Nuclear Engineering PhD Qualifying Exam

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Coal Analyzers

Introduced as a response to regulation, coal analyzers can provide minute-by-minute analysis of sulfur, ash, moisture, and calorific value

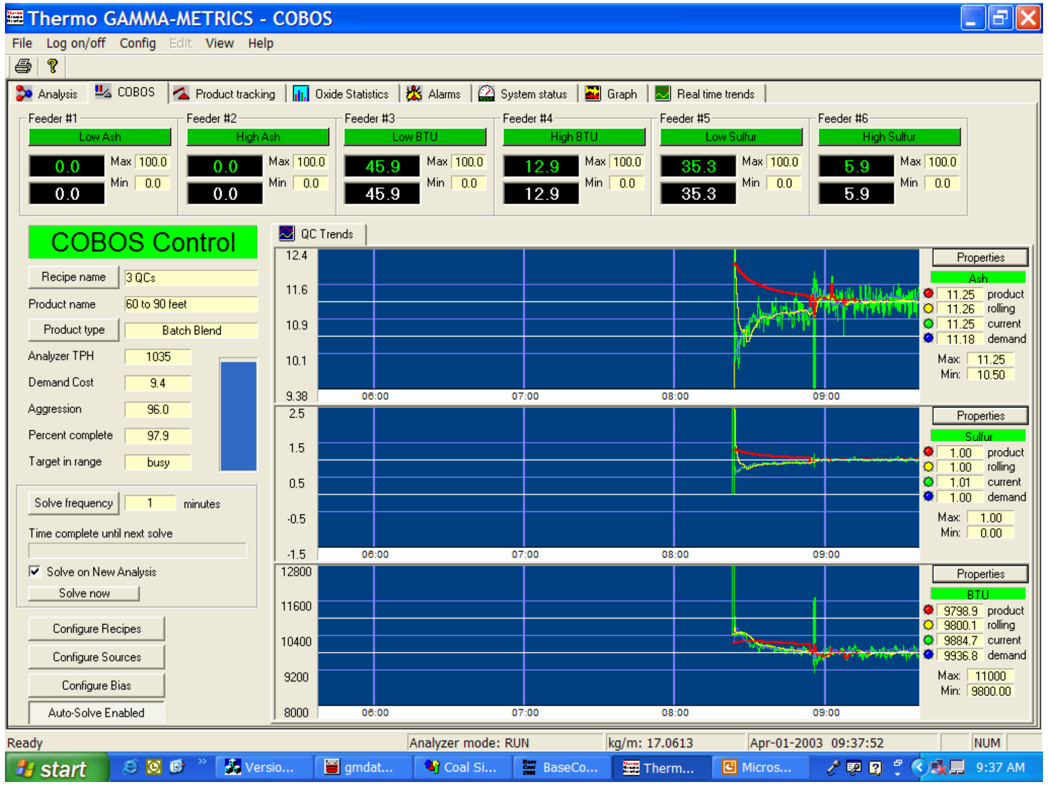
Fixed Geometry (sample-fed)

- No impact from second-by-second changes in belt loading

Cross belt

- Cheaper installation
- 36 to 48 inch belts are ideal
- Requires consistent flow rate and coal topsize no more than 2 inches

Blended Coal



Coal blending is a common practice to meet regulatory requirements

Two, or more, sources of coal are fed from separate storages and combined

Although one type of coal may contain high levels of sulfur, when blended with a low sulfur coal, many properties (BTU/ton) can be retained while reducing harmful SO_2 byproducts

*FROM 1+1=3: MORE FROM YOUR ONLINE COAL ANALYZER, BLACK & VEATCH

Introduction to PGNAA

Prompt Gamma Neutron Activation Analysis (PGNAA) is a nondestructive, real time technique used for bulk material identifications

Neutron inelastic scatter and capture reactions produce characteristic gamma-rays to identify minute amounts of individual elements in a bulk sample

Low cross sections for these reactions, coupled with high natural background, detector activations, and gamma rays from the decay of the neutron source, contribute to a low signal to noise ratio (SNR)

Coincidence counting is applied to counteract these effects

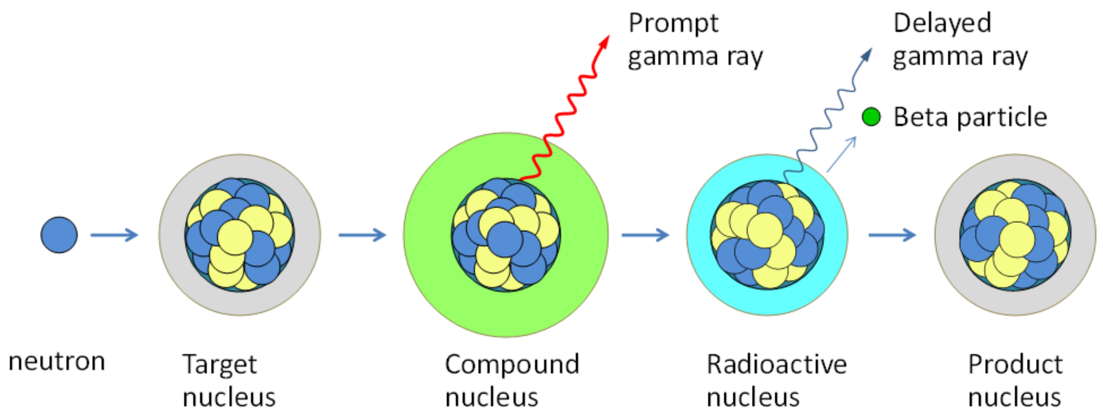
Physics of PGNAA

Neutron Capture

- $^{1}_{0}n + ^{A}_{Z}X \rightarrow ^{A+1}_{Z}X^{*}$

Neutron Inelastic Scatter

- $^{1}_{0}n + ^{A}_{Z}X \rightarrow ^{1}_{0}n' + ^{A}_{Z}X^{*}$
- Threshold energy must be exceeded for inelastic scatter to occur



Of importance:

- Hydrogen only produces 1 gamma ray from neutron capture
  - Does not contribute to a coincidence counting measurement

Development of CEARCPG-CEARPGA I

CEARPGA I is a specific Monte Carlo code developed to analyze bulk materials utilizing the Monte Carlo Linear Least Squares (MCLLS) method

Experiments were performed using a 2 µg ^{252}Cf neutron source and 39% HPGe semiconductor detector

CEARPGA I generates single spectra for use in solving the inverse problem

Main contribution to CEARCPG is due to the many variance reduction techniques employed

CEARPGA I Variance Reduction Techniques

Russian roulette

Truncated exponential PDF

Direction biasing

Discrete importance function

Unscattered detection probability estimator

Expected value technique

Variance Reduction Techniques

Once particle tracking is initiated, a particle is assigned an initial weight

After each interaction, the particle weight is adjusted

Once a particle weight drops below a predetermined value w_{min}, a random number ξ, of value between 0 and 1, compares the weight to the ratio of the particle weight and w_{min}

If ξ ≤ w/ w_{min}, then the particle survives, and the weight will be raised to w_{min}, otherwise the neutron history or photon-tracking is terminated

Russian roulette terminates particles that will not contribute heavily to the solution in an effort to reduce computer run times

Direction biasing is employed to reduce computation time wasted on photons that would not interact with the detector. Each direction is sampled, and only directions that subtend the detector are allowed to continue

Variance Reduction Techniques

The truncated exponential PDF ensures that particles do not exit the system by sampling if the distance to next collision occurs within the system boundary

For particles that will interact before leaving the boundary, the standard exponential probability distribution function is utilized

