Carbonaceous Materials for Facilitating Hydrolysis of Munitions

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Background and Unmet Need

Legacy and insensitive high explosives (IHEs), such as 2,4-dinitroanisole (DNAN) and 2-methyl-1,3,5-trinitrobenzene (TNT), are commonly found in soil at Department of Defense (DoD) testing and training ranges. These ranges maintain very high concentrations of DNAN, which poses a substantial safety concern for personnel as DNAN has been found to possess significant dermal absorption properties.[1] These compounds also are highly water-soluble and can easily migrate from the soil into ground and surface water. This directly threatens aquatic and terrestrial ecosystems, as DNAN is known to be toxic to aquatic organisms, fishes, earthworms, and mammals. As a result, a dynamic pollution risk exists at munitions testing sites that pose an immediate exposure risk to personnel and the health of surrounding ecosystems.

Further, the formation of phenolic products that result from hydrolysis of IHEs raises additional concerns due to their higher toxicity than parent compounds. Therefore, there is a pressing need to maximize the sorption of legacy explosives and IHEs to reduce personnel exposure and minimize their transport from DoD sites into the surrounding environment.

While munition contamination exists worldwide, roughly 1,700 Formerly Used Defense Sites (FUDS) remain contaminated with hazardous substances or military munitions in the United States alone. The cost of remediation has been estimated to be $11.9 billion, and the Military Munitions Response Program (MMRP) makes up 73% of the environmental liabilities within the FUDS program.[2] As a result, there is strong demand for remediation products that provide both an effective and economical solution to sequester and or degrade these contaminents.

The novel modified carbon remediation technology developed by Dr. Xu stands to provide both an effective and cost-efficient in-situ solution for the complex needs of munition remediation.

Opportunity

Dr. Xu has developed novel carbonaceous materials that can be deployed as reactive adsorbents as an in-situ remediation solution for IHEs and other legacy explosives. Although carbon amendments have been widely used for soil and sediment cleanup, this invention is the first reactive carbon amendment that can simultaneously sequester and destroy contaminants, thus significantly reducing the need for amendment regeneration.

Preliminary data suggests the amendment material is not limited to munition remediation but also can sequester anionic compounds such as nitrite, nitrate, and orthophosphate. Dr. Xu believes the technology may be further developed as a platform soil remediation product.

Unlike traditional carbon amendments, DNAN and / or TNT degradation on carbon surfaces will free up adsorption sites, allowing the tailored carbon to sequester DNAN continuously. This functionality will significantly reduce the cost of materials replacement and retreatment. Any munitions, such as 3-Nitio-l,2,4-triazol-5-one (NTO), that are not susceptible to alkaline hydrolysis can be safely entrapped within the carbon amendment, decreasing their bioavailability from the surrounding environment. Further, the developed technology boosts alkaline hydrolysis at near-neutral pH conditions rather than high pH conditions required by current state-of-the-art methods (i.e., lime treatment). As a result, this

[1] *2,4-dinitroanisole, Toxicokinetics, Susceptible Populations, Biomarkers, Chemical Interactions.* Agency for Toxic Substances and Disease Registry., No date.

[2] *Environmental Liabilities: Improvements Needed to Measure Progress of Cleanup of Formerly Used Defense Sites*. U.S. Government Accountability Office, June, 2022.

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technology is ideally positioned to serve the munition response market across multiple global governments.

Dr. Xu's research showed her carbon amendments effectively facilitated DNAN decay, with an average of 98% destruction over ten cycles, suggesting no significant loss of reactivity. Nitrite formation confirmed DNAN decay, which is desired for in-situ remediation of insensitive high explosives. Dr. Xu's material accelerated alkaline hydrolysis over 70-fold while maintaining the amendment's reactivity. These results represent a strong cost-saving advantage, as the number of soil treatments is greatly reduced compared to commercially available technology.

Studies using real soils demonstrated enhanced adsorption affinity (over three orders of magnitude) for highly mobile IHEs, such as (NTO). The amendments maintained their reactivity over consecutive additions of IHE compounds.

The global environmental remediation market was valued at $109.3 billion in 2022 and is expected to grow to $163.4 billion by 2027, with a compound annual growth rate (CAGR) of 8.4%.[3] This represents a healthy market for a solution that is in high demand by Defense agencies worldwide.

Unique Attributes

- Innovative in-situ remediation solution for legacy and insensitive high explosives.
- Reactive absorbent that significantly reduces the need for material regeneration.
- Highly effective and robust materials for rapid IHE retention and destruction.
- Over three orders of magnitude enhancement of compounds' affinity to soil for highly soluble insensitive high explosives in amended soils.
- A platform technology for soil remediation beyond munition contaminants.

Applications

In-situ remediation of legacy and insensitive high explosives, including DNAN and TNT. The material may be deployed as a platform technology to remediate anionic soil contaminants.

Stage of Development

Prototype and Proof of Concept. Prototype ready for testing in relevant use case environments.

Intellectual Property

United States Provisional Patent Application filed January 2024.

Licensing and Collaboration Opportunity

Villanova is seeking a licensee or collaborators to commercialize the invention.

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[3] *Environmental Remediation Market by Environmental Medium*…, Markets and Markets, October, 2022.