Agent Fate Program Overview

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What Is The Objective Of The Agent Fate Program?

Improve model predictions of agent persistence

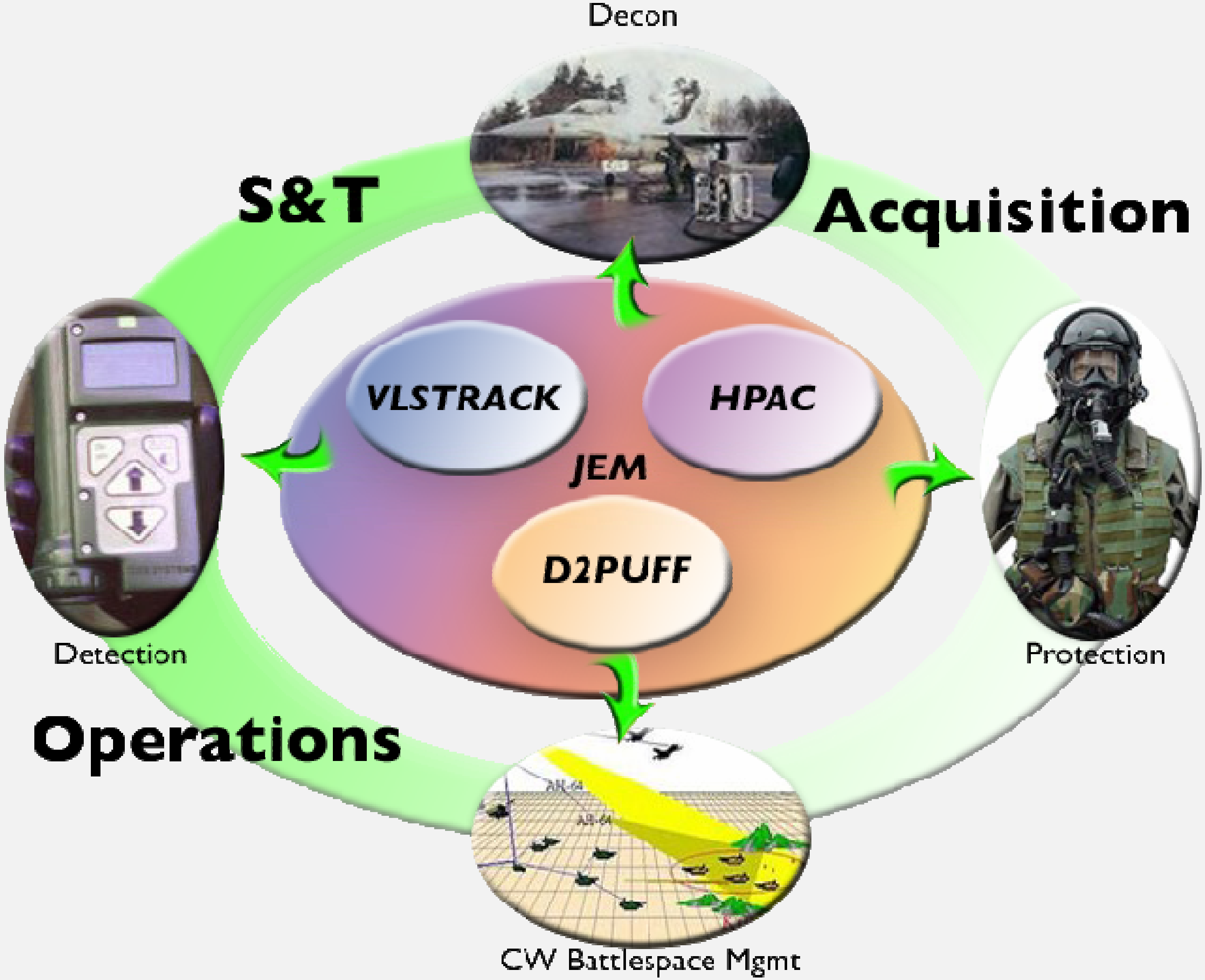
Objectives:

- **Measure and understand the physico-chemical processes of CW agents on surfaces in order to predict their persistence and fate in operational scenarios via agent fate models**

Payoffs:

- **Support research and acquisition decisions of all capability areas: detection, protection, decontamination**
- **Support and improve Operational Risk Management decisions based on inhalation and contact hazard**
- **JFOC - Battle Management: Battlespace Analysis and Planning**
- **Augments operational and mission area analysis tools such as Joint Effects Model (JEM) and Joint Operational Effects Federation (JOEF)**

Role of CB Hazard Models In ChemBio Defense Program



Why Do We Need An Agent Fate Program?

Models give varying and inaccurate persistence predictions

Field manuals and models built from limited data sets & questionable data

CONFLICTING

Concrete/Asphalt		FM 3-4		FM 3-3/ FM 3-7		FM 3-9		CONOPS	
	Temp	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor
GD	10-30°C	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	< 0.2	.5 - 6
HD	10-30°C	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	< 0.2	1 - 4.5
VX	10-30°C	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	Not Avail	< 0.2	1 - 7.5

