Characterizaiton of Pu Separation by PUREX

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NUCLEAR SECURITY SCIENCE & POLICY INSTITUTE

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Outline

Project Goals

- Study and benchmark code predictions against experimental data
- Determine parameters to match MCNP-simulated detector response functions to experimental stilbene measurements
- Add stilbene processing capabilities to DRiFT
- Improve NEUANCE detector array modeling and analysis using new MCNP6 and DRiFT features

Background

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New MCNP6 Features

- New MCNP6 features will include two new event generators
  - Cascading Gamma-Ray Multiplicity with Fission (CGMF)
  - Fission Reaction Event Yield Algorithm (FREYA)
- CGMF and FREYA perform event-by-event Monte Carlo simulations of fission reactions
- Both code packages improve correlated fission and multiplicity models including angular correlations of emitted neutrons
- Project will attempt to benchmark code simulations to differential experimental measurements of fissionable materials

CGMF and FREYA

CGMF

- Uses MC Hauser-Feshbach approach
- Fission fragments are sampled from a joint probability distribution function of: Mass (A), Charge (Z), Total kinetic energy (TKE)
- Neutron/gamma ray competition treated throughout de-excitation process

FREYA

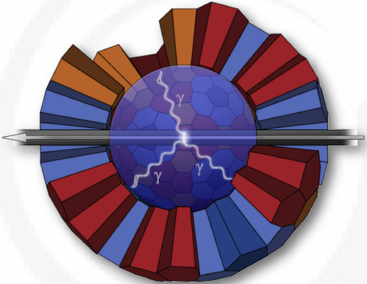
- Fission event generator for LLNL Fission Package
  - Includes tabulated and fitted data for major and minor actinides
- Uses MC Weisskopf approach
  - Neutrons are sampled from Weisskopf spectrum
  - Gamma rays are emitted from residual energy
- More computationally efficient

DRiFT

- **D**etector **R**esponse **F**unction **T**oolkit for MCNP output
- Generates realistic detector response functions for scintillators
- Post-processes MCNP PTRAC files into light output
- User can specify PMT type, quenching data specific to detector material, and trigger threshold
- Future improvements include the addition semiconductor and gas detector response functions

DANCE

- Detector for Advanced Neutron Capture Experiments
- γ-ray calorimeter located at LANSCE
- 160 BaF_2 crystals covering 3.6π solid angle
- Very high efficiency detector array used to measure prompt fission and capture gamma rays
- Inner cavity: 17 cm diameter sphere



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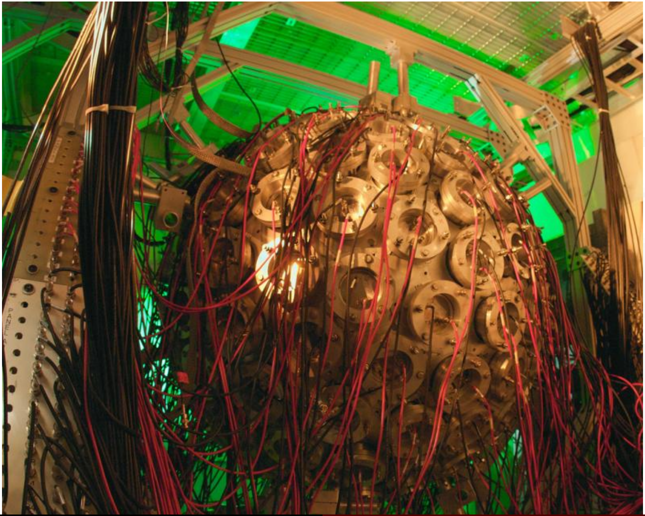

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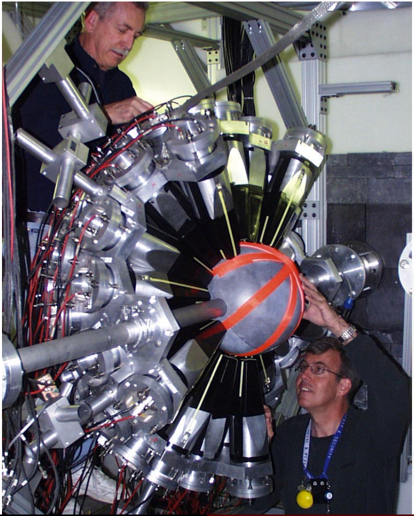
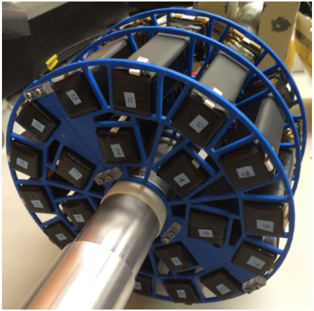


