Calculation of the neutron production in (α,n) reactions with SOURCES4

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Outline

- What are we (low background experiments) looking for?
- Neutron production in (α,n) reactions in SOURCES4 (or how the above can be achieved with SOURCES4?)
- Comparing cross-sections and excitation functions from EMPIRE2.19/3.2.3, TALYS1.9 and experimental data.
- Neutron yields and spectra in different models.
- Conclusions.

This talk is partly based on the paper published in Nucl. Intrum. and Meth. A, 972 (2020) 164095, plus further studies.

- Disclaimer:
  - I am not a nuclear physicist
  - I am not the author of SOURCES4.

What are we looking for?

- Neutron yields and energy spectra.
- Total yields/spectra and partial yields/spectra (for generating parallel gammas but very limited at present).
- Alpha energies up to 9 MeV.
- Materials with low/medium Z (anything above Cu will give a too low neutron yield).
- Materials with high masses present in experiments: SS, Cu, Ti…
- Materials with high neutron yields: F, Al, Si…
- Materials which are part of targets: C, O, N, Ar.
- Primarily reactions above the Coulomb barrier.
- Cross-sections at a level of a few mb or more.
- We would like nuclear physicists to guide us through the process of neutron yield and spectra calculations: which cross-sections and branching ratios to use etc.

SOURCES4

- SOURCES4A/4C: W.B. Wilson, et al., SOURCES4A: a code for calculating (α,n), spontaneous fission, and delayed neutron sources and spectra, Technical Report LA-13639-MS, Los Alamos, 1999;
- Modifications explained in Tomasello et al. NIMA, 595 (2008) 431
- Working historically with SOURCES4A; no noticeable difference for our goals.
- The probability for an alpha particle to produce a neutron by interacting with a nuclide i (N_i is the number density of atoms of nuclide i):

$$P\left(E_\alpha\right)=\int_0^{E_\alpha}\frac{N_i\sigma_i\left(E\right)}{\left(-\frac{dE}{dx}\right)}dE$$

- Stopping power cross-sections from the tables compiled by Ziegler.
- Approximation of thick target.

Modifications to SOURCES4A

- Original versions of SOURCES4A/4C are limited to 6.5 MeV α energies.
- Modifications to SOURCES4A:
  - α energies up to 9.8 MeV.
  - More cross-sections and excitation functions added in 2004-2010, mainly from EMPIRE2.19 (until 2009); M. Herman et al. Nucl. Data Sheets 108 (2007) 2655.
  - Modifications described in Carson et al. Astropart. Phys., 21 (2004) 667; Lemrani et al. NIMA 560 (2006) 454; Tomasello et al. NIMA, 595 (2008) 431; Tomasello et al. Astropart. Phys., 34 (2010) 70.
  - Recent cross-sections from TALYS1.9 (TENDL-2017) and EMPIRE3.2.3 have been added together with new data for some isotopes in 2019-2021.
- The code (modified version) is used by several experiments in dark matter search and neutrino physics.

Advantages and disadvantages

- Advantages
  - Flexible libraries of cross-sections and branching ratios
  - Fast calculation
  - Total neutron spectra; spectra from interactions on individual isotopes and from the variety of radioisotopes in a single calculations; spectra from the ground state and different excited states.
- Disadvantages:
  - Written long time ago (but cross-sections can be added/replaced)
  - Written in Fortran (but no need to intervene if the code works)
  - No gammas generated from de-excitation of final state nuclei (same for most codes)
  - Cannot read ENDF format (but if you know ENDF format, converting the cross-section data into the SOURCES4 format is not a big deal).
  - Cannot deal with 'surface' contaminations/problems.

Other tools

- USD web-based tool: http://neutronyield.usd.edu; Mei et al. NIMA 606 (2009) 651. Cross-sections from TENDL libraries (TALYS code).
- Comparison between SOURCES4A and USD based tool: J. Cooley et al. NIMA 888 (2018) 110-118, arXiv:1705.04736 [physics.ins-det]
- NeuCBOT: S. Westerdale and P.D. Meyers. Nuclear Instr. and Methods in Physics Research, A 875 (2017) 57–64. Neutron spectra are taken from TENDL libraries.
- Comparison of NeuCBOT and SOURCES4: S. Westerdale and P.D. Meyers. Nucl. Instr. and Methods in Physics Research, A 875 (2017) 57–64.
- Results from the USD tool and NeuCBOT are different from SOURCES4A even if cross-sections from TALYS are used; Kudryavtsev et al., Talk at IDM2018. Different versions of TALYS/TENDL, different inputs/models, different energy losses of alphas.
- NEDIS code: Vlaskin et al. Atomic Energy, Vol. 117, No. 5, March 2015.
- Comparison between codes and data: Fernandes et al. EPJ Web of Conferences 153, 07021 (2017).
- GEANT4.10.6 - (α,n) reactions included; E. Mendoza et al. Nucl. Instrum. & Meth. in Phys. Res. A 960 (2020) 163659. arXiv:1906.03903.

Inputs to SOURCES4

- Q-value of the reaction and the energy threshold in the laboratory system (projectile: α particle).
- Cross-section as a function of energy; included in the code library but can be added/changed by a user.
- α lines and intensities (code library).
- Stopping power or energy losses of α's (code library).
- Spontaneous fission spectra (code library).
- Number of atoms of a radioisotope(s) (user defined).
- Material composition (user defined).
- Repository: http://www.oecd-nea.org/tools/abstract/detail/ccc-0661/

