Computational Facilities

Speaker: Cody Peeples; M.S.

Center for Engineering Applications of Radioisotopes
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Objectives

- Education
- Productivity
- Research and Development

Status

- Sun cluster – our first cluster
  - Learning experience
  - Poor performance
  - Decommissioned and dismantled
- ‘Spectral’ – our second cluster
  - Over 1 year of operation
  - Good performance
  - Good utilization
  - Improvements ongoing
- Third cluster on the way
  - Equipment testing/selection
  - Considering multi-core processing

Vision

- Keep up progress in OWL simulation
  - academic partnerships and student direction
  - synergy with homeland security research
- Maintain high-performance Monte Carlo capabilities for MC-DO-LLS approach to various measurement problems

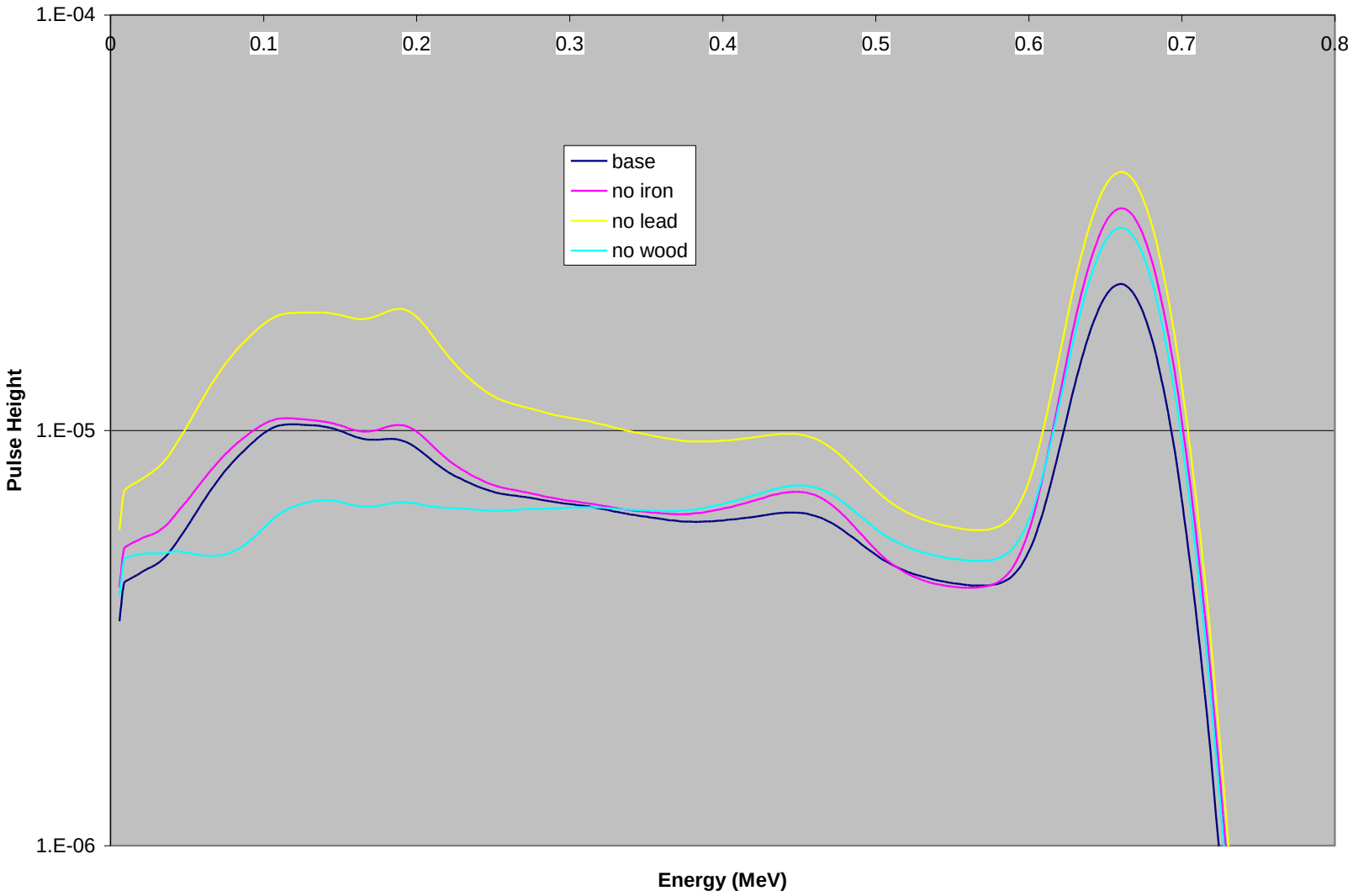
Examples

- Neutron porosity sources
- Portal monitoring DO-LLS
- XRF DO-LLS
- C/O log simulations

