



Laboratory to Field: Characterizing Decontamination Efficacy Through Exposure Assessments



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TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

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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?

Metric

Material Efficacy

How much Agent Remains after Decon

1-

How much Agent you Started With

Health Effects

Do not Exceed Health Effect Toxicity Levels

e.g., toxicity levels: IDLH, AEGL 3 (4 hr, 0.0052 mg/m³)

Objective

Removal of Agent from a **Material**

Returning asset to use will produce no negative health effects

Measurement & Analysis

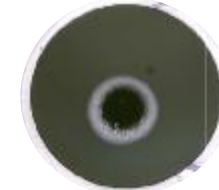
Material Extraction

99.9% Efficacy!

- Measure source terms
- Perform exposure assessments

Context

Laboratory



GD on CARC Panel

Operational



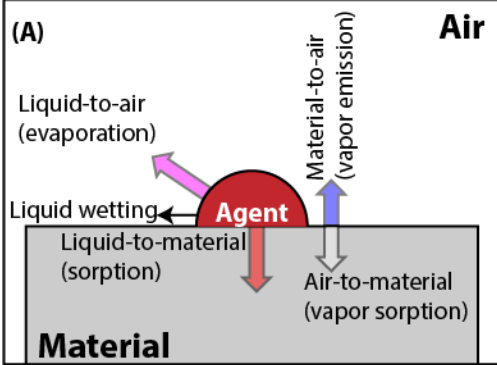
Source Term Scale-up
Exposure Assessment

What is the correlation of efficacy to preventing health effects?

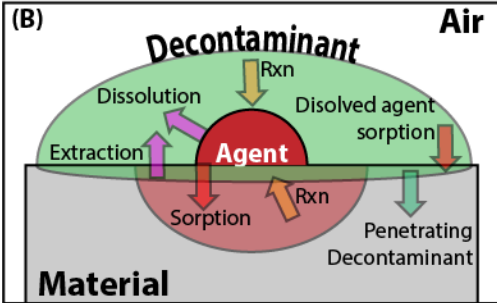
How clean is clean enough?

...it depends on what you want to do with the decontaminated materials.

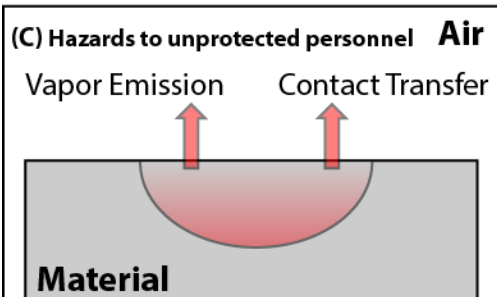
Contamination



Decontamination



Post-Decontamination



Material Efficacy

- 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 ($\text{mg agent m}^{-2} \text{min}^{-1}$)