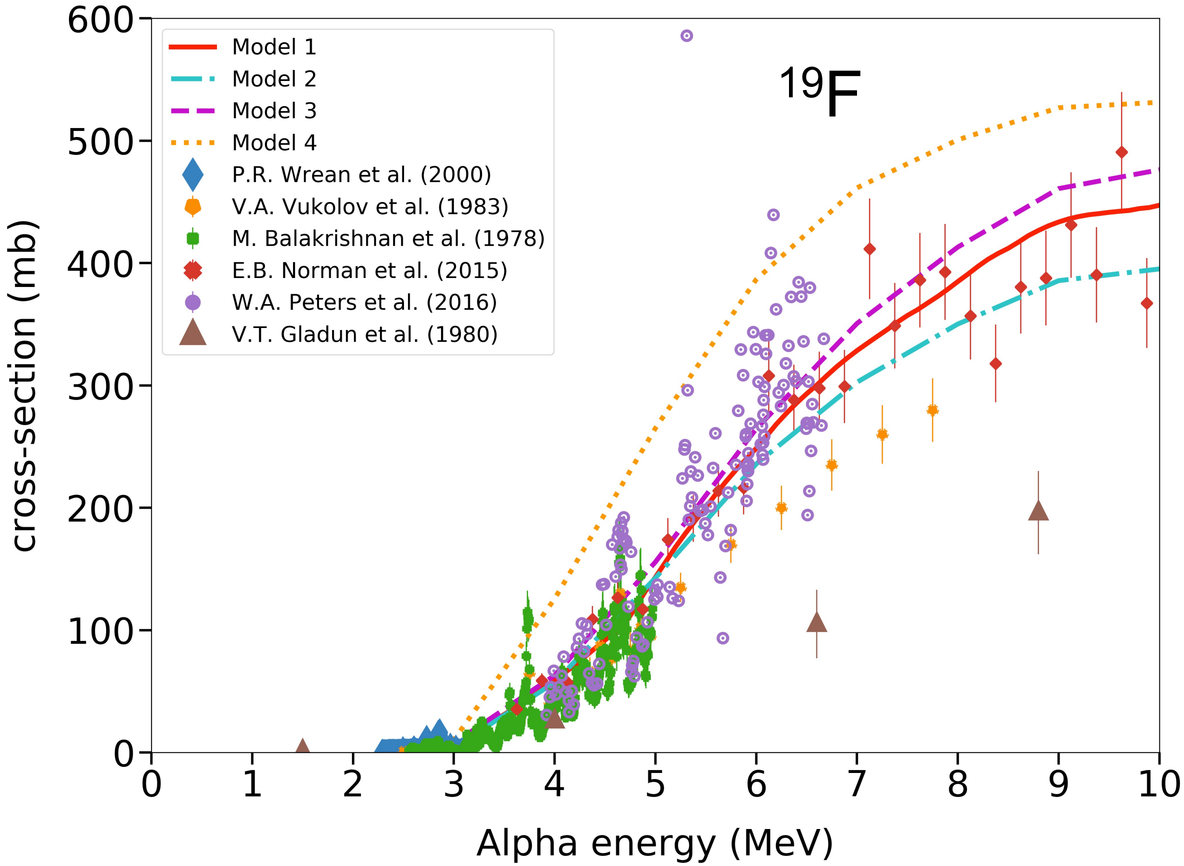
(This is not our code; we have only modified it and support the modified version.)

- Most recent version – SOURCES4C; no difference compared to SOURCES4A (as I am aware of) apart from ^{252}Cf spectrum from SF.

Outputs

- Neutron yields.
- Neutron spectra from SF and (α,n) reactions.
- Spectra for individual radioactive isotopes and for individual isotopes in the target material composition.
- Spectra for the transitions to the ground and different excited states of a final state nucleus (excited states are as given in the code library).

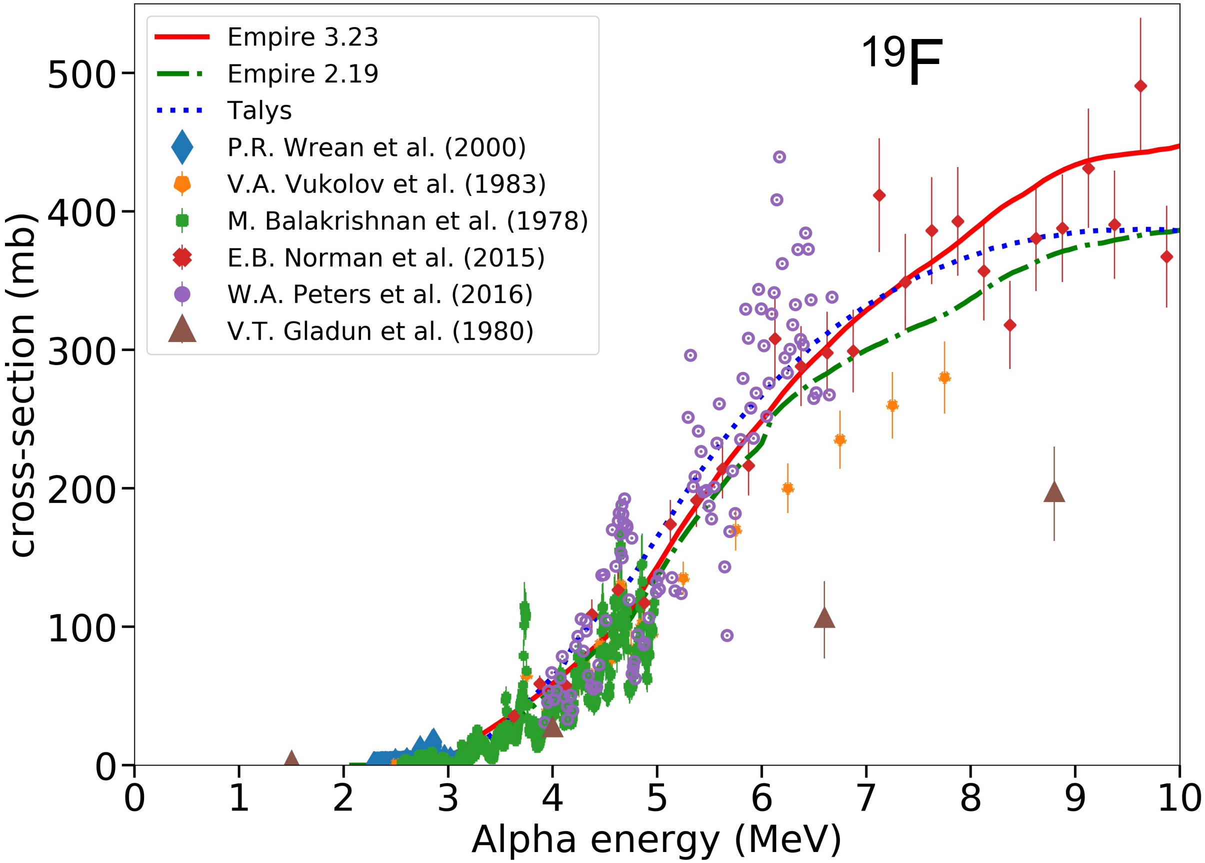
Different models in EMPIRE3.2.3



There are recent data from measurements in 2015-2016.
No new data for branching ratios.