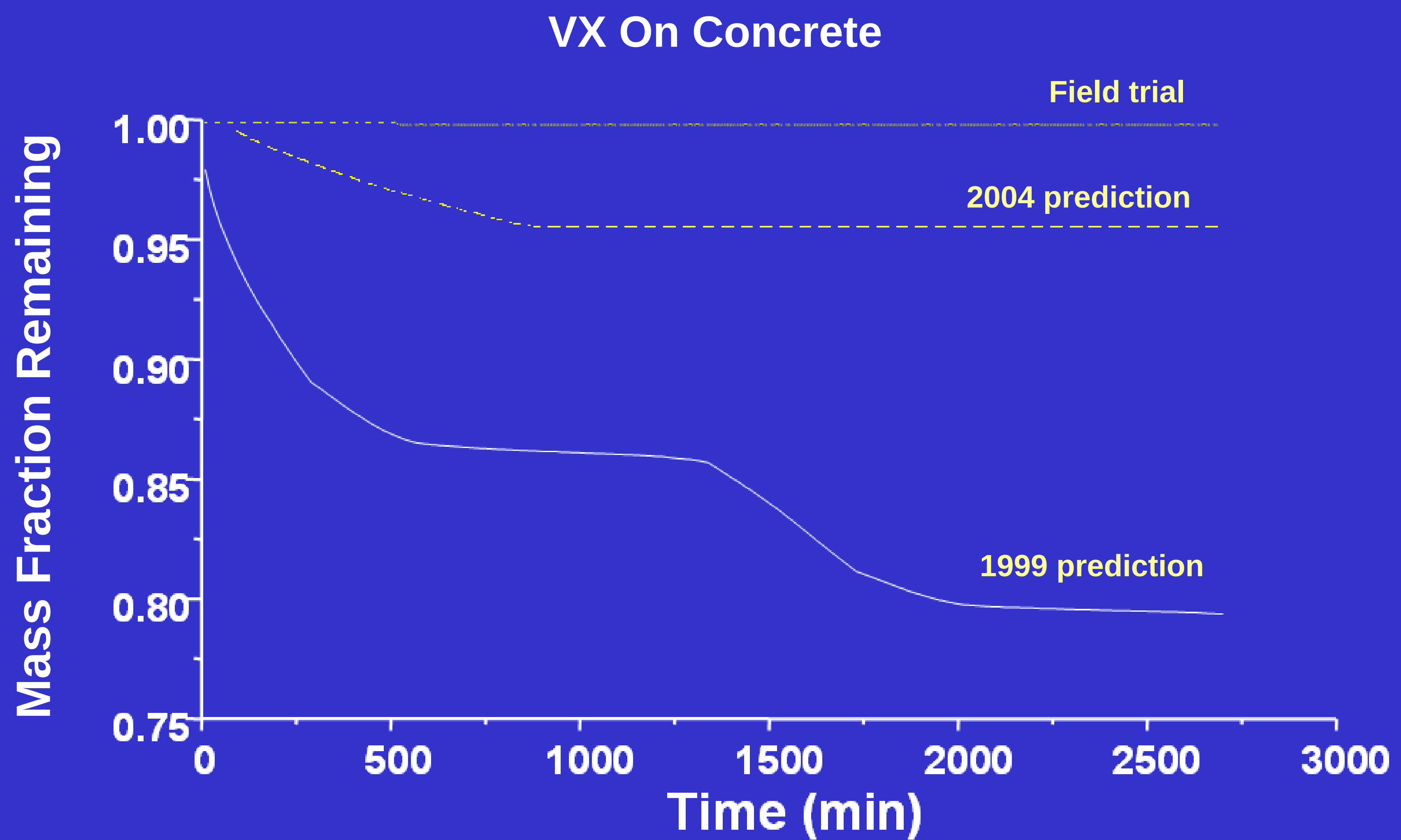
Sand		FM 3-4		FM 3-3/ FM 3-7		FM 3-9		CONOPS	
	Temp	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor
GD	10-30°C	Not Avail	18 - 60+	Not Avail	11 - 44	Not Avail	5 - 48	< 0.2	.5 - 5
HD	10-30°C	Not Avail	60+	Not Avail	3 - 12	Not Avail	6 - 168	< 0.2	.5 - 4
VX	10-30°C	Not Avail	45 - 60+	Not Avail	1085 -7992	Not Avail	1800 -3600	< 0.2	7.5 - 10

Grass		FM 3-4		FM 3-3/ FM 3-7		FM 3-9		CONOPS	
	Temp	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor
GD	10-30°C	Not Avail	7 - 20+	Not Avail	4-17	Not Avail	5 - 48	4*	.5 - 5
HD	10-30°C	Not Avail	20+	Not Avail	1 - 5	Not Avail	6 - 168	4*	.5 - 4
VX	10-30°C	Not Avail	18 - 20+	Not Avail	422 -3108	Not Avail	1800 -3600	4*	7.5 - 10

Temp 10-30 C	FM 3-4 Liquid	FM 3-4 Vapor
GD	Not Avail	7 - 20+
HD	Not Avail	20+
VX	Not Avail	18 - 20+

Temp 10-30 C	FM 3-9 Liquid	FM 3-9 Vapor
GD	Not Avail	5 - 48
HD	Not Avail	6 - 168
VX	Not Avail	1800 -3600

Model Prediction Improvement By Agent Fate Program



Current State of Agent Fate Data

Less than 400 usable live agent fate experiments exist

Circa 1999

- Deficiencies of Existing Data Points:
  - Sparse
  - No coordination between tests
  - Limited test duration
  - No repeatability
  - Missing data
  - Illegible source material
  - Antiquated test equipment
  - Significance versus quantification testing

Agent	Temp (°C)	Surface				
		Grass	Sand	Soil	Concrete	Asphalt
A	≤ 0	no data	no data	no data	no data	no data
	≤ 15	no data	no data	no data	no data	no data
	≤ 30	8	9	no data	2	2
	> 30	no data	6	no data	2	2
B	≤ 0	no data	1	no data	1	no data
	≤ 15	no data	no data	no data	no data	no data
	≤ 30	7	10	no data	2	2
	> 30	no data	6	no data	2	2
C	≤ 0	no data	no data	no data	no data	no data
	≤ 15	no data	1	no data	no data	no data
	≤ 30	16	4	38	1	1
	> 30	1	3	no data	no data	no data
D	≤ 0	no data	no data	no data	no data	no data
	≤ 15	no data	no data	no data	no data	no data
	≤ 30	no data	5	no data	no data	no data
	> 30	no data	2	no data	no data	no data
E	≤ 0	no data	3	no data	no data	no data
	≤ 15	no data	1	no data	no data	no data
	≤ 30	4	49	64	5	1
	> 30	1	23	4	no data	no data
F	≤ 0	no data	no data	no data	16	no data
	≤ 15	2	no data	no data	9	1
	≤ 30	9	1	4	57	2
	> 30	no data	no data	no data	4	no data

Agent Fate Program will start to fill the holes in this matrix (Comprehensive, systematic, and integrated program)

Agent Fate
Concept And Approach

Three Major Thrusts

Lab / Wind Tunnel / Field Trials

- Surface Evaporation
- Substrate Interactions
(vapor flux, temp., wind, RH, agent, substrate, drop size, spread rate, etc.)

