Radiogenic Neutron Code Comparison

USD website and SOURCES4A

Zhang-Mei-Hime code
NIM A606, 651 (2009)
http://neutronyield.usd.edu

4A modified version – Sheffield group
Wilson et al. Sources4A. Technical Report, LA-13639-MS (1999);
Tomasello et al., NIMA 595 (2008) 431.
Outline

• Initial radiogenic neutron spectra from (alpha,n) reactions
  - Input (alpha,n) cross section per material
  - Input alpha decay data
  - Code calculation check against experimental nuclear data
  - Spectra shape and yield integral

• Extensive simulation work to understand how the discrepancies from USD website and SOURCES4 calculations can affect experimental background predictions
  - U and Th in borosilicate seen by an argon detector
  - U and Th in titanium seen by a xenon detector
  - U and Th in copper seen by a germanium detector
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  - U and Th in borosilicate seen by an argon detector
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• Target (alpha,n) cross section
USD: TENDL 2011 and 2012 have been considered as inputs. TENDL is a nuclear data library (validated) which provides the output of the TALYS nuclear model code system.

SOURCES4: cross section input libraries come from EMPIRE calculations and for some isotopes a combination of measurements and EMPIRE calculations. See webpage.

• Alpha particle decay data library
USD: only decays with visible energy larger than 100 keV or branching ratio more than 0.5% are considered.

SOURCES: no threshold.

Good agreement in the (alpha,n) ROI (0-10MeV) for most of the isotope considered.
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  See webpage.

  Checking cross section we found and corrected typos ~25 target isotopes.

• **Alpha particle decay data library**

  USD: only decays with visible energy larger than 100 keV or branching ratio more than 0.5% are considered.

  SOURCES: no threshold.

Good agreement in the (alpha,n) ROI (0-10MeV) for most of the isotope considered.

Neither library fully reproduces experimentally observed resonances, comparisons with experimental data are still important.
Benchmarking calculations against experimental nuclear data.

A validation of SOURCES4 code problems has been detailed [here](#).

We have considered an easy alpha-beam problem to benchmark both SOURCES4C and USD calculations - Alpha Beam (5.5 MeV) on Mg.
Title: Alpha Beam (5.5 MeV) on Mg
Beam problem input (idd = 3)
Magnitudes and spectra computed (id = 2)
Ascending energy structure for output (erg = 1)
Number of elemental constituents: 1
Solid stopping cross-sections used (isg = 0)

Elemental Constituents:

<table>
<thead>
<tr>
<th>Z-value</th>
<th>Atom Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>1.00000000000</td>
</tr>
</tbody>
</table>

Number of neutron spectrum energy groups: 81
Maximum neutron energy is 8.150E+00 MeV.
Minimum neutron energy is 5.000E-02 MeV.

Alpha beam energy is 5.500E+00 Mev.
Number of target nuclides to be used: 2
4000 Alpha energy groups used.

Target Nuclides:

<table>
<thead>
<tr>
<th>ZAID</th>
<th>Atom Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>120250</td>
<td>1.000E-01</td>
</tr>
<tr>
<td>120260</td>
<td>1.101E-01</td>
</tr>
</tbody>
</table>
Fig. 21. Energy-Dependent Neutron Source Strength from 5.5 MeV α-Particles Incident on Magnesium Slab as Calculated by SOURCES 4A and Compared to Measured Data.
Output - 4A(modified) vs 3A(original)

Total (alpha,n) neutron source from all sources and targets: 3.992E+06 n/sec-microamp.
Average (alpha,n) neutron energy: 3.039E+00 MeV.
Portion of Total Neutron Source Rate Accounted for in the Total Energy Spectrum: 99.9%.