If a particle can leave the system, the following expression is used, along with an adjusted weighting of the particle:

- $p(x) = \frac{\Sigma_t \exp(-\Sigma_t x)}{1-\exp(-\Sigma_t D)}, for\ 0 \leq x \leq D$
- $w_{adj} = 1 - \exp(-\Sigma_t D)$

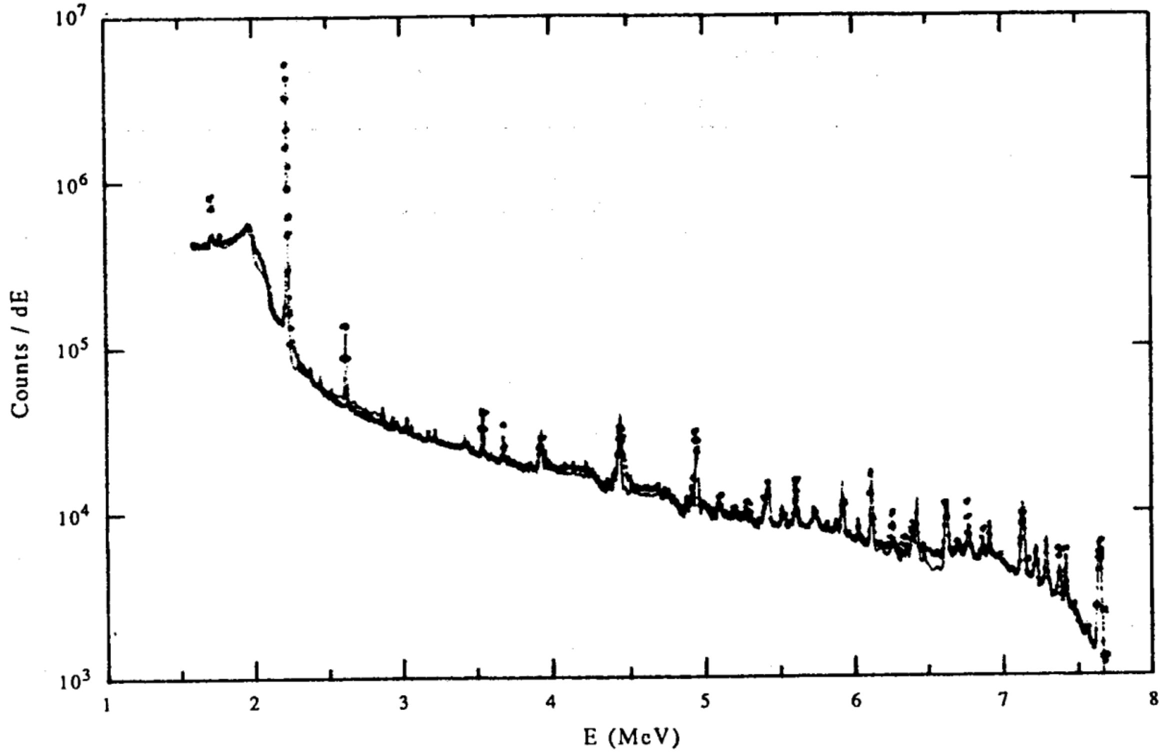
Variance Reduction Techniques

The discrete importance function is used to increase the neutron capture interaction sampling frequency in cases where the capture cross section is less than one tenth of the elastic cross section

Expect value splitting is used to make the gamma ray score at every interaction site by splitting into two parts. One heads directly to the detector without any interaction with the expected weight required, while the other particle will progress normally, interacting multiple times before being terminated by Russian roulette or collecting in the detector

Each of these variance reduction techniques are designed to reduce wasted computation time without deviating from the expected value of each operation

Results (from Shyu et al. 1993)



CEARPGA II

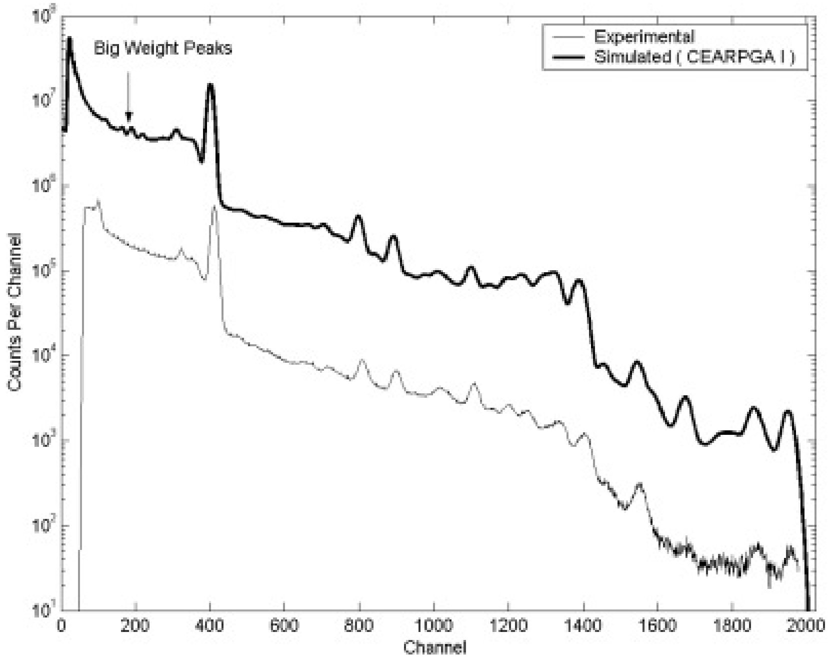
Several deficiencies became apparent when testing CEARPGA I under different conditions

- “Big weight problem”
- Lack of treatment for nonlinear response of detectors common to NaI, BGO, etc…
- Inability to generate background libraries for NaI activation or natural background
- 0.511-MeV annihilation photons generated from pair production outside the detector were not tracked due to a minimum cutoff energy set at 1 MeV
- Improved detector response function (DRF) needed

Many elements of the original code were retained such as:

- Stratified sampling
- Correlated sampling
- Forcing neutron interactions within the system boundary

Big Weight Problem



The “big weight problem” is a result of over sampling gamma rays produced near the detector found in the following equation:

$$P = \int_{v_{min}}^{v_{max}} \int_{p_{min}(v)}^{p_{max}(v)} p_1(v,p) \cdot p_2(v,p) \cdot p_3(v,p) dp dv$$

Where

$p_1(v,p)$ = the probability of scattering or emitting toward the detector through angles (v,p)

$p_2(v,p) = \exp[-\sum_{i=1}^{n} \mu_i l_i(v,p)]$ = the probability that the photon will be transmitted to the detector with the direction angles (v,p) without collision, with μ_i and l_i being the linear attenuation coefficient of zone I and path length through zone i respectively.