Predictive Modeling

Statistical Design of Experiments

- Secondary Evaporation Modeling
- Residual liquid contact & pickup

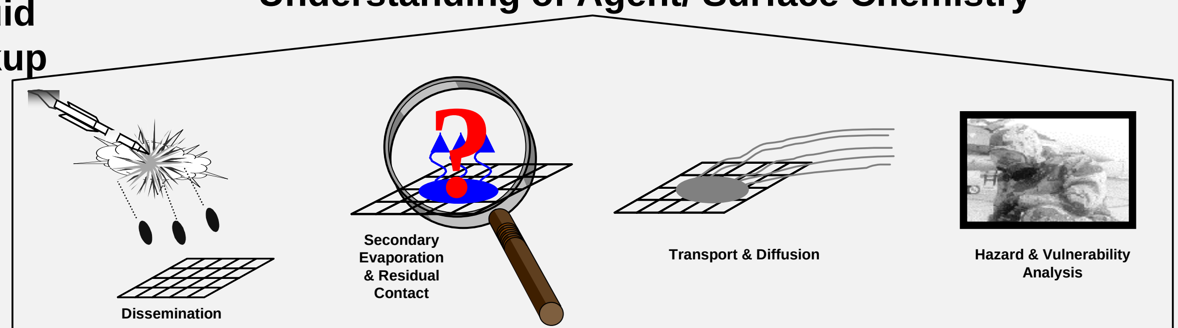
Methodology Development

- NMR
- HS-SPME
- Soil System

Understanding of Agent/ Surface Chemistry

Science Based Predictive Capability for Agent Persistence

- Secondary evap model for JEM
- Interim VLSTRACK
- CHEMRAT/JOEF
- Field Manuals



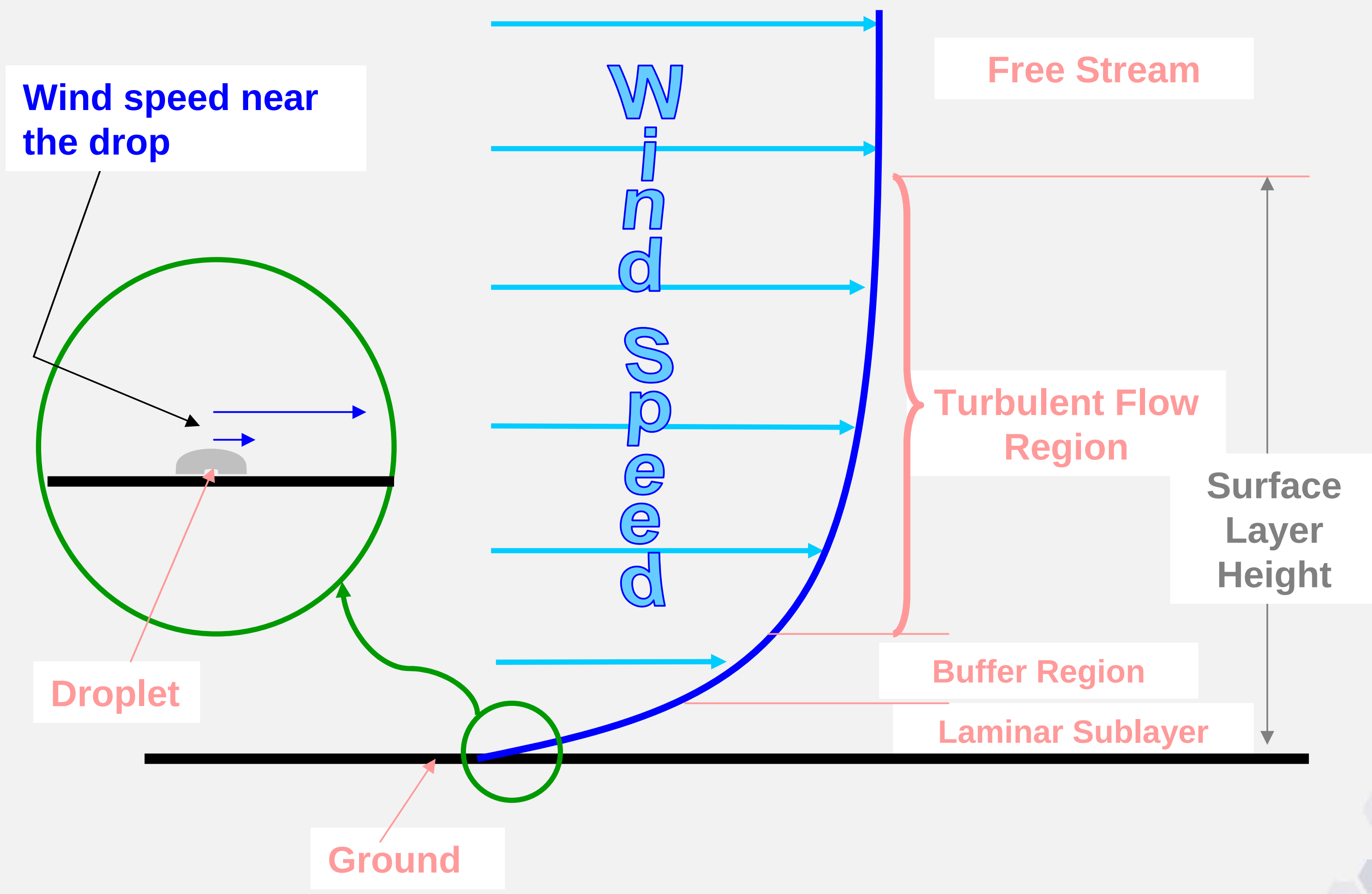
Operational Environment

Testing Matrix

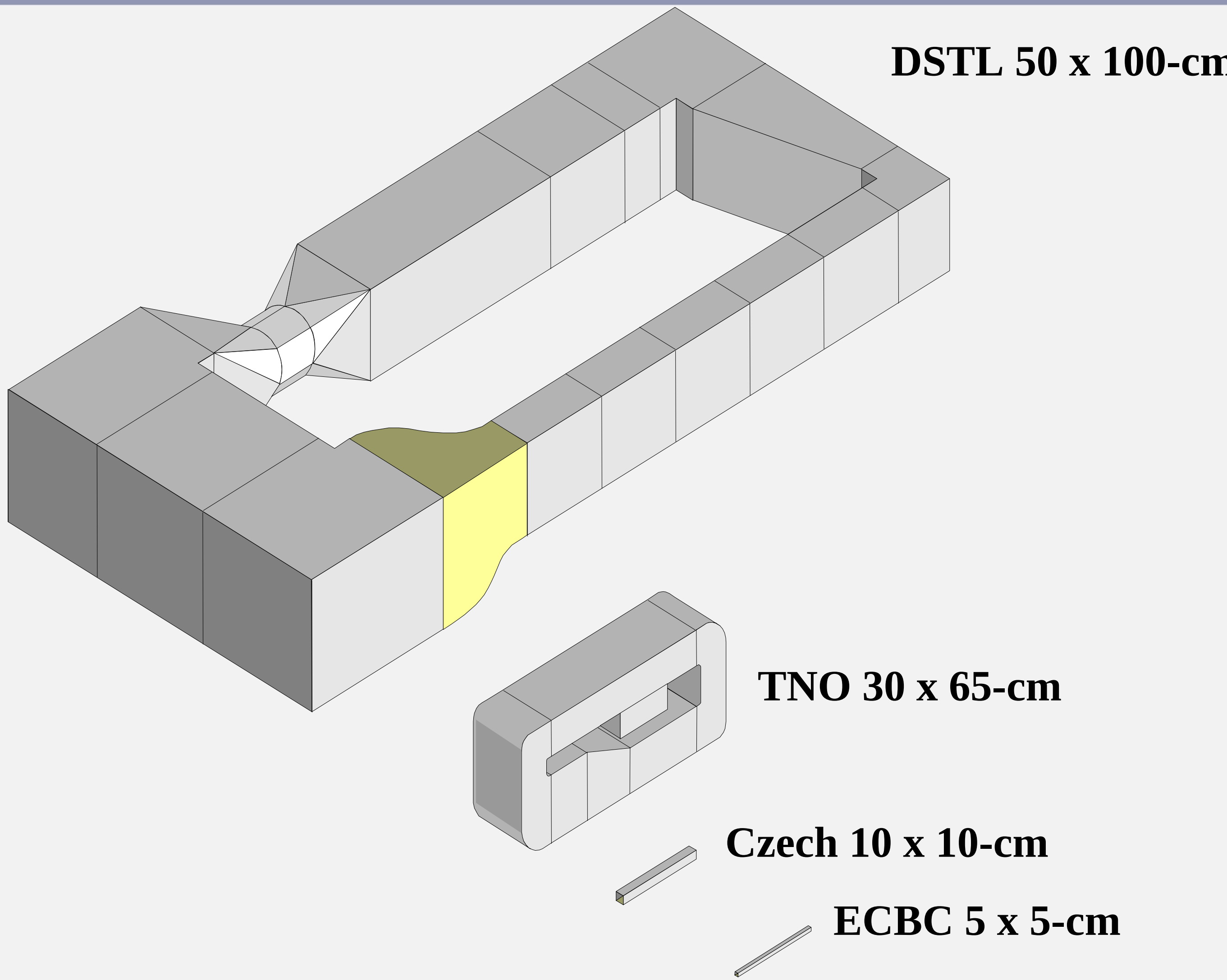
Priorities: 1. non-absorptive, non-reactive
2. absorptive, non-reactive
3. non-absorptive, reactive
4. absorptive, reactive

Agents	**Substrates**	**Test Matrix**
HD	**Glass[1,2]/Teflon[1]**	**Velocity @5mm: 0.2, 1.6, 3.3 m/s**
