SOURCES4 vs USD

Status of (alpha, n) Neutron Yield and Energy Spectrum Comparison

S.Scorza for the Radiogenic WG

Motivation

Reaction due to the alpha particles emitted by uranium, thorium and their daughters interacting with the rocks and in the detectors shielding scheme and components for low background experiments, are an important backgrounds

Validation of the calculations - yield and energy spectrum - are needed

USD website vs SOURCES4 calculations

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.

Calculations details

A homogeneous mixture problem is one in which the α-emitting material sources is intimately mixed with the low-Z target material (i.e., atoms of α-emitting material are directly adjacent to the target atoms)

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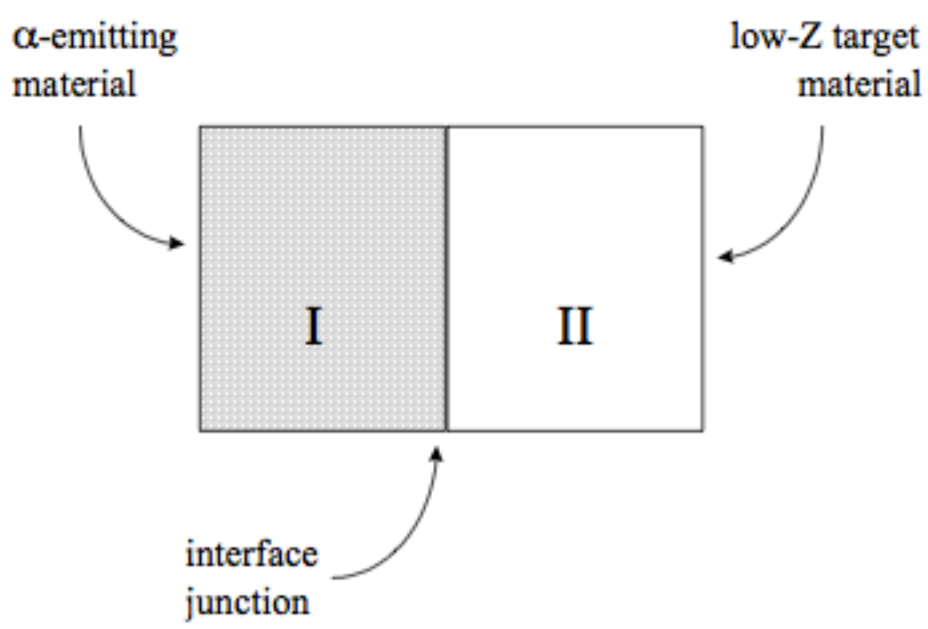
A homogeneous mixture problem is one in which the α-emitting material sources is intimately mixed with the low-Z target material (i.e., atoms of α-emitting material are directly adjacent to the target atoms)

Should we consider **interface problem**?
slab of α-emitting material (e.g. Pu, Po, or Am) is in close contact with a low-Z target material (e.g. Be, C, or Al). In such a geometry, α-particles are emitted from the Region I materials and travel across the interface junction into the Region II materials. Once in Region II, the α-particles can interact through (α,n) reactions and generate a neutron source. It is necessary to assume in all interface problems the thickness of each region is significantly larger than the range of the α-particles within it. It is also assumed that all α-particles travel in a straight-line trajectory from their point of emission (generally an excellent assumption).



Estimating the discrepancies ...

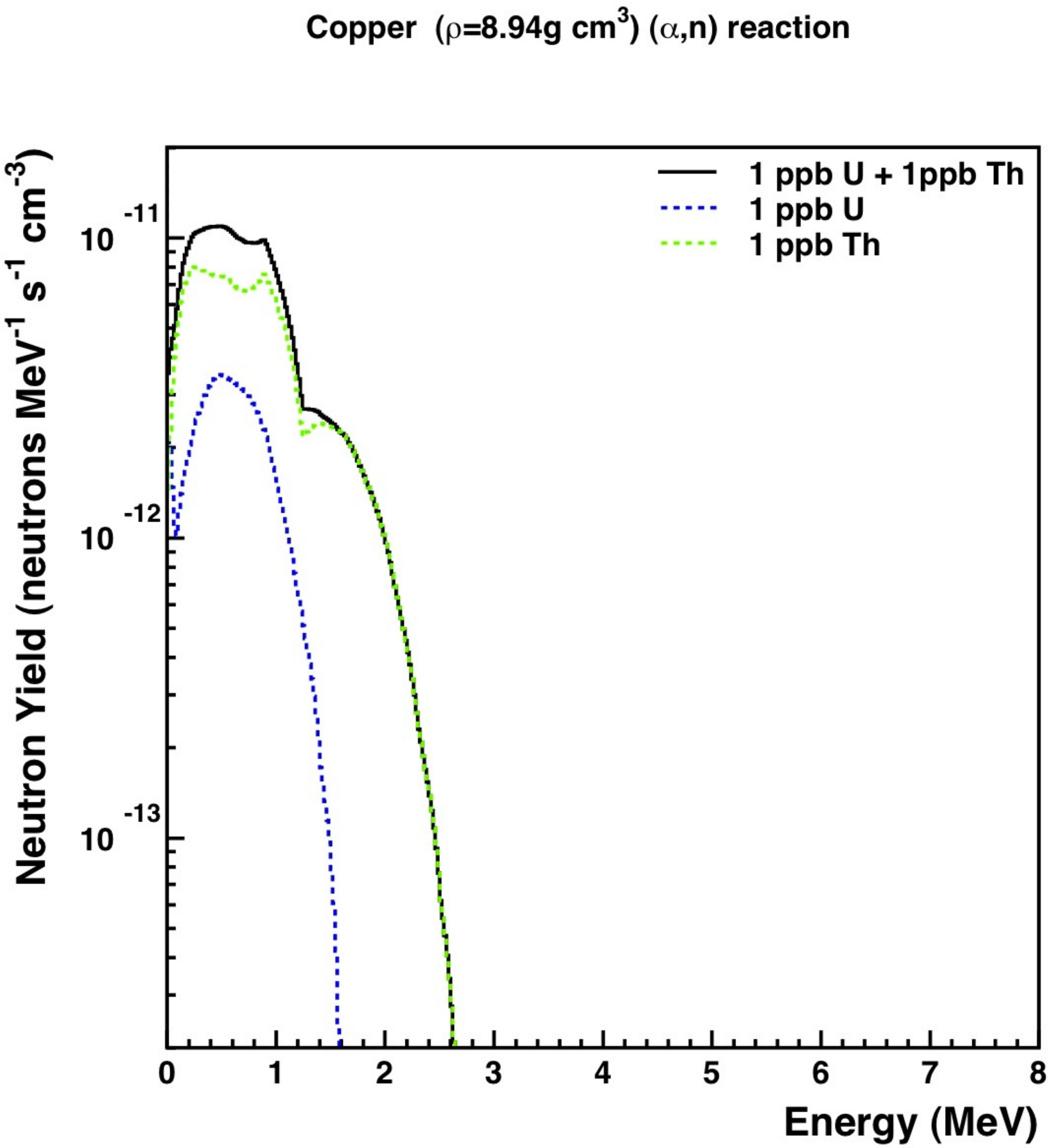
Tab.1 Material definition			
ELEMENT	Z	Name	Atom fraction (%)
Copper rho=8.94 g/cc	29	Cu	100
Titanium rho=4.506 g/cc	81	Ti	100
Polyethylene CH2 rho=0.935 g/cc	1	H	0.667
	6	C	0.333
Steel (from G4) rho=8 g/cc	24	Cr	0.008
	26	Fe	0.74
	28	Ni	0.18
Borosilicate glass (from Miniclean) rho=2.23 g/cc	3	Li	0.0027
	5	B	0.104
	8	O	0.624
	11	Na	0.035
	13	Al	0.035
	14	Si	0.194
	56	Ba	0.0058

