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Motivation – material identification based on elemental reconstruction

The non-destructive search and characterization of materials, which may or may not be accessible within a container, has applications ranging from airport and border crossings to arms control and emergency response. Our system, Material Identification through Resonant Attenuation (MIRA), is capable of reconstructing the elemental densities of hydrogen, carbon, nitrogen, and oxygen, which can in many cases uniquely identify the sample material (see Figure 1: note that our system identifies absolute densities, not only fractions).

Features of the MIRA system are:

- Portability:** only requires the sample container be surrounded by detector units and a d-T neutron generator
- Tunable to scenario:** the desired scan time dictates the number of units surrounding the container.
- In situ characterization:** neutrons are capable of penetrating the sample container

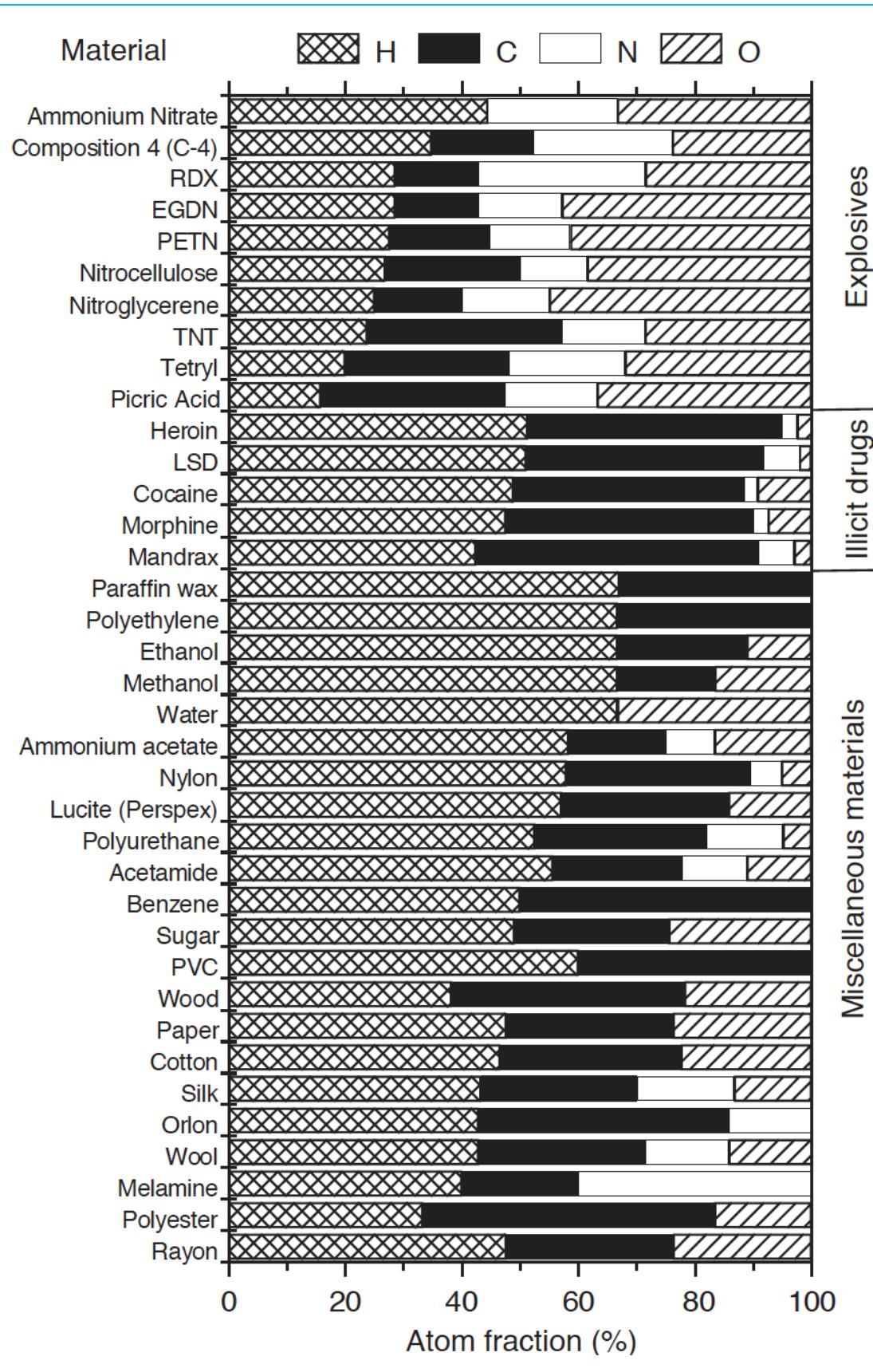


Figure 1: the atomic fraction of several materials, taken from [1].