VX	**Concrete[4]**	**Drop Size: 0.0005, 0.2, 9.0 µL**
GD	**Asphalt[4]**	**Temperature: 0/20, 25, 55 deg. C**
NTA	**Grass[2]**	**RH: 5 to 90%**
Thickened VX	**Sand[2]/Clay[2]**	
Thickened GD		

Atmospheric Surface Layer



Agent Fate Wind Tunnels (to the same scale)



AGENTFATE

Scale Independence of Agent Fate Wind Tunnels

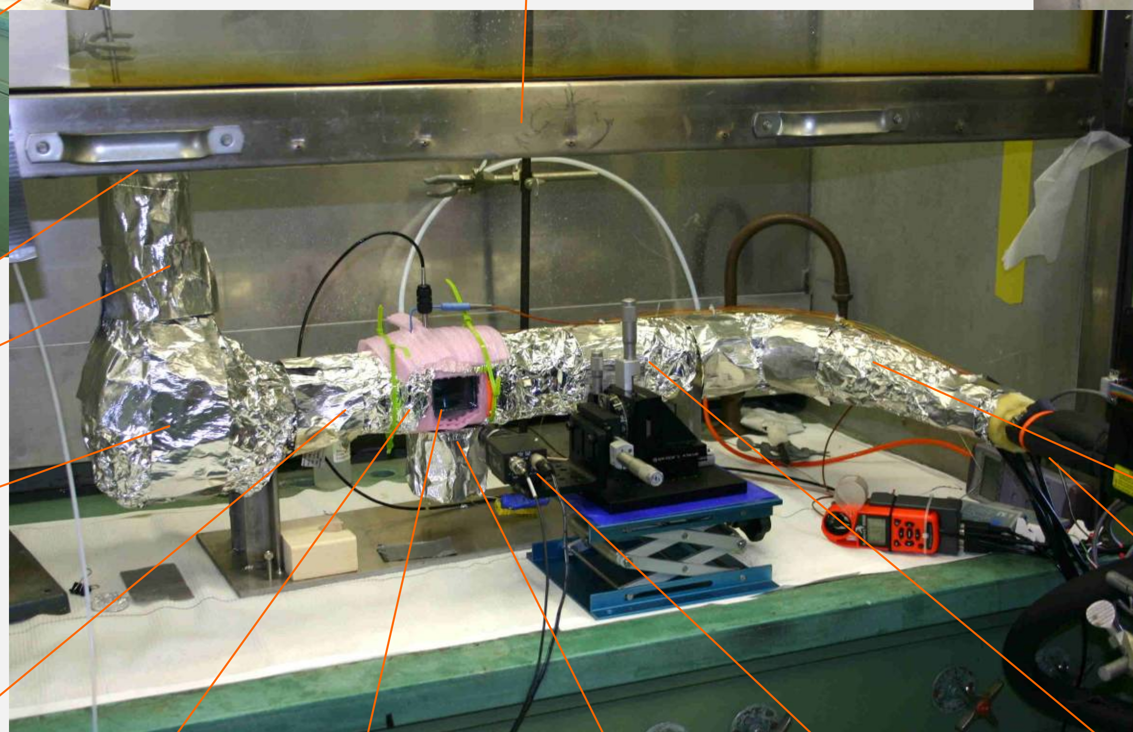
- **No scaling corrections are required** between the various sizes of wind tunnels used in the Agent Fate Program. Since the **tunnels all possess the same velocity profiles** (based on realistic wind conditions), the **agent/substrate combinations** being tested **experience the same air flow** and evaporation environment.

