Calculation of the neutron production induced by radiogenic α-decay chains with Geant4

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Motivation

The simulation of (α,Xn) reactions is required in several fields:

- **Nuclear structure experiments.** Learn about the structure of light nuclei.
- **Nuclear technologies.** α-emitters present in fresh/irradiated nuclear fuels can create a neutron source through (α,Xn) reactions with (light) surrounding nuclei: oxide and carbide fuels, vitrified nuclear waste…
- **Nuclear astrophysics.** Neutron sources in collapsing stars linked to the r-process. E_α below ~1 MeV (around the Gamow peak).
- Neutron background in underground experiments (nuclear astrophysics, **Dark Matter**) due to radiogenic α-decay chains.

For applications, it is necessary to be able to compute **(α,Xn) reaction probabilities**, **particle emission rates** and their associated **energy spectra.**

Can be calculated with the SOURCES-4C code: simple geometries and experimental data for a limited number of isotopes.

$$\textbf{Neutrons} \propto \int \Phi(E)\,\sigma_{(\alpha,Xn)}(E)\,dE$$

Standard Monte Carlo transport codes: **Geant4**, MCNP…

Pros: very detailed geometries,
Cons: large CPU times since EM ion interactions are ~10^6 times more probable than nuclear ones. Model biasing!

Can be calculated independently with Monte Carlo codes like SRIM.

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Can be obtained independently from

a) **Nuclear models** like TALYS and EMPIRE, for a large number of isotopes.
b) **Evaluated cross section files**: cross sections and secondary particles – JENDL and TENDL

NeuCBOT
(SRIM + TALYS)

USD webtool
(SOURCES-4A / EMPIRE)

NEDIS
Similar to SOURCES-4C

Monte Carlo simulations with Geant4

We have investigated the performance of Geant4 when simulating the neutron production induced by α-emitters present in the natural decay chains,

In particular we have:

I. **Methodology**. Investigated **how to run Geant4 safely and efficiently** for this purpose:
   - Is G4ParticleHP it working?
   - Are cross section biasing techniques working? What is the range of usability?

II. **Physics**. Evaluated the **differences between the existing input data libraries**,

III. **Validation. Compared Geant4 with other codes** (NeuCBOT, SOURCES-4C) and **data** for a few selected cases.

I. Development of a Geant4 application and verification

We performed a large number of simulations with 10 MeV alphas interacting with ^{14}N and ^{13}C volumes and the JENDL-AN-2005 library evaluated nuclear data library.

Investigation of different combinations of:

- *StepMax* **(10^{-1} – 10^{-4})** mm
- nuclear cross section biasing factors (1 – 10^{6})

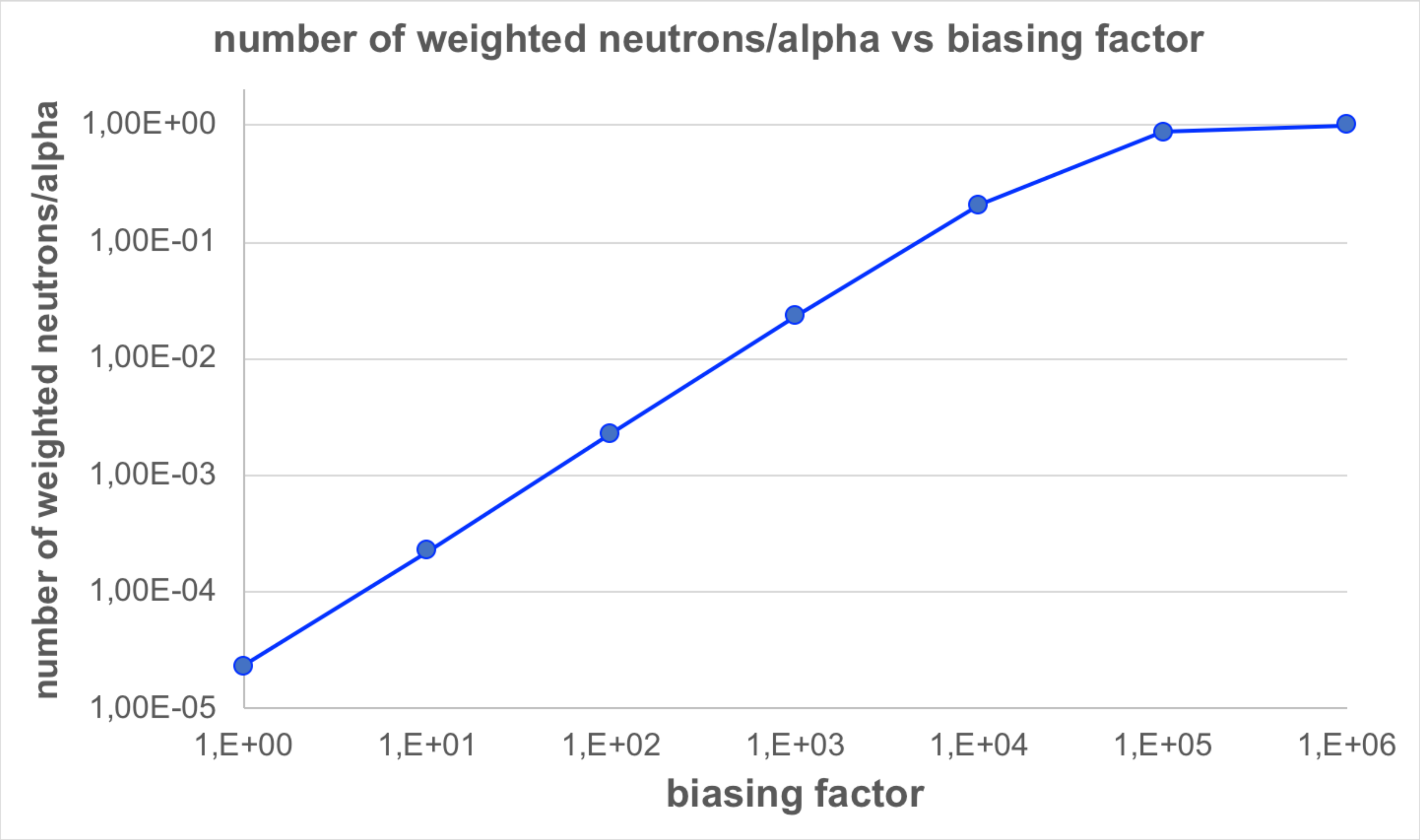
Calculation of the number of neutrons produced by 10^{7} alphas in three different ways:

  - **N1**: simulated neutron yield with biasing,
  - **N2**: neutron yield calculated from the numeric convolution of the "high precision" α flux calculated with GEANT4 and the cross section