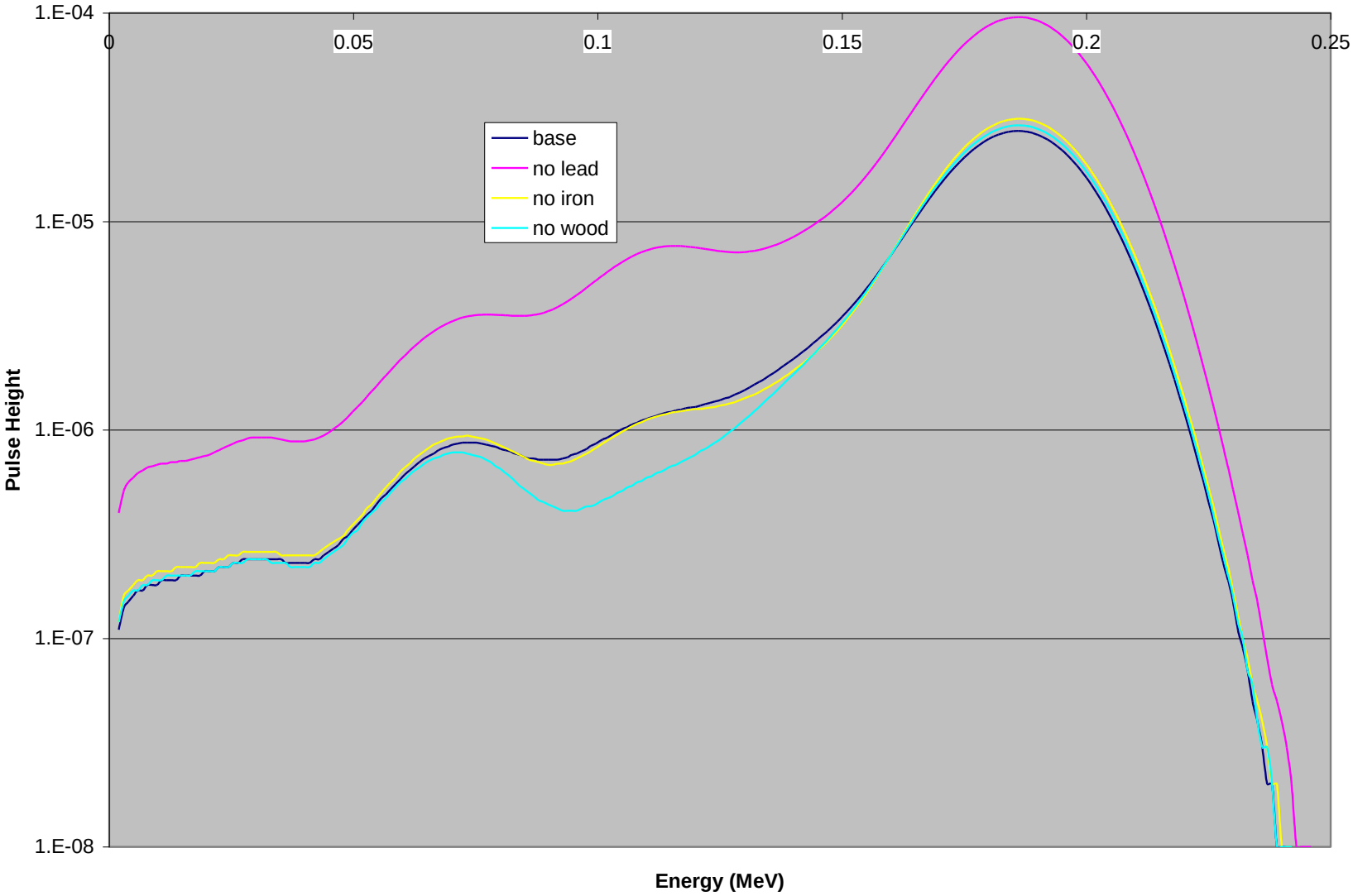
Conclusion

- Education
- Productivity
- Research and Development

Taking out Materials -- Cesium

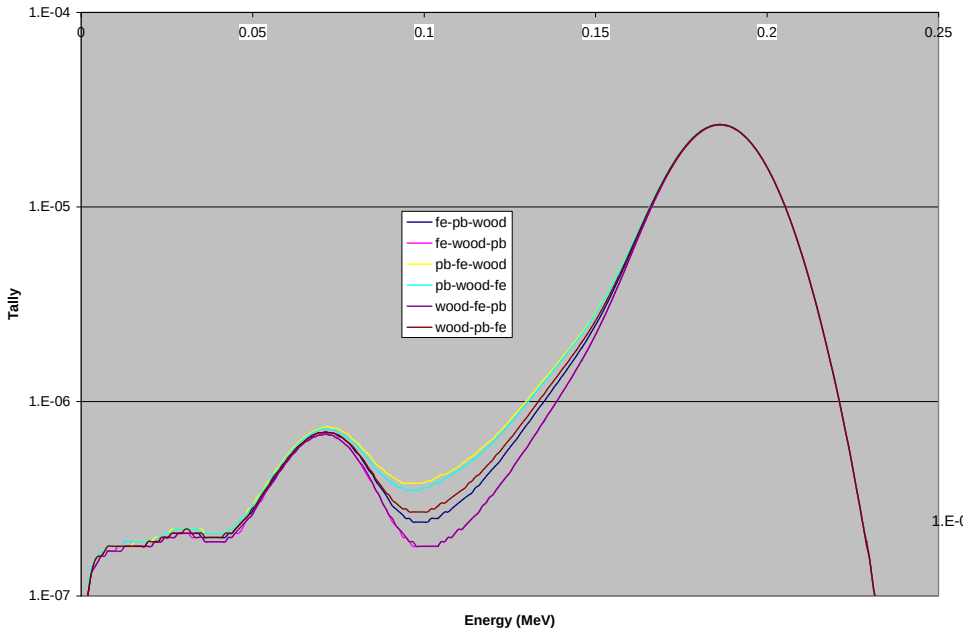


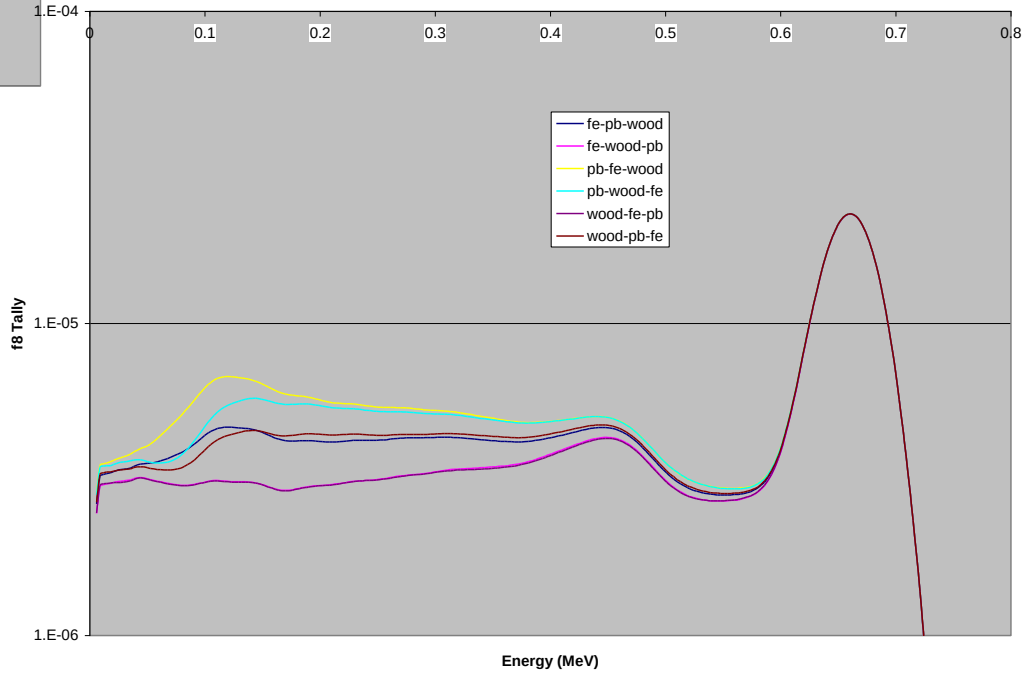
Taking out Materials -- Uranium



Order of Shielding

Order

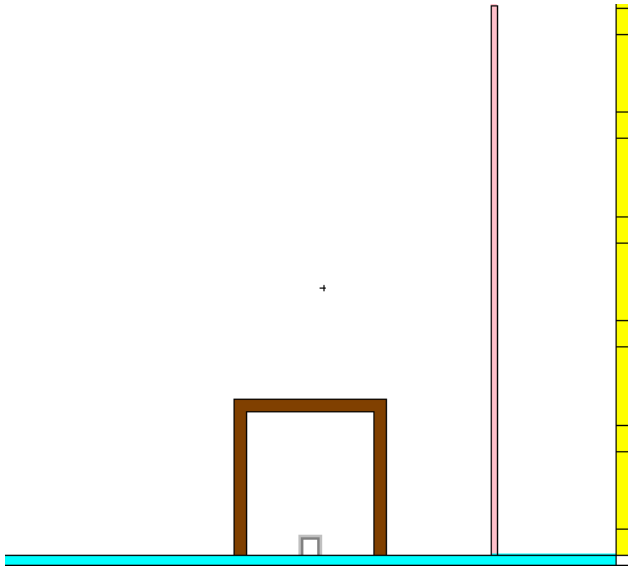

1.E-04
1.E-05
1.E-06
1.E-07
0
0.05
0.1
0.15
0.2
0.25
Tally
Energy (MeV)
fe-pb-wood
fe-wood-pb
pb-fe-wood
pb-wood-fe
wood-fe-pb
wood-pb-fe


1.E-04
1.E-05
1.E-06
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
f8 Tally
Energy (MeV)
fe-pb-wood
fe-wood-pb
pb-fe-wood
pb-wood-fe
wood-fe-pb
wood-pb-fe

Case Studies

Case Studies

- Typical Fertilizer -> NPK mix 15:2:5
- Rice->25% Carbon, 50% Hydrogen, 25% Hydrogen
- Electronics-> 100% Silicon

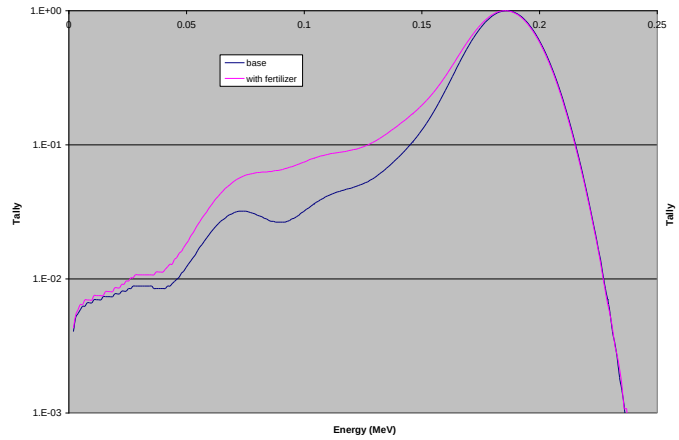


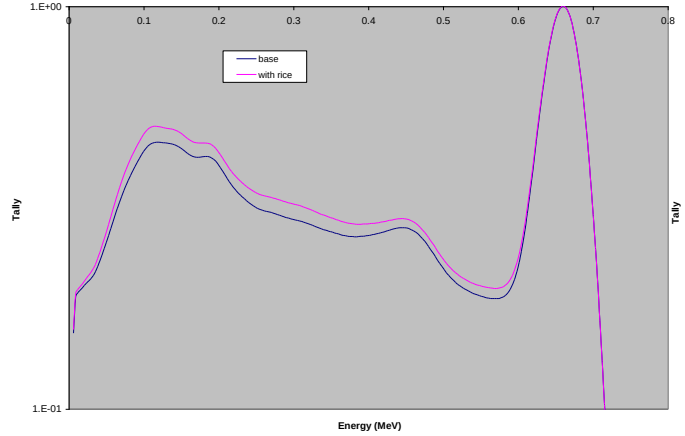
Fertilizer	Chemical composition	S content (%[a])
