(α,n) data for applications
&
SaG4n, an (α,n) simulation tool based on GEANT4

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The MANY collaboration

Motivation

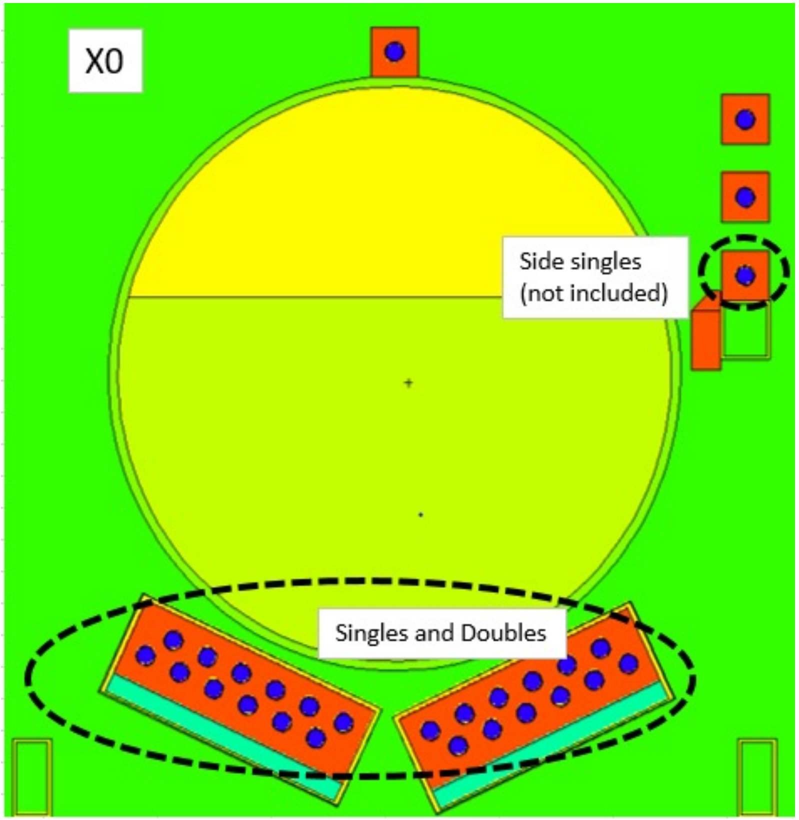
Knowledge on (α,Xn) reactions is required in several fields:

- **Nuclear structure.** Most of our actual experimental knowledge on (α,Xn) reactions comes from nuclear structure experiments between the 50's and the 70's.
- Neutron background in underground experiments (nuclear astrophysics, **Dark Matter**) due to radiogenic α-decay chains.
- **Nuclear astrophysics.** Neutron sources in collapsing stars linked to the r-process. E_α below ~1 MeV (around the Gamow peak).
- **Nuclear technologies, non-proliferation and homeland security.** α-emitters present in fresh/irradiated nuclear fuels can create a neutron source through (α,Xn) reactions with (light) surrounding nuclei: fluorine, oxide and carbide fuels, vitrified nuclear waste…
  - Determination of the ^{235}U enrichment.
  - NDAnalysis of irradiated fuels / fuels enriched in MA / MOX fuels.
  - Neutron source term in the deep geologic repository

  Yesterday's review talk by C. Romano

Contribution of the uncertainty in the nuclear data to the uncertainty budget for UF_6 cylinder measurements

Passive Neutron Enrichment Meter (PNEM)



- Two briefcase size polyethylene pods with twelve ^{3}He tubes at 10 atm.
- Varied enrichments and fraction of UF_6 bound to walls.
- (a,n) source terms built on the Jacobs & Liskien data ('83 and '85), modeled with SOURCES4C
- Included a revaluation of the stopping power.

The total neutron yield has biggest impact. The neutron energies are needed for applying corrections to the neutron detection efficiency.

D.P. Broughton, S. Croft, C. Romano, A. Favalli, **Sensitivity of the simulations of passive neutron emission from UF_6 cylinder to the uncertainties in both ^{19}F(α,n) energy spectrum and thick target yield of ^{234}U in UF_6** (To be submitted to NIM A)

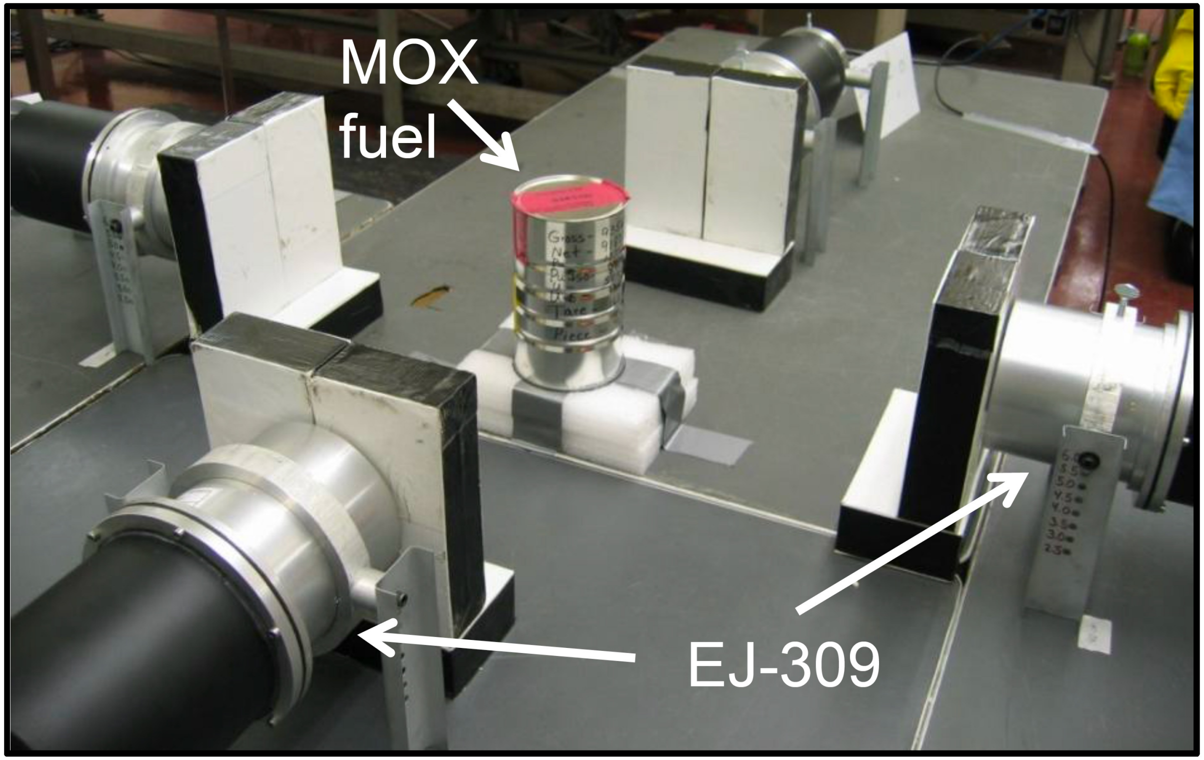
Contribution of the uncertainty in the nuclear data to the uncertainty budget for UF_6 cylinder measurements

Neutrons per s per g ^{234}U (1σ range)	Source
460	(Reilly et al. 1971)
576 ± 7.3% (533-618)	(Sampson 1974)
474 ± 4.4% (453-494)	(Miller et al. 2014)
503 ± ~4% (483-523)	(Kulisek et al. 2017; uncertainty estimated by Croft et al. 2020)
507 ± 1.1% (501-513)	(Croft et al. 2020)
610	SOURCES-4C (Wilson et al. 2002)
604	Modified SOURCES-4C (Wilson et al. 2002; private comm. Croft & Gauld 2020)