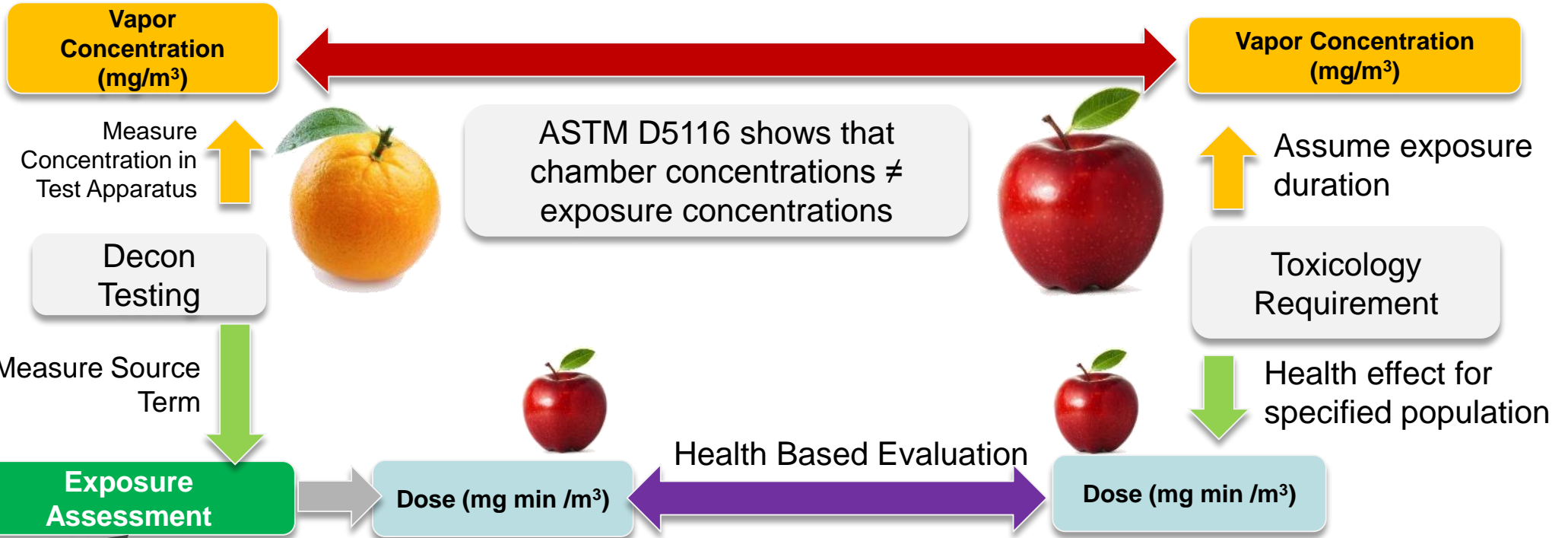
Enables health effect analysis

*Varady et al., *Ind. Eng. Chem. Res.*, **2016**, 55 (11), pp 3139

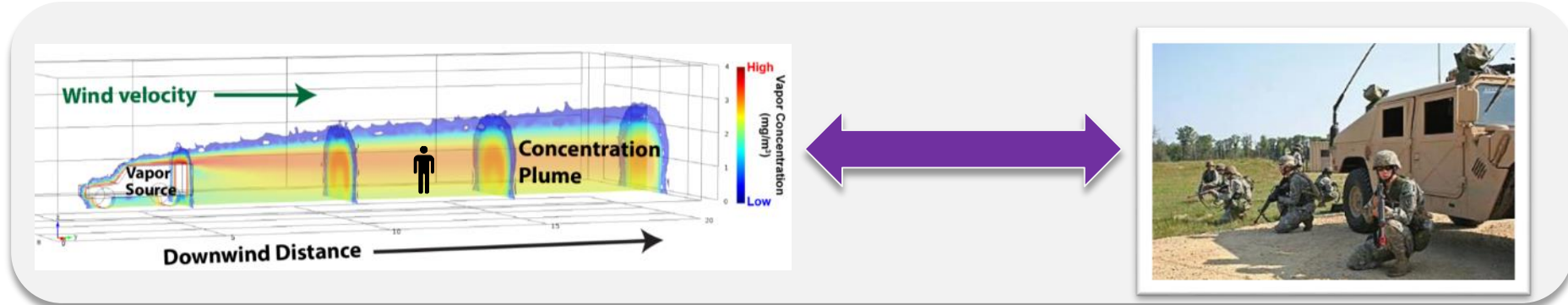
**ECBC-TR-1383 (available at www.dtic.mil)

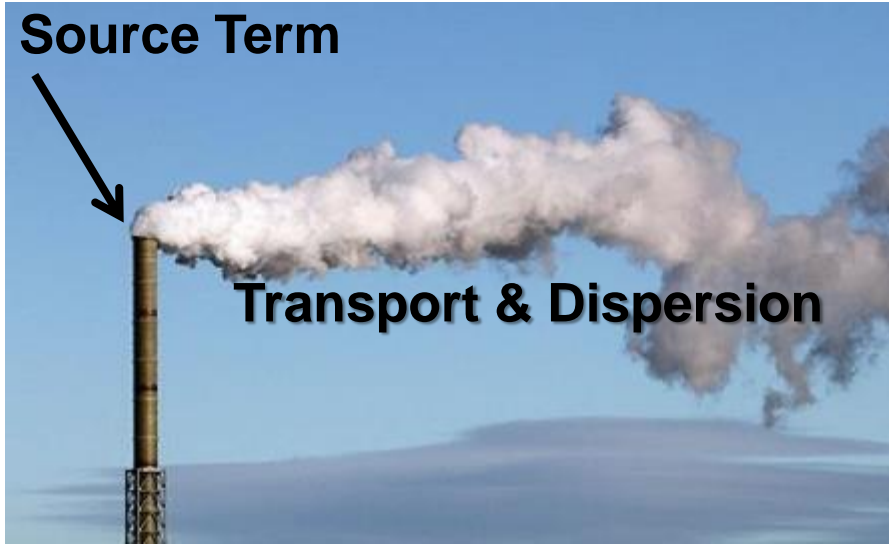


'Asset' in test chamber



Missing Component for 'Clean Enough?'
-Context of asset(s) in a specific environment

