(α,n) and $(\alpha,n\gamma)$ yield calculations with a new version of NeuCBOT for low background experiments

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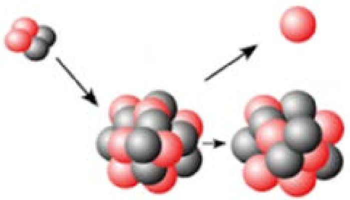

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Importance of (α,n) reactions

Fundamental physics

1. One of the major backgrounds for neutrino experiments and direct search for dark matter (neutrons can mimic nuclear recoils from WIMPs and the inverse β-decay reactions)

2. Nuclear astrophysics, namely the $^{13}C(\alpha,n)^{16}O$ reaction is a neutron source in the s-process

3. Nuclear structure

Applications

1. Fission reactors. To understand energy-dependent neutron interactions with O isotopes in the core the inverse reactions $^{13}C(\alpha,n)^{16}O$ should be studied

2. Nonproliferation, waste management and homeland security applications:
   α-particle interactions with the light fuel compounds produce neutrons that can be used in non-destructive assays of the irradiated fuel to determine the fuel enrichment

3. An important neutron source in deep geological repositories of spent fuel

(α,*n*) background in neutrino and dark matter experiments

1) Contamination of ^{232}Th, ^{235}U, ^{238}U and their daughters in the detector materials and surrounding rock generates α-particles

2) α-particles can induce (α,*n*) reactions on the detector materials and rock and then neutrons can mimic signals from neutrino/DM particles

3) It is necessary to evaluate the (α,*n*) background and at least materials with minimal Th and U contamination should be selected/produced

4) The number of background neutrons N_n from (α,*n*) reactions in a material can be calculated by the equation

$$N_n = (1 - \varepsilon_j)\, m\, T \sum_i A_i Y_i$$

$1 - \varepsilon_j$ is the inefficiency to tag neutrons from a particular detector part j, determined from Monte Carlo simulation

m is the material mass

T is the period of data taking

A_i is the total specific activity (per unit mass of the material), measured with ICP-MS, HPGe, polonium extraction

Y_i is the neutron yield, calculated with a special code using the material composition

i designates a part or complete decay chain (^{232}Th, ^{235}U, ^{238}U upper, middle and lower)

Calculation of neutron yields from (α,n) reactions

For a single interaction

$$Y_i(E_\alpha, E_n) = \int_0^{E_\alpha} \frac{\sigma\,(E'_\alpha, E_n)}{\varepsilon(E'_\alpha)}\, dE'_\alpha$$

Cross section

Stopping power

Outgoing neutron energy

Integral over the α-track (assuming the capture probability is small)

For a specific material and set of α-particles

$$Y_i(E_\alpha, E_n) = \sum_\alpha P_\alpha \sum_m \frac{N_A C_m}{A_m} \int_0^{E_\alpha} \frac{\sigma\,(E'_\alpha, E_n)}{\varepsilon(E'_\alpha)}\, dE'_\alpha$$

Nuclide mass fraction

Avogadro constant

Over all α-particles

α-particle weight (or branching)

Nuclides according to the material composition

Target nucleus mass number

Existing tools for the neutron yield calculations

	Name	References and links	Availability
1	USD (web-based tool)	http://neutronyield.usd.edu; Mei et al. NIMA 606 (2009) 651. arXiv:0812.4307	Publicly available
2	NEDIS-2.0	G. N. Vlaskin and Yu. S. Khomyakov, Atomic Energy, Vol. 130, No. 2, June, 2021 G. N. Vlaskin et al. Atomic Energy, Vol. 117, No. 5, March 2015 G. N. Vlaskin, NEDIS2.0, Prepring VNIINM 06-1 (2006)	Private, but possibly on request
3	SOURCES4A SOURCES4C	W.B. Wilson et al., Technical Report LA-13639-MS, Los Alamos, 1999; Carson et al. Astropart. Phys., 21 (2004) 667; Lemrani et al. NIMA 560 (2006) 454; M. Herman et al. Nucl. Data Sheets 108 (2007) 2655; Tomasello et al. NIMA, 595 (2008) 431; Tomasello et al. Astropart. Phys., 34 (2010) 70 V. A. Kudryavtsev, P. Zakhary, and B. Easeman, NIMA 972 (2020) 164095	Updated version: private, but possibly on request Original version (2002): The SOURCES code package, including documentation, may be obtained from the Radiation Safety Information Computational Center (RSICC), P.O. Box 2008, Oak Ridge, TN 37831-6362 USA (http:/ /www-rsicc.ornl.gov/rsic.html)
4	SaG4n	http://win.ciemat.es/SaG4n/ E. Mendoza et al. NIMA 960 (2020) 163659. arXiv:1906.03903	Publicly available
5	**NeuCBOT**	**https://github.com/shawest/neucbot** **https://github.com/shawest/neucbot/tree/v-3.0** **S. Westerdale and P.D. Meyers. NIMA 875 (2017) 57–64**	**Publicly available**

