Laboratory to Field: Characterizing Decontamination Efficacy Through Exposure Assessments

8 May 2018

Brent Mantooth
Decontamination Sciences Branch
Edgewood Chemical Biological Center (ECBC)

U.S. Environmental Protection Agency (EPA) International Decontamination Research And Development Conference
Objective: Compare the analysis of Efficacy with hazard mitigation for vapor exposure

- Identify the types of measurements to characterize decontaminants
- Demonstrate how to measure vapor source terms and conduct vapor exposure assessments
- Demonstrate correlation of efficacy to vapor source terms
- Through this process see how to progress from lab testing to understanding exposure in the field
Assessing Decontamination Efficacy
Is it Clean Enough?

Example: Decontaminant with 99.7% efficacy used after chemical contamination (e.g., VX).

Would these personnel exhibit acute health effects during their mission if their vehicle, weapons, and radios were just decontaminated?

Could you return an airport to use?
### Purpose of Measurements

<table>
<thead>
<tr>
<th>Metric</th>
<th>Objective</th>
<th>Measurement &amp; Analysis</th>
<th>Context</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Material Efficacy</strong></td>
<td>How much Agent Remains after Decon</td>
<td>Removal of Agent from a Material</td>
<td>Laboratory</td>
</tr>
<tr>
<td></td>
<td>How much Agent you Started With</td>
<td></td>
<td>GD on CARC Panel</td>
</tr>
<tr>
<td><strong>Health Effects</strong></td>
<td>Do not Exceed Health Effect Toxicity Levels</td>
<td>Returning asset to use will produce no negative health effects</td>
<td>Operational</td>
</tr>
<tr>
<td></td>
<td>e.g., toxicity levels: IDLH, AEGL 3 (4 hr, 0.0052 mg/m³)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Objective**

99.9% Efficacy!

**Measurements & Analysis**

- Measure source terms
- Perform exposure assessments

**Context**

- **Laboratory**
  - GD on CARC Panel
- **Operational**
  - Source Term Scale-up
  - Exposure Assessment

What is the correlation of efficacy to preventing health effects?

---

**How clean is clean enough?**

…it depends on what you want to do with the decontaminated materials.
Challenges with Material Decontamination: Transport Limited Rates

- Longer duration contamination allows more absorption
- The decontaminant should remove the absorbed agent from the material to minimize vapor emission or contact transfer
- The decontamination process is rate limited by agent transport to the material surface, or the ability of the decontaminant to penetrate the material*
- The rate limiting process is the primary difference between liquid reactor efficacy (reactivity) and material efficacy (transport)**

Vapor Test

**Output**: Vapor Source Term (mg agent m\(^{-2}\) min\(^{-1}\))

Enables health effect analysis

---


**ECBC-TR-1383 (available at [www.dtic.mil](http://www.dtic.mil))**
**Testing to Vapor Requirements**

- **Vapor Concentration** (mg/m³)
  - Measure Concentration in Test Apparatus

- **Decon Testing**
  - Measure Source Term

- **Exposure Assessment**
  - Health Based Evaluation
  - Dose (mg min /m³)

- **Vapor Concentration** (mg/m³)
  - Assume exposure duration
  - Toxicology Requirement
  - Health effect for specified population

**ASTM D5116 shows that chamber concentrations ≠ exposure concentrations**

- ‘Asset’ in test chamber

- Missing Component for ‘Clean Enough?’
- Context of asset(s) in a specific environment
Vapor Source Terms & Dispersion Models

**Source Term**

- **Vapor Source**
  - Industrial - Smoke stack
  - Military - Vehicle

<table>
<thead>
<tr>
<th>Source Term</th>
<th>Industrial - Smoke stack</th>
<th>Military - Vehicle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source Emission Rate</td>
<td>1000 g/min H₂O</td>
<td>1 mg/min VX from vehicle</td>
</tr>
<tr>
<td>Source Flux (rate/area)</td>
<td>1 g m⁻² min⁻¹</td>
<td>Paint: 1 × 10⁻³ mg VX m⁻² min⁻¹</td>
</tr>
</tbody>
</table>