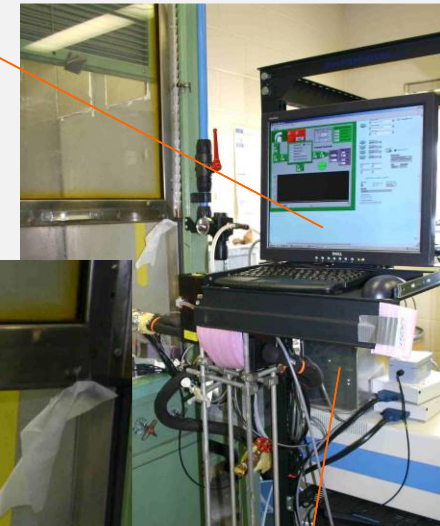
Accordingly, identical data should be obtained for identical agents/substrates tested in any of the tunnels. This finding allows the results from the tunnels to be directly compared and also eliminates the need to perform duplicate tests in the different tunnels.

NO SCALING CORRECTIONS ARE REQUIRED

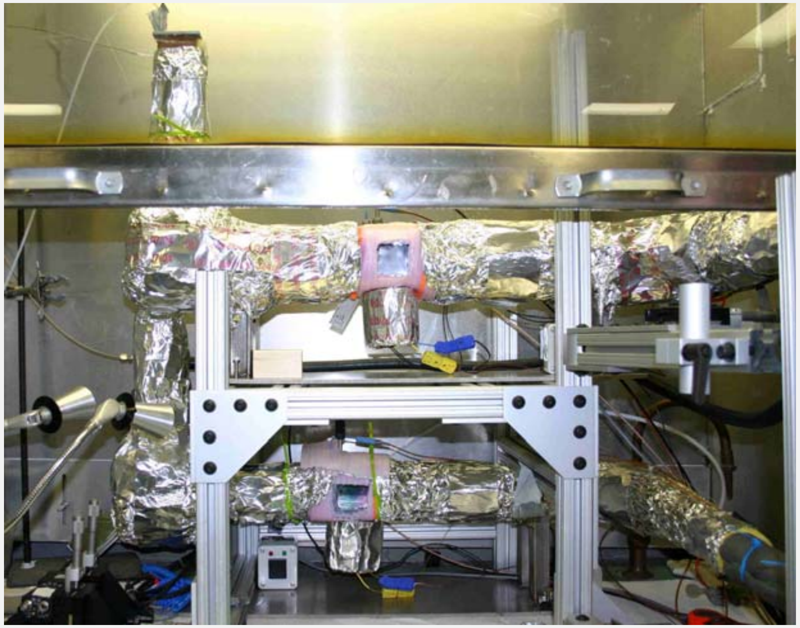
- **Based on assessment by**:
Dr. Klewicki, University of Utah
Recognized expert in theoretical and experimental atmospheric boundary

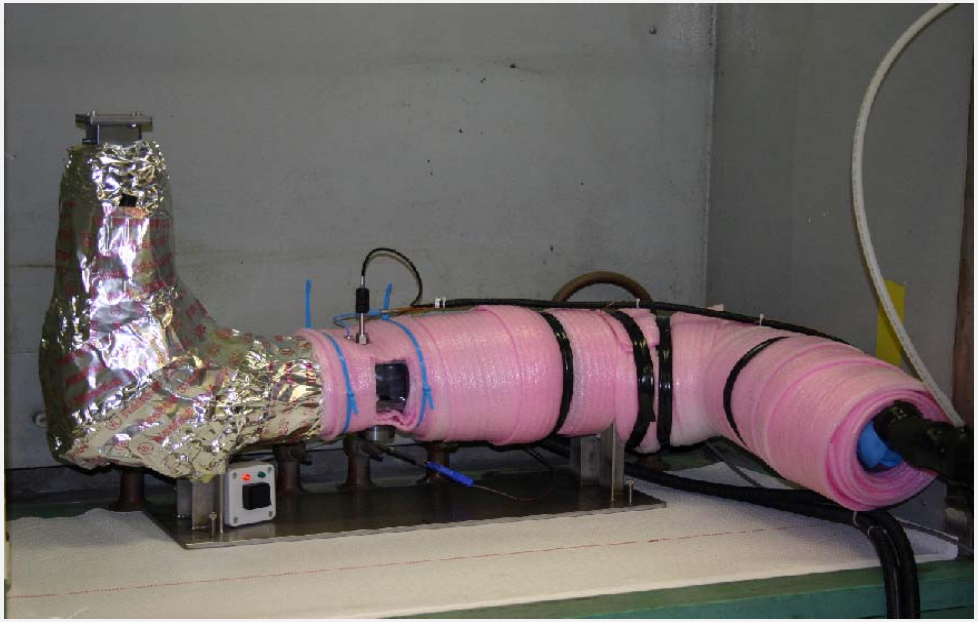
5 x 5-cm Wind Tunnel Operational Arrangement