NeuCBOT

NeuCBOT or **Neu**tron **C**alculator **B**ased **O**n **T**ALYS

- **Goal:** Create a tool that low-background experiments can use for estimating (α,n) neutron backgrounds, providing neutron yields and spectra (the latter if possible)
- Shawn Westerdale is an author of the original version and main contributor
- Three people are currently supporting and developing the project:
  - Shawn Westerdale
  - Maxim Gromov
  - Ivan Goncharenko
- **GitHub repository: https://github.com/shawest/neucbot**
- **References:**
  - S. Westerdale, P.D. Meyers, *Radiogenic Neutron Yield Calculations for Low Background Experiments*, arXiv:1702.02465, 6 Feb 2017
  - S. Westerdale, *A Study of Nuclear Recoil Backgrounds in Dark Matter Detectors*, Ph.D. thesis, Princeton University (2016)
- A new article that includes recent updates, upcoming improvements, new comparisons and estimations of uncertainties is under preparation

NeuCBOT

Advantages	Disadvantages
Easy to use: usable by non-experts out-of-the-box	Consider any material only as bulk, no option for surfaces or thin films
Flexible: usable by experiments with different materials, contaminants, and assumptions about secular equilibrium	No geometry configuration, so no complex objects or multilayer structures, only homogeneous contamination distribution
Fast calculation	No recent experimental data (last few years)
Written in Python, easy to modify and adaptable to different needs	Partial cross sections for excited states of the daughter nucleus are not implemented
Minimal dependencies (Python 3, Bash)	No option to calculate energy lost by the alpha before capturing
A set of libraries that speed up the calculations	
If the TALYS output is used, neutron spectra are available along with yields	
For α energies up to 10 MeV	

NeuCBOT versions

- **NeuCBOT v-1.0** (original version, outdated), NeuCBOT-v1 branch
  - based on TALYS-1.6 (TENDL-2015)
  - written specifically for Python 2.6.6 and 4.1.2
  - only neutron yields and spectra

- **NeuCBOT v-2.0** (current official version), master branch
  - TALYS-1.95 (TENDL-2019)
  - only neutron yields and spectra

- **NeuCBOT v-3.0** (beta, publicly available), v-3.0 branch , tag 3.0
  - also TALYS-1.95 (TENDL-2019)
  - JENDL/AN-2005
  - changing from Python 2 to Python 3 (tested on Python 3.8.10)
  - neutron and gamma yields and spectra

Usage

./neucbot.py –h
Usage: You must specify an alpha list or decay chain file and a target material file.
You may also specify a step size to for integrating the alphas as they slow down in MeV; the default value is 0.01 MeV

-l [alpha list file name]
-c [decay chain file name]
-m [material composition file name]
-s [alpha step size in MeV]
-t (to run TALYS for reactions not in libraries)
-d (download isotopic data for isotopes missing from database)
-d [v1,v2] (specify v1.0 (TALYS 1.6) or v2.0 (TALYS 1.95) database)
-o [output file name]

1) Run only for neutrons (standard option)
./neucbot.py -c Chains/Th232Chain.dat -m Materials/Acrylic.dat -o output.dat

Note: neucbot.py and neucbot_with_gamma.py will be merged shortly

2) Run for neutrons and gammas
./neucbot_with_gamma.py -t -c Chains/Th232Chain.dat -m Materials/Acrylic.dat -o output_with_gamma.dat

Run TALYS-1.95 because the gamma data haven't added to the downloadable libraries yet

User inputs

α source description

α energy list

List of…

α energies in MeV &
Percent relative intensity

```
# Example      Alpha Source
5 100
6 50
```

Isotope list (e.g. decay chains)

List of…

Isotope (e.g. Th232) &
Percent relative abundance

```
# Th232 Decay Chain Alpha-Emitters
Th232 100
Th228 100
Ra224 100
Rn220 100
Po216 100
Bi212 35.94
Po212 64.06
```

Decay info scraped from NuDat and compiled into a local library

Material composition

List of…

Chemical symbol
Mass number (0 means natural abundance)
Percent mass

```
# Example Ar+Xe Mixture
Ar 36 0.167 J
Ar 38 0.032 T
Ar 40 49.802
Xe  0 50 J
```