NEUANCE

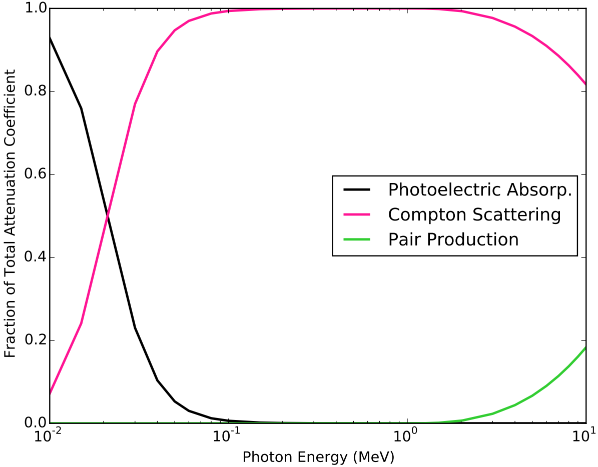
- **NEU**tron detector **A**rray at DA**NCE**
- Designed to fit inside DANCE
- Will study capture cross section of isomeric states of actinides
- EJ-309 and stilbene were tested in earlier prototypes
- Stilbene was chosen due to higher light-output and better PSD performance



Stilbene Detector

- Organic scintillator
- Higher light output and better PSD performance than EJ-309
- NEUANCE detector array will incorporate 21 stilbene crystals
- Approximate size: 2.3 cm x 2.3 cm x 10 cm
- Each crystal will be coupled to a compact photomultiplier tube
- Current efforts include improving modeling accuracy of a single stilbene crystal

Photon Interactions in Stilbene



MCNP6 Settings

MCNP6 Settings

- Gaussian Energy Broadening (GEB)
  - Virtual peak-broadening technique
  - Converts gamma pulse height tally to approximate detector response function
  - No parameters available for stilbene
- DE/DF
  - Converts energy deposited by recoiled protons to electron equivalent energy
  - Equation found in (Hansen, 2002)[**?**]

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GEB Parameters - Iterative Method [Kim, 2015]

- Calculate Compton edge for each peak

$$E_c = E_{e-}|_{(\theta=\pi)} = E_\gamma \left(\frac{2E_\gamma}{m_e c^2 + 2E_\gamma} \right) \quad (1)$$

Compton edges for gamma-ray sources:

Element	E_γ (keV)	Compton Edge (keV)
^{133}Ba	356	207.25
^{137}Cs	662	477.65
^{54}Mn	835	639.36
^{22}Na (P.P.)	511	340.67
^{60}Co	1173	963.42
^{22}Na	1274	1061.18
^{60}Co	1332	1118.10

GEB Parameter - Iterative Method [Baramsai, 2015]

- Calibrate spectra using Compton edge as Compton maximum

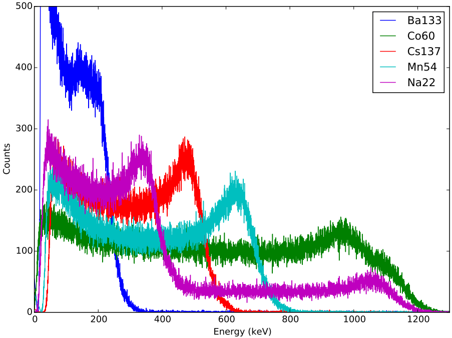

Figure 1: First Calibration, Assumption: Compton Edge = Compton Maximum

GEB Parameters - Iterative Method [Kim, 2015]

- Fit Gaussian function to experimental data using equation 2. [?]

$$f(E) = Ce^{-\left(\frac{2\sqrt{\ln 2}(E-E_0)}{FWHM}\right)^2} \qquad (2)$$

- Set E_0 = Compton maxima
- Fit function to obtain constant (C) and FWHM

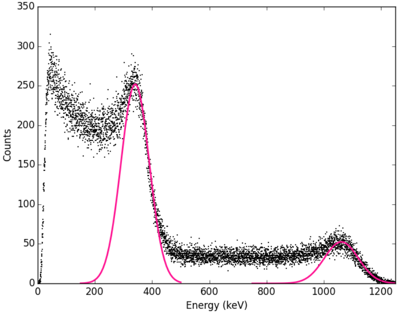

Figure 2: ^{22}Na Gaussian Peak Fit

GEB Parameters - Iterative Method [Kim, 2015]

