



# Post-Decontamination Vapor Testing: Rethinking the Problem



EDGEWOOD CHEMICAL BIOLOGICAL CENTER

**TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.**

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# Vapor Test is a Core Technique to Determine if an Item/Surface May Emit Harmful Vapors



After an item has been decontaminated, the item may still emit harmful agent vapors.



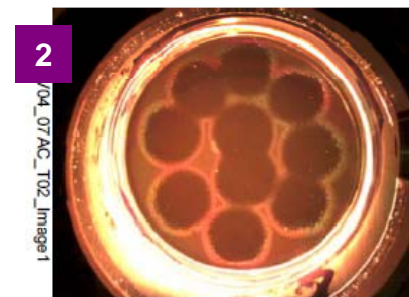
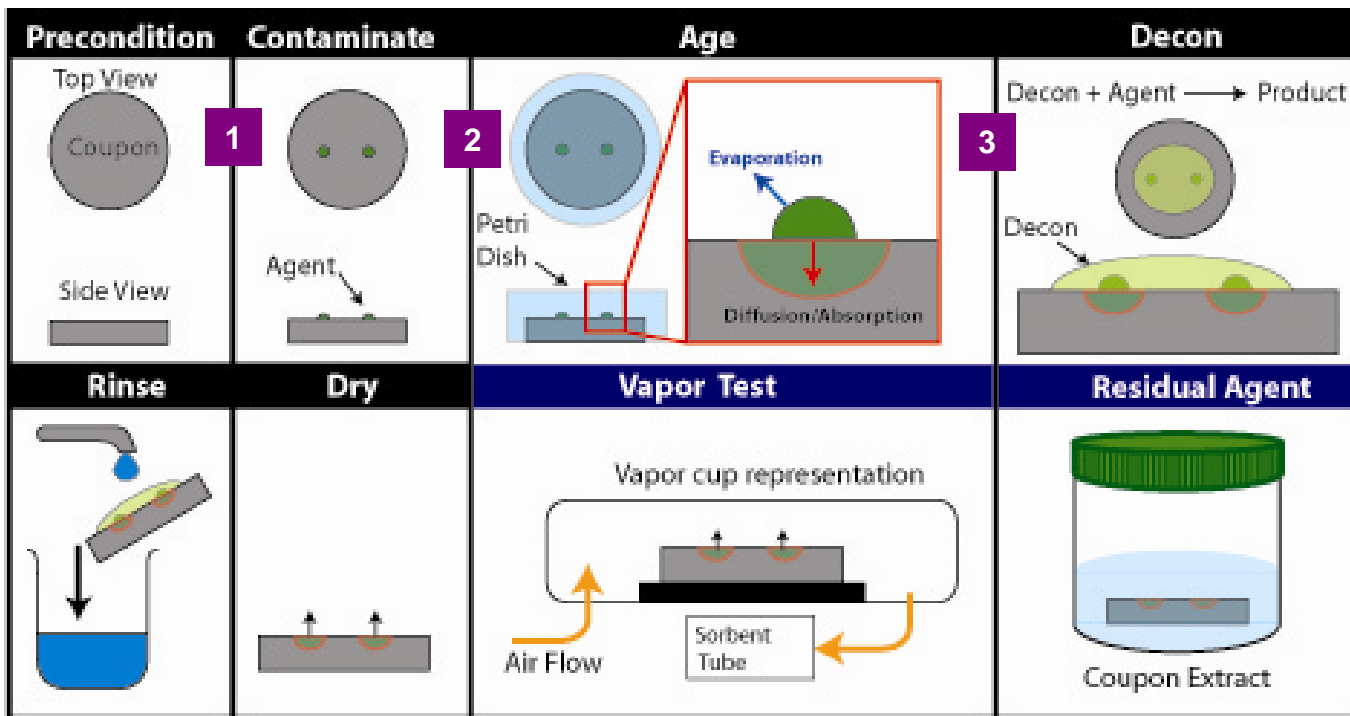
The chemical agent vapor test measures the vapors emitted to determine if there is a potential risk.

The characterization of a vapor emission source requires detailed test methodology, experimental design, and data treatment. Once characterized, the emission factor/rate is a powerful method for scenario-specific risk assessment.