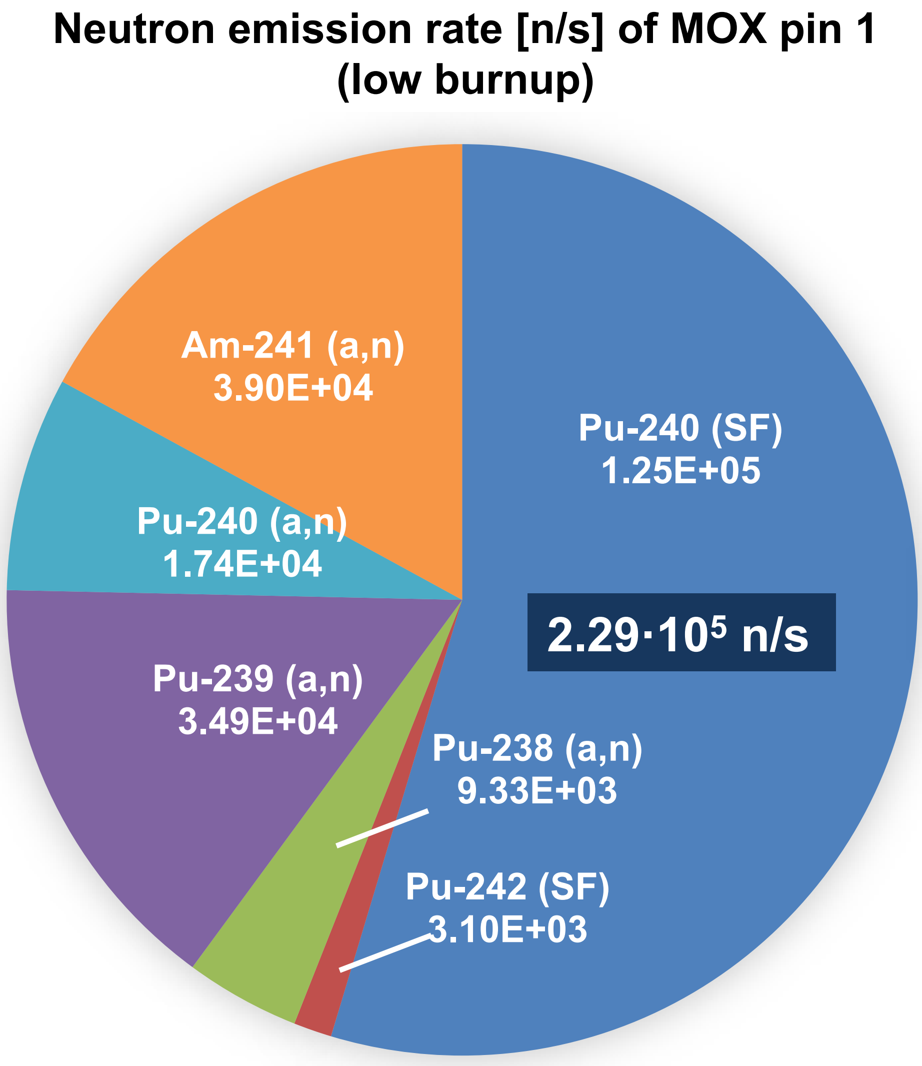
Quantification of ^{239}Pu and other fissile materials in irradiated materials

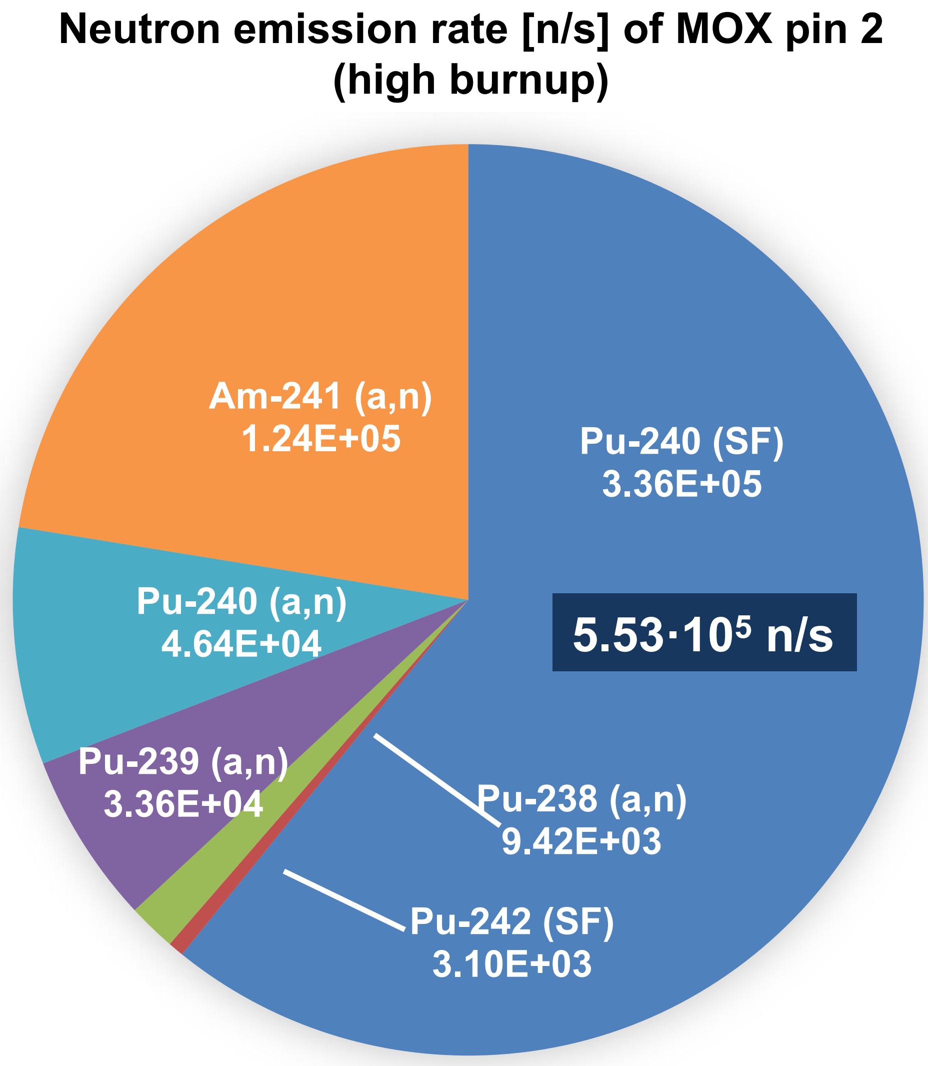
Characterization of different MOX fuel pins via correlated neutron/gamma emission.