- Model 1 is recommended for fluorine: McFadden-Satchler (MS) Optical Model Potential (OMP) with direct reactions.
- Data do not allow us to choose an optimum model for ^{19}F but Model 1 is a good choice and is recommended by the authors.

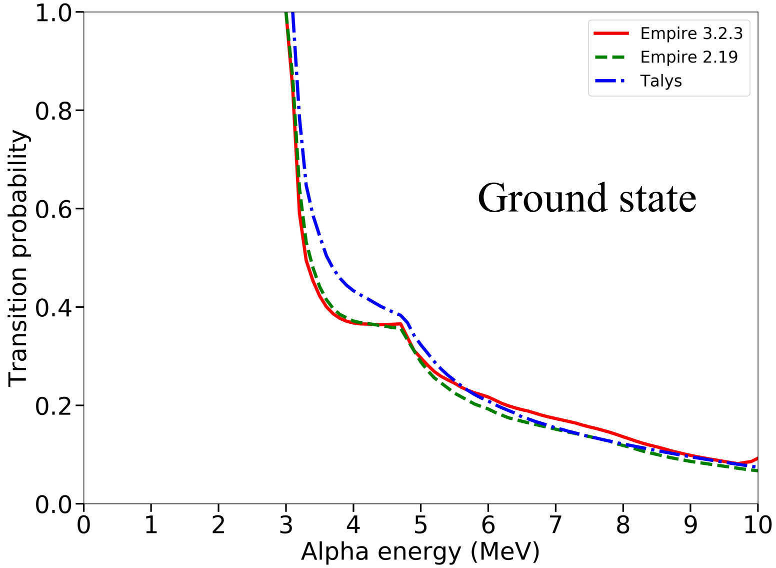
Cross-sections: EMPIRE2.19/3.2.3 vs TALYS1.9

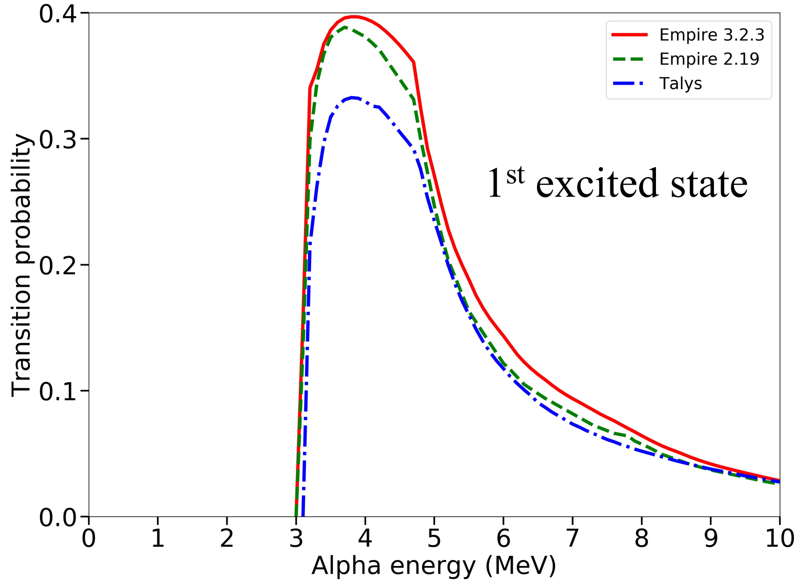


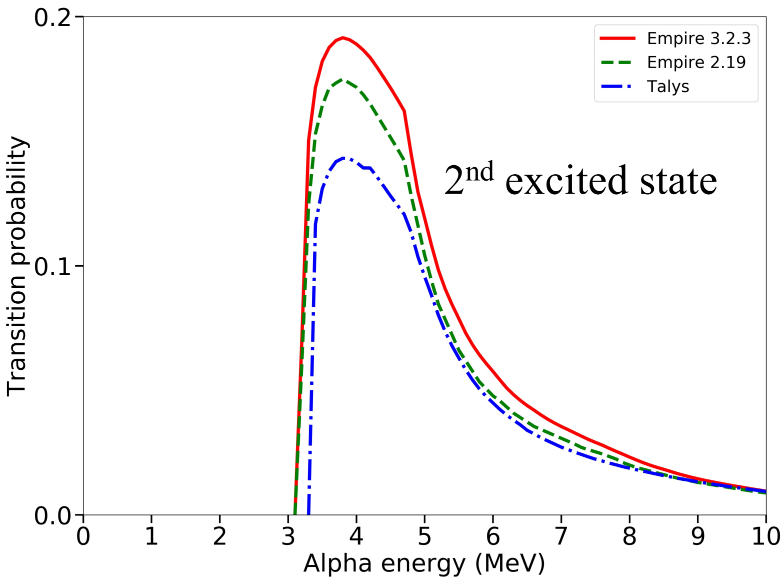
There are recent data from measurements in 2015-2016.
No new data for branching ratios.

