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Alpha Transport in COG

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Auspices

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Alpha Transport in COG

The following outlines how alpha transport is currently implemented in COG. Alpha transport is handled as a two step process …

Step 1: CSDA. Using data and coding borrowed from the AlfaMC code [**1**], a Continuous Slowing Down Approximation for alphas has been implemented in COG. Following the guide of the AlfaMC code, Gaussian or Landau distributed energy straggling is performed, and a simple Fermi small-angle multiple scattering model is adopted. Since for the energy range under consideration (~1 to 20 MeV), the mean free path for nuclear interactions (e.g., (alpha,neutron), (alpha,gamma), etc.) is very much greater than the range of the alpha, the CSDA approach alone is used to track the alpha. That is nuclear interactions are ignored in this step.

Step 2: Nuclear interactions. A fraction (see below) of the CSDA steps are sampled for nuclear reactions – that is, for each step if a random number is less than the fraction, then nuclear reactions are included and any properly weighted secondaries are produced and followed.

How to: In the COG input deck, there is a new block – **alphatrans**. The possible input selections are…

adestep *de*	where *de* is the fractional energy loss per step, default is 0.01
astragflag *flag*	where flag = 0 for gaussian only, = 1 for gaussian, vavilov, or landau depending on energy, default is 0 (option 1 increases running time)
astepmin *stmin1 stmin2 ...*	where *stmin1*, *stmin2*, ... are minimum steps in cm for each material in **mix** block, must be > 1.e-8, default is 1.e-6
astepmax *stmax1 stmax2 ...*	where *stmax1*, *stmax2*, ... are maximum steps in cm for each material in **mix** block, must be < 10., default is 1.e-3
aecut *ecut1 ecut2 ...*	where *ecut1*, *ecut2*, ... are cutoff energies in MeV for each material in **mix** block, must be > 0.001, default is 0.01
afrac *af1*, *af2*, …	where *af1*, *af2*, … are the fraction of CSDA steps, on average, with nuclear reactions, (this factor should be determined by trial and error, too low and you get few, if any, secondaries, too high and you are swamped with secondaries), default is 0.01

Note: The material dependent quantities are entered according to the ordinal material number, i.e. *1* corresponds to the first material defined in the **mix** block, *2* to the second material defined, and so on. If an entry is made for one material it must be entered for each material, otherwise COG doesn't know how to assign values.

Testing Results

Testing Results for Step 1: Included in the AlfaMC package were 4 example problems. I made changes in COG to calculate the same quantities as determined by the AlfaMC program, and ran each example.

> **Example 1):** A pencil beam of 5.48 MeV alphas impinging on a 1000 μm thickness of water. Output is energy deposited vs depth in 'the water. Figure 1 shows a comparison of COG and AlfaMC.