J. L. Dolan et al. Passive measurements of mixed-oxide fuel for nuclear non-proliferation. NIMA 703 (2013) 102–108

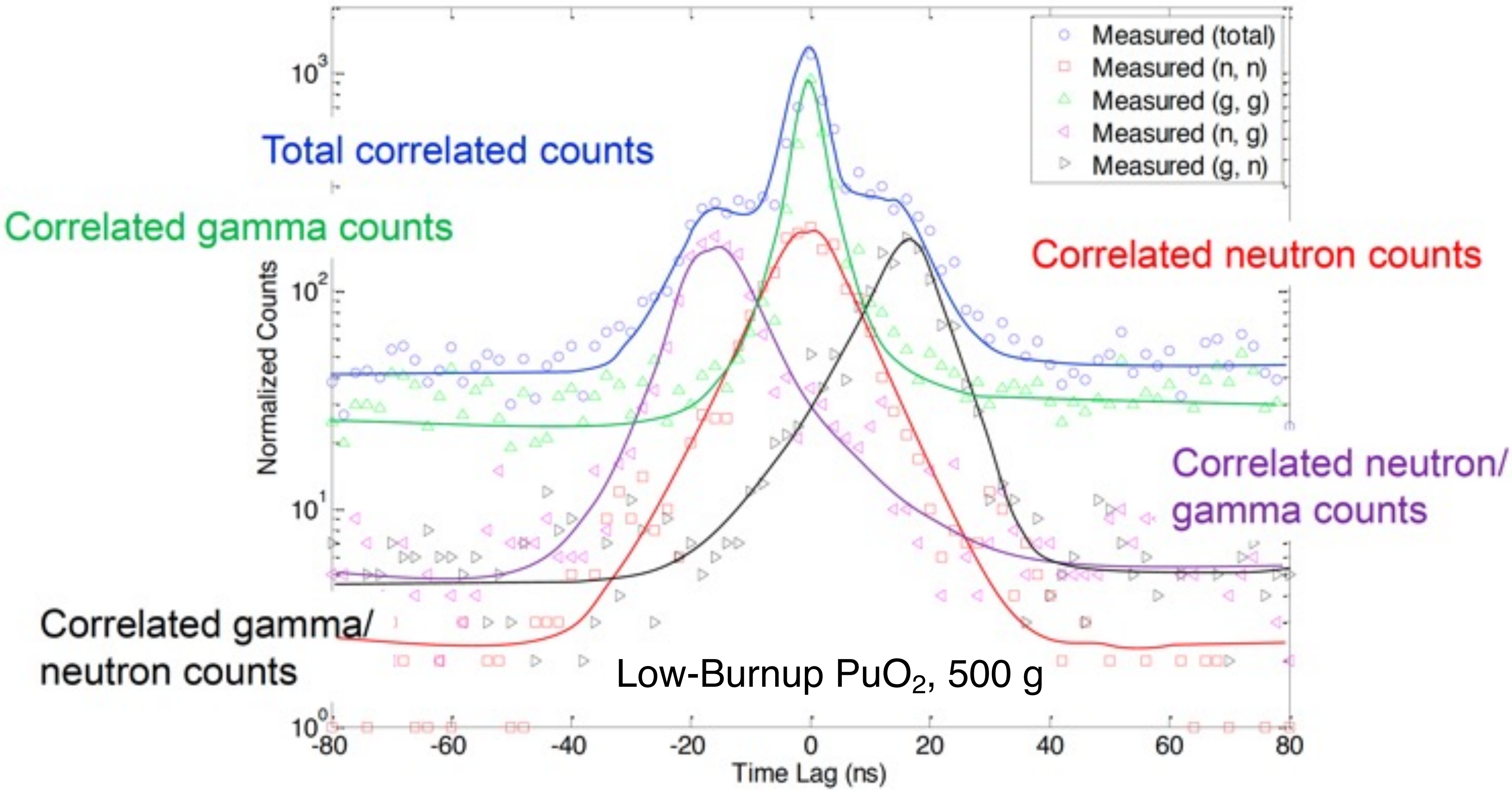


Neutron emission rates for different MOX pins

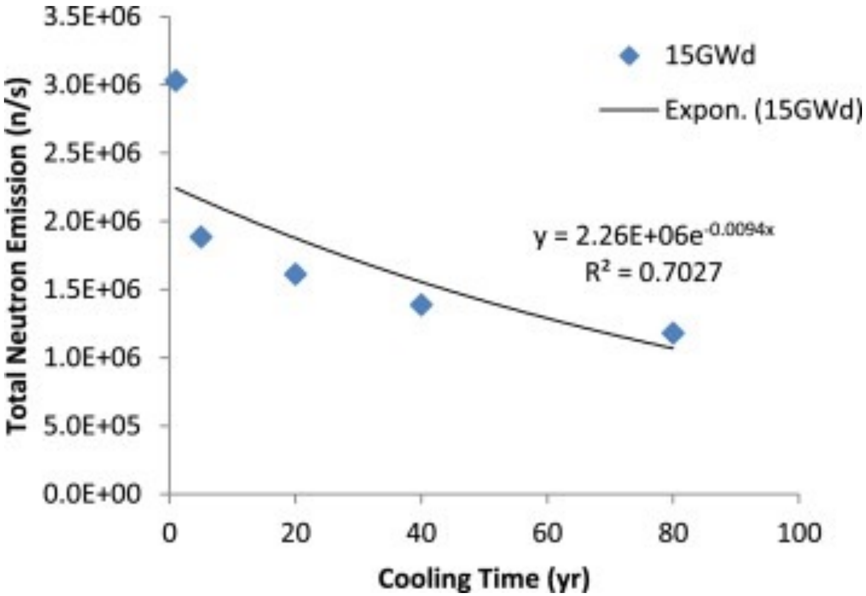


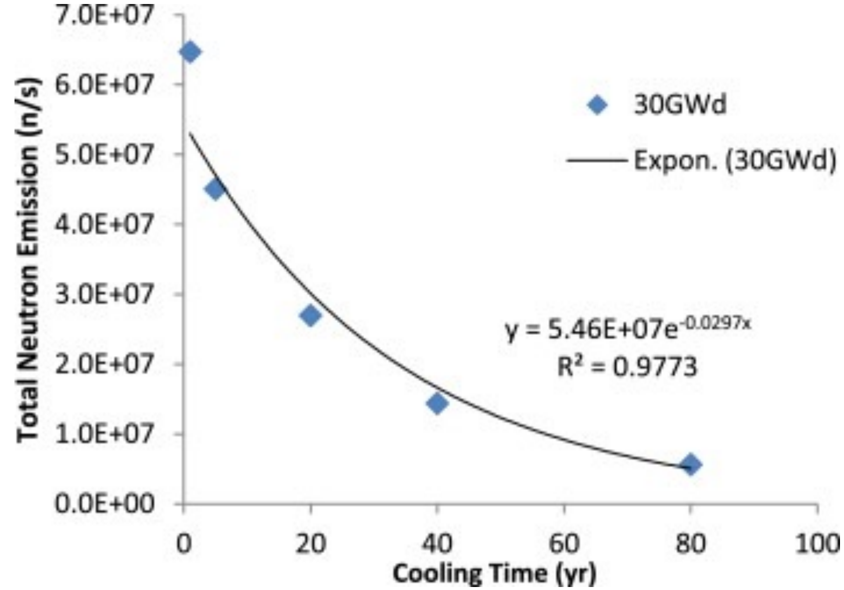


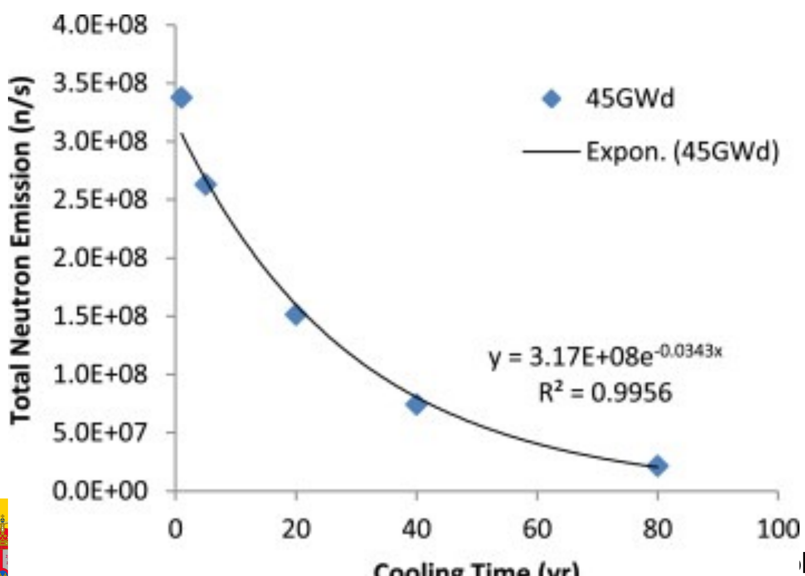
Quantification of ^{239}Pu and other fissile material



Correlation of neutron emission rate, burnup and spent fuel evolution







There is a **correlation between the burnup and neutron emission rates of irradiated nuclear fuel**. During the first 80 years, it is dominated by ^{244}Cm spontaneous fission. After 100 years, (α,n) reactions start to play a role. Relevant as well for **new types of fuels**: ATFs, fuels with high enrichment in minor actinides…

Weldon et al., [Progress in Nuclear Energy Volume 80](), April 2015, Pages 45-73

SaG4n

Simulation of (α,n) reactions with Geant4

E. Mendoza et al., *Neutron production induced by α-decay with Geant4*, Nucl. Instrum. Methods A 960, 163659 (2020)
https://doi.org/10.1016/j.nima.2020.163659

GEANT4 neutron yield and spectra calculator that can be downloaded freely from http://win.ciemat.es/SaG4n/

Calculation of (α,n) neutron yields and spectra

The calculation of the neutrons produced in (α,Xn) reactions in a certain material require:

- The calculation of the α-tracks → stopping powers.
- The cross sections of the neutron production reactions involved.
- The energy - angle distributions of the secondary neutrons.

Geant4	**ICRU 49 report**	**+**	**ENDF-6 format library**	→ **MC**
NeuCBOT	**SRIM**	**+**	**TALYS (Talk by Shawn)**	
NEDIS	**SRIM**	**+**	**own library**	
SOURCES	**SRIM**	**+**	**own library (+ EMPIRE)**	
USD	**ICRU 49 report**	**+**	**TALYS**	

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

Stopping cross section

Why Geant4?