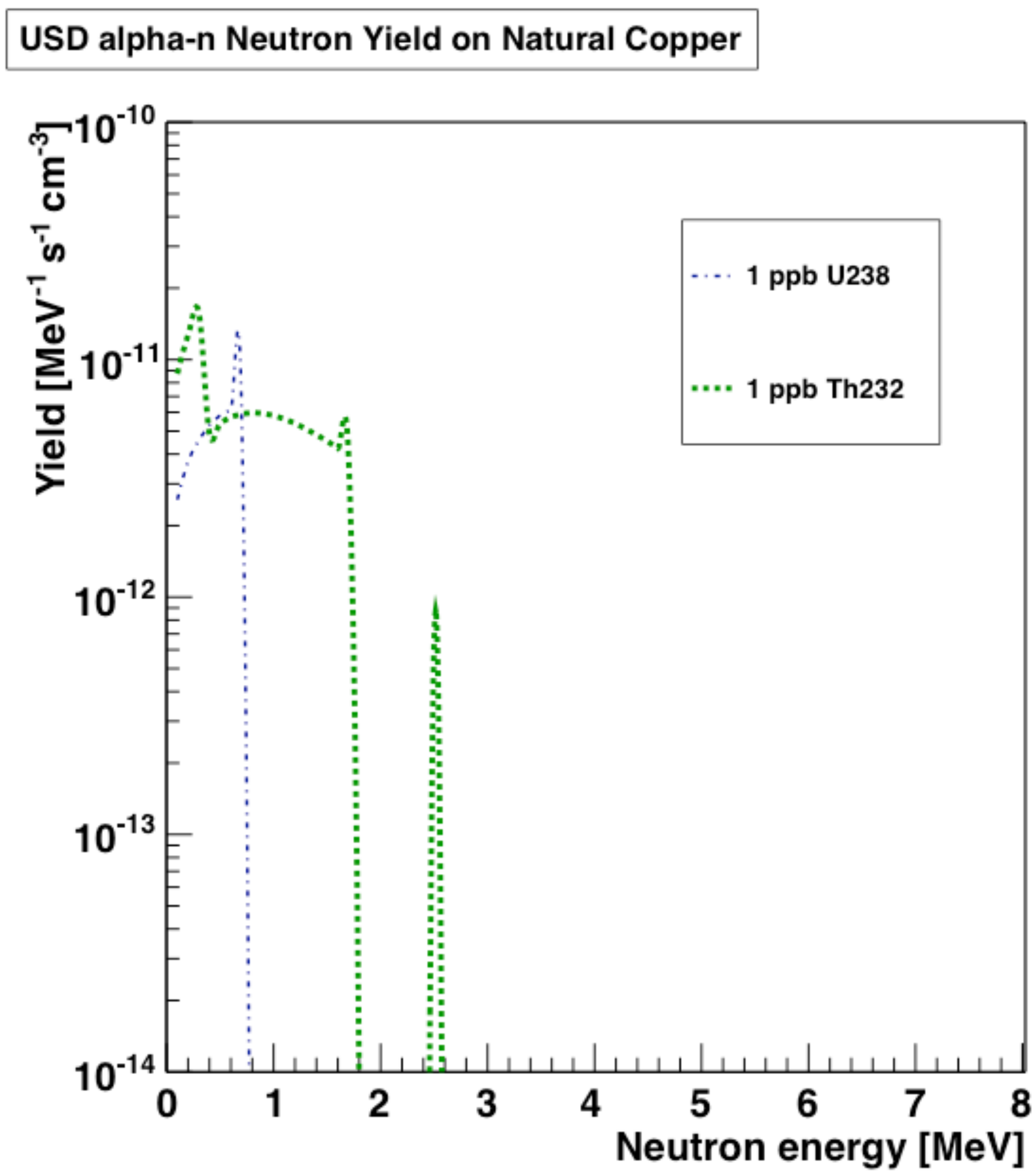
Tab 2. Material and neutron yield (n/s/cm3)			
ELEMENT	Chain	SOURCES4 n/s/cm3	USD n/s/cm3
COPPER	U	2.90 E-12	3.46 E-12
	Th	9.49 E-12	1.11 E-11
	Total	1.24 E-11	1.45 E-11
POLYETHYLENE	U	1.33 E-11	9.56 E-12
	Th	5.28 E-12	2.87 E-12
	Total	1.86 E-11	1.25 E-11
STEEL	U	3.19 E-11	4.28 E-11
	Th	4.05 E-11	4.71 E-11
	Total	7.42 E-11	9.00 E-11
TITANIUM	U	1.65 E-10	1.98 E-10
	Th	9.96 E-11	1.24 E-10
	Total	2.64 E-10	3.22 E-10
BOROSILICATE glass	U	3.63 E-10	2.45 E-10
	Th	1.27 E-10	6.98 E-11
	Total	4.90 E-10	3.15 E-10

material check

webpage

Neutron Spectrum





Understanding the discrepancies ...

Which inputs ?

The data necessary for computing the magnitude of the neutron source due to (α,n) reactions,

1. The energy-dependent α-particle stopping cross section for all elemental constituents (ε^g_i).
2. The energy dependent (α,n) cross-section for all target nuclides (σ^g_i).
3. The intensity for emission of each of the L α-particles (f^{α}_{kl}).
4. The energy of each of the L α-particles (E_l).
5. The source nuclide decay constants (λ_k).

To calculate the neutron source spectrum, it is necessary to have data for:

1. The number of product nuclide levels (M) for all target nuclides.
2. The number of product nuclide level branching data points (M') for all target nuclides.
3. The (α,n) reaction Q-value for all target nuclides.
4. The excitation energy [$E_{ex}(m)$] of product nuclide level m for all target nuclides.
5. The fraction of (α,n) reactions with target i at energy E(m) resulting in the production of product level m.
6. The α-particle, neutron, target, and product nuclei masses.

Within SOURCES4: uncertainties involved in cross-section calculations and measurement can be important.

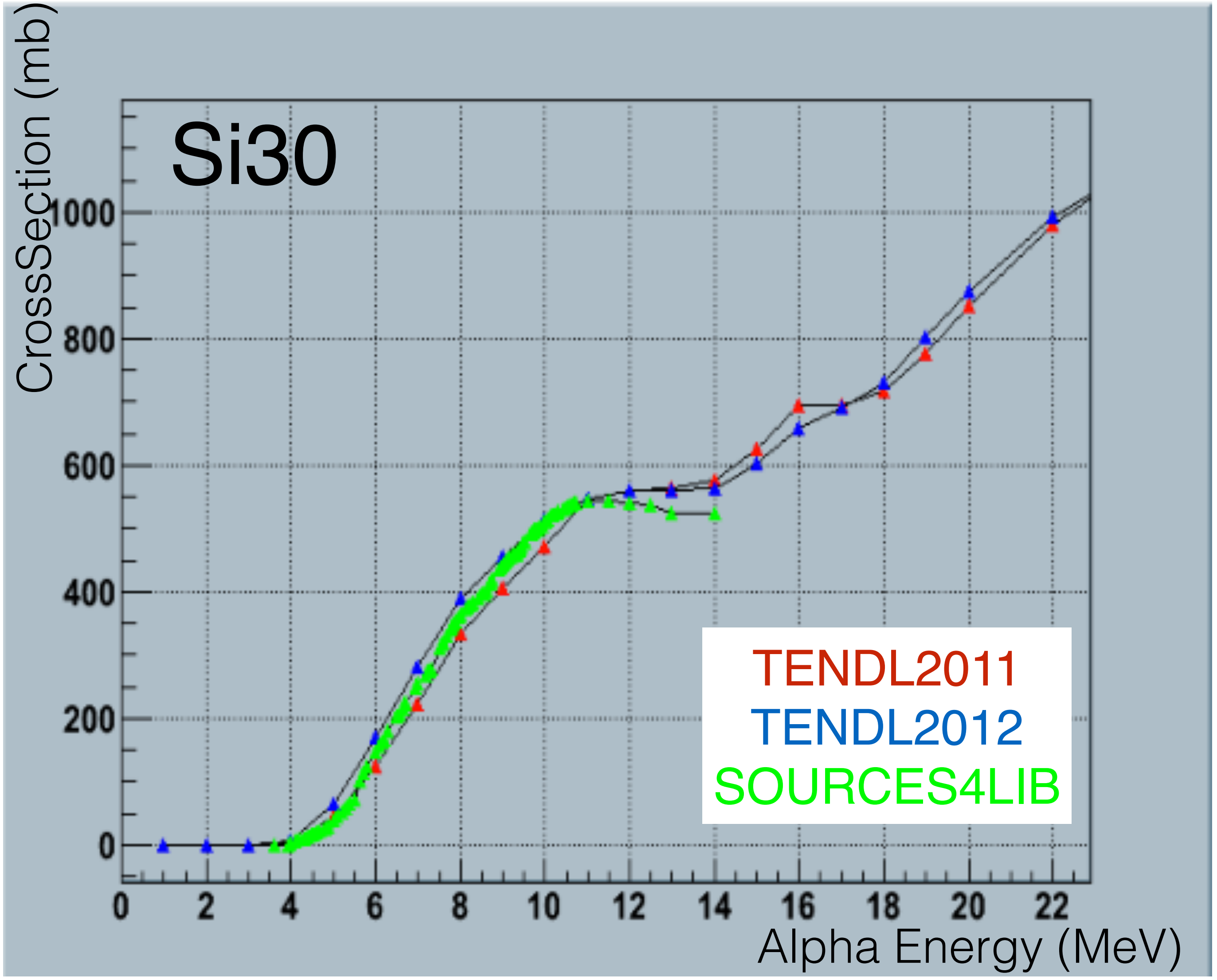
Example: according to the the cross section calculations listed in the library for Ti48 we can get a total neutron contribution from U in Titanium of 2.2E-10 n/s cm3 or 1.76E-10 n/s cm3.