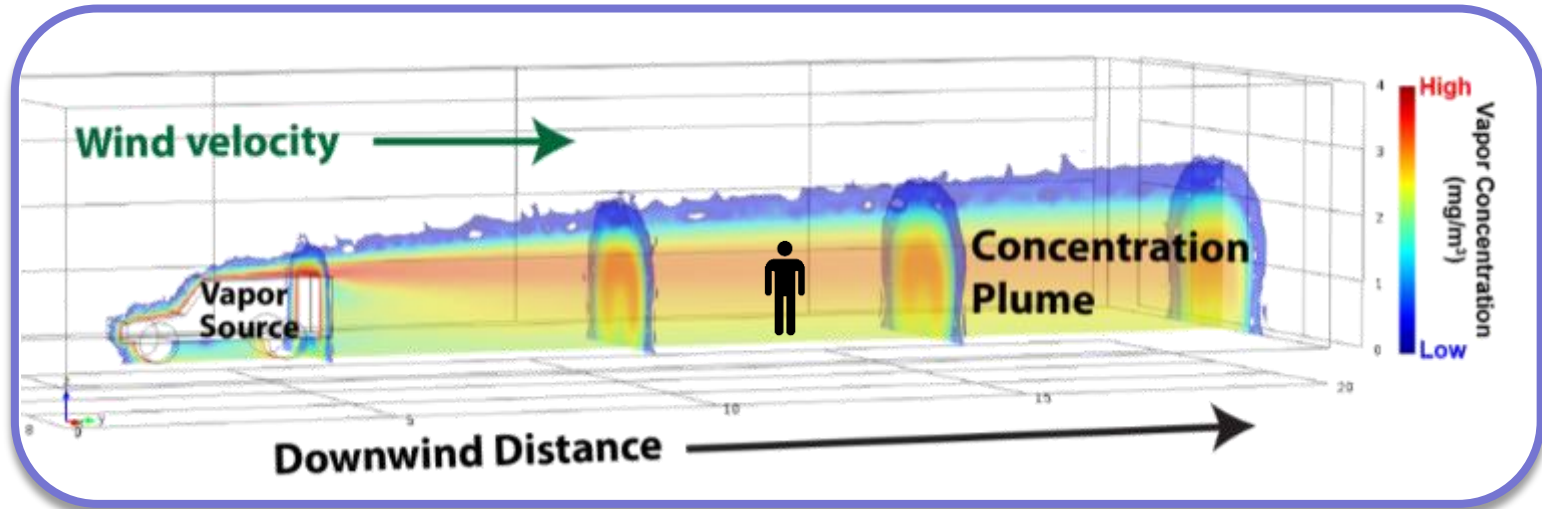




- The vapor source term is a description of how chemicals are introduced into an environment determined by testing* or modeling**
- Exposure is a result of how source terms are carried from asset to personnel via *transport & dispersion* in a vignette

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

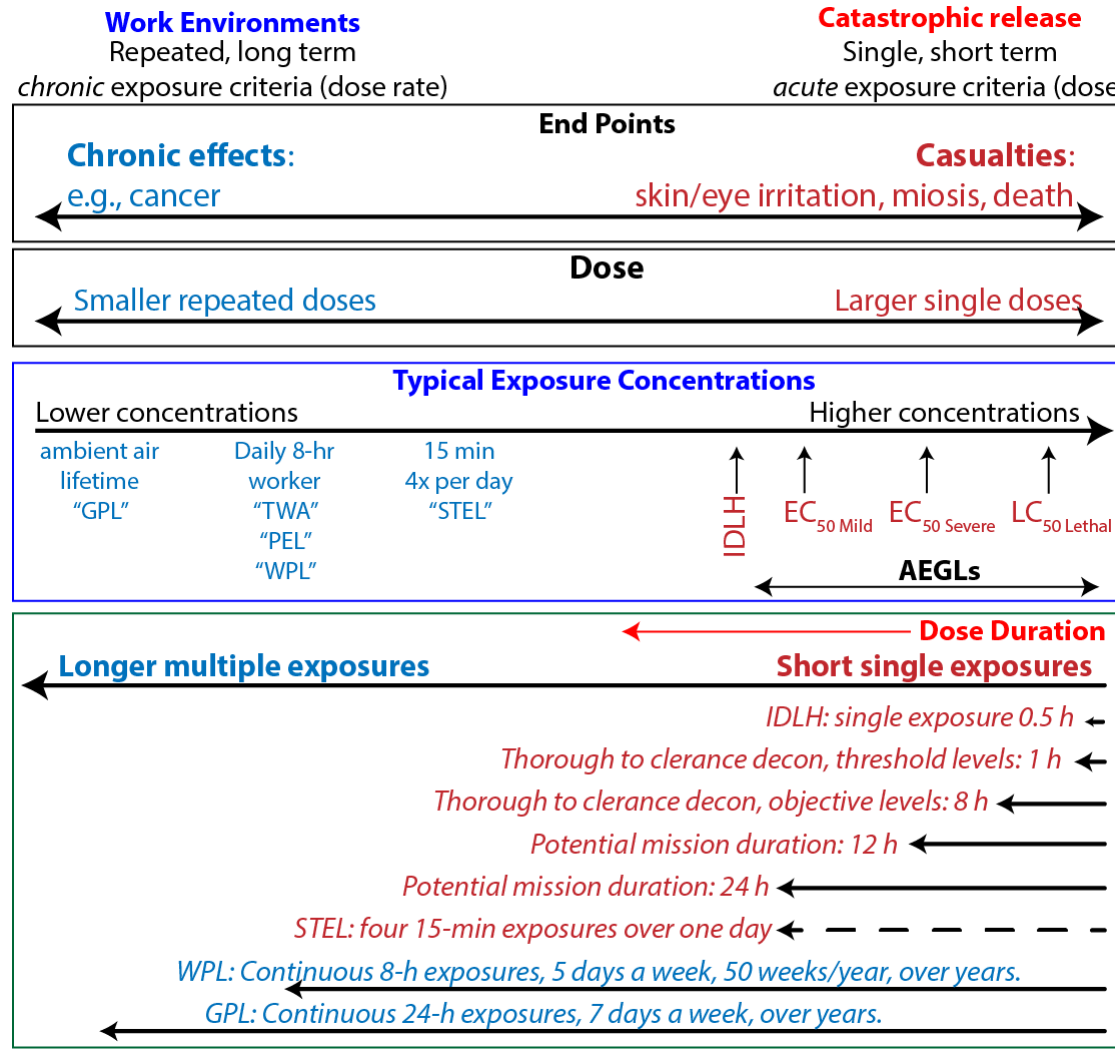
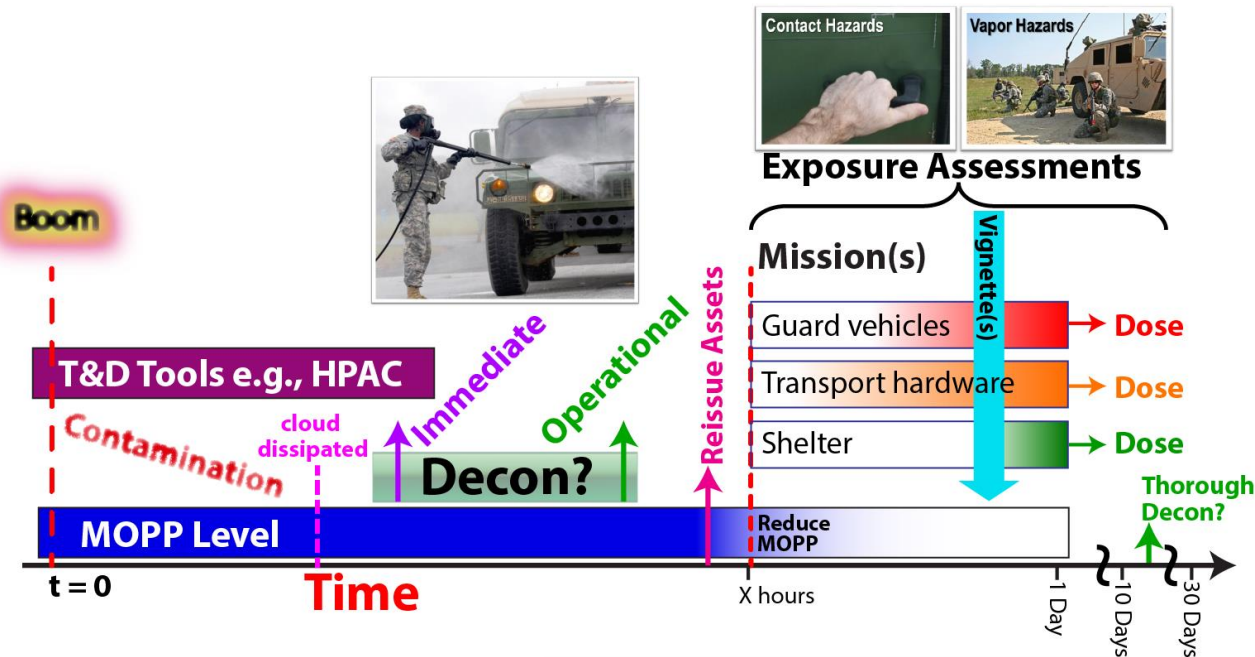
Vapor Source	Industrial - Smoke stack	Military - Vehicle
Source Emission Rate	1000 g/min H ₂ O	1 mg/min VX from vehicle
Source Flux (rate/area)	1 g m ⁻² min ⁻¹	Paint: 1 × 10 ⁻³ mg VX m ⁻² min ⁻¹



