Quantitative Spectrum Analysis using Simulated Neutron Scattering Data

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USDA Internship Project - MINS Simulation and Spectrum Deconvolution

Presentation Outline

Application

- Soil carbon: important for agriculture and emissions
- Lab method: Dry Combustion (accurate, expensive)
- MINS: on-site, non-destructive scanning system
- MINS: Mobile Inelastic Neutron Scattering System
- Role: simulate and analyze MINS neutron data

Figure 1: Soil Core

Figure 2: MINS

Inelastic Neutron Scattering

- Neutrons excite nuclei → emit gamma rays
- Signature peak: Carbon at 4.44 MeV (from 14 MeV neutron)
- Gamma peaks identify elements in soil

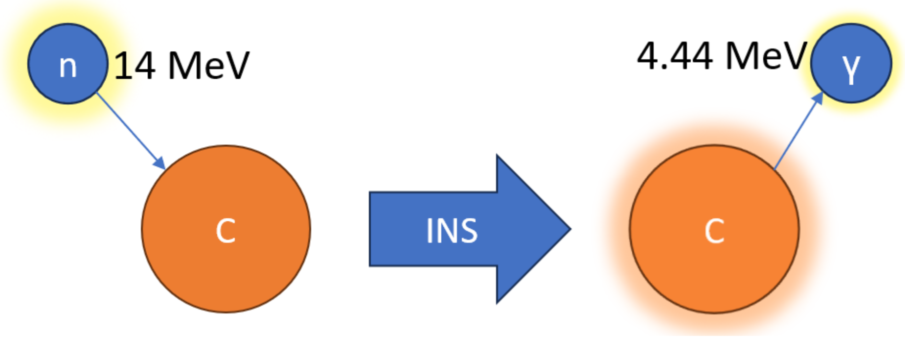

Figure 3: Inelastic Neutron Scattering on Carbon Atom

Carbon Gamma Ray Cross Section

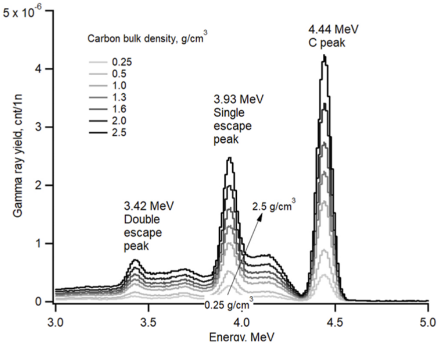

Figure 4: Inelastic Neutron Scattering Cross Section on Carbon Atom

Simulating MINS - 1

- Software: MCNP6.2 (Monte Carlo neutron transport)
- Geometry + material setup for full system

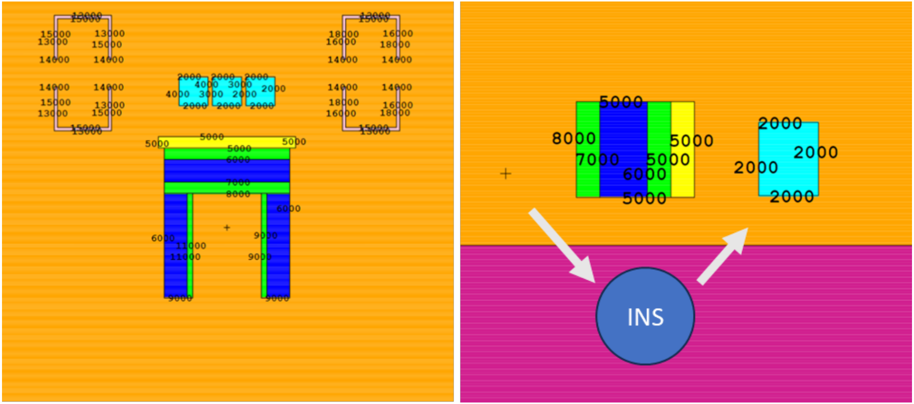

Figure 5: Inelastic Neutron Scattering in MCNP

Simulating MINS - 2

- Fast neutrons interact with soil
- Emitted gamma rays detected and stored

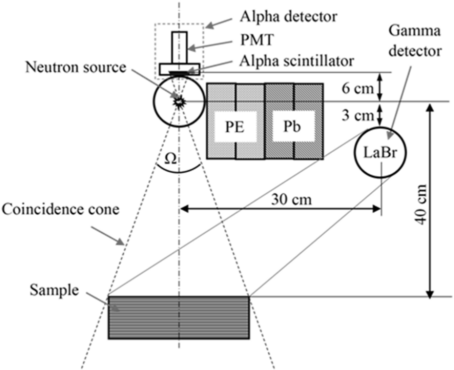

Figure 6: MINS Architecture

Defining Spectrums

- Spectrum: histogram of energy counts
- One "history" = 50 ns neutron event window
- Use 10^9 histories for high resolution
- Normalized spectrum = probability density