220480 157 48Ti 147 points EMPIRE 2.19 calcs
220480 49 ti48 49 points ti48 x-sec from empire-2.19 calcs

The take-home message is that no matter what simulation you do, it's a good first guess, but never a precision statement...

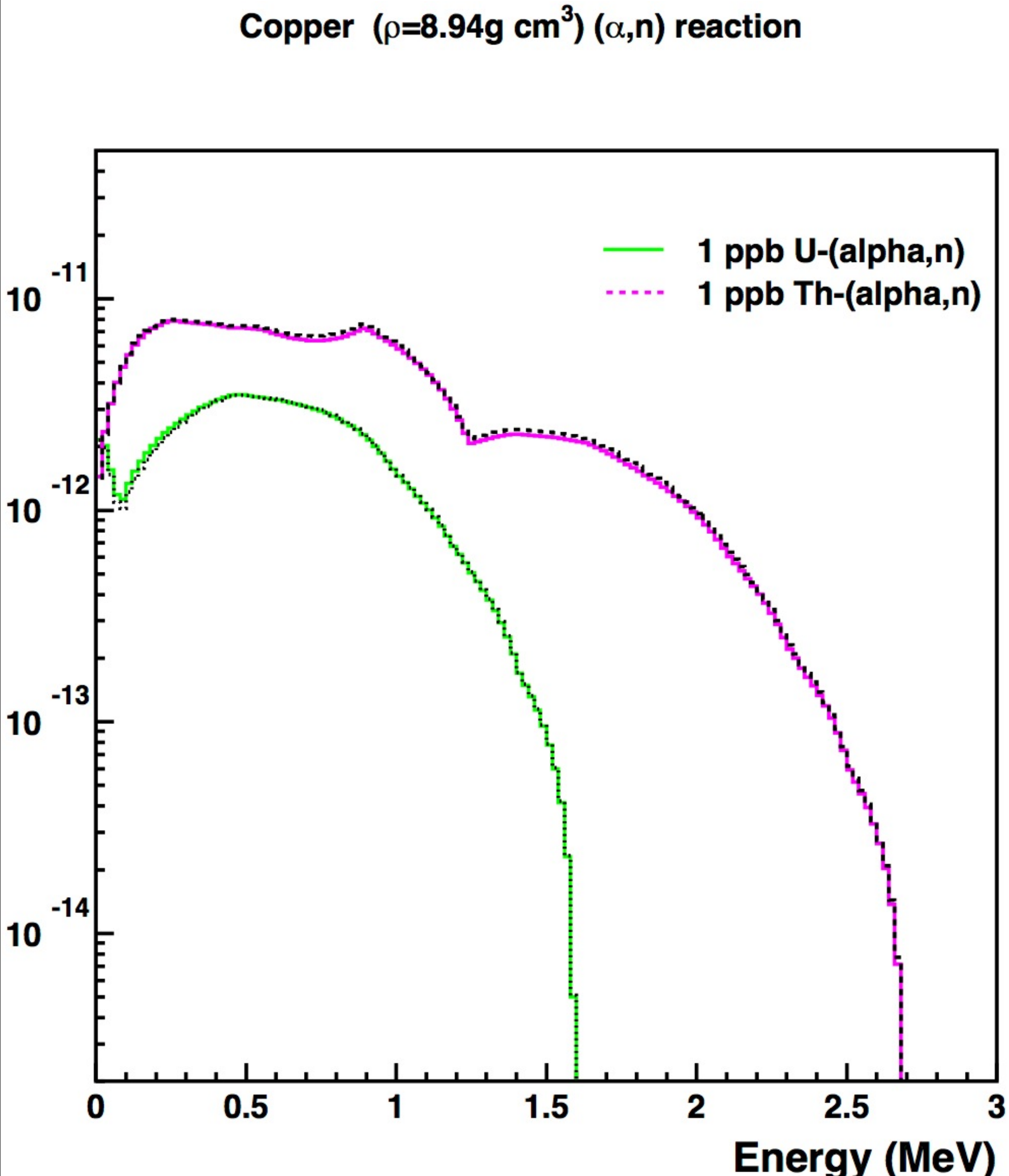
- **Target (alpha,n) cross section**
  USD: TENDL 2011 and 2012 have been considered as inputs. TENDL is a nuclear data library (validated) which provides the output of the TALYS nuclear model code system
  SOURCES4: cross section input libraries come from EMPIRE calculations and for some isotopes a combination of measurements and EMPIRE calculations
  see webpage

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



- **Alpha particle decay data library**
  ONGOING ….
  USD: only decays with visible energy larger than 100 keV or branching ratio more than 0.5% are considered
  SOURCES: no threshold

