0289466
C
M59     59141.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  6.8466628E-11 59   -4  1 for neutrons
C   or FM  6.8466628E-11 59   -5 -6 for photons.
```

Table 174 – Difference between NWC and MatMCNP for Praseodymium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{141}Pr	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.60. Neodymium

Neodymium (Z = 60) has seven naturally occurring isotopes (^{142}Nd, ^{143}Nd, ^{144}Nd, ^{145}Nd, ^{146}Nd, ^{148}Nd, and ^{150}Nd) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 175. The output for neodymium from MatMCNP is shown in Table 176. Finally, the verification of the implementation of neodymium within MatMCNP is found in Table 177. An examination of Table 177 shows that the implementation of neodymium within MatMCNP has been performed correctly.

Table 175 – Neodymium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{142}Nd	0.2715200	-85.9493	141.9077296	0.267127	0.0079443
^{143}Nd	0.1217400	-84.0015	142.9098207	0.120616	0.0035619
^{144}Nd	0.2379800	-83.7473	143.9100936	0.237433	0.0069630
^{145}Nd	0.0829300	-81.4312	144.9125800	0.083316	0.0024264
^{146}Nd	0.1718900	-80.9252	145.9131232	0.173882	0.0050293
^{148}Nd	0.0575600	-77.4068	147.9169004	0.059027	0.0016841
^{150}Nd	0.0563800	-73.6832	149.9208978	0.058600	0.0016496
Density (g/cm^3) = 7.008				FM Conversion = 6.6884107E-11	
Total Atomic Density (atoms/b-cm) = 0.0292586					

Table 176 – MatMCNP Output for Elemental Neodymium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Nd-142       0.271520          0.267127          0.0079443
C  Nd-143       0.121740          0.120616          0.0035619
C  Nd-144       0.237980          0.237433          0.0069630
C  Nd-145       0.082930          0.083316          0.0024264
C  Nd-146       0.171890          0.173882          0.0050293
C  Nd-148       0.057560          0.059027          0.0016841
C  Nd-150       0.056380          0.058600          0.0016496
C
C  The total compound atom density (atom/b-cm):  0.0292587
C
M60     60142.80c   0.271520
        60143.80c   0.121740
        60144.80c   0.237980
        60145.80c   0.082930
        60146.80c   0.171890
        60148.80c   0.057560
        60150.80c   0.056380
C
C  To convert a particle flux to rad[Material]
C  use FM  6.6884109E-11 60   -4  1 for neutrons
C   or FM  6.6884109E-11 60   -5 -6 for photons.
```

Table 177 – Difference between NWC and MatMCNP for Neodymium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{142}Nd	0.000%	0.000%	0.000%	0.000%	0.000%
^{143}Nd	0.000%	0.000%	-0.001%		
^{144}Nd	0.000%	0.000%	0.000%		
^{145}Nd	0.000%	0.000%	-0.001%		
^{146}Nd	0.000%	0.000%	0.001%		
^{148}Nd	0.000%	0.001%	-0.002%		
^{150}Nd	0.000%	0.000%	0.000%		

2.1.61. Promethium

Promethium (Z = 61) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains promethium, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing promethium.

2.1.62. Samarium

Samarium (Z = 62) has seven naturally occurring isotopes (^{144}Sm, ^{147}Sm, ^{148}Sm, ^{149}Sm, ^{150}Sm, ^{152}Sm, and ^{154}Sm) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 178. The output for samarium from MatMCNP is shown in Table 179. Finally, the verification of the implementation of samarium within MatMCNP is found in Table 180. An examination of Table 180 shows that the implementation of samarium within MatMCNP has been performed correctly.

Table 178 – Samarium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{144}Sm	0.0307000	-81.9657	143.9120062	0.029382	0.0009246
^{147}Sm	0.1499000	-79.2657	146.9149048	0.146459	0.0045146
^{148}Sm	0.1124000	-79.3358	147.9148295	0.110567	0.0033852
^{149}Sm	0.1382000	-77.1350	148.9171922	0.136868	0.0041622
^{150}Sm	0.0738000	-77.0504	149.9172830	0.073580	0.0022227
^{152}Sm	0.2675000	-74.7622	151.9197395	0.270263	0.0080564
^{154}Sm	0.2275000	-72.4549	153.9222165	0.232880	0.0068517
Density (g/cm^3) = 7.520				FM Conversion = 6.4159767E-11	
Total Atomic Density (atoms/b-cm) = 0.0301174					

Table 179 – MatMCNP Output for Elemental Samarium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Sm-144       0.030700          0.029382          0.0009246
C  Sm-147       0.149900          0.146459          0.0045146
C  Sm-148       0.112400          0.110567          0.0033852
C  Sm-149       0.138200          0.136868          0.0041622
C  Sm-150       0.073800          0.073580          0.0022227
C  Sm-152       0.267500          0.270263          0.0080564
C  Sm-154       0.227500          0.232880          0.0068517
C
C  The total compound atom density (atom/b-cm):  0.0301174
C
M62      62144.80c   0.030700
         62147.80c   0.149900
         62148.80c   0.112400
         62149.80c   0.138200
         62150.80c   0.073800
         62152.80c   0.267500
         62154.80c   0.227500
C  To convert a particle flux to rad[Material]
C  use FM  6.4159768E-11 62   -4  1 for neutrons
C   or FM  6.4159768E-11 62   -5 -6 for photons.
```

Table 180 – Difference between NWC and MatMCNP for Samarium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{144}Sm	0.000%	-0.001%	-0.001%	0.000%	0.000%
^{147}Sm	0.000%	0.000%	0.000%		
^{148}Sm	0.000%	0.000%	0.000%		
^{149}Sm	0.000%	0.000%	-0.001%		
^{150}Sm	0.000%	0.001%	0.002%		
^{152}Sm	0.000%	0.000%	0.000%		
^{154}Sm	0.000%	0.000%	0.000%		

2.1.63. Europium

Europium (Z = 63) has two naturally occurring isotopes (^{151}Eu and ^{153}Eu) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 181. The output of MatMCNP for europium is shown in Table 182. Finally, the verification of the implementation of europium within MatMCNP is found in Table 183. Table 183 shows that the implementation of europium within MatMCNP has been performed correctly.

Table 181 – Europium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{151}Eu	0.4781000	-74.6517	150.9198581	0.474814	0.0099355
^{153}Eu	0.5219000	-73.3661	152.9212382	0.525186	0.0108457
Density (g/cm^3) = 5.244			FM Conversion = 6.3485078E-11		
Total Atomic Density (atoms/b-cm) = 0.0207812					

Table 182 – MatMCNP Output for Elemental Europium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Eu-151       0.478100           0.474814          0.0099355
C  Eu-153       0.521900           0.525186          0.0108457
C
C  The total compound atom density (atom/b-cm):  0.0207813
C
M63      63151.80c   0.478100
         63153.80c   0.521900
C
C  To convert a particle flux to rad[Material]
C  use FM  6.3485071E-11 63   -4  1 for neutrons
C   or FM  6.3485071E-11 63   -5 -6 for photons.
```

Table 183 – Difference between NWC and MatMCNP for Europium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{151}Eu	0.000%	0.000%	0.000%	0.000%	0.000%
^{153}Eu	0.000%	0.000%	0.000%		

2.1.64. Gadolinium

Gadolinium (Z = 64) has seven naturally occurring isotopes (^{152}Gd, ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, and ^{160}Gd) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 184. The output for gadolinium from MatMCNP is shown in Table 185. Finally, the verification of the implementation of gadolinium within MatMCNP is found in Table 186. An examination of Table 186 shows that the implementation of gadolinium within MatMCNP has been performed correctly.

Table 184 – Gadolinium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{152}Gd	0.0020000	-74.7065	151.9197993	0.001932	0.0000605
^{154}Gd	0.0218000	-73.7055	153.9208739	0.021338	0.0006596
^{155}Gd	0.1480000	-72.0694	154.9226303	0.145808	0.0044781
^{156}Gd	0.2047000	-72.5345	155.922131	0.202969	0.0061938
^{157}Gd	0.1565000	-70.8230	156.9239684	0.156173	0.0047353
^{158}Gd	0.2484000	-70.6891	157.9241121	0.249461	0.0075160
^{160}Gd	0.2186000	-67.9409	159.9270624	0.222318	0.0066143
Density (g/cm^3) = 7.901				FM Conversion = 6.1350332E-11	
Total Atomic Density (atoms/b-cm) = 0.0302577					

Table 185 – MatMCNP Output for Elemental Gadolinium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Gd-152       0.002000           0.001932          0.0000605
C  Gd-154       0.021800           0.021338          0.0006596
C  Gd-155       0.148000           0.145808          0.0044781
C  Gd-156       0.204700           0.202969          0.0061938
C  Gd-157       0.156500           0.156173          0.0047353
C  Gd-158       0.248400           0.249461          0.0075160
C  Gd-160       0.218600           0.222318          0.0066143
C
C  The total compound atom density (atom/b-cm):  0.0302577
C
M64      64152.80c   0.002000
         64154.80c   0.021800
         64155.80c   0.148000
         64156.80c   0.204700
         64157.80c   0.156500
         64158.80c   0.248400
         64160.80c   0.218600
C
C  To convert a particle flux to rad[Material]
C  use FM  6.1350328E-11 64   -4  1 for neutrons
C   or FM  6.1350328E-11 64   -5 -6 for photons.
```

Table 186 – Difference between NWC and MatMCNP for Gadolinium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{152}Gd	0.000%	-0.009%	-0.025%	0.000%	0.000%
^{154}Gd	0.000%	-0.001%	-0.003%		
^{155}Gd	0.000%	0.000%	-0.001%		
^{156}Gd	0.000%	0.000%	0.001%		
^{157}Gd	0.000%	0.000%	-0.001%		
^{158}Gd	0.000%	0.000%	0.000%		
^{160}Gd	0.000%	0.000%	-0.001%		

2.1.65. Terbium

Terbium (Z =65) has only one stable isotope (^{159}Tb) listed in the NWC. The mass defect and Excel computed quantities are found in Table 187. The MatMCNP output for terbium found in Table 188. The terbium verification data for MatMCNP implementation is found in Table 189. An examination of Table 189 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 187 – Terbium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{159}Tb	1.0000000	-69.5315	158.9253549	1.000000	0.0311858
Density (g/cm^3) = 8.23			FM Conversion = 6.0704413E-11		
Total Atomic Density (atoms/b-cm) = 0.0311858					

Table 188 – MatMCNP Output for Elemental Terbium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Tb-159       1.000000          1.000000          0.0311858
C
C  The total compound atom density (atom/b-cm):  0.0311858
C
M65     65159.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  6.0704414E-11 65   -4  1 for neutrons
C   or FM  6.0704414E-11 65   -5 -6 for photons.
```

Table 189 – Difference between NWC and MatMCNP for Terbium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{159}Tb	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.66. Dysprosium

Dysprosium (Z = 66) has seven naturally occurring isotopes (^{156}Dy, ^{158}Dy, ^{160}Dy, ^{161}Dy, ^{162}Dy, ^{163}Dy, and ^{164}Dy) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 190. The output for dysprosium from MatMCNP is shown in Table 191. Finally, the verification of the implementation of dysprosium within MatMCNP is found in Table 192. An examination of Table 192 shows that the implementation of dysprosium within MatMCNP has been performed correctly.

Table 190 – Dysprosium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{156}Dy	0.0005600	-70.5223	155.9242912	0.000537	0.0000177
^{158}Dy	0.0009500	-70.4049	157.9244172	0.000923	0.0000301
^{160}Dy	0.0232900	-69.6711	159.925205	0.022921	0.0007380
^{161}Dy	0.1888900	-68.0541	160.9269409	0.187062	0.0059858
^{162}Dy	0.2547500	-68.1798	161.9268060	0.253852	0.0080729
^{163}Dy	0.2489600	-66.3795	162.9287387	0.249618	0.0078894
^{164}Dy	0.2826000	-65.9663	163.9291823	0.285086	0.0089555
Density (g/cm^3) = 8.551			FM Conversion = 5.9369241E-11		
Total Atomic Density (atoms/b-cm) = 0.0316895					

Table 191 – MatMCNP Output for Elemental Dysprosium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Dy-156       0.000560          0.000537          0.0000177
C  Dy-158       0.000950          0.000923          0.0000301
C  Dy-160       0.023290          0.022921          0.0007380
C  Dy-161       0.188890          0.187062          0.0059858
C  Dy-162       0.254750          0.253852          0.0080729
C  Dy-163       0.248960          0.249618          0.0078894
C  Dy-164       0.282600          0.285086          0.0089555
C
C  The total compound atom density (atom/b-cm):  0.0316895
C
M66     66156.80c   0.000560
        66158.80c   0.000950
        66160.80c   0.023290
        66161.80c   0.188890
        66162.80c   0.254750
        66163.80c   0.248960
        66164.80c   0.282600
C
C  To convert a particle flux to rad[Material]
C  use FM  5.9369239E-11 66   -4  1 for neutrons
C   or FM  5.9369239E-11 66   -5 -6 for photons.
```

Table 192 – Difference between NWC and MatMCNP for Dysprosium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{156}Dy	0.000%	-0.063%	-0.260%	0.000%	0.000%
^{158}Dy	0.000%	-0.027%	-0.017%		
^{160}Dy	0.000%	0.000%	-0.007%		
^{161}Dy	0.000%	0.000%	-0.001%		
^{162}Dy	0.000%	0.000%	0.000%		
^{163}Dy	0.000%	0.000%	0.000%		
^{164}Dy	0.000%	0.000%	0.000%		

2.1.67. Holmium

Holmium (Z =67) has only one stable isotope (^{165}Ho) listed in the NWC. The mass defect and Excel computed quantities are found in Table 193. The MatMCNP output for holmium found in Table 194. The holmium verification data for MatMCNP implementation is found in Table 195. An examination of Table 195 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 193 – Holmium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{165}Ho	1.0000000	-64.8977	164.9303294	1.000000	0.0321134
Density (g/cm^3) = 8.795				FM Conversion = 5.8494216E-11	
Total Atomic Density (atoms/b-cm) = 0.0321134					

Table 194 – MatMCNP Output for Elemental Holmium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ho-165       1.000000           1.000000          0.0321134
C
C  The total compound atom density (atom/b-cm):  0.0321134
C
M67     67165.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  5.8494216E-11 67   -4  1 for neutrons
C   or FM  5.8494216E-11 67   -5 -6 for photons.
```

Table 195 – Difference between NWC and MatMCNP for Holmium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{165}Ho	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.68. Erbium

Erbium (Z = 68) has six naturally occurring isotopes (^{162}Er, ^{164}Er, ^{166}Er, ^{167}Er, ^{168}Er, and ^{170}Er) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 196. The output for erbium from MatMCNP is shown in Table 197. Finally, the verification of the implementation of erbium within MatMCNP is found in Table 198. An examination of Table 198 shows that the implementation of erbium within MatMCNP has been performed correctly.