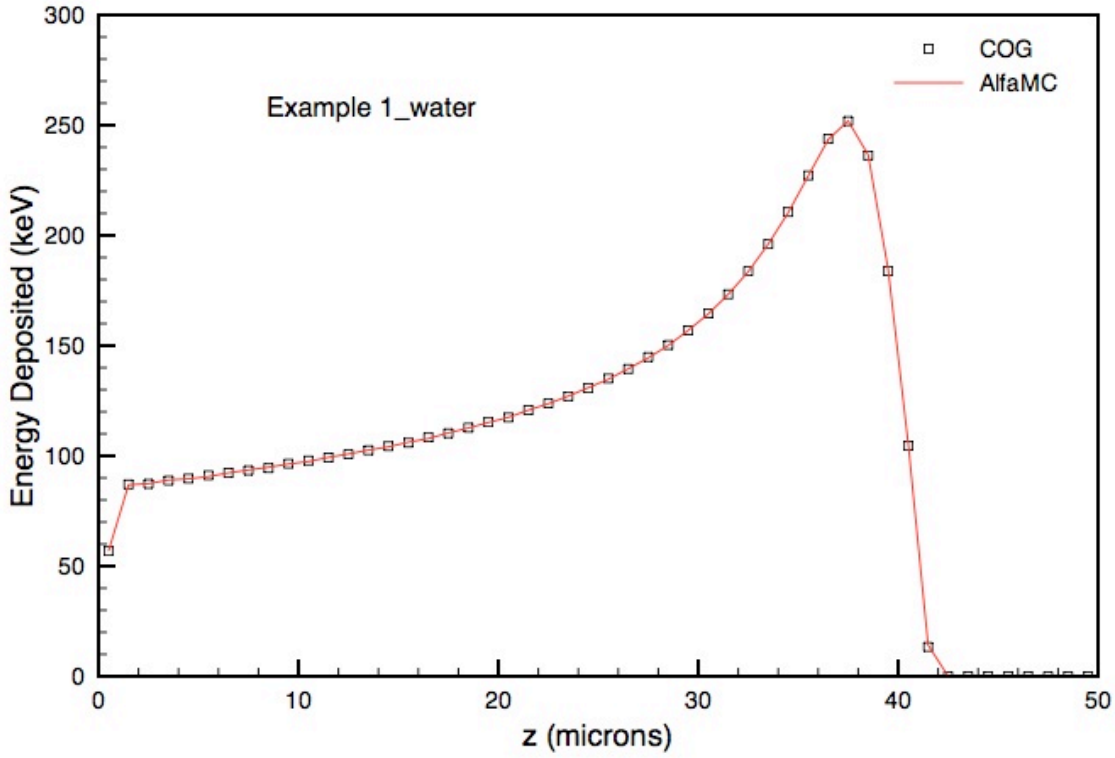

Figure 1

Example 2): A pencil beam of 5.48 MeV alphas impinging on 6 μ mylar foil. Output is the energy transmitted through the foil. Figure 2 shows a comparison of COG and AlfaMC.