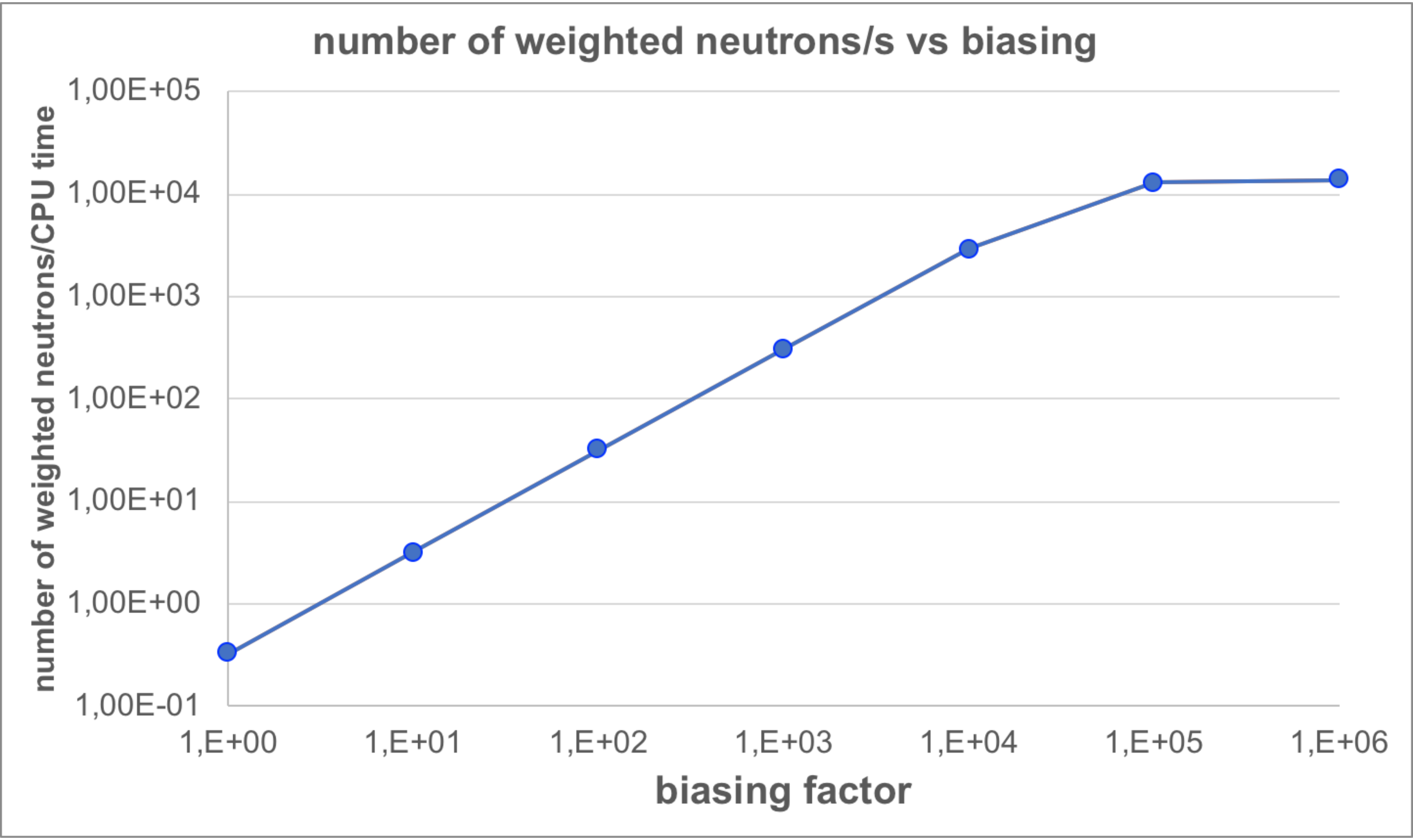
If everything is Ok, **N1=N2**

10 MeV alphas in ^{14}N – JENDL-AN-2005

Step Max (mm)	Biasing Factor	Time (s) [Time/10^7 events]	Neu: #Neutrons generated in the simulation (10^7 events)	Neu/Time (s^{-1})	N1/N2
10^{-1}	1	$7{,}1\cdot10^2$	234	0,33	0,884
10^{-1}	10	$7{,}1\cdot10^2$	2242	3,2	0,847
10^{-1}	10^2	$7{,}0\cdot10^2$	22911	32	0,867
10^{-1}	10^3	$7{,}3\cdot10^2$	229072	310	0,876
10^{-1}	10^4	$7{,}0\cdot10^2$	2057454	2900	0,878
10^{-1}	10^5	$6{,}6\cdot10^2$	8760309	13000	0,878
10^{-1}	10^6	$7{,}1\cdot10^2$	9999996	14000	0,923
10^{-2}	1	$2{,}0\cdot10^3$	241	0,12	0,911
10^{-2}	10	$2{,}0\cdot10^3$	2598	1,3	0,982
10^{-2}	10^2	$2{,}0\cdot10^3$	24228	12	0,917
10^{-2}	10^3	$1{,}8\cdot10^3$	242143	130	0,927
10^{-2}	10^4	$1{,}6\cdot10^3$	2157538	1300	0,925
10^{-2}	10^5	$8{,}6\cdot10^2$	8903461	10000	0,926
10^{-2}	10^6	$7{,}2\cdot10^2$	9999856	14000	0,583
10^{-3}	1	$1{,}5\cdot10^4$	258	0,017	0,975
10^{-3}	10	$1{,}5\cdot10^4$	2607	0,18	0,985
10^{-3}	10^2	$1{,}5\cdot10^4$	26117	1,7	0,988
10^{-3}	10^3	$1{,}5\cdot10^4$	257777	18	0,987
10^{-3}	10^4	$1{,}2\cdot10^4$	2297458	190	0,989
10^{-3}	10^5	$3{,}2\cdot10^3$	9144054	2900	0,988
10^{-3}	10^6	$9{,}7\cdot10^2$	9941846	10000	0,615
10^{-4}	1	$1{,}4\cdot10^5$	282	0,002	1,066
10^{-4}	10	$1{,}4\cdot10^5$	2665	0,019	1,007
10^{-4}	10^2	$1{,}4\cdot10^5$	26486	0,18	1,002
10^{-4}	10^3	$1{,}4\cdot10^5$	259893	1,9	0,995
10^{-4}	10^4	$1{,}2\cdot10^5$	2321998	20	0,999
10^{-4}	10^5	$2{,}5\cdot10^4$	9274608	370	0,999
10^{-4}	10^6	$2{,}9\cdot10^3$	9991875	3500	0,667

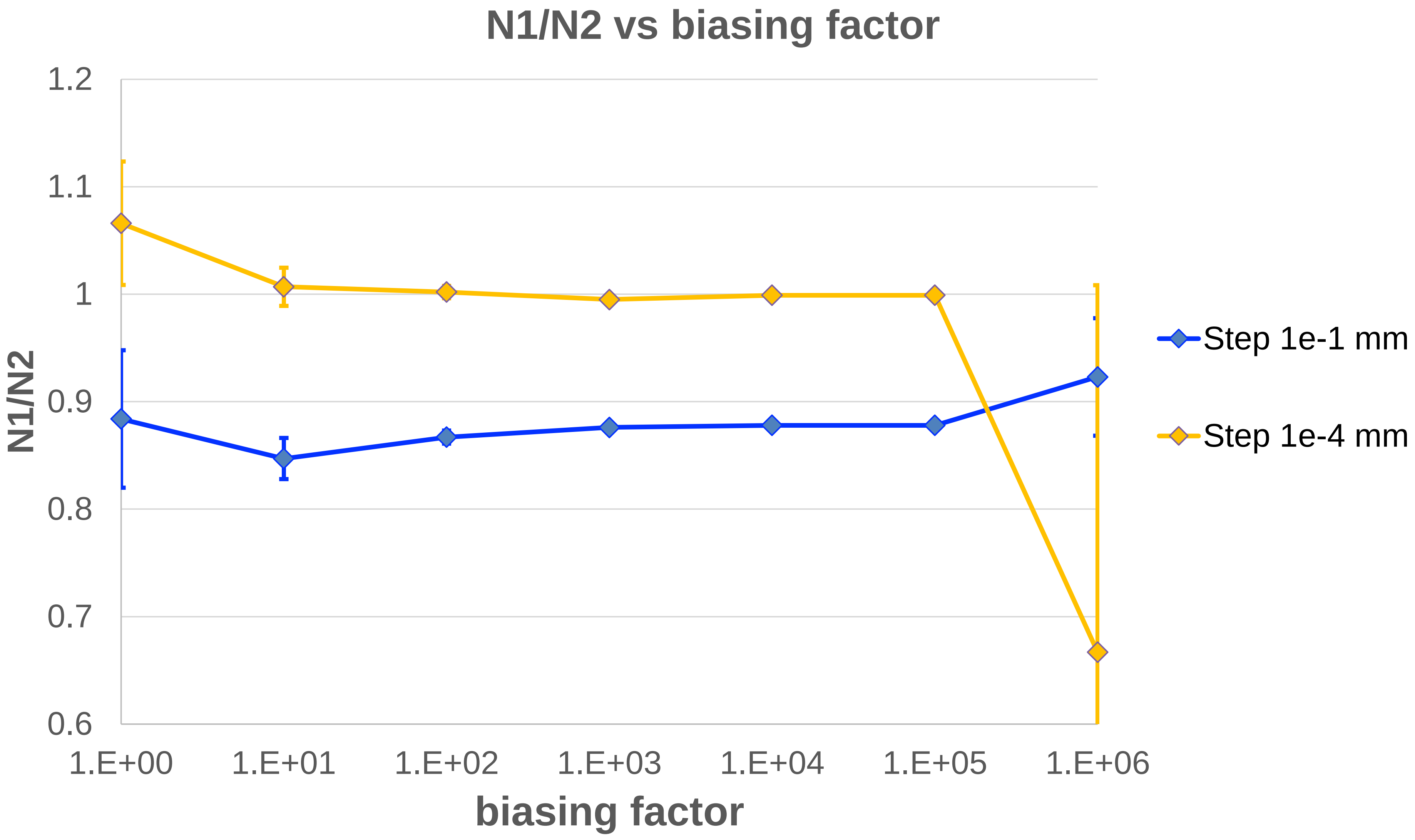


number of weighted neutrons/alpha vs biasing factor
number of weighted neutrons/alpha
1,00E+00
1,00E-01
1,00E-02
1,00E-03
1,00E-04
1,00E-05
1,E+00
1,E+01
1,E+02
1,E+03
1,E+04
1,E+05
1,E+06
biasing factor