Table 196 – Erbium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{162}Er	0.0013900	-66.3329	161.9287887	0.001346	0.0000454
^{164}Er	0.0160100	-65.9415	163.9292089	0.015691	0.0005226
^{166}Er	0.3350300	-64.9245	165.9303007	0.332368	0.0109360
^{167}Er	0.2286900	-63.2897	166.9320557	0.228243	0.0074649
^{168}Er	0.2697800	-62.9897	167.9323778	0.270866	0.0088062
^{170}Er	0.1491000	-60.1080	169.9354714	0.151486	0.0048669
Density (g/cm^3) = 9.066			FM Conversion = 5.7679799E-11		
Total Atomic Density (atoms/b-cm) = 0.0326420					

Table 197 – MatMCNP Output for Elemental Erbium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Er-162       0.001390           0.001346          0.0000454
C  Er-164       0.016010           0.015691          0.0005226
C  Er-166       0.335030           0.332368          0.0109361
C  Er-167       0.228690           0.228243          0.0074649
C  Er-168       0.269780           0.270866          0.0088062
C  Er-170       0.149100           0.151486          0.0048669
C
C  The total compound atom density (atom/b-cm):  0.0326420
C
M68     68162.80c   0.001390
        68164.80c   0.016010
        68166.80c   0.335030
        68167.80c   0.228690
        68168.80c   0.269780
        68170.80c   0.149100
C
C  To convert a particle flux to rad[Material]
C  use FM  5.7679812E-11 68   -4  1 for neutrons
C   or FM  5.7679812E-11 68   -5 -6 for photons.
```

Table 198 – Difference between NWC and MatMCNP for Erbium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{162}Er	0.000%	0.022%	0.061%	0.000%	0.000%
^{164}Er	0.000%	-0.002%	0.000%		
^{166}Er	0.000%	0.000%	0.000%		
^{167}Er	0.000%	0.000%	0.000%		
^{168}Er	0.000%	0.000%	0.001%		
^{170}Er	0.000%	0.000%	0.000%		

2.1.69. Thulium

Thulium (Z =69) has just one stable isotope (^{169}Tm) listed in the NWC. The mass defect and Excel computed quantities are found in Table 199. The MatMCNP output for thulium found in Table 200. The thulium verification data for MatMCNP implementation is found in Table 201. An examination of Table 201 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 199 – Thulium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{169}Tm	1.0000000	-61.2745	168.9342191	1.000000	0.0332273
Density (g/cm^3) = 9.321			FM Conversion = 5.7107852E-11		
Total Atomic Density (atoms/b-cm) = 0.0332273					

Table 200 – MatMCNP Output for Elemental Thulium (Excerpt)

```
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Tm-169       1.000000          1.000000          0.0332274
C
C  The total compound atom density (atom/b-cm):  0.0332274
C
M69     69169.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  5.7107853E-11 69   -4  1 for neutrons
C   or FM  5.7107853E-11 69   -5 -6 for photons.
```

Table 201 – Difference between NWC and MatMCNP for Thulium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{169}Tm	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.70. Ytterbium

Ytterbium (Z = 70) has seven naturally occurring isotopes (^{168}Yb, ^{170}Yb, ^{171}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb, and ^{176}Yb) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 202. The output for ytterbium from MatMCNP is shown in Table 203. Finally, the verification of the implementation of ytterbium within MatMCNP is found in Table 204. An examination of Table 204 shows that the implementation of ytterbium within MatMCNP has been performed correctly. The FM value for converting fluence to dose is not computed by MatMCNP for ytterbium. [*NOTE: The ytterbium implementation within MatMCNP does not result in a material card because there are no suitable cross sections available for ytterbium.*]

Table 202 – Ytterbium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{168}Yb	0.0012300	-61.5804	167.9338907	0.001194	0.0000295
^{170}Yb	0.0298200	-60.7636	169.9347676	0.029282	0.0007163
^{171}Yb	0.1409000	-59.3068	170.9363315	0.139176	0.0033847
^{172}Yb	0.2168000	-59.2550	171.9363871	0.215400	0.0052079
^{173}Yb	0.1610300	-57.5510	172.9382165	0.160922	0.0038682
^{174}Yb	0.3202600	-56.9443	173.9388678	0.321897	0.0076932
^{176}Yb	0.1299600	-53.4885	175.9425777	0.132129	0.0031219
Density (g/cm^3) = 6.903				FM Conversion = 5.5748275E-11	
Total Atomic Density (atoms/b-cm) = 0.0240219					

Table 203 – MatMCNP Output for Elemental Ytterbium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Yb-168       0.001230           0.001194         0.0000295
C  Yb-170       0.029820           0.029282         0.0007163
C  Yb-171       0.140900           0.139176         0.0033847
C  Yb-172       0.216800           0.215400         0.0052079
C  Yb-173       0.161030           0.160922         0.0038682
C  Yb-174       0.320260           0.321897         0.0076932
C  Yb-176       0.129960           0.132129         0.0031219
C
C  The total compound atom density (atom/b-cm):  0.0240219
C
C
C  One or more of the elements in the compound does not have a cross-section
C  and therefore the MCNP Card will not be created.
```

Table 204 – Difference between NWC and MatMCNP for Ytterbium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{168}Yb	0.000%	0.033%	-0.159%	0.000%	Not computed by MatMCNP
^{170}Yb	0.000%	-0.002%	-0.004%		
^{171}Yb	0.000%	0.000%	0.001%		
^{172}Yb	0.000%	0.000%	-0.001%		
^{173}Yb	0.000%	0.000%	-0.001%		
^{174}Yb	0.000%	0.000%	0.000%		
^{176}Yb	0.000%	0.000%	0.001%		

2.1.71. Lutetium

Lutetium (Z = 71) has two naturally occurring isotopes (^{175}Lu and ^{176}Lu) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 205. The output of MatMCNP for lutetium is shown in Table 206. Finally, the verification of the implementation of lutetium within MatMCNP is found in Table 207. Table 207 shows that the implementation of lutetium within MatMCNP has been performed correctly.

Table 205 – Lutetium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{175}Lu	0.9740100	-55.1661	174.9407768	0.973865	0.0329912
^{176}Lu	0.0259900	-53.3828	175.9426912	0.026135	0.0008803
Density (g/cm^3) = 9.841				FM Conversion = 5.5138857E-11	
Total Atomic Density (atoms/b-cm) = 0.0338715					

Table 206 – MatMCNP Output for Elemental Lutetium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Lu-175       0.974010           0.973865          0.0329912
C  Lu-176       0.025990           0.026135          0.0008803
C
C  The total compound atom density (atom/b-cm):  0.0338715
C
M71     71175.80c   0.974010
        71176.80c   0.025990
C
C  To convert a particle flux to rad[Material]
C  use FM  5.5138855E-11 71   -4  1 for neutrons
C   or FM  5.5138855E-11 71   -5 -6 for photons.
```

Table 207 – Difference between NWC and MatMCNP for Lutetium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{175}Lu	0.000%	0.000%	0.000%	0.000%	0.000%
^{176}Lu	0.000%	0.000%	0.000%		

2.1.72. Hafnium

Hafnium (Z = 72) has six naturally occurring isotopes (^{174}Hf, ^{176}Hf, ^{177}Hf, ^{178}Hf, ^{179}Hf, and ^{180}Hf) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 208. The output for hafnium from MatMCNP is shown in Table 209. Finally, the verification of the implementation of hafnium within MatMCNP is found in Table 210. An examination of Table 210 shows that the implementation of hafnium within MatMCNP has been performed correctly.

Table 208 – Hafnium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{174}Hf	0.0016000	-55.8455	173.9400474	0.001559	0.0000719
^{176}Hf	0.0526000	-54.5769	175.9414093	0.051850	0.0023622
^{177}Hf	0.1860000	-52.8850	176.9432256	0.184393	0.0083530
^{178}Hf	0.2728000	-52.4396	177.9437038	0.271973	0.0122510
^{179}Hf	0.1362000	-50.4673	178.9458211	0.136552	0.0061165
^{180}Hf	0.3508000	-49.7838	179.9465549	0.353673	0.0157538
Density (g/cm^3) = 13.31				FM Conversion = 5.4052002E-11	
Total Atomic Density (atoms/b-cm) = 0.0449083					

Table 209 – MatMCNP Output for Elemental Hafnium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Hf-174       0.001600           0.001559          0.0000719
C  Hf-176       0.052600           0.051850          0.0023622
C  Hf-177       0.186000           0.184393          0.0083530
C  Hf-178       0.272800           0.271973          0.0122510
C  Hf-179       0.136200           0.136552          0.0061165
C  Hf-180       0.350800           0.353673          0.0157539
C
C  The total compound atom density (atom/b-cm):  0.0449084
C
M72      72174.80c   0.001600
         72176.80c   0.052600
         72177.80c   0.186000
         72178.80c   0.272800
         72179.80c   0.136200
         72180.80c   0.350800
C
C  To convert a particle flux to rad[Material]
C  use FM  5.4052002E-11 72   -4  1 for neutrons
C   or FM  5.4052002E-11 72   -5 -6 for photons.
```

Table 210 – Difference between NWC and MatMCNP for Hafnium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{174}Hf	0.000%	-0.017%	0.065%	0.000%	0.000%
^{176}Hf	0.000%	-0.001%	0.001%		
^{177}Hf	0.000%	0.000%	0.001%		
^{178}Hf	0.000%	0.000%	0.000%		
^{179}Hf	0.000%	0.000%	0.000%		
^{180}Hf	0.000%	0.000%	0.000%		

2.1.73. Tantalum

Tantalum (Z = 73) has two naturally occurring isotopes (^{180m}Ta and ^{181}Ta) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 211. The output of MatMCNP for tantalum is shown in Table 212. Finally, the verification of the implementation of tantalum within MatMCNP is found in Table 213. Table 213 shows that the implementation of tantalum within MatMCNP has been performed correctly.

Table 211 – Tantalum Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{180m}Ta	0.0001201	-48.8594	179.9475473	0.000119	0.0000066
^{181}Ta	0.9998799	-48.4419	180.9479955	0.999881	0.0545744
Density (g/cm^3) = 16.4			FM Conversion = 5.3316295E-11		
Total Atomic Density (atoms/b-cm) = 0.0545809					

Table 212 – MatMCNP Output for Elemental Tantalum (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ta-180       0.000120           0.000119          0.0000066
C  Ta-181       0.999880           0.999881          0.0545744
C
C  The total compound atom density (atom/b-cm):  0.0545810
C
M73     73180.80c   0.000120
        73181.80c   0.999880
C
C  To convert a particle flux to rad[Material]
C  use FM  5.3316296E-11 73   -4  1 for neutrons
C   or FM  5.3316296E-11 73   -5 -6 for photons.
```

Table 213 – Difference between NWC and MatMCNP for Tantalum

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{180m}Ta	-0.083%	-0.365%	0.684%	0.000%	0.000%
^{181}Ta	0.000%	0.000%	0.000%		

2.1.74. Tungsten

Tungsten (Z = 74) has five naturally occurring isotopes (^{180}W, ^{182}W, ^{183}W, ^{184}W, and ^{186}W) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 214. The output for tungsten from MatMCNP is shown in Table 215. Finally, the verification of the implementation of tungsten within MatMCNP is found in Table 216. An examination of Table 216 shows that the implementation of tungsten within MatMCNP has been performed correctly.

Table 214 – Tungsten Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{180}W	0.0012000	-49.6365	179.946713	0.001175	0.0000759
^{182}W	0.2650000	-48.2475	181.9482042	0.262270	0.0167537
^{183}W	0.1431000	-46.3671	182.9502229	0.142406	0.0090470
^{184}W	0.3064000	-45.7075	183.9509310	0.306582	0.0193710
^{186}W	0.2843000	-42.5109	185.9543627	0.287567	0.0179738
Density (g/cm^3) = 19.3				FM Conversion = 5.2477029E-11	
Total Atomic Density (atoms/b-cm) = 0.0632213					

Table 215 – MatMCNP Output for Elemental Tungsten (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   W-180       0.001200           0.001175          0.0000759
C   W-182       0.265000           0.262271          0.0167537
C   W-183       0.143100           0.142406          0.0090470
C   W-184       0.306400           0.306582          0.0193710
C   W-186       0.284300           0.287567          0.0179738
C
C  The total compound atom density (atom/b-cm):  0.0632214
C
M74     74180.80c   0.001200
        74182.80c   0.265000
        74183.80c   0.143100
        74184.80c   0.306400
        74186.80c   0.284300
C
C  To convert a particle flux to rad[Material]
C  use FM  5.2477033E-11 74   -4  1 for neutrons
C   or FM  5.2477033E-11 74   -5 -6 for photons.
```

Table 216 – Difference between NWC and MatMCNP for Tungsten

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{180}W	0.000%	0.036%	0.045%	0.000%	0.000%
^{182}W	0.000%	0.000%	0.000%		
^{183}W	0.000%	0.000%	0.000%		
^{184}W	0.000%	0.000%	0.000%		
^{186}W	0.000%	0.000%	0.000%		

2.1.75. Rhenium

Rhenium (Z = 75) has two naturally occurring isotopes (^{185}Re and ^{187}Re) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 217. The output of MatMCNP for rhenium is shown in Table 218. Finally, the verification of the implementation of rhenium within MatMCNP is found in Table 219. Table 219 shows that the implementation of rhenium within MatMCNP has been performed correctly.