In v3.0

JENDL/AN-2005 library (J)

TENDL library (T)
(also if no symbol)

Example output

From integrating cross sections directly

```
# Total neutron yield =  9.71666685097e-07  n/decay
c12.0 0.0
c13.0 8.55700532908e-07
h1.0 0.0
h2.0 0.0
o16.0 0.0
o17.0 1.23641936001e-08
o18.0 1.03601958589e-07
# Integral of spectrum =  9.89634575434e-07  n/decay 0
2.62220094277e-13
100 2.72591038813e-10
200 1.68369480721e-10
300 1.26346507089e-10
[...]
```

Contributions from different isotopes

Neutron energy spectrum in keV

From integrating sum of the neutron spectrum

v-3.0: The similar output is produced for gammas along with the neutron output in case of $(\alpha, n\gamma)$ reactions

Databases: downloaded by default

- NeuCBOT comes with some data automatically and generates a local database with additional data as needed

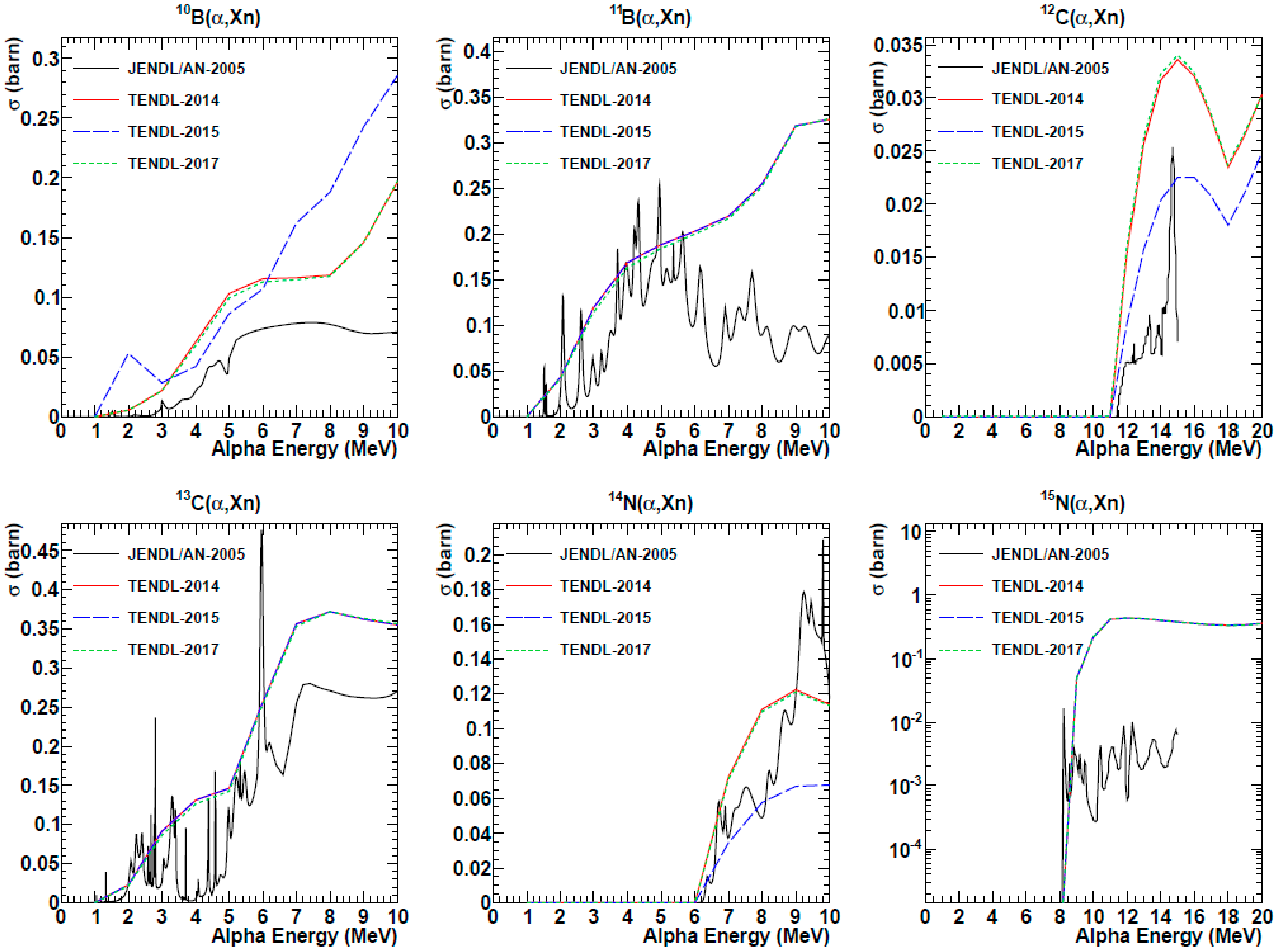
- Elemental isotopic abundance in **./Data/abundances.dat:**
  - From P. De Biévre and P.D.P. Taylor, "Table of the isotopic compositions of the elements", Int. J. Mass Spectrom. Ion Processes, 123 (2) (1993) 149-166
  - Used for determining default abundances when "0" is specified for the mass number in the material file – relevant for slowing and capturing α's