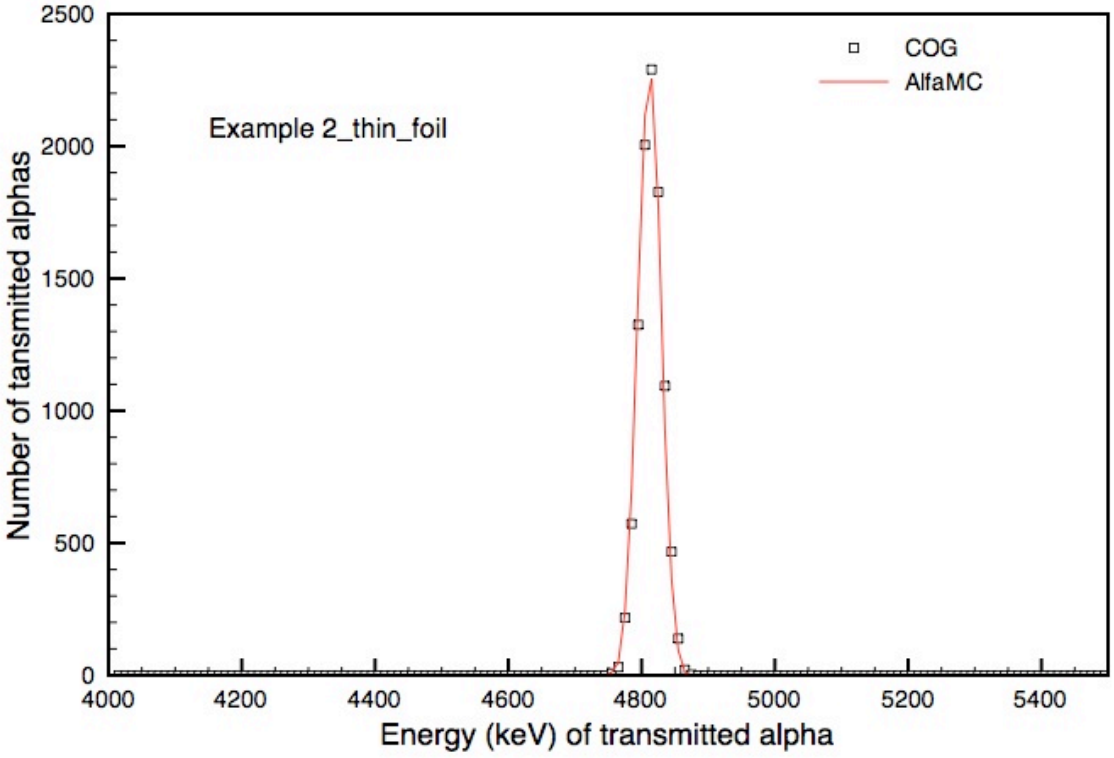

Figure 2

Example 3): An isotropic point source of 5.304 MeV alphas passing through a 6 μm Al foil and a 1 cm vacuum chamber to impinge on a detector consisting of 0.05 μm Au window and 0.03 cm Si wafer. Output is the energy deposited in the Al foil and the Si wafer. Figures 3 and 4 show comparisons of COG and AlfaMC.