ALI: Correction of the “Big Weight Problem”

The Analog Linear Interpolation (ALI) approach was formulated in an effort to address the “big weight problem” through the following steps:

- Choose a proper pseudo gamma ray
- Optimize the gamma ray sampling number, determined to be 100 by trial and error
- Tallying the scores of pseudo gamma rays
- Calculate the average neutron capture cross section
- Interpolate using generated energy-score tables
- Generate the spectra for prompt gamma rays

Detector Response Function

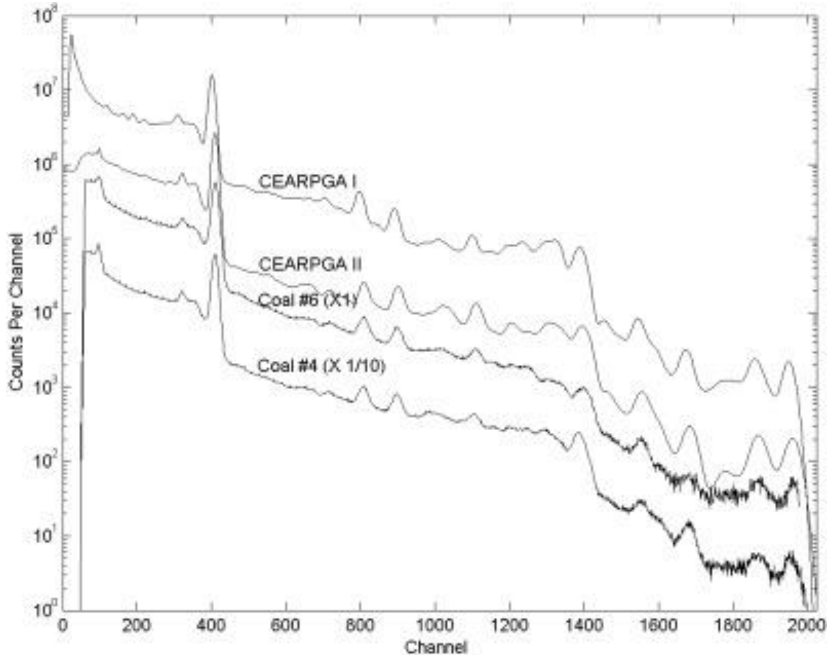
CEARPGA II incorporates the G03 code developed by Dr. Avneet Sood during his PhD work

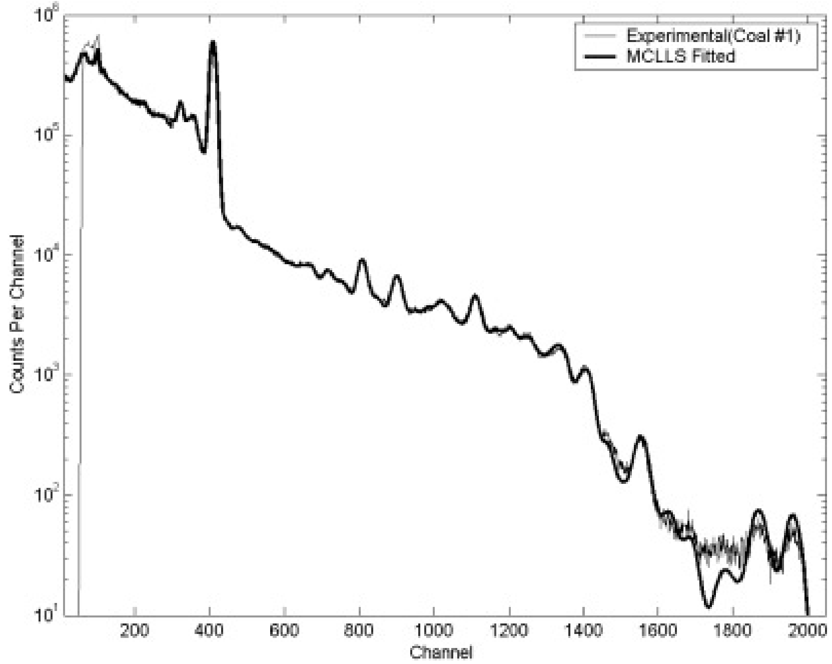
G03 uses a combination of physical principles and semi-empirical models to fit

- Full energy peak determined by pair production, Compton scattering, and photoelectric effect
- Compton continuum is treated semi-empirically, to address the "flat-continuum problem"
- Gaussian broadening parameters can be determined experimentally, increasing the accuracy over GEB treatment used by MCNP

Using surface flux tallies as opposed to energy deposition inside the detector, G03 is found to improve computation time by over 50% while maintaining or improving accuracy

CEARPGA II Results





CEARCPG

CEARCPG is a specific purpose Monte Carlo Code with the capabilities of simulating coincidence, anti-coincidence, time-of-flight, and standard (non-coincidence) PGNAA simulations

Input cards are used to supply user-guided instructions to turn on variance reduction techniques, define the neutron source, and provide detailed geometries

- Input cards for materials and geometry are the same format as MCNP5, allowing for practical development using visual software such as VisED

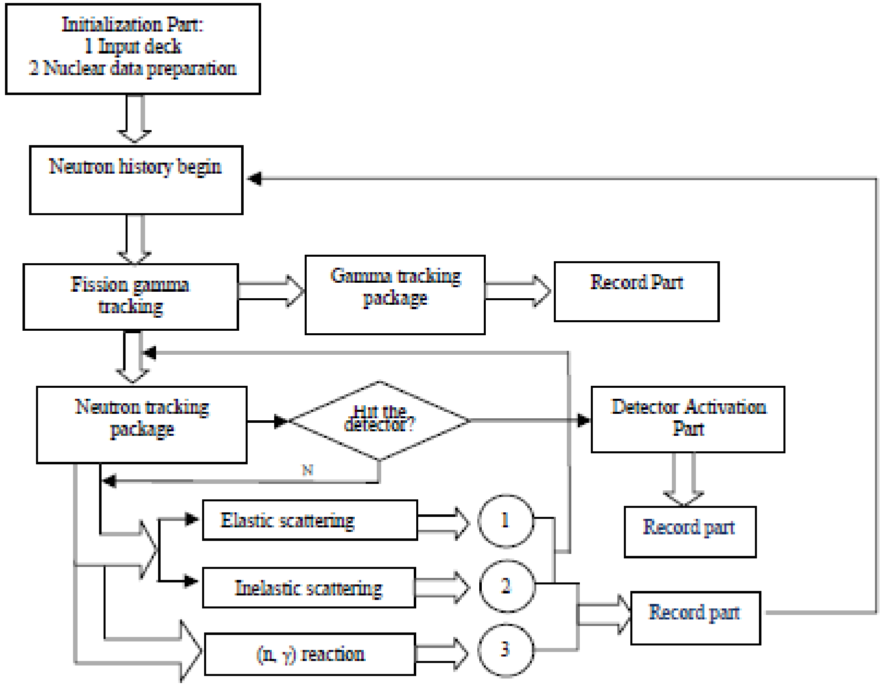
Cross section libraries include:

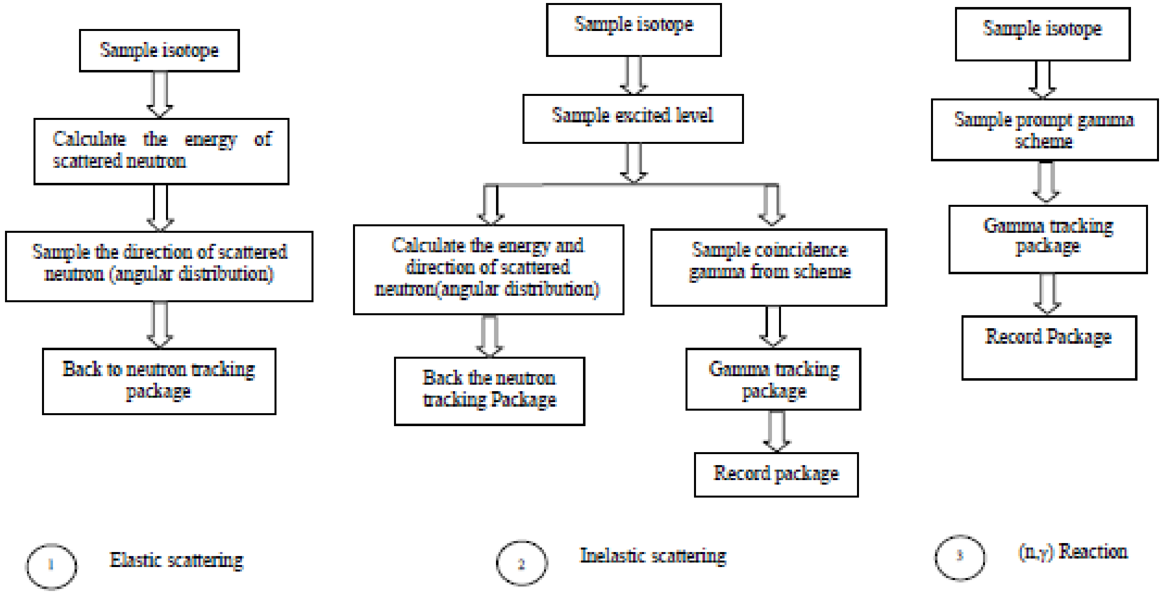
- Neutron libraries from ENDF/B-VI 8300K and JENDL-3 3300K databases
- Gamma ray libraries include elements Z=1 to 100, from the EPDL97 library