- Elemental stopping powers **./Data/StoppingPowers/[Chemical Symbol].dat:**
  - Contains SRIM stopping power tables for α's in pure element from 10 keV to 10 MeV

Databases: populated as needed

- **Isotope decay data ./Data/Decays/ensdf[Isotope].dat:**
  -Populated when NeuCBOT is run with an isotope list retrieving ENSDF files NNDC's website
  - Contains α-decay data about the isotope (energy and branching ratio)
- **Cross section and neutron spectrum calculation ./Data/Isotopes/[Ele]/[Isotope]/…**
  - **Gspectra/** : Gamma energy spectrum, generated by TALYS
  - **NSpectra/** : Neutron energy spectrum, generated by TALYS
  - **TalysInputs/** : auto-generated input files for running TALYS, currently using default model parameters
  - **TalysOut/** : detailed TALYS output file describing α reactions, outgoing γ's and excited daughters
  - **JendlOut/**: extracted (α,n) cross sections from JENDL/AN-2005
  - **Database generation options:**
    Auto-generated with local TALYS installation (-t option)
    Pulled from a pre-generated database (-d option): available for all natural isotopes for α energies up to 10 MeV
    - NeuCBOT-v1.0 uses database generated with TALYS-1.6 (checkout branch to access)
    - NeuCBOT-v2.0 uses database generated with TALYS-1.95 (currently default, master)
    - NeuCBOT-v3.0 uses database generated with TALYS-1.95 (checkout v-3.0 branch , tag 3.0)

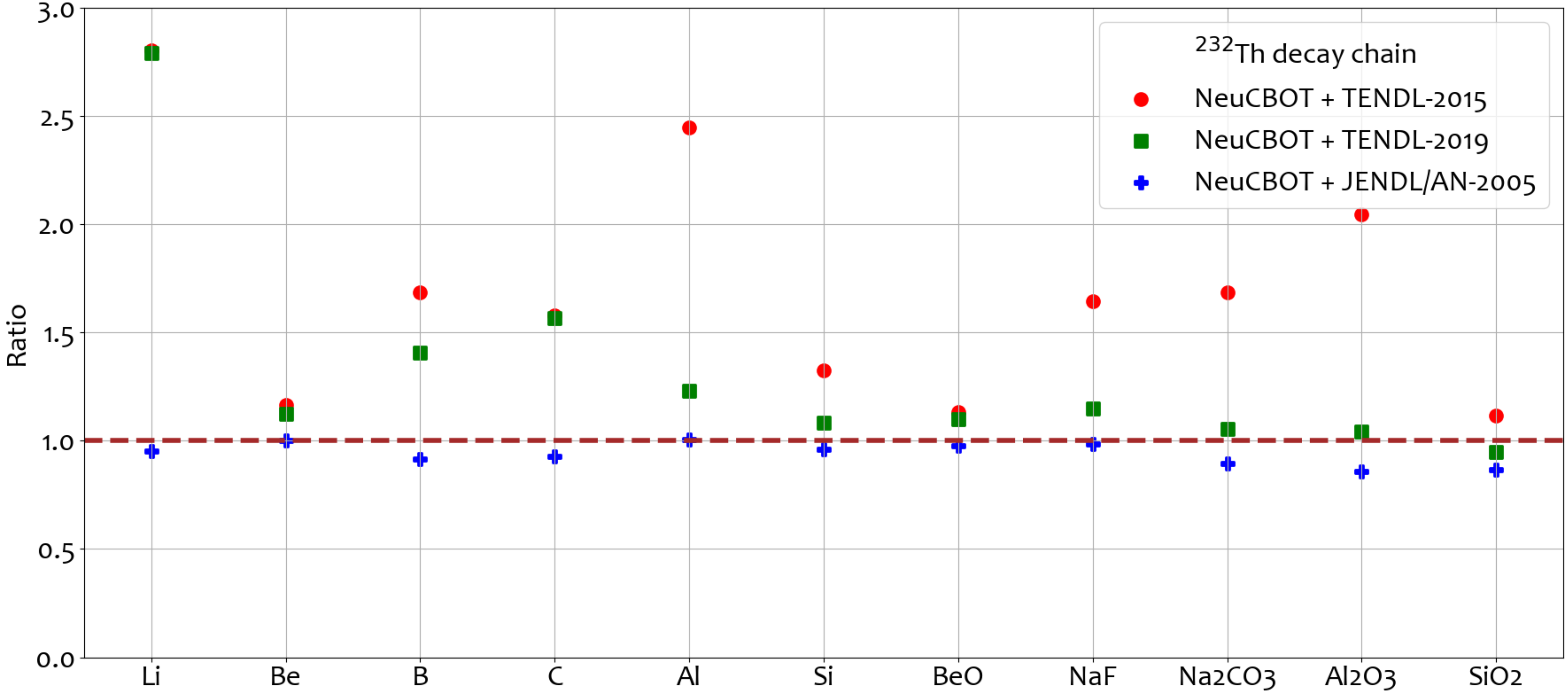
Issue: cross sections for different isotopes and libraries