*ECBC-TR-980 (available at www.dtic.mil)

**Varady et al. *Ind. Eng. Chem. Res.*, 2017, 56, 10911

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

Decon?

Domestic Exposure (chronic?)

→



Communications



Vehicles



Fixed Sites

- 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 μ L droplet applied to material (2.8 mg HD)

Contamination Age Time: 1 h, 12 h duration

Material: Polymer

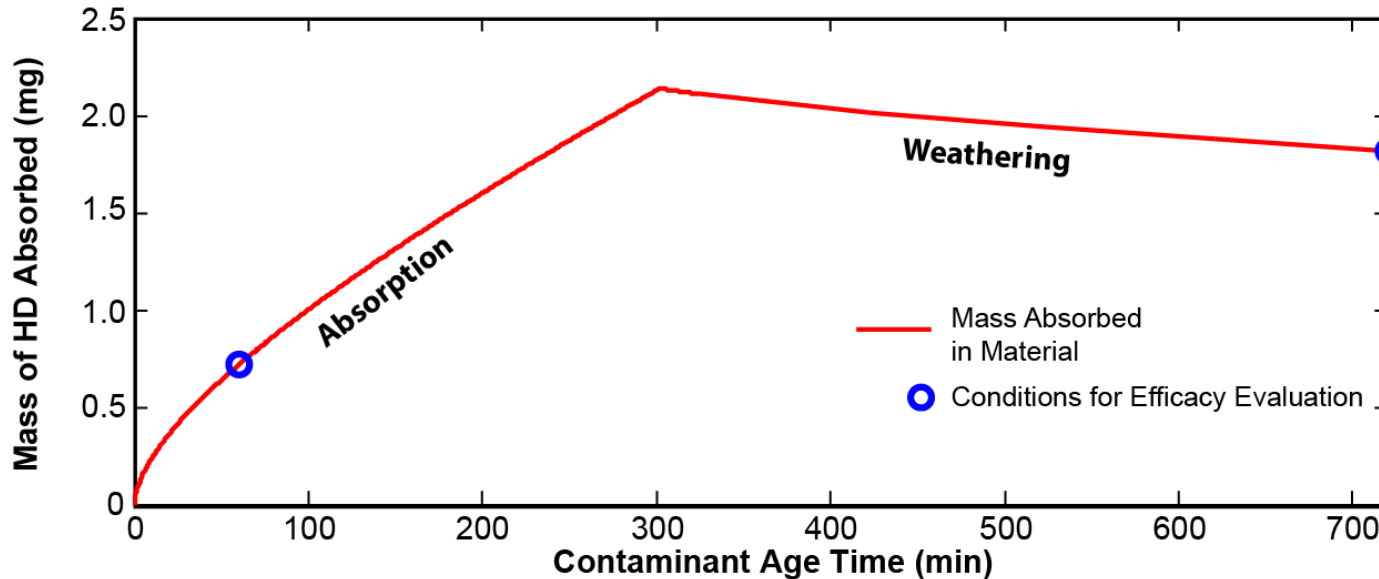
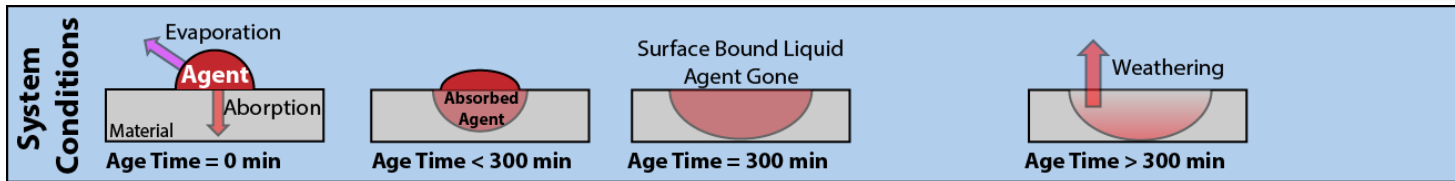
Decontamination: Soapy Water Wash and immerse panel in decontaminant for 30 min