number of weighted neutrons/s vs biasing
number of weighted neutrons/CPU time
1,00E+05
1,00E+04
1,00E+03
1,00E+02
1,00E+01
1,00E+00
1,00E-01
1,E+00
1,E+01
1,E+02
1,E+03
1,E+04
1,E+05
1,E+06
biasing factor

N2=26,5 neutrons for 10^7 alphas with 10 MeV in ^{14}N



The results obtained in the tested cases indicate that:

- **Maximum allowed step size**: the best results correspond to the smaller values (~10^{-4} mm). Larger values allow to perform faster simulations (up to more than 100 times faster), and the obtained results deviate, in general, a few percent (up to 10-15%).

- **Biasing Factor**: the model biasing technique works fine up to almost one nuclear interaction per simulated event. If the biasing factor is increased above this “saturated” value then the obtained results are not correct.

- We have verified that the amount of neutrons produced in the simulations is the same as the one expected from the input cross sections.

- We have verified that the resulting energy spectra are the same as the ones in the input data libraries, with and without biasing.

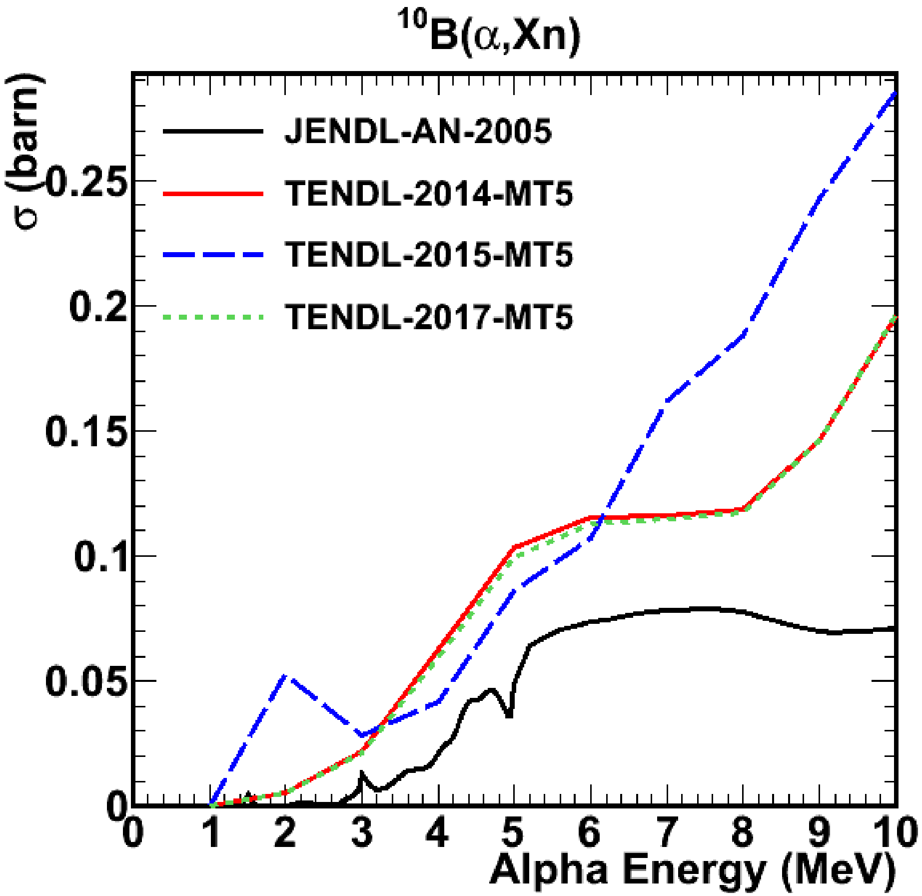
II. Differences between the ENDF-6 format libraries

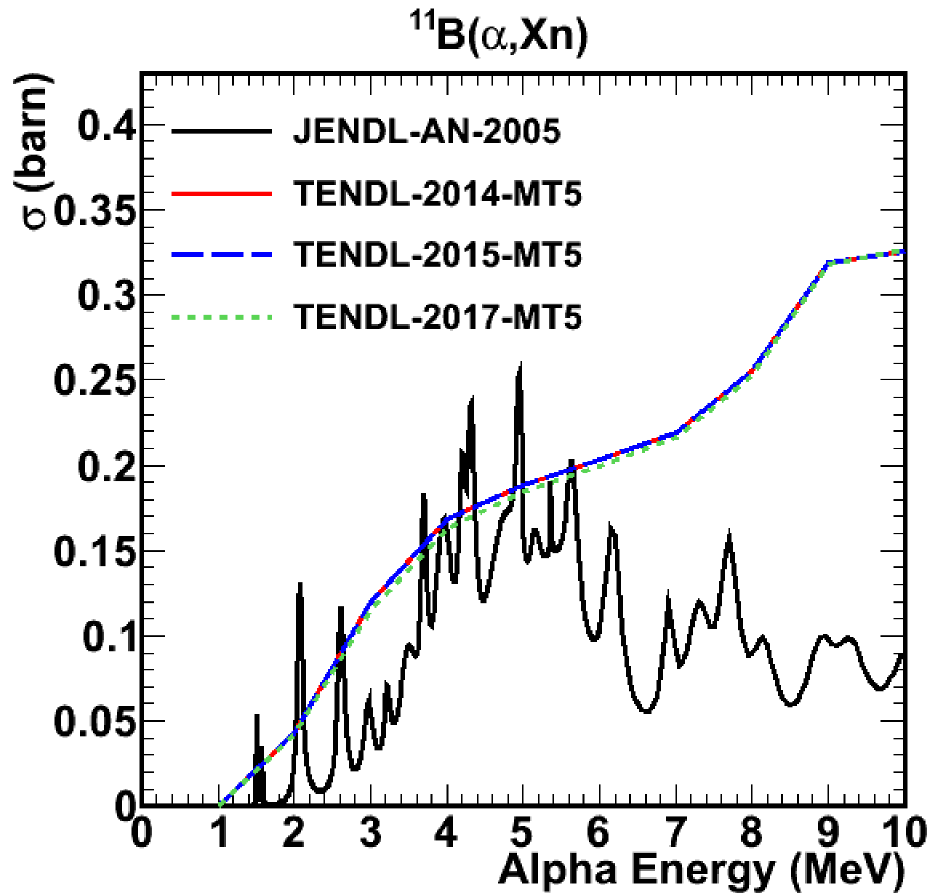
The ENDF-6 α-incident data libraries available are:

JENDL-AN-2005: this is an evaluated library (experimental data + theoretical calculations). There are only 17 isotopes: ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{12,13}C, ^{14,15}N, ^{17,18}O, ^{19}F, ^{23}Na, ^{27}Al, ^{28,29,30}Si.

