Reactions on Zorflex Activated Carbon Cloth with Chemical Warfare Agents Measured Using NMR, GC, and MS Techniques

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Introduction

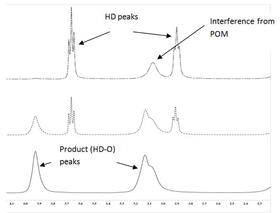
Integrated Protective Fabric System (IPFS) Program materials are being studied for garment systems that will provide improved water and thermal transport while also providing improved protection for the Warfighter against chemical warfare agent (CWA) and biological agent permeation. Zorflex® activated carbon cloth (Calgon Carbon) 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 performed against the agents HD, GD, and VX, and the simulant CEES. 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 solids and liquids nuclear magnetic resonance (NMR).

Studies of permeation of CWA through the fabric were performed with a novel headspace gas chromatograph (GC) method using a vial inside a vial. Samples of fabric were also solvent extracted to determine residual CWA and to identify reaction products using GC/mass spectroscopy (MS) and liquid chromatography (LC)/MS. Reactions of reagents in solution were done to determine kinetics in a homogeneous system. Reactions were also studied in the presence of common battlefield contaminants, in particular JP8 fuel, which can saturate the carbon cloth.

NMR Methods:

- Solids NMR using a high-speed rotor were employed to study reaction of neat CWA on solid materials.
- CWA can also be deposited on solid, solvent extracted, and then run by liquids NMR to perform quantitation of starting reagents and products.
- Reactivity of reagents was studied in solution to determine kinetics.
- Extracts are also run by GC/MS and LC/MS.
- Kinetics can be determined from multiple NMR runs on the same sample.
- Reaction was observed even when the fabric was saturated with JP8 fuel.



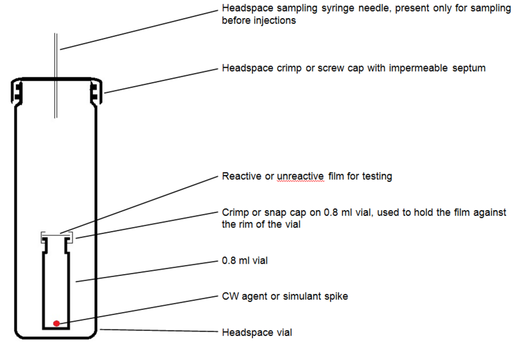
Reaction of HD with Polyoxometalate (POM) in solution.

POM on activated carbon cloth: Calgon Zorflex™ carbon film was received from Natick Soldier Research, Development, and Engineering Center (NSRDEC). POM compounds were obtained from Prof. Craig Hill and Dr. Zhen Luo of Emory University. POM was applied to the Zorflex fabric at Natick.

See also: Polyoxometalate deposition on activated carbon cloth via supercritical CO_2 for CWA decontamination, by Nick Dugan, Michelle Fasolino , Weiwei Guo, Craig T. Hill, Val Krukonis, Zhen Luo, Natalie Pomerantz, John Walker, also being presentated at this conference.

GC Methods:

The headspace vial-in-vial method has been developed for determining permeation through a film of reactive material. CWA is placed in the inner vial, and permeates through the film into the outer vial. It is sampled and analyzed by headspace GC.

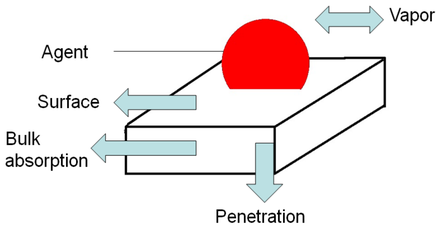


Nanoparticles on activated carbon cloth: Metal oxide nanoparticles were deposited using proprietary methods and tested for reactivity.

See also: "Redox Nanoparticle Enhanced Activated Carbon Fabrics" by Natalie Pomerantz, Nick Dugan, Wayne Lavocah, Jacquelyn Andrews, Patrick Morgan, Robert Kaiser, Michelle Fasolino, presentation at this conference.

Conclusion:

A large number of fabric systems have been tested to determine performance with CWA in ways that give consistent results. Multiple analytical methods are needed to study reactions on solid materials. The CWA can be distributed in multiple locations:



Vapor and penetration are the main immediate hazards to the wearer. But the bulk absorption and reactions raise questions about long-term safety.

More alternate spectroscopic methods are needed to determine 100% mass balance and fate of the agent.

High throughput, *in operando* methods are under consideration to obtain more information about the distribution of the CWA throughout the material under different environmental and operational conditions. Methods will be developed for acceptance testing and quality control of the materials.

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