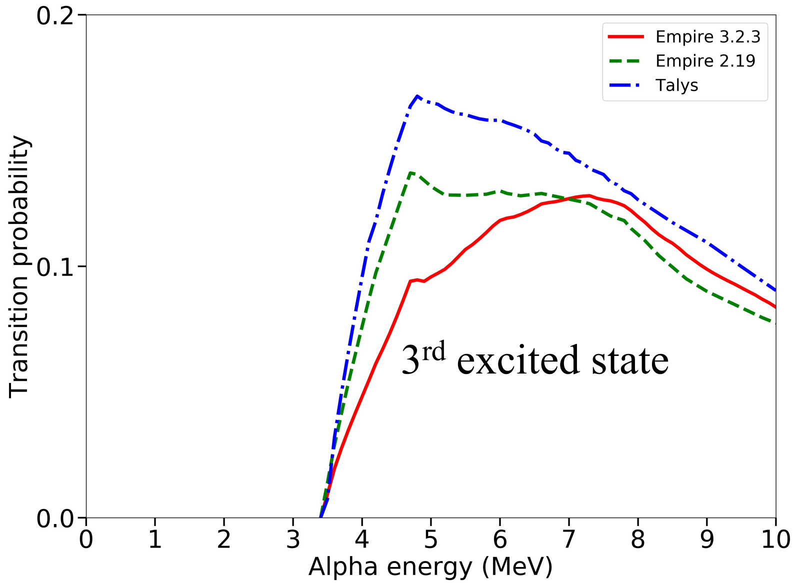
- Data do not allow us to choose the optimum model for ^{19}F.
- Data can be used in SOURCES4A (possibly in combination with another model). The results are quite different depending on a specific measurement.

