

Baseline Evaluation of CNO Composition Analysis Using Detector-Specific Pure-Element Gamma Signatures under 14 MeV Neutron Irradiation

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1. Introduction

Neutron-induced prompt gamma-ray spectroscopy enables non-destructive analysis of elemental composition and can therefore be applied to material identification. Previous studies used an unfolding algorithm to estimate elemental contributions by decomposing measured gamma-ray spectra into linear combinations of pure-element gamma signatures. For organic materials, the resulting relative proportions of C, N, and O were used to distinguish explosives, narcotics, and benign materials [1,3]. However, elemental analysis based on individual characteristic gamma-ray peaks is limited when spectral peaks overlap. In particular, the 4.439 MeV gamma ray from C and the 4.442 MeV gamma ray from N cannot be resolved with the energy resolution of NaI(Tl) detectors [1,2]. In this study, the baseline performance of this previously reported CNO-based unfolding approach was examined, and the effects of detector characteristics on the analysis results were compared. Rather than modeling the detailed chemical composition of a specific explosive or narcotic, a simple C:N:O = 1:1:1 mixture by mass (CNOMIX) containing all three target elements was adopted as a baseline test case. The same analysis procedure was applied under NaI(Tl), CsI(Tl), and HPGe detector conditions, and the resulting CNO composition estimates were compared.

2. Methods

2.1 MCNP Model

To evaluate the baseline performance of the unfolding algorithm under idealized conditions, a geometry consisting of a neutron source, sample, and detector was modeled, as shown in Fig. 1. For each detector, the same nuclear data and geometry were used for the pure-element and CNOMIX calculations.

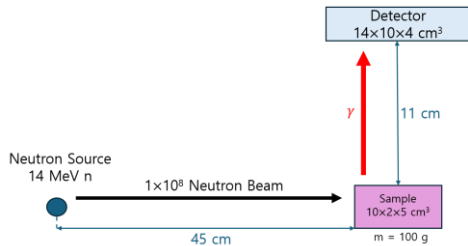


Fig. 1. MCNP geometry for CNO signature generation and CNOMIX analysis.

2.2 Detector Modeling

The detector energy-deposition spectra were calculated using the MCNP F8 pulse-height tally for NaI(Tl), CsI(Tl), and HPGe detectors, with their respective material and density properties included in the model. To account for detector energy resolution, Gaussian Energy Broadening (GEB) was applied. The FWHM is given by Eq. (1), where E is the gamma-ray energy and a , b , and c are detector-specific coefficients.

$$FWHM = a + b\sqrt{E} + cE^2 \quad (1)$$

The GEB coefficients for each detector were determined based on energy-resolution data reported in the literature [4-6] and are listed in Table 1.

Table I. GEB coefficients for each detector.

Detector	a	b	c
NaI(Tl)	-0.01392	0.06968	-0.05862
CsI(Tl)	-0.00328	0.07395	0.00675
HPGe	5.868×10^{-4}	3.951×10^{-4}	7.46793

2.3 Pure-Element Gamma Signatures and Unfolding Algorithm

Detector-specific pure-element gamma signatures for C, N, and O were generated from the F8 spectra calculated for pure-element samples. The F8 spectra of carbon, nitrogen, and oxygen were each divided by the simulated sample mass of 100 g and defined as $L_C(E)$, $L_N(E)$, and $L_O(E)$, respectively. This allowed the linear-combination coefficients obtained from the unfolding algorithm to be interpreted as the equivalent mass contribution of each element. The overall spectral shape was used in the unfolding algorithm, and the spectrum $S(E)$ of a sample containing C, N, and O was approximated by equation (2).

$$S(E) \approx a_C \cdot L_C(E) + a_N \cdot L_N(E) + a_O \cdot L_O(E) \quad (2)$$

Here, a_C , a_N , and a_O represent the estimated mass contributions of C, N, and O, respectively. The coefficients were determined by minimizing the sum of squared residuals between the fitted spectrum and the sample spectrum over the 0.5–8 MeV range. The low-energy region below 0.5 MeV was excluded from the analysis because the influence of low-energy deposition

components is relatively large. The relative mass fractions within CNO were calculated by equation (3).