Sample Input Deck

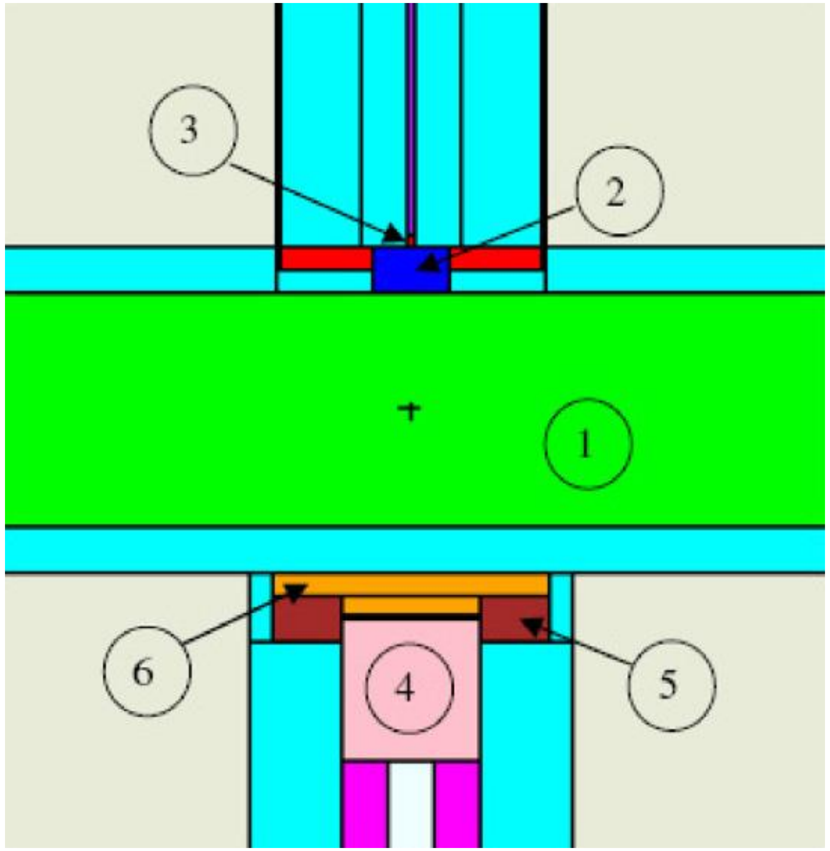
```
Created on: Monday, December 29, 2003 at 22:50
    1     1  -11.34     -1  2  -4  5  -6  7
    2     1  -11.34     5  -4  -2  40  7  -6  8
        ......
   44     6  -1.06      -41  35  -27  30
   45     6  -1.06      -42  33  -27  29

    1        pz       23.5
    2        pz         23
    3        pz       13.3
        ......
   41       c/z         14           0        8.3
   42       c/z        -14           0        8.3

m1    82000             -1.0
        ......
m8    13027             -1
imp  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
     1 1 1 1 1 1 1 1 0 0 0 1 1 1
sdef   cf x=0.0  y=0.0  z=18  icel=3
nps    300000
number_detector 2
detector  -14.0 0 -25.8  7.62  15.24  16
          12.73 0 -24.53 7.62  15.24  21
sample   12
wcut 1d-6 1d-7 1d-10 1d-11 0.02
spect    2048 512 0 0  0.0055575  18000  0.0055575 0.02223
detcoin 1 ( 16 : 21 )
```

CEARCPG Code Flow Chart





Bulk Coal Sample Experimental Setup



Geometry configuration of the ETI prototype

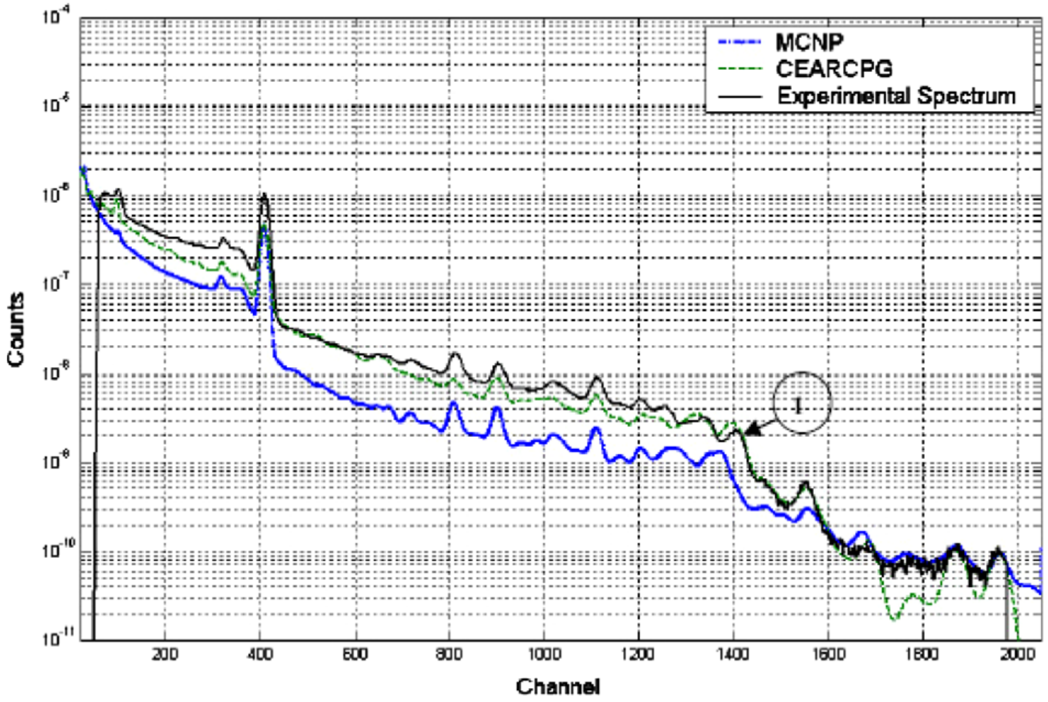
Detector: NaI (4)

Source: Californium (3)

Sample: Coal (1)