Material Efficacy

How much Agent Remains after Decon

$$1 - \frac{\text{How much Agent Remains after Decon}}{\text{How much Agent you Started With}}$$

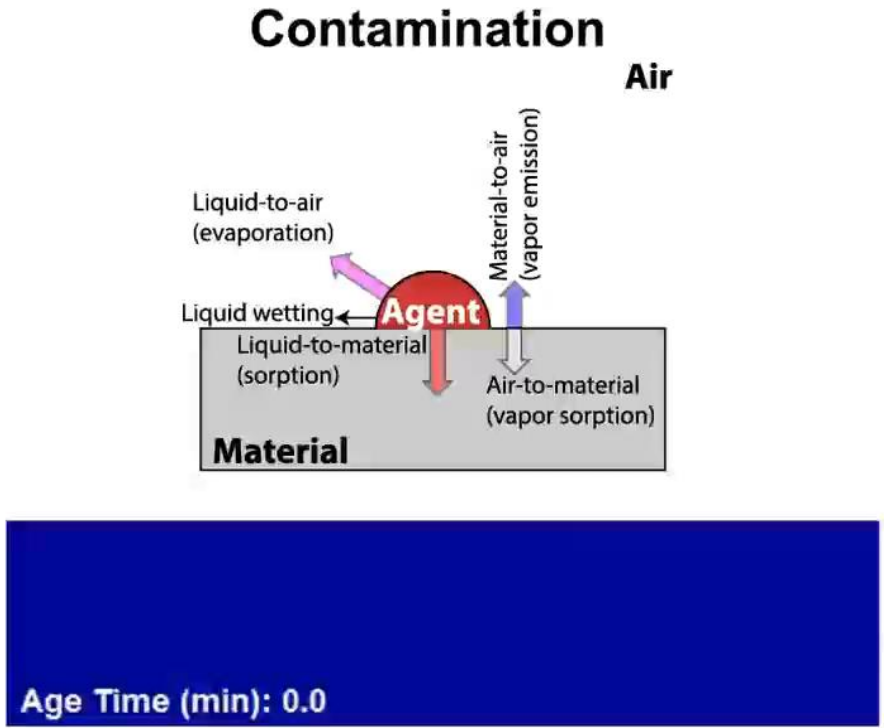
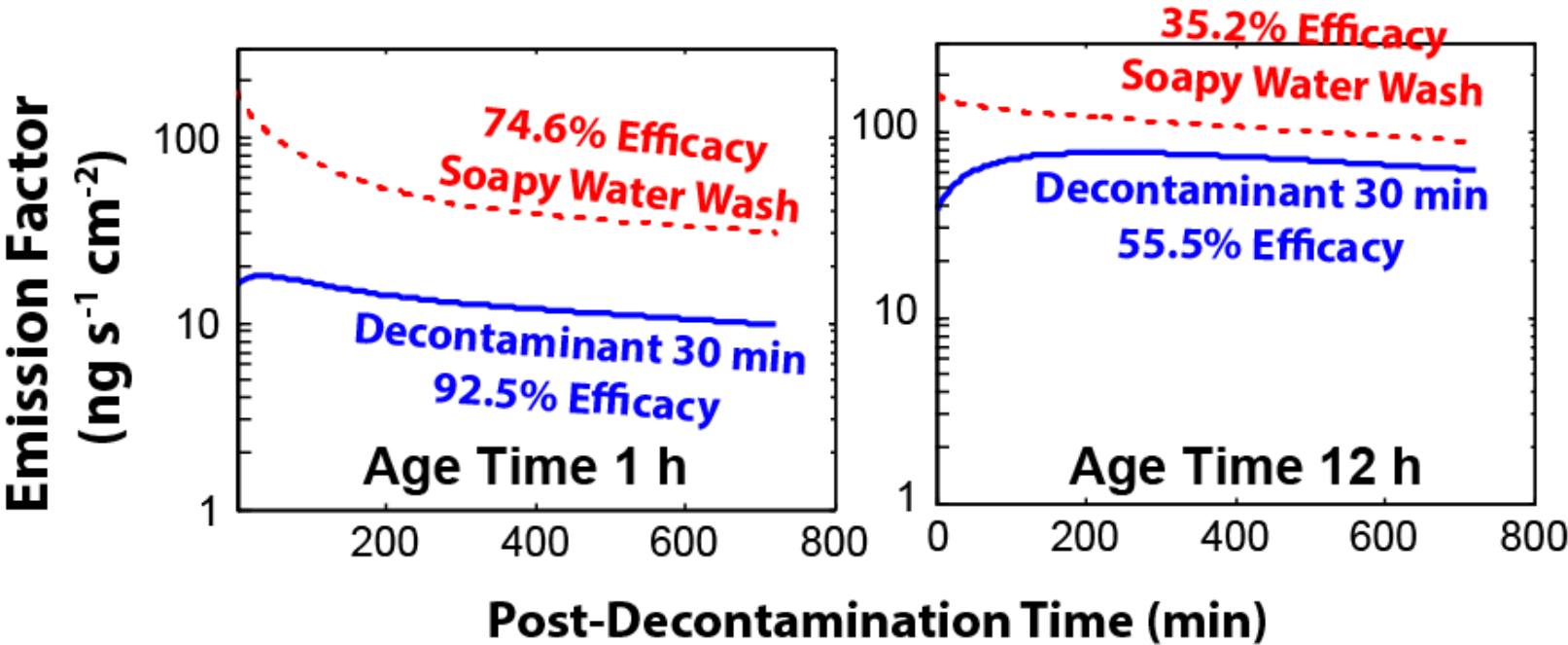
Contamination Duration establishes the *initial condition* for the agent distribution and how much agent is absorbed