S Fertilizers		
Elemental S	S	99.6
Agric-S	S	90.0
Gypsum	$CaSO_4 \cdot 2H_2O$	18.6
Commercial gypsum	$CaSO_4 \cdot 2H_2O$ + impurities	13–14
Pyrites	FeS_2	53.5
N Fertilizers		
Ammonium sulfate	$(NH_4)_2SO_4$	23.7
Urea sulfur		10
Ammonium phosphate sulfate	$(NH_4)_2SO_4 + NH_4H_2PO_4 + (NH_4)_2HPO_4$	15.5
P Fertilizers		
Ordinary superphosphate (OSP)	$Ca(H_2PO_4)_2 + CaSO_4 \cdot 2H_2O$	13.9
Concentrated superphosphate (CSP)	$Ca(H_2PO_4)_2$	1.5
Ammoniated OSP		12
Ammoniated CSP		1.4
K Fertilizers		
Potassium sulfate	K_2SO_4	17.6
Potassium magnesium sulfate	$K_2SO_4 \cdot 2\ MgSO_4$	22.0
Others		
Copper sulfate	$CuSO_4 \cdot 5H_2O$	12.8
Zinc sulfate	$ZnSO_4 \cdot H_2O$	17.8
Manganese sulfate	$MnSO_4 \cdot 4H_2O$	14.5
Magnesium sulfate (Epsom salt)	$MgSO_4 \cdot 7H_2O$	13.0
Ammonium thiosulfate	$(NH_4)_2S_2O_3$	43.3

[a] Commercial grades generally contain somewhat lesser values.

