

Universal Oxidation for CBW Decontamination: L-Gel System Development and Deployment

*M. Hoffman, A. Alcaraz, D. Shepley, J. Elliot, P. Krauter
and E. Garcia*

December 16, 1999

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

Work performed under the auspices of the U. S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

This report has been reproduced
directly from the best available copy.

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831
Prices available from (423) 576-8401
<http://apollo.osti.gov/bridge/>

Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.,
Springfield, VA 22161
<http://www.ntis.gov/>

OR

Lawrence Livermore National Laboratory
Technical Information Department's Digital Library
<http://www.llnl.gov/tid/Library.html>

Universal Oxidation for CBW Decontamination: L-Gel System Development and Deployment

**Ellen Raber
Ray McGuire**

Co-Investigators:

*Mark Hoffman, Armando Alcaraz, Don Shepley,
Jeff Elliot, Paula Krauter, Emilio Garcia,*

December 16, 1999

Universal Oxidation for CBW Decontamination: L-Gel System Development and Deployment

Ellen Raber
Lawrence Livermore National Laboratory
(925) 423-3985
raber1@llnl.gov

Ray McGuire,
Lawrence Livermore National Laboratory
(925) 422-7791
m McGuire4@llnl.gov

Co-Investigators: Mark Hoffman, Armando Alcaraz, Don Shepley, Jeff Elliot, Paula Krauter, Emilio Garcia, Lawrence Livermore National Laboratory



Objectives

The general philosophy of this work is to develop an integrated set of decontamination methods and tools that will work on the major CBW threat agents. The work includes some near term techniques that can be demonstrated within a year and implemented soon thereafter as well as longer term research objectives. It is recognized that there is a balance between somewhat less effective methods which can be demonstrated quickly and more effective ones which may require a much longer time to fruition. The optimum goal of this study is to find a single decontamination system for chemical and biological agents which is non-toxic, non-corrosive, and easily deployable.

One of the goals is to have decontamination systems that might be used by first responders as well as more complete systems to be used by specialized decontamination teams. Therefore, the overall project goal is to develop better decontamination methods that can be quickly implemented by these organizations. This includes early demonstrations and field work with companies or other government agencies who can identify implementation concerns and needs. The approach taken in this work is somewhat different than the standard military approach to decontamination. In a battlefield scenario, it is critical to decontaminate to a useful level in a very short time so the soldiers can continue their mission. In a domestic, urban scenario, time is of less consequence but collateral damage and recertification (public perception and stakeholder acceptance) are of much greater importance.

The specific objective of the LLNL work to date has been to evaluate various oxidizer systems as reagents to allow for detoxification and/or degradation to non-toxic environmentally acceptable components rather than necessitate complete destruction. Detoxification requires less reagent material than total oxidation, thereby reducing the logistic burden for a decontamination team. Since we also wanted to maximize the contact time between the decontaminating reagent and the contaminant agent, we selected gelled reagents as the primary carrier material. Gels have the additional advantage of adhering to vertical and even the underside of horizontal surfaces such as ceilings and walls. Lawrence Livermore National Laboratory,

over a period of twenty years from the late 1960's to the late 1980's, developed a series of extrudable high explosives based on the gelling of polar energetic liquids. While never going into production, this development served as an experience base for formulation, characterization and dispersal system design and fabrication. It was a logical step, therefore, to adapt this work to the gelling of aqueous oxidizers for candidate BW/CW decontaminants.