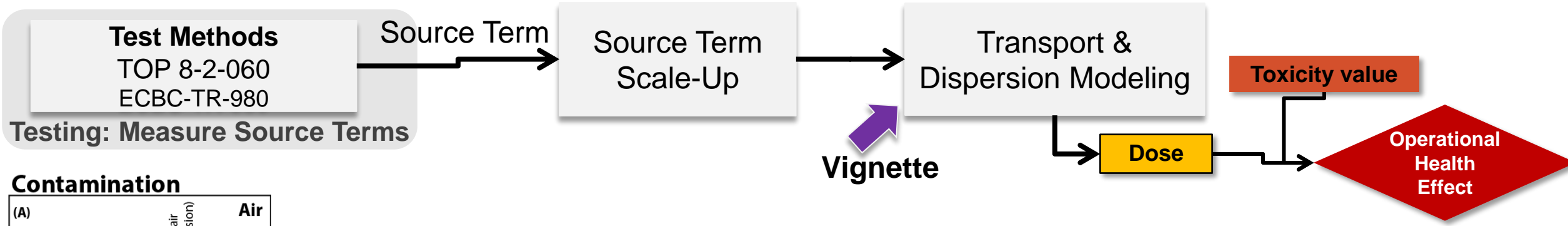


Applied Mass: 2.8 mg HD

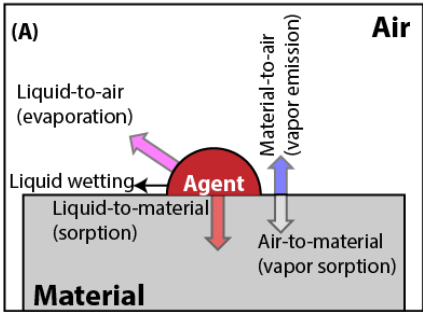
	Soapy Water Wash	Efficacy
1 h	0.712 mg HD	74.6%
12 h	1.815 mg HD	35.2%
	Decon 30 min	Efficacy
1 h	0.208 mg HD	92.5%
12 h	1.245 mg HD	55.5%