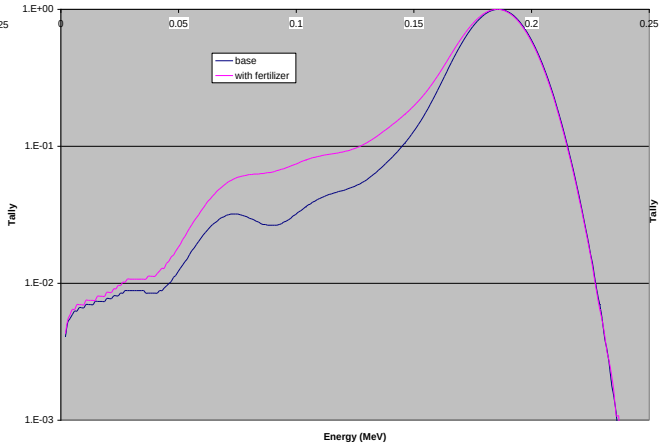
Case studies

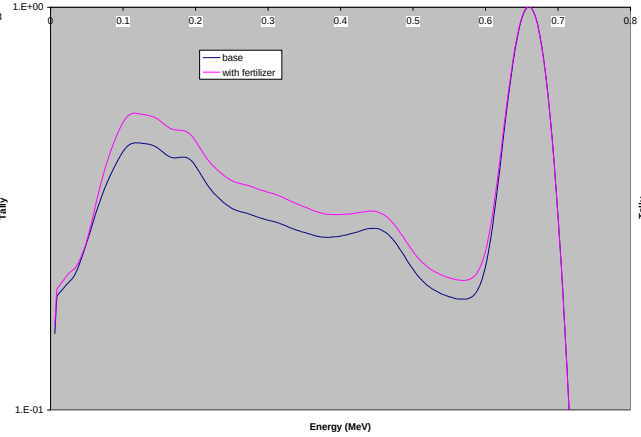
Rice



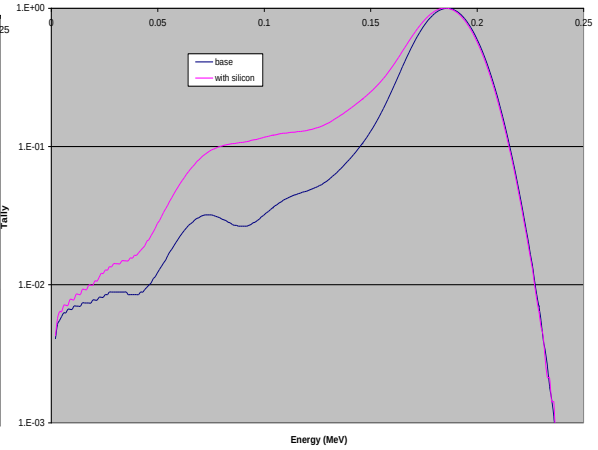


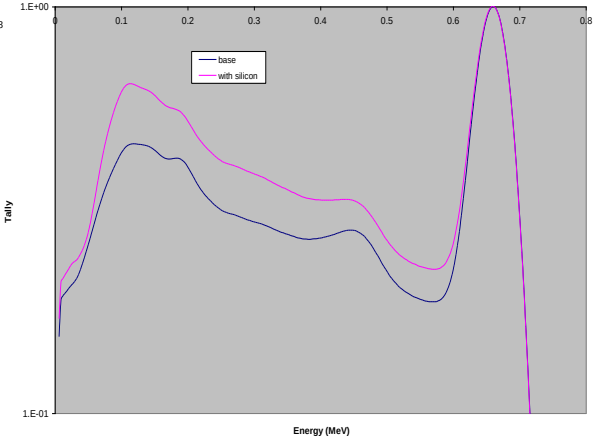
Fertilizer



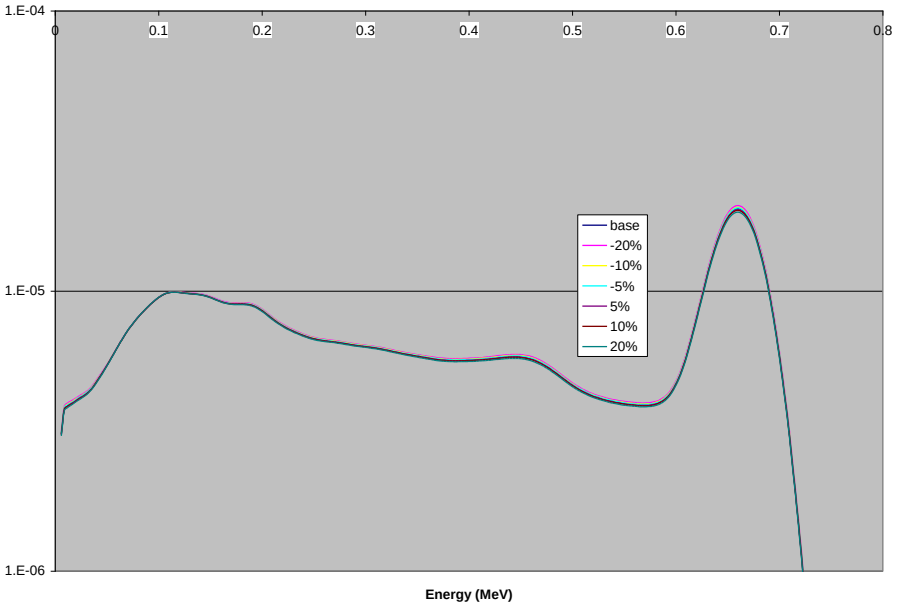


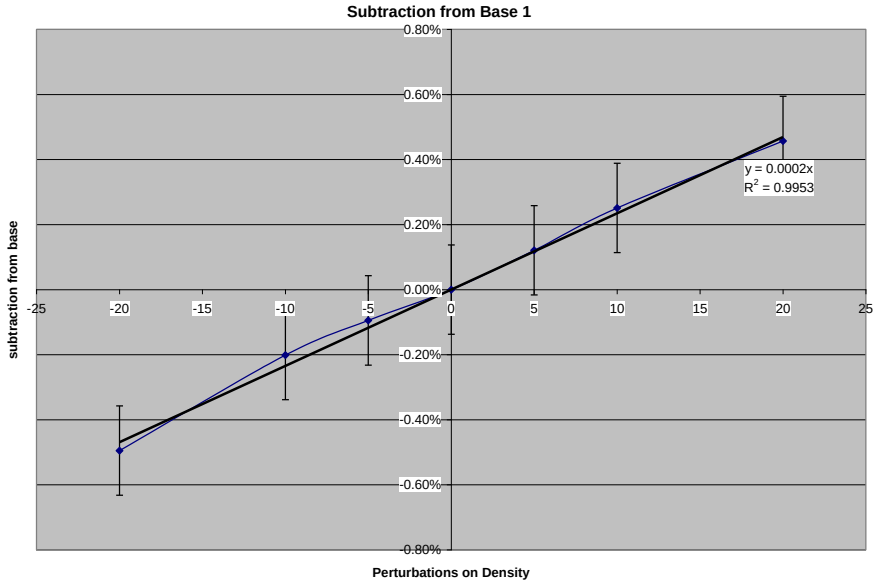