Table 217 – Rhenium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{185}Re	0.3740000	-43.8225	184.9529546	0.371482	0.0251588
^{187}Re	0.6260000	-41.2184	186.9557502	0.628518	0.0421107
Density (g/cm^3) = 20.8				FM Conversion = 5.1810542E-11	
Total Atomic Density (atoms/b-cm) = 0.0672696					

Table 218 – MatMCNP Output for Elemental Rhenium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Re-185       0.374000           0.371482          0.0251588
C  Re-187       0.626000           0.628518          0.0421108
C
C  The total compound atom density (atom/b-cm):  0.0672696
C
M75     75185.80c   0.374000
        75187.80c   0.626000
C
C  To convert a particle flux to rad[Material]
C  use FM  5.1810545E-11 75   -4  1 for neutrons
C   or FM  5.1810545E-11 75   -5 -6 for photons.
```

Table 219 – Difference between NWC and MatMCNP for Rhenium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{185}Re	0.000%	0.000%	0.000%	0.000%	0.000%
^{187}Re	0.000%	0.000%	0.000%		

2.1.76. Osmium

Osmium (Z = 76) has seven naturally occurring isotopes (^{184}Os, ^{186}Os, ^{187}Os, ^{188}Os, ^{189}Os, ^{190}Os, and ^{192}Os) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 220. The output for osmium from MatMCNP is shown in Table 221. Finally, the verification of the implementation of osmium within MatMCNP is found in Table 222. An examination of Table 222 shows that the implementation of osmium within MatMCNP has been performed correctly. The FM value for converting fluence to dose is not computed by MatMCNP for osmium. [*NOTE: The osmium implementation within MatMCNP does not result in a material card because there are no suitable cross sections available for osmium.*]

Table 220 – Osmium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{184}Os	0.0002000	-44.2566	183.9524886	0.000193	0.0000143
^{186}Os	0.0159000	-43.0023	185.9538351	0.015543	0.0011369
^{187}Os	0.0196000	-41.2209	186.9557475	0.019263	0.0014015
^{188}Os	0.1324000	-41.1392	187.9558352	0.130821	0.0094674
^{189}Os	0.1615000	-38.9883	188.9581443	0.160425	0.0115482
^{190}Os	0.2626000	-38.7093	189.9584439	0.262232	0.0187774
^{192}Os	0.4078000	-35.8838	191.9614772	0.411523	0.0291601
Density (g/cm^3) = 22.587			FM Conversion = 5.0716139E-11		
Total Atomic Density (atoms/b-cm) = 0.0715059					

Table 221 – MatMCNP Output for Elemental Osmium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Os-184       0.000200           0.000193         0.0000143
C  Os-186       0.015900           0.015543         0.0011369
C  Os-187       0.019600           0.019263         0.0014015
C  Os-188       0.132400           0.130821         0.0094674
C  Os-189       0.161500           0.160425         0.0115482
C  Os-190       0.262600           0.262232         0.0187775
C  Os-192       0.407800           0.411523         0.0291601
C
C  The total compound atom density (atom/b-cm):  0.0715060
C
C
C  One or more of the elements in the compound does not have a cross-section
C  and therefore the MCNP Card will not be created.
```

Table 222 – Difference between NWC and MatMCNP for Osmium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{184}Os	0.000%	-0.210%	-0.008%	0.000%	Not computed by MatMCNP
^{186}Os	0.000%	0.000%	-0.004%		
^{187}Os	0.000%	-0.001%	-0.001%		
^{188}Os	0.000%	0.000%	0.000%		
^{189}Os	0.000%	0.000%	0.000%		
^{190}Os	0.000%	0.000%	0.000%		
^{192}Os	0.000%	0.000%	0.000%		

2.1.77. Iridium

Iridium (Z = 77) has two naturally occurring isotopes (^{191}Ir and ^{193}Ir) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 223. The output of MatMCNP for iridium is shown in Table 224. Finally, the verification of the implementation of iridium within MatMCNP is found in Table 225. Table 225 shows that the implementation of iridium within MatMCNP has been performed correctly.

Table 223 – Iridium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{191}Ir	0.3730000	-36.7107	190.9605894	0.370564	0.0263662
^{193}Ir	0.6270000	-34.5382	192.9629217	0.629436	0.0443206
Density (g/cm^3) = 22.562				FM Conversion = 5.0190763E-11	
Total Atomic Density (atoms/b-cm) = 0.0706868					

Table 224 – MatMCNP Output for Elemental Iridium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ir-191       0.373000           0.370564          0.0263662
C  Ir-193       0.627000           0.629436          0.0443207
C
C  The total compound atom density (atom/b-cm):  0.0706869
C
M77     77191.80c   0.373000
        77193.80c   0.627000
C
C  To convert a particle flux to rad[Material]
C  use FM  5.0190768E-11 77   -4  1 for neutrons
C   or FM  5.0190768E-11 77   -5 -6 for photons.
```

Table 225 – Difference between NWC and MatMCNP for Iridium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{191}Ir	0.000%	0.000%	0.000%	0.000%	0.000%
^{193}Ir	0.000%	0.000%	0.000%		

2.1.78. Platinum

Platinum (Z = 78) has six naturally occurring isotopes (^{190}Pt, ^{192}Pt, ^{194}Pt, ^{195}Pt, ^{196}Pt, and ^{198}Pt) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 226. The output for platinum from MatMCNP is shown in Table 227. Finally, the verification of the implementation of platinum within MatMCNP is found in Table 228. An examination of Table 228 shows that the implementation of platinum within MatMCNP has been performed correctly. [*NOTE: The platinum implementation within MatMCNP uses the elemental cross section (78000.42c) rather than an isotopic description. Also, the platinum cross section selected within MatMCNP does not utilize the ENDF/B-VII Release 1 cross section because it is not available.*]

Table 226 – Platinum Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{190}Pt	0.0001200	-37.3251	189.9599299	0.000117	0.0000079
^{192}Pt	0.0078197	-36.2921	191.9610388	0.007694	0.0005178
^{194}Pt	0.3285869	-34.7625	193.9626809	0.326697	0.0217573
^{195}Pt	0.3377865	-32.7962	194.9647918	0.337579	0.0223665
^{196}Pt	0.2520899	-32.6468	195.9649522	0.253228	0.0166921
^{198}Pt	0.0735971	-29.9056	197.9678950	0.074685	0.0048732
Density (g/cm^3) = 21.45				FM Conversion = 4.9452759E-11	
Total Atomic Density (atoms/b-cm) = 0.0662148					

Table 227 – MatMCNP Output for Elemental Platinum (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Pt-190       0.000120           0.000117          0.0000079
C  Pt-192       0.007820           0.007694          0.0005178
C  Pt-194       0.328587           0.326697          0.0217573
C  Pt-195       0.337786           0.337579          0.0223665
C  Pt-196       0.252090           0.253228          0.0166921
C  Pt-198       0.073597           0.074685          0.0048732
C
C  The total compound atom density (atom/b-cm):  0.0662148
C
M78     78000.42c   1.000000
C
C  Caution: The natural zaid is used for Platinum.
C
C  To convert a particle flux to rad[Material]
C  use FM  4.9452765E-11 78   -4  1 for neutrons
C   or FM  4.9452765E-11 78   -5 -6 for photons.
```

Table 228 – Difference between NWC and MatMCNP for Platinum

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{190}Pt	0.004%	0.134%	-0.572%	0.000%	0.000%
^{192}Pt	0.004%	-0.006%	0.004%		
^{194}Pt	0.000%	0.000%	0.000%		
^{195}Pt	0.000%	0.000%	0.000%		
^{196}Pt	0.000%	0.000%	0.000%		
^{198}Pt	0.000%	0.000%	0.000%		

2.1.79. Gold

Gold (Z = 79) has just one stable isotope (^{197}Au) listed in the NWC. The mass defect and Excel computed quantities are found in Table 229. The MatMCNP output for gold found in Table 230. The gold verification data for MatMCNP implementation is found in Table 231. An examination of Table 231 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 229 – Gold Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{197}Au	1.0000000	-31.1409	196.9665689	1.000000	0.0590086
Density (g/cm^3) = 19.3				FM Conversion = 4.8980243E-11	
Total Atomic Density (atoms/b-cm) = 0.0590086					

Table 230 – MatMCNP Output for Elemental Gold (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Au-197       1.000000           1.000000          0.0590087
C
C  The total compound atom density (atom/b-cm):  0.0590087
C
M79     79197.80c   1.000000
C  To convert a particle flux to rad[Material]
C  use FM  4.8980243E-11 79   -4  1 for neutrons
C   or FM  4.8980243E-11 79   -5 -6 for photons.
```

Table 231 – Difference between NWC and MatMCNP for Gold

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{197}Au	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.80. Mercury

Mercury (Z = 80) has seven naturally occurring isotopes (^{196}Hg, ^{198}Hg, ^{199}Hg, ^{200}Hg, ^{201}Hg, ^{202}Hg, and ^{204}Hg) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 232. The output for mercury from MatMCNP is shown in Table 233. Finally, the verification of the implementation of mercury within MatMCNP is found in Table 234. An examination of Table 234 shows that the implementation of mercury within MatMCNP has been performed correctly.

Table 232 – Mercury Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{196}Hg	0.0015000	-31.8267	195.9658326	0.001465	0.0000610
^{198}Hg	0.0997000	-30.9548	197.9667687	0.098392	0.0040544
^{199}Hg	0.1687000	-29.5464	198.9682806	0.167328	0.0068604
^{200}Hg	0.2310000	-29.5035	199.9683267	0.230274	0.0093939
^{201}Hg	0.1318000	-27.6629	200.9703027	0.132044	0.0053598
^{202}Hg	0.2986000	-27.3456	201.9706433	0.300641	0.0121429
^{204}Hg	0.0687000	-24.6902	203.9734940	0.069856	0.0027938
Density (g/cm^3) = 13.546				FM Conversion = 4.8093272E-11	
Total Atomic Density (atoms/b-cm) = 0.0406661					

Table 233 – MatMCNP Output for Elemental Mercury (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Hg-196       0.001500           0.001465          0.0000610
C  Hg-198       0.099700           0.098392          0.0040544
C  Hg-199       0.168700           0.167328          0.0068604
C  Hg-200       0.231000           0.230274          0.0093939
C  Hg-201       0.131800           0.132044          0.0053598
C  Hg-202       0.298600           0.300642          0.0121429
C  Hg-204       0.068700           0.069856          0.0027938
C
C  The total compound atom density (atom/b-cm):  0.0406661
C
M80     80196.80c   0.001500
        80198.80c   0.099700
        80199.80c   0.168700
        80200.80c   0.231000
        80201.80c   0.131800
        80202.80c   0.298600
        80204.80c   0.068700
C
C  To convert a particle flux to rad[Material]
C  use FM  4.8093269E-11 80   -4  1 for neutrons
C   or FM  4.8093269E-11 80   -5 -6 for photons.
```

Table 234 – Difference between NWC and MatMCNP for Mercury

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{196}Hg	0.000%	-0.024%	0.001%	0.000%	0.000%
^{198}Hg	0.000%	0.000%	0.000%		
^{199}Hg	0.000%	0.000%	0.000%		
^{200}Hg	0.000%	0.000%	0.000%		
^{201}Hg	0.000%	0.000%	0.000%		
^{202}Hg	0.000%	0.000%	0.000%		
^{204}Hg	0.000%	0.001%	0.001%		

2.1.81. Thallium

Thallium (Z = 81) has two naturally occurring isotopes (^{203}Tl and ^{205}Tl) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 235. The output of MatMCNP for thallium is shown in Table 236. Finally, the verification of the implementation of thallium within MatMCNP is found in Table 237. Table 237 shows that the implementation of thallium within MatMCNP has been performed correctly. (*NOTE: The NWC atomic abundances sum to 100.004. The numbers below and within MatMCNP take that into account.*)

Table 235 – Thallium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{203}Tl	0.2952282	-25.7620	202.9723434	0.293190	0.0103082
^{205}Tl	0.7047718	-23.8215	204.9744266	0.706810	0.0246078
Density (g/cm^3) = 11.85				FM Conversion = 4.7202818E-11	
Total Atomic Density (atoms/b-cm) = 0.0349159					

Table 236 – MatMCNP Output for Elemental Thallium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Tl-203       0.295240           0.293202          0.0103086
C  Tl-205       0.704760           0.706798          0.0246074
C
C  The total compound atom density (atom/b-cm):  0.0349159
C
M81     81203.80c   0.295240
        81205.80c   0.704760
C  To convert a particle flux to rad[Material]
C  use FM  4.7202825E-11 81   -4  1 for neutrons
C   or FM  4.7202825E-11 81   -5 -6 for photons.
```

Table 237 – Difference between NWC and MatMCNP for Thallium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{203}Tl	0.004%	0.004%	0.004%	0.000%	0.000%
^{205}Tl	-0.002%	-0.002%	-0.001%		

2.1.82. Lead

Lead (Z = 82) has four naturally occurring isotopes (^{204}Pb, ^{206}Pb, ^{207}Pb, and ^{208}Pb) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 238.

The output for lead from MatMCNP is shown in Table 239. Finally, the verification of the implementation of lead within MatMCNP is found in Table 240. An examination of Table 240 shows that the implementation of lead within MatMCNP has been performed correctly.

Table 238 – Lead Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{204}Pb	0.0140000	-25.1105	203.9730428	0.013781	0.0004618
^{206}Pb	0.2410000	-23.7862	205.9744645	0.239555	0.0079495
^{207}Pb	0.2210000	-22.4527	206.9758960	0.220743	0.0072898
^{208}Pb	0.5240000	-21.7492	207.9766513	0.525921	0.0172843
Density (g/cm^3) = 11.35				FM Conversion = 4.6557351E-11	
Total Atomic Density (atoms/b-cm) = 0.0329854					

Table 239 – MatMCNP Output for Elemental Lead (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Pb-204       0.014000           0.013781          0.0004618
C  Pb-206       0.241000           0.239555          0.0079495
C  Pb-207       0.221000           0.220743          0.0072898
C  Pb-208       0.524000           0.525921          0.0172843
C
C  The total compound atom density (atom/b-cm):  0.0329854
C
M82     82204.80c   0.014000
        82206.80c   0.241000
        82207.80c   0.221000
        82208.80c   0.524000
C  To convert a particle flux to rad[Material]
C  use FM  4.6557352E-11 82   -4  1 for neutrons
C   or FM  4.6557352E-11 82   -5 -6 for photons.
```