Branching ratios for fluorine

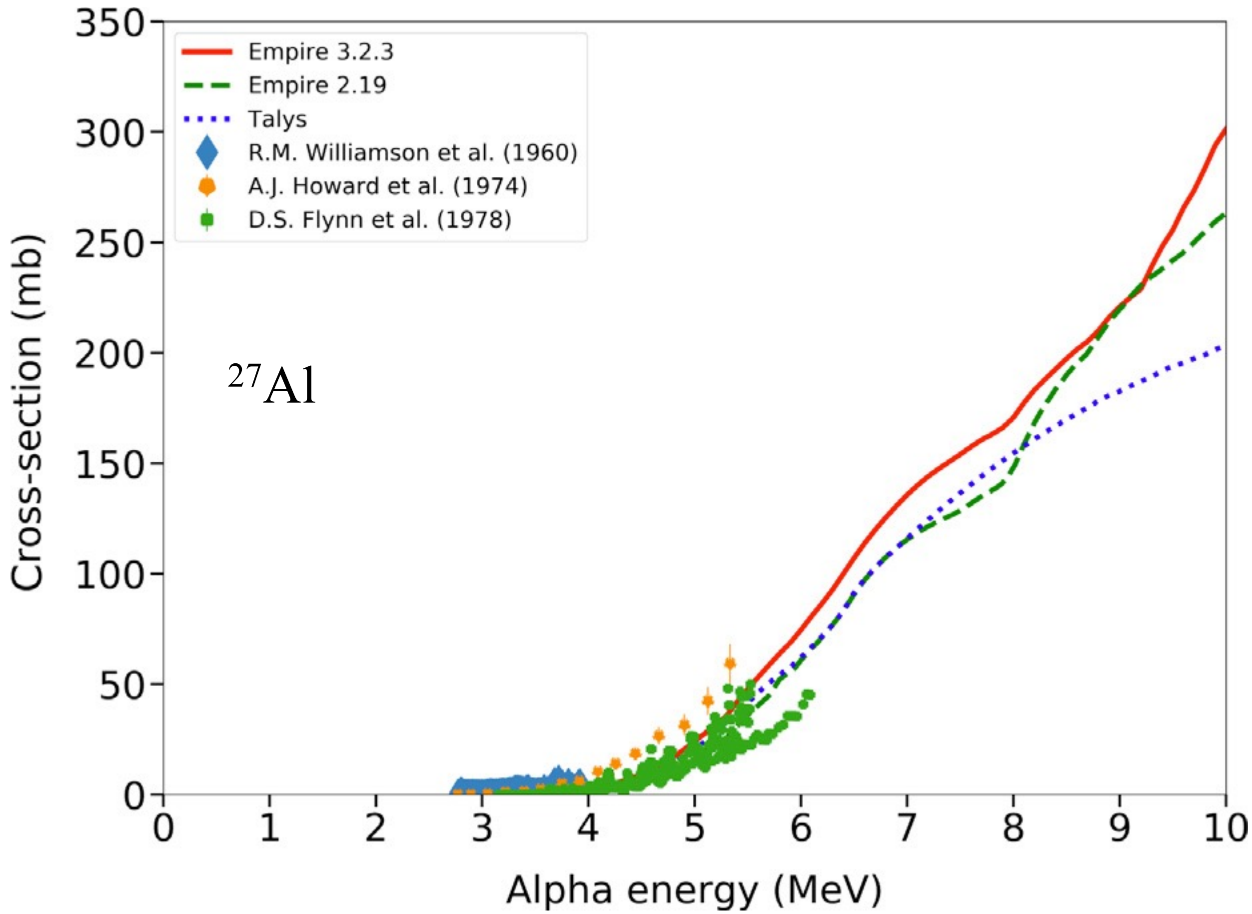






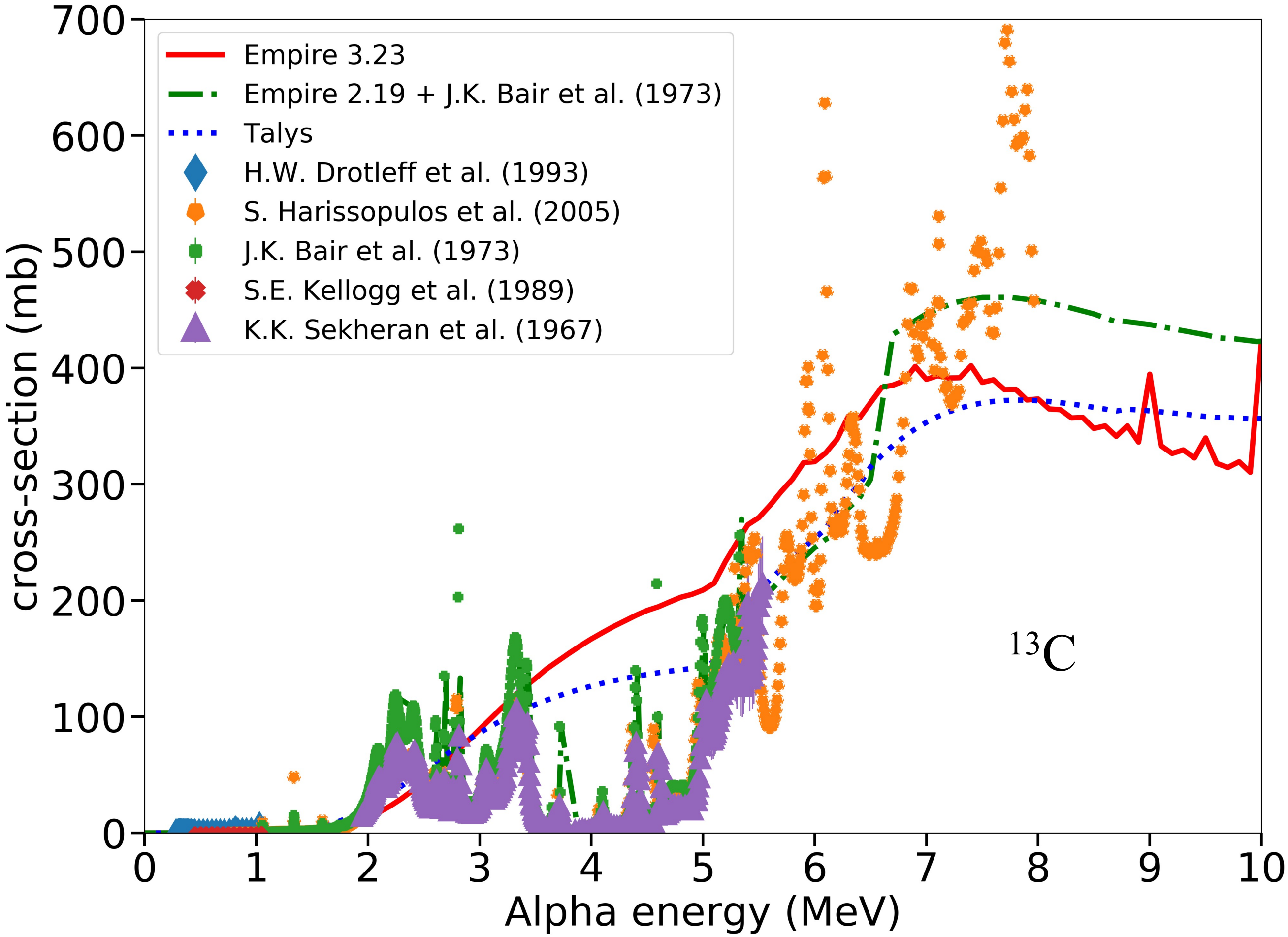


Cross-sections for aluminium



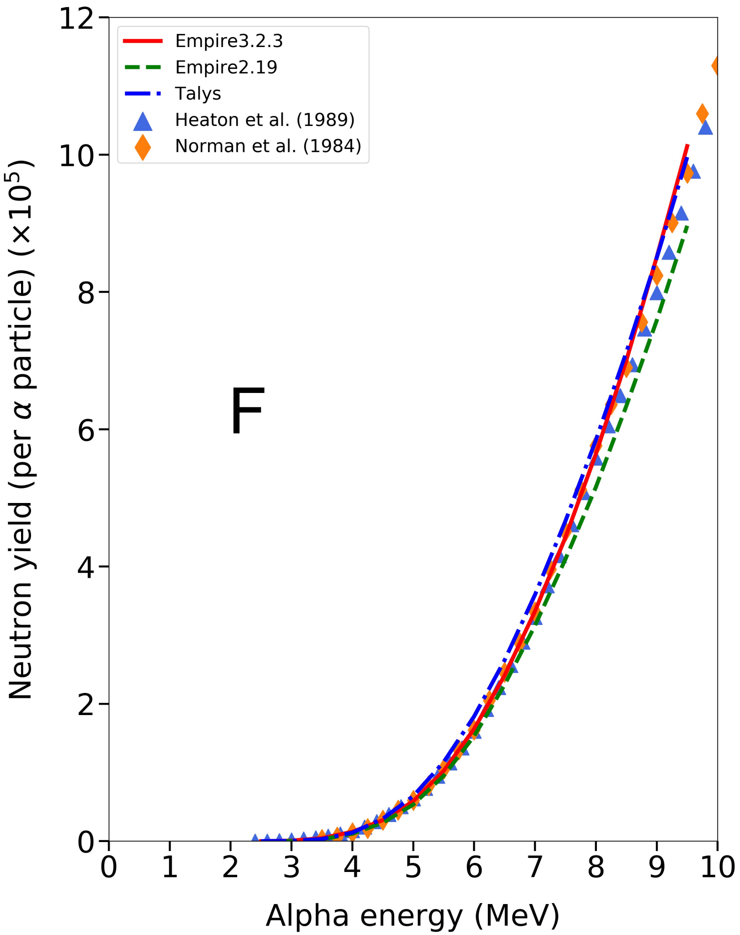
- Data are limited (quite old) and cannot help with the choice of the model. Using measured cross-sections leads to large variation in the neutron yield, depending on a specific measurements.