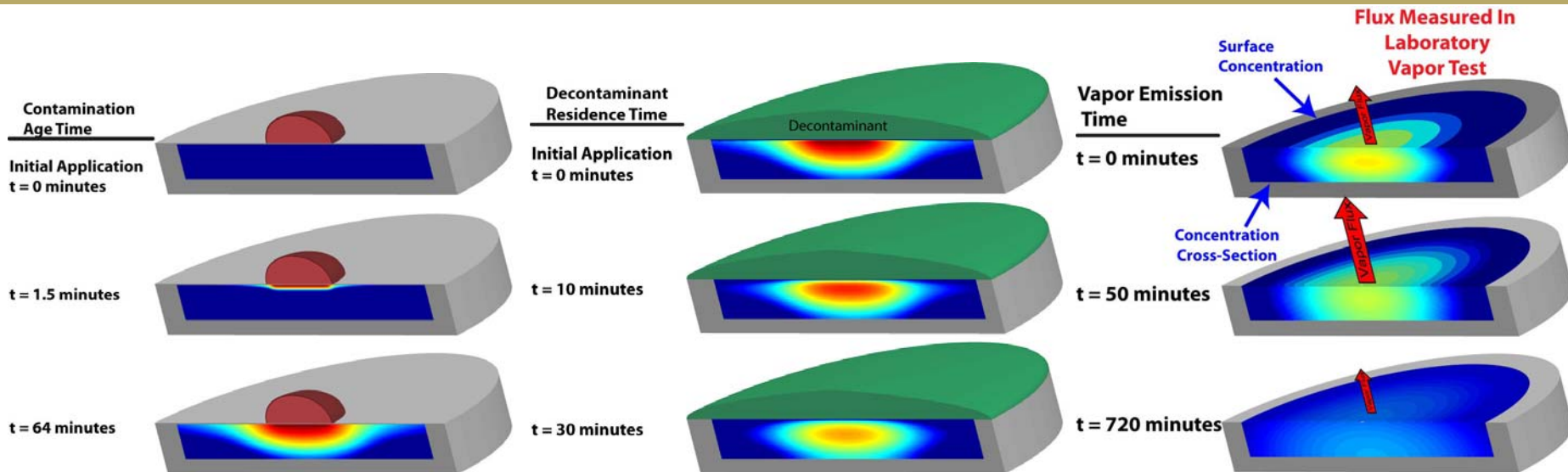
Live chemical agent test data for small items is used in this presentation to illustrate the impact of the paradigm shift through updated test methodology that enables scenario-based risk assessments.

# New Methodology Focuses on High Impact Variables of Agent-Material-Decon Interactions

Over the past 4 years the new methodology has focused on identification, measurement and documentation of the high impact variables. All of these high impact variables are related to mass transport processes of the agent-material-decontaminant interaction.



# Mass Transport is Fundamental Basis of Agent-Material-Decon Interactions

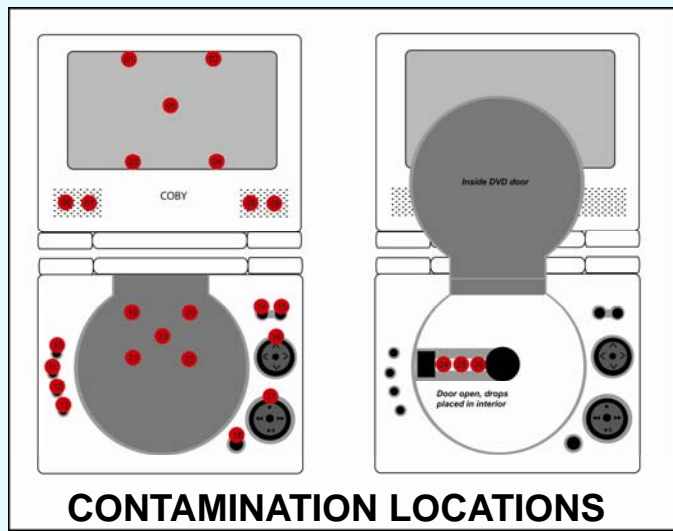


- Decontamination testing involves multiple types of mass transport that determine agent concentration and distribution in the material.
- Small variations in any decon process, such as contaminant spreading may affect the agent distribution in the material resulting in different vapor hazards.
- Vapor (emission) hazards are a result of the agent mass transport out of the material that was not removed by the decon.

# Data Comparison Case Study: Evaluation of Test Results for Similar Items

Decontamination vapor test data is used for risk assessments and to identify potential technologies for fielding. Test data is typically compared to vapor requirements that identify the acceptable vapor exposure risk level for unprotected personnel. The case study uses actual live agent on small item test data.