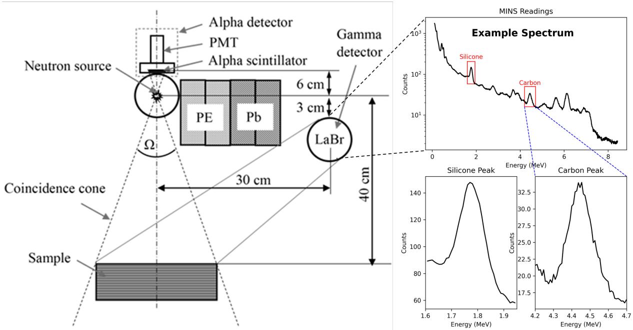

Figure 7: Architecture to Spectrum

Spectrum Analysis

- Peaks correspond to element emissions
- Goal: Deconvolve mix to get composition

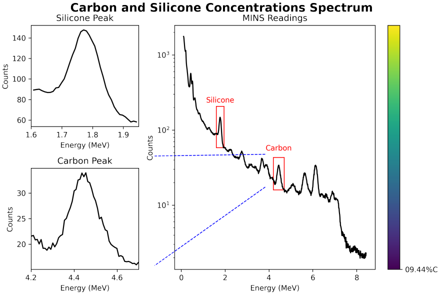

Figure 8: Example Spectrum

Data Generation

- Simulate samples: 0–30% carbon + silicon base
- 10^9 histories per sample

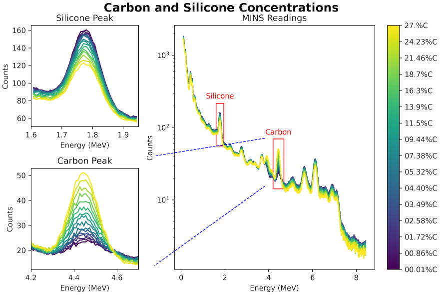

Figure 9: Carbon and Silicon Concentrations

Analysis Methods

- Five methods: from classical to advanced
- Focus: identify carbon peak + baseline

Classical Methods

- Perpendicular Drop (PD): flat baseline from minimum
- Tangent Skim (TS): tangent line across valley
- Field data is noisy → limitations arise

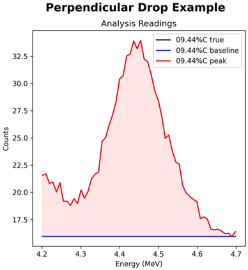

Figure 10: PD Example

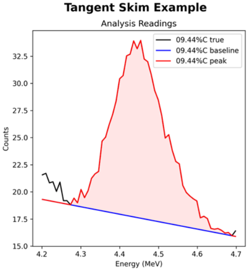

Figure 11: TS Example

Peak Fitting - Linear Baseline

- Gaussian peak + linear baseline
- Fit using Levenberg-Marquardt algorithm

Peak and Baseline Function

$$f_{peak}(x) = Ae^{-\frac{(x-B)^2}{2C^2}} \quad (1)$$

$$f_{baseline}(x) = mx + b \quad (2)$$

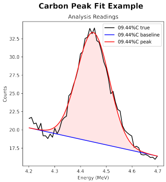

Figure 12: Linear Peak Fitting Example

L-M Algorithm

- Solves non-linear least squares
- Combines Gauss-Newton + gradient descent
- Robust curve fitting tool

Least Squares Minimzation

$$\text{minimize } ||y - f(x, params)||^2 \tag{3}$$

$$\text{where } y = \text{data}, f(x) = \text{model}$$

Levenberg-Marquardt algorithm

$$\text{L-M: } \Delta x = (J^T J + \lambda I)^{-1} J^T r \tag{4}$$

$$\text{where } J = \text{Jacobian}, r = y - f(x)$$

$$\text{and } \lambda = \text{damping factor}$$

Peak Fitting - Exponential Falloff Baseline

- Use exponential falloff for better background modeling
- Bounds constrain peak within target window

Exponential Falloff Function

$$f_{baseline}(x) = Ae^{-B(x-C)} + D \quad (5)$$

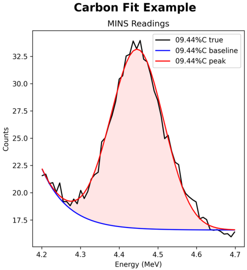

Figure 13: Peak Fitting Example

Prediction

- Peak area → carbon content
- Train linear regression on outer values
- Mean Squared Error: 7.56223e-06