<table>
<thead>
<tr>
<th>target</th>
<th>atom frac.</th>
<th>source</th>
<th>energy /microamp</th>
<th>p(e)</th>
<th>neut/alpha /microamp</th>
</tr>
</thead>
<tbody>
<tr>
<td>mg 25</td>
<td>1.0000E-01</td>
<td>beam</td>
<td>5.500</td>
<td>3.1209E+12</td>
<td>5.2789E-07</td>
</tr>
<tr>
<td>mg 26</td>
<td>1.1010E-01</td>
<td>beam</td>
<td>5.500</td>
<td>3.1209E+12</td>
<td>7.5131E-07</td>
</tr>
</tbody>
</table>
+        |            |        |                  |      |                      |
Total (all targets): 3.9923E+06

Total (alpha,n) neutron source from all sources and targets: 3.613E+06 n/sec-microamp.
Average (alpha,n) neutron energy: 2.897E+00 MeV.
Portion of Total Neutron Source Rate Accounted for in the Total Energy Spectrum: 95.6%.

<table>
<thead>
<tr>
<th>target</th>
<th>atom frac.</th>
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<td>3.1209E+12</td>
<td>4.5949E-07</td>
</tr>
<tr>
<td>mg 26</td>
<td>1.1010E-01</td>
<td>beam</td>
<td>5.500</td>
<td>3.1209E+12</td>
<td>6.9817E-07</td>
</tr>
</tbody>
</table>
+        |            |        |                  |      |                      |
Total (all targets): 3.6129E+06
Fig. 21. Energy-Dependent Neutron Source Strength from 5.5 MeV α-Particles Incident on Magnesium Slab as Calculated by SOURCES 4A and Compared to Measured Data.
Some discrepancies in shape...but good agreement

USD: 11.7249e-07 per alpha decay.
SOURCES4A: 11.5766e-07 per alpha decay
Extensive comparison for material giving important alpha,n reactions (Cu, Ti, Borosilicate glass, SS, PE, PTFE, Al$_2$O$_3$, ...)

Spectra calculated via:

- USD code,
- SOURCES4A spectrum with original input crossX
- USD input cross section (TALYS) into SOURCES4A
Polyethylene

C13 alpha input cross section shows discrepancies at low energy

USD SOURCES4A

C13_SOURCES4A: ba73b fig. 3 13c(a,n) x sec + EMPIRE2.19
Polyethylene

Different input CrossX

Alpha-n Neutron Yield on PE - 1ppb $^{238}$Uranium

USD into SOURCES4A crashes

Alpha-n Neutron Yield on PE - 1ppb $^{232}$Thorium

Polyethylene

Different input CrossX

USD into SOURCES4A crashes
Alpha-n Neutron Yield on PE - 1ppb $^{238}$Uranium

Alpha-n Neutron Yield on PE - 1ppb $^{232}$Thorium

USD into SOURCES4A crashes

Alpha cross sections matters

Polyethylene
Different input CrossX

$\text{USD}$

$\text{SOURCES4A}$

$\text{USD input into SOURCES4A}$

$\text{USD}$ into SOURCES4A crashes

Alpha cross sections matters

$\text{n/s/cm}^3$

9.6e-12
1.3e-11
1.6e-11

$\text{n/s/cm}^3$

2.9e-12
5.3e-12

Neutron energy [MeV]

Neutron energy [MeV]
Copper

Check code calculation for matching USD and SOURCES4A input alpha cross sections
Alpha-n Neutron Yield on Natural Copper - 1ppb $^{235}$Uranium

Neutron energy [MeV] vs. Yield [n/s/cm$^3$]

- SOURCES4A
- USD
- USD input into SOURCES4A

Alpha-n Neutron Yield on Natural Copper - 1ppb $^{232}$Thorium

Neutron energy [MeV] vs. Yield [n/s/cm$^3$]

- SOURCES4A
- USD
- USD input into SOURCES4A

n/s/cm$^3$
- 3.5e-12
- 2.8e-12
- 2.9e-12

n/s/cm$^3$
- 1.1e-11
- 9.5e-12
- 9.2e-12
<table>
<thead>
<tr>
<th>Material</th>
<th>Decay Chain</th>
<th>Neutron/s/cm³</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>USD</td>
<td>SOURCES4A</td>
</tr>
<tr>
<td>Cu</td>
<td>238U</td>
<td>3.46E-12</td>
<td>2.84E-12</td>
</tr>
<tr>
<td></td>
<td>232Th</td>
<td>1.11E-11</td>
<td>9.49E-12</td>
</tr>
<tr>
<td>PE</td>
<td>238U</td>
<td>9.56E-12</td>
<td>1.26E-11</td>
</tr>
<tr>
<td></td>
<td>232Th</td>
<td>2.87E-12</td>
<td>5.28E-12</td>
</tr>
</tbody>
</table>

- Looking at the first ratio column: SOURCES4 code differs by factor <2 USD calculation

- Looking at the second ratio column: different input cross section may account up to 20% in calculation
GEANT4 neutron propagation studies

by KJPalladino

What do these input radiogenic neutron spectra differences mean for experimentalists?

