Threat Agent Science Capability Area CBIS 2007

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Threat Agent Science CAPO

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Agent Fate enhances predictive tools with data, quantifying the fate of chemical agents within operationally significant climates and surfaces.

International Partners: CZ, POL, NLD, UK, and SGP

Wind Tunnel Testing

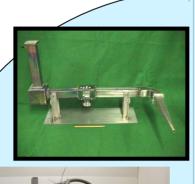
Measures evaporation of agent from surface at realistic climactic conditions. Main data input stream for predictive models

Uses combinations of vapor sampling & gravimetric analysis

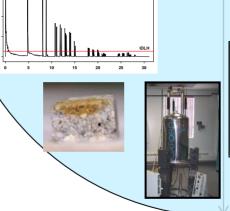
Agent/Substrate Interactions

Agent/Substrate interactions are critical component to determinations of fate.

Studies use highest fidelity methods including NMR, SPME, vapor resurgence, extractions quantitative imaging and fundamental property measurements











6 - 168

1800 -3600

4

Outdoor Testing

Validates model developed with wind tunnels data

Provides "ground truth" of behavior in environment

Modeling

Improves hazard prediction tool accuracy

Transitions information to warfighter in a usable format.



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Physiological Effects CWA Operational Exposure Hazard Assessment Research

Purpose and Goal: Operationally-relevant health effects of exposure to the class of chemical warfare agents (CWAs) to include those termed "Non-Traditional Agents (NTAs)".

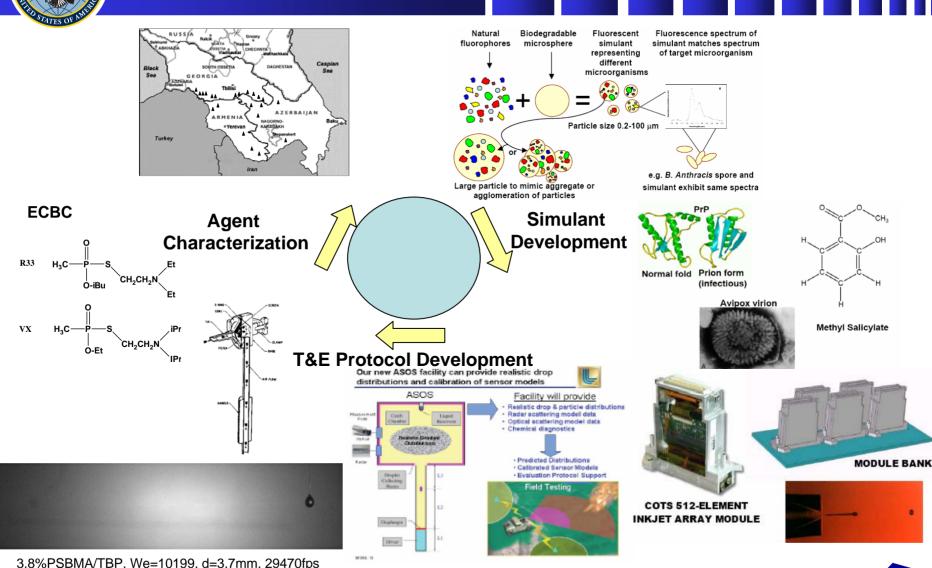
Integration Studies Exposure Studies Route Extrapolation • Inhalation dose-response Human effects Percutaneous contact o:15:0 Mission/Hazard Profiling 0:05:00 0:07:30 0:10:00 0:12:30 Time (minutes) 0.2 **PAYOFFS** 0.06 ²⁰ Exposure Time (min) and Standards **Health Effects** • JPID Sub-Clinical effect Delayed/Persistant Toxicity Repeated exposures • JFM/JOFF

- Operational Requirements
 - FM 3-11.9
 - AFMAN 1026-02
- Operability Modeling

 - Agent Fate Link
- Reachback Expertise

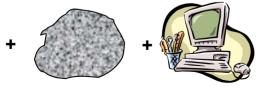


Agent Characterization/ Simulant Development





Computational Chemistry provides fundamental understanding



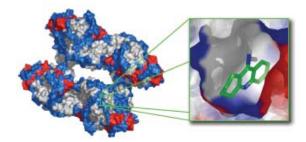
CWA

solid adsorbent quantumchemical

• interaction parameters
• chemical properties

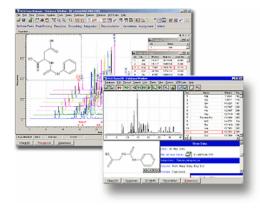
• environmental stability

modeling
Intelligent Design of
Materials & Simulants

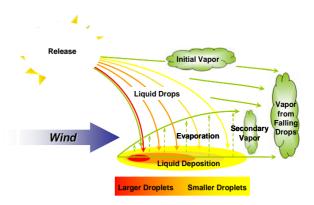


Tetramer of human acetylcholinesterase

Tacrine bound in one active site of acetylcholinesterase



In-silico simulant selection For CWA T&E



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We provide data, models, and reachback expertise coordinated across the community