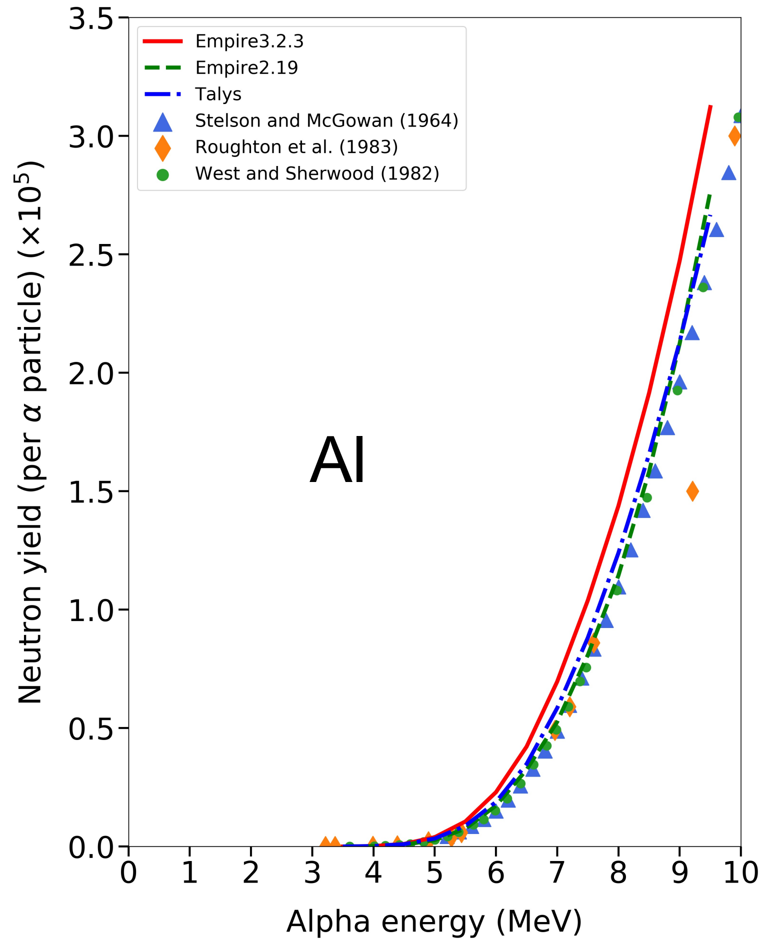
Cross-sections for carbon



- ^{12}C does not contribute (high threshold). Only ^{13}C contributes to the neutron yield (but small abundance).

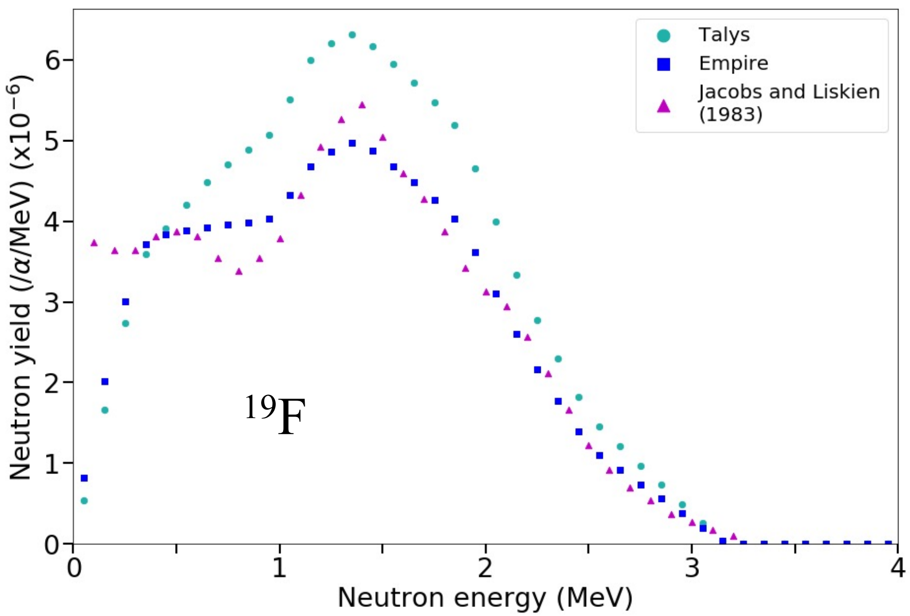
Neutron yield: EMPIRE versus data

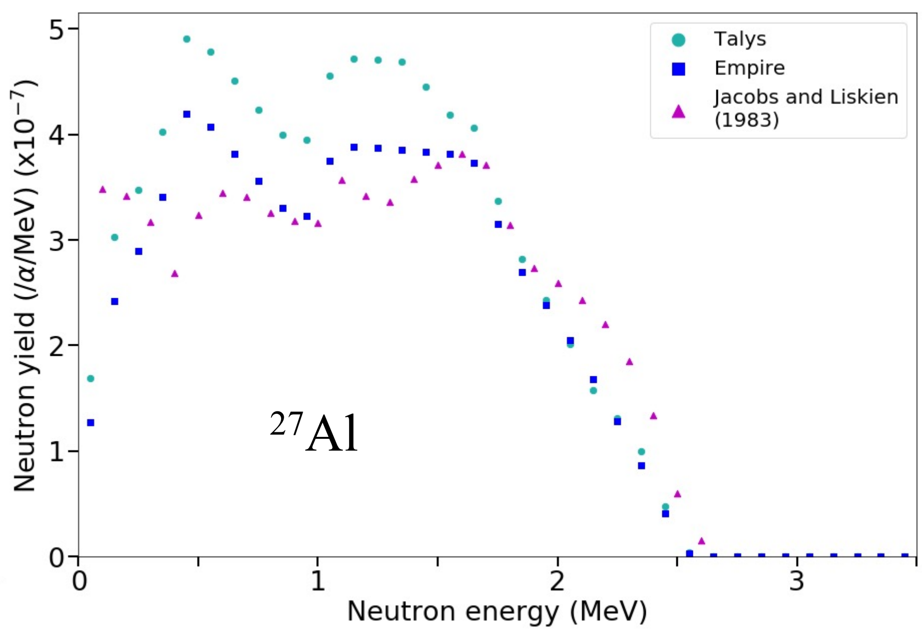




- Neutron yield as a function of alpha energy for fluorine (left) and aluminium (right). The agreement is quite good.