Table 240 – Difference between NWC and MatMCNP for Lead

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{204}Pb	0.000%	0.001%	0.001%	0.000%	0.000%
^{206}Pb	0.000%	0.000%	0.000%		
^{207}Pb	0.000%	0.000%	0.000%		
^{208}Pb	0.000%	0.000%	0.000%		

2.1.83. Bismuth

Bismuth (Z = 83) has just one stable isotope (^{209}Bi) listed in the NWC. The mass defect and Excel computed quantities are found in Table 241. The MatMCNP output for bismuth found in Table 242. The bismuth verification data for MatMCNP implementation is found in Table 243. An examination of Table 243 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 241 – Bismuth Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{209}Bi	1.0000000	-18.2593	208.9803978	1.000000	0.0280877
Density (g/cm^3) = 9.747			FM Conversion = 4.6164475E-11		
Total Atomic Density (atoms/b-cm) = 0.0280877					

Table 242 – MatMCNP Output for Elemental Bismuth (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Bi-209       1.000000           1.000000          0.0280877
C
C  The total compound atom density (atom/b-cm):  0.0280877
C
M83     83209.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  4.6164478E-11 83   -4  1 for neutrons
C   or FM  4.6164478E-11 83   -5 -6 for photons.
```

Table 243 – Difference between NWC and MatMCNP for Bismuth

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{209}Bi	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.84. Polonium

Polonium (Z = 84) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains polonium, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing polonium.

2.1.85. Astatine

Astatine (Z = 85) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains astatine, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing astatine.

2.1.86. Radon

Radon (Z = 86) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains radon, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing radon.

2.1.87. Francium

Francium (Z = 87) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains francium, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing francium.

2.1.88. Radium

Radium (Z = 88) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains radium, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing radium.

2.1.89. Actinium

Actinium (Z = 89) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains actinium, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing actinium.

2.1.90. Thorium

Thorium (Z = 90) has just one stable isotope (^{232}Th) listed in the NWC. The mass defect and Excel computed quantities are found in Table 244. The MatMCNP output for thorium found in Table 245. The thorium verification data for MatMCNP implementation is found in Table 246. An examination of Table 246 reveals that the MatMCNP results agree within the precision of the Excel values chosen for all quantities examined.

Table 244 – Thorium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{232}Th	1.0000000	35.4526	232.0380599	1.000000	0.0304172
Density (g/cm^3) = 11.72				FM Conversion = 4.1577103E-11	
Total Atomic Density (atoms/b-cm) = 0.0304172					

Table 245 – MatMCNP Output for Elemental Thorium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Th-232       1.000000          1.000000          0.0304172
C
C  The total compound atom density (atom/b-cm):  0.0304172
C
M90     90232.80c   1.000000
C
C  To convert a particle flux to rad[Material]
C  use FM  4.1577110E-11 90   -4  1 for neutrons
C   or FM  4.1577110E-11 90   -5 -6 for photons.
```

Table 246 – Difference between NWC and MatMCNP for Thorium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{232}Th	0.000%	0.000%	0.000%	0.000%	0.000%

2.1.91. Protactinium

Protactinium (Z = 91) has no naturally occurring isotopes listed in the NWC. MatMCNP will process a material that contains protactinium, but no atom fractions, weight fractions, or atom densities are calculated. Essentially, the program will exit gracefully when given a material containing protactinium.

2.1.92. Uranium

Uranium (Z = 92) has three naturally occurring isotopes (^{234}U, ^{235}U, and ^{238}U) listed in the NWC. The abundances, mass defects, and Excel computed quantities are found in Table 247. The output of MatMCNP for uranium is shown in Table 248. Finally, the verification of the implementation of uranium within MatMCNP is found in Table 249. An examination of Table 249 shows that the implementation of uranium within MatMCNP has been performed correctly.

Table 247 – Uranium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{234}U	0.0000540	38.1480	234.0409536	0.000053	0.0000026
^{235}U	0.0072040	40.9218	235.0439314	0.007114	0.0003481
^{238}U	0.9927420	47.3100	238.0507894	0.992833	0.0479723
Density (g/cm^3) = 19.1				FM Conversion = 4.0530666E-11	
Total Atomic Density (atoms/b-cm) = 0.0483230					

Table 248 – MatMCNP Output for Elemental Uranium (Excerpt)

```
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  U-234        0.000054           0.000053          0.0000026
C  U-235        0.007204           0.007114          0.0003481
C  U-238        0.992742           0.992833          0.0479723
C
C  The total compound atom density (atom/b-cm):  0.0483231
C
M92      92234.80c   0.000054
         92235.80c   0.007204
         92238.80c   0.992742
C
C  To convert a particle flux to rad[Material]
C  use FM  4.0530666E-11 92   -4  1 for neutrons
C   or FM  4.0530666E-11 92   -5 -6 for photons.
```

Table 249 – Difference between NWC and MatMCNP for Uranium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{234}U	0.000%	-0.179%	-0.362%	0.000%	0.000%
^{235}U	0.000%	0.005%	-0.006%		
^{238}U	0.000%	0.000%	0.000%		

2.2. Compounds and Mixtures

In this section, a selection of different compounds or mixtures is verified. It is impossible to validate MatMCNP for every mixture or compound. In Section 2.1, each individual element (Z =

1 – 92) was verified within the code. Compounds and mixtures are verified by performing example calculations for compounds (or mixtures) using the equations in Section 1.3. Those calculations are compared to the results from MatMCNP. MatMCNP allows materials to be entered as either atomic or weight fraction. The verification process takes materials specified in both atomic or weight fractions to ensure that the techniques used by the code provide the correct answer with either specification. (*NOTE: The example below will utilize "Atomic Fraction", "Weight Fraction", and "Isotopic Mass" columns from the appropriate tables in Section 2.1 above to compute the elemental weights that go into the compounds. Additionally, the final values computed below are shown as approximate due to round-off.*)

2.2.1. Examples Using Atomic Fractions

Water

Water (H_2O) is commonly used in radiation transport particularly in reactor analysis, shielding calculations, and criticality safety analysis. It is easy to specify in MatMCNP simply using the atomic formula (2 H and 1 O) because the code will normalize the results. We will use a density of 1.0 g/cm^3. First, we compute the elemental atomic fractions:

$$(a/o)_H = \left(\frac{2}{3}\right) \approx 0.66666667$$

$$(a/o)_O = \left(\frac{1}{3}\right) \approx 0.33333333$$

Next, we must compute the molecular mass:

$$M_H = \frac{1}{100}\left[(99.9885)\cdot(1.007824956) + (0.0115)\cdot(2.014101755)\right] \approx 1.007940678$$

$$M_O = \frac{1}{100}\left[(99.757)\cdot(15.99491462) + (0.038)\cdot(16.99913182) + (0.205)\cdot(16.99913182)\right] \approx 15.99940493$$

$$M_{H_2O} = 2\cdot M_H + 1\cdot M_O = \left(2\cdot 1.007940678\right) + \left(1\cdot 15.99940493\right) \approx 18.01528628$$

Next, we compute the weight fractions of each element:

$$(w/o)_H = \left(\frac{2\cdot 1.007940678}{18.01528628}\right) \approx 0.11189838$$

$$(w/o)_O = \left(\frac{1\cdot 15.99940493}{18.01528628}\right) \approx 0.88810162$$

Next, we compute the isotopic atomic fractions:

$$(a/o)_{^1H} = 0.999885 \cdot 0.66666667 \approx 0.66659000$$
$$(a/o)_{^2H} = 0.000115 \cdot 0.66666667 \approx 0.00007667$$
$$(a/o)_{^{16}O} = 0.99757 \cdot 0.33333333 \approx 0.33252333$$
$$(a/o)_{^{17}O} = 0.00038 \cdot 0.33333333 \approx 0.00012667$$
$$(a/o)_{^{18}O} = 0.00205 \cdot 0.33333333 \approx 0.00068333$$

Next, we compute the isotopic weight fractions:

$$(w/o)_{^1H} = 0.999770 \cdot 0.11189838 \approx 0.11187267$$
$$(w/o)_{^2H} = 0.000230 \cdot 0.11189838 \approx 0.00002571$$
$$(w/o)_{^{16}O} = 0.997290 \cdot 0.88810162 \approx 0.88569489$$
$$(w/o)_{^{17}O} = 0.000404 \cdot 0.88810162 \approx 0.00035857$$
$$(w/o)_{^{18}O} = 0.002306 \cdot 0.88810162 \approx 0.00204816$$

Now, we compute the number density for the molecule as well as the elemental atom density (in [number/b-cm]):

$$N_{H_2O} = \frac{\rho_{H_2O} \cdot N_A}{M_{H_2O}} = \frac{1.0 \cdot \left(6.02214129 \times 10^{23} \cdot 1 \times 10^{-24}\right)}{18.01528628} \approx 0.033427952 \ \left(\text{molecules}/\text{barn-cm}\right)$$
$$N_H = 2 \cdot 0.033427952 \approx 0.066855904 \ \left(\text{atoms}/\text{barn-cm}\right)$$
$$N_O = 1 \cdot 0.033427952 \approx 0.033427952 \ \left(\text{atoms}/\text{barn-cm}\right)$$
$$N_{H_2O\ (\text{Total Atoms})} = 0.066855904 + 0.033427952 \approx 0.100283856 \ \left(\text{atoms}/\text{barn-cm}\right)$$

Finally, the isotopic number density is computed (in atoms/b-cm):

$$N_{^1H} = \left[(a/o)_{^1H}\right] \cdot \left[N_{H_2O\ (\text{Total Atoms})}\right] = 0.66659000 \cdot 0.100283856 \approx 0.06684822$$
$$N_{^2H} = \left[(a/o)_{^2H}\right] \cdot \left[N_{H_2O\ (\text{Total Atoms})}\right] = 0.00007667 \cdot 0.100283856 \approx 0.00000769$$
$$N_{^{16}O} = \left[(a/o)_{^{16}O}\right] \cdot \left[N_{H_2O\ (\text{Total Atoms})}\right] = 0.33252333 \cdot 0.100283856 \approx 0.03334672$$
$$N_{^{17}O} = \left[(a/o)_{^{17}O}\right] \cdot \left[N_{H_2O\ (\text{Total Atoms})}\right] = 0.00012667 \cdot 0.100283856 \approx 0.00001270$$
$$N_{^{18}O} = \left[(a/o)_{^{18}O}\right] \cdot \left[N_{H_2O\ (\text{Total Atoms})}\right] = 0.00068333 \cdot 0.100283856 \approx 0.00006853$$

The input and output of MatMCNP for water is found in Appendix B. The verification data for water calculated by MatMCNP is found in Table 250. All of the ratios are within 1.1% of unity and most are even closer (round off for the very low abundance of ^{2}H causes the "large" difference [1.1% for weight fraction] for that isotope).

Table 250 – MatMCNP Verification of Water

Isotope	Atom Fraction Ratio	Weight Fraction Ratio	Atom Density Ratio	Total Atom Density Ratio
^{1}H	1.00000	1.00000	1.00000	1.00000
^{2}H	0.99567	0.98900	0.99850	
^{16}O	1.00000	1.00000	1.00000	
^{17}O	0.99738	0.99879	1.00021	
^{18}O	1.00049	1.00008	1.00040	
The ratios are the "hand calculation" divided by the MatMCNP result.				

Gallium Arsenide

Gallium Arsenide (GaAs) is commonly used by Sandia National Laboratories (SNL) in studies of radiation effects on electronic devices. Again, this compound is easy to specify in MatMCNP simply using the atomic formula (1 Ga and 1 As). We will use a density of 5.32 g/cm^3 [5]. First, we compute the elemental atomic fractions:

$$(a/o)_{Ga} = \left(\frac{1}{2}\right) = 0.50$$

$$(a/o)_{As} = \left(\frac{1}{2}\right) = 0.50$$

Next, we must compute the molecular mass:

$$M_{Ga} = \frac{1}{100}\left[(60.108)\cdot(68.92557365) + (39.892)\cdot(70.92470268)\right] \approx 69.72306620$$

$$M_{As} = \frac{1}{100}\left[(100.0)\cdot(74.92159509)\right] = 74.92159509$$

$$M_{GaAs} = M_{Ga} + M_{As} = (69.7230662) + (74.92159509) \approx 144.64466130$$

Next, we compute the weight fractions of each element:

$$(w/o)_{Ga} = \left(\frac{1\cdot 69.72306620}{144.64466130}\right) \approx 0.482030001$$

$$(w/o)_{As} = \left(\frac{1\cdot 74.92159509}{144.64466130}\right) \approx 0.517969999$$

Next, we compute the isotopic atomic fractions:

$$(a/o)_{^{69}Ga} = 0.60108\cdot 0.50 = 0.30054$$

$$(a/o)_{^{71}Ga} = 0.39892\cdot 0.50 = 0.19946$$

$$(a/o)_{^{75}As} = 1.00000\cdot 0.50 = 0.50000$$

Next, we compute the isotopic weight fractions:

$$(w/o)_{^{69}Ga} = 0.594205 \cdot 0.482030001 \approx 0.28642456$$
$$(w/o)_{^{71}Ga} = 0.405795 \cdot 0.482030001 \approx 0.19560544$$
$$(w/o)_{^{75}As} = 1.000000 \cdot 0.517969999 \approx 0.51797000$$

Now, we compute the number density for the molecule as well as the elemental atom density (in [number/b-cm]):

$$N_{GaAs} = \frac{\rho_{GaAs} \cdot N_A}{M_{GaAs}} = \frac{5.32 \cdot \left(6.02214129 \times 10^{23} \cdot 1 \times 10^{-24}\right)}{144.64466130} \approx 0.022149308 \left(\text{molecules}/\text{barn-cm}\right)$$
$$N_{Ga} = 1 \cdot 0.022149308 \approx 0.022149308 \left(\text{atoms}/\text{barn-cm}\right)$$
$$N_{As} = 1 \cdot 0.022149308 \approx 0.022149308 \left(\text{atoms}/\text{barn-cm}\right)$$
$$N_{GaAs\ (\text{Total Atoms})} = 0.022149308 + 0.022149308 \approx 0.044298616 \left(\text{atoms}/\text{barn-cm}\right)$$

Finally, the isotopic number density is computed (in atoms/b-cm):

$$N_{^{69}Ga} = \left[(a/o)_{^{69}Ga}\right] \cdot \left[N_{GaAs\ (\text{Total Atoms})}\right] = 0.30054 \cdot 0.044298616 \approx 0.01331351$$
$$N_{^{71}Ga} = \left[(a/o)_{^{71}Ga}\right] \cdot \left[N_{GaAs\ (\text{Total Atoms})}\right] = 0.19946 \cdot 0.044298616 \approx 0.00883580$$
$$N_{^{75}As} = \left[(a/o)_{^{75}As}\right] \cdot \left[N_{GaAs\ (\text{Total Atoms})}\right] = 0.50000 \cdot 0.044298616 \approx 0.02214931$$

The input and output of MatMCNP for gallium arsenide is found in Appendix B. The verification data for gallium arsenide calculated by MatMCNP is found in Table 251. All of the ratios compute to unity for a minimum of 5 decimal places.