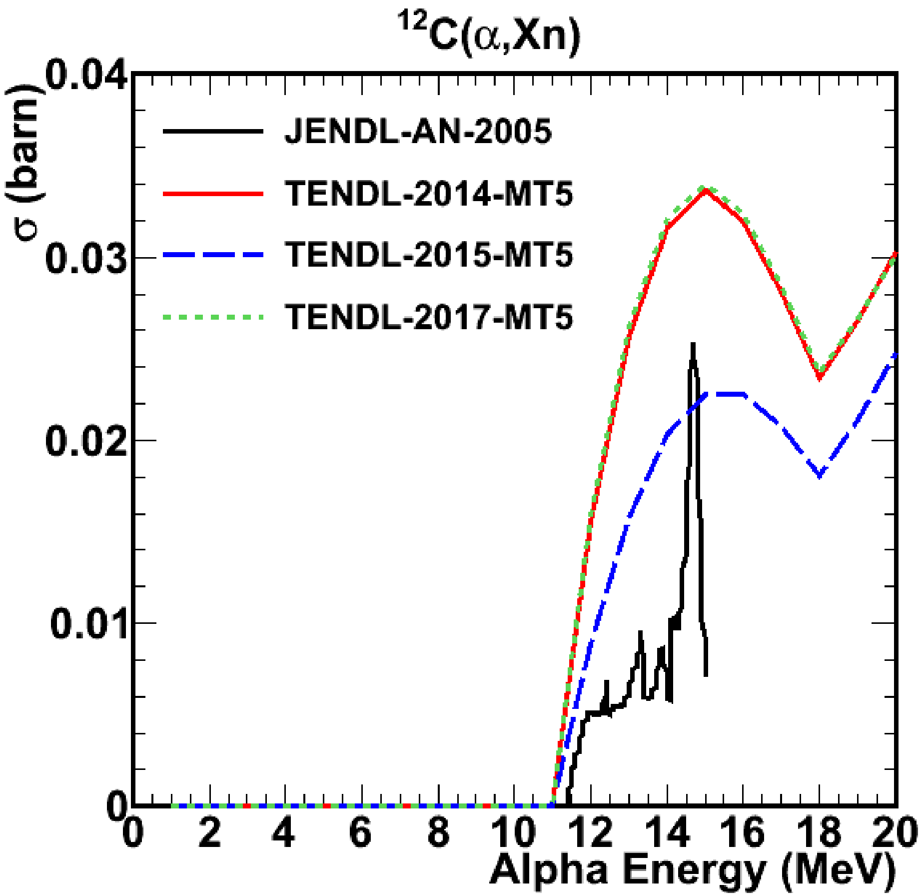
TENDL libraries: they have been made with the results of the TALYS code. We have performed calculations with TENDL-2014, TENDL-2015 and TENDL-2017 (there is no TENDL-2016). They contain a large amount of isotopes.

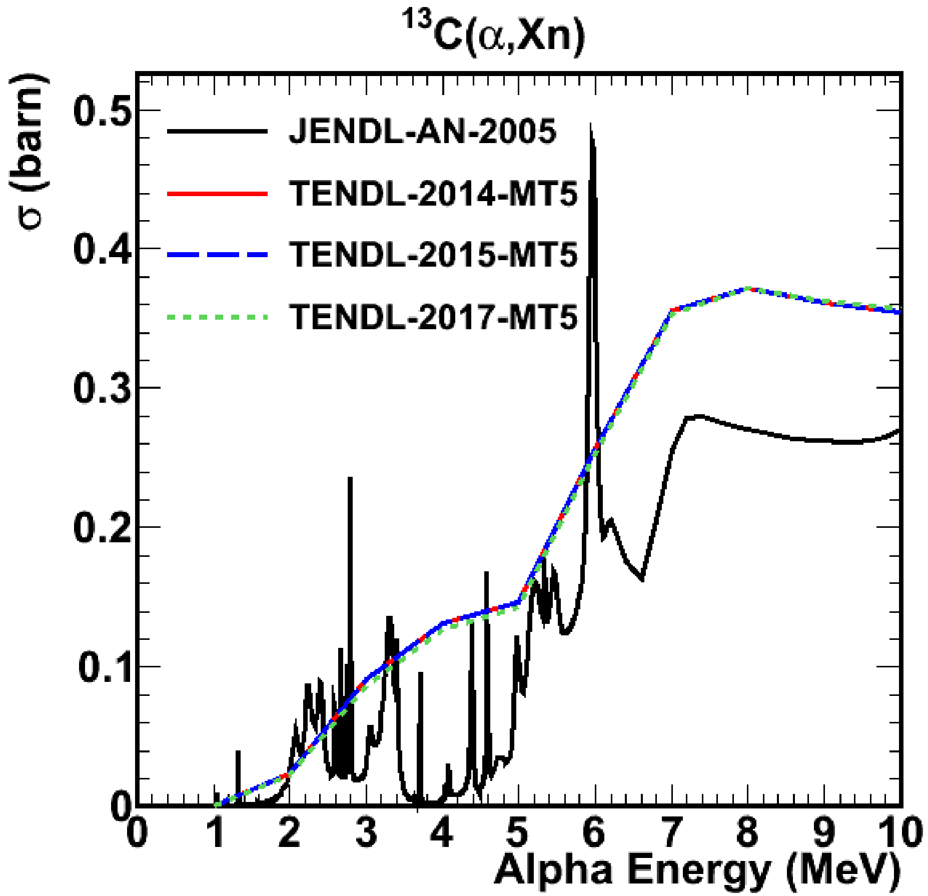
Comparison between JENDL-AN-2005 and TENDL-MT5



