Chemical Warfare Agent (CWA) Simulant Project

Mr. Frank Palya, NIOSH
PI: Dr. Donald Rivin, RDECOM
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Background

- April 2001 NIOSH Public Meeting, 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

- Literature search revealed studies on the permeation effects of CWA simulants through barrier materials, however, inadequate data available to derive a reliable correlation between the simulants and CWA

- Jun 02 CWA Simulant Project began [Phase I]
Accomplishments of Phase I

1.) Developed an inexpensive permeation system with a new cell design for testing both hard and soft barrier materials up to at least 1 cm thick.

- **Goal:** Low cost, rapid, simulant screening method for determining agent barrier performance

- Flooded Cell Technique for Testing Liquid Permeation Through Nonporous Barrier Polymers which was incorporated into the interim NIOSH Test Method
NIOSH Test Method Technical Details

Permeation Test System

Air / Nitrogen → Flow Controller → Perm. Cell → Detector → Analog to Digital Acquisition Board → Trap → Thermostat → Computer

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Liquid Permeation Cell Component

Side View

Teflon Gasket

Agent

Specimen

Air or N₂

Detector

Top View

Liquid Well

2 ¼”
Permeation Cell Photographs
Accomplishments of Phase I (Cont.)

2.) Based on correlation, identified four (4) simulants that can be used to estimate CWA permeation through barrier materials:

- Nominal HD Simulants
  DCH - 1,6-Dichlorohexane
  CEPS - 2-Chloroethyl phenyl sulfide

- Nominal GB Simulants
  DEMP - Diethyl methanephosphonate
  DIMP - Diisopropyl methylphosphonate
The Selection of CWA Simulants Based on:

Testing of 3 Materials:
The test materials with specimen thickness selected for convenient breakthrough time were:

Butyl Rubber: 12 mil
EPDM: 30 mil
Silicone Rubber: 125 mil

Note: Permeation and immersion testing was conducted on seven reinforced, cured elastomer compounds known to span a wide range in barrier properties. These 3 were chosen as standard materials for comparative testing with CWA (HD, GB) and simulants.

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Accomplishments of Phase I (Cont.)

3.) Developed an Interim NIOSH Test Method to be made available to stakeholders

**Test Method:**

- Describes required equipment, procedures, and data analysis techniques; Also, will include mechanical drawings of Permeation Cell

- Interim Test Method will be made available in Draft form on NIOSH/NPPTL WebSite in Dec 2003

- Test Method will be published in the future as an official NIOSH Numbered Document
Permeation Test
Phase II

Primary Goals

• Improve estimation reliability of Flooded Cell Technique by testing additional simulants with other barrier materials

• Determine quantitative relationship between Flooded Cell Technique and traditional test loading (5-10 g/m²)

• Determine CWA/simulant sorption/desorption of representative barrier materials

• Identify critical properties of permeants and barrier materials that control permeation

• Develop capability to predict barrier permeation based on available chemical and physical properties of barrier polymers and permeating molecule
Potential Benefits of CWA Simulant Project (Phases I and II) will:

1. Assist manufacturers in selection of barrier materials based on scientific information and reduce product development time and cost

2. Expedite availability of new respirators and materials technology for the users

3. Determine quantitative relationship between Flooded Cell Technique and traditional test loading (5-10 g/m²)

4. Determine CWA/simulant sorption/desorption of representative barrier materials

5. Identify critical properties of permeants and barrier materials that control permeation
Summary/Conclusion

- Developed a rapid, relatively low cost laboratory procedure that can be used to estimate CWA permeation through barrier materials

- Identified four (4) CWA simulants for permeation testing

- Wrote an Interim NIOSH Test Method that describes equipment, test procedures, and data analysis techniques: Draft form will be made available on NIOSH/NPPTL WebSite in Dec 2003

- Initiated Phase II of the CWA Simulant Project

- NIOSH or RDEC does not guarantee that simulants identified will be suitable for all materials, nor does passage of manufacturer’s pretest with a simulant guarantee passage of the official NIOSH certification testing
Liquid Permeation of EPDM With DIMP

- **Signal (V)**
  - 0.3
  - 0.2
  - 0.1
  - 0.0

- **Time (s)**
  - 0
  - 10000
  - 20000
  - 30000
  - 40000
  - 50000

**Key Elements**

- **$T_{1/2}$**: Time at $1/2$ the steady state penetration is reached.
- **$T_s$**: Beginning of steady state penetration.
- **$T$**: Time at Initial Break.

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PERMEATION in BUTYL RUBBER (12 mil)