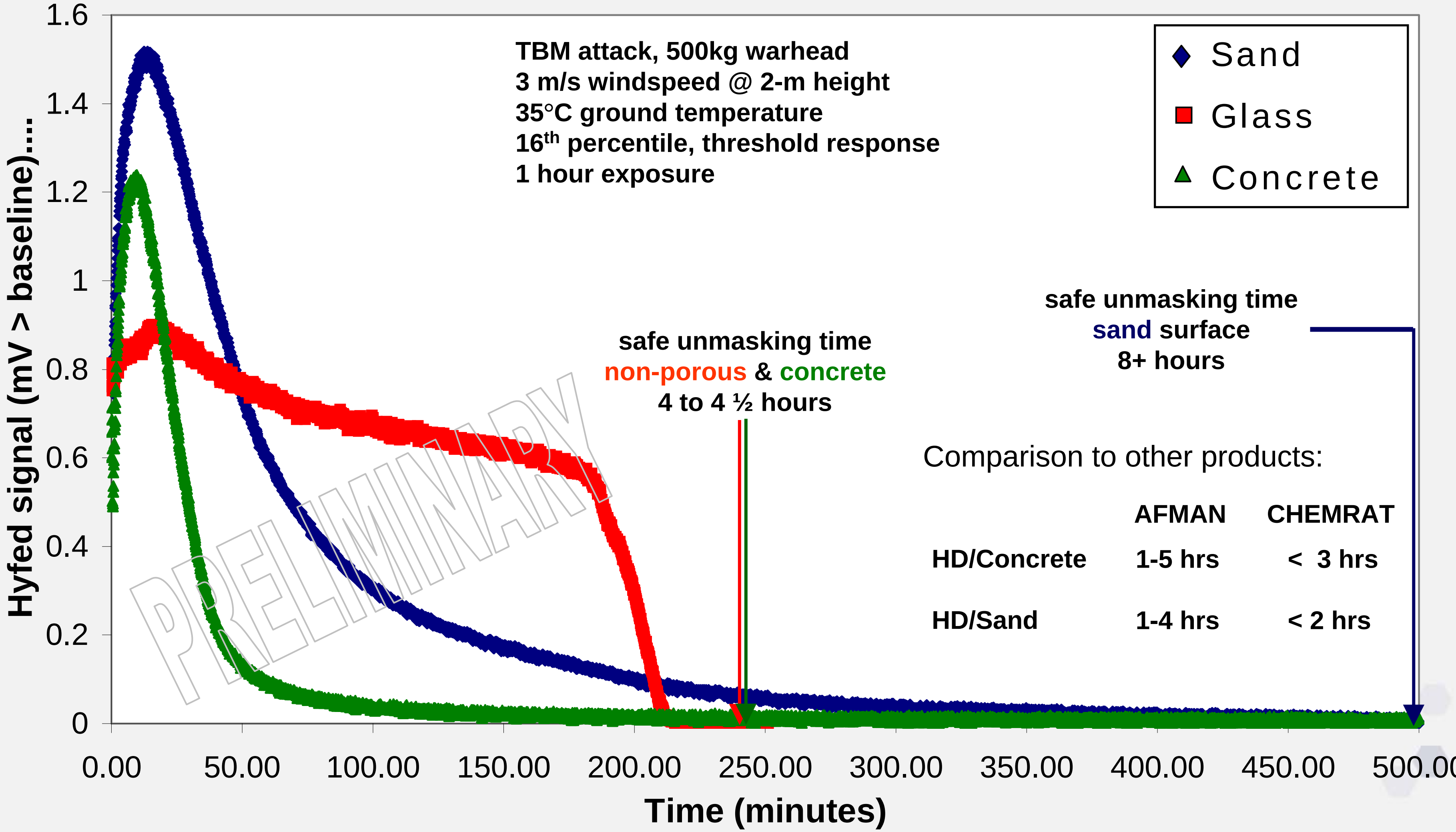
5-cm Wind Tunnels





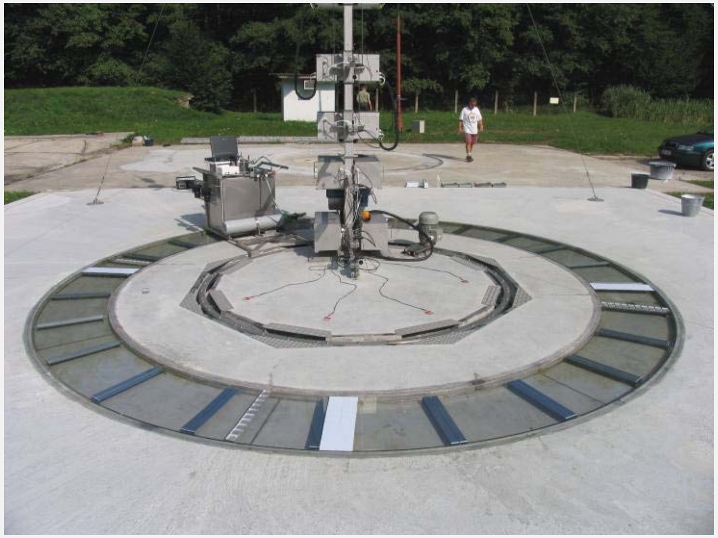
Sub-ambient ECBC windtunnel

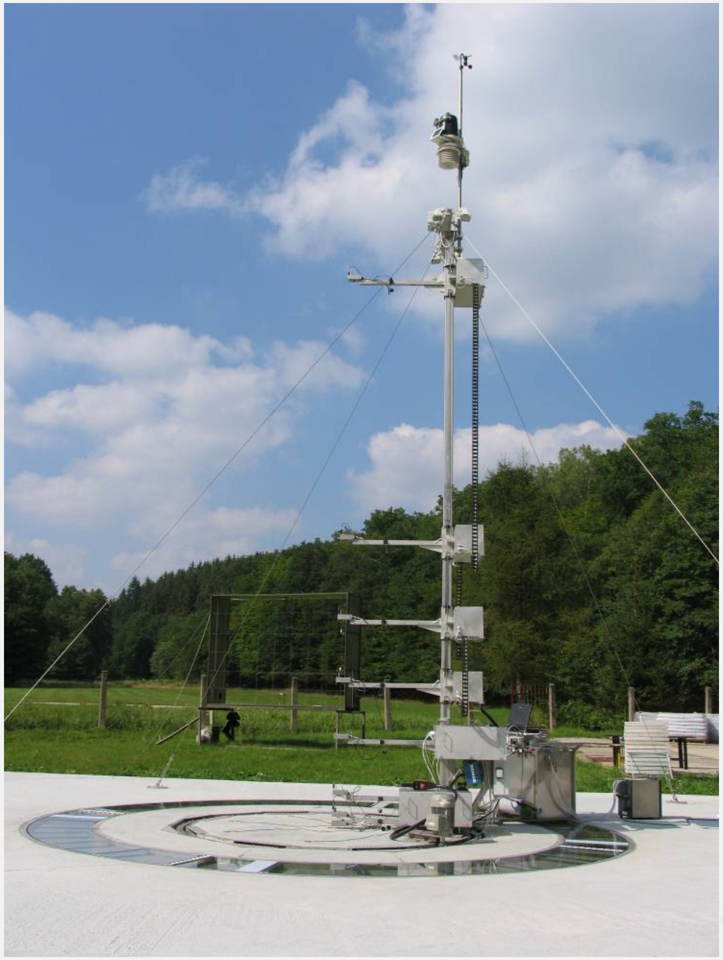
Persistence Estimates
HD On Concrete/Sand Vapor Hazard



Open Air Field Trials
Improved Test Pad

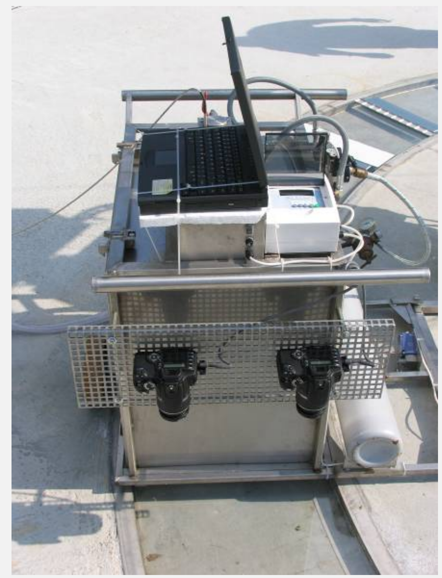
- Track-driven system to regulate dissemination device speed
- New concrete pad
- New sampling mast, arms, and sampling hardware/equipment