- Use FWHM from Eq. 2 to find fitting parameters (a, b, c)

$$FWHM(E_o) = a + b\sqrt{E_o + cE_o^2} \tag{3}$$

After 1^{st} iteration:

- a = -0.049702
- b = 0.267462
- c = -0.526174

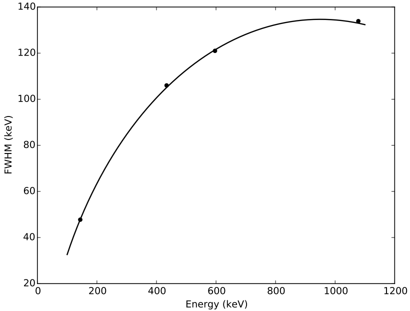

Figure 3: FWHM Curve for Stilbene

GEB Parameters - Iterative Method

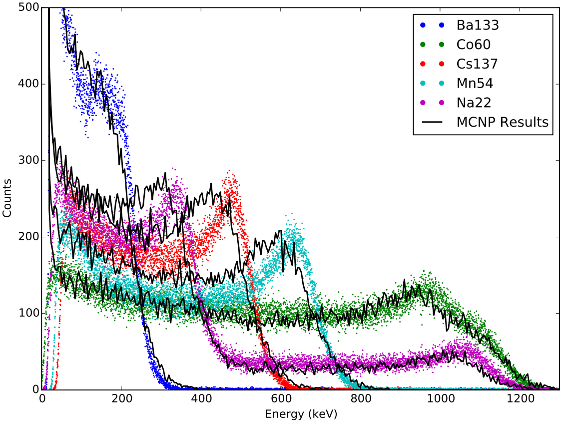

Figure 4: 1^{st} MCNP Iteration

GEB Parameters - Iterative Method [Kim, 2015]

- Re-calibrate spectra using Compton maxima from MCNP
- Fit Gaussian functions to each peak
- Fit parameters:

$$FWHM(E_o) = a + b\sqrt{E_o + cE_o^2}$$

After 2^{nd} iteration:

- a = -0.057192
- b = 0.249732
- c = -0.432120

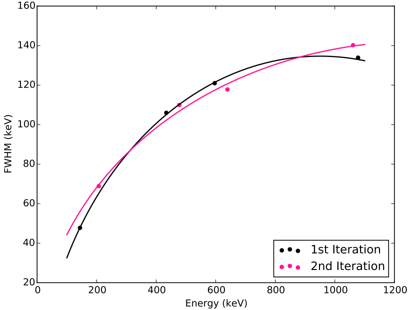

Figure 5: FWHM Curves for Stilbene

GEB Parameters - Iterative Method

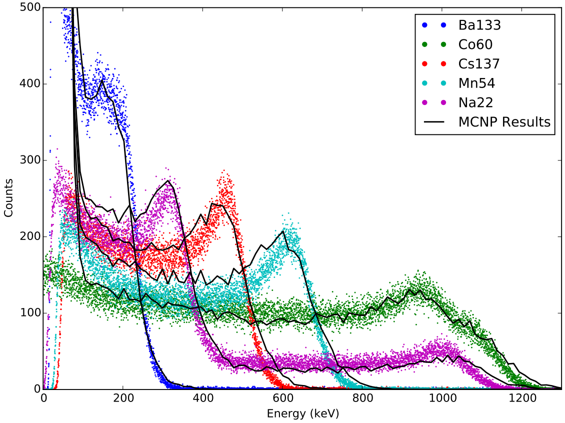

Figure 6: 2^{nd} MCNP Iteration

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DE and DF Cards [Hansen, 2002]

- Non-linear light output function for stilbene:

$$L = aE_p - b[1 - exp(-cE_p^d)] \tag{4}$$

- Converts recoil proton energy (E_p), to light output due to energy deposited by the effective electron equivalent energy (L)

Optimization constants found in [Hansen, 2002]:

- a=0.693
- b=3.0
- c= 0.2
- d=0.965

Simulation Results: ^{252}Cf

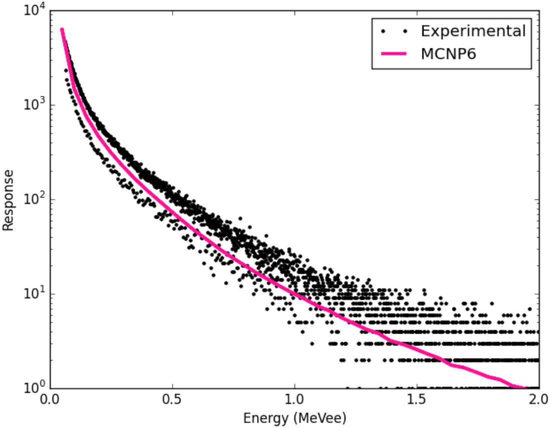

Figure 7: MCNP6 vs Experimental measurements using the DE/DF tally treatment

DRiFT

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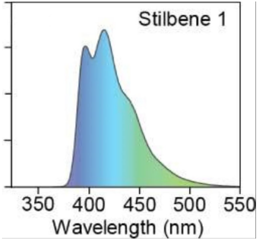
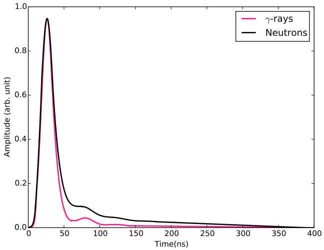
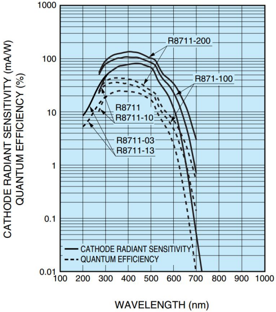
DRiFT

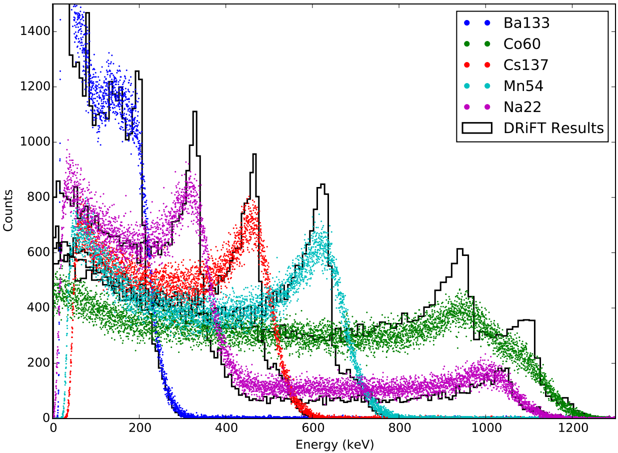
- Stilbene processing capabilities have been added to DRiFT
  - Light output function (Equation 4)
  - Light emission spectrum (Left)
  - Neutron and gamma pulse shapes - in progress (Center)
  - PMT Quantum Efficiency(Right)



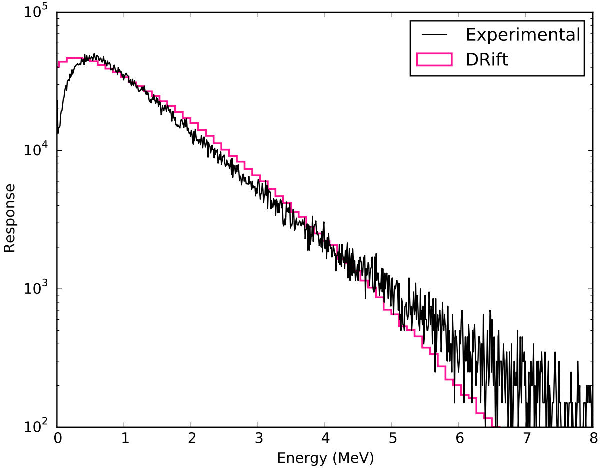




Preliminary DRiFT Results: Gamma Rays



Preliminary DRiFT Results - Neutrons



Future Work

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Future Work

- Continue improving stilbene modeling parameters and capabilities in DRiFT
  - PSD using waveforms
  - Low-energy photon detection improvements

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- Begin modeling multiple stilbene detectors in different angle configurations
- Model full NEUANCE detector array
- Study detector cross-talk
- Compare MCNP6/DRiFT simulations using CGMF/FREYA against experimental measurements
  - ^{252}Cf: spontaneous fission
  - ^{239}Pu and ^{235}U: neutron-induced fission

Questions?

References I