Working with Geant4.9.5.p02 in the simulation package RAT, propagate alpha-n neutrons for the various U238 and Th232 spectra from SOURCES and TALYS-USD.

NeutronHP handles neutrons < 20MeV with cross sections from ENDF.

Create generalized direct dark matter detectors of common materials (argon, xenon and germanium) along with external vetoes.

LRT 2105
Neutrons in copper from $^{238}\text{U}$

From 1ppb of U238, USD calculations give a neutron yield of $3.46 \times 10^{-12}$ n/s/cm$^3$ while SOURCES gives a neutron yield of $2.90 \times 10^{-12}$ n/s/cm$^3$, 19% lower.

USD spectrum cuts off at half the energy of SOURCES.
Ge Detector Simulation

- 250,000 neutrons isotropic from copper for each simulation
- Neutron recoil threshold of 5 keVnr used in analysis
- 1 keVee threshold for EM deposits to veto event in argon
- Neutron capture in plastic scintillator needed to externally veto event

![Nested cylinders geometry](image)

- 10 cm Lead shield cylinder
  - 31 cm radius, 1.75m tall
- 15 cm polyethylene down to 6 cm radius,
  - 1.5 m tall
- 1 cm copper to 5 cm radius
- Germanium
  - 10 cm diameter, 1.2m tall
Ge recoils

Shape and yield effects cause an 80% higher prediction of single scatters from USD than SOURCES

<table>
<thead>
<tr>
<th></th>
<th>Summed nuclear recoils over 5 keV</th>
<th>Single nuclear recoil over 5 keV</th>
<th>Single recoils over 5 keV no capture in veto</th>
<th>Single recoils over 5 keV no electron scatter &gt;1 keV</th>
<th>Ratio of Multiple scatters: single scatters no threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>TALYS-USD % of initial sim</strong></td>
<td>14.2 +/- 0.07%</td>
<td>10.2 +/- 0.06%</td>
<td>2.4 +/- 0.03%</td>
<td>8.87 +/- 0.06%</td>
<td>3.42 +/- 0.017</td>
</tr>
<tr>
<td><strong>SOURCES % of initial sim</strong></td>
<td>8.3 +/- 0.06%</td>
<td>6.71 +/- 0.05%</td>
<td>1.6 +/- 0.02%</td>
<td>5.8 +/- 0.05%</td>
<td>3.17 +/- 0.076</td>
</tr>
<tr>
<td><strong>TALYS-USD n/s/cm³/ppb</strong></td>
<td>(4.92 +/- 0.02)E-13</td>
<td>(3.53 +/- 0.02)E-13</td>
<td>(8.32 +/- 0.01)E-13</td>
<td>(3.07 +/- 0.02)E-13</td>
<td>(2.04 +/- 0.003)E-12: (0.59 +/- 0.003)E-12</td>
</tr>
<tr>
<td><strong>SOURCES n/s/cm³/ppb</strong></td>
<td>(2.41 +/- 0.02)E-13</td>
<td>(1.50 +/- 0.07)E-13</td>
<td>(4.56 +/- 0.07)E-13</td>
<td>(1.69 +/- 0.01)E-13</td>
<td>(1.17 +/- 0.002)E-12: (0.37 +/- 0.004)E-12</td>
</tr>
</tbody>
</table>
Shape considerations lead to 64% more single scatters from USD than SOURCES.
Conclusions

- Exhaustive comparison code study has been carried out.

- Extensive simulation work has been performed to check the influence of radiogenic neutron spectrum for experimentalist.

- Wrap everything up in a paper