Open Air Field Trials
Agent Dissemination Device

- 2005 Objectives were to minimize:
  - Variance in circumferental deposition density
  - Variance in annular deposition density (more uniform density)
  - Droplet overlap and droplet size distribution
- Objectives met with new dissemination device (goose)
- New goose performance allows for more accurate
  - Mass balance
  - Determination of evaporation rate



HD On Glass (15 Sep 2005)

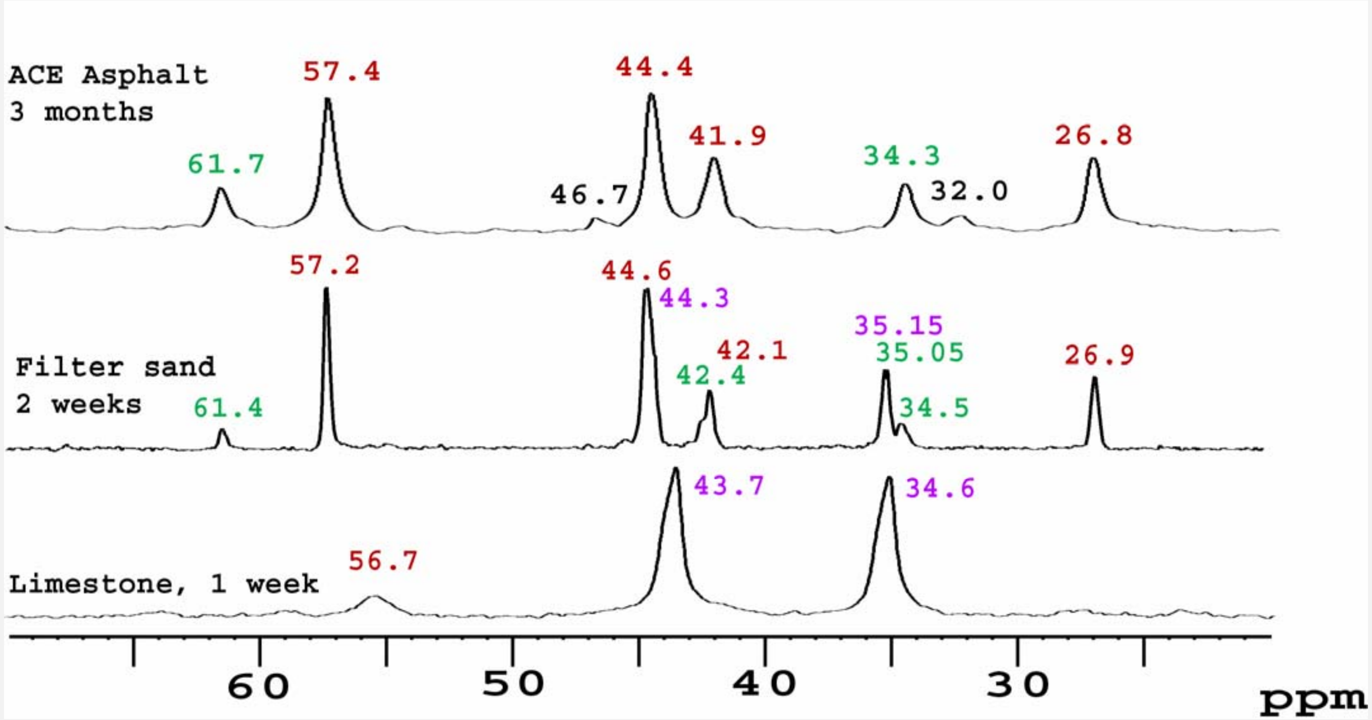
Methodology Development

Results: Degradation of HD* on Ambient Substrates

• Limestone:	No reaction in 7 months
• Asphalt:	No reaction in 2 months
• Sand:	No reaction in 7 months
• Mortars:	Half-lives of weeks to years.
• Concrete:	Half-lives of weeks to years.

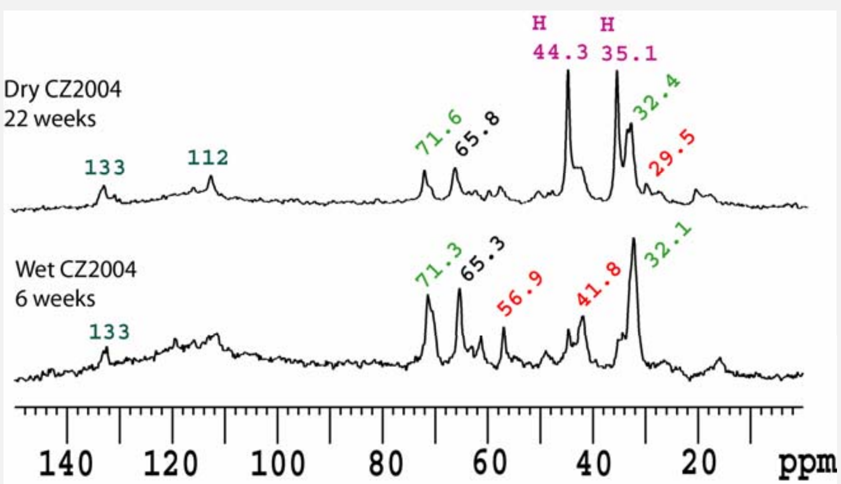
HD* and Water on Asphalt, Sand & Limestone

- The sulfonium ion H-2TG (toxic) was the major product, >75%.
- An alcohol – thiodiglycol (non-toxic) and/or chlorohydrin - was also formed.
- Half-lives: ~1 month for asphalt and limestone, 1-2 weeks for sand.