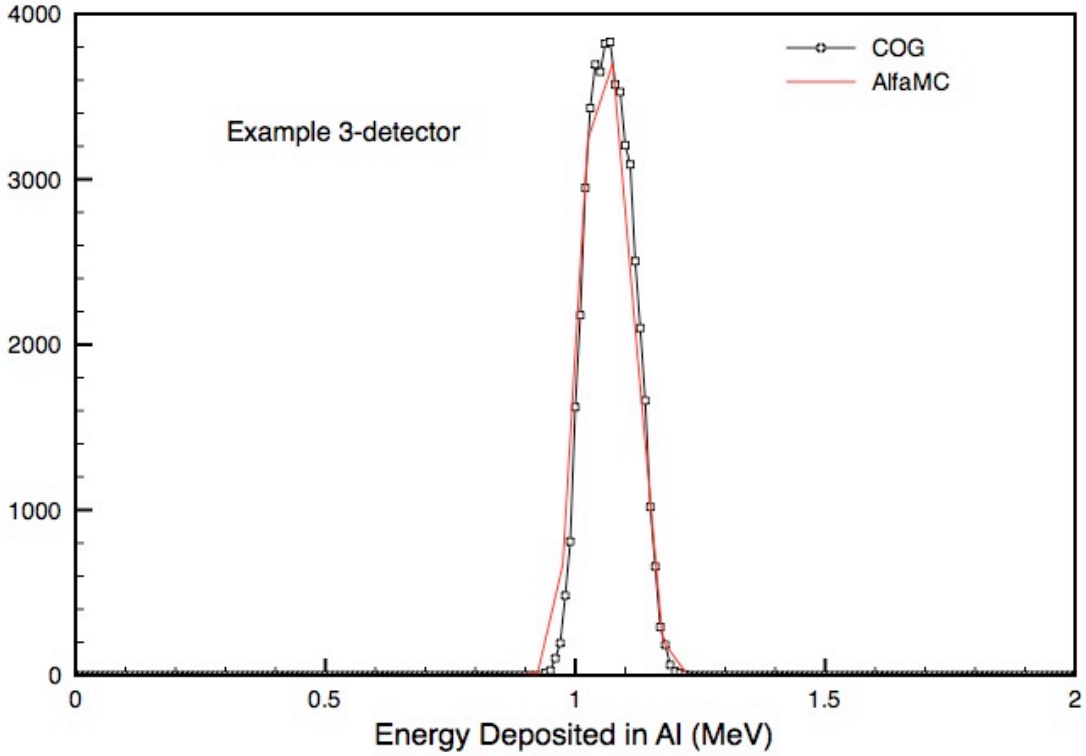

Figure 3

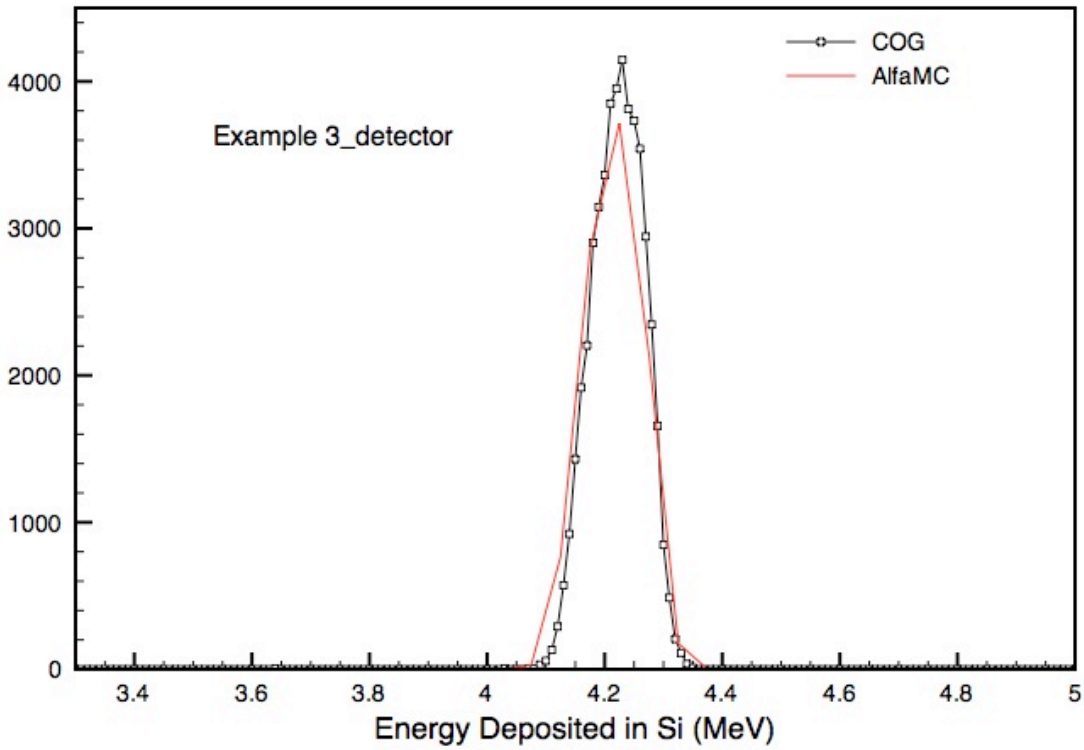
COG
AlfaMC
Example 3_detector
4000
3000
2000
1000
0
3.4
3.6
3.8
4
4.2
4.4
4.6
4.8
5
Energy Deposited in Si (MeV)

Figure 4

Example 4): An isotropic point source of alphas from the U232 decay chain passing through a 1 cm vacuum chamber to impinge on a detector consisting of 0.05 μm Au window and 0.03 cm Si wafer. Output is the energy deposited in the Au window and the Si wafer. Figures 5 and 6 show comparisons of COG and AlfaMC.