Methods – measuring elemental composition of materials through resonant absorption

Figure 2 shows the spectrum of neutron interaction cross sections for Hydrogen, Carbon, Nitrogen, and Oxygen from the ENDF/B-VII.0 database [2]. These unique resonant “fingerprints” in the attenuation can be used to quantify their density within a sample:

- Two scans over the 0.5-9 MeV range, one with the sample present and one without, provides an attenuation spectrum unique to the particular elemental ratios of the sample.
- Although hydrogen does not have resonant features, its energy dependence of its cross section does enable its molar density to be determined as well

In order to utilize this signature, we require a neutron source with a broad energy range, as well as a neutron spectrometer with a reasonable energy resolution. Our system meets both requirements with its geometrical layout

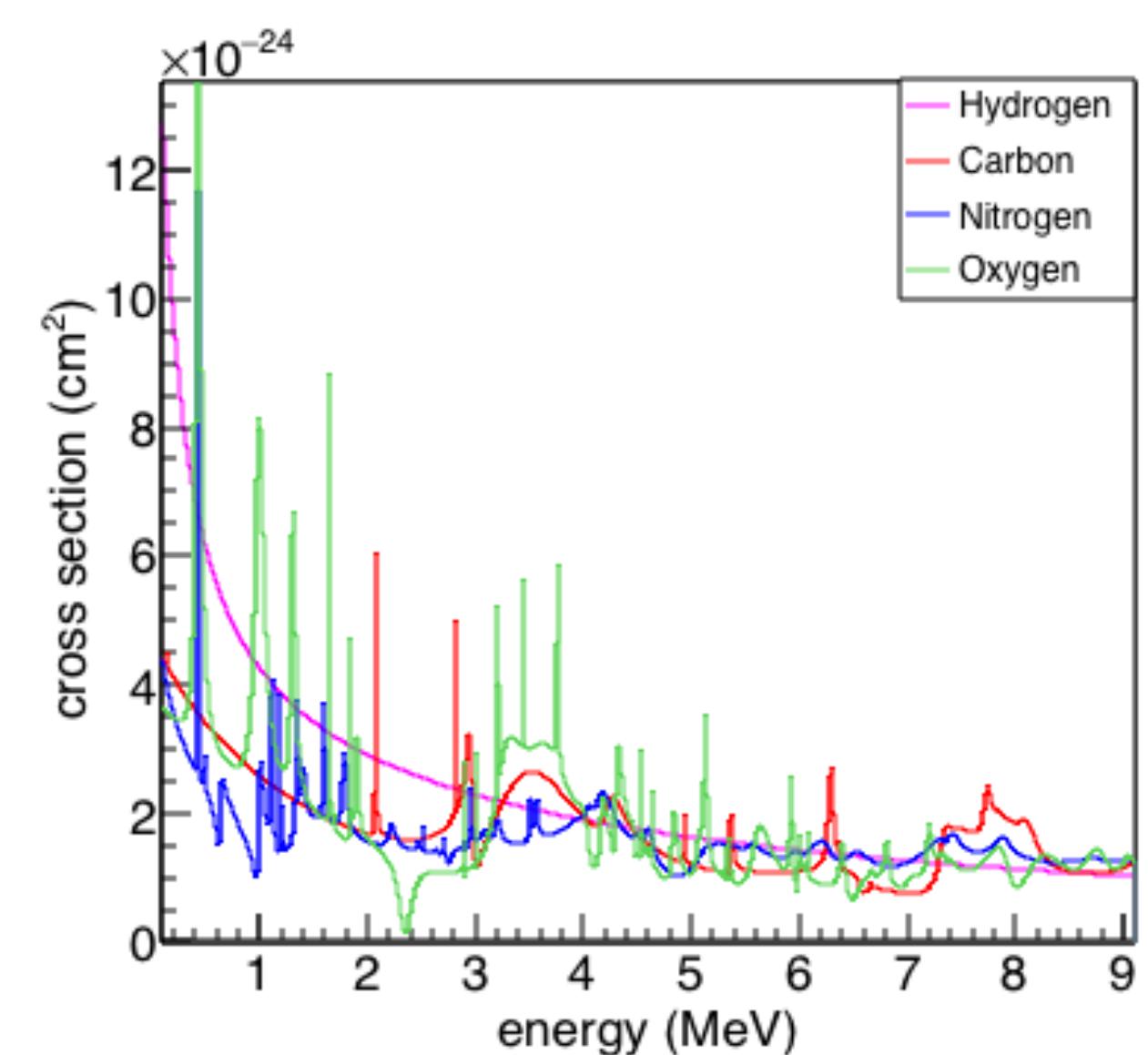