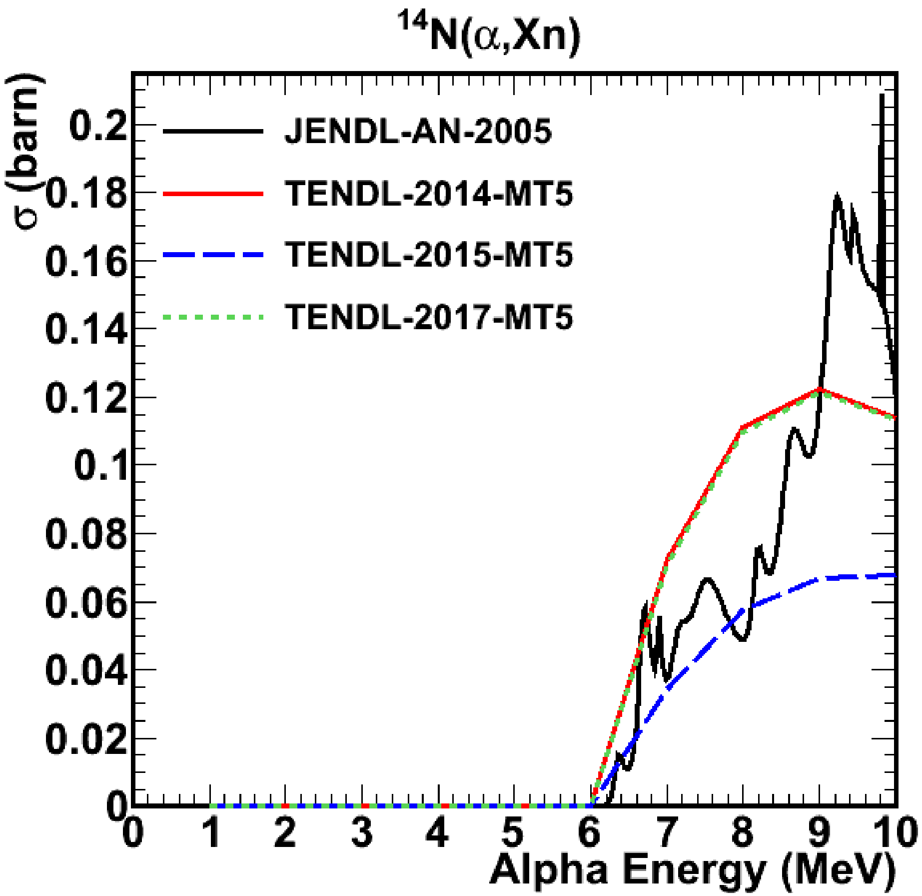


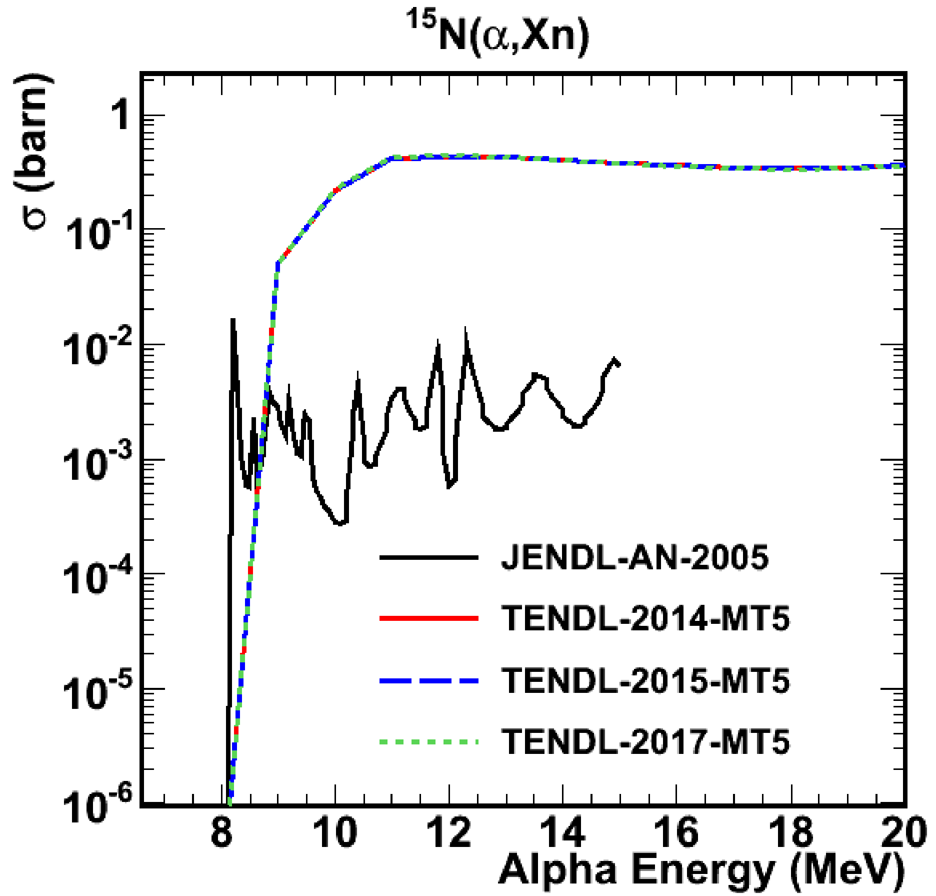
Comparison between JENDL-AN-2005 and TENDL-MT5





Comparison between JENDL-AN-2005 and TENDL-MT5





- The different versions of the TENDL libraries do not differ so much.

- The neutron production in TENDL (i.e. average behavior without resonant structure) is larger than in JENDL in most of the cases.

III. Comparison to other codes and experimental data

NeuCBOT – *S. Westerdale et al. , P. Meyers, Nucl. Inst. and Meth. A 875, 57 (2017)*
SOURCES – *W. Wilson et al., Progress in Nuclear Energy 51, 608 (2009)*
NEDIS – *G. N. Vlaskin et al. , Atomic Energy 117, 357 (2015)*
USD – *D.M. Mei, Nucl. Inst. and Meth. A 606, 651 (2009)*

All these codes calculate the neutron yields according to:

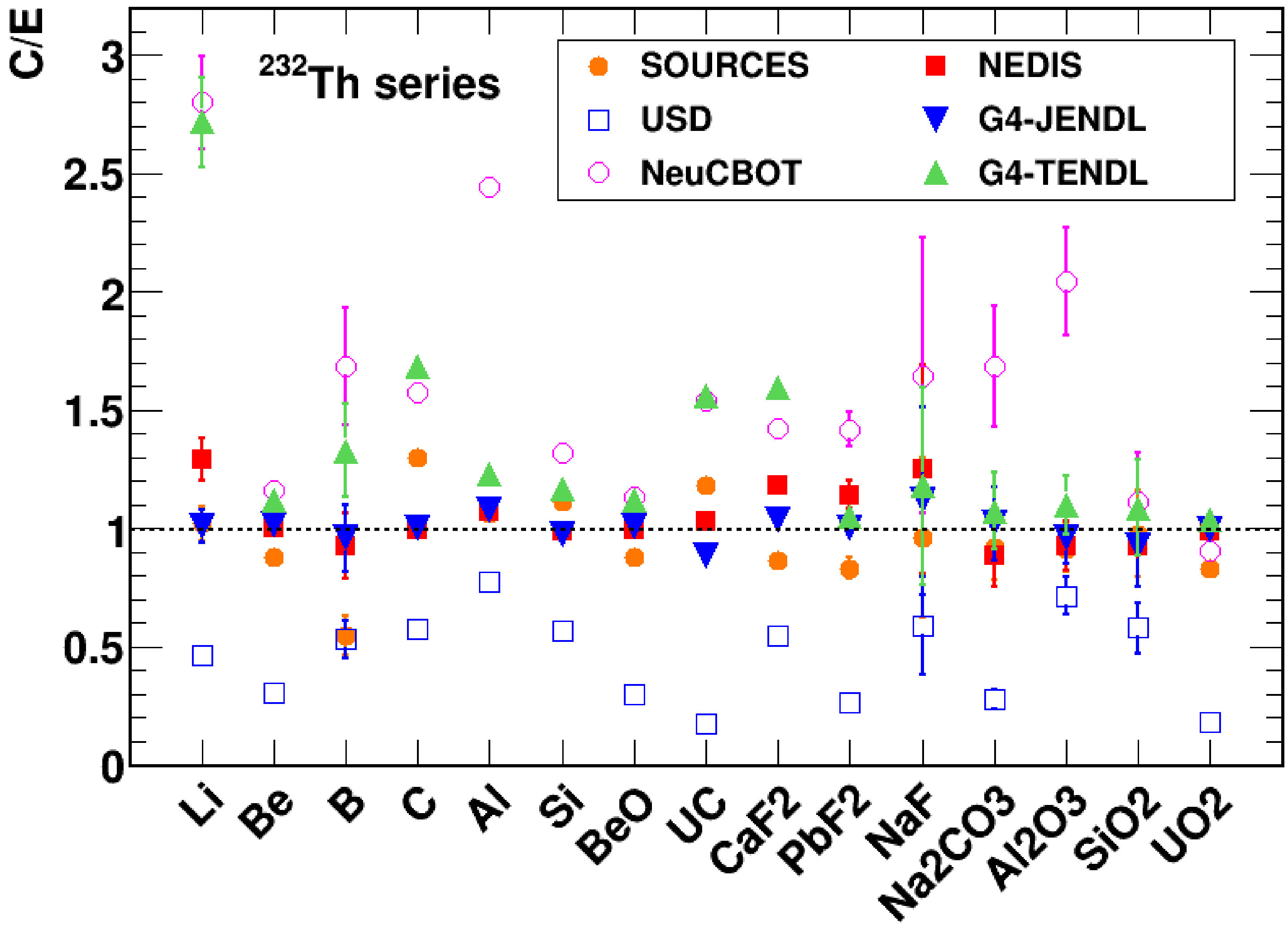
$$Y(E_\alpha) = \int_0^{E_\alpha} \frac{\sigma_{(\alpha,Xn)}(E)}{S(E)} dE$$

where E_α is the initial energy of the α particle, $\varepsilon(E)$ is the mass stopping power of the material, and $\sigma_{(\alpha,Xn)}(E)$ is the neutron production cross section.

SOURCES and NEDIS → own databases with neutron production cross sections and secondary energy spectra.