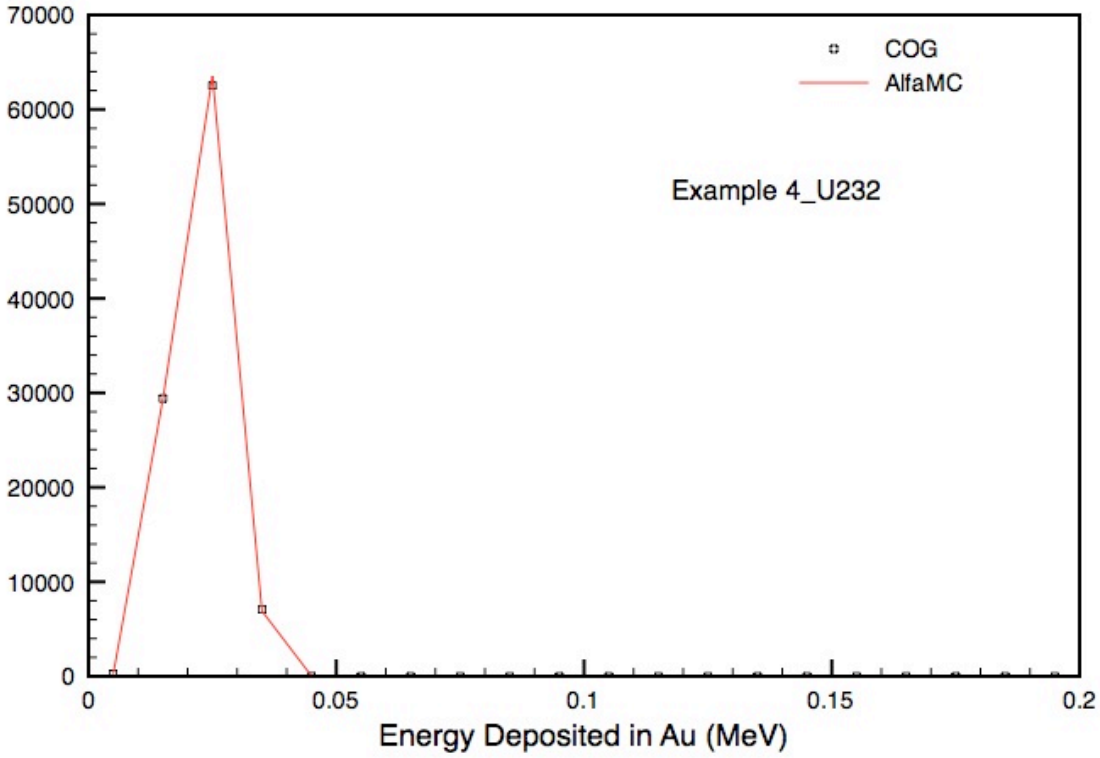

Figure 5

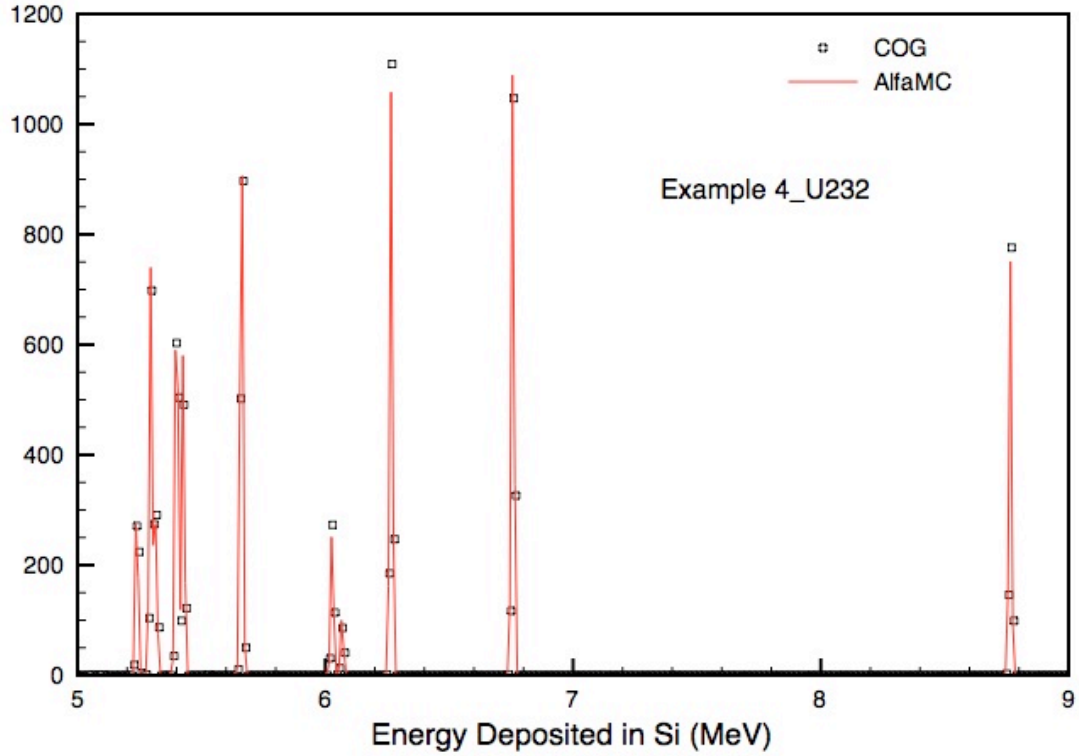

Figure 6

The comparisons range from very good to excellent. On to the next step, include alpha reactions to allow neutron production by the alphas.

