OpenAGS: an Online Analysis Program for Prompt & Delayed Gamma Activation Spectra

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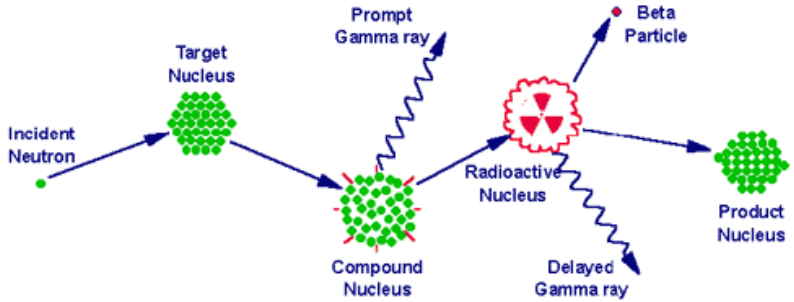
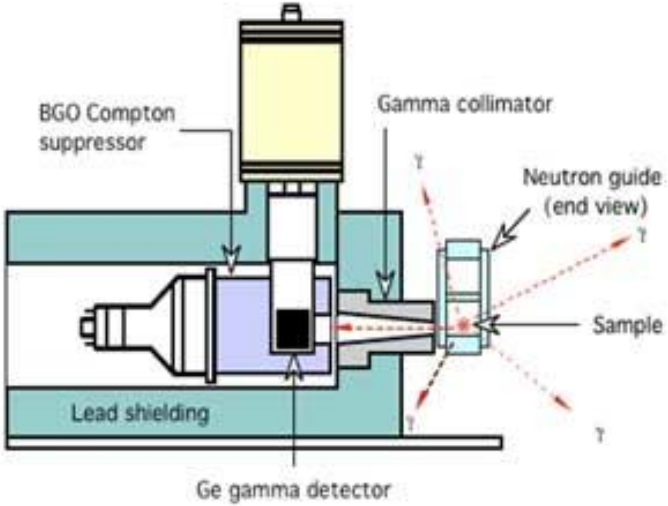
Why PGAA?

- Detecting boron at concentrations ~10ppb
  - Only method with this level of precision for boron
- Detecting chlorine within concrete
  - Can pose failure risks even at small conc.
- So how does it work?





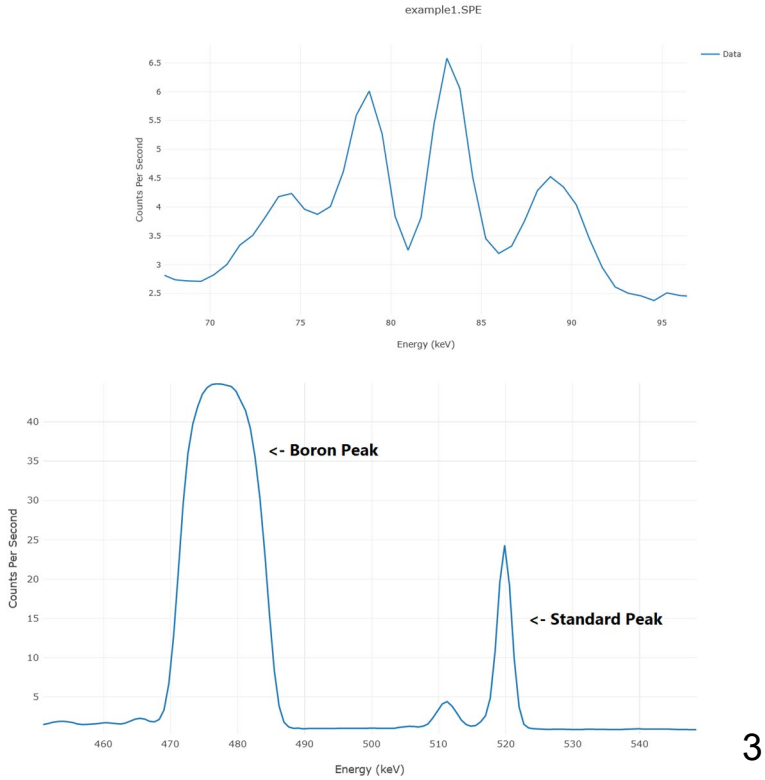
Data Analysis for PGAA

- Peak area is directly related to elemental mass
- Calculate a sensitivity value using a known mass (Counts per Second / mg)
- Use this sensitivity to determine an unknown mass based on area of new peak
- Example:
  - Irradiate 100mg of Calcium-41
  - Find peak area, say 10 cps
  - Sensitivity = .1 cps/mg.
  - Irradiate unknown sample
  - Find peak area, say 15cps
  - 15cps/(.1 cps/mg) = 150 mg
- Create Sensitivity Table