E. Mendoza et al., Neutron production induced by α-decay with Geant4, [NIMA 960 (2020) 163659](), [arXiv:1906.03903]()

Results of implementation of the JENDL/AN-2005 library

Calculated-to-experimental ratios for the ^{232}Th decay chain and different NeuCBOT versions



The measured values and those of SOURCES, NEDIS and USD are from
A. C. Fernandes, A. Kling and G. N. Vlaskin, Comparison of thick-target (alpha,n) yield calculation codes, EPJ Web Conf. 153 (2017) 07021.

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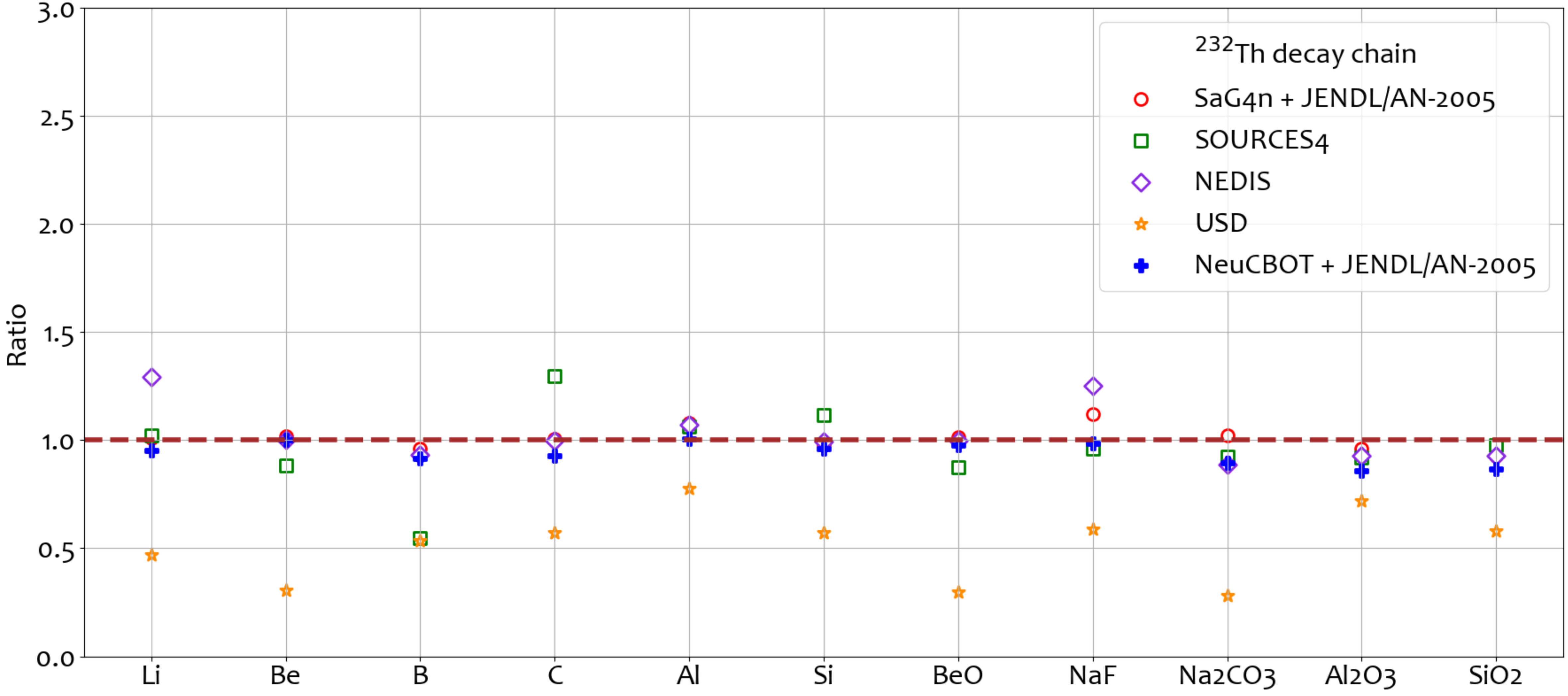
The SaG4n results are taken from
E. Mendoza et al., Neutron production induced by α-decay with Geant4, NIMA 960 (2020) 163659, arXiv:1906.03903.