- 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

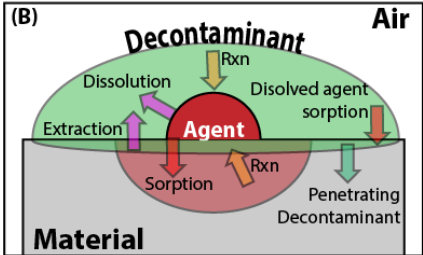




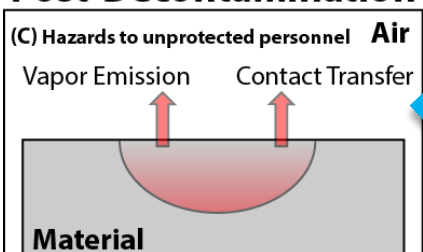
Contamination



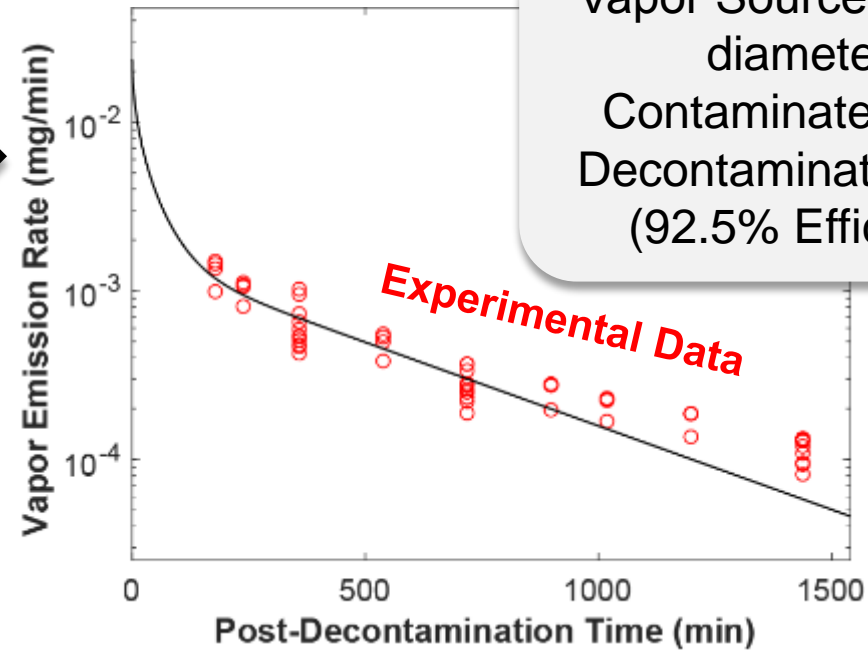
Decontamination

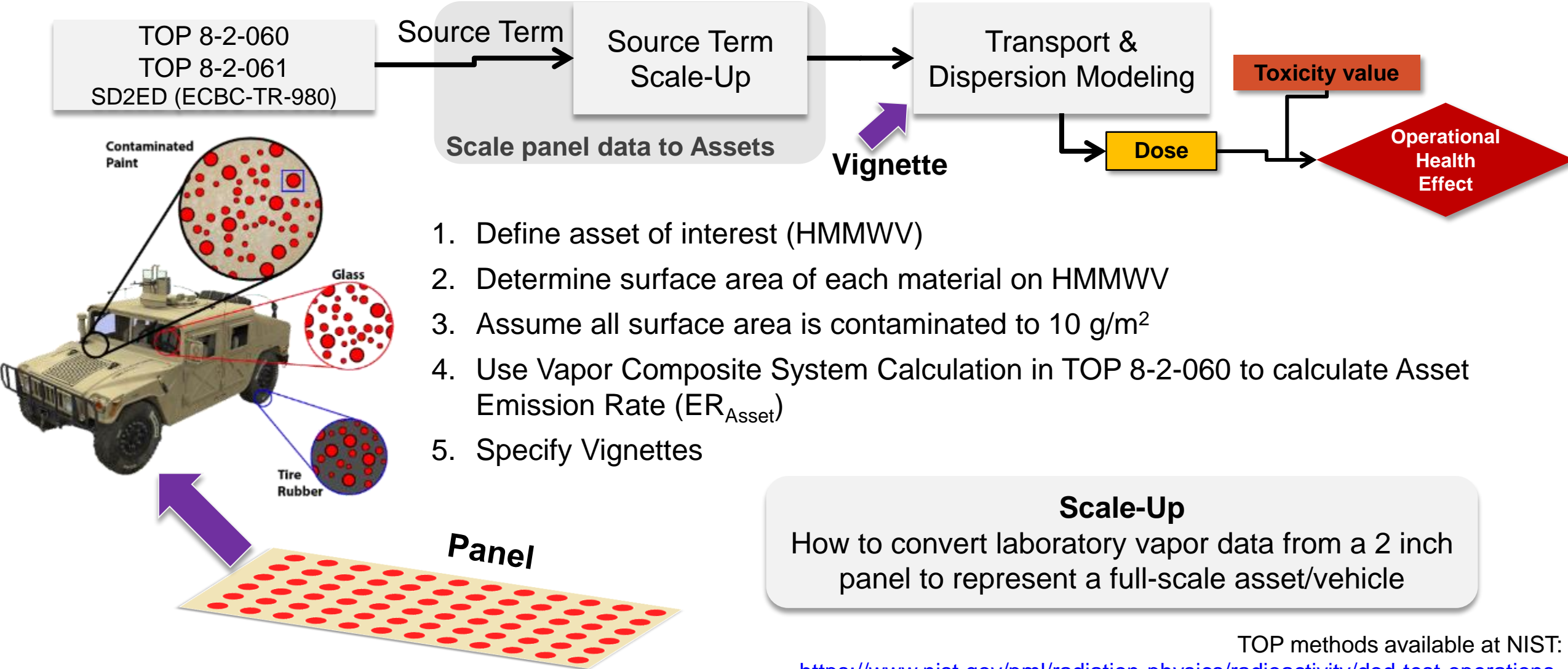


Post-Decontamination



Vapor Microchamber





TOP 8-2-060
TOP 8-2-061
SD2ED (ECBC-TR-980)