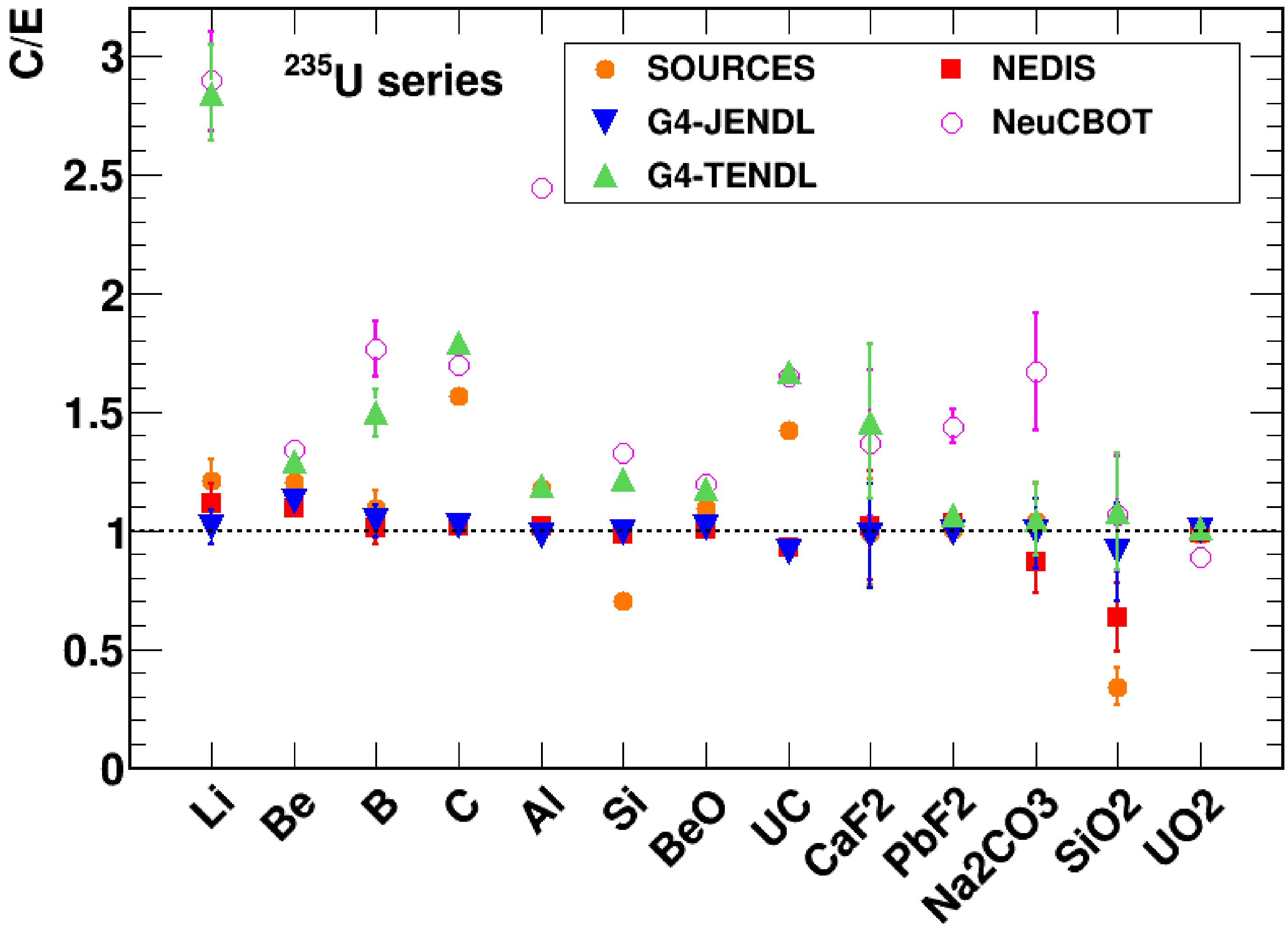
NeuCBOT and USD → TALYS

Comparison: neutron yields



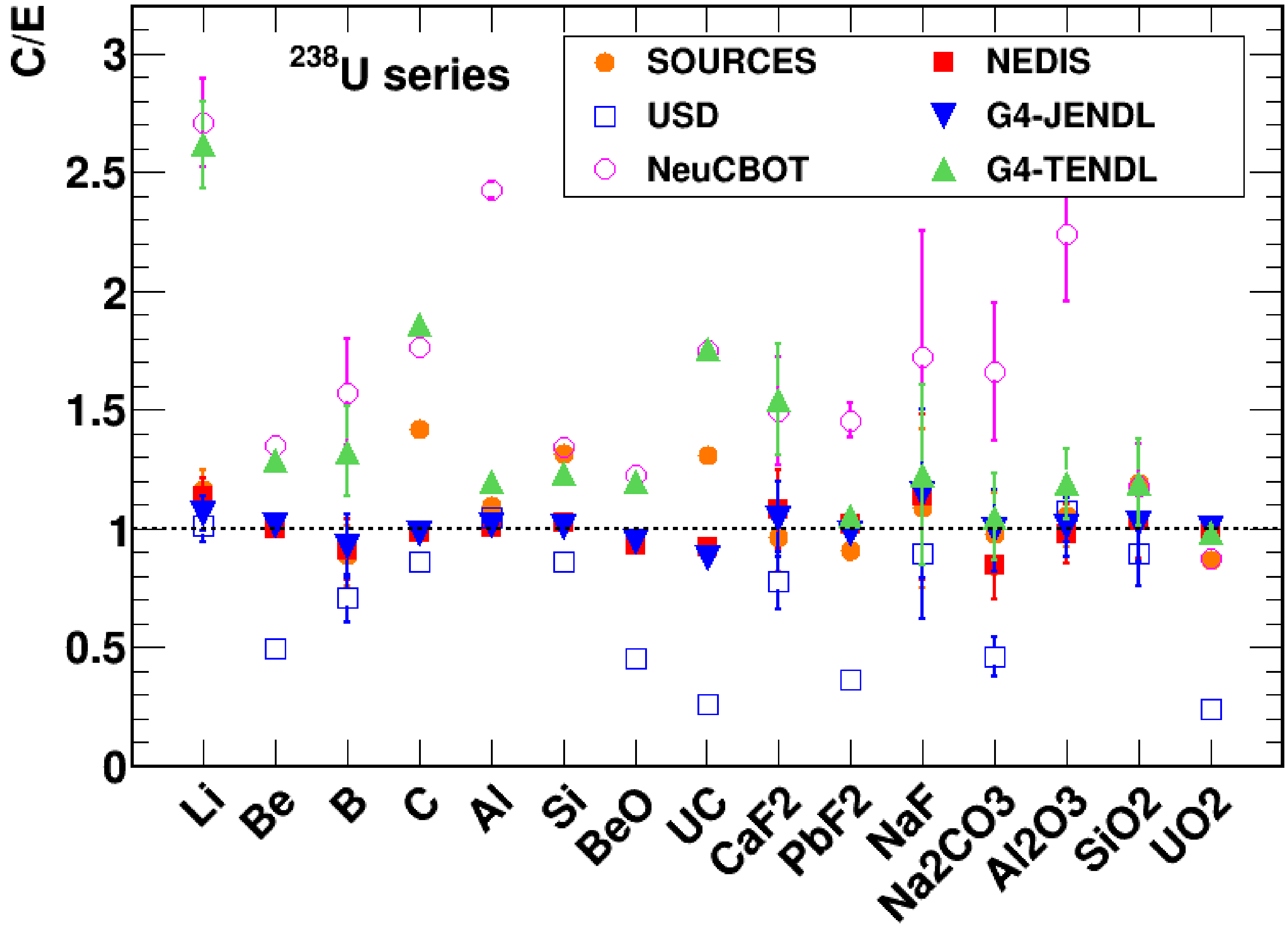
Source: *A. C. Fernandes, A. Kling, G. N. Vlaskin, EPJ Web Conf. 153, 07021 (2017).*