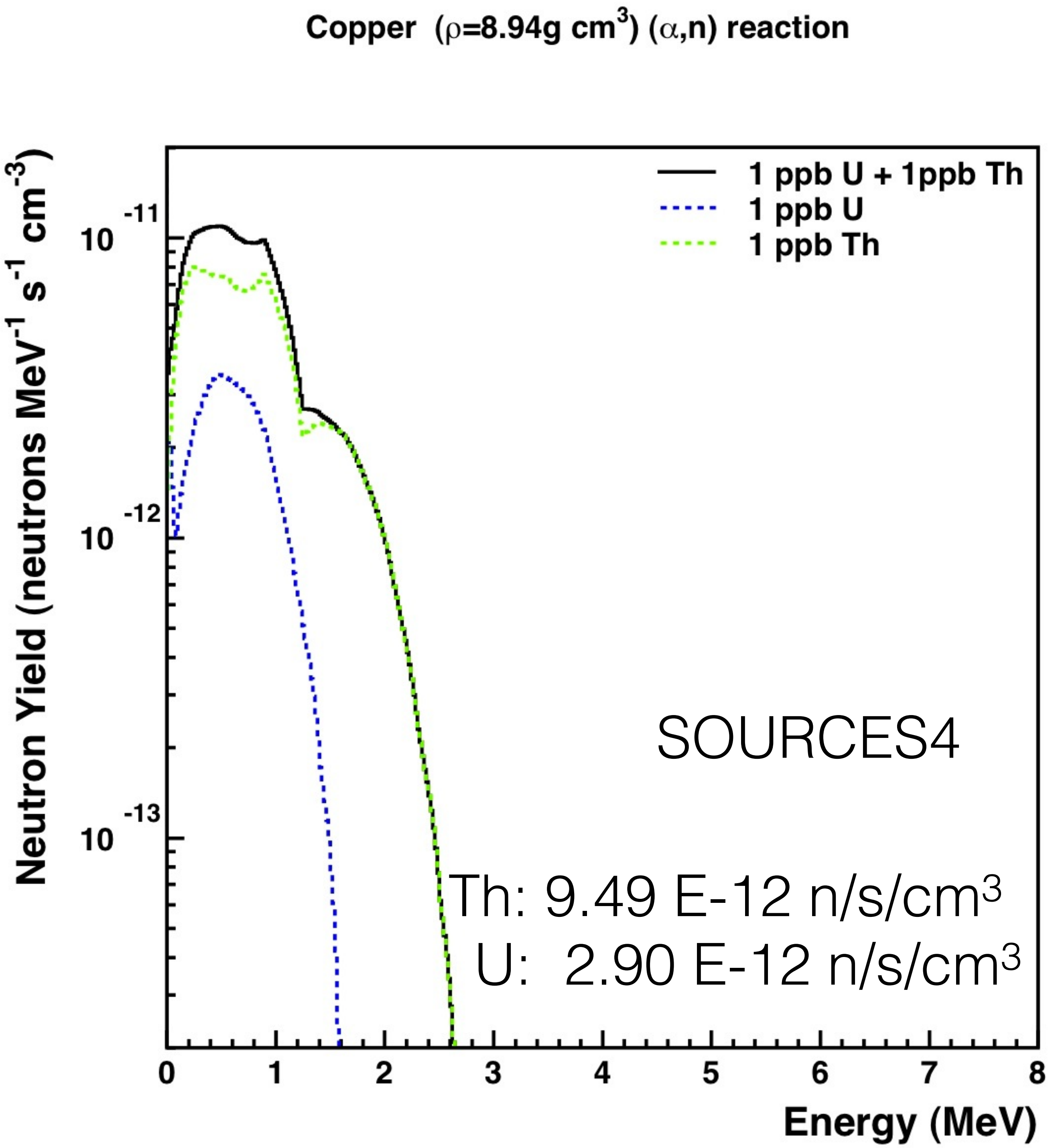
USD cross section into SOURCES4 code

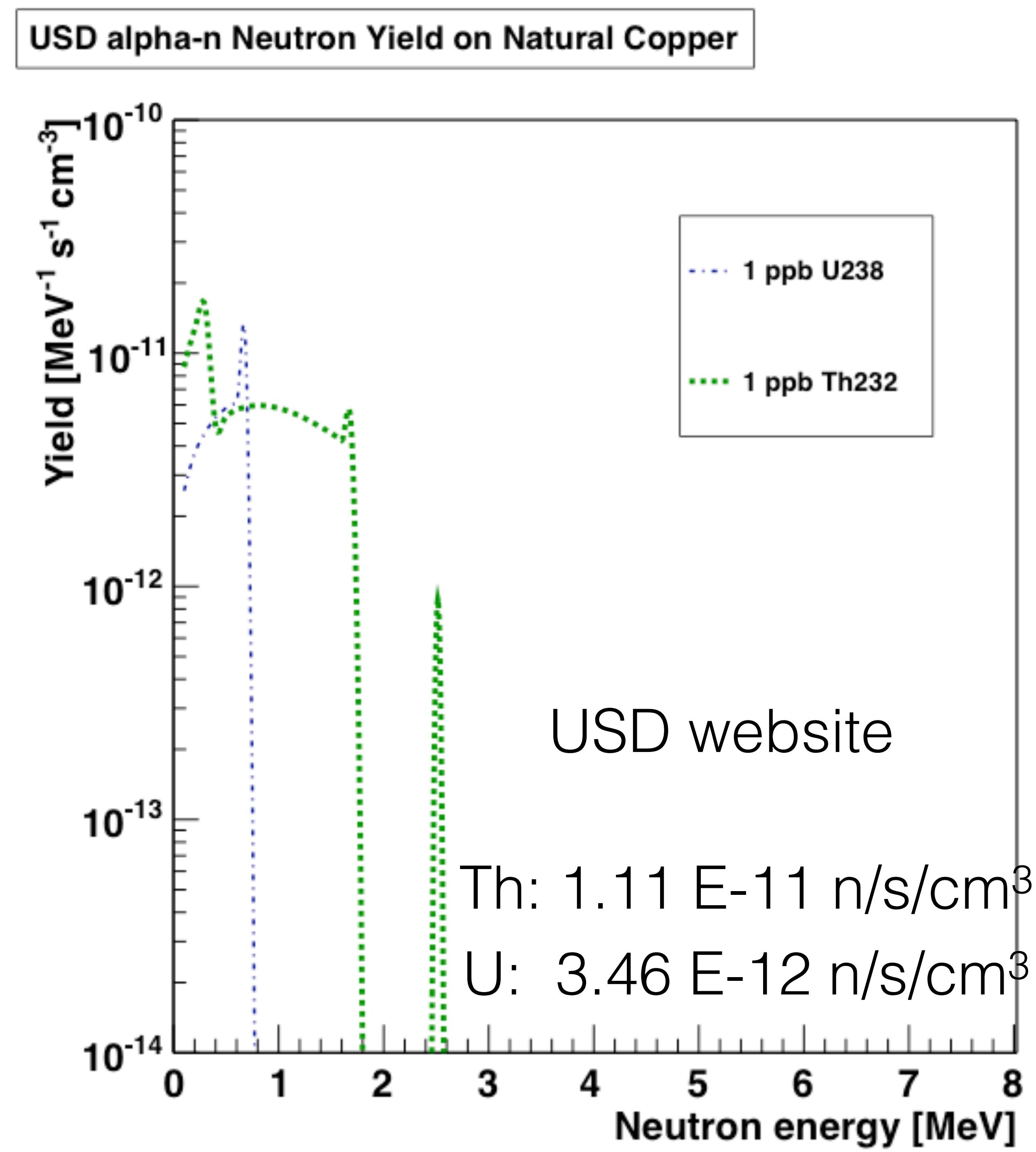


Good agreement!

Dotted black line: USD
Colored plain lines: SOURCES4

Copper Check





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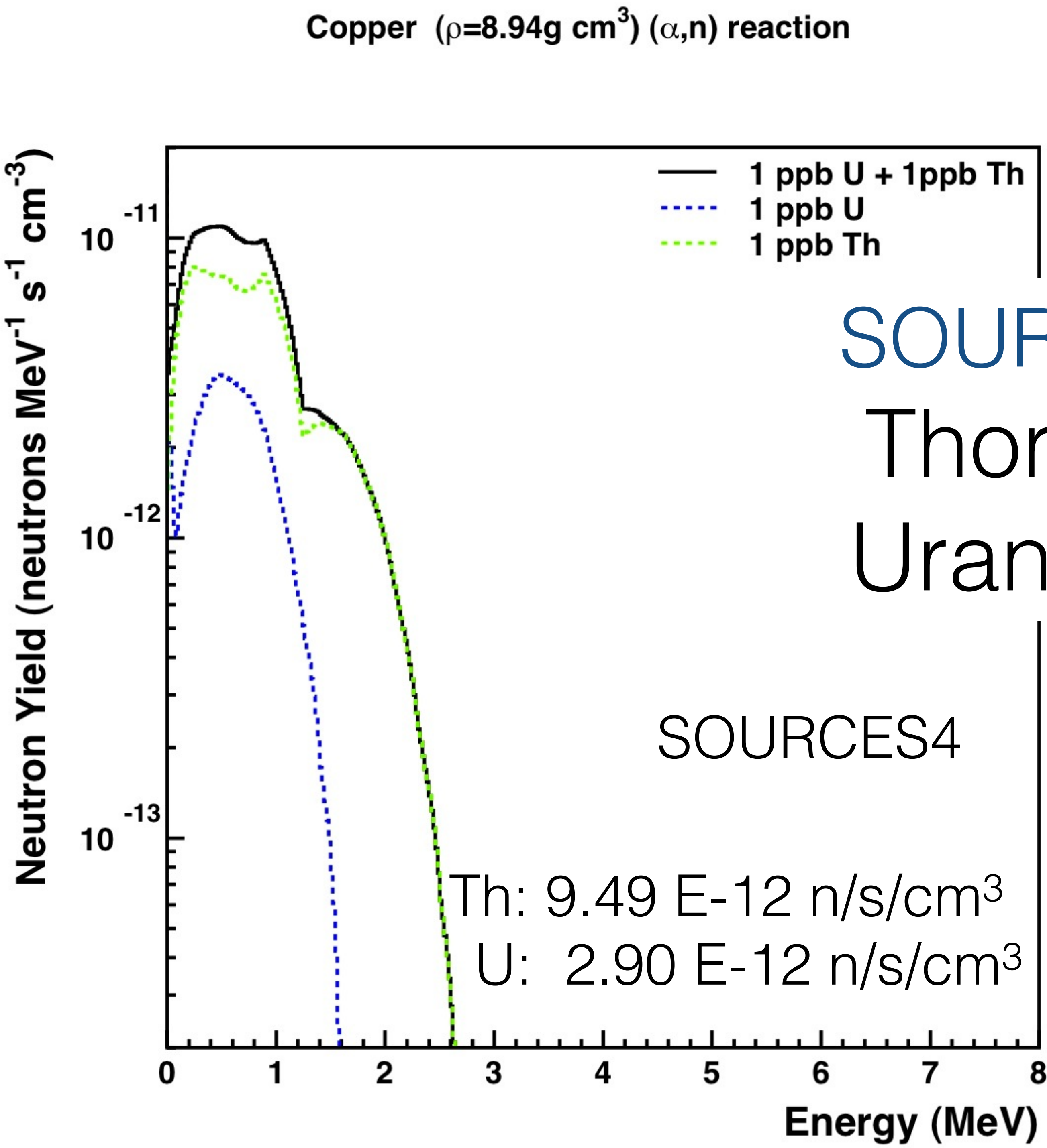
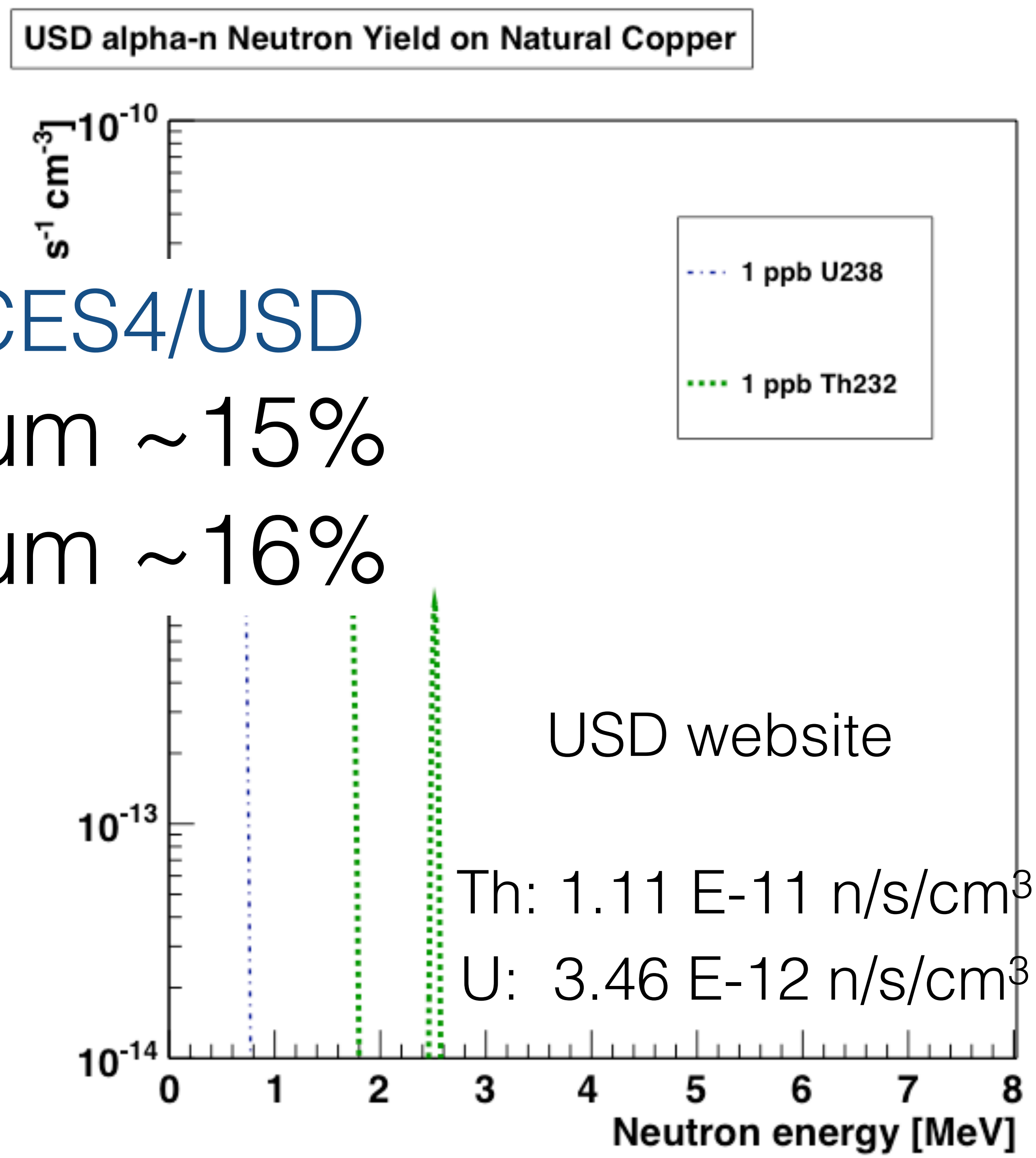