Geant4 operates in a different way from the other codes → Complete Monte Carlo

Pros:

- Modelling complex geometries and material inhomogeneities
- Use of evaluated nuclear data libraries JENDL-AN-2005, TENDL, others coming?…
- Possibility of using event generators: correlated γ-ray and neutron emission
- Same code for generating and transporting the neutron and simulating a detection system
- Possibility of using various alfa transport models (in GEANT4)
- Open-source distribution with software maintenance (GEANT4 collaboration)
- Widely used

Cons:

- Slow → large CPU times, even with particle biasing techniques (1 n/10 alphas)

SaG4n input - powerful but simpe geometry treatment

```
# VOLUMES:
VOLUME 1 BigBox   7 2 0 - 20 10 10 0 0 0
VOLUME 2 MedBox01 7 2 0 - 4 6 10 12 -2 0
VOLUME 3 MedBox02 7 2 0 - 0.5  2.5 10 14.25  -3.75 0
VOLUME 4 Wheels01 8 3 0 - 2 1 -7 -5 6
VOLUME 4 Wheels02 8 3 0 - 2 1 +7 -5 6
VOLUME 4 Wheels03 8 3 0 - 2 1 -7 -5 -6
VOLUME 4 Wheels04 8 3 0 - 2 1 +7 -5 -6
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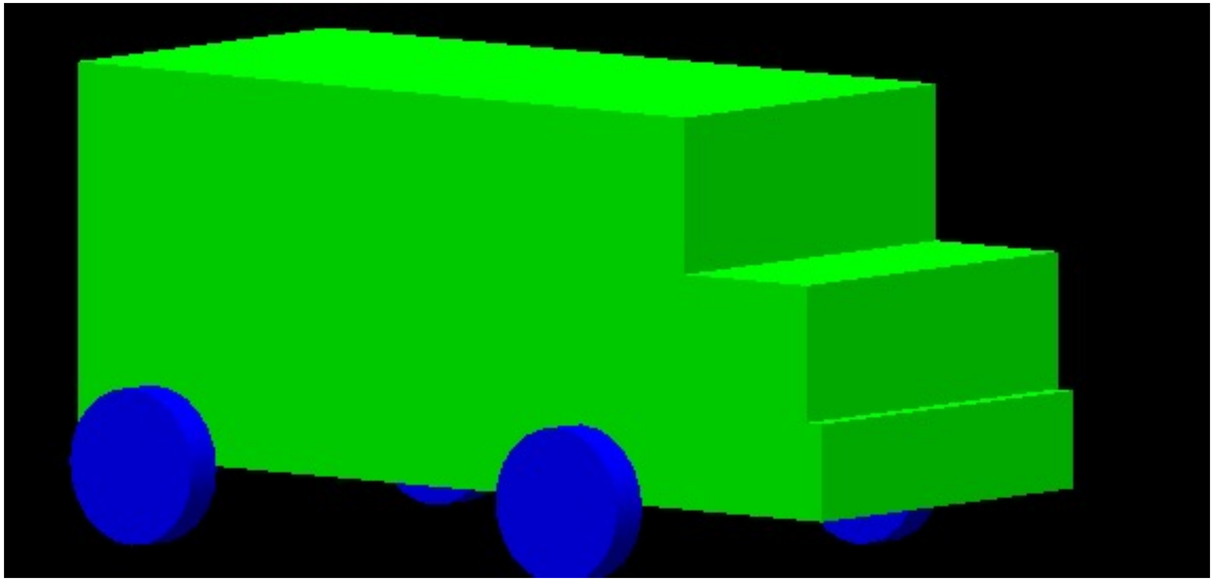

SaG4n comes with a manual and examples!

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Available “standard” evaluated nuclear data libraries

The following ”evaluated” libraries are available:

JENDL-AN-2005: this is an evaluated library (**experimental data** + theoretical calculations), Data a available for a small number of 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: generated with TALYS in an “automatic” way. The latest releases are TENDL-2014, TENDL-2015 and TENDL-2017 and more recently the TENDL-2019 (not yet revised by us)

There are two versions of each TENDL library:

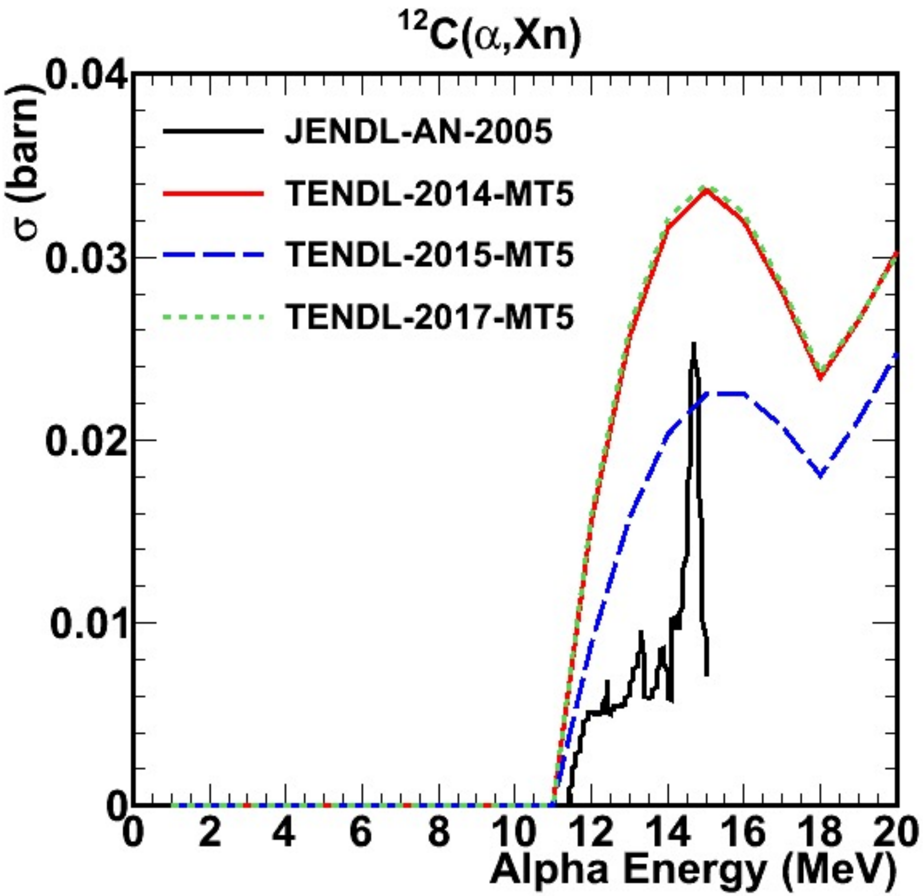
- One version with all the non-elastic channels added in a single channel (MT=5, (z,x) reaction).