Non-coincidence example

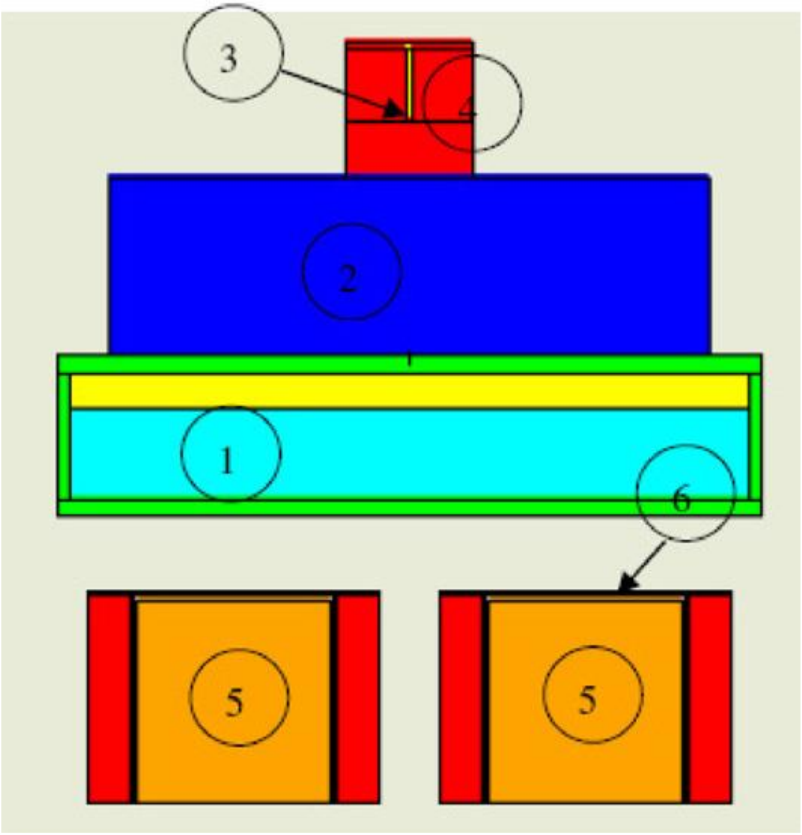
Results



Results are normalized at the nitrogen peak

Label 1 demonstrates the inability of MCNP to accurately simulate the activation of the NaI detector

Pure Sulfur Sample Experimental Setup



Geometry configuration of the sulfur sample arrangement

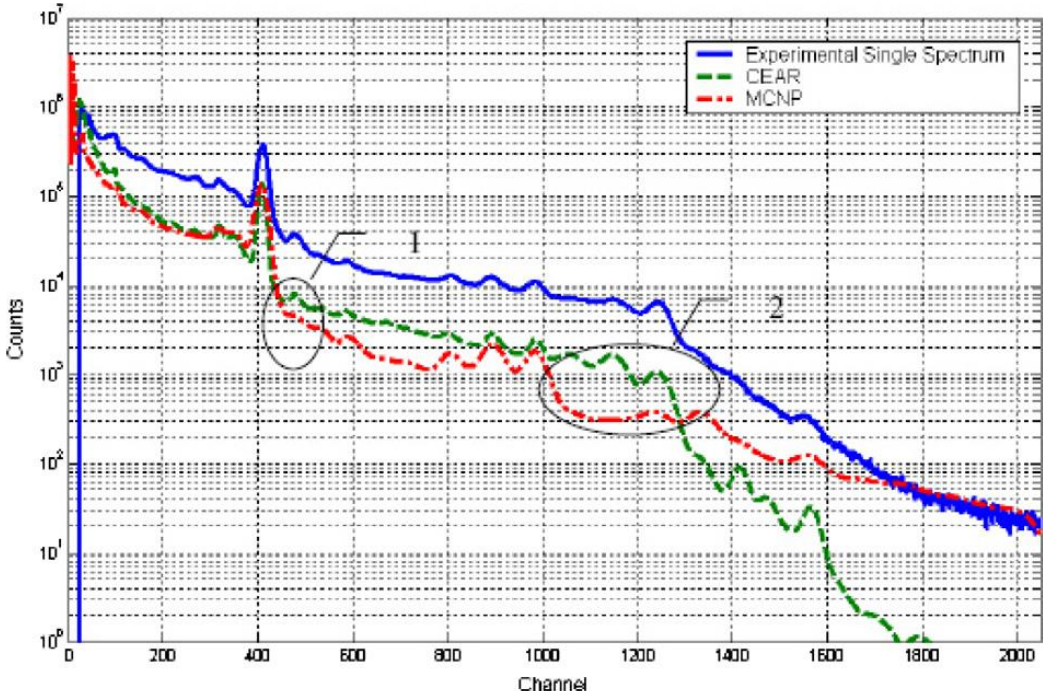
Detector: NaI (5)

Source: Californium (3)

Sample: Sulfur (1)

Coincidence example

Results



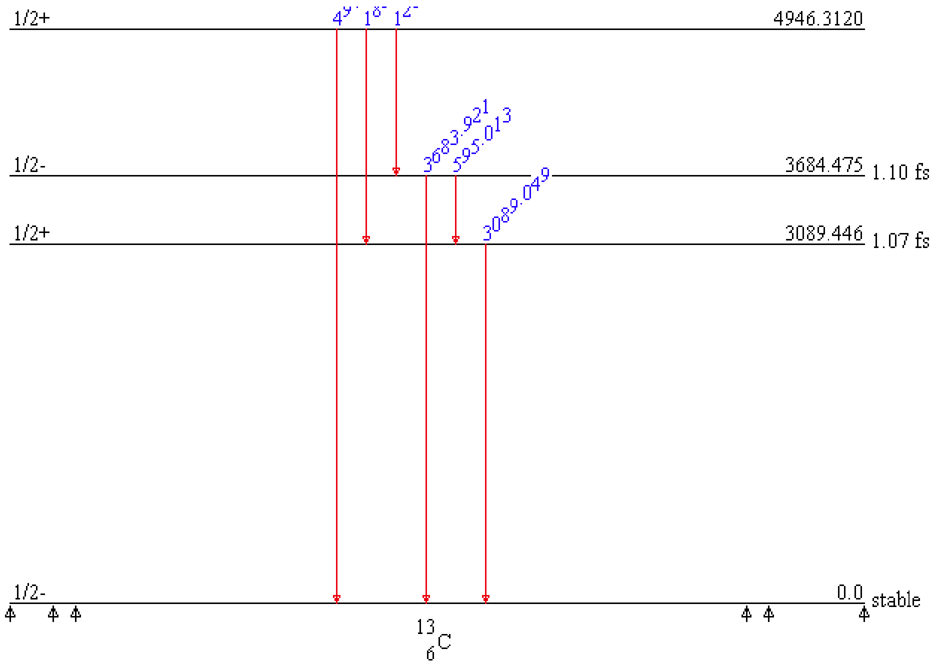
Single spectra results are normalized at the hydrogen peak for MCNP and CEARCPG only

The treatment of background libraries can be seen as the difference in region 1 for MCNP and CEARCPG

NaI activation gamma rays are not accounted for by MCNP, resulting in the differences in region 2

The high energy differences between MCNP and CEARCPG are determined to be from the number of overall histories run by each code