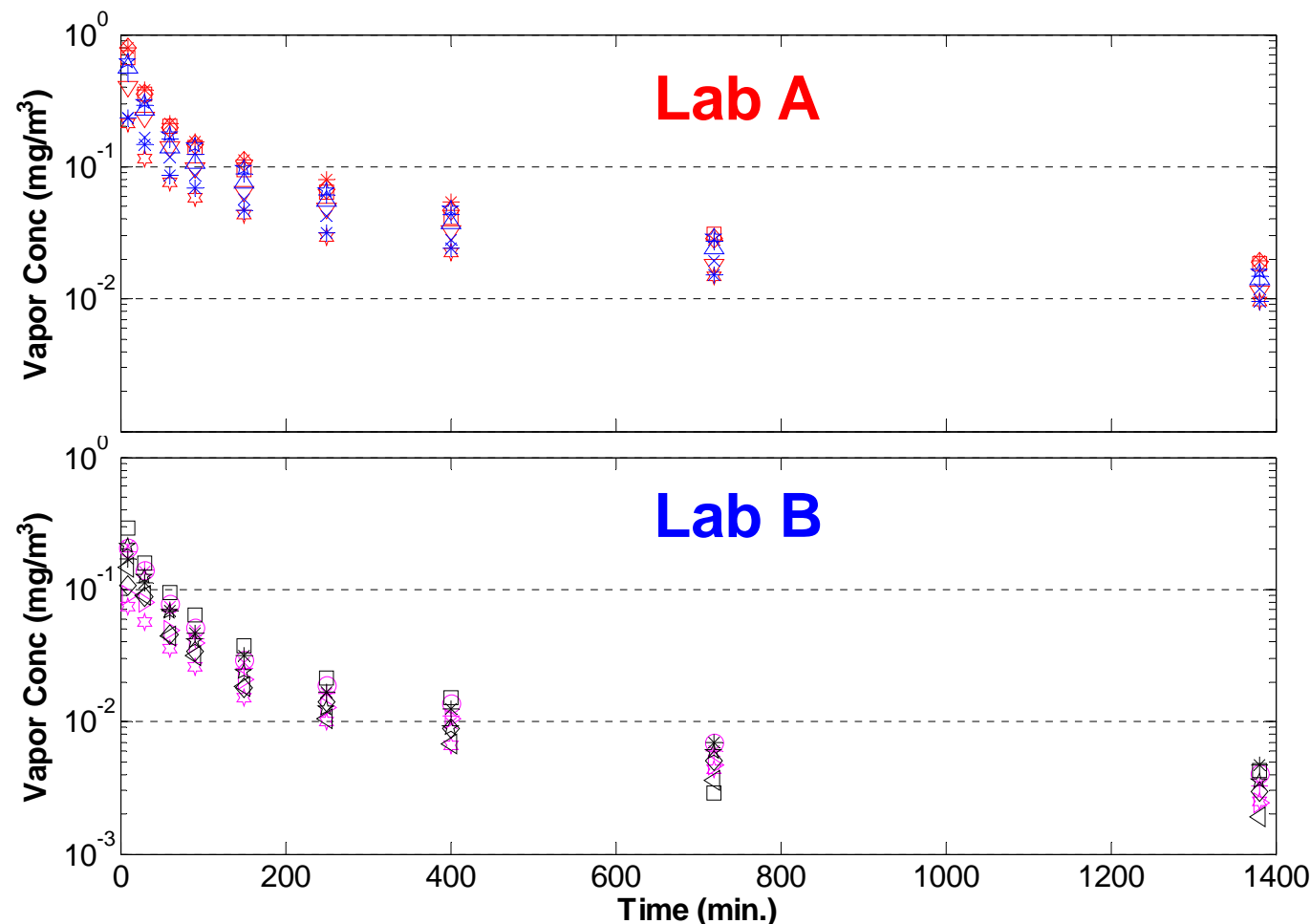
## Case study\*



20 surrogate small items (DVD players) were contaminated with 26 1-uL drops of HD as shown. The items were aged 5 min. in a chemical fume hood prior to vapor sampling. For the case study, the items were split between “Lab A” and “Lab B” for vapor testing.

\*note: data is actually from a single lab, presented as Lab A, Lab B.

# Data Comparison Case Study: Vapor Test Chamber Concentration Results



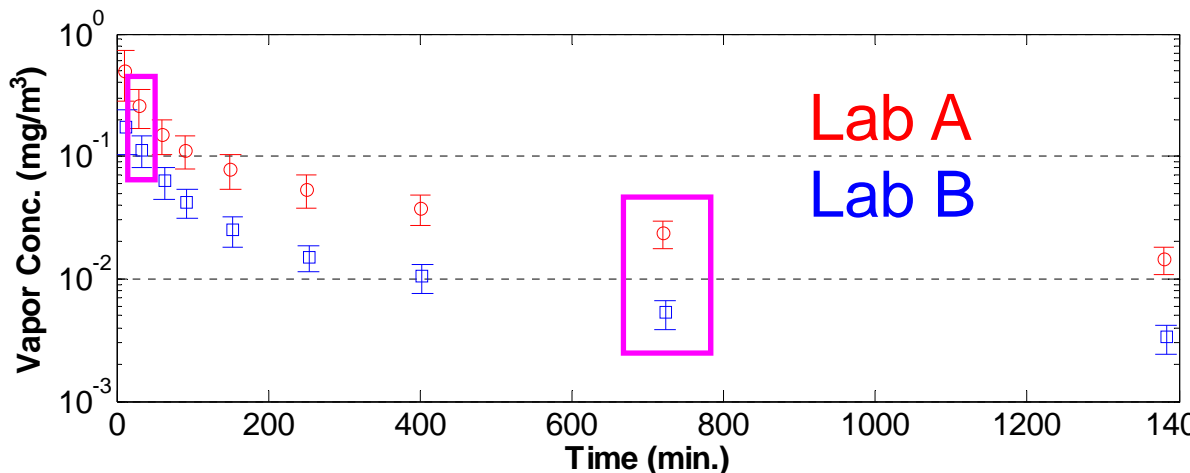
**Data:** 10 DVD players analyzed by each lab.

Each DVD player sampled using 9 solid sorbent tubes over the course of 24 hours.

**Observation:** Lab A vapor concentration is 5 times higher than Lab B.

**Question:**  
*How do Lab A & Lab B data compare for the analysis of similar items?*

# Data Comparison Case Study: Comparing Chamber Concentrations



## Answer – Data Comparison

- Similarity and difference are determined by ANOVA test at 95% confidence.
- Coefficient of Variation (CV) represents the relative error in a measurement.

1. Labs have similar CV (variability) within groups.
2. Labs have different ave. conc. between groups.
3. CV for combined Lab A&B is large compared to each lab.

