NMR Analysis of Chemical Agent Reactions with Dynamic Multifunctional Materials for a Second Skin

David J. McGarvey, Ph.D.[1] William R. Creasy, Ph.D.[2] Lev Bromberg[3], T. Alan Hatton[3]

[1]Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD, [2]Leidos, P.O. Box 68, Gunpowder Branch, Aberdeen Proving Ground, MD 21010,
[3] Massachusetts Institute of Technology, Cambridge, MA 02139

Introduction

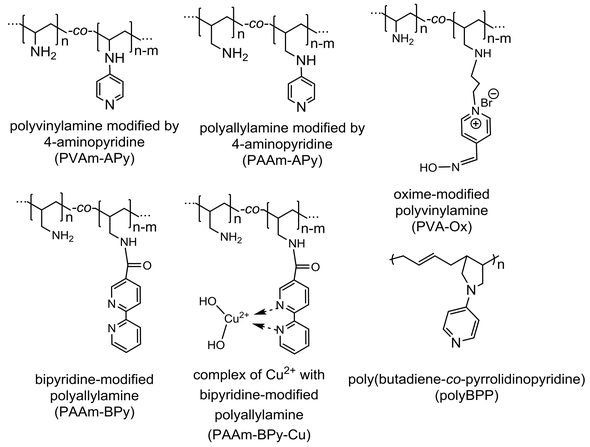
It is the goal of the Chemical and Biological Defense Program to "equip the force to successfully conduct military operations to prevent, protect, and respond to CBRN threats and effects." (2014 Department of Defense Chemical and Biological Defense Annual Report to Congress, March 2014) Warfighters may be required to operate in contaminated environments, and it is the goal of the Dynamic Multifunctional Materials for a Second Skin project to improve the survivability of the Warfighters in these scenarios by developing a suit that can detect and neutralize a chemical or biological threat. Soldiers performing operations in the field may not know they have been contaminated. They might be going through a foliage area that had been previously contaminated, something might brush off on the uniform, or they might be in a position where logistically they can't get to a decontamination area -- either because of the mission or because there isn't a decontamination setup available. We are trying to increase Soldier survivability through improved suit capabilities.

Materials are being studied for garment systems that will provide improved water and thermal transport, while also providing improved protection for the warfighter against chemical weapons agent (CWA) and biological agent permeation. Zorflex® activated carbon cloth (Calgon Carbon, Pittsburgh, PA) is a woven cloth that allows water and air permeation but has high absorption and surface area to absorb organic molecules. Performance is improved by adding reactive components to the cloth that will react with CWA to cause decontamination. Studies of cloth treated with several reactive compounds were done against the agents HD, GD, and VX, and the simulant CEES (chloroethyl ethylsulfide).

Analytical Approach

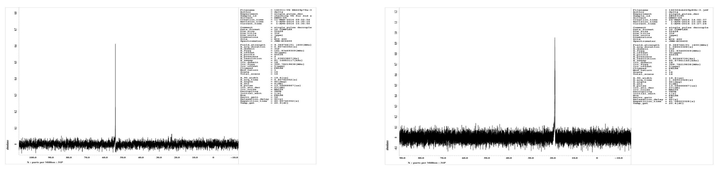
Determining the reactivity on cloth requires a number of complementary methods since the strong absorption on the cloth can prevent analysis of analytes. The reactivity was studied by using solid and liquid nuclear magnetic resonance (NMR). Studies of permeation of CWA through the fabric were studied with a novel headspace GC method using a vial in a vial. Samples of fabric were also solvent extracted to determine residual CWA and to identify reaction products using GC/MS and LC/MS. Reactions of reagents in solution were done to determine kinetics in a homogeneous system

Polymers Synthesized at MIT



Agent Testing at ECBC

Reaction of Soman (GD) with Polyvinylamine, modified with 4-aminopyridine. After just two minutes, more than 75% of the agent has been neutralized.



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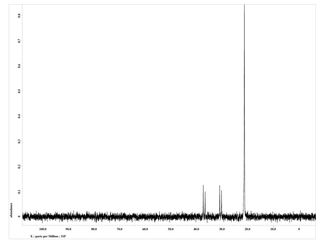
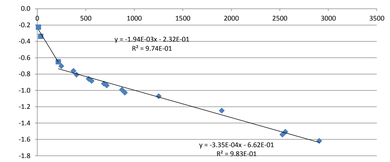


Kinetic data for the reaction of HD with polyvinylamine modified with 4-aminopyridine, measured by proton NMR. The time axis is in minutes, and the y-axis is a natural log of the ratio of HD to HD+products



Conclusion

Reactive polymers have been shown to quickly decontaminate all the major classes of chemical weapons, to include difficult-to-decontaminate materials not shown here. The ability to effectively decontaminate chemical weapons of greatly varied structure and mechanism of action is difficult to achieve in a system that lacks severely reactive materials such as strong caustic or acidic chemicals that would clearly be incompatible with placement on a soldier uniform.