Table 251 – MatMCNP Verification of Gallium Arsenide

Isotope	Atom Fraction Ratio	Weight Fraction Ratio	Atom Density Ratio	Total Atom Density Ratio
^{69}Ga	1.00000	1.00000	1.00000	1.00000
^{71}Ga	1.00000	1.00000	1.00000	
^{75}As	1.00000	1.00000	1.00000	
The ratios are the “hand calculation” divided by the MatMCNP result.				

If additional verification data is desired, contact the author (krdepri@sandia.gov) for more cases that are described by atomic fractions.

2.2.2. Example Using Weight Fractions

Stainless Steel 301

Stainless steel is commonly used in radiation transport particularly in reactor analysis, shielding calculations, and criticality safety analysis. For this example, stainless steel alloy 301 will be utilized. The composition by weight is as follows: 0.15% carbon, 17.00% chromium, 7.00% nickel, 2.00% manganese, and 73.85% iron [6]. First, we need to compute the atom fractions from the weight percentages:

$$(Normalization)_{SS304} = \left.\frac{0.0015}{12.0107359}\right|_{C} + \left.\frac{0.1700}{51.9961318}\right|_{Cr} + \left.\frac{0.0200}{54.9380439}\right|_{Mn} + \left.\frac{0.0700}{58.6933472}\right|_{Ni} + \left.\frac{0.7385}{55.8451446}\right|_{Fe}$$

$$(Normalization)_{SS304} \approx 0.01817512$$

$$(a/o)_{C} = \frac{0.00012489}{0.01817512} \approx 0.00687139$$
$$(a/o)_{Cr} = \frac{0.00326947}{0.01817512} \approx 0.17988738$$
$$(a/o)_{Mn} = \frac{0.00036405}{0.01817512} \approx 0.02002994$$
$$(a/o)_{Ni} = \frac{0.00119264}{0.01817512} \approx 0.06561936$$
$$(a/o)_{Fe} = \frac{0.01322407}{0.01817512} \approx 0.72759194$$

Next, we compute the isotopic atomic fractions:

$$(a/o)_{^{12}C} = 0.9893 \cdot 0.00687139 \approx 0.00679786$$
$$(a/o)_{^{13}C} = 0.0107 \cdot 0.00687139 \approx 0.00007352$$
$$(a/o)_{^{50}Cr} = 0.04345 \cdot 0.17988738 \approx 0.00781611$$
$$(a/o)_{^{52}Cr} = 0.83789 \cdot 0.17988738 \approx 0.15072583$$
$$(a/o)_{^{53}Cr} = 0.09501 \cdot 0.17988738 \approx 0.01709110$$
$$(a/o)_{^{54}Cr} = 0.02365 \cdot 0.17988738 \approx 0.00425434$$
$$(a/o)_{^{55}Mn} = 1.0000 \cdot 0.02002994 \approx 0.02002994$$
$$(a/o)_{^{58}Ni} = 0.680770 \cdot 0.06561936 \approx 0.04467169$$
$$(a/o)_{^{60}Ni} = 0.262230 \cdot 0.06561936 \approx 0.01720736$$
$$(a/o)_{^{61}Ni} = 0.011399 \cdot 0.06561936 \approx 0.00074800$$
$$(a/o)_{^{62}Ni} = 0.036346 \cdot 0.06561936 \approx 0.00238500$$
$$(a/o)_{^{64}Ni} = 0.009255 \cdot 0.06561936 \approx 0.00060731$$
$$(a/o)_{^{54}Fe} = 0.05845 \cdot 0.72759194 \approx 0.04252775$$
$$(a/o)_{^{56}Fe} = 0.91754 \cdot 0.72759194 \approx 0.66759471$$
$$(a/o)_{^{57}Fe} = 0.02119 \cdot 0.72759194 \approx 0.01541767$$
$$(a/o)_{^{58}Fe} = 0.00282 \cdot 0.72759194 \approx 0.00205181$$

Next, we compute the isotopic weight fractions:

$$\begin{aligned}
(w/o)_{^{12}C} &= 0.988416 \cdot 0.0015 \approx 0.00148262 \\
(w/o)_{^{13}C} &= 0.011584 \cdot 0.0015 \approx 0.00001738 \\
(w/o)_{^{50}Cr} &= 0.041737 \cdot 0.1700 \approx 0.00709527 \\
(w/o)_{^{52}Cr} &= 0.836994 \cdot 0.1700 \approx 0.14228892 \\
(w/o)_{^{53}Cr} &= 0.096736 \cdot 0.1700 \approx 0.01644510 \\
(w/o)_{^{54}Cr} &= 0.024534 \cdot 0.1700 \approx 0.00417072 \\
(w/o)_{^{55}Mn} &= 1.0000 \cdot 0.0200 = 0.0200 \\
(w/o)_{^{58}Ni} &= 0.671978 \cdot 0.0700 \approx 0.04703847 \\
(w/o)_{^{60}Ni} &= 0.267759 \cdot 0.0700 \approx 0.01874310 \\
(w/o)_{^{61}Ni} &= 0.011834 \cdot 0.0700 \approx 0.00082835 \\
(w/o)_{^{62}Ni} &= 0.038349 \cdot 0.0700 \approx 0.00268445 \\
(w/o)_{^{64}Ni} &= 0.010080 \cdot 0.0700 \approx 0.00070563 \\
(w/o)_{^{54}Fe} &= 0.056456 \cdot 0.7385 \approx 0.04169245 \\
(w/o)_{^{56}Fe} &= 0.919015 \cdot 0.7385 \approx 0.67869279 \\
(w/o)_{^{57}Fe} &= 0.021604 \cdot 0.7385 \approx 0.01595432 \\
(w/o)_{^{58}Fe} &= 0.002925 \cdot 0.7385 \approx 0.00216044
\end{aligned}$$

Now, compute the “molecular mass” of the stainless steel:

$$M_{SS301} = \frac{1}{100}\begin{bmatrix} (0.15)\cdot(12.0107359) + (17.00)\cdot(51.9961318) + \\ (2.00)\cdot(54.9380439) + (7.00)\cdot(58.6933472) + \\ (73.85)\cdot(55.8451446) \end{bmatrix} \approx 55.0202806$$

The number or atom density can be calculated next:

$$N_{SS301} = \frac{\rho_{SS301}\cdot N_A}{M_{SS301}} = \frac{8.0272\cdot\left(6.02214129\times10^{23}\cdot 1\times10^{-24}\right)}{55.0202806} \approx 0.08786021\ \left(\text{atoms}/\text{barn-cm}\right)$$

Finally, the isotopic number density is computed (in atoms/b-cm):

$$N_{^{12}C} = 0.00679786 \cdot 0.08786021 \approx 0.00059726$$
$$N_{^{13}C} = 0.00007352 \cdot 0.08786021 \approx 0.00000646$$
$$N_{^{50}Cr} = 0.00781611 \cdot 0.08786021 \approx 0.00068672$$
$$N_{^{52}Cr} = 0.15072583 \cdot 0.08786021 \approx 0.01324280$$
$$N_{^{53}Cr} = 0.01709110 \cdot 0.08786021 \approx 0.00150163$$
$$N_{^{54}Cr} = 0.00425434 \cdot 0.08786021 \approx 0.00037379$$
$$N_{^{55}Mn} = 0.02002994 \cdot 0.08786021 \approx 0.00175983$$
$$N_{^{58}Ni} = 0.04467169 \cdot 0.08786021 \approx 0.00392486$$
$$N_{^{60}Ni} = 0.01720736 \cdot 0.08786021 \approx 0.00151184$$
$$N_{^{61}Ni} = 0.00074800 \cdot 0.08786021 \approx 0.00006572$$
$$N_{^{62}Ni} = 0.00238500 \cdot 0.08786021 \approx 0.00020955$$
$$N_{^{64}Ni} = 0.00060731 \cdot 0.08786021 \approx 0.00005336$$
$$N_{^{54}Fe} = 0.04252775 \cdot 0.08786021 \approx 0.00373650$$
$$N_{^{56}Fe} = 0.66759471 \cdot 0.08786021 \approx 0.05865501$$
$$N_{^{57}Fe} = 0.01541767 \cdot 0.08786021 \approx 0.00135460$$
$$N_{^{58}Fe} = 0.00205181 \cdot 0.08786021 \approx 0.00018027$$

The input and output of MatMCNP for stainless steel 301 is found in Appendix B. The verification data for stainless steel 301 calculated by MatMCNP is found in Table 252. All of the ratios are well within the accuracy needed for producing material cards for MCNP.

Table 252 – MatMCNP Verification of Stainless Steel 301

Isotope	Atom Fraction Ratio	Weight Fraction Ratio	Atom Density Ratio	Total Atom Density Ratio
^{12}C	0.99998	0.99975	0.99994	1.00000
^{13}C	0.99357	1.02214	0.99382	
^{50}Cr	1.00001	1.00004	1.00004	
^{52}Cr	1.00000	1.00000	1.00000	
^{53}Cr	1.00001	1.00001	1.00002	
^{54}Cr	1.00008	0.99993	0.99996	
^{55}Mn	1.00000	1.00000	1.00002	
^{58}Ni	0.99999	1.00001	1.00000	
^{60}Ni	1.00000	1.00000	1.00000	
^{61}Ni	0.99998	1.00002	1.00000	
^{62}Ni	0.99991	1.00020	0.99985	
^{64}Ni	0.99999	1.00001	0.99999	
^{54}Fe	1.00002	1.00001	1.00003	
^{56}Fe	0.99999	1.00042	1.00029	
^{57}Fe	1.00000	1.00017	1.00022	
^{58}Fe	1.00051	0.99947	0.99922	
The ratios are the "hand calculation" divided by the MatMCNP result.				

The stainless steel 301 was the only verification performed using materials described by weight percent. If additional verification data is desired, contact the author (krdepri@sandia.gov) for more cases that are described by weight fractions.

2.3. Enriched Materials

MatMCNP allows the specification of enriched materials for the special cases of lithium, boron, and uranium. While the user is allowed to specify the material in terms of atomic fractions, the enrichment must always be specified in terms of enriched weight percent.

2.3.1. Enriched ^{6}Li

Lithium is commonly used in thermoluminescent dosimeters (TLDs) to monitor radiation exposures to personnel using LiF. However, ^{6}Li is particularly sensitive to neutrons with a large thermal cross for an (n, α) reaction. Both the enriched ^{6}Li material and "depleted" material are used to estimate the proportion of personnel dose that is attributed to neutrons. As an example calculation, the MatMCNP output for 90% enriched ^{6}Li material is found in Table 253. Examination of the table and simple hand calculations will verify that MatMCNP accurately modifies the natural lithium description to produce the correct description for the enriched material.

Table 253 – MatMCNP Output for Lithium Enriched to 90 w/o ^{6}Li

```
C
C  Lithium Enriched to 90 w/o Li-6
C
C   Lithium from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     Li-6        7.59%             14.0868
C     Li-7       92.41%             14.9070
C
C   Atomic Weight:  6.94 g/mol
C         Density:  0.534 g/cc
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   Li-6        0.913025           0.900000          0.0481161
C   Li-7        0.086975           0.100000          0.0045836
C
C  The total compound atom density (atom/b-cm):  0.0526996
C
M3      03006.80c   0.913025
        03007.80c   0.086975
C
C  To convert a particle flux to rad[Material]
C  use FM  1.5809889E-09 3    -4  1 for neutrons
C   or FM  1.5809889E-09 3    -5 -6 for photons.
C
```

2.3.2. Enriched ^{10}B

Boron is commonly used as a neutron shielding material. The key neutron absorber is ^{10}B because of its large thermal cross for an (n, α) reaction. As an example calculation, the MatMCNP output for 75% enriched ^{10}B material is found in Table 254. Examination of the table and simple hand calculations will verify that MatMCNP accurately modifies the natural boron description to produce the correct description for the enriched material.

Table 254 – MatMCNP Output for Boron Enriched to 75 w/o ^{10}B

```
C
C  Boron Enriched to 75 w/o B-10
C
C   Boron from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     B-10        19.9%             12.0507
C     B-11        80.1%              8.6679
C
C   Atomic Weight:  10.81 g/mol
C         Density:  2.34 g/cc
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   B-10        0.767362           0.750000          0.1055520
C   B-11        0.232638           0.250000          0.0319998
C
C  The total compound atom density (atom/b-cm):  0.1375518
C
M5      05010.80c   0.767362
        05011.80c   0.232638
C
C  To convert a particle flux to rad[Material]
C  use FM  9.4170083E-10 5    -4  1 for neutrons
C   or FM  9.4170083E-10 5    -5 -6 for photons.
C
```

2.3.3. Enriched ^{235}U

Uranium is commonly used in nuclear engineering. The key isotope to examine is ^{235}U because it is tracked as fissile material for nuclear power and weapons. As an example calculation, the MatMCNP output for 50% enriched ^{235}U material is found in Table 255 (the input specified as the enriched uranium as 0.01% ^{234}U, 50% ^{235}U, and 49.99% ^{238}U). Examination of the table and simple hand calculations will verify that MatMCNP accurately modifies the natural uranium description to produce the correct description for the enriched material.