Lab	Average CV (stdev / Avg)	Avg. Conc. at 30 min. (mg/m <sup>3</sup> )	Avg. Conc. at 720 min. (mg/m <sup>3</sup> )
A	0.316 <b>1</b> similar	0.262 <b>2</b> different	0.0237 <b>2</b> different
B	0.283	0.113	0.00527
A&B	0.637 <b>3</b>		

**Question:**

*What was different?*

# Data Comparison Case Study: Test Setting Affect Concentration

**Answer:** Chamber volume and chamber air flow rate which significantly impact chamber concentration.

Laboratory	A	B
Chamber Free Air Volume, $V$ (m <sup>3</sup> )	0.01878	0.1661
Chamber Air Flow, $Q$ (L/min)	1.250	5.500
$C(t=720)$ , $C$ (mg/m <sup>3</sup> )	0.0237	0.00527

Lab B tested the same emitting item as Lab A but:

- Chamber was 8.8 times bigger.
- Air flow rate was 4.4 times higher.
- Resulting in concentrations 5 times lower.

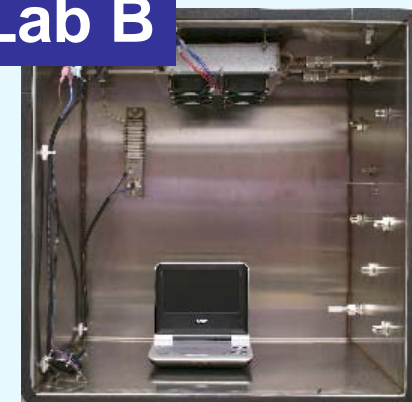
Both chambers meet the requirement of ASTM D5116  
Historical methods did not require measuring or using these variables in the data calculations.

**Question:** Which chamber concentration should be used to assess risk?

Lab A



Lab B

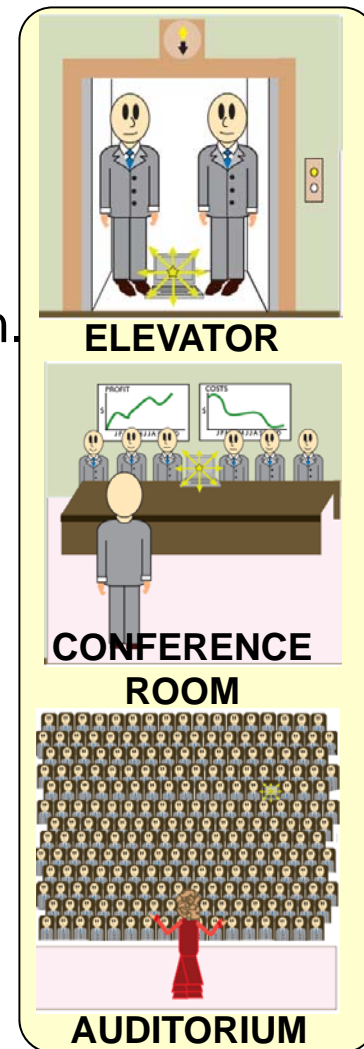


## Paradigm Shift

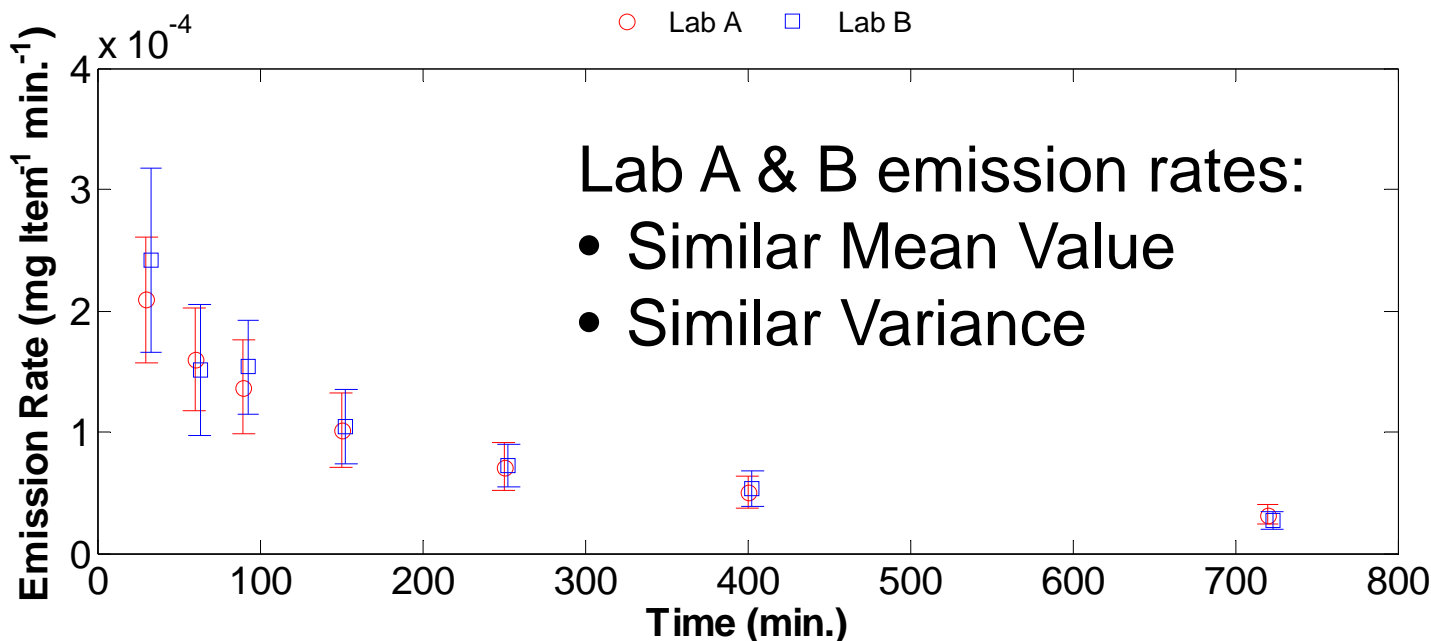
**New Approach:** characterize the emission source - how the item emits agent vapors; determining the *item emission rate*.

