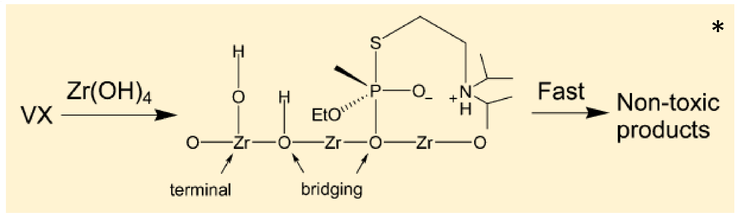
Optimization of a Zirconium Hydroxide Slurry Decontaminant Using Experimental Design

Joseph Myers, Jay Davies, Matthew Shue, and Gregory Peterson
Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD

Background

Zirconium Hydroxide ($Zr(OH)_4$) is a reactive solid metal oxyhydroxide found in filter materials that rapidly hydrolyzes chemical warfare agents into non-toxic by-products*.

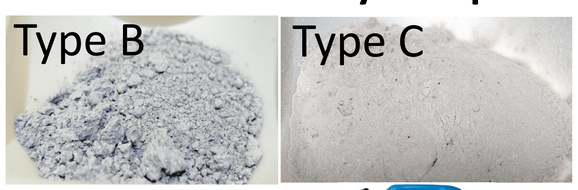


The Decontamination Sciences Branch, working in collaboration with the CBR Filtration Branch have developed a sprayable decontaminant formulation for material surfaces using two types of $Zr(OH)_4$ (B and C), water, and kerosene as the carrier liquid.

Objective

Experimental design was used to optimize the mixture of the components to enhance decontaminant efficacy and maximize the efficiency of the evaluation. A single decontaminant formulation could be deployed to the warfighter at a lower cost than several decontaminants (one formulation for each contaminant) resulting in better logistics.

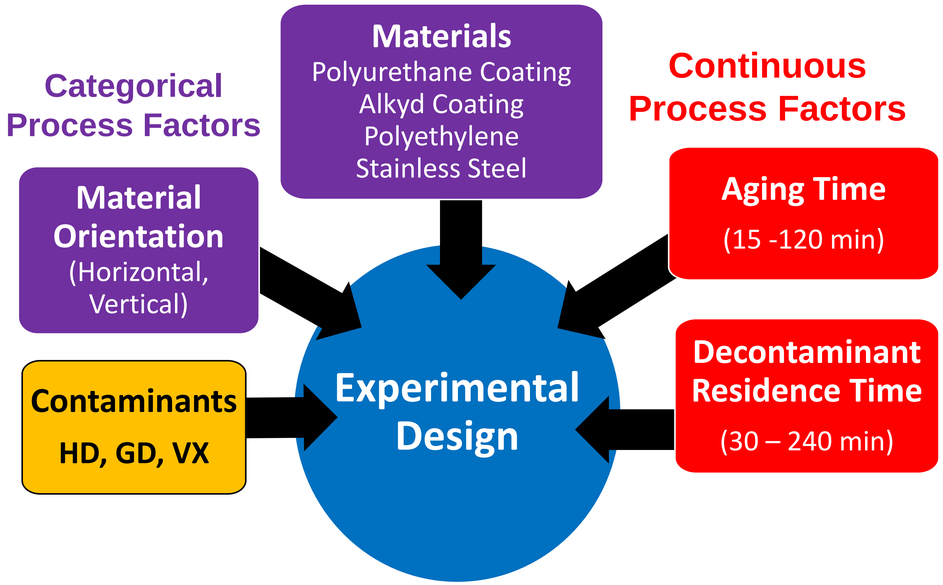
Decontaminant Slurry Components



Hydration Kerosene

Approved for Public Release

Experimental Design

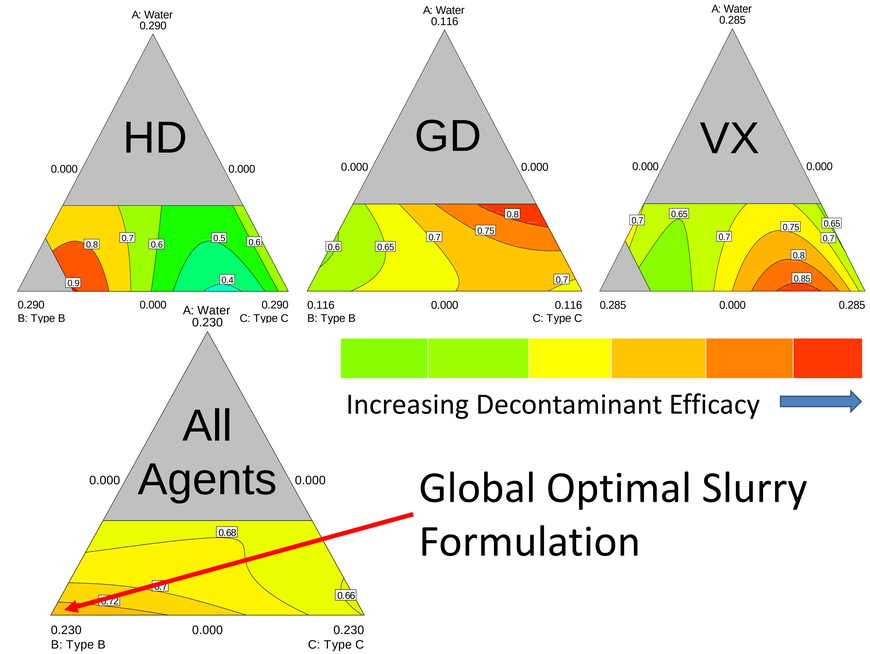


Experimental design, also known as design of experiments (DOE), uses statistical modeling to improve the efficiency of an evaluation. A mixture-process experimental design was used to build a predictive model for each of the 3 contaminants (HD, GD, and VX). The models included terms for the 4 components of the $Zr(OH)_4$ decontaminant slurry, 2 categorical process factors (materials and orientations), and 2 continuous process factors (aging and decontaminant residence times).

Five experimental sessions were required to generate the predictive performance models for all tested contaminants. A Multi-Objective Optimization was performed using statistical software packages (SAS JMP©, DesignExpert©) to find a global optimal formulation that provided the best overall performance against all three contaminants on all materials and across all process conditions.

Results and Conclusions

- The Global Optimal Slurry Formulation was predicted via statistical modeling to provide optimal decontaminant efficacy against all three contaminants.
- The performance of the predictive models used to determine the formulation was experimentally confirmed.
- DOE produced MORE information than a full-factorial evaluation of the decontaminant technology for a fraction of the cost. *(DOE = ~96% less experimentation than full factorial)*
- The Decontaminant slurry had an increased efficacy on sorptive materials (coatings) at short aging times (limits sorption into the material) and increased efficacy with long decontaminant residence times (increased time to react with and detoxify the contaminants).



References: *Bandosz, et. al., Reactions of VX, GD, and HD with $Zr(OH)_4$: Near Instantaneous Decontamination of VX. J. Phys. Chem. C 2012, 116, 11606-11614, 2012.

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