$$w_i = \frac{a_i}{a_C + a_N + a_O}, \quad i = C, N, O \quad (3)$$

3. Results

The unfolding algorithm was applied to CNOMIX using the detector-specific pure-element gamma signatures of C, N, and O. Fig. 2 compares the directly calculated CNOMIX spectrum with the spectrum fitted as a linear combination of the C, N, and O pure-element gamma signatures using the coefficients obtained from the unfolding algorithm. For all three detectors, the major peak positions and overall spectral structures were reproduced.

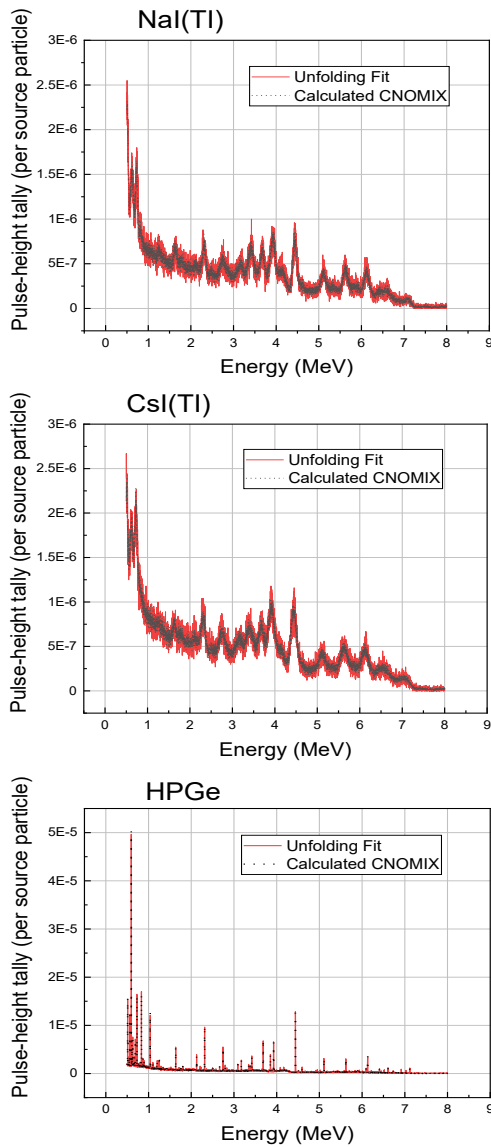


Fig. 2. Comparison of calculated and fitted CNOMIX spectra.

For CNOMIX, the reference mass fraction of each element was 33.33%. Table 2 summarizes the estimated C, N, and O mass fractions and the corresponding MAE

for each detector. The MAE was below 1 percentage point for all three detectors under the present CNOMIX condition.

Table II. Estimated CNO mass fractions of CNOMIX.

Detector	C (%)	N (%)	O (%)	MAE(%p)
NaI(Tl)	32.78	33.35	33.88	0.37
CsI(Tl)	32.54	33.51	33.95	0.53
HPGe	33.04	33.97	32.99	0.43

4. Conclusions

In this study, the same procedure, from the generation of pure-element gamma signatures to the application of the unfolding algorithm, was applied to each detector to examine the basic feasibility of CNO composition analysis. Since only one CNOMIX composition was evaluated, MAE was used as a preliminary indicator of composition estimation accuracy, and its variation with composition could not be assessed. The MAE values were below 1 percentage point for all three detectors, indicating that the estimated compositions were close to the reference values under the present idealized conditions. Although this result does not establish the overall performance of the method, it supports its basic feasibility at the conceptual design stage. For further evaluation, spectral fitting performance may also be examined in addition to composition accuracy. R^2 and NRMSE can provide additional information on overall spectral agreement and normalized fitting error, respectively. Future work will evaluate the method over a wider range of CNO compositions and extend the validation to more realistic inspection conditions.

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