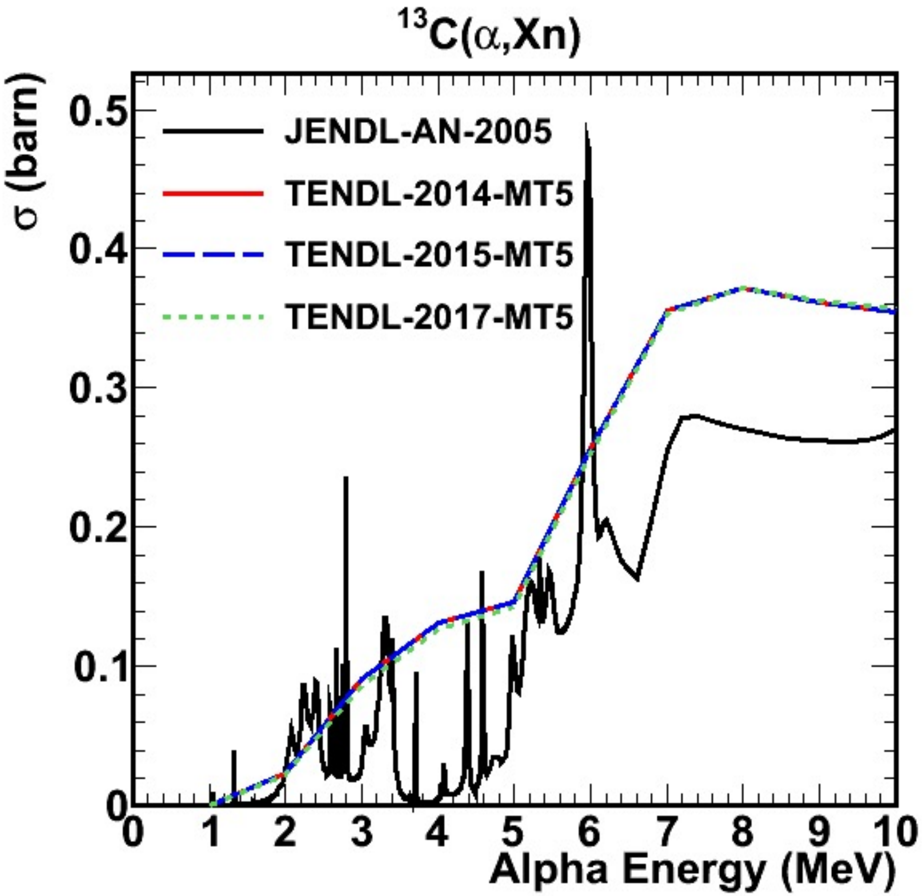
  → TENDL-XXXX-MT5

- Other version with individual channel cross sections up to 30 MeV.

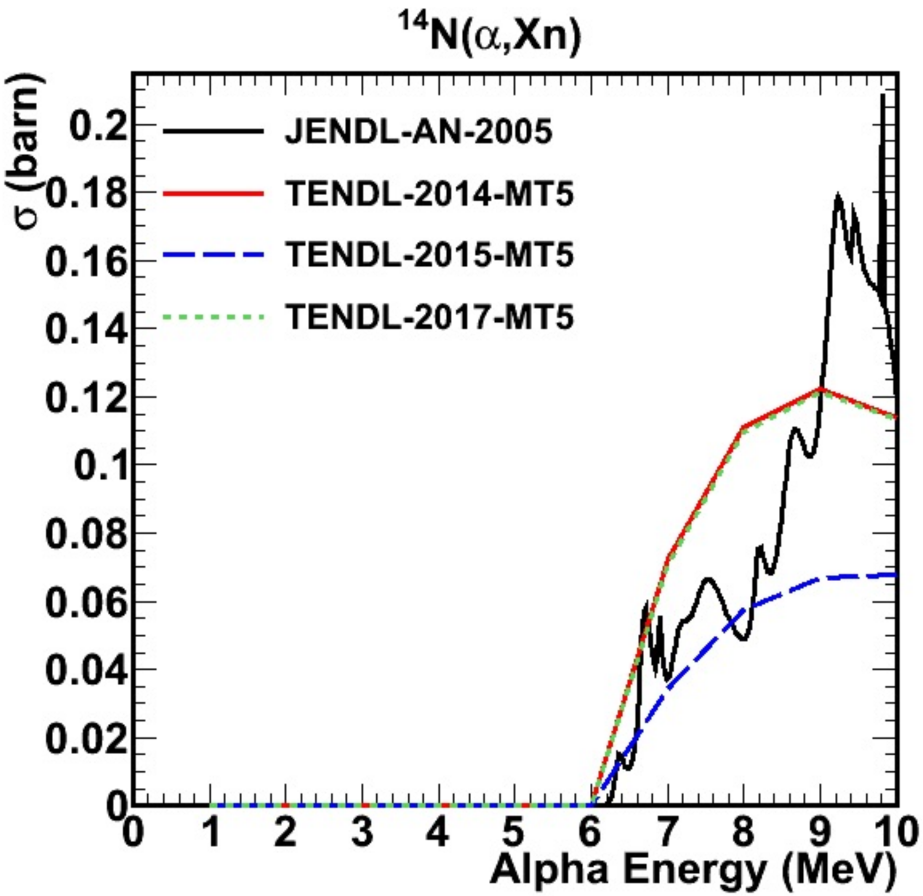
  → TENDL-XXXX-AllMT

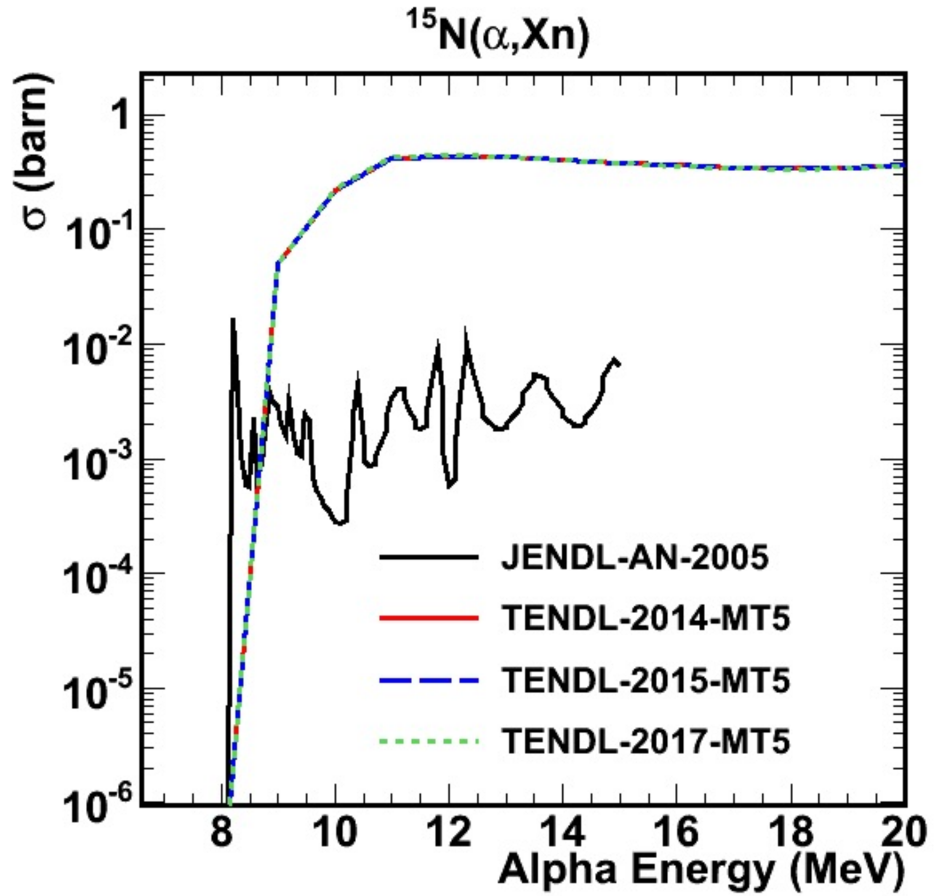
Comparison between JENDL-AN-2005 and TENDL-MT5



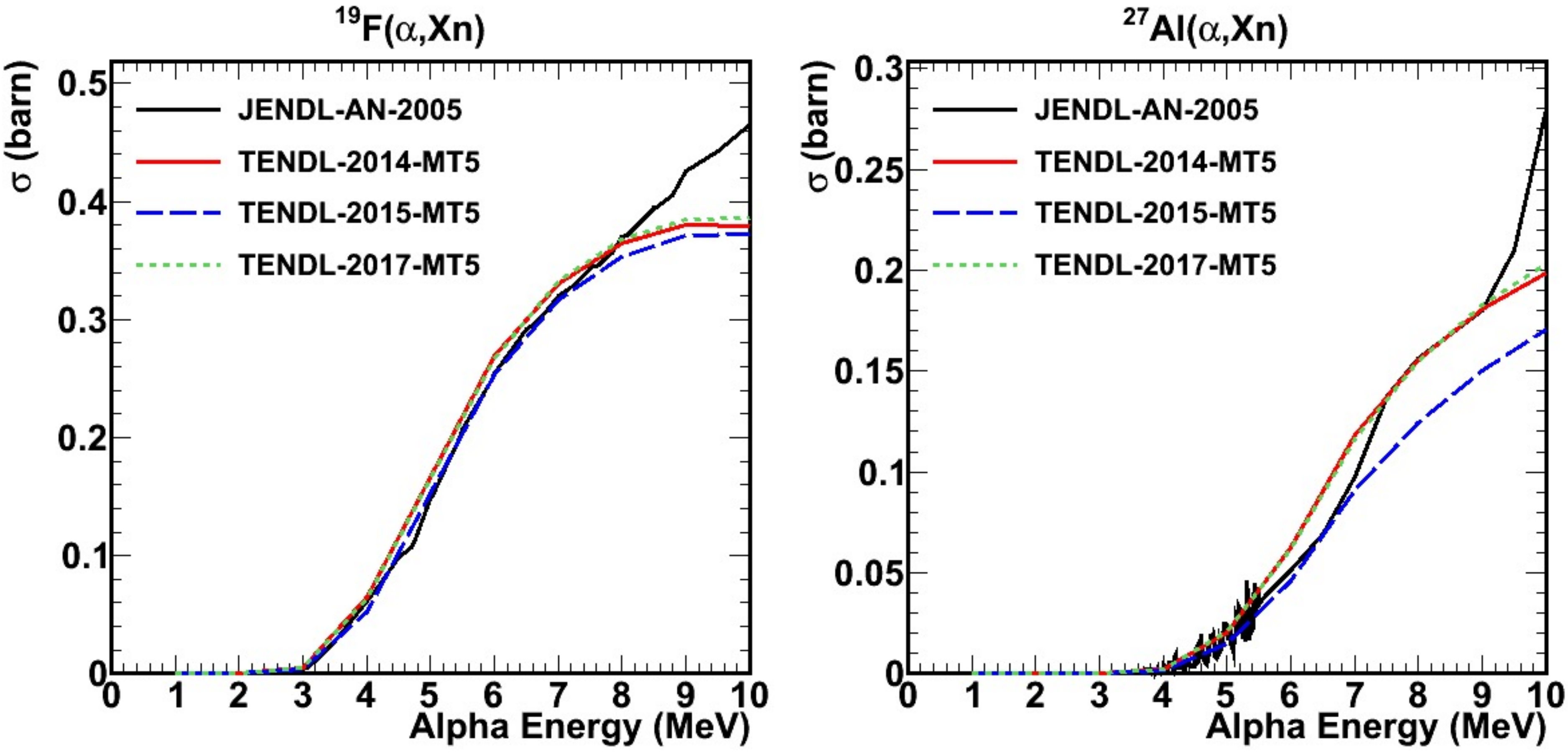


Comparison between JENDL-AN-2005 and TENDL-MT5

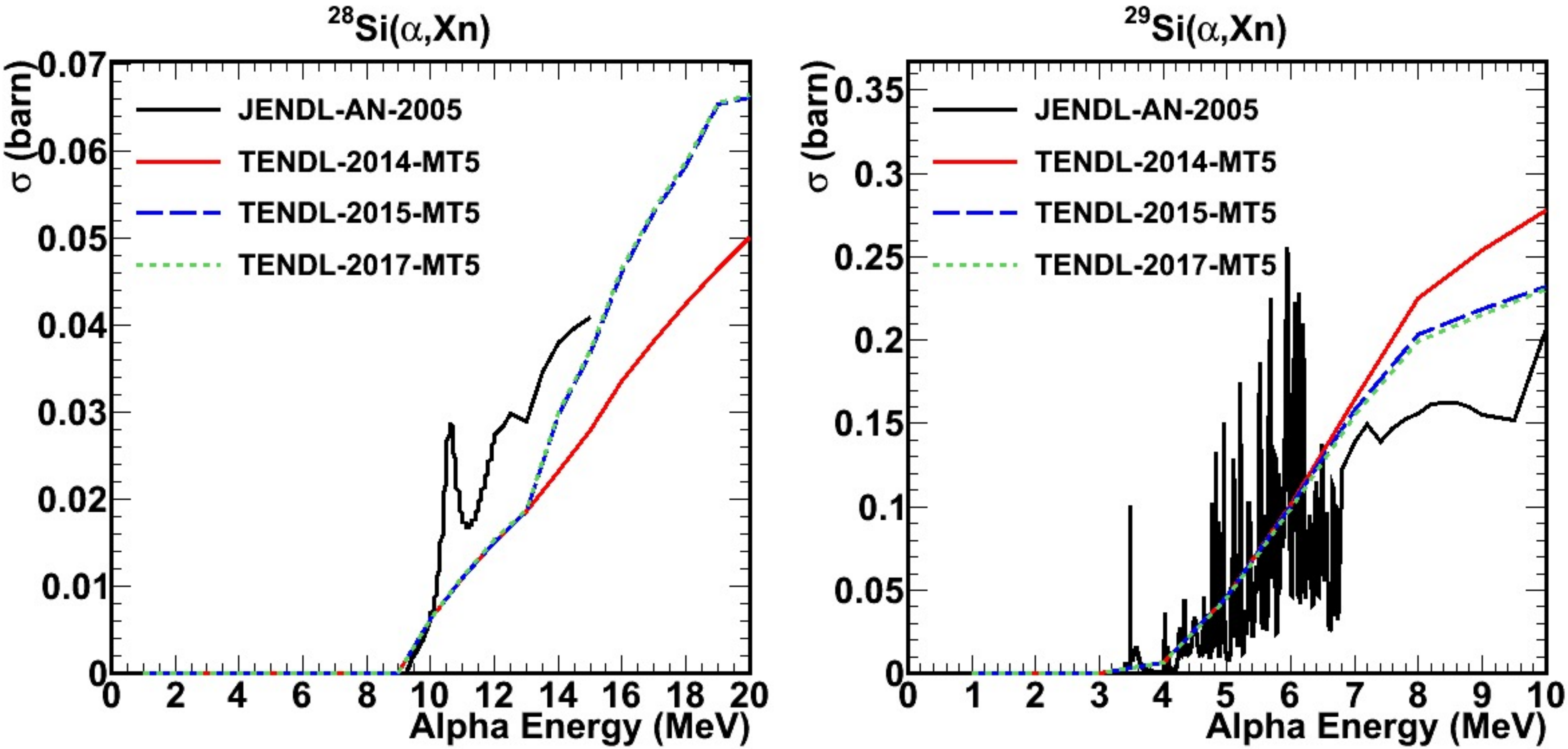




Comparison between JENDL-AN-



Comparison between JENDL-AN-2005 and TENDL-MT5



Observations

- JENDL-AN-2005 VS TENDL-MT5: there are sizeable differences between the cross sections (< 1 order of magnitude) with the exception of ^{15}N (which has a threshold at ~8 MeV). TENDL does not reproduce (by construction) the resonance behavior of the real cross section.

- TENDL-MT5: the recent releases of TENDL do not differ so much. In all the cases tested but $^{28,29}Si$ TENDL-2014-MT5 and TENDL-2017-MT5 are very similar.

Neutron spectra

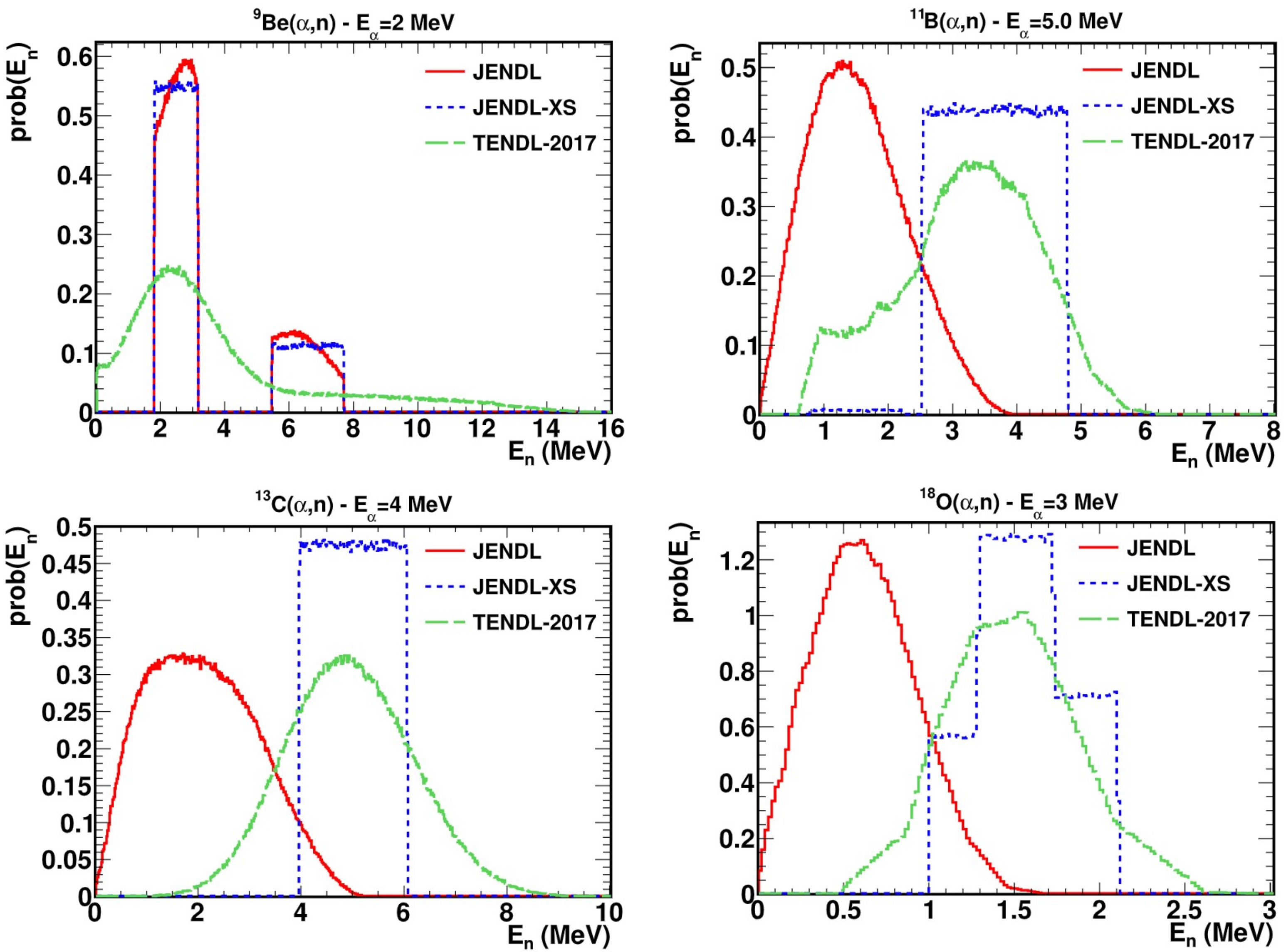
JENDL/AN-2005 has information on the individual (α,n_i) channels for some isotopes (example in next slide) and information about the neutron spectra.

Comment: the neutron spectra can be computed with two body kinematics in this case if the angular distribution is used (or assumed to be isotropic in the CM system). According to the JENDL evaluators, the mEXIFON and EGNASH-2 code were used for producing the enegy-angle neutron emission distributions.

The **TENDL** library used had only information about one single **(α,n)** channel.

Comparison of three simulations with GEANT4 for 4 isotopes for which **(α,n_i)** partial cross sections and spectra are provided:

- JENDL as it is.
- JENDL-XS. The neutron spectra are computed from 2-body kinematics.
- TENDL as it is (no information on the partial cross sections).