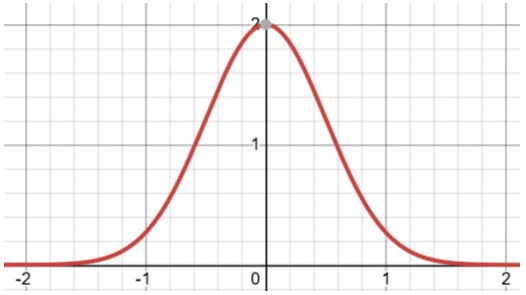
	A	B	C	D
1	Isotope	Energy (keV)	Sensitivity (cps/mg)	
2	Yb-175	41.218	1.2907	
3	As-76	44.425	1.702192	
4	Eu-152	48.31	301.5848	
5	Rh-104	51.5	42.12355	
6	I-128	58.11	0.662855	
7	Re-186	59.01	8.974821	
8	Sb-122	61.413	1.924258	
9	Re-188	63.582	13.71547	
10	Tb-160	63.686	2.935628	
11	Th-233	63.81	14.76416	
12	Tb-160	64.11	2.424496	
13	W-187	72.002	2.455623	

Complexities with Data Analysis

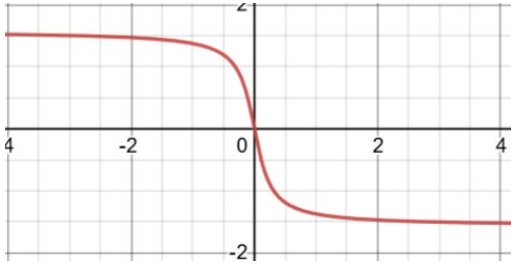
- The Boron Peak
  - Different decay path
  - B-10 + n → B-11* → Li-7* + a
  - Li-7* → Li-7 + γ
  - No analytical solution
- Overlapping Peaks
- Low SNR
- Compton Scattering
  - Background must compensate

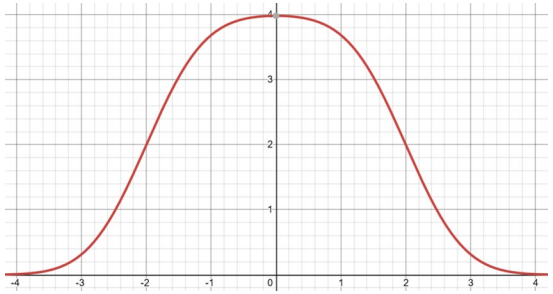


Model Function Choices



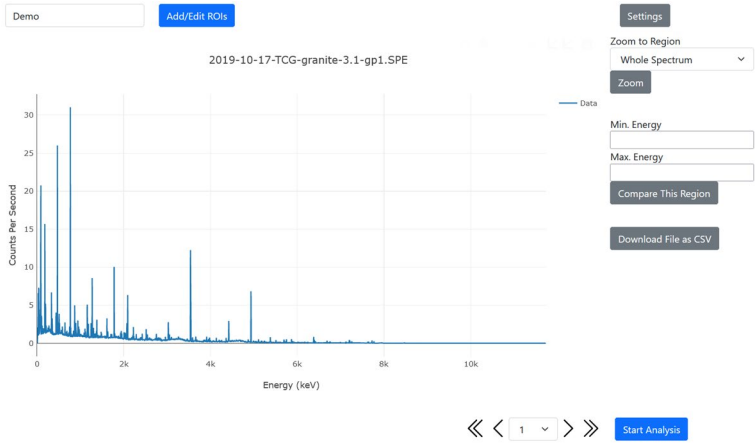
- Peaks
  - Simple Gaussian
  - Complex Gaussian-like model (accounts for charge carrier build-up)
  - Boron peak approximation (difference of 2 error functions)
  - Physical Boron peak model (requires numerical convolution)
- Backgrounds
  - Linear
  - Quadratic
  - Arctan