Q-Value Summing



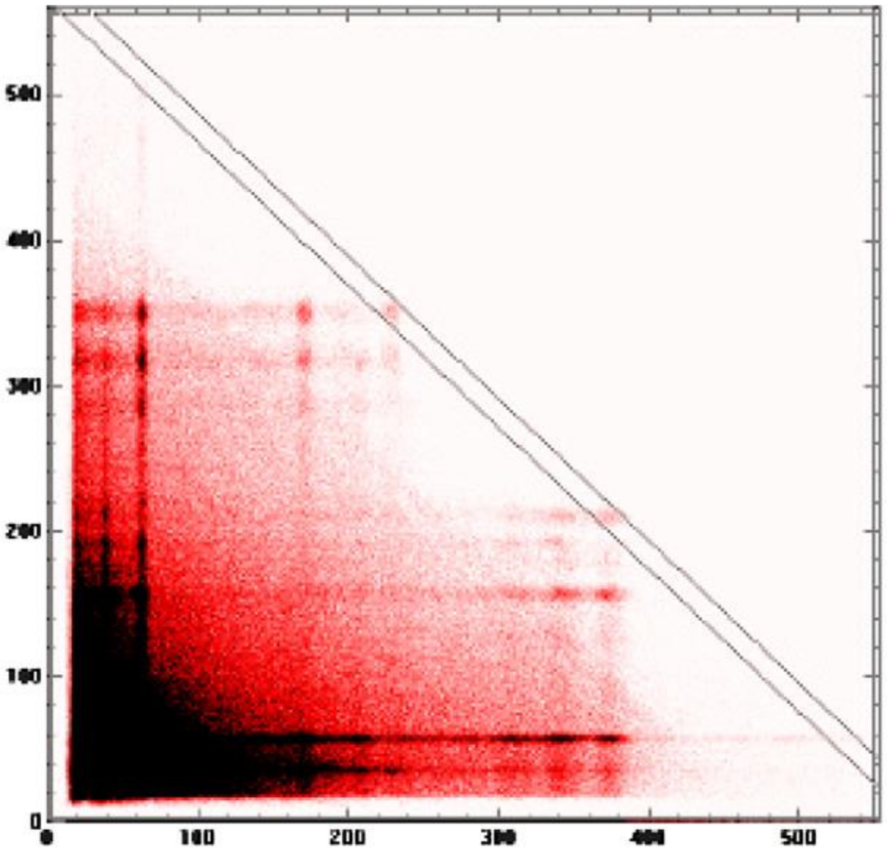
Q-value for Carbon is 4.946 MeV

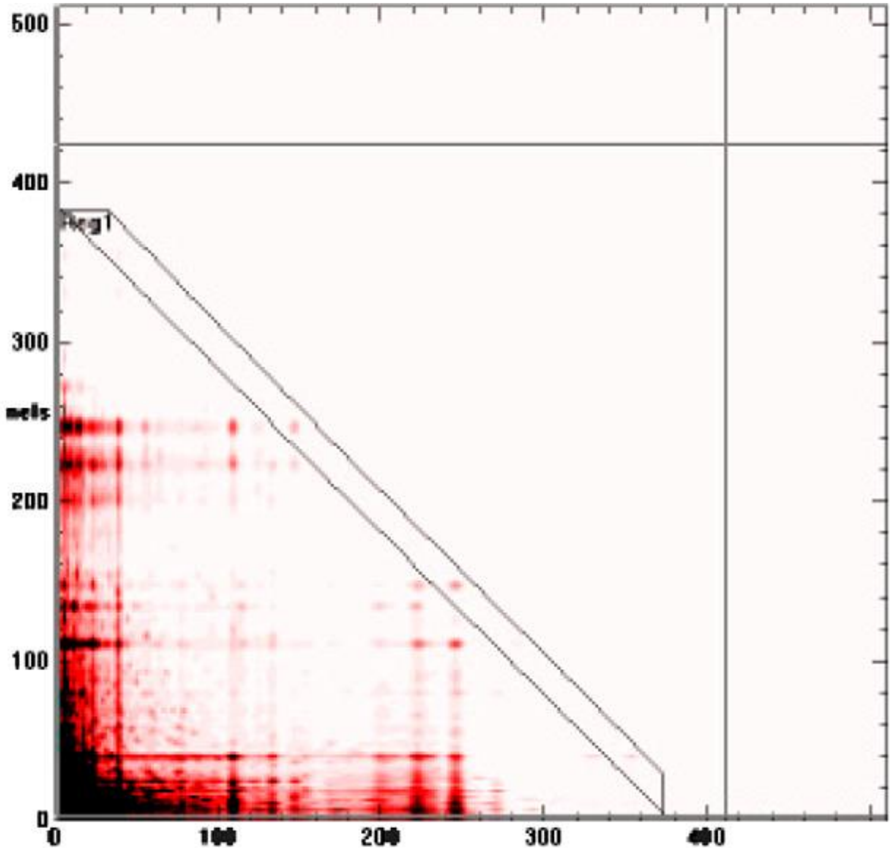
Using multiple detectors and timing bins, Q-value summing can be used to detect gamma rays ejected in coincidence that sum to 4.946 MeV

KMAX generates a 2D coincidence spectrum, allowing for projected diagonal summing to be used

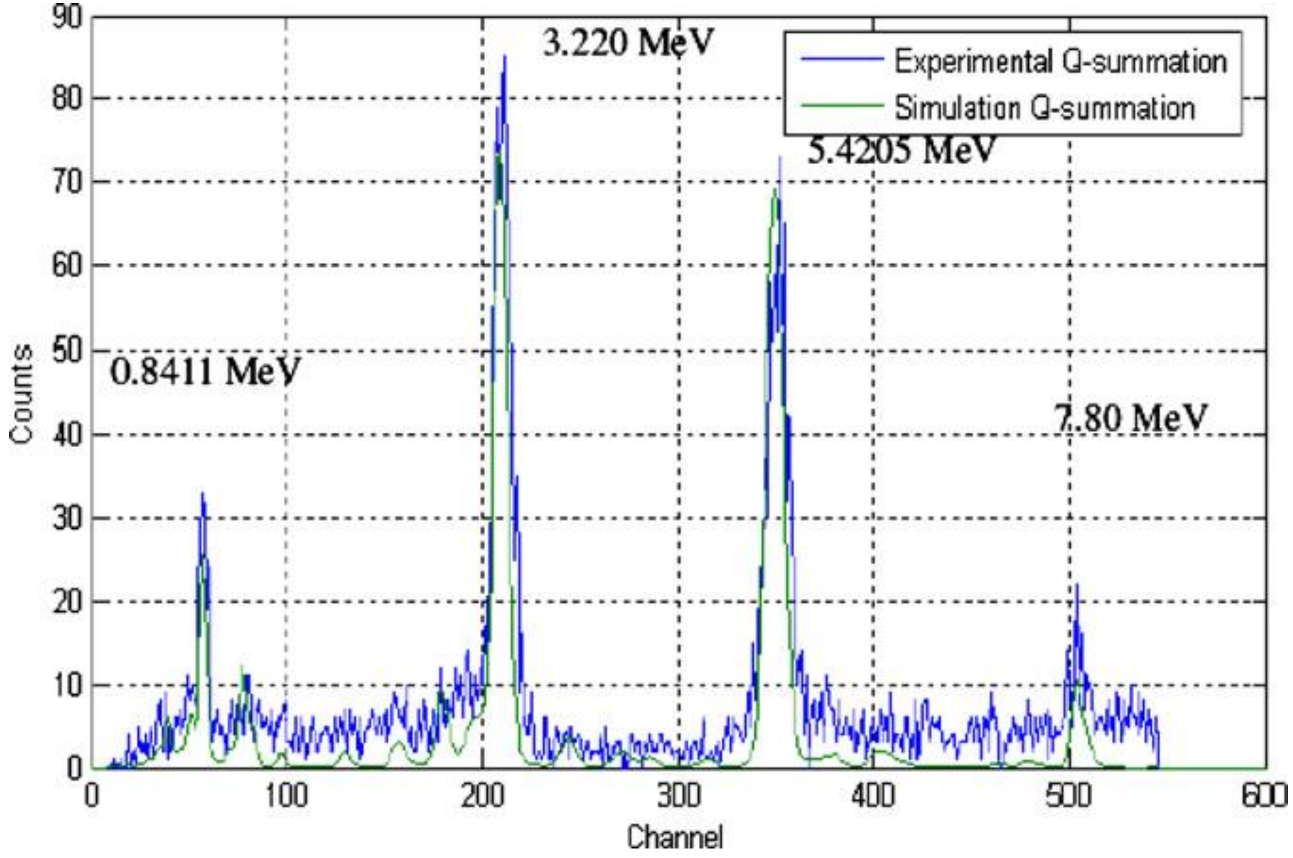
Energy(MeV)	Relative ratio(%)	Structure	
		Begin (level)	End (level)
3.089	0.43	2	1
0.595	0.24	3	2
3.683	32.14	3	1
1.261	32.36	4	3
1.856	0.16	4	2
4.945	67.47	4	1