Table 255 – MatMCNP Output for Uranium Enriched to 50 w/o ^{235}U

```
C
C  Uranium Enriched to 50 w/o U-235
C
C   Uranium from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C    U-234          0.0054          38.1480
C    U-235          0.7204          40.9218
C    U-238         99.2742          47.3100
C
C   Atomic Weight:  238.02891 g/mol
C         Density:  19.1 g/cc
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  U-234        0.000101           0.000100          0.0000049
C  U-235        0.503177           0.500000          0.0244684
C  U-238        0.496722           0.499900          0.0241545
C
C  The total compound atom density (atom/b-cm):  0.0486278
C
M92     92234.80c   0.000101
        92235.80c   0.503177
        92238.80c   0.496722
C
C  To convert a particle flux to rad[Material]
C  use FM  4.0786239E-11 92   -4  1 for neutrons
C   or FM  4.0786239E-11 92   -5 -6 for photons.
C
```

3. USER GUIDE

3.1. Obtaining MatMCNP

Obtaining the MatMCNP program can be done by performing a “git clone” operation. If you are at Sandia National Laboratories and you have git installed on your machine, you can perform these commands from a command prompt (terminal or DOS command window) to obtain a full development git repository of the MatMCNP program. (*NOTE: All lines below that start with “#” are comments. The example script below assumes the user has access to the SNL weed server.*)

```
#
#Create a working space for the program
#
Cmd prompt> mkdir mcnpmaterials
#
#
#Change directory to the working space
#
Cmd prompt> cd mcnpmaterials
#
#
#Perform the git clone operation
#
Cmd prompt> git clone ssh://weed.sandia.gov/export/git/N-codes/MatMCNP.git
#
#Now, you have a full repository in a directory called MatMCNP located
# at /../mcnpmaterials/MatMCNP
#
```

3.2. Installing MatMCNP

Within the git repository for MatMCNP, there is a bin subdirectory. The bin directory contains both a Linux executable (xmatmcnp) and a Windows executable (MatMCNP.exe). In most cases, these files will be suitable for use on your machine. However, we have included the option of building your own executable from the Fortran 90 source files. The following sections will outline how to build the code using the provided tools. The Linux build requires a Fortran 90 compatible compiler and a version of perl built on the system.

3.2.1. Building a Linux Version

In order to build the Linux version, we have included a simple perl script to compile the program using the native Fortran 90 (this build assumes compiler is aliased to “f90”) compiler on a Linux system. The MatMCNP program is simple enough that a Makefile to build it seemed like overkill. We can include conversion to a Makefile system for building if there is a request for it. Here are the steps to build MatMCNP:

```
#
#The next two steps assume that you have perl and an f90 compiler
# available to you on the Linux machine.
#
#Change to the Fortran source directory
#
Linux prompt> cd /../mcnpmaterials/MatMCNP/source
#
#Compile MatMCNP using the perl script
#
Linux prompt> ./compile-MatMCNP.pl
#
#Now, you should have an executable called "xmatmcnp" located in the
# /../mcnpmaterials/MatMCNP/bin directory
#
```

3.3. Running MatMCNP

3.3.1. Linux

In the Linux environment, the MatMCNP program uses a C shell (csh) and a perl script as wrappers to run input files and change the name of the output files. The perl script requires that a version of perl be installed on the machine. The C shell (MatMCNP) and perl script (matmcnp.pl) are located in the main directory while the executable (xmatmcnp) is located in the bin subdirectory (see above sections for more detail). Input files (described below) should be saved in the main directory as filename.inp where filename is chosen by the user. The following command line illustration demonstrates running MatMCNP on a Linux machine:

```
#
#Run MatMCNP from the main directory /../mcnpmaterials/MatMCNP/
#
Linux prompt> MatMCNP filename
#
```

The wrapper scripts associated with the MatMCNP program will copy filename.inp to matmcnp.inp (the default input file for MatMCNP), execute the MatMCNP program, and move the default output file (matmcnp.out) to filename.out. The output file produced by the wrapper scripts (filename.out) can be opened with any ASCII text editor.

3.3.2 Windows

In the Windows environment, the MatMCNP program uses a DOS batch file and a perl script as wrappers to run input files and change the name of the output files. The perl script requires that a version of perl be installed on the machine (we tend to install ActivePerl, http://www.activestate.com/, on our machines at SNL). The batch files (MatMCNP.bat) and perl script (matmcnp-PC.pl) are located in the main directory while the executable (MatMCNP.exe) is located in the bin subdirectory (see above sections for more detail). As with the Linux installation, input files (described below) should be saved in the main directory as filename.inp where filename is chosen by the user. The following command line illustration demonstrates running MatMCNP on a Windows machine:

```
#
#Run MatMCNP from the main directory \..\mcnpmaterials\MatMCNP\
#
Windows prompt> MatMCNP filename
#
```

The wrapper scripts associated with the MatMCNP program will copy filename.inp to matmcnp.inp (the default input file for MatMCNP), execute the MatMCNP program, and move the default output file (matmcnp.out) to filename.out. The output file produced by the wrapper scripts (filename.out) can be opened with any ASCII text editor.

3.4. MatMCNP Input Format

The MatMCNP input file is a simple ASCII text file that provides the program with the needed information. The program does not have an interactive mode, so all the information must be supplied through the input file (matmcnp.inp is the default name of the input file if you choose to run the program without the wrapper scripts). The following sections detail the information that must be present in a MatMCNP input file.

3.4.1. Title

The first line of the input file is the title of the compound or mixture that will be calculated. The title will be printed at the top of the output file to help with identification. The title can be a maximum of 65 characters. Title lengths greater than 65 characters are truncated.

3.4.2. Comment Cards

The second line of the input deck displays the number of comment cards that are present. The user provides information he or she wants displayed in the output file. Since this information will help the user identify the compound, it should include important information such as the density of the mixture, whether atom or weight fractions are being used in the element information, and whether the natural or enriched abundances are being used. Each comment line has a maximum length of 72 characters. Comment card lengths greater than 72 characters are truncated.

3.4.3. Density

The density of the mixture or compound follows the comment cards. The density should be provided in g/cm^3.

3.4.4. Fraction Type

Following the density of the compound, the user decides whether the mixture will be specified in atom fraction ("atomic") or weight fraction ("weight"). This specification allows MatMCNP to calculate the atom and weight fractions properly. This is a fixed format read that will eventually be modified to allow for more freedom. At this time, you must specify "atomic" or "weight" in all lower case in the first six characters of this input line. The input is case sensitive, but only reads the first six characters.

3.4.5. Number of Elements

The number of elements in the mixture or compound follows the fraction type. At present, MatMCNP allows a maximum of 92 elements in the mixture. However, it does not allow for transuranic elements (Z > 92) even if the total number of elements is less than or equal to 92.

3.4.6. Element Information

The description of each of the elements in the compound or mixture follows the number of elements entry. There are three parts to the elemental information. First, the user specifies whether that element uses natural isotopic abundances or is an enriched material ("nat" or "enr"). Again, the user should use all lowercase for this specification. Second, the user enters the atomic number or Z of the element. Uranium (Z = 92) is the heaviest allowed element. In addition, the artificial or short-lived naturally occurring elements in Table 256 are not allowed. The final piece of information about the element is the atomic or weight fraction (depending on the fraction type set) for the specified element in the mixture.

Table 256 – Artificial or Short-Lived Naturally Occurring Elements

Element	Z
Technetium	42
Promethium	61
Polonium	84
Astatine	85
Radon	86
Francium	87
Radium	88
Actinium	89
Protactinium	91

3.4.7. MCNP Material Number

The MCNP material number follows the elemental information. The MCNP material number can range from 1 to 99999 and is formatted in the output to go directly into an MCNP input file. The program is reading the material number as a character string, so numbers greater than 99999 are truncated to five characters.

3.4.8. Example Input

The elemental information for an enriched material requires additional information (see below). In order to visualize a MatMCNP input file with natural isotopic abundances, we labeled the various parts of the input file example in Table 257.

Table 257 – Input Example with Natural Isotopic Abundances

```
Boron Nitride
8
*1
*2 There are 8 comment cards for this input deck.
*3 The atom fraction of boron nitride (BN) is used
*4 The natural abundances are used for each element
*5 The density of BN is 2.142 g/cc
*6 The MCNP material (100) is found after the material.
*7 The line below "*8" gives the density
*8
2.142
atomic
2
nat 5  0.5
nat 7  0.5
100
```

Title

Number of Comments

Density

Atom fraction will be input

Number of Elements

Element Information

MCNP Material Number

3.4.9. Enriched Isotopes

Currently, MatMCNP allows the user to specify enriched isotopic abundances for just three materials: Lithium, Boron, and Uranium. If one (or more) of the elements in the mixture has enriched isotopes, the input must still contain all of the element information ("enr", Z, and atomic or weight fraction). If an element is enriched, then the isotopic information must be supplied on the next lines of the input. The isotopic information takes the form of the mass number and the weight fraction. MatMCNP replaces the pre-calculated weight percent with the user specified amount. The user must supply the weight fraction for each of the naturally occurring isotopes of the element. Each isotope is placed on an individual line. Table 258 shows an input example for a compound with enriched lithium (increase in ^{6}Li) material, Table 259 displays an input example for a compound with boron enrichment (increase in ^{10}B), and Table 260 shows an example with an enriched uranium (^{235}U at 20 weight percent) material.

Table 258 – Input Example with Enriched Lithium Isotopes

```
Lithium Fluoride
7
*1
*2 There are 7 comment cards for this input deck.
*3 The atom fraction of lithium fluoride (LiF) is used
*4 Lithium is enriched to 90 w/o Li-6
*5 The density of LiF is 2.64 g/cc
*6 The MCNP material (100) is found after the material.
*7
2.64
atomic
2
enr 3  0.5
  6    0.90
  7    0.10
nat 9  0.5
100
```

Title

Number of Comments

Density

Atom fraction will be input

Number of Elements

Enrichment Information

MCNP Material Number

Table 259 – Input Example with Enriched Boron Isotopes

```
Boron Carbide (B4C)
6

 The weight fraction of boron carbide (B4C) is used
 Boron is enriched to 75 w/o B-10
 The density of B4C is 2.48 g/cc
 The MCNP material (999) is found after the material.

2.48
atomic
2
enr 5  0.8
  10    0.75
  11    0.25
nat 6  0.2
999
```

Atom fraction will be input

Enrichment Information

Table 260 – Input Example with Enriched Uranium Isotopes

```
U-10Moly 20 w/o LEU
2
   This is 20 w/o U-235 alloyed with 10 w/o Molybdenum.
   The density of U-10Moly is 17.08 g/cc.
17.08
weight
2
nat  42  0.1
enr  92  0.90
  234   0.0
  235   0.20
  238   0.80
100
```

Weight fraction will be input

Enrichment Information

3.5. Output File from MatMCNP

The output file from MatMCNP displays all the information that the program calculates for the user. The program prints the title of the compound, the comment cards, and, in a table format, each isotope in the compound with its atom fraction, weight fraction, and atom density in atoms/b-cm. The output file also contains the atom density for the entire compound, the MCNP material number, and the information needed to create material cards for MCNP input decks. This information contains the ZAID and atom fraction for each isotope.

There are some elements that are still problematic from a cross section data perspective (see Table 261). There are a few that do not have a ZAID (or MCNP material identifier) while some use an elemental or natural material identifier. If the user selects one of these elements, MatMCNP provides a warning in the output file. A list of all the isotopes contained in the Nuclear Wallet Card database within MatMCNP and their MCNP material identifier (ZAID) can be found in Appendix C.

Table 261 – Problematic Elements for Cross Section Data

Elemental zaid Utilized	No MCNP Cross Section Data
Carbon	Neon (Cross Section for Ne-20 exists)
	Osmium
Platinum	Ytterbium

Table 262 shows an example output from a MatMCNP calculation. The table shows that MatMCNP alerts the user that the specified material contains an element that often must have a thermal scattering cross section [S(α, β)] material modifier to calculate the neutron transport correctly. However, MatMCNP does not supply the S(α, β) card because that is specific to the MCNP calculation that will use the material card.

Table 262 – Output Example from MatMCNP Calculation

```
C
C  Boron Carbide (B4C)
C   6 Comment Cards
C
C
C   The weight fraction of boron carbide (B4C) is used
C   Boron is enriched to 75 w/o B-10
C   The density of B4C is 2.48 g/cc
C   The MCNP material (999) is found after the material.
C
C
C   Summary of MatMCNP Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   C-12       0.1978600          0.2240362          0.0278830
C   C-13       0.0021400          0.0026257          0.0003016
C   B-10       0.6138896          0.5800036          0.0865110
C   B-11       0.1861104          0.1933345          0.0262272
C
C  The total compound atom density (atom/b-cm):  0.14092277
C
C  This material contains an isotope that is often
C  modified by an S(alpha,beta).  Check MCNP
C  Manual Appendix G to see if an
C  S(alpha,beta) is required.
C
C  MCNP Material 999
C
M999    06000.80c  0.2000000
        05010.80c  0.6138896
        05011.80c  0.1861104
C
C  Caution: The natural zaid is used for Carbon.
C
C  If the natural zaid is used for any element, the atom fractions of each isotope
C  of that element are added together and listed with the natural zaid just once.
C
C  To convert a particle flux to rad[Material]
C  use FM  9.10555020E-10 999  -4 1 for neutrons
C   or FM  9.10555020E-10 999  -5 -6 for photons.
```

4. SUMMARY

A code for generating MCNP material cards (MatMCNP) has been written and verified for naturally occurring, stable isotopes. The program allows for material specification as either atomic or weight percent (fractions). MatMCNP also permits the specification of enriched lithium, boron, and/or uranium. In addition to producing the material cards for MCNP, the code calculates the atomic (or number) density in atoms/barn-cm and calculates the multiplier that should be used to convert neutron and gamma fluences to kerma (or dose under certain conditions) in the material. Questions about the MatMCNP code should be directed to K. Russell DePriest (krdepri@sandia.gov).

5. REFERENCES

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5. Brian D. Hehr. Private communication, 2014.