Testing Results for Step 2: I included nuclear reactions by sampling a fraction (default or input by material, as described above) of the CSDA steps, forcing nuclear reactions to occur within the selected step, and then following the appropriate, properly weighted secondaries. This scheme allows for nuclear reactions along the entire path and so includes effects of alpha positioning and energy loss. Also, the number of secondaries to follow can be adjusted by setting the fraction of CSDA steps to be sampled.

Wilson, Bozian, and Perry [**2**] , describe a scheme to calculate alpha-induced thick target neutron yields. Table 2 of the reference compares their calculations (SOURCES) to various measurements (Ja83, We82,…). I set out to reproduce these calculations using COG and met with several limitations. Alpha transport in COG is modeled after the AlfaMC code, and so uses the AlfaMC database, which does not include Li, B, F, Na, or Mg. Alpha nuclear reactions are available using primarily the JENDL-AN-2005 data library which does not include O16 or Ne. In Table 1 below I reproduce a truncated (reflecting the above limitations) version of Wilson, Bozian, and Perry's Table 2. I've added columns representing COG calculations using JENDL2005 and TENDL2013 alpha cross sections.

Thick Target (α,n) Neutron Yields, neutrons/10^6 α's															
		Calculation			Measured Values										
Target	E (MeV)	COG-JENDL	COG-TENDL	SOURCES	Ja83	We82	Ge80	Sm80	Ba79	Bu79	Ge75	An71	Go62	Ru56	Ro44
Be	2.0	3.62	2.65	3.16											
	2.5	8.15	8.56	7.73											
	3.0	11.60	18.54	12.30					9.79			10.05			
	3.5	15.45	31.99	15.40					12.79			14.4			
	4.0	23.34	48.72	22.86		22.86			19.88			21.1			
	4.5	38.04	67.85	39.35					33.27			34.8			
	5.0	57.28	89.11	56.89		56.78			49.43			35.5			
	5.3	71.93	102.8	70.35			73		63		64	69	84.4		80
	5.48	81.27	110.5	79.28			82	70						74	
	5.5	82.44	111.6	80.31					71.81		80				
	5.79	98.59	125.2	96.56			100								
	6.0	111.7	135.1	108.5		109.5		99.2							
	6.1	117.0	140.6	113.9			118							112	
	6.5	140.3	157.7	136.0				126.2							
C	3.0	0.020	0.028	0.029					0.024						
	3.5	0.036	0.053	0.051					0.040						
	4.0	0.038	0.087	0.057	0.039	0.043			0.042						
	4.5	0.044	0.126	0.065	0.046				0.047						
	5.0	0.060	0.172	0.081	0.061	0.065			0.063						
	5.3	0.087	0.205	0.114									0.113		0.09
	5.5	0.107	0.232	0.142	0.101				0.11						
	6.0	0.186	0.318	0.224		0.172			0.170						
	6.5	0.260	0.428	0.325					0.252						
N	6.5	0.156	0.424	0.484											
Al	3.5	0.0016	0.0031	0.0008					0.0012						
	4.0	0.0152	0.0237	0.0158	0.019				0.0169						
	4.5	0.0865	0.120	0.0828	0.087				0.0802						
	5.0	0.324	0.392	0.281	0.260				0.2643						
	5.3	0.567	0.698	0.495									0.76		0.64
	5.5	0.830	0.973	0.697	0.747				0.6967						
	6.0	1.701	2.070	1.468					1.438						
	6.5	2.993	3.770	2.855					2.780						
Si	4.0	0.004	0.007	0.011	0.004	0.004									
	4.5	0.018	0.028	0.032	0.014				0.016						
	5.0	0.056	0.076	0.080	0.058	0.067			0.052						
	5.3	0.086	0.124	0.118									0.168		0.15
	5.5	0.120	0.166	0.146	0.113				0.114						
	6.0	0.263	0.306	0.277		0.249			0.231						
	6.5	0.435	0.508	0.411					0.385						

Table 1

To more easily make comparisons I divided each column by the COG-JENDL column, the results are given in Table 2. I also included a color coding: ± 10% are black; ± 20% are green; ± 30% are blue; and > ± 30% are red.