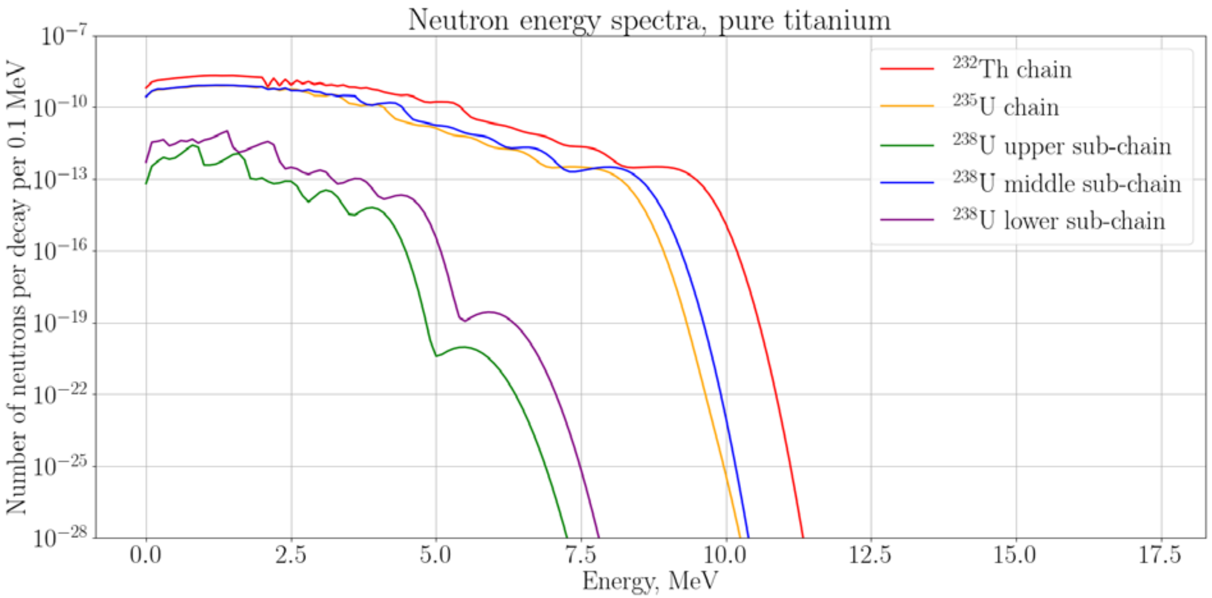
Calculated-to-experimental ratios for the ^{232}Th decay chain and different codes