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APPENDIX A: ARTIFICIAL DENSE GAS VERIFICATION

Hydrogen

Table 263 – Artificially Dense Hydrogen Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{1}H	0.999885	7.2889	1.007824956	0.999770	0.5974006
^{2}H	0.000115	13.1357	2.014101755	0.000230	0.0000687
Density (g/cm^3) = 1.0			FM Conversion = 9.5714664E-09		
Total Atomic Density (atoms/b-cm) = 0.5974694					

Table 264 – MatMCNP Output for Artificially Dense Hydrogen

```
C
C  Hydrogen
C
C   Hydrogen from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     H-1        99.9885%            7.289
C     H-2         0.0115%           13.136
C
C   Atomic Weight:  1.008 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   H-1         0.999885           0.999770          0.5974011
C   H-2         0.000115           0.000230          0.0000687
C
C  The total compound atom density (atom/b-cm):  0.5974698
C
C
C  This material contains an isotope that is often modified by
C  an S(alpha,beta). Check MCNP Manual Appendix G to see if an
C  S(alpha,beta) card (i.e., an MTn card) is required.
C
M1      01001.80c   0.999885
        01002.80c   0.000115
C
C  To convert a particle flux to rad[Material]
C  use FM  9.5714681E-09 1    -4  1 for neutrons
C   or FM  9.5714681E-09 1    -5 -6 for photons.
C
```

Table 265 – Difference between NWC and MatMCNP for Artificially Dense Hydrogen

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{1}H	0.000%	0.000%	0.000%	0.000%	0.000%
^{2}H	0.000%	0.088%	-0.013%		

Helium

Table 266 – Artificially Dense Helium Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{3}He	0.00000134	14.9312	3.016029303	0.000001	0.0000002
^{4}He	0.99999866	2.4249	4.002603237	0.999999	0.1504553
Density (g/cm^3) = 1.0			FM Conversion = 2.4102997E-09		
Total Atomic Density (atoms/b-cm) = 0.1504555					

Table 267 – MatMCNP Output for Elemental Artificially Dense Helium (Excerpt)

```
C
C  Helium
C
C   Helium from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     He-3        0.000134%         14.9312
C     He-4       99.999866%          2.4249
C
C   Atomic Weight:  4.002602 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   He-3        0.000001           0.000001          0.0000002
C   He-4        0.999999           0.999999          0.1504555
C
C  The total compound atom density (atom/b-cm):  0.1504557
C
M2      02003.80c   0.000001
        02004.80c   0.999999
C
C  To convert a particle flux to rad[Material]
C  use FM  2.4103000E-09 2    -4  1 for neutrons
C   or FM  2.4103000E-09 2    -5 -6 for photons.
C
```

Table 268 – Difference between NWC and MatMCNP for Artificially Dense Helium

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{3}He	-25.373%	-0.962%	-0.799%	0.000%	0.000%
^{4}He	0.000%	0.088%	0.000%		

Nitrogen

Table 269 – Artificially Dense Nitrogen Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{14}N	0.9963600	2.8634	14.00307399	0.996102	0.0428382
^{15}N	0.0036400	0.1014	15.00010886	0.003898	0.0001565
Density (g/cm^3) = 1.0				FM Conversion = 6.8877524E-10	
Total Atomic Density (atoms/b-cm) = 0.0429947					

Table 270 – MatMCNP Output for Artificially Dense Nitrogen

```
C
C  Nitrogen
C
C   Nitrogen from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     N-14        99.636%            2.8634
C     N-15         0.364%            0.1014
C
C   Atomic Weight:  14.007 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   N-14        0.996360           0.996102          0.0428382
C   N-15        0.003640           0.003898          0.0001565
C
C  The total compound atom density (atom/b-cm):  0.0429947
C
M7      07014.80c   0.996360
        07015.80c   0.003640
C
C  To convert a particle flux to rad[Material]
C  use FM  6.8877531E-10 7    -4  1 for neutrons
C   or FM  6.8877531E-10 7    -5 -6 for photons.
C
```

Table 271 – Difference between NWC and MatMCNP for Artificially Dense Nitrogen

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{14}N	0.000%	0.000%	0.000%	0.000%	0.000%
^{15}N	0.000%	-0.004%	0.000%		

Oxygen

Table 272 – Artificially Dense Oxygen Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{16}O	0.9975700	-4.7370	15.99491462	0.997290	0.0375483
^{17}O	0.0003800	-0.8087	16.99913182	0.000404	0.0000143
^{18}O	0.0020500	-0.7828	17.99915963	0.002306	0.0000772
Density (g/cm^3) = 1.0			FM Conversion = 6.0298932E-10		
Total Atomic Density (atoms/b-cm) = 0.0376398					

Table 273 – MatMCNP Output for Artificially Dense Oxygen

```
C
C  Oxygen
C
C   Oxygen from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     O-16         99.757%          -4.7370
C     O-17          0.038%          -0.8087
C     O-18          0.205%          -0.7828
C
C   Atomic Weight:  15.999 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   O-16        0.997570           0.997290          0.0375483
C   O-17        0.000380           0.000404          0.0000143
C   O-18        0.002050           0.002306          0.0000772
C
C  The total compound atom density (atom/b-cm):  0.0376398
C
C
C  This material contains an isotope that is often modified by
C  an S(alpha,beta). Check MCNP Manual Appendix G to see if an
C  S(alpha,beta) card (i.e., an MTn card) is required.
C
M8      08016.80c   0.997570
        08017.80c   0.000380
        08016.80c   0.002050
C
C  Caution: The O-18 has been set to O-16.
C
C  To convert a particle flux to rad[Material]
C  use FM  6.0298933E-10 8    -4  1 for neutrons
C   or FM  6.0298933E-10 8    -5 -6 for photons.
C
```

Table 274 – Difference between NWC and MatMCNP for Artificially Dense Oxygen

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{16}O	0.000%	0.000%	0.000%	0.000%	0.000%
^{17}O	0.000%	0.063%	-0.022%		
^{18}O	0.000%	-0.010%	0.050%		

Neon

Table 275 – Artificially Dense Neon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{20}Ne	0.9048000	-7.0419	19.99244021	0.896388	0.0000243
^{21}Ne	0.0027000	-5.7317	20.99384677	0.002809	0.0000001
^{22}Ne	0.0925000	-8.0247	21.99138513	0.100803	0.0000025
Density (g/cm^3) = 1.0				FM Conversion = 4.7806978E-10	
Total Atomic Density (atoms/b-cm) = 0.0298420					

Table 276 – MatMCNP Output for Artificially Dense Neon

```
C
C  Neon
C
C   Neon from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     Ne-20        90.48%           -7.0419
C     Ne-21         0.27%           -5.7317
C     Ne-22         9.25%           -8.0247
C
C   Atomic Weight:  20.1797 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ne-20        0.904800           0.896388          0.0270011
C  Ne-21        0.002700           0.002809          0.0000806
C  Ne-22        0.092500           0.100803          0.0027604
C
C  The total compound atom density (atom/b-cm):  0.0298421
C
C
C  One or more of the elements in the compound does not have a cross-section
C  and therefore the MCNP Card will not be created.
```

Table 277 – Difference between NWC and MatMCNP for Artificially Dense Neon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{20}Ne	0.000%	0.000%	0.000%	0.000%	Not computed by MatMCNP
^{21}Ne	0.000%	0.004%	0.033%		
^{22}Ne	0.000%	0.000%	0.000%		

Argon

Table 278 – Artificially Dense Argon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{36}Ar	0.0033360	-30.2315	35.96754515	0.003004	0.0000503
^{38}Ar	0.0006290	-34.7147	37.96273223	0.000598	0.0000095
^{40}Ar	0.9960350	-35.0398	39.96238323	0.996399	0.0150152
Density (g/cm^3) = 0.0150750				FM Conversion = 2.4150193E-10	
Total Atomic Density (atoms/b-cm) = 0.0000269					

Table 279 – MatMCNP Output for Artificially Dense Argon

```
C
C  Argon
C
C   Argon from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     Ar-36        0.3336%          -30.2315
C     Ar-38        0.0629%          -34.7147
C     Ar-40       99.6035%          -35.0398
C
C   Atomic Weight:  39.948 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ar-36        0.003336           0.003004          0.0000503
C  Ar-38        0.000629           0.000598          0.0000095
C  Ar-40        0.996035           0.996399          0.0150153
C
C  The total compound atom density (atom/b-cm):  0.0150750
C
M18      18036.80c   0.003336
         18038.80c   0.000629
         18040.80c   0.996035
C
C  To convert a particle flux to rad[Material]
C  use FM  2.4150193E-10 18   -4  1 for neutrons
C   or FM  2.4150193E-10 18   -5 -6 for photons.
C
```

Table 280 – Difference between NWC and MatMCNP for Artificially Dense Argon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{36}Ar	0.000%	0.013%	0.019%	0.000%	0.000%
^{38}Ar	0.000%	0.043%	0.188%		
^{40}Ar	0.000%	0.000%	0.000%		

Krypton

Table 281 – Artificially Dense Krypton Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{78}Kr	0.0035500	-74.1795	77.92036503	0.003301	0.0000255
^{80}Kr	0.0228600	-77.8925	79.91637896	0.021801	0.0001643
^{82}Kr	0.1159300	-80.5902	81.91348286	0.113323	0.0008331
^{83}Kr	0.1150000	-79.9900	82.91412720	0.113787	0.0008264
^{84}Kr	0.5698700	-82.4393	83.91149777	0.570642	0.0040954
^{86}Kr	0.1727900	-83.2656	85.91061070	0.177146	0.0012418
Density (g/cm^3) = 1.0				FM Conversion = 1.1512769E-10	
Total Atomic Density (atoms/b-cm) = 0.0071865					

Table 282 – MatMCNP Output for Artificially Dense Krypton

```
C  Krypton
C
C   Krypton from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C     Kr-78         0.355          -74.1795
C     Kr-80         2.286          -77.8925
C     Kr-82        11.593          -80.5902
C     Kr-83        11.500          -79.9900
C     Kr-84        56.987          -82.4393
C     Kr-86        17.279          -83.2656
C
C   Atomic Weight:  83.798 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Kr-78        0.003550           0.003301          0.0000255
C  Kr-80        0.022860           0.021801          0.0001643
C  Kr-82        0.115930           0.113323          0.0008331
C  Kr-83        0.115000           0.113787          0.0008264
C  Kr-84        0.569870           0.570642          0.0040954
C  Kr-86        0.172790           0.177146          0.0012418
C
C  The total compound atom density (atom/b-cm):  0.0071865
C
M36     36078.80c   0.003550
        36080.80c   0.022860
        36082.80c   0.115930
        36083.80c   0.115000
        36084.80c   0.569870
        36086.80c   0.172790
C  To convert a particle flux to rad[Material]
C  use FM  1.1512771E-10 36   -4  1 for neutrons
C   or FM  1.1512771E-10 36   -5 -6 for photons.
```

Table 283 – Difference between NWC and MatMCNP for Artificially Dense Krypton

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{78}Kr	0.000%	0.000%	-0.047%	0.000%	0.000%
^{80}Kr	0.000%	0.000%	0.010%		
^{82}Kr	0.000%	0.000%	-0.004%		
^{83}Kr	0.000%	0.000%	-0.006%		
^{84}Kr	0.000%	0.000%	0.001%		
^{86}Kr	0.000%	0.000%	0.004%		

Xenon

Table 284 – Artificially Dense Xenon Data from NWC and Excel

Isotope	Atomic Fraction	Δ (MeV)	Isotopic Mass (u)	Weight Fraction	Atom Density (atom/barn-cm)
^{124}Xe	0.0009520	-87.6612	123.9058918	0.000898	0.0000044
^{126}Xe	0.0008900	-89.1462	125.9042976	0.000853	0.0000041
^{128}Xe	0.0191021	-89.8602	127.9035311	0.018609	0.0000876
^{129}Xe	0.2640071	-88.6960	128.9047809	0.259205	0.0012109
^{130}Xe	0.0407102	-89.8804	129.9035094	0.040279	0.0001867
^{131}Xe	0.2123208	-88.4136	130.9050841	0.211694	0.0009739
^{132}Xe	0.2690871	-89.2789	131.9041552	0.270340	0.0012342
^{134}Xe	0.1043574	-88.1245	133.9053945	0.106434	0.0004787
^{136}Xe	0.0885734	-86.4291	135.9072145	0.091686	0.0004063
Density (g/cm^3) = 1.0				FM Conversion = 7.3480595E-11	
Total Atomic Density (atoms/b-cm) = 0.0045868					

Table 285 – MatMCNP Output for Artificially Dense Xenon (Excerpt)

```
C  Xenon
C
C   Xenon from Nuclear Wallet Cards - Electronic Version
C    Isotope   atomic abundance    delta (MeV)
C    Xe-124        0.0952          -87.6612
C    Xe-126        0.0890          -89.1462
C    Xe-128        1.9102          -89.8602
C    Xe-129       26.4006          -88.6960
C    Xe-130        4.0710          -89.8804
C    Xe-131       21.232           -88.4136
C    Xe-132       26.9086          -89.2789
C    Xe-134       10.4357          -88.1245
C    Xe-136        8.8573          -86.4291
C
C   Atomic Weight:  131.293 g/mol
C         Density:  1.0 g/cc (artificially high)
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Xe-124       0.000952           0.000898          0.0000044
C  Xe-126       0.000890           0.000853          0.0000041
C  Xe-128       0.019102           0.018609          0.0000876
C  Xe-129       0.264007           0.259205          0.0012109
C  Xe-130       0.040710           0.040279          0.0001867
C  Xe-131       0.212321           0.211694          0.0009739
C  Xe-132       0.269087           0.270340          0.0012342
C  Xe-134       0.104357           0.106434          0.0004787
C  Xe-136       0.088573           0.091686          0.0004063
C
C  The total compound atom density (atom/b-cm):  0.0045868
C
M54     54124.80c   0.000952
        54126.80c   0.000890
        54128.80c   0.019102
        54129.80c   0.264007
        54130.80c   0.040710
        54131.80c   0.212321
        54132.80c   0.269087
        54134.80c   0.104357
        54136.80c   0.088573
C  To convert a particle flux to rad[Material]
C  use FM  7.3480604E-11 54   -4  1 for neutrons
C   or FM  7.3480604E-11 54   -5 -6 for photons.
```