Conclusion: there seems to be some issue with JENDL energy spectra.

Recommended data library for SaG4n

Recommended for SaG4n: the **JENDLTENDL01** library

- The **17 isotopes of JENDL/AN-2005** with modifications: The data tables concerning the energy-angular distributions of the neutrons from (α,n) reactions (MT=4) on ^{6,7}Li, ^{10,11}B, ^{13}C, ^{14,15}N and ^{17,18}O have been removed. These energy-angular distributions are then computed by GEANT4 from the information of the excited state of the residual nucleus (information provided by the library). An isotropic neutron angular distribution in the CM system is assumed, and the energy of the emitted neutrons is obtained from two-body kinematics.

- TENDL-2017 for all the rest of isotopes.

We will updated it son with the TENDL-2019 or 2021.

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Validation and verification of SaG4n

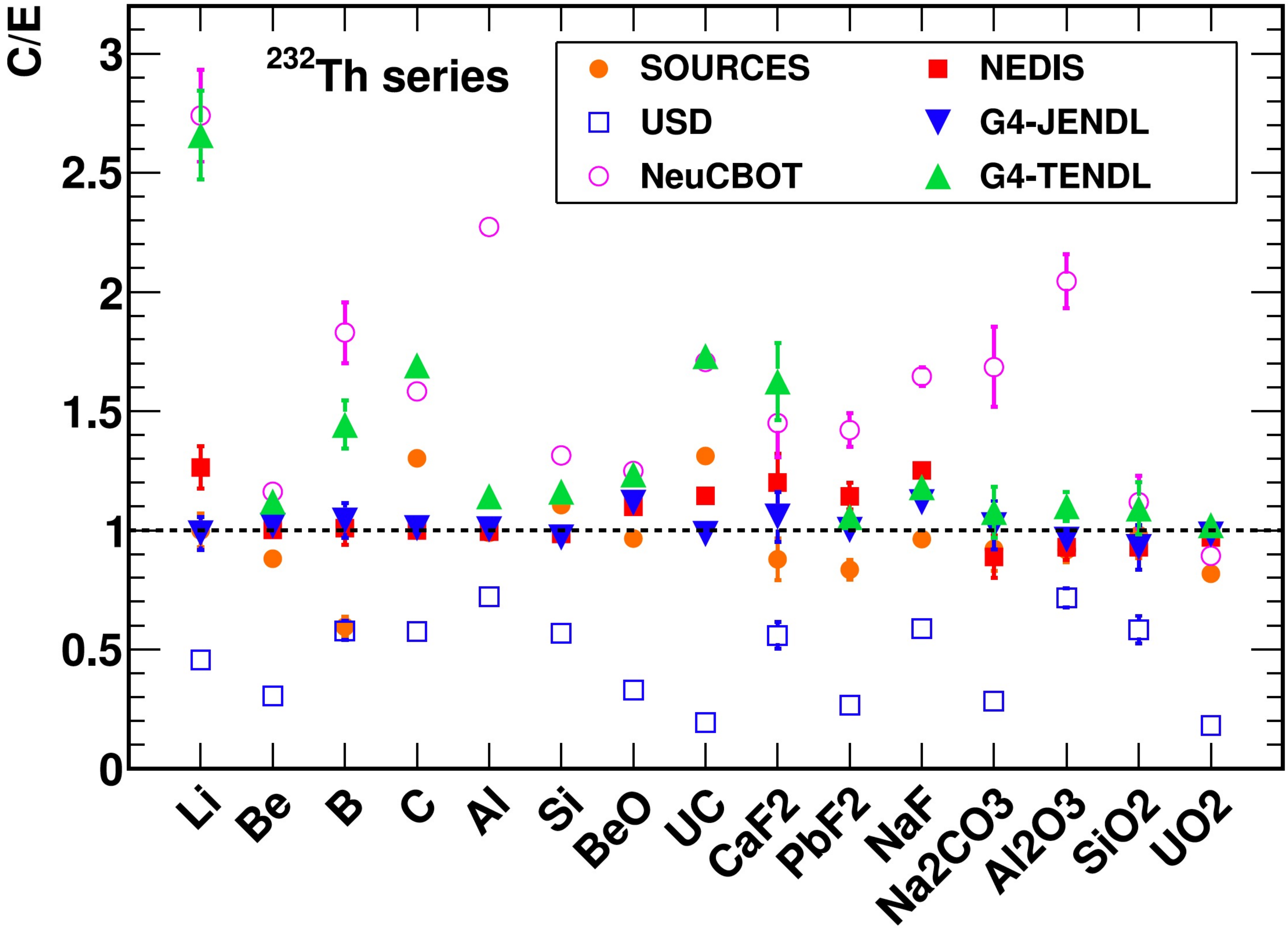
(α,xn) thick target yields for α's from the natural decay chains in secular equilibrium:

- SaG4n with JENDL and TENDL
- NeuCBOT
- USD
- NEDIS

USD and NEDIS: values from Fernandes et al. EPJ Web Conf., 153 (2017) 10.1051/epjconf/201715307021

Experimental data:

- Gorshkov G.V. and Tsvetkov O.S., Sov. At. Energy, 14 (6) (1964), pp. 573-577 ^{232}Th and ^{238}U decay series data for Be, B, C, O, F, Na, Mg, Al and Si.
- West, A. Sherwood, Ann. Nucl. Energy 9 (11) (1982) 551–577
- http://dx.doi.org/10.1016/0306-4549(82)90001-9.
- J.K. Bair, J.G. del Campo, Nucl. Sci. Eng. 71 (1) (1979) 18–28, http://dx.doi.org/10.13182/NSE71-18.
- E. Norman, T. Chupp, K. Lesko, P. Grant, G. Woodruff, Appl. Radiat. Isot. 103 (2015) 177–178, http://dx.doi.org/10.1016/j.apradiso.2015.04.018.
- Y. Feige, B.G. Oltman, J. Kastner, Production rates of neutrons in soils dueto natural radioactivity, J. Geophys. Res. 73 (10) (1968) 3135–3142, https://doi.org/10.1029/JB073i010p03135