**Why:** For the same emitting item, conditions affect concentration.

- The chamber concentration is a response to the item emission rate, the chamber free air volume **AND** chamber air flow rate.
  - For the same emitting item, different chamber volumes and air flow rates (scenarios) result in different agent vapor concentrations.
- Hazards are a response to the agent vapor concentration generated in the scenario by the item.
  - Risk assessment for health-based criteria is based on the exposure of unprotected personnel to a vapor concentration generated by the emitting item and is scenario specific.



# The Emission Rate Method Enables Reproducible Characterization of Similar Items

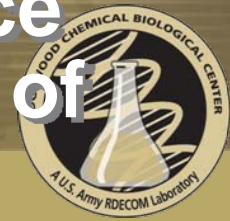


## Labs A and B measured similar Emission Rates even though:

- Four different vapor test chambers (2 small, 2 large) were used.
- Different chamber operating parameters were used.
- Different operators were used.
- Multiple analytical platforms were used.
- Data was collected over several weeks of testing.
- Different chamber concentrations were measured.

*Multiple sources of variance were introduced into this study*

# Characterization of the Emission Source Enables Reproducible Characterization of Similar Items



**New approach accounts for the key variables to properly characterize the emission source.**

## Chamber Concentration:

Data	Average CV (stdev / Avg)	Avg. Conc. at 30 min. (mg/m <sup>3</sup> )	Avg. Conc. at 720 min. (mg/m <sup>3</sup> )
<b>A</b>	0.316	0.262	0.0237
<b>B</b>	0.283 <span style="background-color: #d9ead3;">similar</span>	0.113 <span style="background-color: #f1c40f;">different</span>	0.00527 <span style="background-color: #f1c40f;">different</span>
<b>A&amp;B</b>	<span style="color: red;">0.637</span> <span style="background-color: #f1c40f;">different</span>	0.187	0.0145

## Conclusions:

1. Concentration comparison (chamber response) illustrated that A & B were not similar.
2. Emission rate calculation showed A and B measured similar emission rates.
3. The CV (variance) shows emission rate variance is similar but concentration variance is different.
4. One source of variation in historical data may be due to different test conditions.

## Emission Rate (new method):

Data	Average CV (stdev / Avg)	Avg. Emission Rate at 30 min. (mg item <sup>-1</sup> min <sup>-1</sup> )	Avg. Emission Rate at 720 min. (mg item <sup>-1</sup> min <sup>-1</sup> )
<b>A</b>	0.269 <span style="background-color: #d9ead3;">similar</span>	2.09 E-4 <span style="background-color: #d9ead3;">similar</span>	3.19 E-5 <span style="background-color: #d9ead3;">similar</span>
<b>B</b>	0.285	2.42 E-4 <span style="background-color: #d9ead3;">similar</span>	2.74 E-5 <span style="background-color: #d9ead3;">similar</span>
<b>A&amp;B</b>	<span style="color: red;">0.274</span> <span style="background-color: #d9ead3;">similar</span>	2.25 E-4	2.97 E-5

# Emission Rate Calculation Methodology Overview



Characterizing a vapor emission source involves determination of the emission rate function,  $E(t)$ , as described by the mass balance equation.

$E(t)$  is the agent mass emitted per item per time ( $\text{mg item}^{-1} \text{min}^{-1}$ ) as a function of time.

$$\frac{dC}{dt} = E(t) \frac{Z}{V} - C(t) \frac{Q}{V}$$

$C$  measured vapor concentration, ( $\text{mg}/\text{m}^3$ )

$V$  Chamber Free Air Volume, ( $\text{m}^3$ )

$Q$  Chamber Air Flow, ( $\text{L}/\text{min}$ )

$Z$  Num. items in chamber, (item)

$l = Z / V$  Loading Factor, ( $\text{item}/\text{m}^3$ )

$n = Q / V$  Air Change, ( $1/\text{min}$ )

# Emission Rate Calculation Methodology Overview

- Approximate the mass balance differential equation using Euler method.

$$C_{\text{model}}(t) = lE(t)\delta t - nC(t - \delta t)\delta t + C(t - \delta t)$$

