

Chemical Warfare Agent Simulants Project

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Draft for Discussion



Project Overview

- Background
- Purpose/Objective
 - Category 1. Adsorption CWA simulants
 - Category 2. Permeation CWA simulants
- Permeation Study Details
- Potential Benefits



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Background

- NIOSH Public Meeting held in April 2001, some respirator manufacturers requested that NIOSH identify simulants for CBRN respirator standards.
- International Safety Equipment Association (ISEA) letter to NIOSH, January 22, 2002 requested NIOSH develop surrogate test agents.
- Although large number of studies on the permeation effects of CWA simulants through barrier materials, inadequate data available to derive a reliable correlation between the simulants and CWA.
- Two categories of Simulants being addressed: 1) Adsorption on activated carbon. 2) Permeation through barrier materials.
- The correlation coefficient of a simulant to a CWA may be different on another barrier material (Correlation Coefficient Material Dependent).



Background (Continued)

- Reviewed database, developed matrix; simulants vs. barrier material vs. agent.
– Screening Tool
- SBCCOM Agent Simulant Knowledge (ASK) Advisory Office identifies past work with simulants.
- ASK search revealed 8 reports that can be made available on request.
- Ten permeation simulants were identified in the 8 reports revealed from the ASK Advisory Office literature search:
 - CEES - 2-Chlorethethyl Sulfide
 - CEMS - 2-Chloroethylmethyl Sulfide
 - CPTA - 3-Chloropropylthiolacetate
 - DBS - Dibutyl sulfide
 - DEEP - Diethylethyl Phosphonate
 - DFP - Diisopropylfluro Phosphonate
 - DIMP - Diisopropylmethyl Phosphonate
 - DMHP - Dimehtylhydrogen Phosphonate
 - MAL - Malathion
 - MS - Methyl Salicylate



Project Purpose / Objective

- Category 1; Adsorption Simulants:

- Purpose:

Identify a chemical compound(s) that simulates the adsorption of Sarin (GB) nerve agent and Sulfur Mustard (HD) blister agent on activated carbon.

- Objective:

To identify through research chemical compound(s) that can be used as adsorption simulants and to identify pertinent reports that are available to the public.



Project Purpose / Objective (continue)

- Category 2; Purpose of Simulant Permeation Study:
Through research and testing, identify chemical compounds to simulate the penetration and permeation effects of GB and HD through barrier materials.
- Objective:
Identify simulants and laboratory procedures that can be used by manufacturers for estimating GB and HD blister agent permeation through barrier materials used to manufacture respirators.



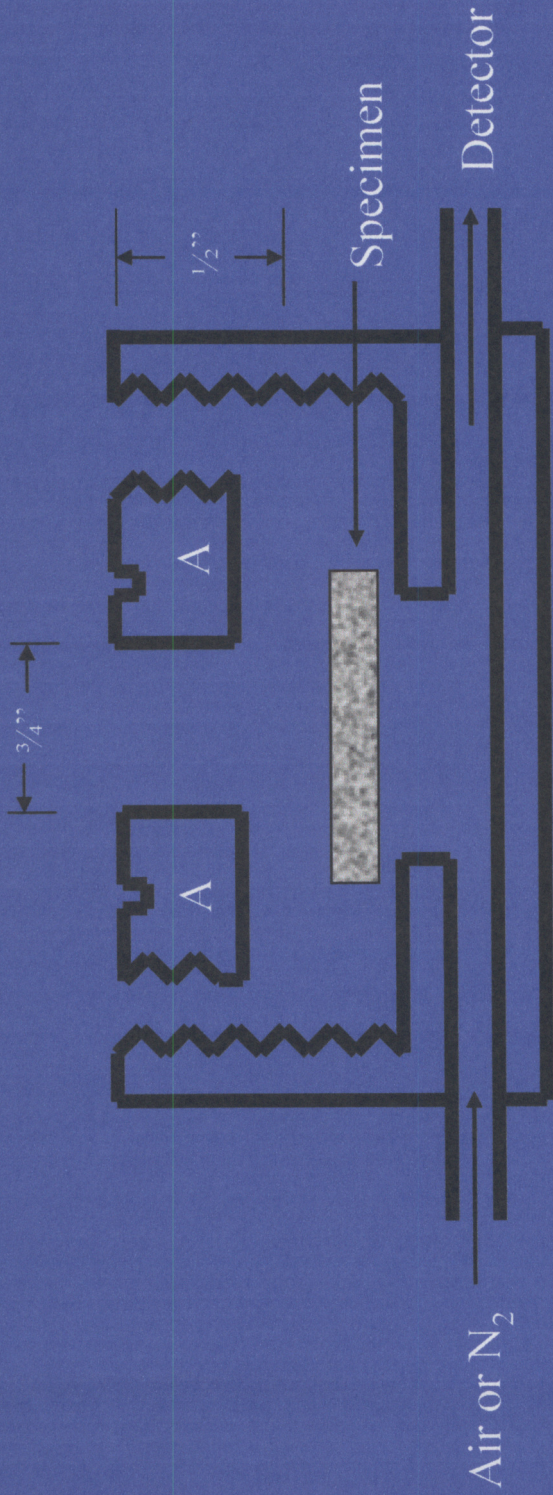
Simulant Permeation Study Details

1. Identify 2 simulants for GB and HD for 3 different barrier materials.
2. Design experiment and perform liquid permeation tests on the 3 barrier materials and solubility tests with the simulants.
3. Perform solubility tests with GB and HD on the 3 barrier materials.
4. Perform permeation tests on the 3 barrier materials with GB and HD.
5. Write a NIOSH Guidance Document that describes test procedures, simulants and results of agent permeation tests.