Electronics

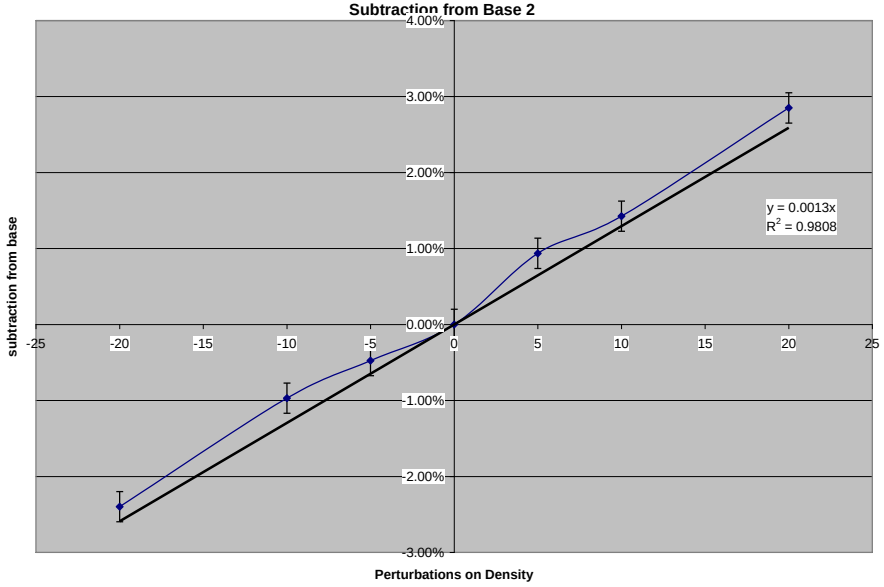


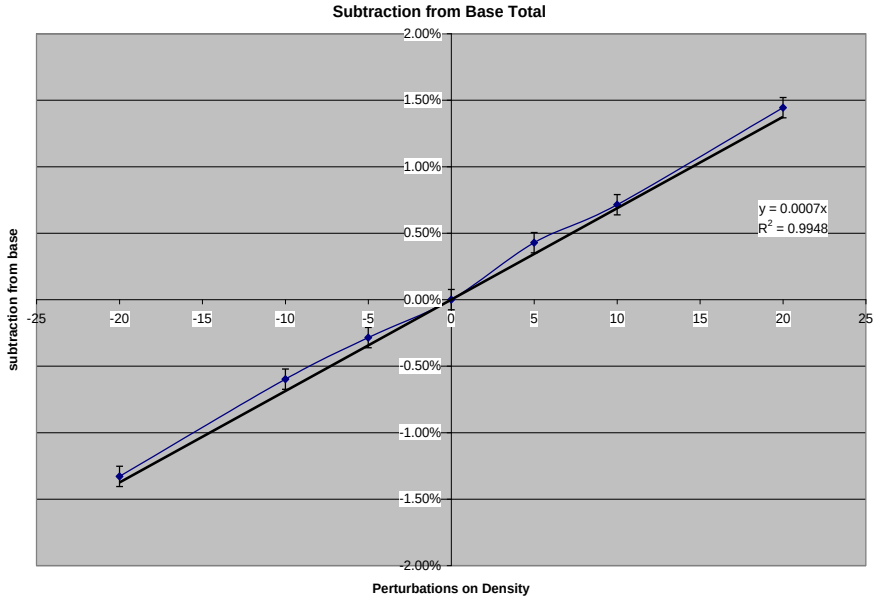


Rice Perturbation







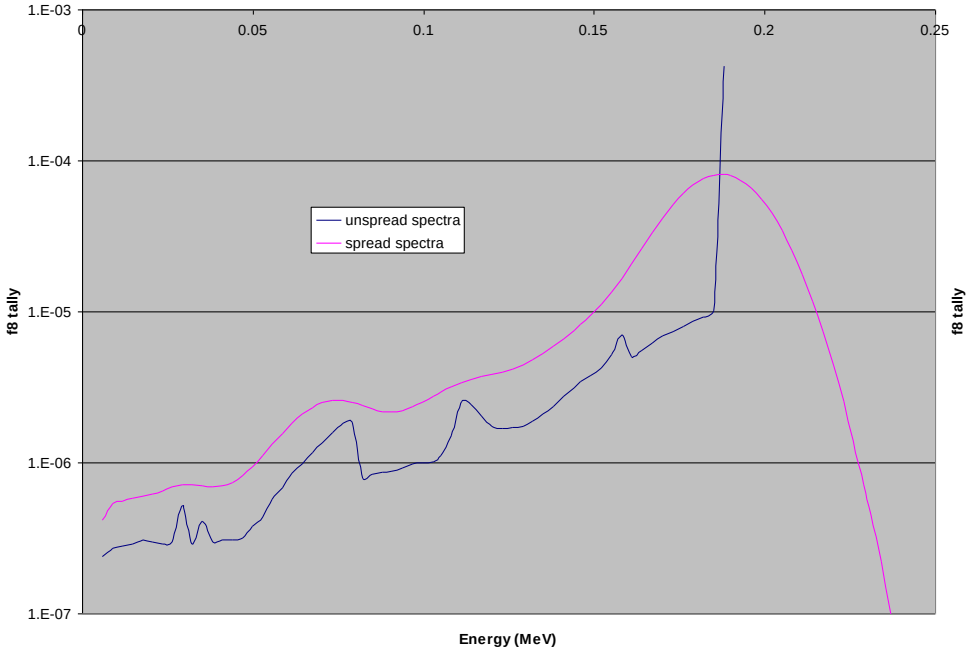


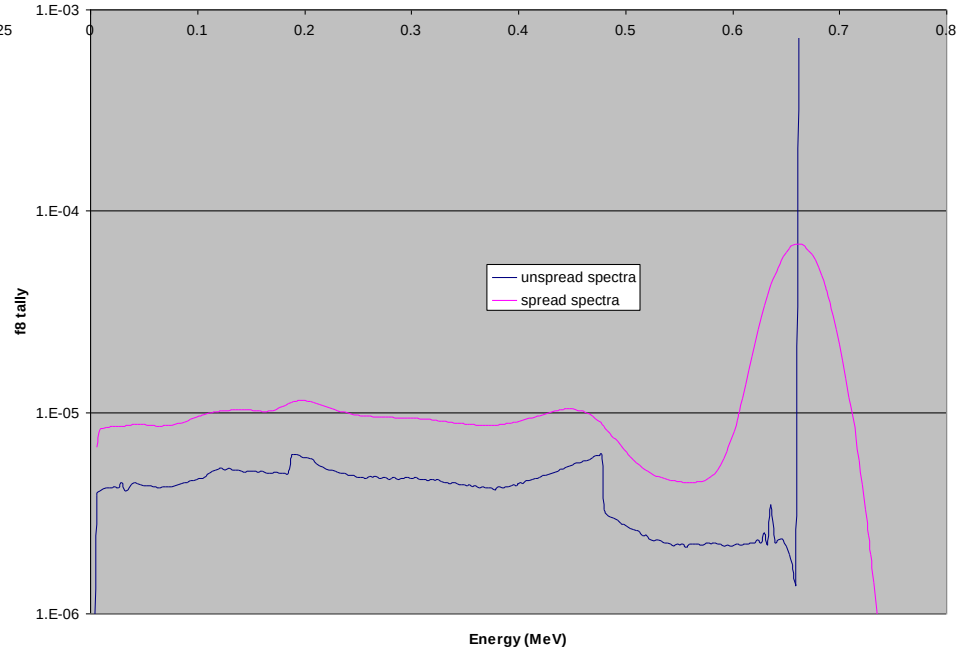
Differential Operator File Setup

MCNP runs

- Reference spectra for the thickness of lead, iron, and wood are 0.1, 0.1442, and 0.71 cm respectively for both energies
- Unknown spectra that has 0.108, 0.146, and 0.68 cm shielding of lead, iron and wood respectively for both energies
- +/- 5% density for lead, iron and wood for both energies at reference file thickness