Source Term

Source Term
Scale-Up

Transport &
Dispersion Modeling

Toxicity value

Dose

Operational
Health
Effect

Scale panel data to Assets

Vignette

Contaminated
Paint

Glass

Tire
Rubber

Panel

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

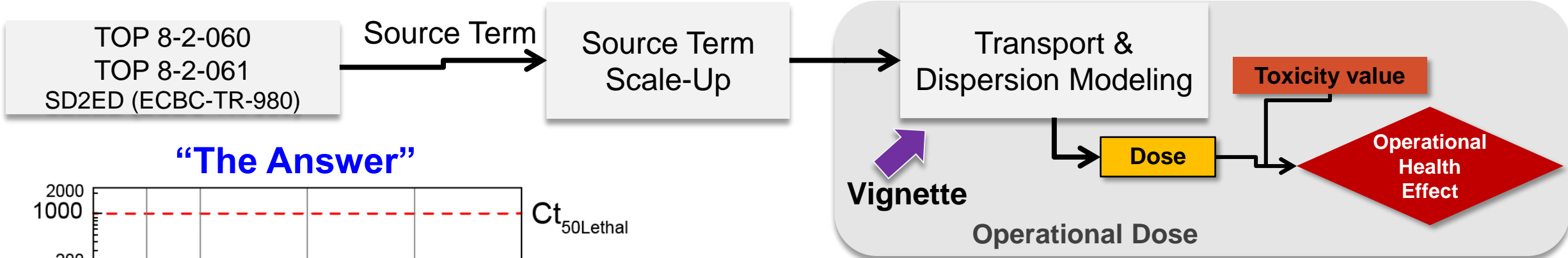
Scale-Up

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

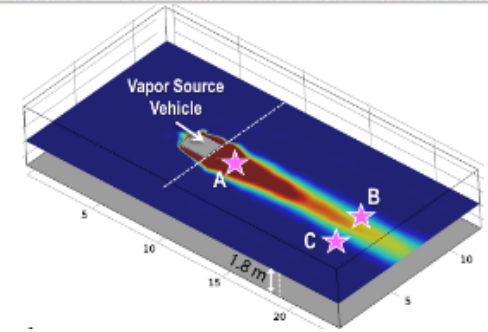
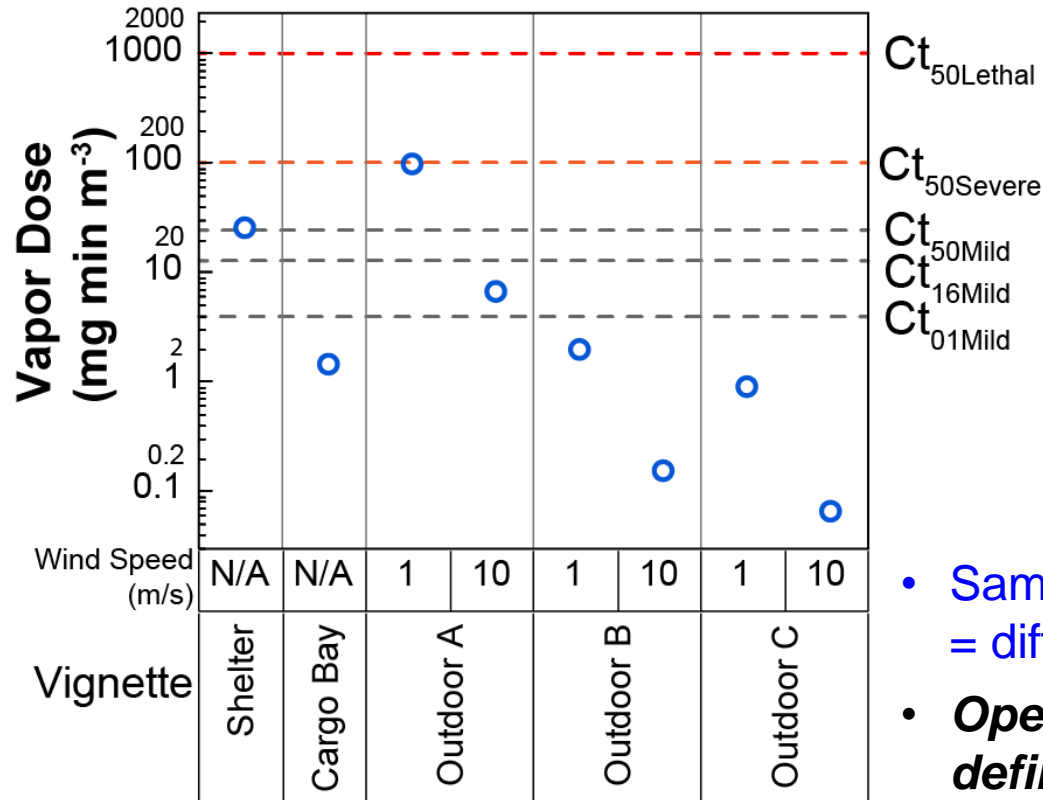
TOP methods available at NIST:

<https://www.nist.gov/pml/radiation-physics/radioactivity/dod-test-operations-procedures-documents/decontamination>

Exposure Dose Changes with Vignette



“The Answer”

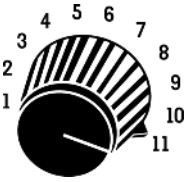


- Same asset, same decon, different vignette = different dose, different health effect
- **Operational health effects vary with the defined operation (combination of material effects and operational inputs)**

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



Connects and accounts for *material effects* and *operational inputs*

Material Effects



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

Timing



Source Terms

Exposure calculation

Dose

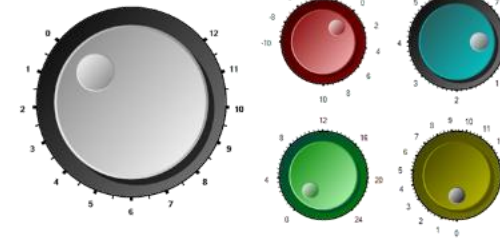
Operational Inputs

- Contamination density
- % of asset contaminated



- What personnel do with contaminated assets
- Environment: temperature, wind speed, etc.

Vignettes



Vignettes

Health Effect

Contamination

- 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

- 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



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Research Team



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Kevin Ulmes

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