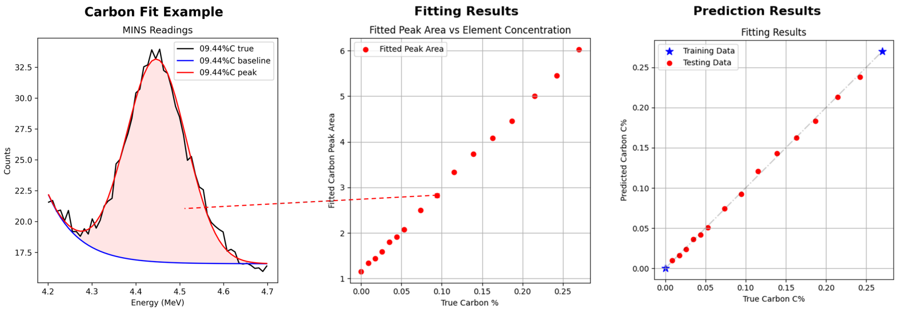

Figure 14: Peak Fitting Results

Limitations

- Requires manual element window per element
- Peaks may overlap $\rightarrow$ difficult for generalization

Paper Review

- GEANT4-based study on tagged neutron method (TNM)
- Goal: detect explosives via C/N/O signature

Modeling of tagged neutron method for explosive detection using GEANT4

Saroj Bishnoi [a,d,*], R.G. Thomas [b,d], Arnab Sarkar [c,d], P.S. Sarkar [a,d], Amar Sinha [d], Alok Saxena [d], S.C. Gadkari [d]

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GEANT4
Pure element spectra

ABSTRACT

The study has been focused on modeling the capabilities of tagged neutron method (TNM) for detection and identification of explosive materials using an approximated experimental configuration. The underlying principle is to use D-T (14.1 MeV) neutrons tagged by its associated charged particle and incorporating neutron time-of-flight technique to identify explosives by estimating carbon, nitrogen and oxygen contents and their ratios. This research was carried out to facilitate the design and construction of a prototype laboratory based TNM system and a simulation model was developed in the GEANT4 framework. The model has established an environment for (a) simulating production of D-T tagged neutrons, their transport and interactions with an object to induce emission, detection of characteristic gamma-rays and (b) image reconstruction (3D) of the interrogated object using time-of-

Figure 15: Paper Review

Tagged Neutron Method

- Uses alpha-neutron coincidence
- Measures within a known cone of interaction

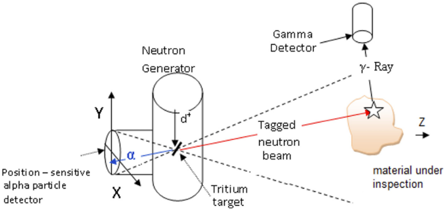


Figure 16: Schematic of Tagged Neutron Method

Component Fitting - Training

- Generate pure-element spectra
- Use as reference basis for decomposition

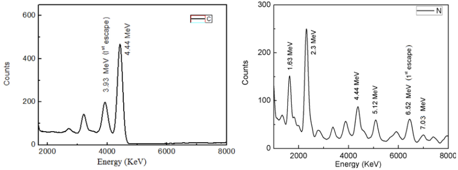


Figure 17: Simulated Spectra

Component Fitting - Testing

- Fit unknown spectrum as weighted sum
- Coefficients = estimated element ratios
- Fit optimized with L-M algorithm

Fitting Function

$$f_{fit}(x) = \sum_{i=1}^{n} w_i f_i(x) \tag{6}$$

where w_i = weight of element i

and $f_i(x)$ = pure element spectrum

Paper Results

- $\tilde{6}$% error in elemental estimates
- Effective for simulated detection of explosives

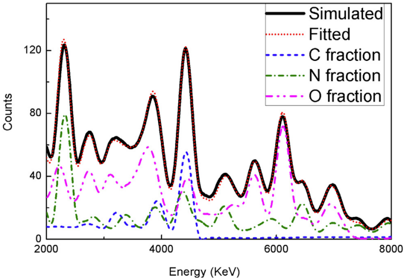


Figure 18: Simulated Spectra and Components

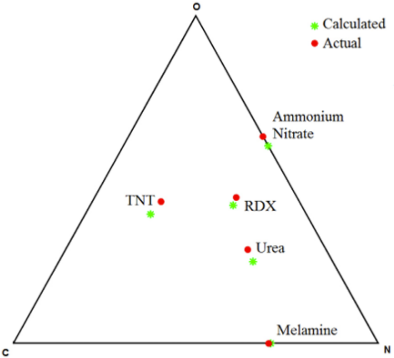


Figure 19: TNM Results

Applying to MINS Data

- Simulated spectra: C, Si, Al_2O_3, C/Si mix
- Initial weights: 1/n for each element