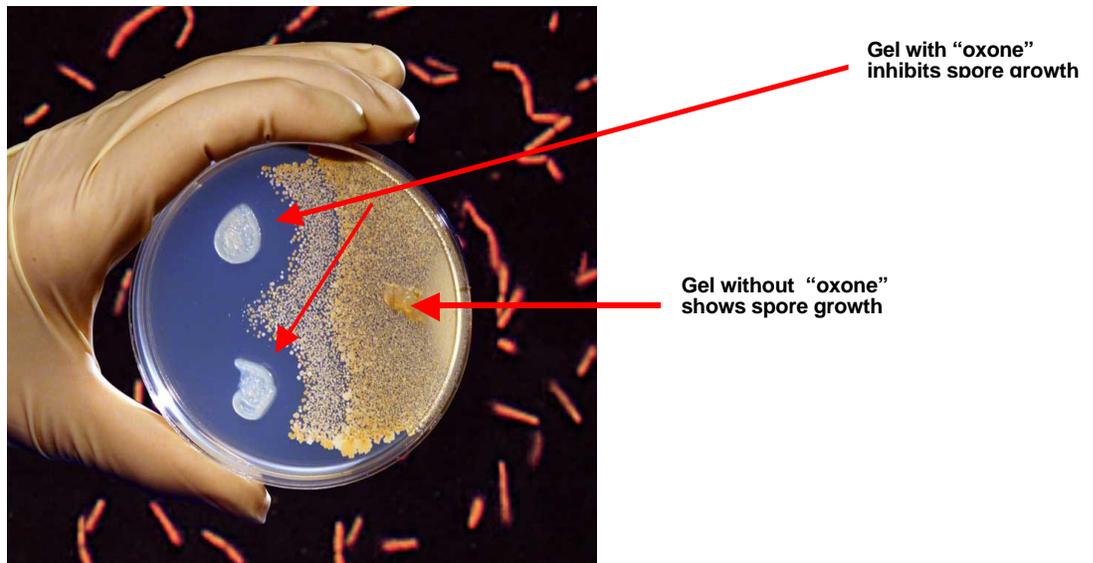
Recent Progress

Various aqueous phase oxidizers were evaluated to include potassium permanganate, peroxydisulfate, peroxymonosulfate, hydrogen peroxide as well as both acidic and basic hypochlorite. These types of materials allow for various dispersal and/or application methods, depending on the particular scenario (i.e., Outdoors, Semi-enclosed, or Indoor). These oxidizer systems can be deployed in various carriers such as compatible liquid, and water-based spray systems, or incorporated into compatible gels to meet deployment needs.

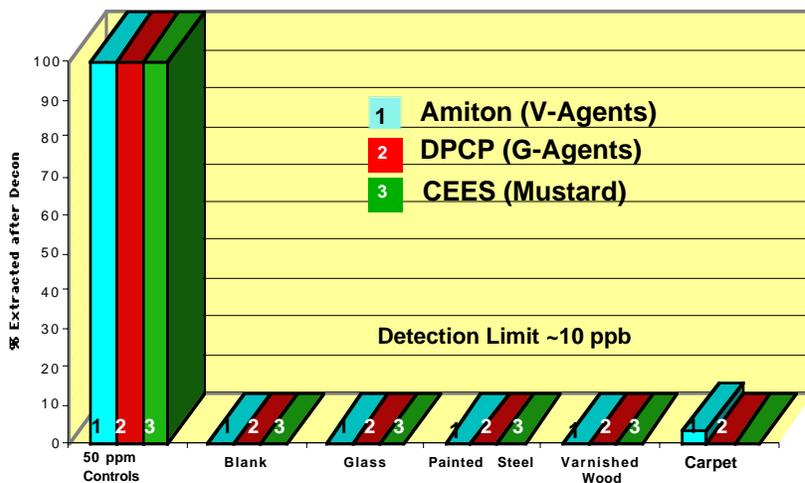
Experimental testing at LLNL has shown that RO• (peroxyl) oxidizers are the most effective for complete CW and BW decontamination. The primary decontamination system now under development at LLNL is based on the commercial oxidizer "oxone" manufactured by DuPont. The active ingredient is potassium peroxymonosulfate. Our work built on previous research at Edgewood Chemical and Biological Center (ECBC) which demonstrated the effectiveness of aqueous Oxone in decomposing both VX and Mustard type agents. While, decomposition of "G" agents occurred, the reaction was very slow because of the low pH of the system. The acidic pH is necessary, however, in the case of VX, where it leads to the protonation of the amino nitrogen and enhances the oxidation of the sulfur. Once the sulfur is oxidized the P-S bond is easily and irreversibly hydrolyzed, detoxifying the "V" agent. A similar oxidation of the sulfur in Mustard facilitates the hydrolysis of the C-Cl bonds.

LLNL has incorporated an amorphous fumed silica gelling agent into the oxone solution. Experimental testing on both surrogates and real chemical agents has further shown that only RO• (peroxyl) oxidizers are effective for complete CW decontamination. This formulation was also found to be effective for all biological surrogates/spores as well as live vaccine strains (*B. anthracis* Sterne). These types of gels have the advantage of being compatible with strong oxidizing agents as well as having the added advantage of maximizing contact time due to their thixotropic nature. The viscosity of the system can be varied depending on the application. Under shear forces they have very low viscosity, when there is no shear they become very viscous. This allows the gel to be sprayed using an atomizing nozzle and when the gel is dry (1-6 hrs) it can simply be vacuumed up and discarded. The final formulation is relatively noncorrosive (pH approx. equal to vinegar) and EPA testing on the residual materials from surrogate experiments shows residues to be non hazardous.