Pure Sulfur Coincidence Results

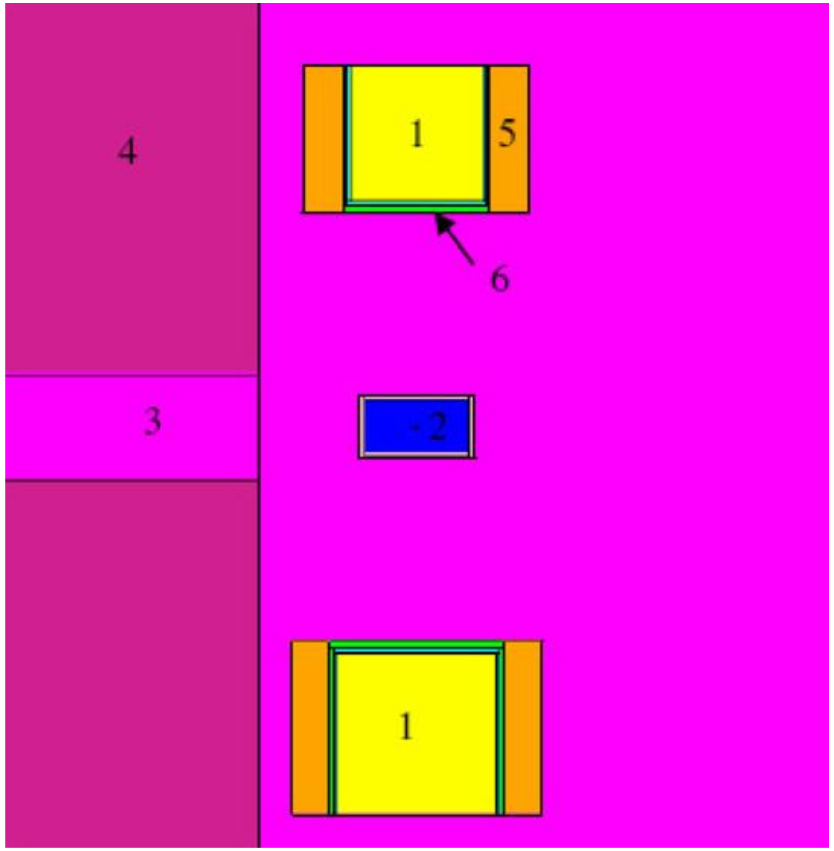




Pure Sulfur Q-Value Summing



Pure Mercury Sample Experimental Setup



Geometry configuration of the Mercury sample arrangement

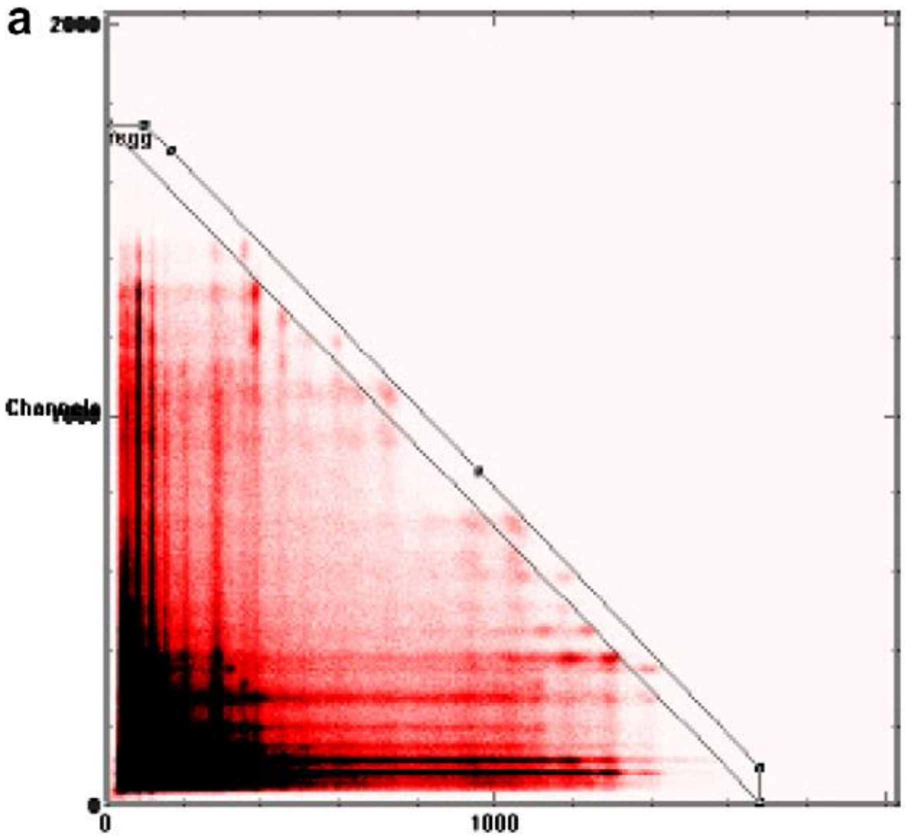
Detector: NaI (1)

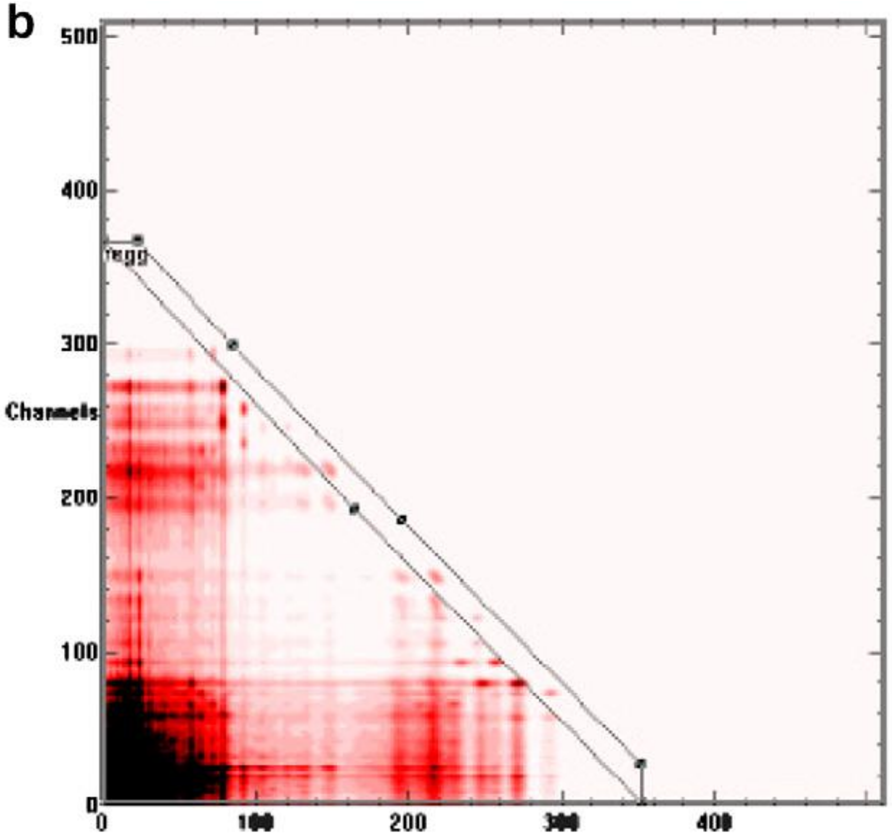
Source: PULSTAR Neutron Beam (3)