- The vapor source term is a description of how chemicals are introduced into an environment determined by testing* or modeling**
- Exposure is a result of how source terms are carried from asset to personnel via *transport & dispersion* in a vignette

**Vignette** – Description of environment, asset, and personnel during mission

*ECBC-TR-980 (available at [www.dtic.mil](http://www.dtic.mil))


**TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.**
Exposure Durations: Acute Through Chronic

- Toxicological endpoint of interest drives timing and approach to collecting source terms for exposure assessment
- Timing of contamination, decontamination, and exposure significantly influence efficacy and source terms
Focus: Asset/Material vs. Personnel

- Material Efficacy (e.g., 99.9%) focuses on a material response in a laboratory context.
- Typically, decontamination assessments have focused on evaluating individual assets to toxicology-based levels.
- Health effects result from the aggregate dose due to interacting with all contaminated materials in a vignette during the mission.
- Exposure is a function of how personnel interact with all contaminated items.
- Key Change: Move focus from assets to how personnel interact with multiple assets in the context of their use of the assets.
- For simplicity, next demonstrations will focus on a single asset.
**Agent:** HD, 1 x 2 µL droplet applied to material (2.8 mg HD)

**Contamination Age Time:** 1 h, 12 h duration

**Material:** Polymer

**Decontamination:** Soapy Water Wash and immerse panel in decontaminant for 30 min

Contamination Duration establishes the *initial condition* for the agent distribution and how much agent is absorbed

---

**Applied Mass:** 2.8 mg HD

<table>
<thead>
<tr>
<th>Time</th>
<th>Mass Absorbed (mg)</th>
<th>Efficacy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 h</td>
<td>0.712 mg HD</td>
<td>74.6%</td>
</tr>
<tr>
<td>12 h</td>
<td>1.815 mg HD</td>
<td>35.2%</td>
</tr>
</tbody>
</table>

**Soapy Water Wash**

**Decon 30 min**

<table>
<thead>
<tr>
<th>Time</th>
<th>Mass Absorbed (mg)</th>
<th>Efficacy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 h</td>
<td>0.208 mg HD</td>
<td>92.5%</td>
</tr>
<tr>
<td>12 h</td>
<td>1.245 mg HD</td>
<td>55.5%</td>
</tr>
</tbody>
</table>
• Efficacy changes with age time and indicates how much agent remains
• Vapor source term magnitude and time evolution are influenced by the distribution of the agent in the material
From Testing To Health Effects: Source Term Measurement

Test Methods
TOP 8-2-060
ECBC-TR-980

Vapor Source Term for a 2” diameter panel
Contaminated for 60 min
Decontaminated for 30 min
(92.5% Efficacy Case)

Contamination
(A) Liquid-to-air (evaporation)
Liquid wetting
Liquid-to-material (sorption)
Air
Material

Decontamination
(B) Liquid-to-material (sorption)
Dissolution
Dissolved agent sorption
Penetrating Decontaminant
Sorption
Penetration
Extraction
Agent
Decontaminant
Air
Material

Post-Decontamination
(C) Hazards to unprotected personnel
Vapor Emission
Contact Transfer
Air

Vapor Microchamber

Test Methods: Measure Source Terms

Source Term
Scale-Up

Transport & Dispersion Modeling

Vignette

Toxicity value

Operational Health Effect

Experimental Data

Vapor Emission Rate (mg/min)

0 10^-2 10^-3 10^-4

Post-Decontamination Time (min)

0 500 1000 1500

Dose
1. Define asset of interest (HMMWV)
2. Determine surface area of each material on HMMWV
3. Assume all surface area is contaminated to 10 g/m²
4. Use Vapor Composite System Calculation in TOP 8-2-060 to calculate Asset Emission Rate (ER_{Asset})
5. Specify Vignettes

Scale-Up
How to convert laboratory vapor data from a 2 inch panel to represent a full-scale asset/vehicle

Exposure Dose Changes with Vignette

- Same asset, same decon, different vignette = different dose, different health effect
- Operational health effects vary with the defined operation (combination of material effects and operational inputs)