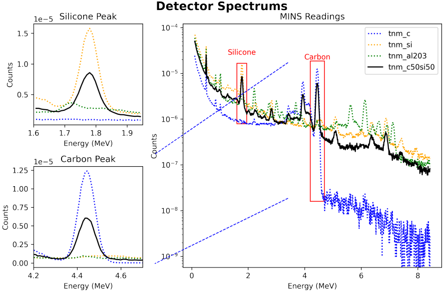


Figure 20: Detector Spectrums

Single Result

- Fit: C + Si = C/Si mix
- 0.4392∗C + 0.5415∗ Si = C/Si mix

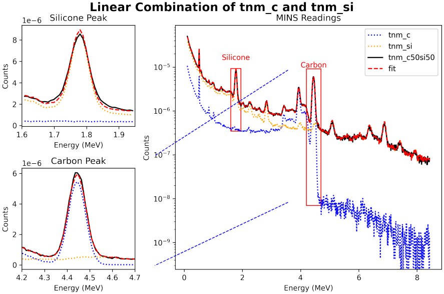


Figure 21: Linear Combination of TNM C and Si

Ghost Element Issue

- Including Al_2O_3 falsely contributes $\tilde{1}4\%$
- Caution when selecting training data
- $0.3821 * C + 0.4448 * Si + 0.1434 * Al_2O_3 = C/Si$ mix

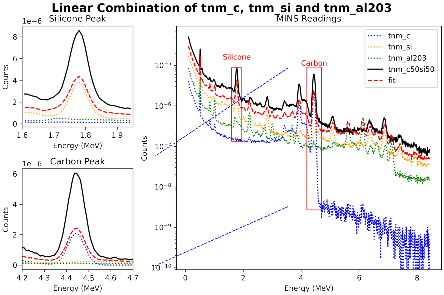


Figure 22: Linear Combination of TNM C and Si with Al_2O_3

Limiting to Windows

- using windows gives better Results
- $0.4466 * \mathrm{C} + 0.5063 * \mathrm{Si} + 0.1014 * \mathrm{Al_2O_3} = \mathrm{C/Si}$ mix

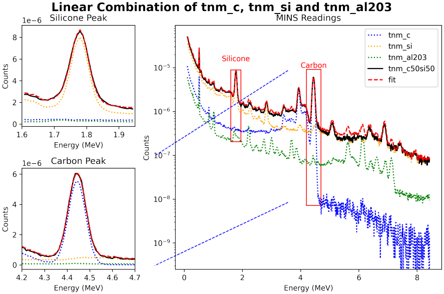
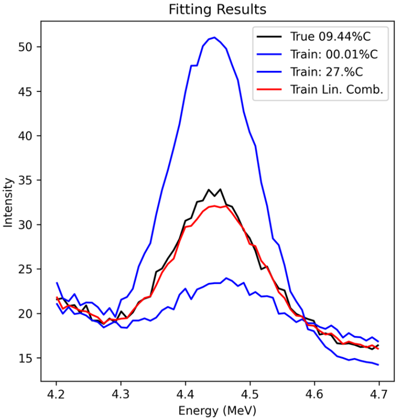


Figure 23: Linear Combination of TNM C and Si with $\mathrm{Al_2O_3}$ using Windows

Results

- Balances peak accuracy with generalization
- Promising method for element quantification

Component Fitting



Full Results

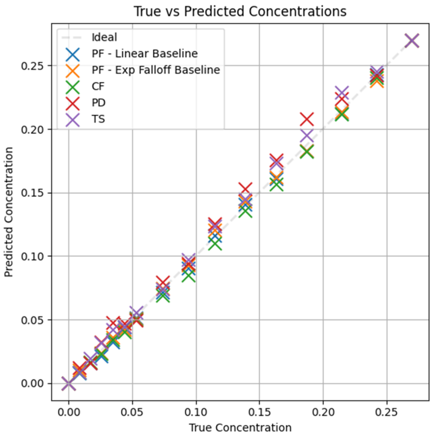


Figure 25: Full Results

MAE comparison

Spectrum Analysis Method	MSE
Peak Fitting Linear Baseline	6.00647×10^{-6}
Peak Fitting Exponential Baseline	7.56223×10^{-6}
Component Fitting	1.89773×10^{-5}
Perpendicular Drop	0.00741817
Tangent Skim	0.00504626

Table 1: Mean Squared Error (MSE) by Spectrum Analysis Method

Conclusion

- Explored spectral deconvolution paper
- Applied curve-fitting method to project data
- Compared with other methods
- Promising for real-time field analysis
- Flexible alternative to peak-based approaches

Future Work

- Simulations take long time (5 days for 10^9 histories)
- Atlas HPC: run 20 jobs at once, still long wait
- Future: reverse deconvolution method
- Generate spectrum from known mixture
- Test accuracy of deconvolution methods

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