Spreading Spectra

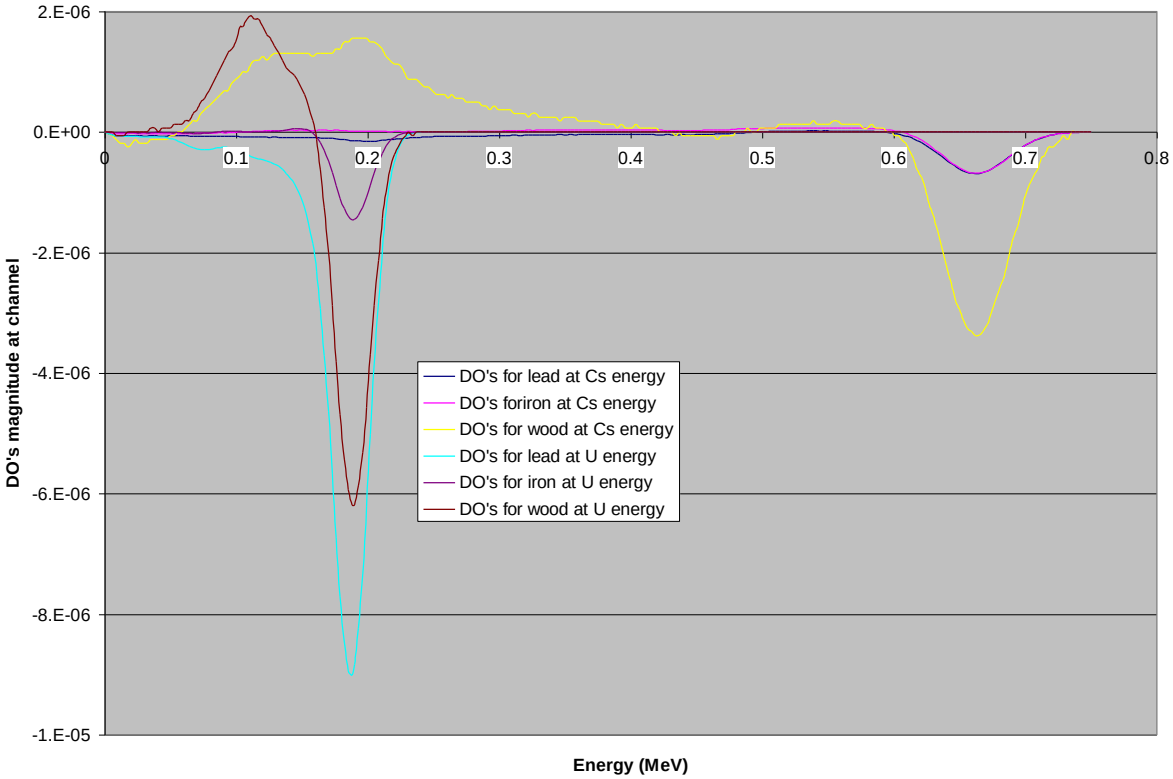




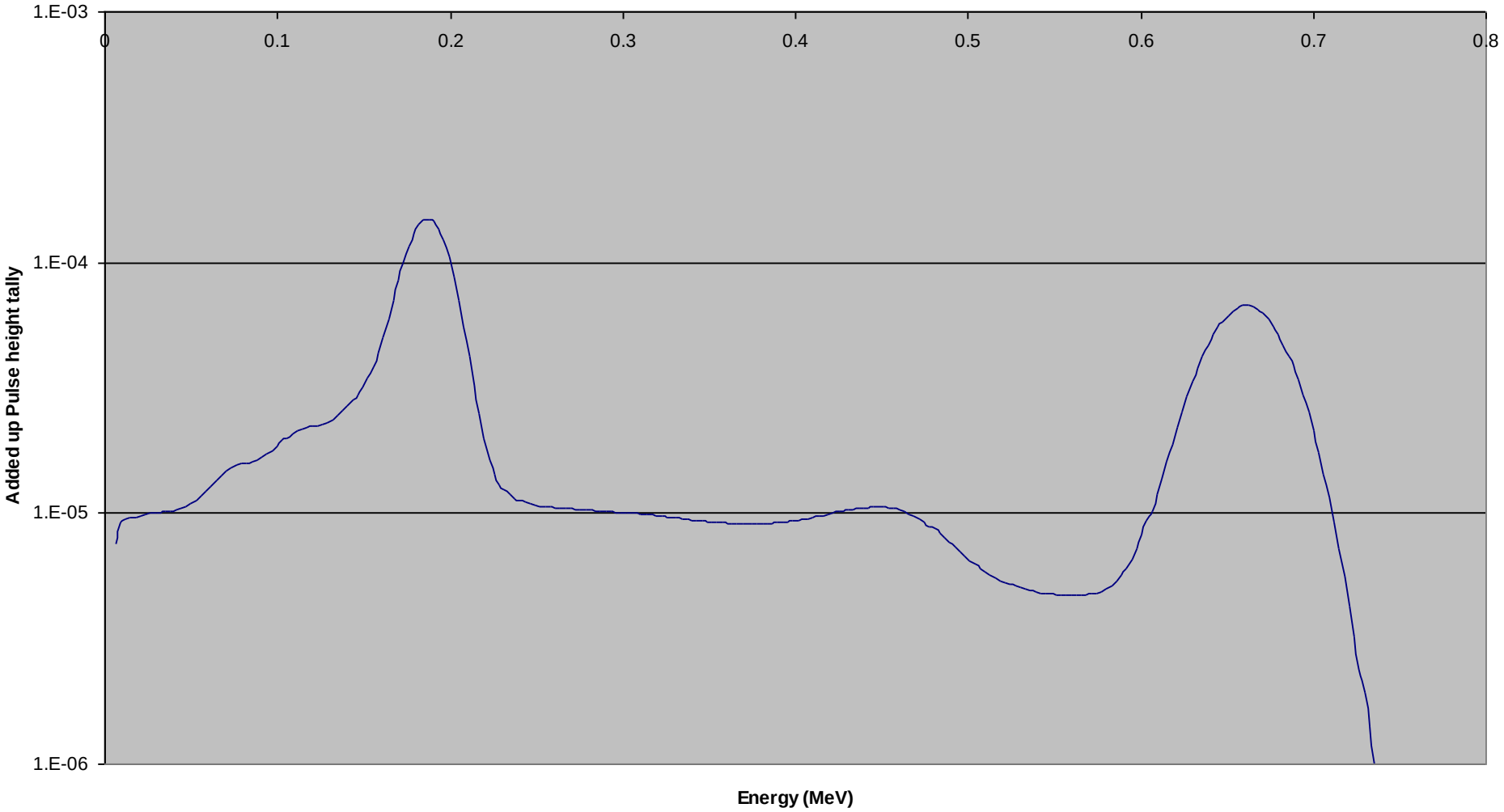
DO Derivation

$$D.O._{ref-5\%} = \frac{R_{ref} - R_{-5\%}}{\rho_{ref} - \rho_{-5\%}}$$

$$D.O._{+5\%-ref} = \frac{R_{+5\%} - R_{ref}}{\rho_{-5\%} - \rho_{ref}}$$



Unknown Spectra



Setup Verification File

						Cs			U
chan #	Uknown added	ref lib Cs	ref lib U	DO for Pb	DO for Fe	DO for Wo	DO for Pb	DO for Fe	DO for Wo
1	0.00E+00	0	0	0.00E+00	0	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2	7.53E-06	6.7E-06	4.2E-07	-4.85E-08	-1.91E-08	-6.25E-08	-4.85E-08	-6.35E-09	0.00E+00
3	9.27E-06	8.22E-06	5.4E-07	-5.73E-08	-2.54E-08	-1.25E-07	-6.17E-08	-6.35E-09	-6.25E-08
4	9.48E-06	8.37E-06	5.6E-07	-5.73E-08	-2.54E-08	-1.87E-07	-6.17E-08	-6.35E-09	-6.25E-08
5	9.58E-06	8.43E-06	5.8E-07	-5.73E-08	-2.54E-08	-1.87E-07	-6.61E-08	-6.35E-09	-6.25E-08
6	9.67E-06	8.46E-06	6E-07	-6.17E-08	-2.54E-08	-2.50E-07	-7.05E-08	-6.35E-09	0.00E+00
7	9.77E-06	8.5E-06	6.2E-07	-5.73E-08	-1.91E-08	-1.87E-07	-7.05E-08	-6.35E-09	0.00E+00
8	9.87E-06	8.52E-06	6.5E-07	-5.73E-08	-2.54E-08	-1.25E-07	-7.05E-08	-6.35E-09	0.00E+00
9	9.98E-06	8.54E-06	6.9E-07	-6.17E-08	-3.18E-08	-1.87E-07	-7.93E-08	-1.27E-08	0.00E+00
10	1.01E-05	8.54E-06	7.2E-07	-6.61E-08	-2.54E-08	-1.87E-07	-7.93E-08	-6.35E-09	0.00E+00
11	1.01E-05	8.55E-06	7.2E-07	-6.61E-08	-3.18E-08	-1.87E-07	-7.93E-08	-1.27E-08	0.00E+00
12	1.01E-05	8.59E-06	7.1E-07	-6.17E-08	-3.18E-08	-1.25E-07	-7.93E-08	-6.35E-09	6.25E-08
13	1.02E-05	8.65E-06	6.9E-07	-6.17E-08	-3.18E-08	-1.25E-07	-7.93E-08	-6.35E-09	6.25E-08
14	1.03E-05	8.71E-06	7E-07	-6.61E-08	-3.18E-08	-1.25E-07	-7.93E-08	0.00E+00	0.00E+00
15	1.04E-05	8.73E-06	7.4E-07	-6.61E-08	-3.18E-08	-1.25E-07	-8.37E-08	-6.35E-09	6.25E-08
16	1.06E-05	8.72E-06	8.2E-07	-6.61E-08	-2.54E-08	-1.25E-07	-9.25E-08	-6.35E-09	6.25E-08
17	1.09E-05	8.69E-06	9.4E-07	-6.17E-08	-2.54E-08	-6.25E-08	-1.10E-07	-6.35E-09	6.25E-08
18	1.13E-05	8.65E-06	1.11E-06	-6.17E-08	-2.54E-08	-6.25E-08	-1.28E-07	-1.27E-08	1.25E-07