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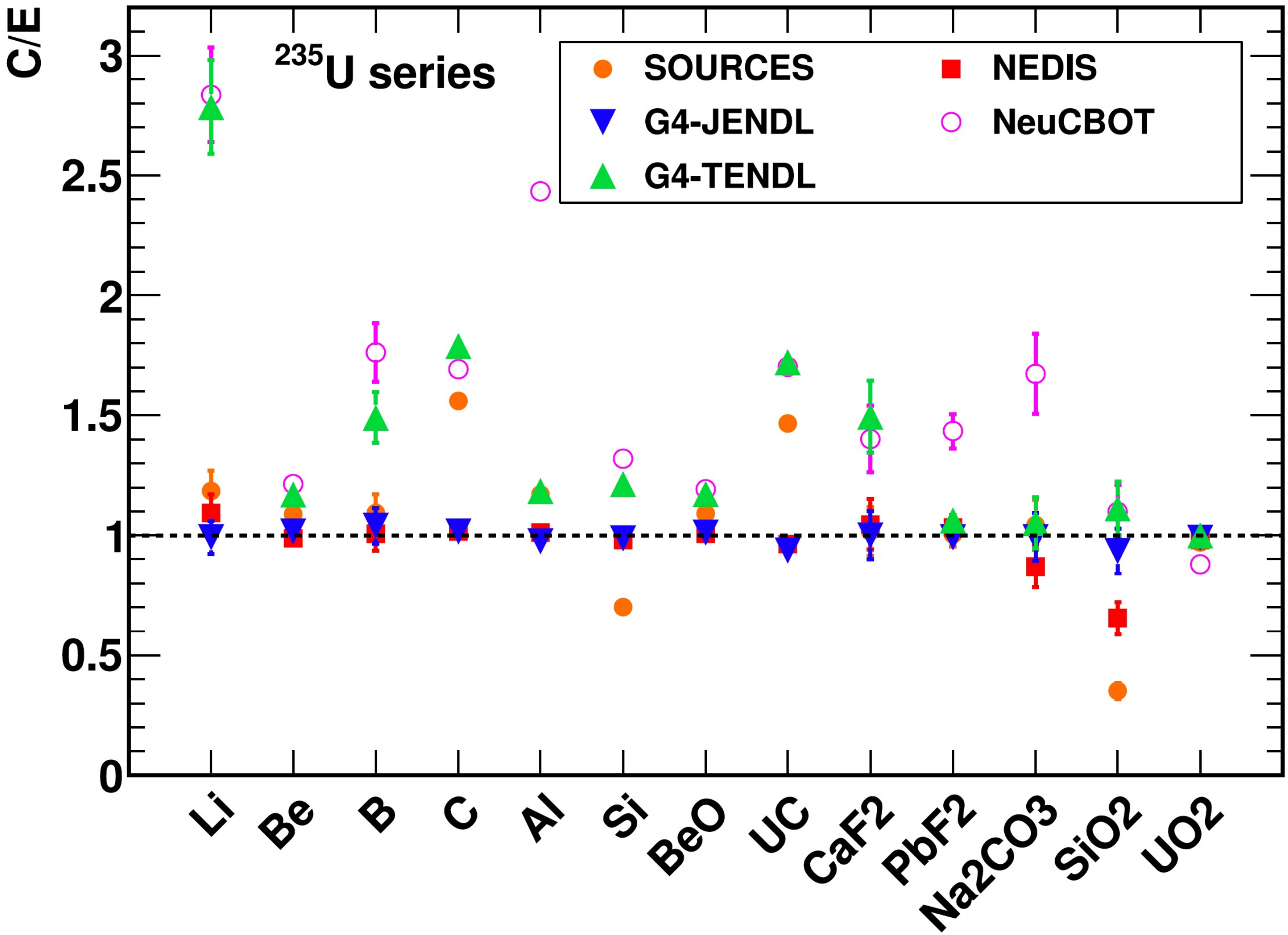

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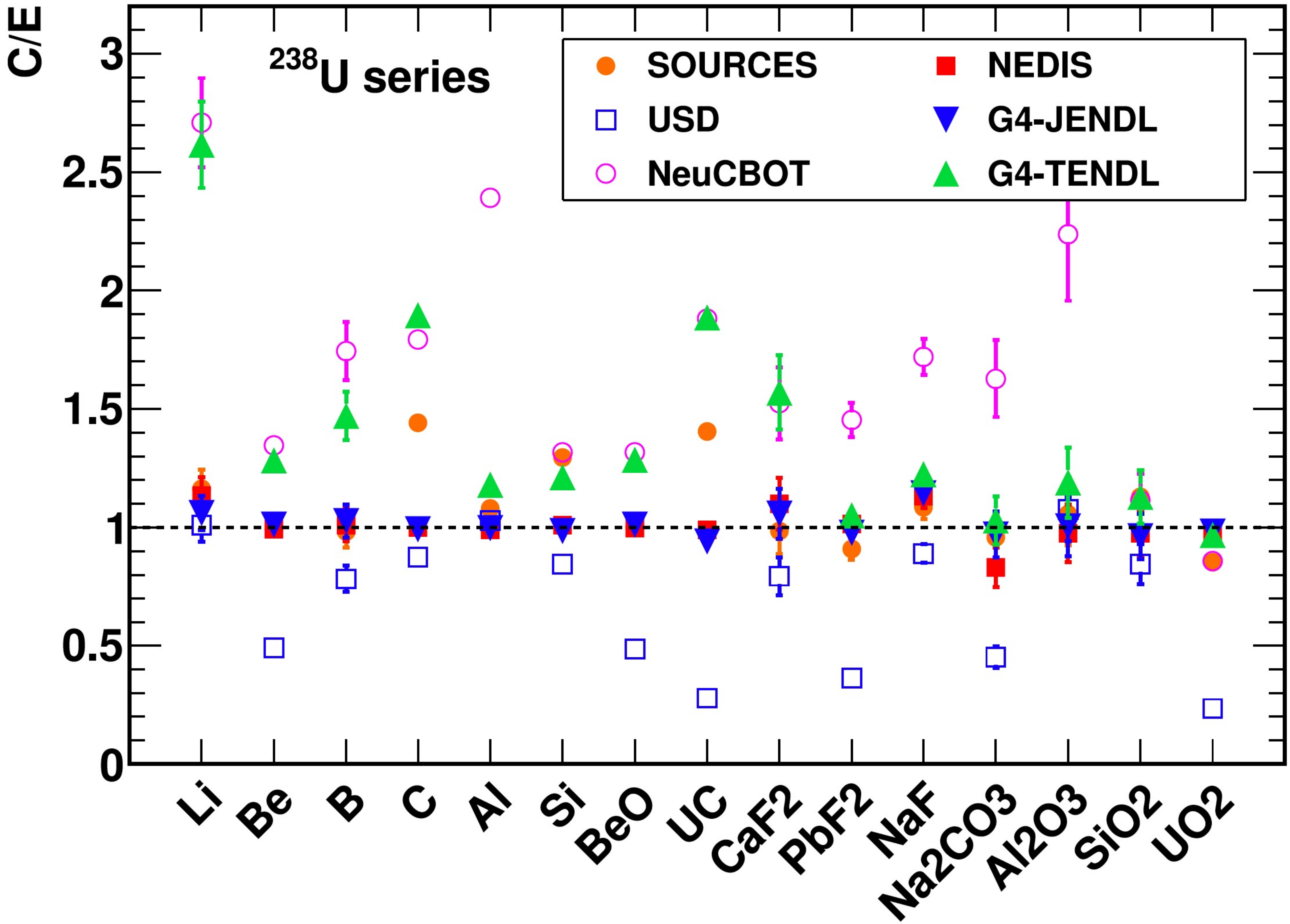

C/E
^{238}U series
SOURCES
NEDIS
USD
G4-JENDL
NeuCBOT
G4-TENDL
0
0.5
1
1.5
2
2.5
3
Li
Be
B
C
Al
Si
BeO
UC
CaF2
PbF2
NaF
Na2CO3
Al2O3
SiO2
UO2

Conclusions

NEDIS and G4-JENDL (Geant4 using the JENDL/AN-2005 library) are the results which better reproduce the experimental values, with an agreement better than 10% in most cases.

The values of SOURCES (taken from Fernandes et al.) agree within 20% with the experimental data for most materials.

USD gives neutron yields below the experimental values in almost all the tested cases, being the discrepancies as large as 80%

NeuCBOT and G4-TENDL (Geant4 using the TENDL-2017 library) give yields which are, on average, 60% and 40% larger than the measured values, respectively.

http://win.ciemat.es/SaG4n/ SaG4n

Simulation of (α,xn) reactions with Geant4

Emilio Mendoza, Daniel Cano-Ott, Vicente Pesudo, Roberto Santorelli

SaG4n is a Geant4 tool developed to calculate neutron production due to (α,xn) reactions in different materials. Once compiled, SaG4n takes from an input file written by the user all the information necessary to define the geometry of the problem, the source, parameters of the physics, the type of output, etc... The program uses the electromagnetic models implemented in Geant4 to perform an explicit transport of the incident α particles through the geometry, and data libraries originally written in ENDF-6 format to model the (α,xn) reactions.

The SaG4n code, together with different (α,xn) data libraries can be downloaded from the present webpage. Documentation concerning how the code works and how to use it is provided as well.