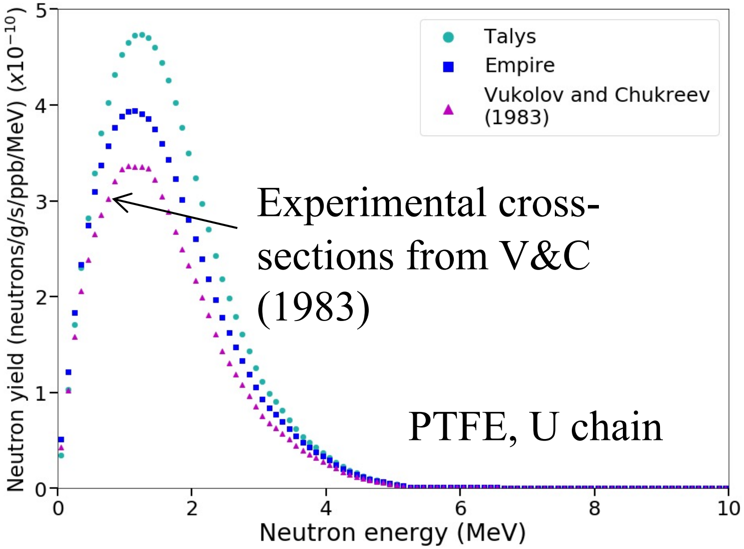
Neutron spectra: SOURCES4A vs measurements

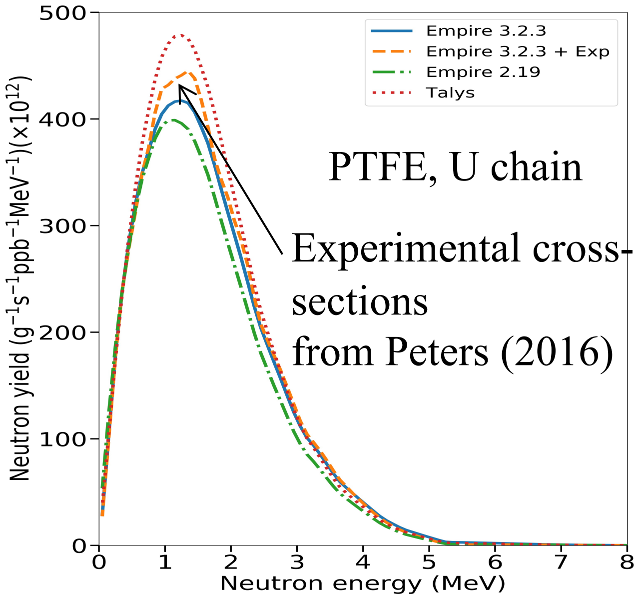




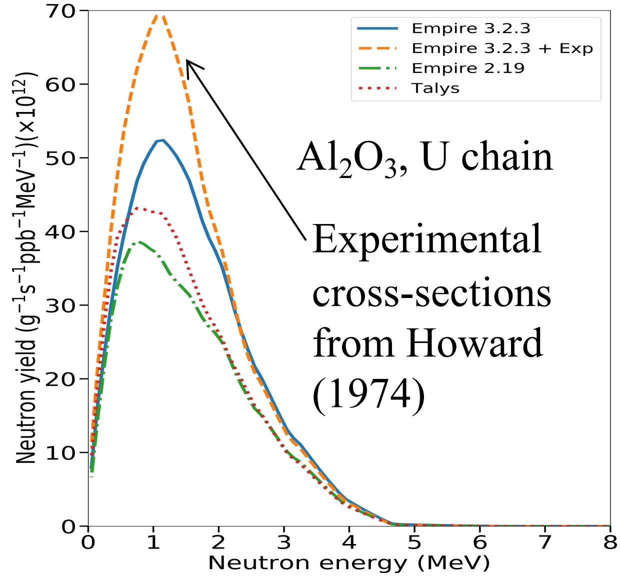
- Neutron spectra from 5.5 MeV alphas in fluorine and aluminium.
- SOURCES4A uses either EMPIRE2.19 or TALYS1.9 cross-sections.

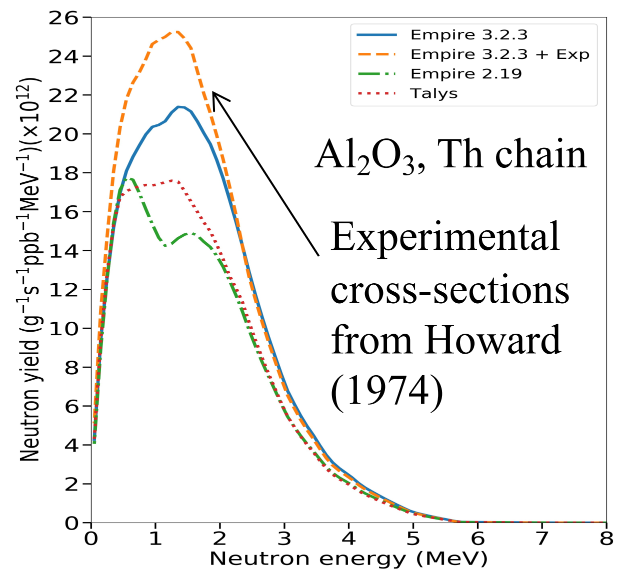
Neutron spectra from decay chains: C_2F_4 (PTFE) and Al_2O_3





Neutron spectra from U/Th decay chains in equilibrium using cross-sections from TALYS1.9, EMPIRE2.19/ 3.2.3 and measurements.





SOURCES4A: total neutron yields from U/Th chains

Material	Cross-section	$^{238}U + ^{235}U$	^{232}Th
Aluminium	TALYS1.9	1.86×10^{-10}	9.05×10^{-11}
	EMPIRE2.19	1.69×10^{-10}	8.59×10^{-11}
	EMPIRE3.2.3	2.20×10^{-10}	1.07×10^{-10}
Al_2O_3	TALYS1.9	9.48×10^{-11}	4.56×10^{-11}
	EMPIRE2.19	8.59×10^{-11}	4.32×10^{-11}
	EMPIRE3.2.3	11.42×10^{-11}	5.45×10^{-11}
Howard, 1974	EMPIRE3.2.3 +Experiment	13.55×10^{-11}	6.04×10^{-11}
PTFE	TALYS1.9	10.21×10^{-10}	4.03×10^{-10}
	EMPIRE2.19	8.72×10^{-10}	3.50×10^{-10}
	EMPIRE3.2.3	9.39×10^{-10}	3.78×10^{-10}
	EMPIRE3.2.3 +Experiment	9.68×10^{-10}	3.91×10^{-10}

Units: neutrons/g/s/ppb of the parent isotope. Only (α, n) reactions, no SF.