SOURCES4/USD

Thorium ~15%

Uranium ~16%

Simulation check

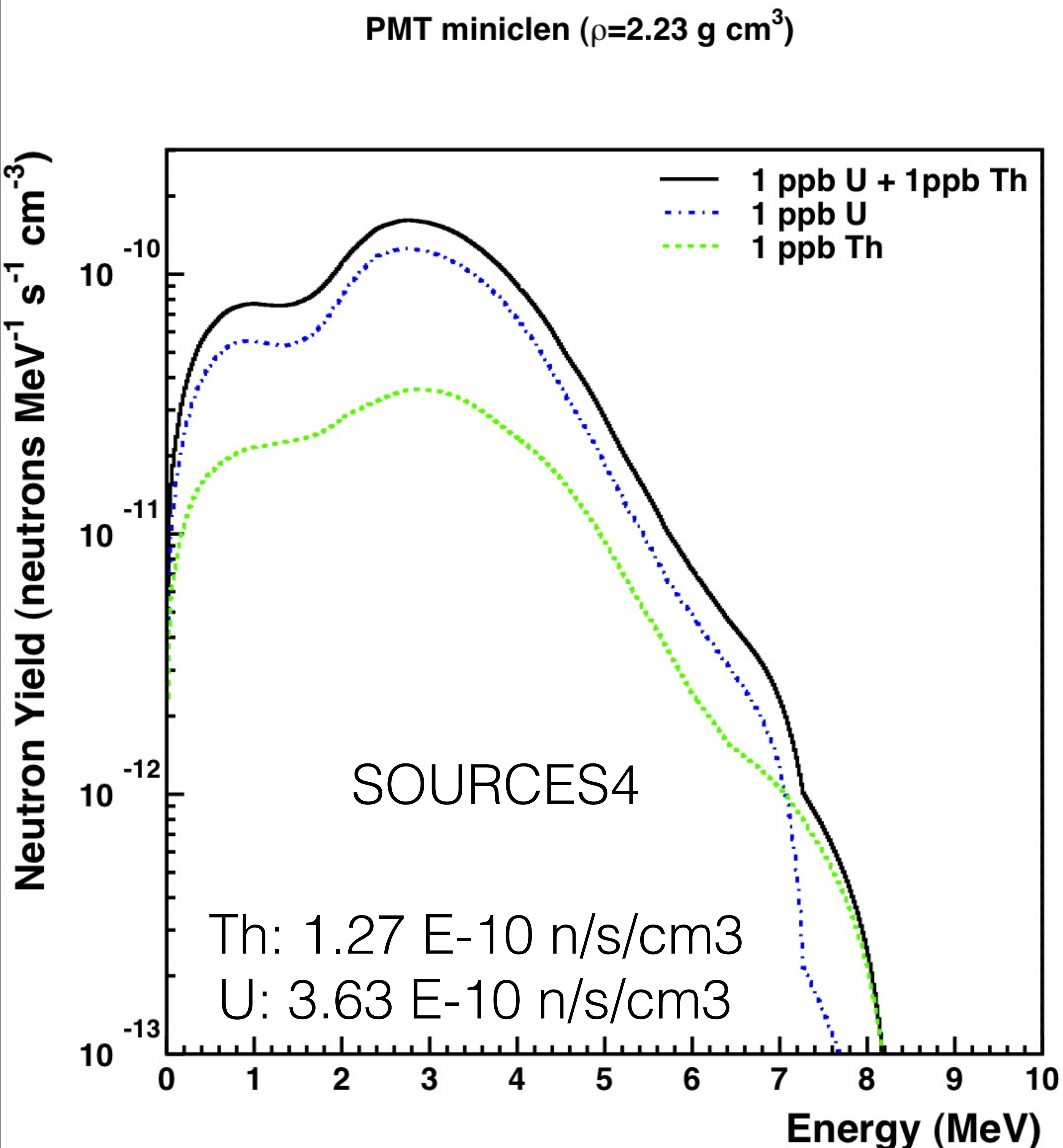
We have performed some quick simulations: propagate both USD and SOURCES4 Cu radiogenic neutron spectra in the same experimental geometry to check the background neutron rate
1 Cu can (21760.6 cm3) around 100kg of germanium detector.
Cu contamination level:Th: 0.02mBq/kg , U: 0.1 mBq/kg