Table 286 – Difference between NWC and MatMCNP for Artificially Dense Xenon

Isotope	Atom Fraction (% Difference)	Weight Fraction (% Difference)	Atom Density (% Difference)	Total Atom Density (% Difference)	FM Value (% Difference)
^{124}Xe	0.000%	-0.049%	0.764%	0.000%	0.000%
^{126}Xe	0.000%	-0.056%	0.434%		
^{128}Xe	0.000%	0.000%	-0.020%		
^{129}Xe	0.000%	0.000%	-0.004%		
^{130}Xe	0.000%	-0.001%	-0.016%		
^{131}Xe	0.000%	0.000%	0.003%		
^{132}Xe	0.000%	0.000%	-0.004%		
^{134}Xe	0.000%	0.000%	0.007%		
^{136}Xe	0.000%	0.000%	0.008%		

APPENDIX B: EXAMPLE INPUT/OUTPUT

Water

Input

```
Water
3
H2O at a density of 1 g/cm3
- Chemical formula (atom fraction) used
- MatMCNP will normalize to 1.0
1.0
atomic
2
nat  1   2.0
nat  8   1.0
100
```

Output

```
C
C  Water
C
C  H2O at a density of 1 g/cm3
C  - Chemical formula (atom fraction) used
C  - MatMCNP will normalize to 1.0
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   H-1         0.666590           0.111873          0.0668482
C   H-2         0.000077           0.000026          0.0000077
C   O-16        0.332523           0.885695          0.0333467
C   O-17        0.000127           0.000359          0.0000127
C   O-18        0.000683           0.002048          0.0000685
C
C  The total compound atom density (atom/b-cm):  0.1002839
C
C
C  This material contains an isotope that is often modified by
C  an S(alpha,beta). Check MCNP Manual Appendix G to see if an
C  S(alpha,beta) card (i.e., an MTn card) is required.
C
M100    01001.80c   0.666590
        01002.80c   0.000077
        08016.80c   0.332523
        08017.80c   0.000127
        08016.80c   0.000683
C
C  Caution: The O-18 has been set to O-16.
C
C  To convert a particle flux to rad[Material]
C  use FM  1.6065476E-09 100  -4  1 for neutrons
C   or FM  1.6065476E-09 100  -5 -6 for photons.
C
```

Gallium Arsenide

Input

```
GaAs
1
Gallium Arsenide @ 5.32 g/cm3 (per email from B. D. Hehr)
5.32
atomic
2
nat  31  0.5
nat  33  0.5
5
```

Output

```
C
C  GaAs
C
C  Gallium Arsenide @ 5.32 g/cm3 (per email from B. D. Hehr)
C
C   Summary of MatMCNP (Version 2.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C  Ga-69       0.3005400          0.2864246          0.0133135
C  Ga-71       0.1994600          0.1956054          0.0088358
C  As-75       0.5000000          0.5179700          0.0221493
C
C  The total compound atom density (atom/b-cm):  0.04429858
M5      31069.80c  0.3005400
        31071.80c  0.1994600
        33075.80c  0.5000000
C
C  To convert a particle flux to rad[Material]
C  use FM  1.33403399E-10 5    -4  1 for neutrons
C   or FM  1.33403399E-10 5    -5 -6 for photons.
C
```

Stainless Steel 301

Input

```
SS301
11
Stainless Steel 301
- Specs taken from Comet Metals Stainless Steel Alloy Guide
- Composition is provided in w/o
- Density 0.290 lb/in**3 -> 8.0272 g/cm**3

Element   Weight Percent
  C            0.15
  Cr          17.00
  Ni           7.00
  Mn           2.00 MAX [Use max value for composition]
  Fe          73.85 [Computed as the remainder]
8.0272
weight
5
nat 6   0.15
nat 24 17.00
```

```
nat 25  2.00
nat 26 73.85
nat 28  7.00
301
```

Output

```
C
C  SS301
C
C  Stainless Steel 301
C  - Specs taken from Comet Metals Stainless Steel Alloy Guide
C  - Composition is provided in w/o
C  - Density 0.290 lb/in**3 -> 8.0272 g/cm**3
C
C  Element   Weight Percent
C    C            0.15
C    Cr          17.00
C    Ni           7.00
C    Mn           2.00 MAX [Use max value for composition]
C    Fe          73.85 [Computed as the remainder]
C
C   Summary of MatMCNP (Version 3.0) Calculations:
C
C  Isotope  Number Fraction    Weight Fraction       Atoms/b-cm
C   C-12        0.006798           0.001483         0.0005973
C   C-13        0.000074           0.000017         0.0000065
C  Cr-50        0.007816           0.007095         0.0006867
C  Cr-52        0.150726           0.142289         0.0132428
C  Cr-53        0.017091           0.016445         0.0015016
C  Cr-54        0.004254           0.004171         0.0003738
C  Mn-55        0.020030           0.020000         0.0017598
C  Fe-54        0.042528           0.041692         0.0037365
C  Fe-56        0.667595           0.678693         0.0586550
C  Fe-57        0.015418           0.015954         0.0013546
C  Fe-58        0.002052           0.002160         0.0001803
C  Ni-58        0.044672           0.047038         0.0039249
C  Ni-60        0.017207           0.018743         0.0015118
C  Ni-61        0.000748           0.000828         0.0000657
C  Ni-62        0.002385           0.002684         0.0002095
C  Ni-64        0.000607           0.000706         0.0000534
C
C  The total compound atom density (atom/b-cm):  0.0878602
C
C
C  This material contains an isotope that is often modified by
C  an S(alpha,beta). Check MCNP Manual Appendix G to see if an
C  S(alpha,beta) card (i.e., an MTn card) is required.
C
M301    06000.80c   0.006871
        24050.80c   0.007816
        24052.80c   0.150726
        24053.80c   0.017091
        24054.80c   0.004254
        25055.80c   0.020030
        26054.80c   0.042528
        26056.80c   0.667595
        26057.80c   0.015418
        26058.80c   0.002052
        28058.80c   0.044672
        28060.80c   0.017207
        28061.80c   0.000748
        28062.80c   0.002385
```

```
        28064.80c   0.000607
C
C  Caution: The natural zaid is used for Carbon.
C
C  To convert a particle flux to rad[Material]
C  use FM  1.7534393E-10 301  -4  1 for neutrons
C   or FM  1.7534393E-10 301  -5 -6 for photons.
C
```

APPENDIX C: MATMCNP CROSS SECTION SPECIFICATIONS

Isotope	MatMCNP ZAID	Isotope	MatMCNP ZAID
H-1	1001.80c	Ca-42	20042.80c
H-2	1002.80c	Ca-43	20043.80c
He-3	2003.80c	Ca-44	20044.80c
He-4	2004.80c	Ca-46	20046.80c
Li-6	3006.80c	Ca-48	20048.80c
Li-7	3007.80c	Sc-45	21045.80c
Be-9	4009.80c	Ti-46	22046.80c
B-10	5010.80c	Ti-47	22047.80c
B-11	5011.80c	Ti-48	22048.80c
C-12	6000.80c	Ti-49	22049.80c
C-13	6000.80c	Ti-50	22050.80c
N-14	7014.80c	V-50	23050.80c
N-15	7015.80c	V-51	23051.80c
O-16	8016.80c	Cr-50	24050.80c
O-17	8017.80c	Cr-52	24052.80c
O-18	8016.80c	Cr-53	24053.80c
F-19	9019.80c	Cr-54	24054.80c
Ne-20	10020.42c	Mn-55	25055.80c
Ne-21	---	Fe-54	26054.80c
Ne-22	---	Fe-56	26056.80c
Na-23	11023.80c	Fe-57	26057.80c
Mg-24	12024.80c	Fe-58	26058.80c
Mg-25	12025.80c	Co-59	27059.80c
Mg-26	12026.80c	Ni-58	28058.80c
Al-27	13027.80c	Ni-60	28060.80c
Si-28	14028.80c	Ni-61	28061.80c
Si-29	14029.80c	Ni-62	28062.80c
Si-30	14030.80c	Ni-64	28064.80c
P-31	15031.80c	Cu-63	29063.80c
S-32	16032.80c	Cu-65	29065.80c
S-33	16033.80c	Zn-64	30064.80c
S-34	16034.80c	Zn-66	30066.80c
S-36	16036.80c	Zn-67	30067.80c
Cl-35	17035.80c	Zn-68	30068.80c
Cl-37	17037.80c	Zn-70	30070.80c
Ar-36	18036.80c	Ga-69	31069.80c
Ar-38	18038.80c	Ga-71	31071.80c
Ar-40	18040.80c	Ge-70	32070.80c
K-39	19039.80c	Ge-72	32072.80c
K-40	19040.80c	Ge-73	32073.80c
K-41	19041.80c	Ge-74	32074.80c
Ca-40	20040.80c	Ge-76	32076.80c

Isotope	MatMCNP ZAID	Isotope	MatMCNP ZAID
As-75	33075.80c	Pd-104	46104.80c
Se-74	34074.80c	Pd-105	46105.80c
Se-76	34076.80c	Pd-106	46106.80c
Se-77	34077.80c	Pd-108	46108.80c
Se-78	34078.80c	Pd-110	46110.80c
Se-80	34080.80c	Ag-107	47107.80c
Se-82	34082.80c	Ag-109	47109.80c
Br-79	35079.80c	Cd-106	48106.80c
Br-81	35081.80c	Cd-108	48108.80c
Kr-78	36078.80c	Cd-110	48110.80c
Kr-80	36080.80c	Cd-111	48111.80c
Kr-82	36082.80c	Cd-112	48112.80c
Kr-83	36083.80c	Cd-113	48113.80c
Kr-84	36084.80c	Cd-114	48114.80c
Kr-86	36086.80c	Cd-116	48116.80c
Rb-85	37085.80c	In-113	49113.80c
Rb-87	37087.80c	In-115	49115.80c
Sr-84	38084.80c	Sn-112	50112.80c
Sr-86	38086.80c	Sn-114	50114.80c
Sr-87	38087.80c	Sn-115	50115.80c
Sr-88	38088.80c	Sn-116	50116.80c
Y-89	39089.80c	Sn-117	50117.80c
Zr-90	40090.80c	Sn-118	50118.80c
Zr-91	40091.80c	Sn-119	50119.80c
Zr-92	40092.80c	Sn-120	50120.80c
Zr-94	40094.80c	Sn-122	50122.80c
Zr-96	40096.80c	Sn-124	50124.80c
Nb-93	41093.80c	Sb-121	51121.80c
Mo-92	42092.80c	Sb-123	51123.80c
Mo-94	42094.80c	Te-120	52120.80c
Mo-95	42095.80c	Te-122	52122.80c
Mo-96	42096.80c	Te-123	52123.80c
Mo-97	42097.80c	Te-124	52124.80c
Mo-98	42098.80c	Te-125	52125.80c
Mo-100	42100.80c	Te-126	52126.80c
Ru-96	44096.80c	Te-128	52128.80c
Ru-98	44098.80c	Te-130	52130.80c
Ru-99	44099.80c	I-127	53127.80c
Ru-100	44100.80c	Xe-124	54124.80c
Ru-101	44101.80c	Xe-126	54126.80c
Ru-102	44102.80c	Xe-128	54128.80c
Ru-104	44104.80c	Xe-129	54129.80c
Rh-103	45103.80c	Xe-130	54130.80c
Pd-102	46102.80c	Xe-131	54131.80c

Isotope	MatMCNP ZAID	Isotope	MatMCNP ZAID
Xe-132	54132.80c	Dy-160	66160.80c
Xe-134	54134.80c	Dy-161	66161.80c
Xe-136	54136.80c	Dy-162	66162.80c
Ce-133	55133.80c	Dy-163	66163.80c
Ba-130	56130.80c	Dy-164	66164.80c
Ba-132	56132.80c	Ho-165	67165.80c
Ba-134	56134.80c	Er-162	68162.80c
Ba-135	56135.80c	Er-164	68164.80c
Ba-136	56136.80c	Er-166	68166.80c
Ba-137	56137.80c	Er-167	68167.80c
Ba-138	56138.80c	Er-168	68168.80c
La-138	57138.80c	Er-170	68170.80c
La-139	57139.80c	Tm-169	69169.80c
Ce-136	58136.80c	Yb-168	---
Ce-138	58138.80c	Yb-170	---
Ce-140	58140.80c	Yb-171	---
Ce-142	58142.80c	Yb-172	---
Pr-141	59141.80c	Yb-173	---
Nd-142	60142.80c	Yb-174	---
Nd-143	60143.80c	Yb-176	---
Nd-144	60144.80c	Lu-175	71175.80c
Nd-145	60145.80c	Lu-176	71176.80c
Nd-146	60146.80c	Hf-174	72174.80c
Nd-148	60148.80c	Hf-176	72176.80c
Nd-150	60150.80c	Hf-177	72177.80c
Sm-144	62144.80c	Hf-178	72178.80c
Sm-147	62147.80c	Hf-179	72179.80c
Sm-148	62148.80c	Hf-180	72180.80c
Sm-149	62149.80c	Ta-180	73180.80c
Sm-150	62150.80c	Ta-181	73181.80c
Sm-152	62152.80c	W-180	74180.80c
Sm-154	62154.80c	W-182	74182.80c
Eu-151	63151.80c	W-183	74183.80c
Eu-153	63153.80c	W-184	74184.80c
Gd-152	64152.80c	W-186	74186.80c
Gd-154	64154.80c	Re-185	75185.80c
Gd-155	64155.80c	Re-187	75187.80c
Gd-156	64156.80c	Os-184	---
Gd-157	64157.80c	Os-186	---
Gd-158	64158.80c	Os-187	---
Gd-160	64160.80c	Os-188	---
Tb-159	65159.80c	Os-189	---
Dy-156	66156.80c	Os-190	---
Dy-158	66158.80c	Os-192	---

Isotope	MatMCNP ZAID	Isotope	MatMCNP ZAID
Ir-191	77191.80c	Hg-202	80202.80c
Ir-193	77193.80c	Hg-204	80204.80c
Pt-190	78000.42c	Tl-203	81203.80c
Pt-192	78000.42c	Tl-205	81205.80c
Pt-194	78000.42c	Pb-204	82204.80c
Pt-195	78000.42c	Pb-206	82206.80c
Pt-196	78000.42c	Pb-207	82207.80c
Pt-198	78000.42c	Pb-208	82208.80c
Au-197	79197.80c	Bi-209	83209.80c
Hg-196	80196.80c	Th-232	90232.80c
Hg-198	80198.80c	U-234	92234.80c
Hg-199	80199.80c	U-235	92235.80c
Hg-200	80200.80c	U-238	92238.80c
Hg-201	80201.80c		

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