Source code

The last release of the SaG4n source code, release 1.2 (January 2021), can be downloaded from here.

Documentation

The user's manual for SaG4n can be downloaded from here.

More information concerning the performance of the code can be found in:

E. Mendoza et al., *Neutron production induced by α-decay with Geant4*, Nucl. Instrum. Methods A 960, 163659 (2020) [https://doi.org/10.1016/j.nima.2020.163659].

The authors would appreciate that their work is acknowledged properly. Please use this publication to reference SaG4n.

Previous releases of SaG4n

Release 1.1 (February 2020) can be downloaded from here, and the associated manual from here.

Release 1.0 (January 2020) can be downloaded from here, and the associated manual from here.

Summary and conclusions

- (α,Xn) cross section data and neutron energy spectra are relevant for several nuclear technology applications.
- Neutron yield and spectra (α,Xn) calculators are widely used. SaG4n, a new tool based on GEANT4, has been made available. It combines the powerful GEANT4 simulation capabilities with the use of standard nuclear data evaluated libraries.
- The code has been verified with other common neutron yield calculators and validated with experimental data.
  - SaG4n + JENDL and NEDIS are the codes **more compatible** (~10% average deviation) with the data for isotopes and materials investigated.
  - The performance of SOURCES is similar (~15% average deviation).
  - USD tends to underestimate the neutron yields.
  - TALYS based calculations with NeuCBOT and SaG4n + TENDL-2017 lead to 60% and 40% overestimations, respectively.
- Correlated and accurate neutron / gamma information is necessary for modelling the right neutron spectra. It is not the case in JENDL and TENDL.
- New data and evaluations are necessary.