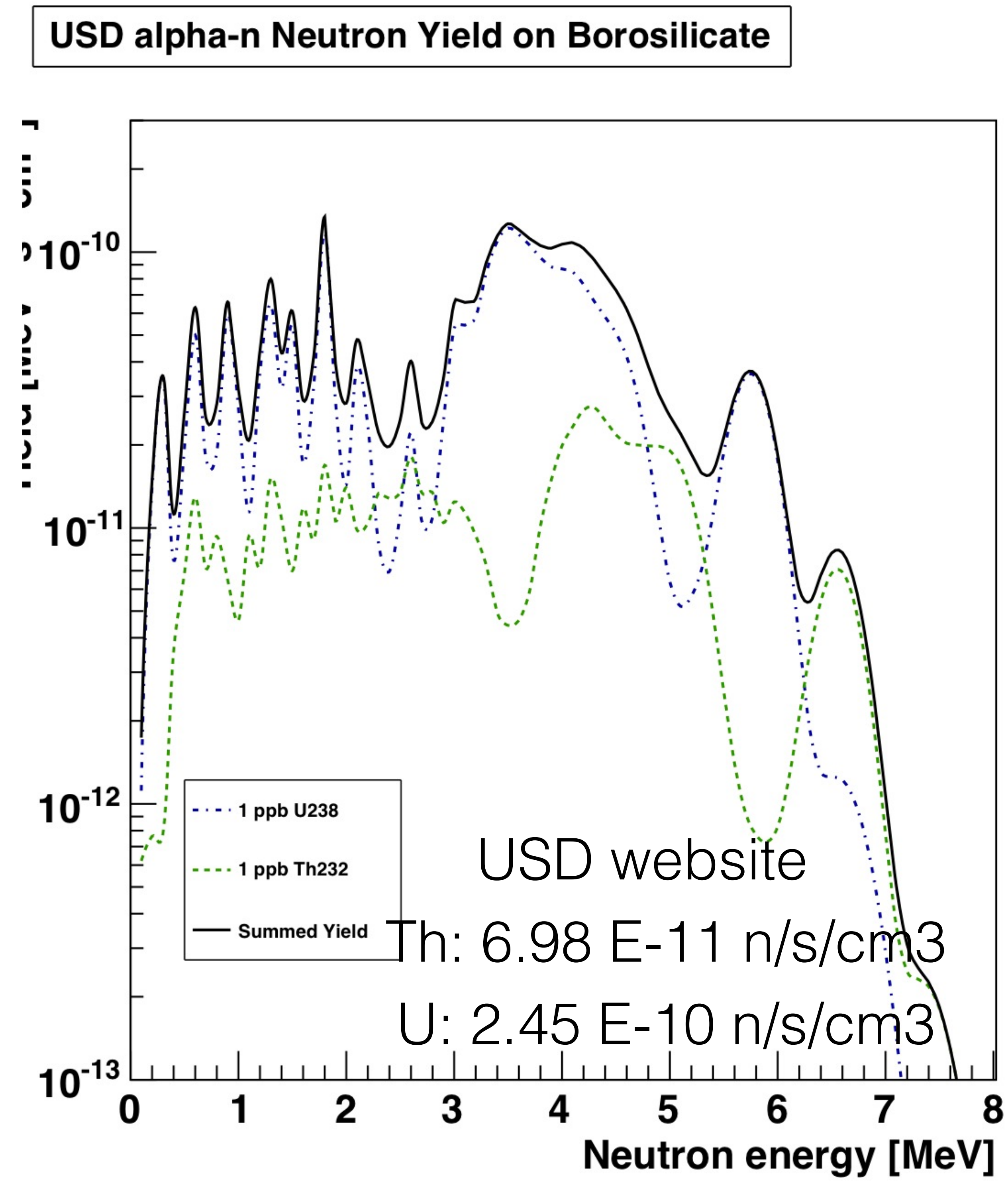
	# Simulated	**Events 10-100 keV**	**MC multiple scatters 10-100keV**	**MC single scatters 10-100keV**
USD	1000000	298035	198539	99496
Sources	1000000	289848	189941	99907

Copper Conclusion:

Shape differences are not a large effect, the MC singles are compatible within stat error.
Looking at the rate (which consider the yield integral) SOURCES4 produces a slightly smaller detection rate than USD but still within stat errors (2.30E-05n/kg/y vs 2.67n/kg/y)

Borosilicate glass check





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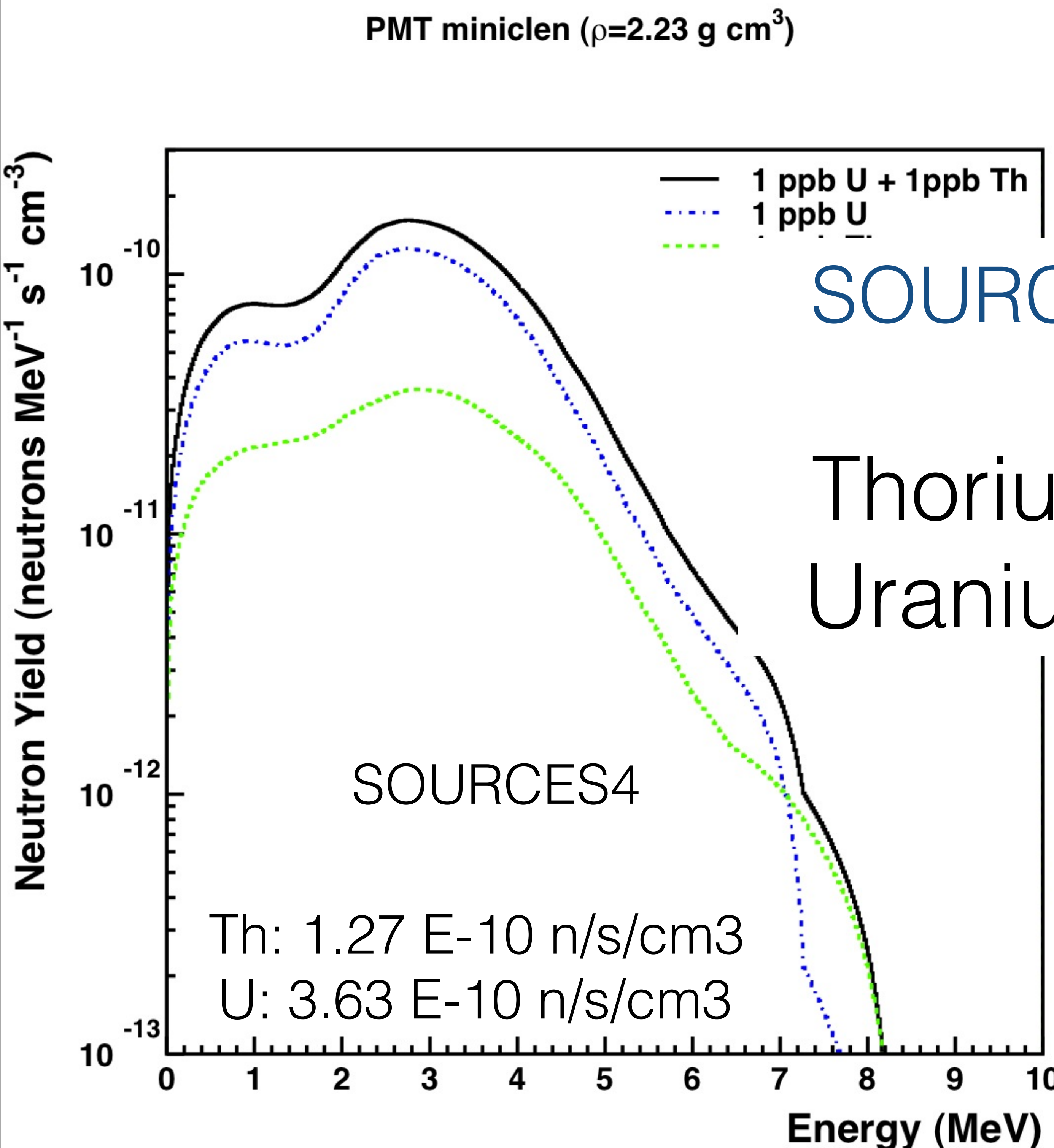
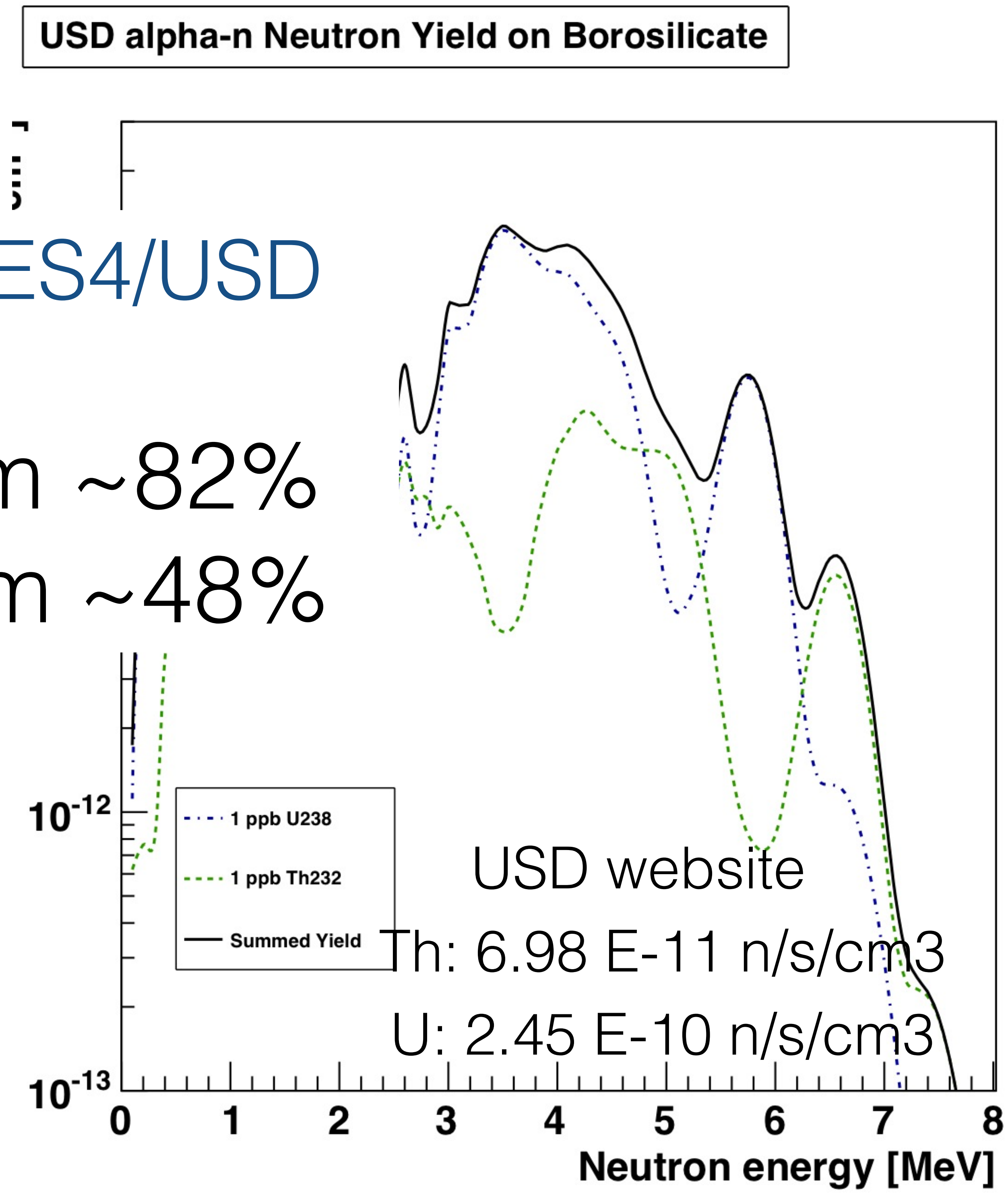