Comparison: neutron yields



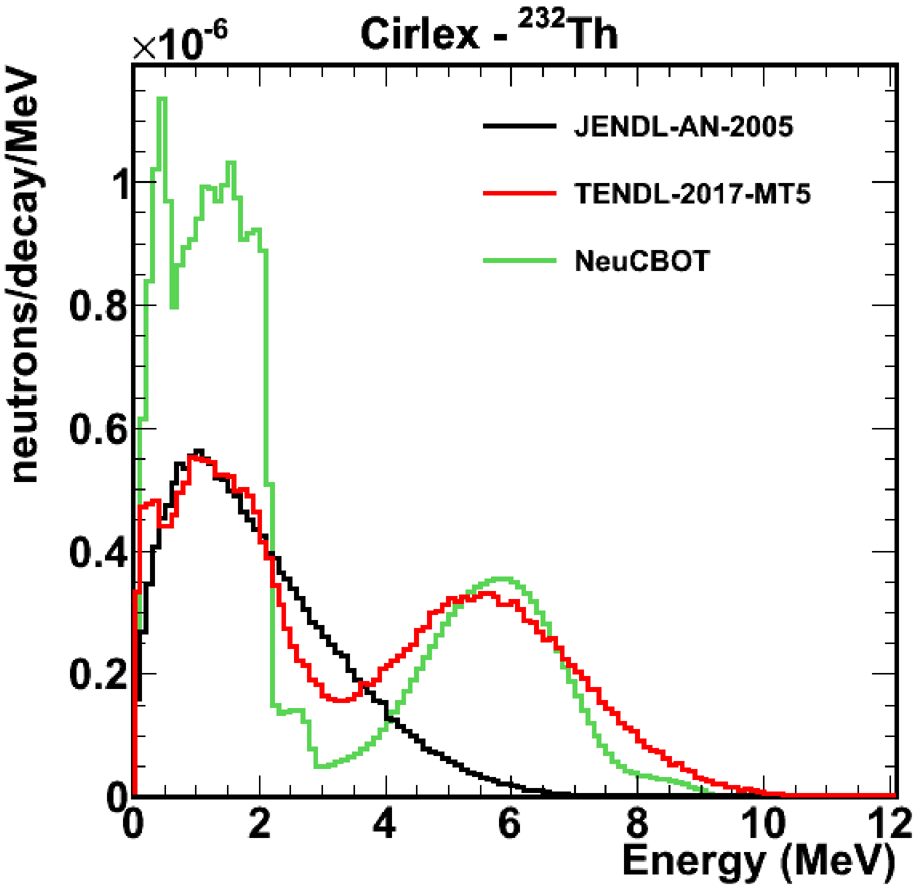
<u>Source</u>: *A. C. Fernandes, A. Kling, G. N. Vlaskin, EPJ Web Conf. 153, 07021 (2017).*

Comparison: neutron yields

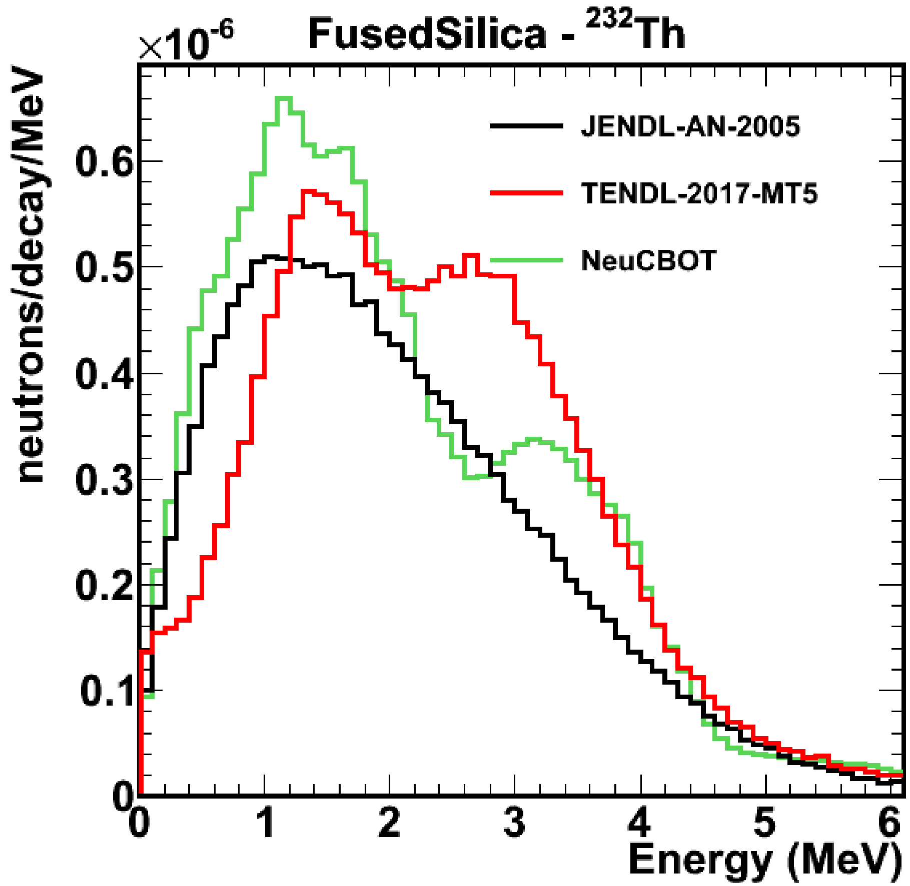


Source: *A. C. Fernandes, A. Kling, G. N. Vlaskin, EPJ Web Conf. 153, 07021 (2017).*