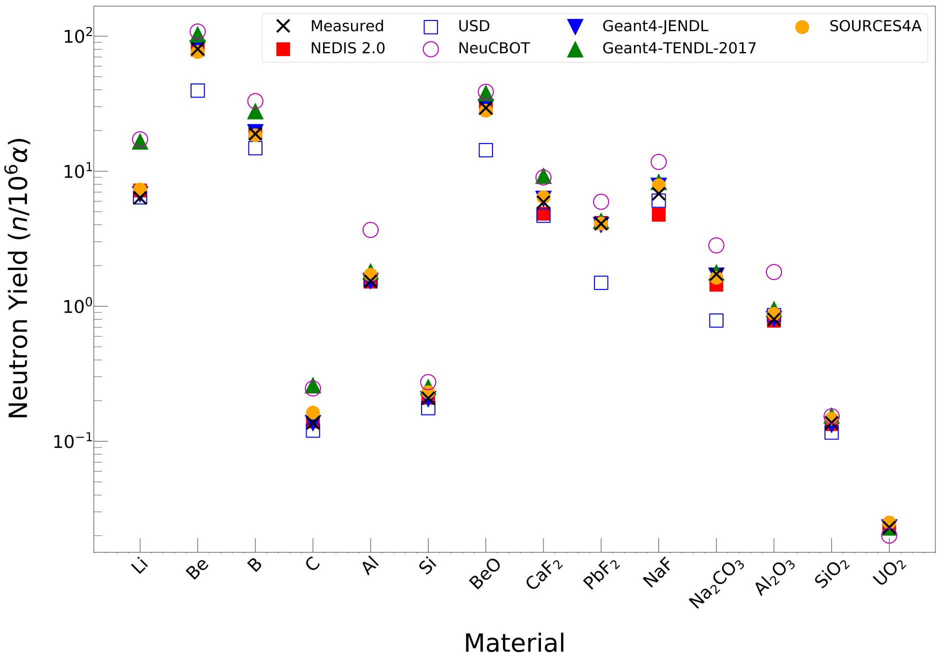
SOURCES4A: total neutron yields from U/Th chains

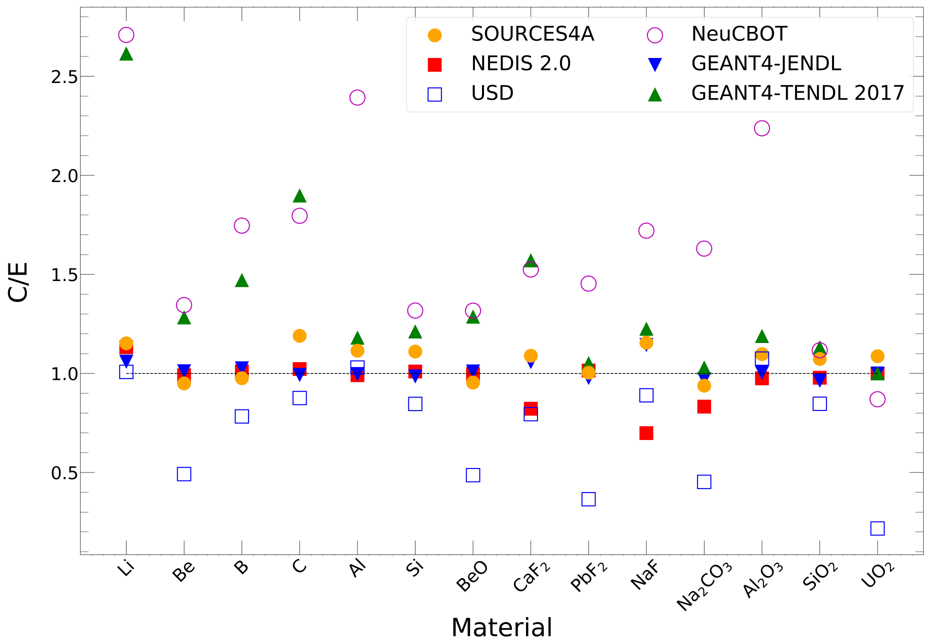
Material	Cross-section	$^{238}U + ^{235}U$	^{232}Th
SiO_2	TALYS1.9	1.54×10^{-11}	6.75×10^{-12}
	EMPIRE2.19	1.59×10^{-11}	7.03×10^{-12}
	EMPIRE3.2.3	2.07×10^{-11}	8.61×10^{-12}
	EMPIRE3.2.3 +Experiment	1.35×10^{-11}	6.21×10^{-12}
Ti	TALYS1.9	2.80×10^{-11}	2.33×10^{-11}
	EMPIRE2.19	2.55×10^{-11}	2.15×10^{-11}
	EMPIRE3.2.3	3.39×10^{-11}	2.48×10^{-11}
	EMPIRE3.2.3 +Experiment	3.39×10^{-11}	2.46×10^{-11}

Units: neutrons/g/s/ppb of the parent isotope. Only (α, n) reactions, no SF.

SOURCES4A: total neutron yields from U chain

- It may be the best option to use experimental data if available and reliable and complement them with a model.
- Branching ratio: we still need a model.
- Recent work: use measurements and the model.
- Graphs are for U chain and a selection of materials used also in other publications.
- 'Experimental data': combination of neutron yields from individual alphas on individual isotopes in a material.





Conclusions

- Recommended models (TALYS1.9 and EMPIRE2.19/3.2.3) give similar cross-sections (within 20-30%), at least for most critical isotopes and most energies of interest.
- Cross-sections:
  - Data on cross-sections are not sufficient to choose the best code/model – large variations exist among experimental cross-sections.
  - Using measured cross-sections makes the neutron yields bigger or smaller than the yield based purely on a model (depending on the data and the model used).
- Neutron yields:
  - For most tested isotopes, EMPIRE3.2.3 and TALYS1.9 cross-sections give slightly higher neutron yields than EMPIRE2.19.
  - Comparison with data does not allow us to select the best code/model.
  - Different models for the cross-sections result in 20-25% difference between neutron yields (SOURCES4A is used for all neutron yield calculations).
- A good option for neutron yield calculation is use the data if available and reliable and add a model which best matches the data.
- First results show a good agreement with experimental data.