SOURCES4/USD

Thorium ~82%

Uranium ~48%



Borosilicate Simulations

- Simulations done within RAT, utilizing Geant4.9.5, and a cylindrical 45T liquid argon single phase detector surrounded by borosilicate glass mimicking PMTs as well as stainless steel and a water veto
- Simulation done with 1.65 times more thorium than uranium matching assayed values of glass (and old simulations)

	# Simulated	Events 12-25 keVee	& >65 cm from wall	& PSD cut	MC single scatters in ROI
USD	5000000	11651	211	9	2
Sources	5000000	12133	217	10	2

Borosilicate Conclusion:

Shape differences are not a large effect, but at this assay value SOURCES would have 1.8x more neutrons produced than the USD code

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

SOURCES4 - 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:

Z-value	Atom Fraction
12	1.0000000000

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:

ZAID	Atom Fraction
120250	1.000E-01
120260	1.101E-01

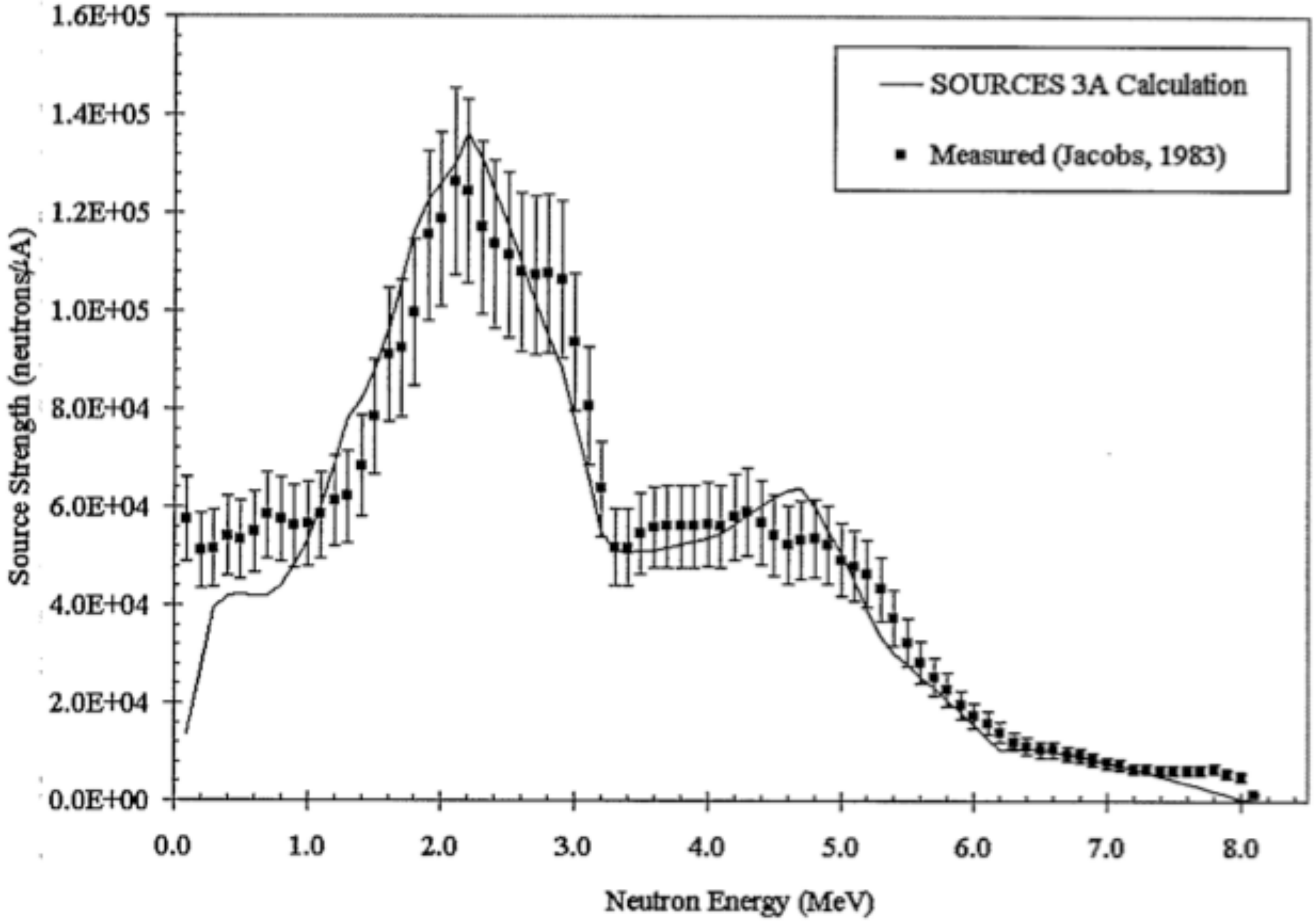


Fig. 21. Energy-Dependent Neutron Source Strength from 5.5 MeV α-Particles Incident on Magnesium Slab as Calculated by SOURCES 4A and Compared to Measured Data.