---

### “The Answer”

<table>
<thead>
<tr>
<th>Vignette</th>
<th>Source Term</th>
<th>Top 8-2-060</th>
<th>Top 8-2-061</th>
<th>SD2ED (ECBC-TR-980)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Wind Speed (m/s)</th>
<th>N/A</th>
<th>N/A</th>
<th>1</th>
<th>10</th>
<th>1</th>
<th>10</th>
<th>1</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shelter</td>
<td>N/A</td>
<td>N/A</td>
<td>Ct</td>
<td>Ct</td>
<td>Ct</td>
<td>Ct</td>
<td>Ct</td>
<td>Ct</td>
</tr>
<tr>
<td>Cargo Bay</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Outdoor A</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Outdoor B</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Outdoor C</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Vapor Dose (mg min m⁻³)
- Ct₅₀Lethal
- Ct₅₀Severe
- Ct₅₀Mild
- Ct₀₁Mild

---

Transport & Dispersion Modeling

Dose

Operational Health Effect

Vignette

Operational Dose

Toxicity value

---

Technology Driven. Warfighter Focused.
Exposure & Health Effects are a Response to Many Factors

Material Hardness
- Resistance to agent sorption
- Agent spread on material

Decontaminant Performance
- Chemical reactivity
- Material penetration

Material Effects

Operational Inputs
- Contamination density
- % of asset contaminated

Timing
- When decontamination occurs (min, hours, days) after contamination
- When exposure occurs (min, hours, days) after decontamination

Source Terms

Vignettes
- Agent spread on material
- Environment: temperature, wind speed, etc.

Exposure calculation

Dose

Health Effect

Connects and accounts for material effects and operational inputs

- Exposure is a ‘systems’ level output and is influenced by multiple inputs
- Health effects are a convolution of decontaminant performance, material hardness, and operational inputs
- The only factor a decontamination technology/process influences is the ability to Reduce source terms
Conclusions

- Material decontamination is rate limited by transport, typically by rate of agent transport to material surface.
- Efficacy changes with test conditions (such as contamination duration).
- The ability to determine health effects requires the measurement of source terms and exposure assessments.
- The same assets used in a different vignette/context may produce different exposures.
- Efficacy is a measure of decontaminant performance in the context of individual materials.
- “Is it Clean Enough?” requires Source Term measurement and Exposure Assessments.
Acknowledgements

**DTRA Funding**
John Hannan
Eric Lowenstein
John Cusano

Charles Bass
Glenn Lawson
Mark Morgan

**Research Team**
Mark Varady, Tom Pearl, Stefan Bringuier, Shawn Stevenson, Joe Myers, Stefanie Smallwood, Janlyn Eikenberg, Michelle Sheahy, Mandy Schenning, Larry Procell, Jennifer Piesen, Brian Luthardt, Michael Chesebrough, Dave Gehring, Jill Ruth, Matt Shue, Patrick Riley, Janet Fouse

**DUSA-TE**
Decon CAPAT

Dr. Stuart Notman

Dr. Sharon Reutter-Christy (ECBC Op. Tox)
Doug Sommerville (ECBC MS&A)
Dr. Stephen Channel (Air Force)
Dr. Candace Coyle (ECBC Eng.)
Monicia Hall (ECBC Eng.)

Kevin Ulmes

JRO: Scott Robinson, Greg Marshall

JPEO-CBD – Mark Thomas
JPM-P – Erica Howell
DoD Public Release Reports (available via https://www.dtic.mil)

- ECBC-TR-980 – Chemical Contaminant and Decontamination Source Document 2nd Edition Test Methodologies
- ECBC-TR-1384 - Interpretation of Liquid Reactor Results
- ECBC-TR-1383 - Relationship of Liquid Reactor to Material Testing

Peer Reviewed Literature

- *Journal of Physical Chemistry B, 2018*, 122, 2155 – Multi-species transport related to removing contaminants from materials
- *Industrial & Engineering Chemistry Research, 2017*, 56, 10911 - Agent to Simulant Relationships for vapor emission
- *Industrial & Engineering Chemistry Research, 2016*, 55(11), 3139 – Material decontamination dynamics for VX from a polymer
- *ACS Appl. Mater. Interfaces, 2014*, 6, 16289 – Chemical depth profiling in coatings