19	1.17E-05	8.62E-06	1.33E-06	-6.17E-08	-3.18E-08	0.00E+00	-1.50E-07	-6.35E-09	1.25E-07
20	1.23E-05	8.59E-06	1.57E-06	-6.17E-08	-3.18E-08	7.94E-23	-1.76E-07	-1.27E-08	1.25E-07
21	1.29E-05	8.58E-06	1.83E-06	-6.17E-08	-2.54E-08	6.25E-08	-2.03E-07	-1.91E-08	1.88E-07
22	1.35E-05	8.57E-06	2.1E-06	-6.61E-08	-3.18E-08	1.25E-07	-2.38E-07	-1.91E-08	1.88E-07
23	1.41E-05	8.58E-06	2.32E-06	-6.61E-08	-2.54E-08	1.88E-07	-2.64E-07	-2.54E-08	3.13E-07
24	1.47E-05	8.6E-06	2.5E-06	-6.61E-08	-1.91E-08	1.87E-07	-2.82E-07	-3.18E-08	3.75E-07
25	1.52E-05	8.63E-06	2.59E-06	-6.61E-08	-1.91E-08	3.12E-07	-2.91E-07	-2.54E-08	5.00E-07
26	1.55E-05	8.68E-06	2.6E-06	-7.05E-08	-1.91E-08	3.75E-07	-2.95E-07	-1.91E-08	5.63E-07
27	1.58E-05	8.74E-06	2.52E-06	-7.05E-08	-1.27E-08	4.38E-07	-2.91E-07	-1.27E-08	6.88E-07
28	1.59E-05	8.81E-06	2.41E-06	-7.05E-08	-1.27E-08	5.00E-07	-2.78E-07	-6.35E-09	8.13E-07
29	1.61E-05	8.89E-06	2.28E-06	-7.05E-08	-1.27E-08	5.63E-07	-2.60E-07	0.00E+00	9.38E-07
30	1.64E-05	8.99E-06	2.19E-06	-7.05E-08	-6.35E-09	6.25E-07	-2.56E-07	6.35E-09	1.06E-06
31	1.67E-05	9.1E-06	2.17E-06	-7.05E-08	-1.27E-08	6.88E-07	-2.51E-07	1.27E-08	1.19E-06
32	1.72E-05	9.22E-06	2.22E-06	-7.05E-08	-6.35E-09	6.87E-07	-2.60E-07	1.27E-08	1.31E-06
33	1.79E-05	9.35E-06	2.34E-06	-7.05E-08	-6.35E-09	8.12E-07	-2.73E-07	1.27E-08	1.38E-06
34	1.86E-05	9.48E-06	2.52E-06	-7.49E-08	-6.35E-09	8.75E-07	-3.00E-07	1.27E-08	1.50E-06
35	1.95E-05	9.63E-06	2.78E-06	-7.93E-08	0	9.38E-07	-3.30E-07	1.27E-08	1.75E-06
36	2.00E-05	9.72E-06	2.94E-06	-7.93E-08	0	1.00E-06	-3.52E-07	6.35E-09	1.75E-06
37	2.08E-05	9.82E-06	3.18E-06	-7.93E-08	6.35E-09	1.00E-06	-3.79E-07	6.35E-09	1.88E-06
38	2.13E-05	9.91E-06	3.39E-06	-8.37E-08	6.35E-09	1.13E-06	-4.05E-07	6.35E-09	1.94E-06

Results

- Recall that the reference values were 0.1, 0.14, and 0.7 cm
- The calculated shield thicknesses were 0.1009, 0.2265, and 0.6258 with standard deviations of ~2.4%, ~6.5%,~2.4%
- The calculated radioisotope amounts were 0.9956 and 0.9103 with standard deviations of 0.0690%, and 0.269%.