Figure 2: the total neutron interaction cross section for hydrogen, carbon, nitrogen, and oxygen, from ENDF/B-VII.0 [2]

Methods – detector system and Geant4 model

The MIRA demonstration system consists of:

- 32 channels of 3x3 inch right cylindrical liquid scintillator cells
- two 16-cell planar arrays on either side of the sample
- d-T neutron generator moving through an arc with axis centered on the “front” plane (red array)

A range of scattering angles results in neutrons with 0.5-14 MeV energies exiting the front array:

- scattering in the front array starts time-of-flight clock
- neutrons depositing energy in the back detector array stop time-of-flight clock: these are neutrons that have passed through the sample without scattering

This system has been modeled in Geant4. Depositions are convoluted in both time and position to account for the detector size and the expected time resolution (Figure 4).

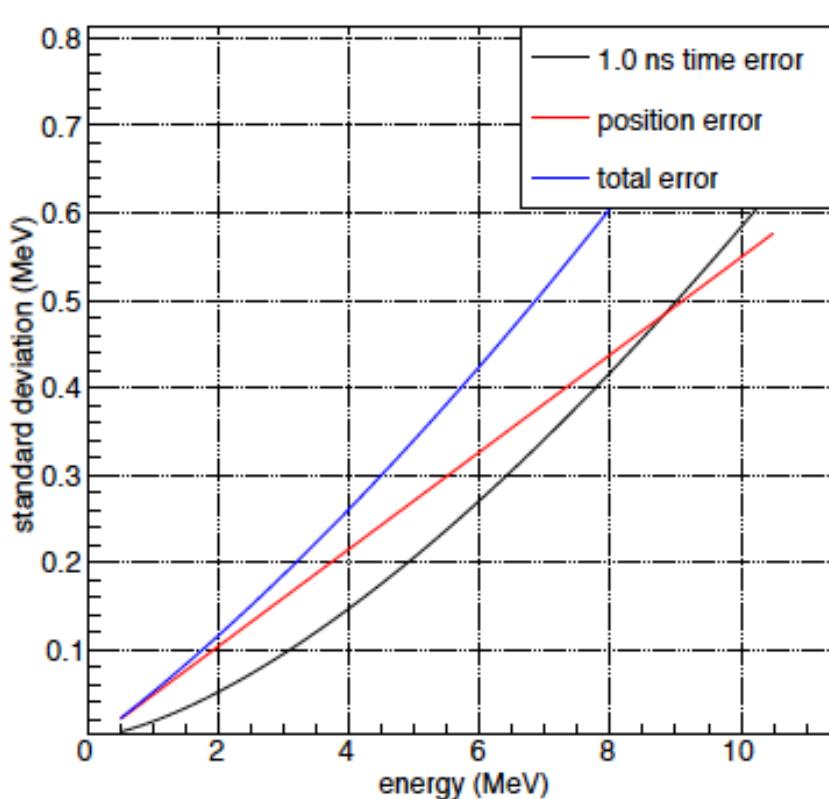
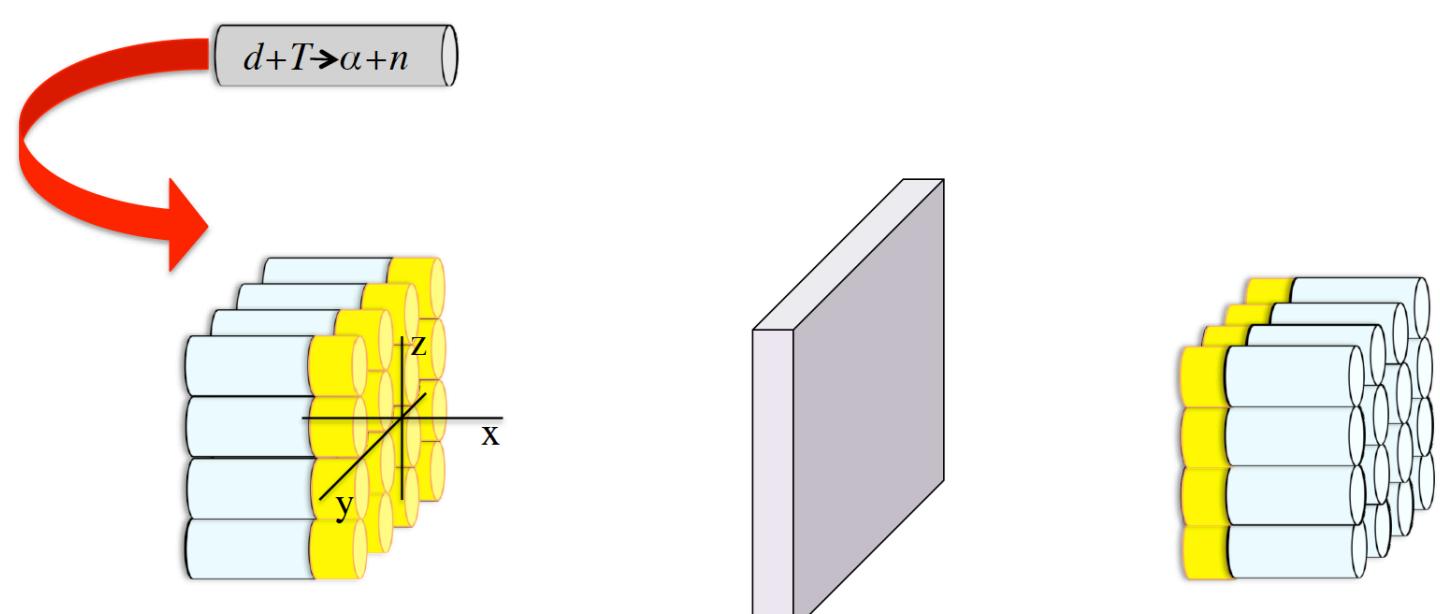


