# Using Graphite in Degradation of Explosives

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**Graphite powder can promote the degradation of DNAN, an insensitive but toxic explosive widely deployed at Department of Defense military training sites. High pressure liquid chromotography was used to determine the efficiency of graphite powder in the extraction of DNAN from a solution. A standard curve was calculated as well as extraction efficiency from numerous trials. This investigation will continue due to the inconsistency of the initial stock solution used.**

## Introduction

Insensitive high explosives (IHE) are widely deployed at Department of Defense (DoD) military training sites to replace conventional energetic compounds such as TNT. IHEs such as 2,4-dinitroanisole ($C_7H_6N_2O_5$, also known as DNAN), an energetic nitroaromatic compound, have become more frequently used due to their insensitivity to accidental stimuli while maintaining high performance (1). However, DNAN is more toxic than TNT and is negatively charged and highly water soluble. At environmentally relevant conditions it weakly interacts with soil particles and can seep into the groundwater through the soil. IHEs are often found in high concentrations at these military training sites (1) causing potential health risks and harmful environmental contamination. Alkaline hydrolysis is a possible pathway to degrade IHEs such as DNAN in soil but causes concerns as it requires raising soil pH to elevated pH conditions (>pH 11). Hydrolysis of DNAN promoted by pyrogenic carbonaceous matter (PCM) is promising because it can occur under environmental pH conditions (pH 7) (2). In this study we examined the efficiency of a model PCM, graphite powder, in the degradation of DNAN at different pH values.

## Methods

Vials of water, graphite powder, an acidic buffer and various concentrations of DNAN (4, 8, 16, 32, and 64 μM) were prepared. We used High Pressure Liquid Chromatography (HPLC-UV) to analyze the concentrations of DNAN and develop a standard curve (Figure 1). We then prepared, incubated and rotated vials of DNAN and graphite. An acidic buffer and distilled water were added, and the vials were centrifuged and separated. HPLC-UV and the standard curve equation were used to determine the extraction efficiency of graphite powder.

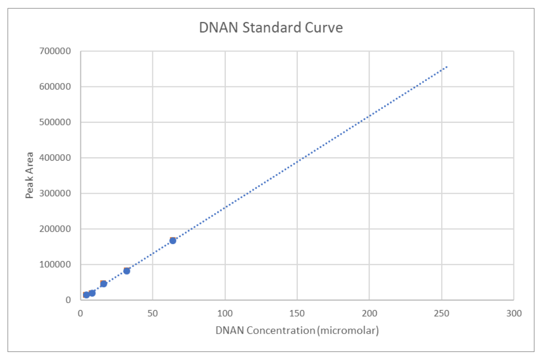


**Figure 1.** DNAN Standard Curve Showing DNAN Concentration vs. Peak Area from High Pressure Liquid Chromatography. y =2583.6x + 1873.7; $R^2$ = 0.9983

## Results & Conclusion

The DNAN constructed standard curve demonstrates a strong linear correlation between peak areas and DNAN concentrations (Figure 1). Using linear regression, any sample's DNAN concentration (x) can be calculated by substituting peak areas (y) in the equation: y =2583.6x + 1873.7. DNAN extraction efficiencies from the graphite surface were then calculated. This is an essential step allowing us to discern adsorption from reaction. That is, we should be able to recover DNAN back from the solid phase if no reaction occurs; otherwise, it indicates that DNAN undergoes degradation on graphite surface. Our calculated extraction efficiencies (Table 1) widely ranged from 3 to 35%. The large variation is likely due to operational error, which should improve as I become more familiar with the procedure. Another strategy I will explore to reduce the variation is to use

| | Mass of DNAN in Extracted Solvents (μmoles) | Extraction Efficiency (%) |
|---|---|---|
| DNAN Tube #1 | 47.55 | 23.07 |
| DNAN Tube #2 | 6.79 | 3.27 |
| DNAN Tube #3 | 20.85 | 10.01 |
| DNAN Tube #4 | 14.49 | 6.85 |
| DNAN Tube #5 | 72.05 | 34.69 |
| DNAN Tube #6 | 39.51 | 18.99 |

**Table 1.** Calculated extraction efficiencies for DNAN in the presence of 21 g/L of graphite at 25 °C.

more concentrated stock to minimize the amount of solvent introduced into the reaction system.

After determining a reliable extraction efficiency, we will continue to understand the pH effect on PCM-promoted hydrolysis and explore the implementation conditions for this technology in soil remediation for DoD sites. Specifically, we will use biochar for such application, a solid residue produced from incomplete biomass waste combustion. Biochar's performance will be compared with activated carbon, a benchmark PCM. We will also consider environmental impact by including life cycle analysis. The ultimate goal is determining a suitable PCM to not only retain but also degrade IHEs.

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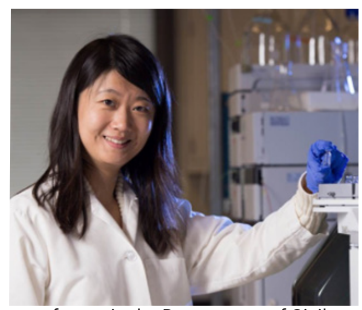
### Author

### Megan Fitzpatrick

Megan Fitzpatrick is a Presidential Scholar in the Villanova Class of 2023. She is pursuing a major in Civil Engineering and minors in Spanish and Sustainability. She is focusing on environmental engineering, and her ambition is to provide clean water for underdeveloped communities around the world. Through the Villanova Match Research Program, she worked with her mentor, Dr. Wenqing Xu, and a team of postdoctorates and graduate students on the DNAN contamination project. Outside of research and academics, Megan is extremely active on Villanova's campus. She is a peer minister, freshman retreat leader, RUIBAL leader and the Social Chair of NOVANoise, Villanova's tap dance club. She is also a member of Villanova Student Musical Theatre, NOVAdance morale committee, ASCE, SWE, and the Sophomore Service Learning Community.



### Mentor

### Dr. Wenqing Xu

Dr. Wenqing Xu is an associate professor in the Department of Civil and Environmental Engineering at Villanova University. She is actively engaged in both research and teaching. Her group has demonstrated that pyrogenic carbonaceous matter (black carbon, activated carbon) can facilitate various environmental reactions, which have implications for accelerating pollutant degradation and remediating contaminated soil and water. Xu received B.S. and M.S. degrees in environmental engineering from Nankai University in China (2007) and Johns Hopkins University (2009), respectively, and a Ph.D. degree in environmental engineering from Yale University (2014). She is a recipient of various awards, including the NSF CAREER award (2018) and University Scholarly Achievement Award (2020).