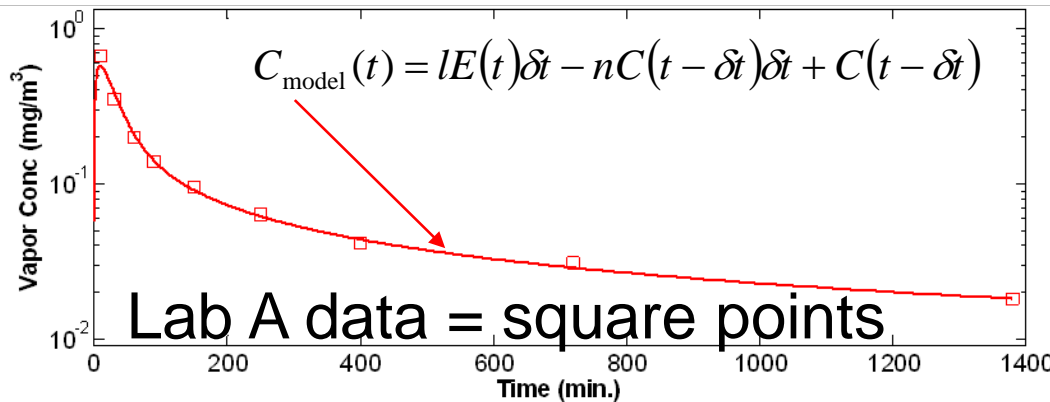
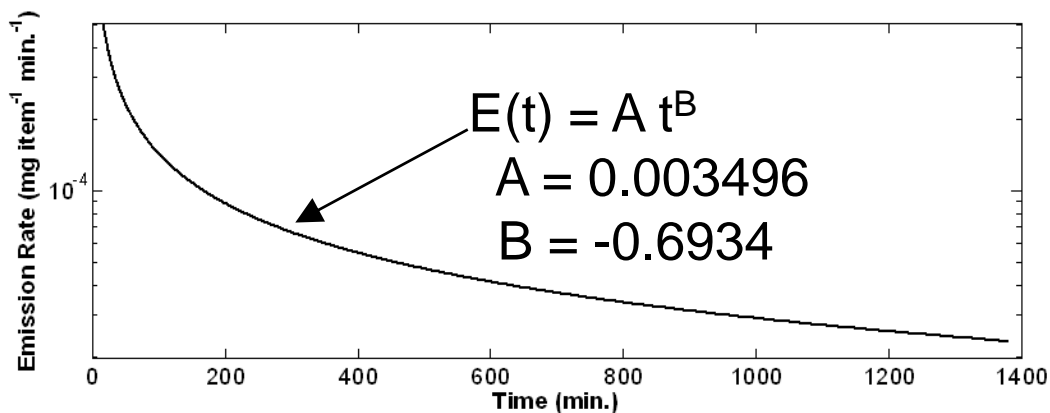
- Select best empirical function for  $E(t)$

- Calculate  $C_{\text{model}}(t)$  using  $E(t)$  and test conditions ( $l, n$ ).

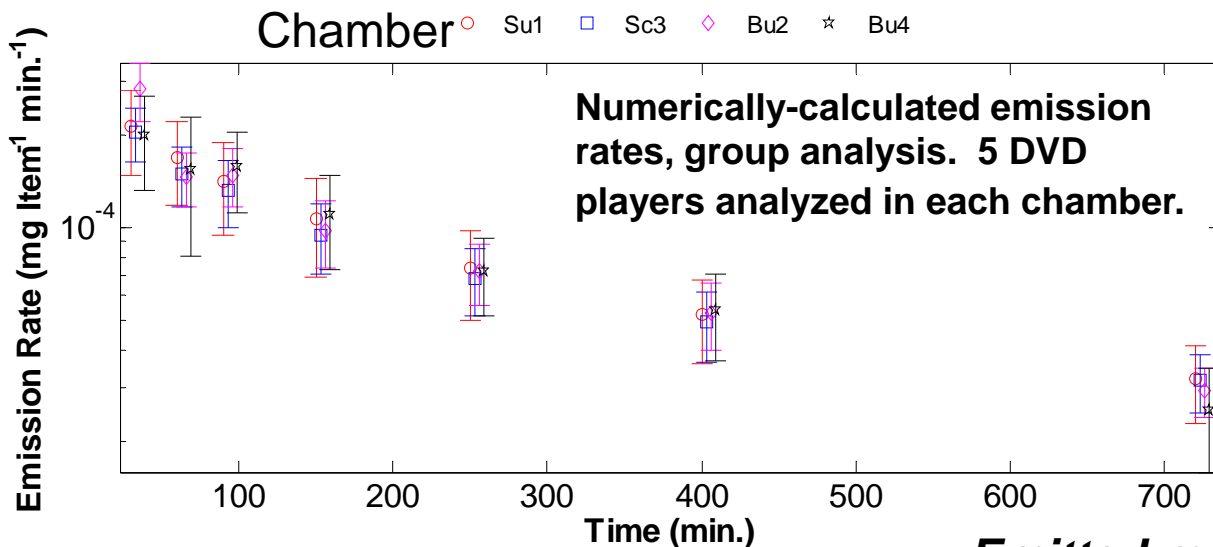
- Evaluate model error by comparing  $C_{\text{model}}(t)$  to  $C_{\text{measured}}(t)$

$$\chi = \sum_i \frac{|C_{\text{measured}}(t_i) - C_{\text{model}}(t_i)|}{C_{\text{measured}}(t_i)}$$