Figure 4: the total neutron time-of-flight energy error for our system. The error in the position, $f(E)$, is inferred from the Monte Carlo, and the error in time is calculated by the time-dependence of the energy calculation:

$$\frac{\sigma_E}{E} = \sqrt{\left(\frac{f(E)}{E}\right)^2 + 4\left(\frac{1}{t}\right)^2 \sigma_t^2}$$

Methods – reconstruction technique

The attenuated spectrum is used to reconstruct the molar concentration of hydrogen, carbon, nitrogen, and oxygen. Beer’s law is used to calculate the expected number of transmitted particles in a particular energy bin, e , and for a particular detector pair, d :

$$\lambda_{e,d} = N_{e,d}^{\text{empty}} e^{-N_{A,l_d} \sum_{i=HCNO} M_i <\sigma_i, E>},$$

- $N_{e,d}^{\text{empty}}$ is the measured number of counts without the sample present,
- M_i is the molar fraction of each element $i=HCNO$, in units of moles/cm³, and
- l_d is the detector-dependent path length through the sample.

We maximize the negative log-likelihood, calculated from the measured value, $n_{e,d}^{\text{sample}} = N_{e,d}^{\text{sample}} / N_{e,d}^{\text{empty}}$, using the Minuit [3] package included in ROOT [4]:

$$\log \mathcal{L} = \sum_{e=0}^{n_e} \sum_{d=0}^{n_d} n_{e,d} \log(\lambda_{e,d}) - \lambda_{e,d}$$