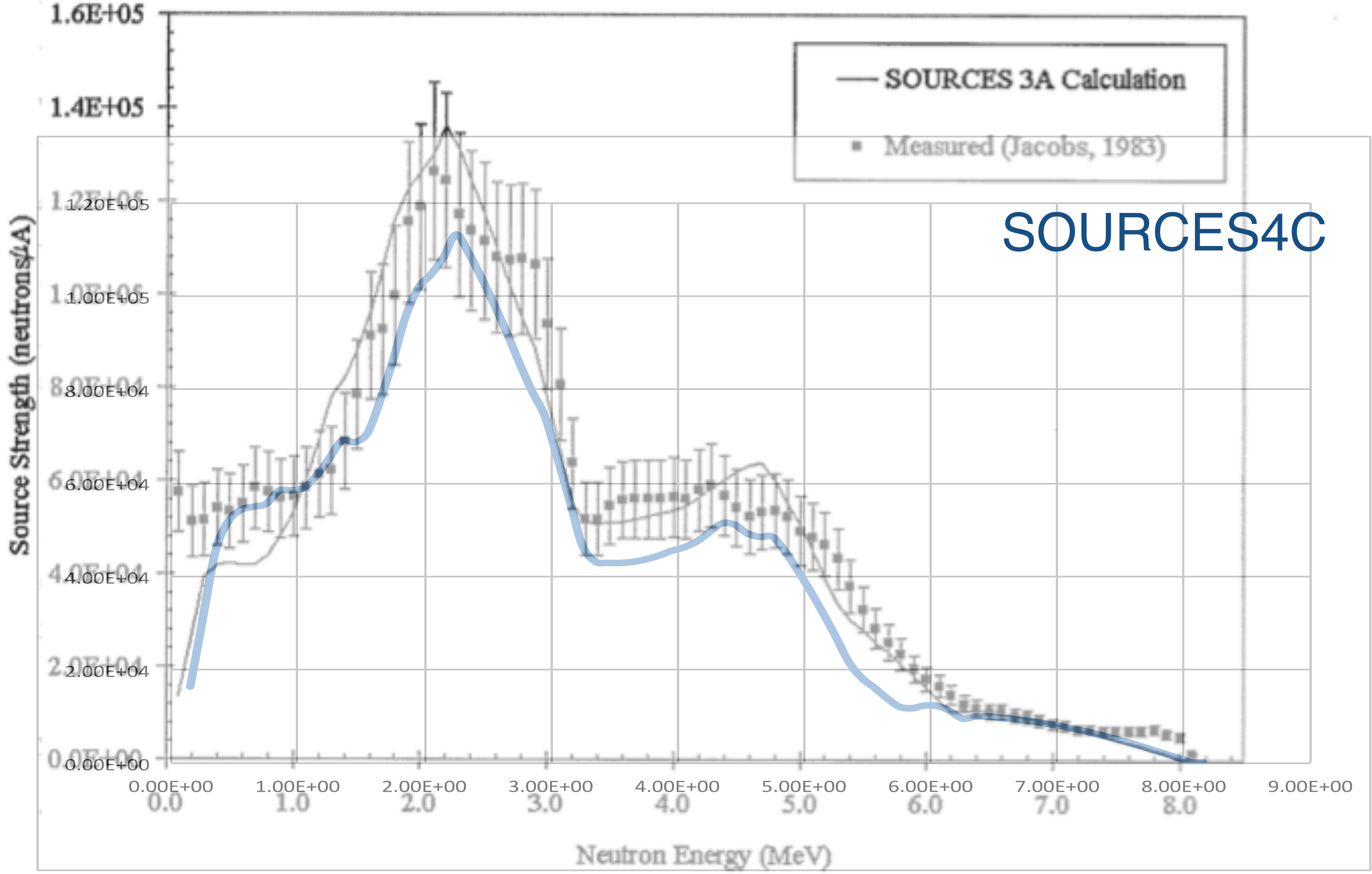
Output - 4A(modified) vs 3A(original)

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%.

target	target atom frac.	alpha source	alpha energy	alphas/sec /microamp	p(e) neut/alpha	neuts/sec /microamp
mg 25	1.0000E-01	beam	5.500	3.1209E+12	5.2789E-07	1.6475E+06
mg 26	1.1010E-01	beam	5.500	3.1209E+12	7.5131E-07	2.3448E+06
					Total (all targets):	3.9923E+06

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

target	target atom frac.	alpha source	alpha energy	alphas/sec /microamp	p(e) neut/alpha	neuts/sec /microamp
mg 25	1.0000E-01	beam	5.500	3.1209E+12	4.5949E-07	1.4340E+06
mg 26	1.1010E-01	beam	5.500	3.1209E+12	6.9817E-07	2.1789E+06
					Total (all targets):	3.6129E+06



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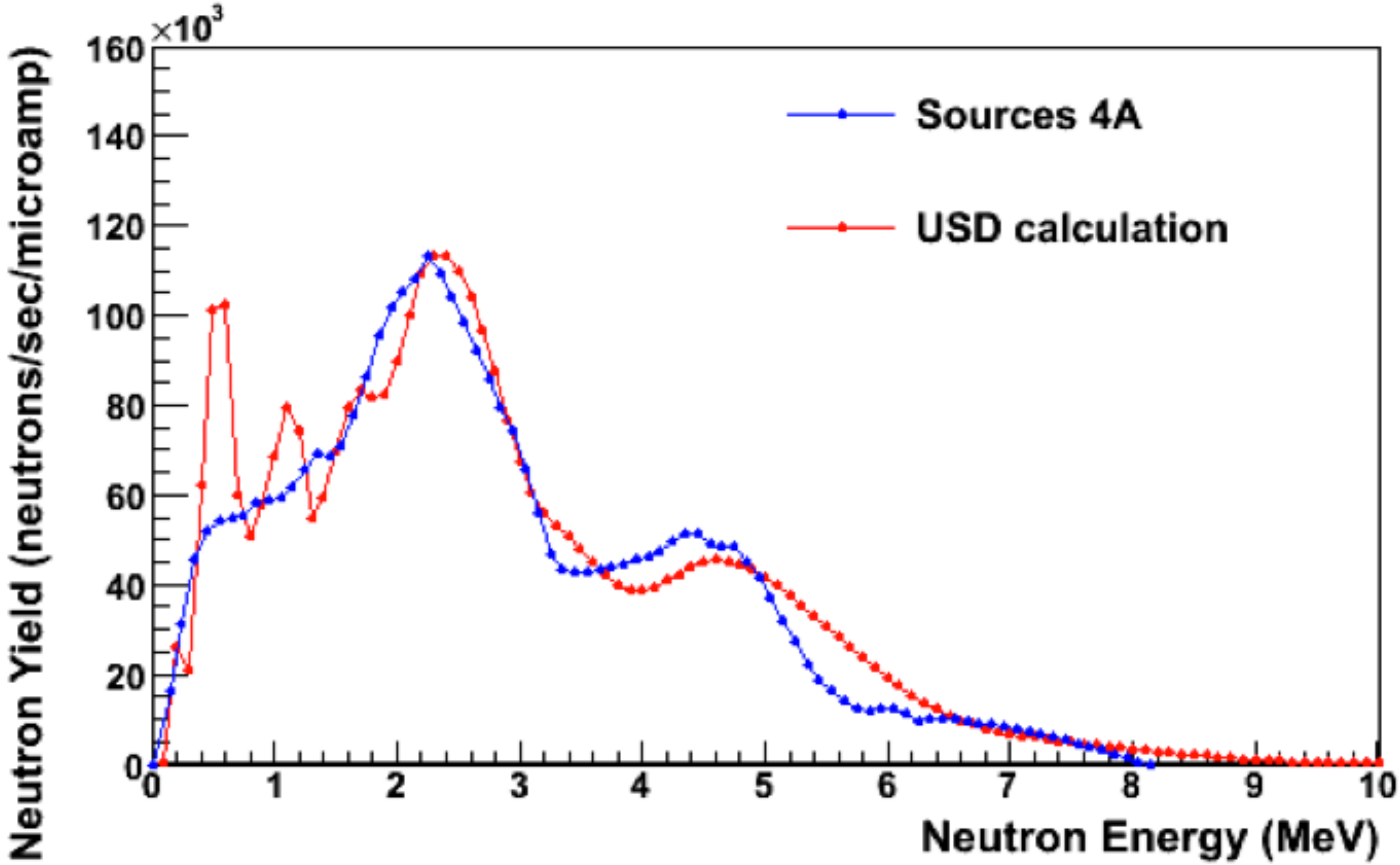

Still some discrepancies…but good agreement

USD: 11.7249e-07 per alpha decay.

SOURCES4: 11.5766e-07 per alpha decay

Conclusion

- USD website and SOURCES4 calculations are compatible within a factor <2
- Validation of some input parameters
  - cross sections
  - alpha decay data - *in fieri*
  - codes against experimental nuclear data

Conclusion

- USD website and SOURCES4 calculations are compatible within a factor <2
- Validation of some input parameters
    - cross sections — check other materials than Cu such as poly and stainless steel which show resonances in their radiogenic neutron spectra
    - alpha decay data - *in fieri*
    - codes against experimental nuclear data — other experimental data?

- “Universal” radiogenic spectrum library for different materials ?
- Are we happy ?!