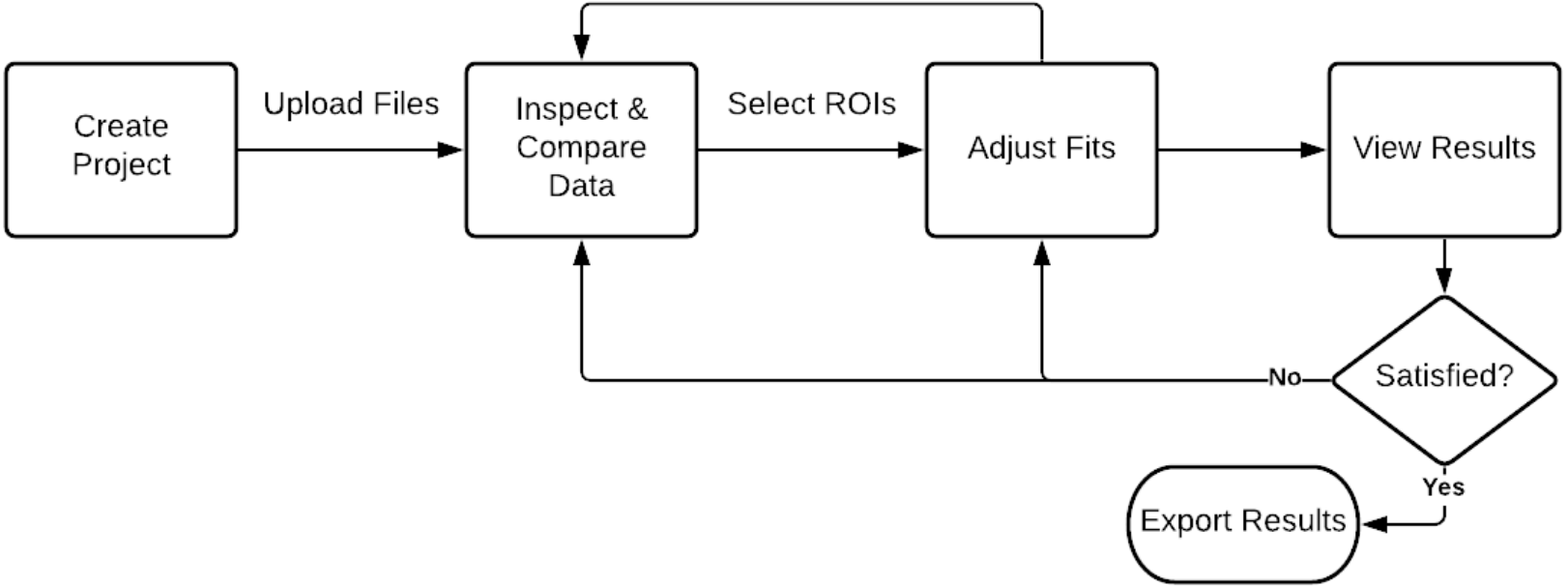


My Approach

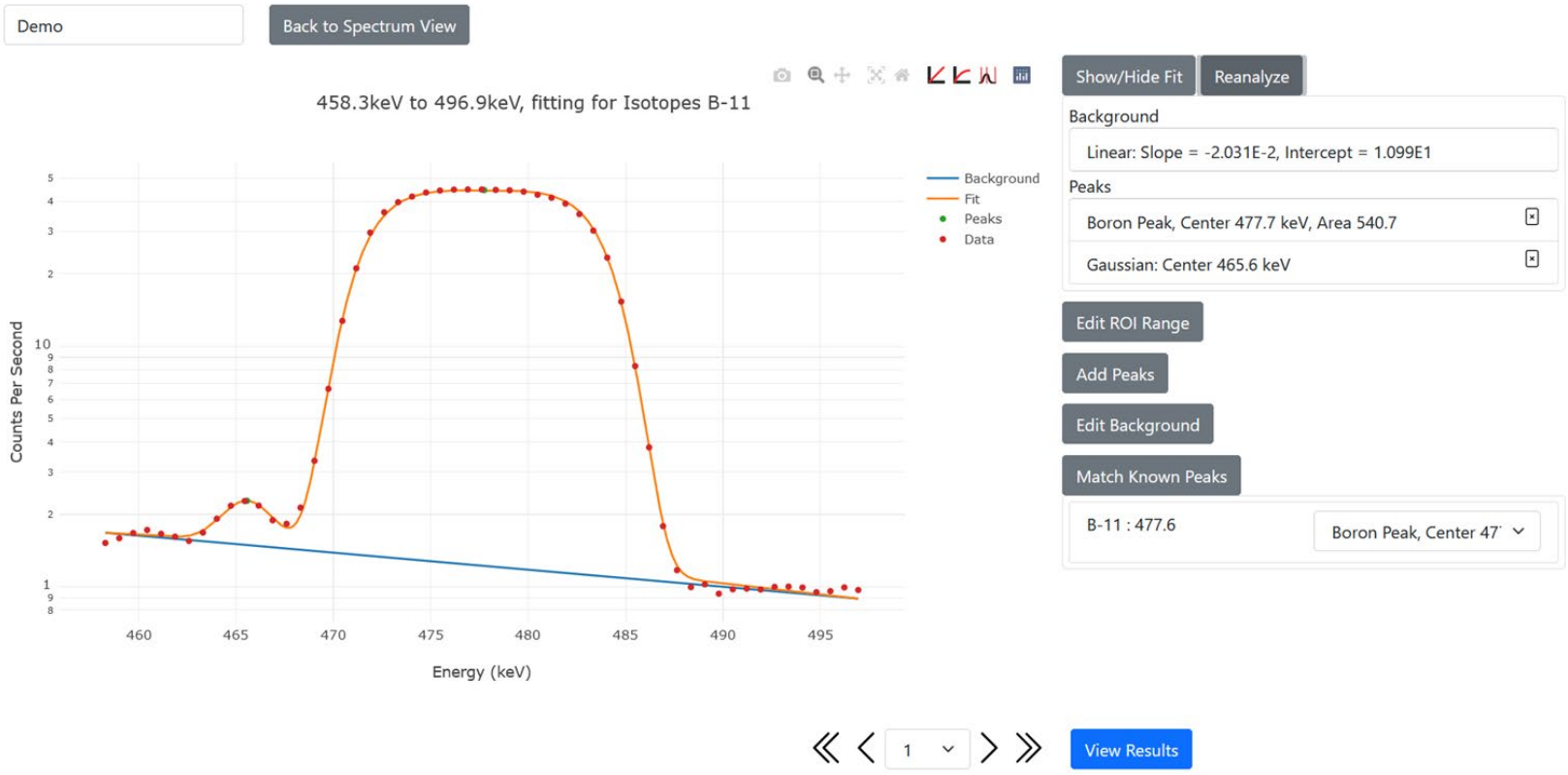
- Nonlinear least squares (LM) fitting
- User chooses peak/background models to use
  - This lets them balance # of fitter params and physical accuracy of models
- User then selects regions to fit
- Program finds and fits peaks
- User adjusts fit
- Program outputs results
  - .xlsx and .csv formats



Program Flow



The Data Analysis Process: A Demo



Comparison to Existing Solution

Program	Availability	Peak Fitting	ROI Editing	Batch Processing	Collaborative
OpenAGS	Free & Open-Source	Fit with multiple peaks, user chooses type	Simultaneous, can manually adjust region and peaks	Yes	Yes (link sharing)
PeakEasy	Proprietary, only available to US Gov.	Predetermined fit with 1-2 Gaussians	Silmultaneous, can manually adjust region	Yes	Files must be emailed back and forth

- Both programs support reading proprietary spectrum file formats
- Both also support several output formats (including CSV)

Acknowledgements

- Dr. Heather Chen-Mayer
- Paul Kienzle

Questions?

References

- Paul, R. L., & Lindstrom, R. M. (2000). Prompt Gamma-Ray Activation Analysis: Fundamentals and Applications. Journal of Radioanalytical and Nuclear Chemistry, 243(1), 181–189. https://doi.org/10.1023/a:1006796003933
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- https://github.com/wojdyr/xylib