The L-Gel system has been tested on a variety of different materials as would be expected in an actual decontamination scenario. To date, the gelled system has been tested with a complete suite of CW (Amiton, DPCP, CEES) and BW (*Bacillus Globigii*, *Erwinia Herbicula*) surrogates on substrates of fiberglass, varnished wood, painted steel (acrylic paint), and indoor/outdoor carpet. The surrogate is placed on the test material and the reagent gel added to the surface and allowed to dry. In every case but one, no surrogate material was detected after treatment. (A small amount, ~5%, of the Amiton was detected after extraction from the carpet material.) Similarly, none BW surrogates were detected. All experiments were done with appropriate laboratory controls and standards.



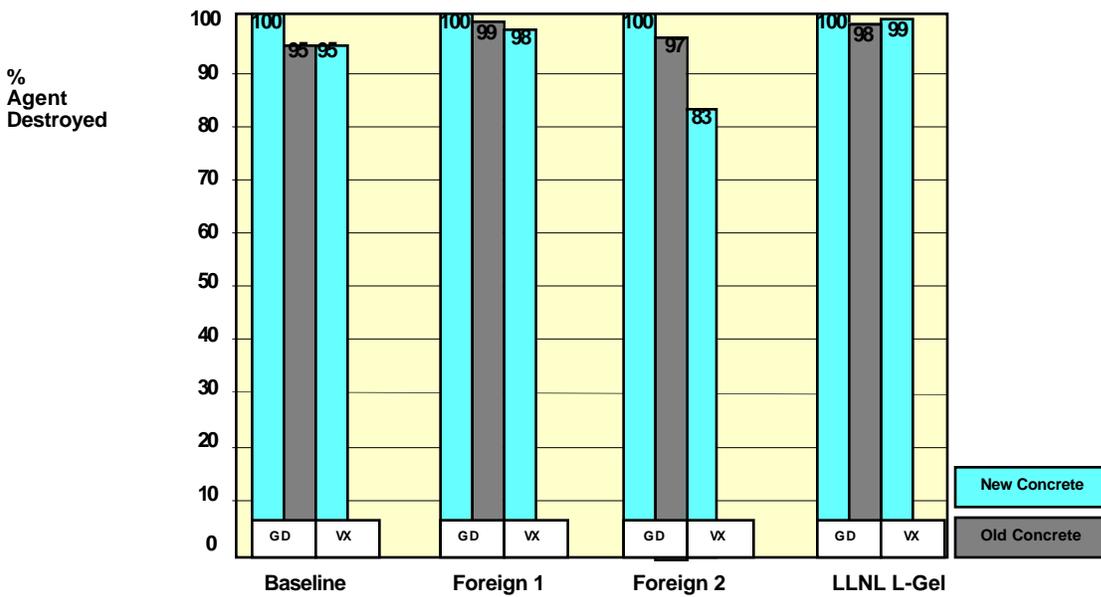
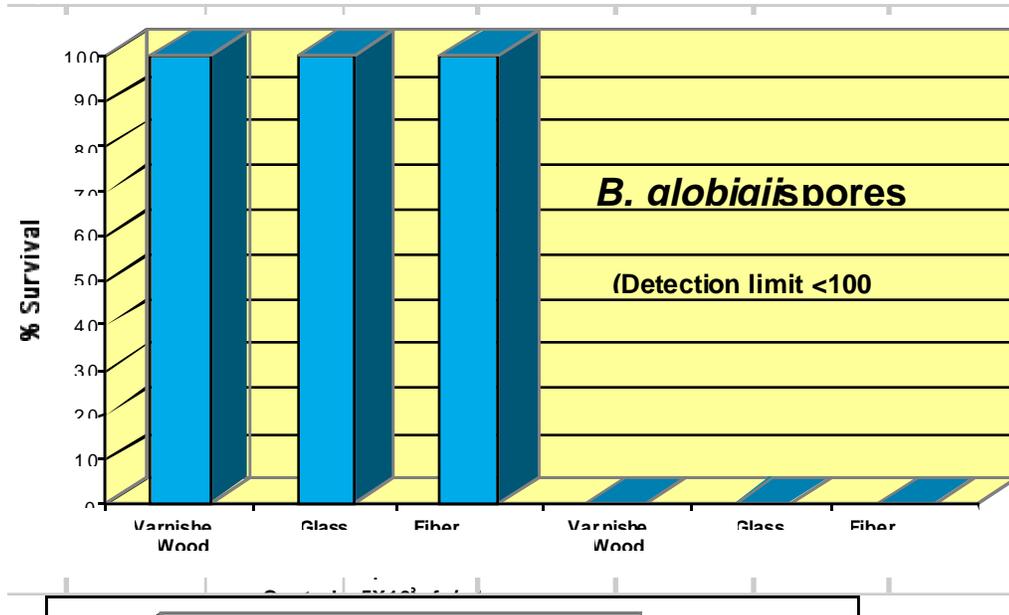
The U.S. Edgewood Chemical and Biological Center (ECBC) has been involved in the laboratory evaluation and field testing of L-Gel. Real CW agent laboratory testing has been completed by the ECBC on the above described surrogate materials. The L-Gel reduced VX, HD and GD to below detectable limits on all surfaces tested with residuals of GD found on the painted surfaces. Agent concentration used for experimental testing was 25 – 50 gms per square meter. Required gel material for complete decontamination is about 200gms/square meter at a thickness of ~5 mils. The most significant finding and advantage