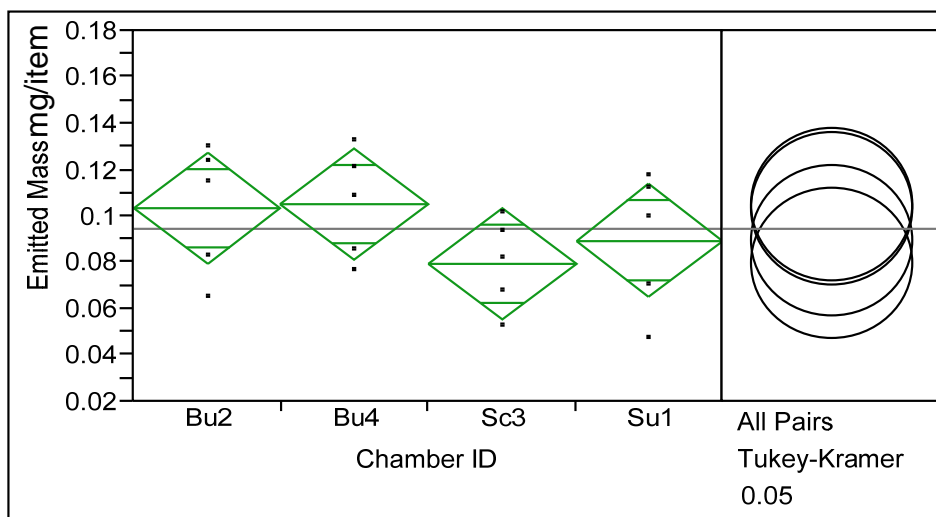
- Optimize  $E(t)$  parameters  $A$  and  $B$  until the model error is minimized achieving the best fit  $E(t)$  model.



# Emission Rate Applications in Decontamination Technology Development and Performance Evaluations



**Test data comparisons even if different conditions were used. One comparison uses emission rates to determine the emitted mass.**



**Emitted mass is a scenario-independent metric that indicates the total mass of agent that was emitted during the vapor test duration calculated as the integral of the emission factor model over time.**

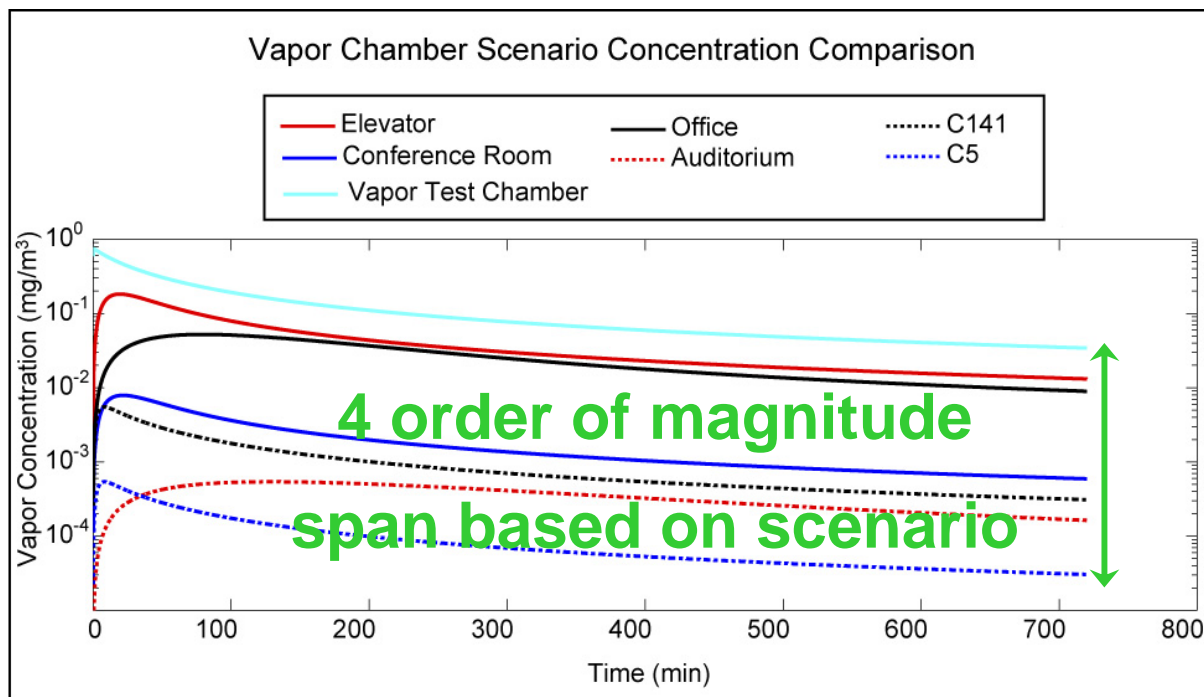
**A higher emitted mass will typically produce higher vapor concentrations and vapor exposure values.**

# Emission Rate Applications

## Scenario Vapor Concentration Calculations

Emission rates can be used to calculate scenario vapor concentrations and scenario-based risk assessments.

$$C_{\text{scenario}}(t) = l_{\text{scenario}} E_{\text{Item}}(t) \delta t - n_{\text{scenario}} C(t - \delta t) \delta t + C(t - \delta t)$$



Scenarios provide better representation of the decon. performance and potential hazard compared to test chamber data as loading factor and air change rate have a large effect on the final hazard.

Scenario calculations can also be used for scenarios where it is not feasible to conduct live agent testing.

\*Scenarios shown are hypothetical for educational purposes. These scenarios have not been approved for data analysis and comparison to requirements.

# Emission Rate Applications

## Toxic Load Calculations

### Background Information

**Toxic load** is a metric to measure vapor exposure. Toxic load is the current method accepted by the Department of Defense to evaluate vapor exposures and the likelihood of a toxicological response (i.e., hazards).

Vapor concentration fluctuations may have nonlinear effect on toxicological response.

Toxic load modeling accounts for fluctuations in concentration and exposure time.