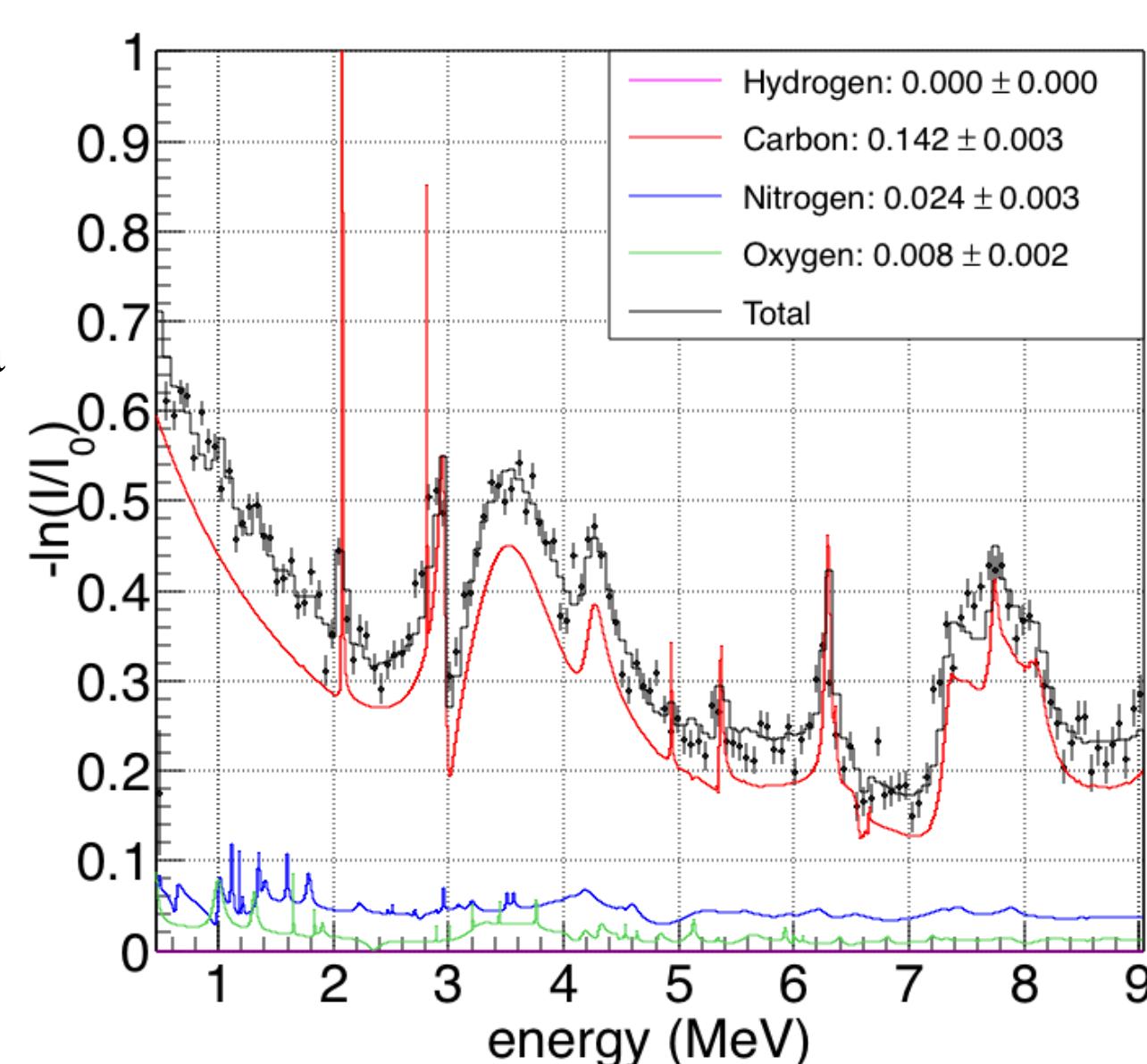


Figure 5: the attenuated energy spectrum for a 2x30.48x30.48 cm graphite sample and 2 hours of sample run time, including only events which did not scatter in the sample and with no detector response applied. The reconstructed molar concentration for all four elements are shown in the legend, and the corresponding contribution to the total attenuated spectrum is plotted. The errors quoted are one standard deviation, output from the error matrix of Minuit.