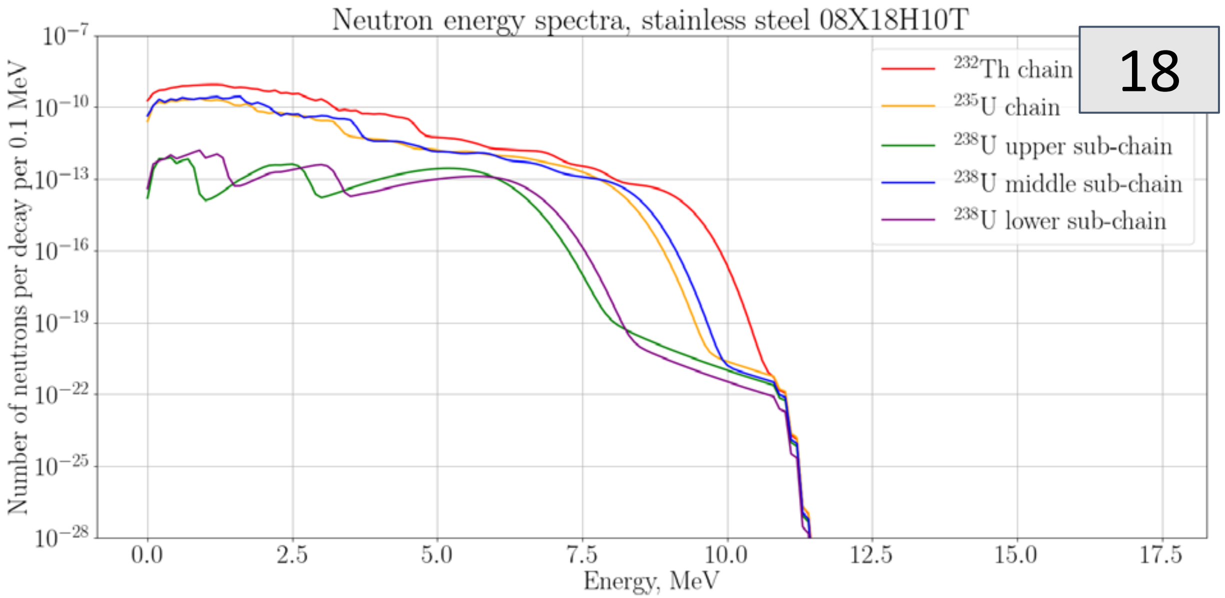


Material	Neutron yield, 10^{-8} neutrons per decay of the parent nucleus				
	^{232}Th	^{235}U	^{238}U upper	^{238}U middle	^{238}U lower
Cu	27	1.3	0	2.7	0
Cu20Ti80	510	180	0.15	200	0.7
Ti	620	220	0.18	240	0.9
VT1-00	625	230	0.4	240	1.1
VT1-0	630	230	0.6	250	1.45
Stainless steel 08X18H10T	190	39	0.13	51	0.18

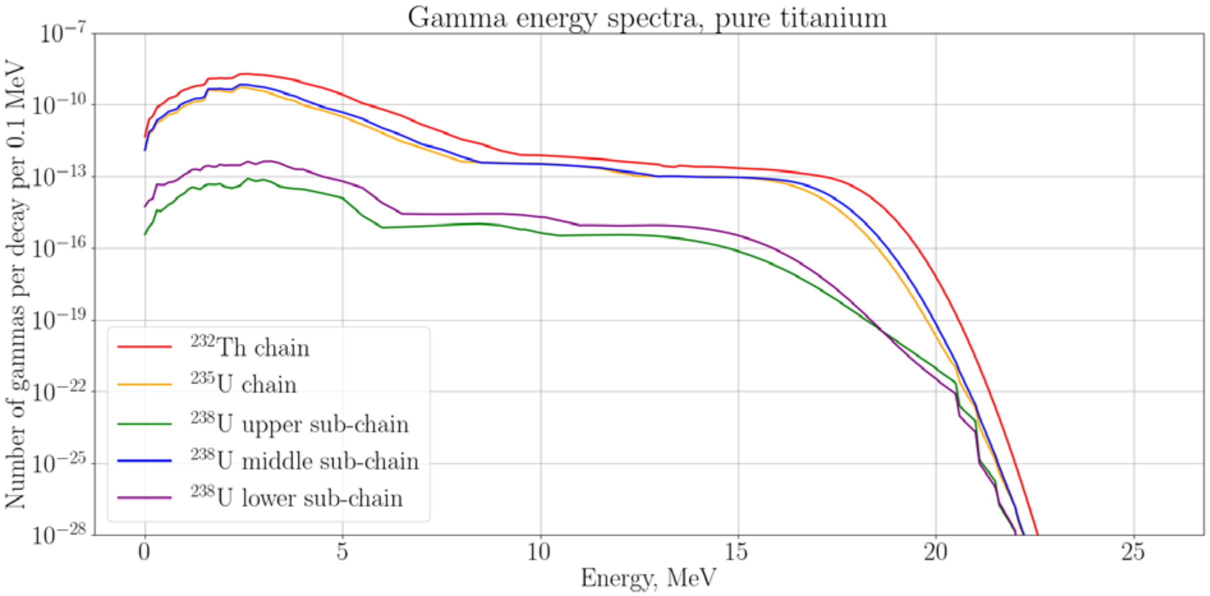
Material	Gamma yield, 10^{-10} gammas decay of the parent nucleus				
	^{232}Th	^{235}U	^{238}U upper	^{238}U middle	^{238}U lower
Cu	62	29.5	0.02	23	0.16
Cu20Ti80	72	29	0.06	29	0.18
Ti	74	29	0.07	30	0.19
VT1-00	74	29	0.11	30	0.23
VT1-0	74	30	0.16	30	0.27
Stainless steel 08X18H10T	32	23	0.4	16.4	1.3