of the L-Gel material is surface catalysis effected by the gelling agent on "G" agent hydrolysis. The rate of hydrolysis of "G" agents by the gelled aqueous Oxone, at pH ~2, is nearly as great as normally observed in aqueous base. This property allows the decontamination of "G" agents, "V" agents and Mustard to be effectively decontaminated with a single reagent.

L-Gel has an effective shelf life of 6 to 8 months, allowing it to be premixed. L-Gel is thixotropic (i.e., it liquefies upon vibration and solidifies when left standing). Therefore, after liquefaction by manual or mechanical shaking, it can be applied using any commercially available paint sprayer. L-Gel clings to walls and ceilings and does not harm carpets or painted surfaces. L-Gel has been independently tested against all classes of chemical agents and has been found to be as effective as the best military

decontaminants. L-GEL has also been shown to be as effective against biological materials, including spores, as the best available commercial disinfectants.



L-Gel system was more effective against VX and GD than the baseline U.S. military method (HTH)

Future Outlook

During this next year we will finalize all laboratory and field testing on live CW and BW agents. Laboratory testing is underway on live vaccine-strain biological agents to verify our surrogate findings. Similar, preliminary tests show that the L-Gel is effective against the toxin surrogate ovalbumin. Real toxin decontamination also needs to be verified in a follow-on field test.

Efforts are also underway to begin technology transfer activities for the L-Gel formulation to a commercial and/or military partner. Work continues to address potential new gas and/or aerosol phase systems to meet other technical requirements.

Experiments/Field Testing

DOD Commodity Area Field Tests, January 1999. Field experiments in the Czech Republic on VX and GD validated laboratory findings for those types of agents on both concrete and asphalt surfaces. Even though contact time was limited to 30 minutes, the L-Gel system was more effective against VX and GD than standard military methods (i.e., HTH). The L-Gel was successful sprayed using an electric paint sprayer.

Dugway Proving Ground BW Field Test, December 1999. The test objectives were to (1) develop optimal techniques for biological warfare agent stimulant contamination of six type of material surfaces, (2) develop techniques for sampling/recovery of BWA stimulant contamination of materials surfaces, and (3) compare the ability of several decontamination materials to inactivate a BWA stimulant. LLNL tested the L-gel formulation and results are still pending.

Citations

"Oxone Based Decontamination" Raymond R. McGuire, et al., Proceedings of International Workshop on Decontamination in a Chemical or Biological Warfare Environment, Durham, UK, 7-9 September, 1999

"Oxidative Decontamination" Raymond R. McGuire, et al., NATO/ISTC Advanced Research Workshop on "Environmental Aspects of Converting CW Facilities to Peaceful Purposes and Derivative Technologies in Modeling, Medicine and Monitoring" KLUWER Academic Publishers, 1999, (in press)

"The Results of Agent Testing of a Decontaminating Gel", Proceedings of the 1999 Joint Service Chemical and Biological Decontamination Conference, Nashville, TN, June 8-10, 1999, Raymond R. McGuire, et al (in press)