Geant4 Results – expected detector performance

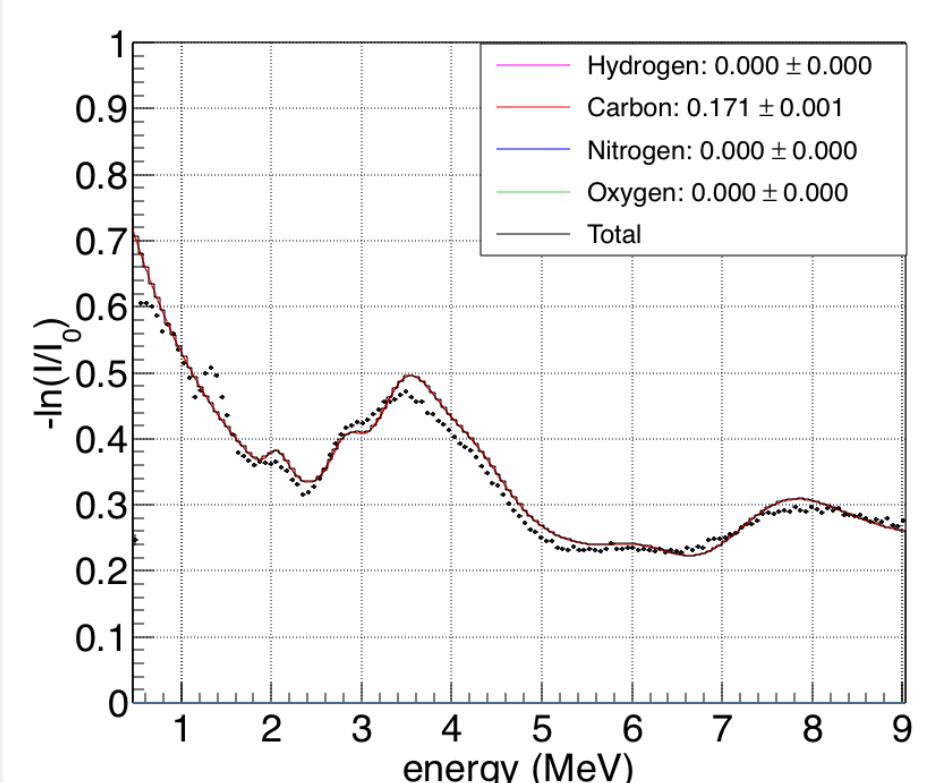


Figure 6: The same as Figure 5, but with the position and time response of the detectors applied. The total neutron cross sections of each element have also been convoluted with the expected time-of-flight energy resolution.