Thick Target (α,n) Neutron Yields, neutrons/10^6 α's															
		Calculation			Measured Values										
Target	E (MeV)	COG-JENDL	COG-TENDL	SOURCES	Ja83	We82	Ge80	Sm80	Ba79	Bu79	Ge75	An71	Go62	Ru56	Ro44
Be	2.0	1.000	0.732	0.873											
	2.5	1.000	1.050	0.948											
	3.0	1.000	1.598	1.060					0.844			0.866			
	3.5	1.000	2.071	0.997					0.828			0.932			
	4.0	1.000	2.087	0.979		0.979			0.852			0.904			
	4.5	1.000	1.784	1.034					0.875			0.915			
	5.0	1.000	1.556	0.993		0.991			0.863			0.620			
	5.3	1.000	1.429	0.978			1.015		0.876		0.890	0.959	1.17		1.11
	5.48	1.000	1.360	0.976			1.009	0.861						0.91	
	5.5	1.000	1.354	0.974					0.871		0.970				
	5.79	1.000	1.270	0.979			1.014								
	6.0	1.000	1.209	0.971		0.980		0.888							
	6.1	1.000	1.202	0.974			1.009							0.96	
	6.5	1.000	1.124	0.969				0.900							
C	3.0	1.000	1.400	1.450					1.200						
	3.5	1.000	1.472	1.417					1.111						
	4.0	1.000	2.289	1.500	1.026	1.132			1.105						
	4.5	1.000	2.864	1.477	1.045				1.068						
	5.0	1.000	2.867	1.350	1.017	1.083			1.050						
	5.3	1.000	2.356	1.310									1.3		1.03
	5.5	1.000	2.168	1.327	0.944				1.028						
	6.0	1.000	1.710	1.204		0.925			0.914						
	6.5	1.000	1.646	1.250					0.969						
N	6.5	1.000	2.718	3.103											
Al	3.5	1.000	1.938	0.500					0.750						
	4.0	1.000	1.559	1.039	1.250				1.112						
	4.5	1.000	1.387	0.957	1.006				0.927						
	5.0	1.000	1.210	0.867	0.802				0.816						
	5.3	1.000	1.231	0.873									1.34		1.13
	5.5	1.000	1.172	0.840	0.900				0.839						
	6.0	1.000	1.217	0.863					0.845						
	6.5	1.000	1.260	0.954					0.929						
Si	4.0	1.000	1.558	2.558	0.930	0.930									
	4.5	1.000	1.588	1.808	0.791				0.904						
	5.0	1.000	1.371	1.441	1.045	1.207			0.937						
	5.3	1.000	1.453	1.379									1.95		1.74
	5.5	1.000	1.388	1.220	0.944				0.952						
	6.0	1.000	1.162	1.054		0.947			0.879						
	6.5	1.000	1.167	2.683					0.885						

Table 2

Comparing COG-JENDL to COG-TENDL shows the TENDL2013 alpha cross sections yield consistently, and significantly, higher neutron yields. Comparing COG-JENDL to SOURCES shows a mixed bag; the Be comparisons are mostly ± 10%, the others range from a few at ± 10% to mostly > ±30%. Comparison of COG-JENDL with measurements is considerably better. Of the 73 measurements included in Table 2, 39 are at ± 10%, 26 at ± 20%, 4 at ± 30%, and 4 at >± 30%.

References:

[**1**] L. Peralta and A. Louro, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 737, 11 February 2014, Pages 163–169

[**2**] W. B. Wilson, M. Bozian, and R. T. Perry, LA-UR-88-1976