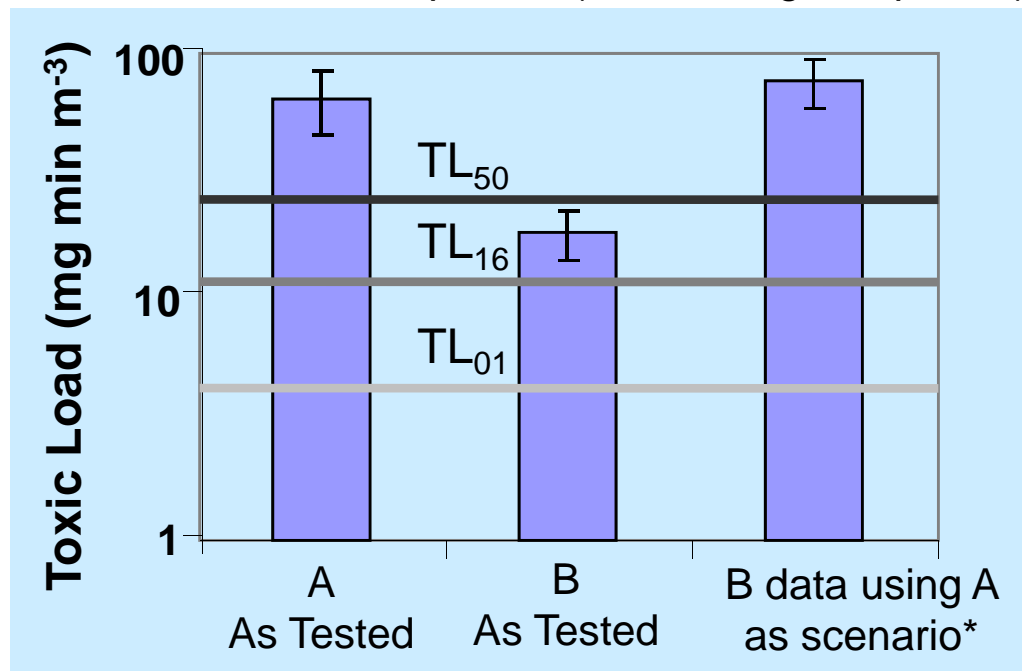
Toxic load exponents are reported by USACHPPM and in FM 3-11.9.

$$TL = \int C_{Scenario}(t)^{TLE} dt$$

TL = toxic load ( $mg^n \text{ min}/m^{3n}$ )

C(t) = concentration as a function of time ( $mg/m^3$ )

TLE = toxic load exponent (unitless, agent specific)



$$*C_{A \text{ Scenario}}(t) = l_{\text{Lab A}} E_{\text{Lab B}}(t) \delta t - n_{\text{Lab A}} C(t - \delta t) \delta t + C(t - \delta t)$$

# In Summary, Vapor Testing Should Characterize the Vapor Source

## Paradigm Shift: Characterize Item Emission Rate

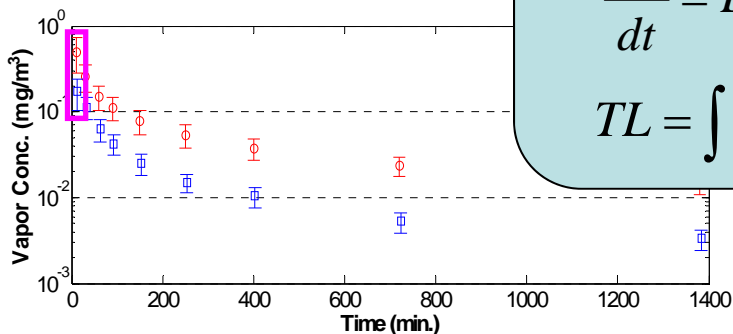
- Characterize item emission rate rather than chamber concentration response.
- Emission characterization enables data comparison and scenario specific risk assessment.

2007 Source Document & Small Item Methods

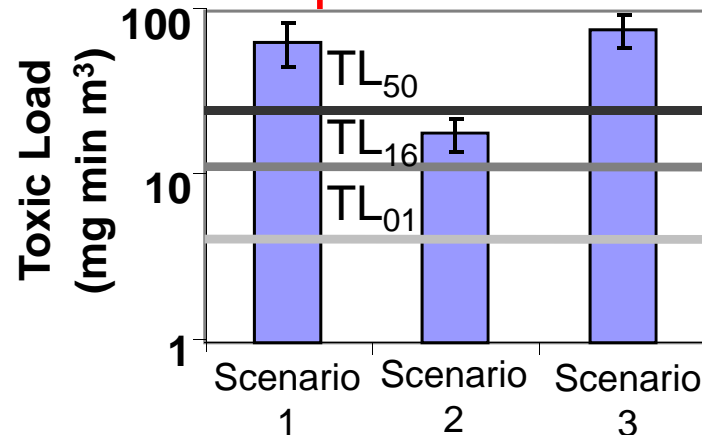
$$\frac{dC}{dt} = E(t) \frac{Z}{V} - C(t) \frac{Q}{V}$$

$$TL = \int C_{Scenario}(t)^{TLE} dt$$

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## Vapor Hazards



## Risk Assessment

- Scenarios can influence vapor concentration and toxic load by **orders of magnitude**.
- Same item may be hazardous in some scenarios but not others.

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## Research Team



Decon Sciences: Dr. Teri Lalain, Dr. Brent Mantooh, Tom Lynn, Dave Gehring, Zach Zander, Matt Shue, Michelle Hover.



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Michelle Sheahy.

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