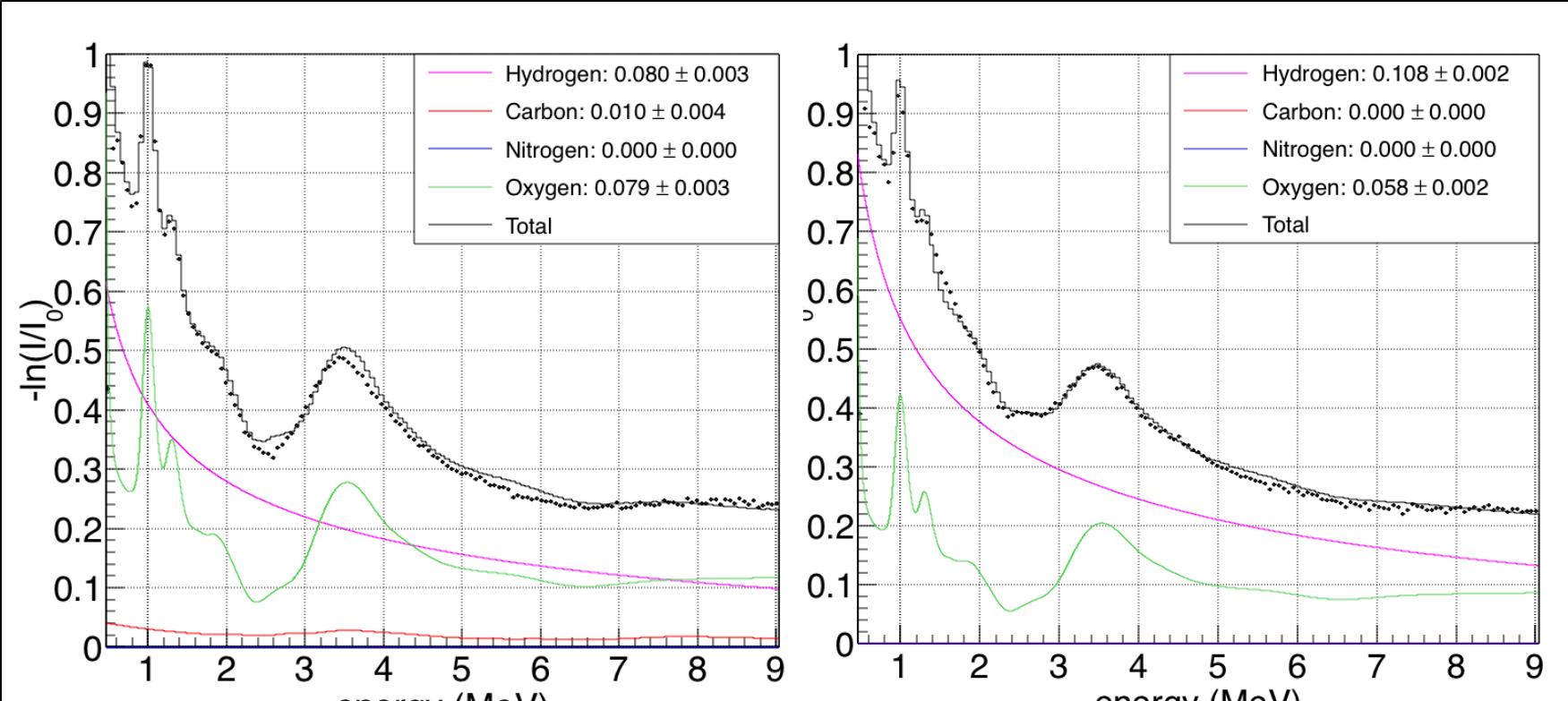


Figure 7: The attenuated energy spectra and reconstruction results for a 2x30.48x30.48 cm sample of pure hydrogen peroxide (left) and water (right). The accuracy compared to the true molar concentration is 7% or less for all elements. This degree of accuracy is sufficient to distinguish pure hydrogen peroxide from water.

Results and Next Steps

Based on the results in Table 2, we expect our system will perform with an accuracy sufficient to identify and characterize a number of different samples of interest. Detector characterization of the current system is underway, and a data campaign will commence soon. Samples such as water, HDPE, hydrogen peroxide, and various concentrations of sugar water will be studied.

Sample	ρ (g/cm ³)	Hydrogen (M/cm ³)	Carbon (M/cm ³)	Nitrogen (M/cm ³)	Oxygen (M/cm ³)
Ammonium Nitrate	1.725	0.086	0.00	0.043	0.065
Graphite	2.09	0.00	0.174	0.00	0.00
HDPE	0.94	0.134	0.067	0.00	0.00
Hydrogen Peroxide	1.45	0.085	0.00	0.00	0.085
Water	1.00	0.111	0.00	0.00	0.056

Table 1: The true molar concentration and total density for all samples studied.

Sample	ρ (g/cm ³) (%)	H (M/cm ³) (%)	C (M/cm ³) (%)	N (M/cm ³) (%)	O (M/cm ³) (%)
Ammonium Nitrate	1.73 ± 0.064 (1.7)	0.084 ± 0.002 (2.3)	0.000 ± 0.000 (0.0)	0.051 ± 0.003 (19)	0.058 ± 0.003 (11)
Graphite	2.05 ± 0.012 (0.1)	0.000 ± 0.000 (0.0)	0.171 ± 0.001 (1.7)	0.000 ± 0.000 (0.0)	0.000 ± 0.000 (0.0)
HDPE	0.95 ± 0.036 (0.9)	0.131 ± 0.003 (2.2)	0.068 ± 0.003 (1.5)	0.000 ± 0.000 (0.0)	0.000 ± 0.000 (0.0)
Hydrogen Peroxide	1.46 ± 0.048 (0.6)	0.080 ± 0.003 (5.8)	0.010 ± 0.004 (n/a)	0.000 ± 0.000 (0.0)	0.079 ± 0.003 (1.2)
Water	1.07 ± 0.032 (6.7)	0.108 ± 0.002 (2.7)	0.000 ± 0.000 (0.0)	0.000 ± 0.000 (0.0)	0.058 ± 0.002 (7.1)

Table 2: The reconstructed molar concentration of hydrogen, carbon, nitrogen, and oxygen for several materials. These results are from two hours of runtime, using the Geant4 application and with our expected detector response applied. The parameter errors are one standard deviation errors from the error matrix of Minuit, and the value in parentheses are the percent error of the value compared to the true values from Table 1.

References:

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