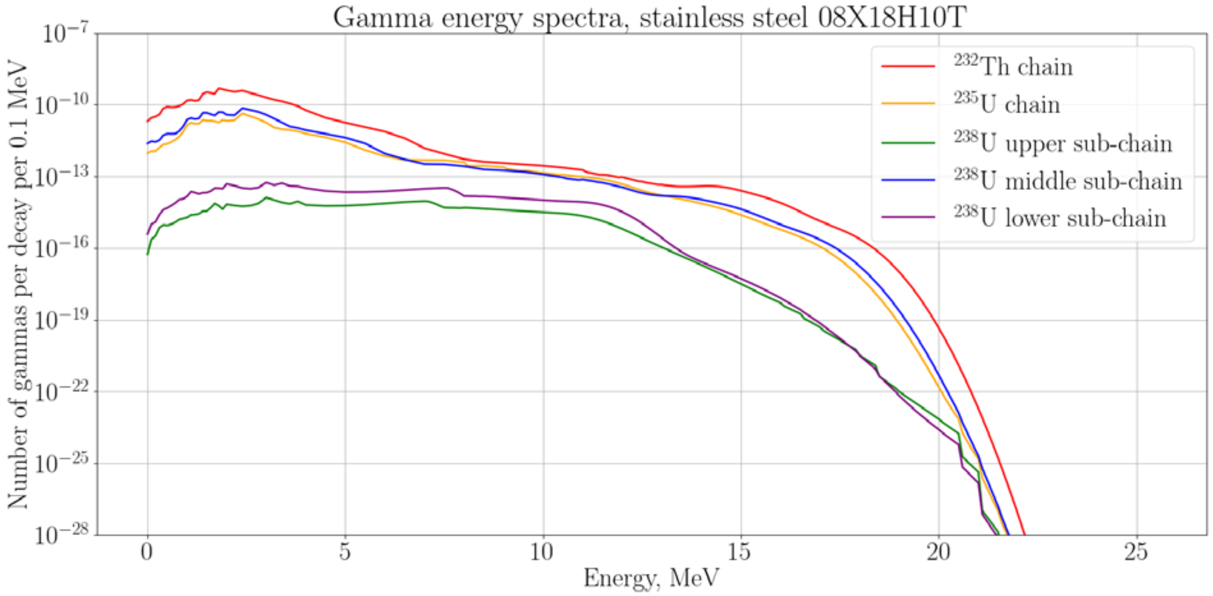
(α,$n\gamma$) reactions are subdominant with respect to (α,n) reactions (as expected)





Some examples of neutron and gamma spectra





Calculation examples: plastics doped by gadolinium

Material	Neutron yield, 10^{-7} neutrons per decay of the parent nucleus				
	^{232}Th	^{235}U	^{238}U upper	^{238}U middle	^{238}U lower
PMMA	13.18	14.02	2.11	8.47	1.16
PMMA + Gd_2O_3 (1.5 wt% Gd)	13.10	13.94	2.09	8.42	1.15
PMMA + $Gd(C_5H_7O_2)_3$ (1.5 wt% Gd)	13.12	13.96	2.10	8.44	1.15
PMMA + GdF_3 (1.5 wt% Gd, ≈0.5 wt% F)	18.41	19.41	2.50	11.74	1.51

Calculated with NeuCBOT + TALYS-1.95

More details are available in the following article

M. Zykova et al., Hybrid Ultra-Low-Radioactive Material for Protecting Dark Matter Detector from Background Neutrons, Materials **2021**, *14*(13), 3757

Planned new features

- **Data-driven corrections** to (α,n) cross sections and α stopping powers with uncertainty estimate
  - Including options to choose between SRIM and ICRU 49 calculations, and to include Core and Bond corrections
- **Further optimizing the TALYS model parameters**
- **Alternative cross section libraries,** where available
  - ENDF/B-VIII, EMPIRE, User-added (especially in case of recent publications)
- **Use of partial cross sections** for excited states of the daughter nucleus
- **Total α energy loss** calculations prior to capture
- **Non-homogeneous** contamination distribution yield calculations
- **Graphical interface**
- **Ability to visualize and compare spectra**

Conclusions

- The updated version of NeuCBOT (v3.0) is about to be released
  Its beta version is already available on GitHub
- NeuCBOT-v3.0 shows significantly better agreement with experimental data if the JENDL/AN-2005 library is used
- Now one can get gamma yields and spectra along with neutron yields and spectra
- The transition from Python 2 to Python 3 is done

- A lot of new and interesting features are planned. Feel free to contribute!
- Understanding the systematic uncertainties in these (α,n) yield calculations is one of the next important steps
- Multiple, independent tools for calculating (α,n) yields will allow us to more thoroughly understand the range of possible yields, given the substantial uncertainties

Thank you for your attention!