Sample: Mercury (2)

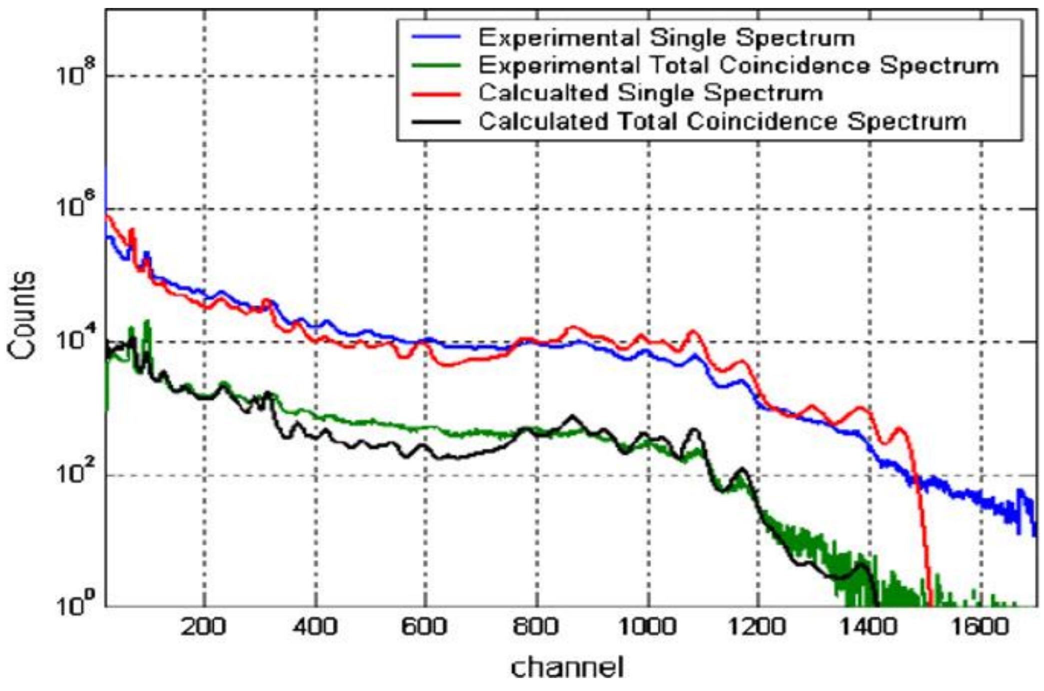
Coincidence example

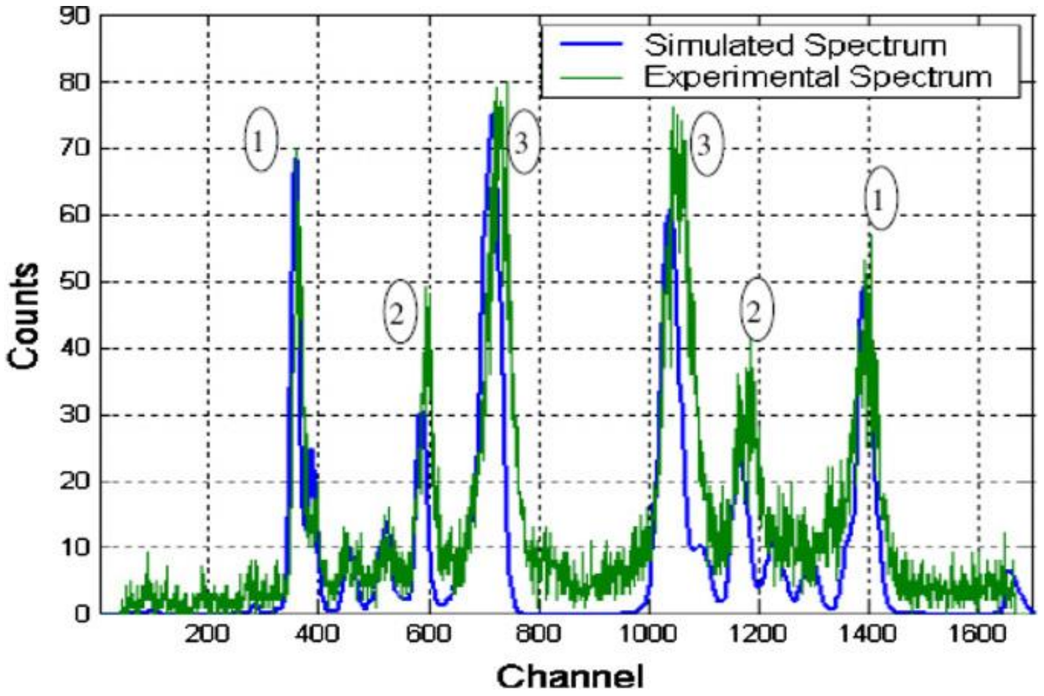
Pure Mercury Coincidence Results





Pure Mercury Coincidence Results



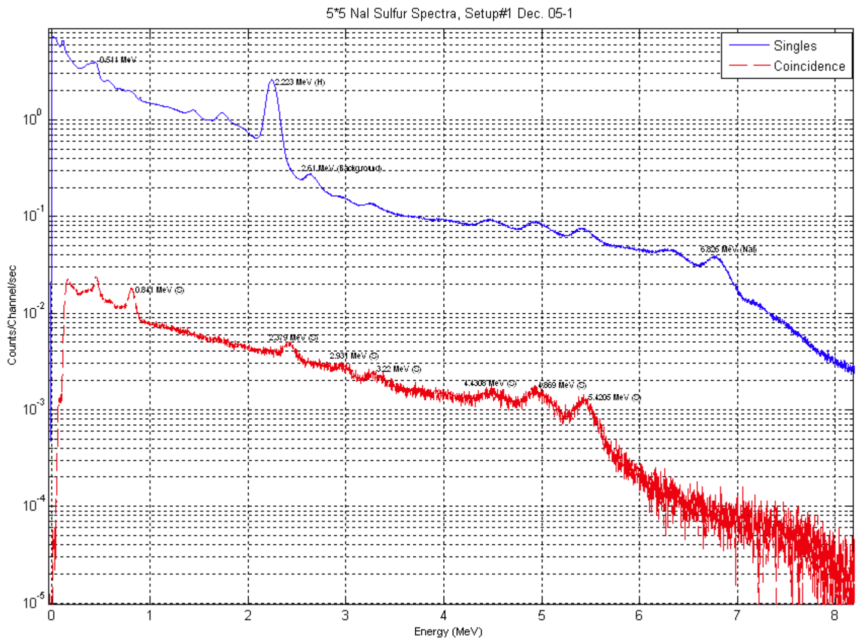


Conclusions

CEARCPG demonstrated the ability to generate accurate spectra for analysis using either single or coincidence measurements

Coincidence methods successfully demonstrated the ability to reduce noise from background sources, and fission induced gamma rays, and the extreme hydrogen dominating peak

Updates could be made by introducing new neutron sources (DT generators), new detectors (LaBr, CeBr), and updated cross section libraries



Discussion

Questions?

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