Comparison: neutron energy spectra

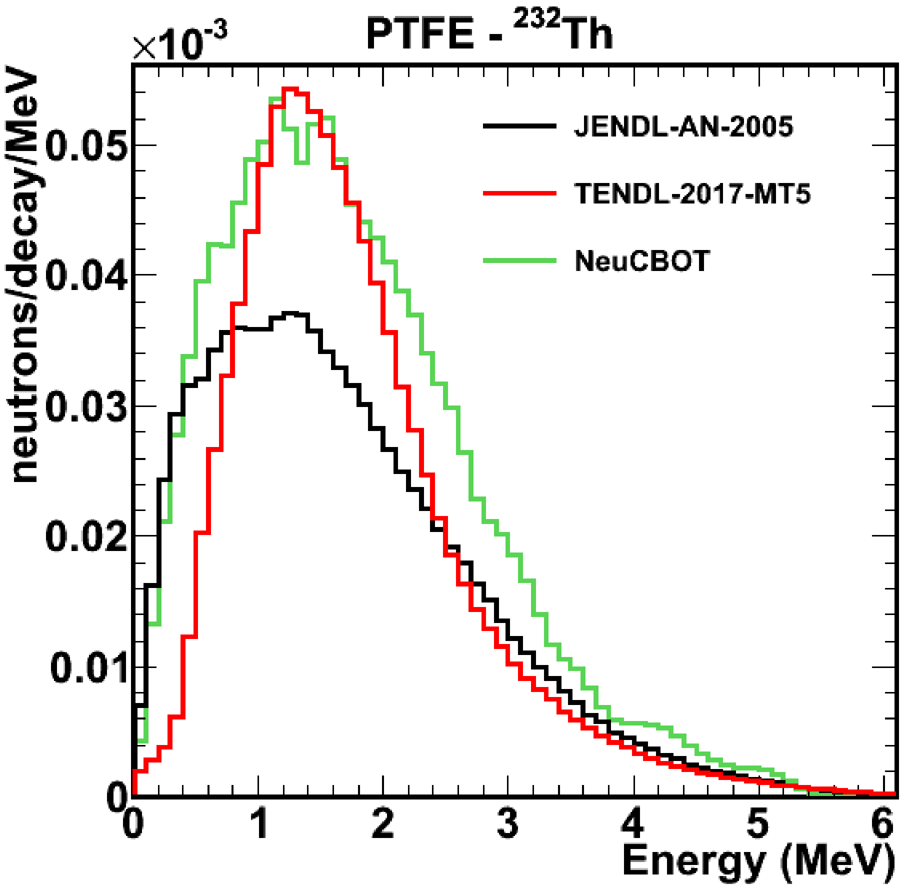


H:25.4%, C:56.6%
N:5.1%, O:12.9%

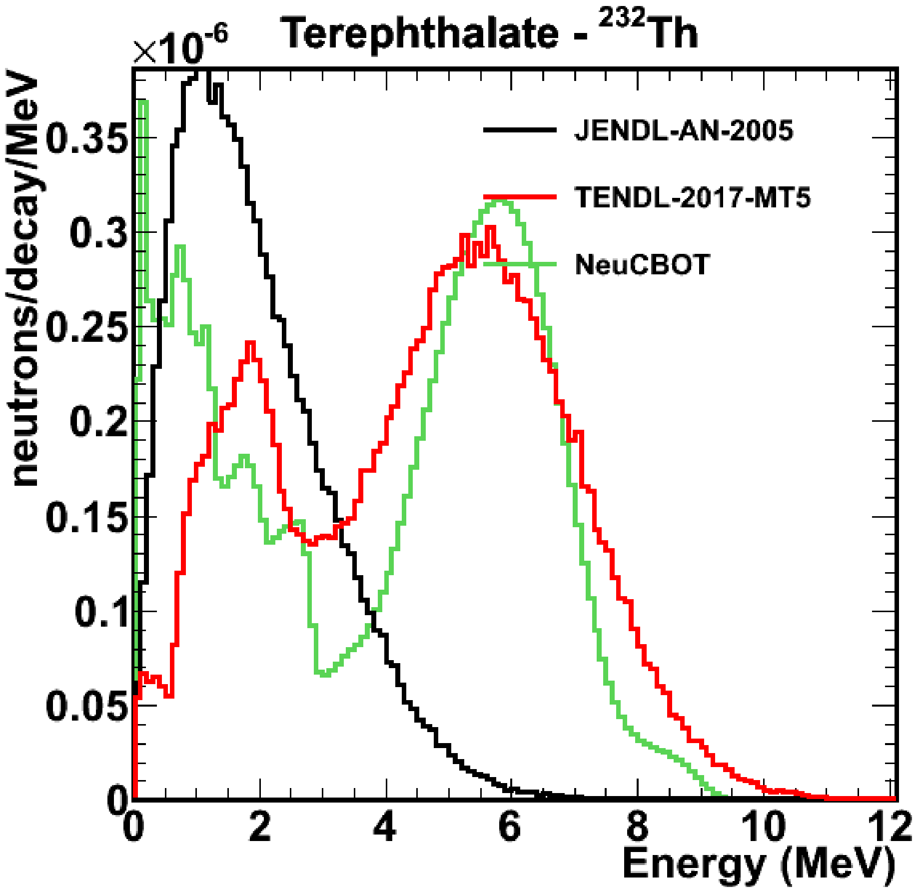


SiO_2

Comparison: neutron energy spectra

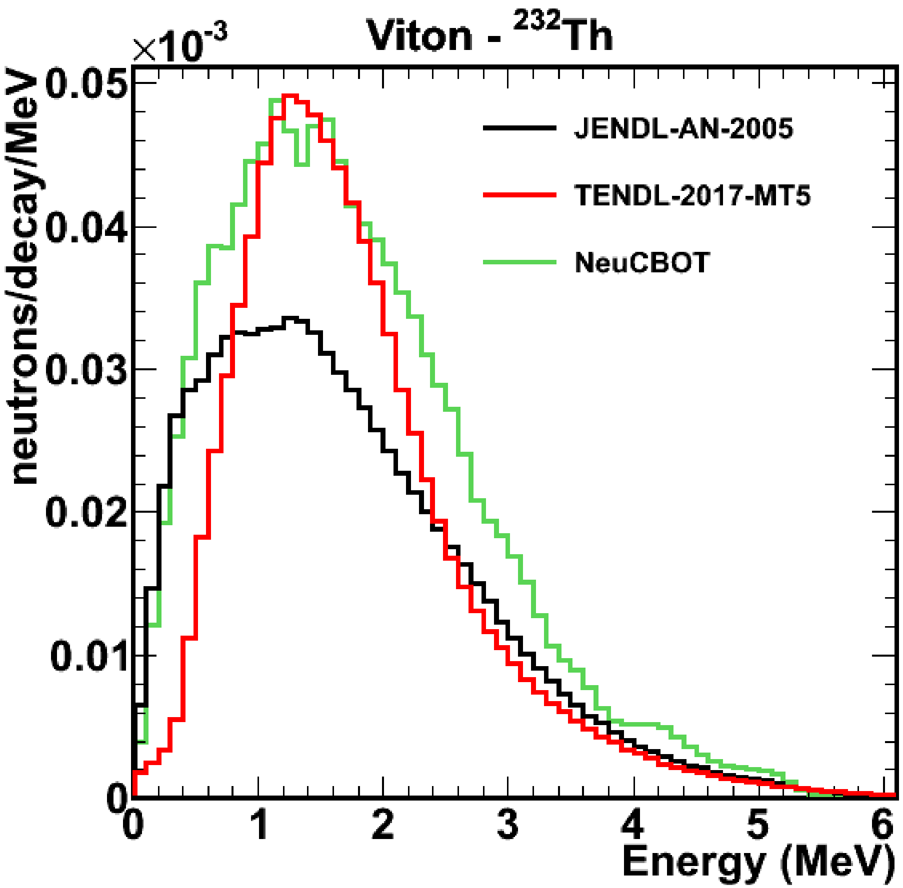


CF_2

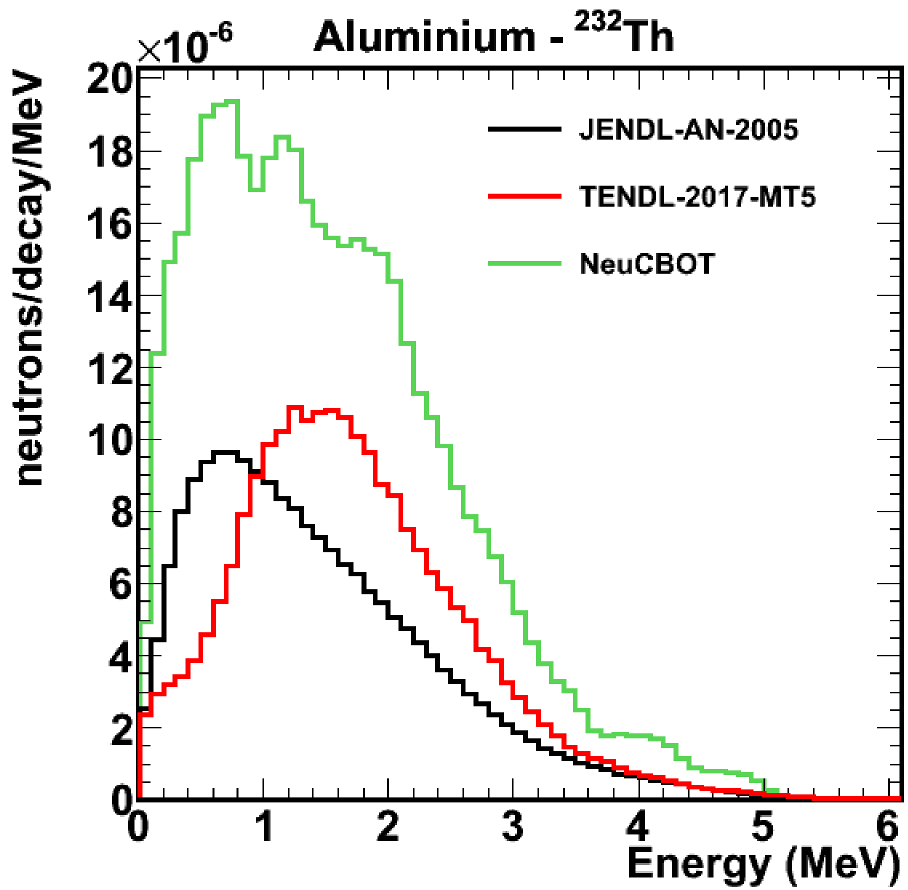


$H_4C_5O_2$

Comparison: neutron energy spectra



$H_2C_5F_8$



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Summary and conclusions

We have built a Geant4 application capable of calculating neutron yields in (α,xn) reactions, i.e. we have verified that it is possible to use Geant4 to model neutron production induced by alpha decay.

We have performed a verification study of GEANT4 (ParticleHP + biasing). New classes have been written and will be distributed in future code releases.

We have translated various ENDF-6 incident alpha data libraries into the G4NDL format. We have performed a comparison between GEANT4 using these libraries with other codes and with experimental data:

- GEANT4 calculated (α,Xn) neutron yields for different materials are in excellent agreement with experimental data (JENDL library).

- The neutron spectra obtained with the different libraries do not agree. There neutron spectra in JENDL tend to underestimate the energy of the produced neutrons.

Advantages of GEANT4 over other codes:

- Complex geometries
- Event generator: gamma rays in coincidence with neutrons.
- Same code for generating and for transporting the neutrons.