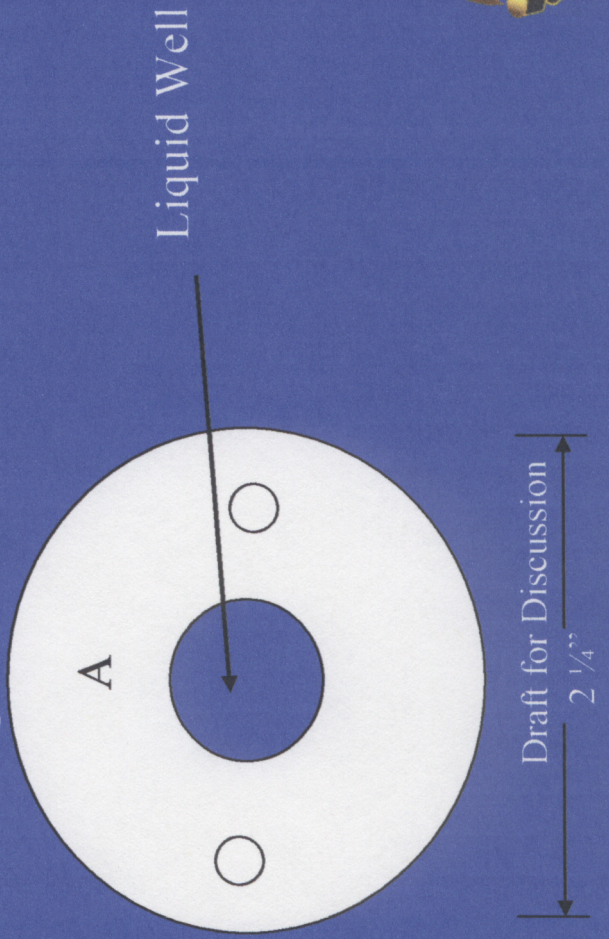


Prototype Liquid Permeation Cell

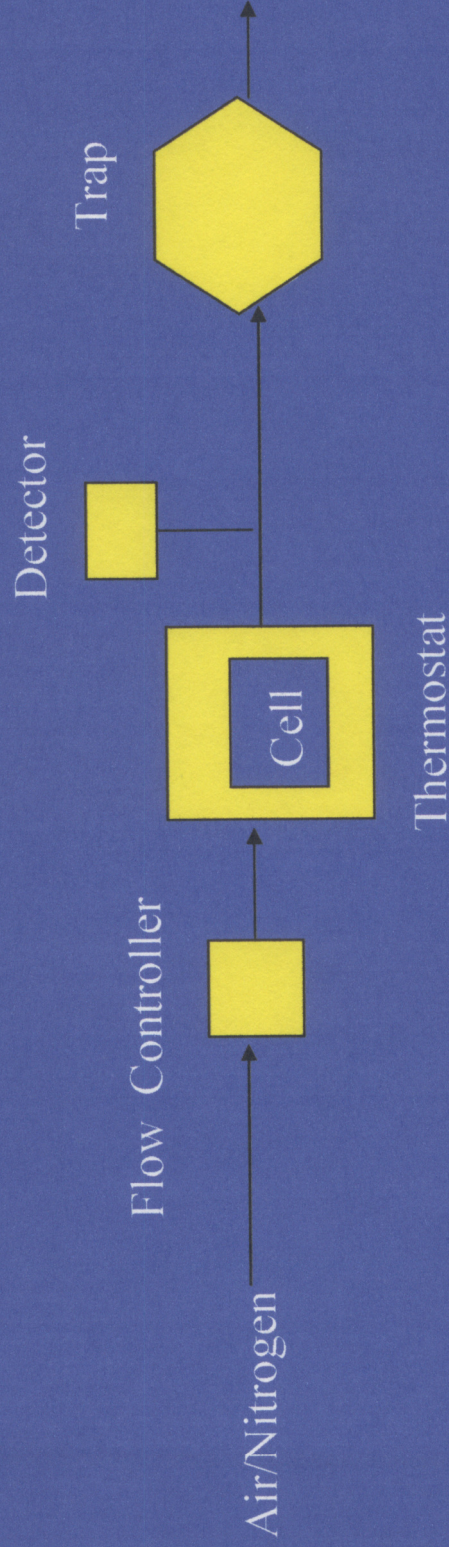
Side View



Top View



Permeation System



Material Permeability (P)

$$P = D \cdot S \cdot L^{-1}$$

D = f (Molecular Size, Concentration, Temperature)

S = f (Chemical Interaction, Concentration, Temperature)

D = Diffusion Coefficient

S = Solubility Coefficient



Potential Benefits of Simulant Permeation Study:

1. Provides data so manufacturers can make a determination on potential pretest simulants.
2. Assists manufacturers in their decision of selecting barrier materials based on scientific information; reducing product development times and costs.
3. Expedites availability of new respirators and materials technology for the users.



Summary/Conclusion

- To identify through research chemical compound(s) that can be used as adsorption simulants and to identify pertinent reports that are available to the public.
- Identify simulants and laboratory procedure that can be used by manufacturers for estimating CWA permeation through barrier materials.
- Write a draft NIOSH Guidance Document that describes test procedures, simulants and results of agent permeation tests.
- NIOSH or SBCCOM will not guarantee the simulants identified will work on all materials and their correlation coefficient to CWA.
- Passage of manufacturer's pretest with the simulant does not guarantee passage of the official NIOSH certification testing.



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