HD* and Water on Concrete

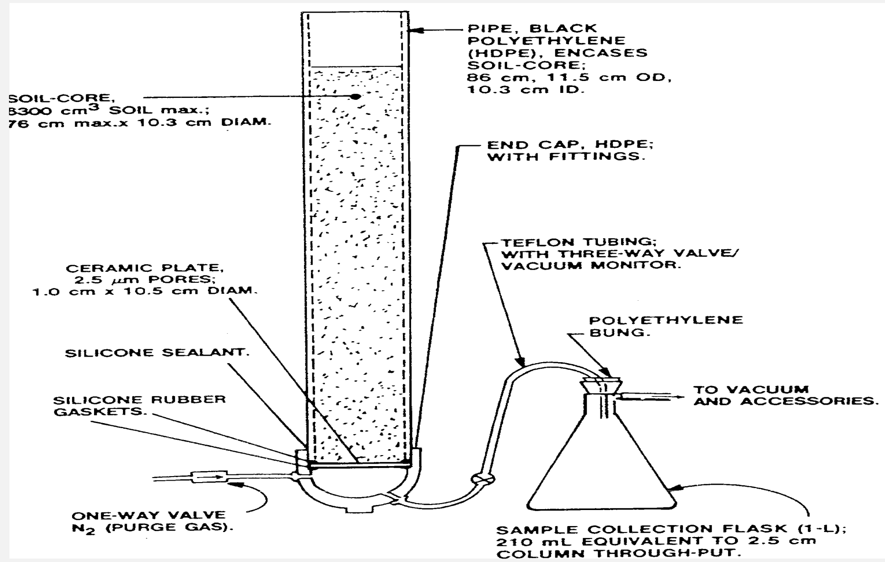
- The product distribution varied from sample to sample.
  - The sulfonium ion H-2TG (toxic) was a minor product, 0-30%.
  - 2-chloroethyl vinyl sulfide, minor product, 10–15%
  - Thiodiglycol (non-toxic) was also formed, 5 – 25%.
  - Product tentatively identified as 1,4-oxathiane, ~30%
  - Unknown at 65.5 ppm, 25-50%
- Half-lives: 3 – 9 days for wet concrete and mortar samples.
- Non-toxic products in green; toxic in red.



Comparison of HD* on ambient concrete (“dry”) and with added water (“wet”).

The same products were formed; water decreased the half-life from months to days.

Soil System Unit



General Schematic

References

USEPA. 1987. Soil-Core Microcosm Test. Fed. Reg. 52, 36363-36371.

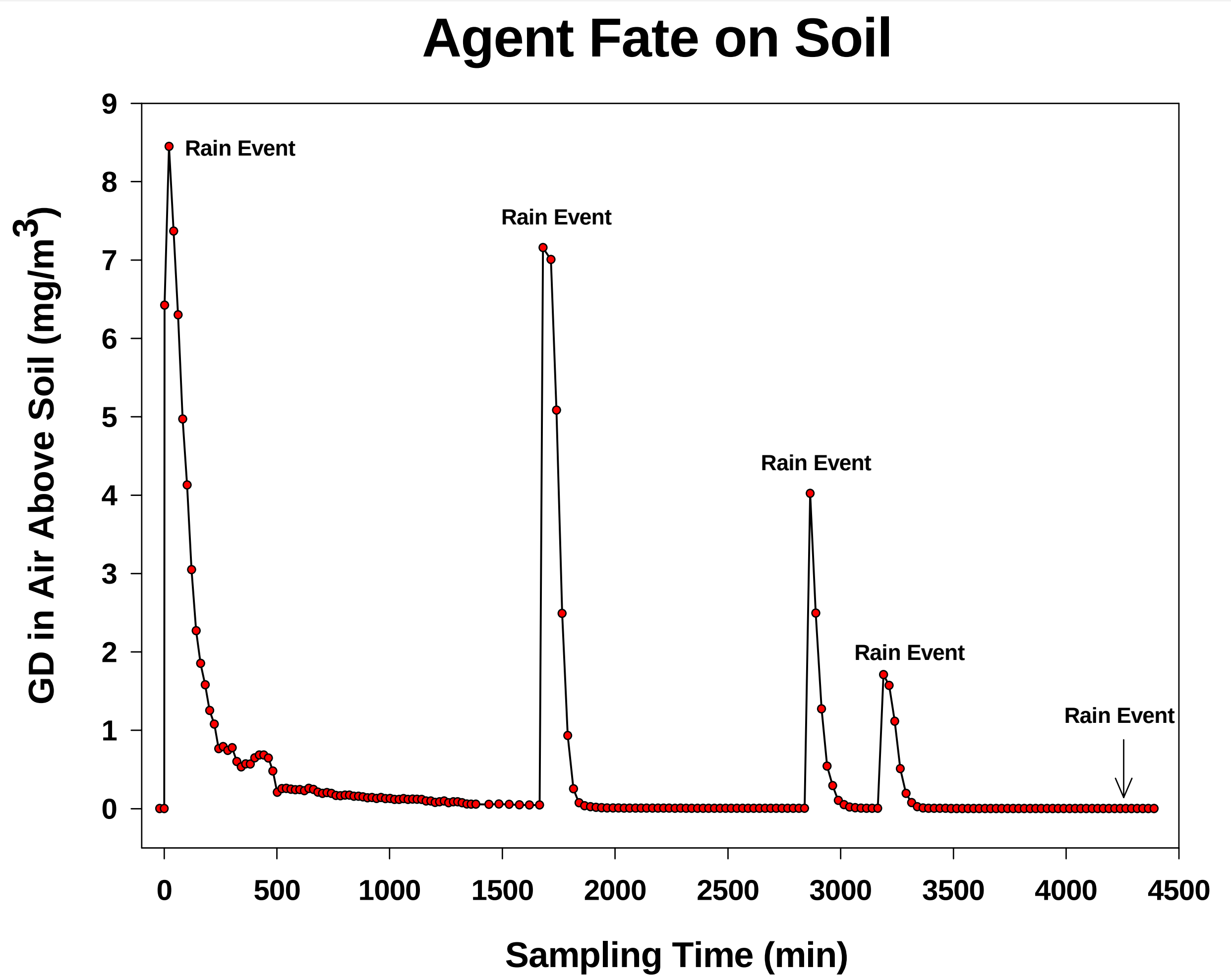
Checkai, R.T., Wentsel, R.S., Phillips, C.T., Yon, R.L. 1993. Controlled Environment Soil-Core Microcosm Unit for Investigating Fate, Migration, and Transformation of Chemicals in Soils. J. Soil Contam. 2(3):229-243.

USEPA. 1996. Ecological Effects Test Guidelines: Terrestrial Soil-Core Microcosm Test. EPA712–C–96–143. Office of Prevention, Pesticides & Toxic Substances, Washington, DC.

Environmental Analysis of Contaminated Sites. 2002. Sunahara, G., Renoux, A., Thellen, C., Gaudet, C., Pilon, A., Eds. John Wiley & Sons, New York, NY.

Checkai, R.T., et al. 2004. Innovative Methods for Investigating the Fate of Chemical Warfare Agents in Soil. 24th Army Science Conference. Accepted for presentation and publication.

Simulated Rain Event On Soil

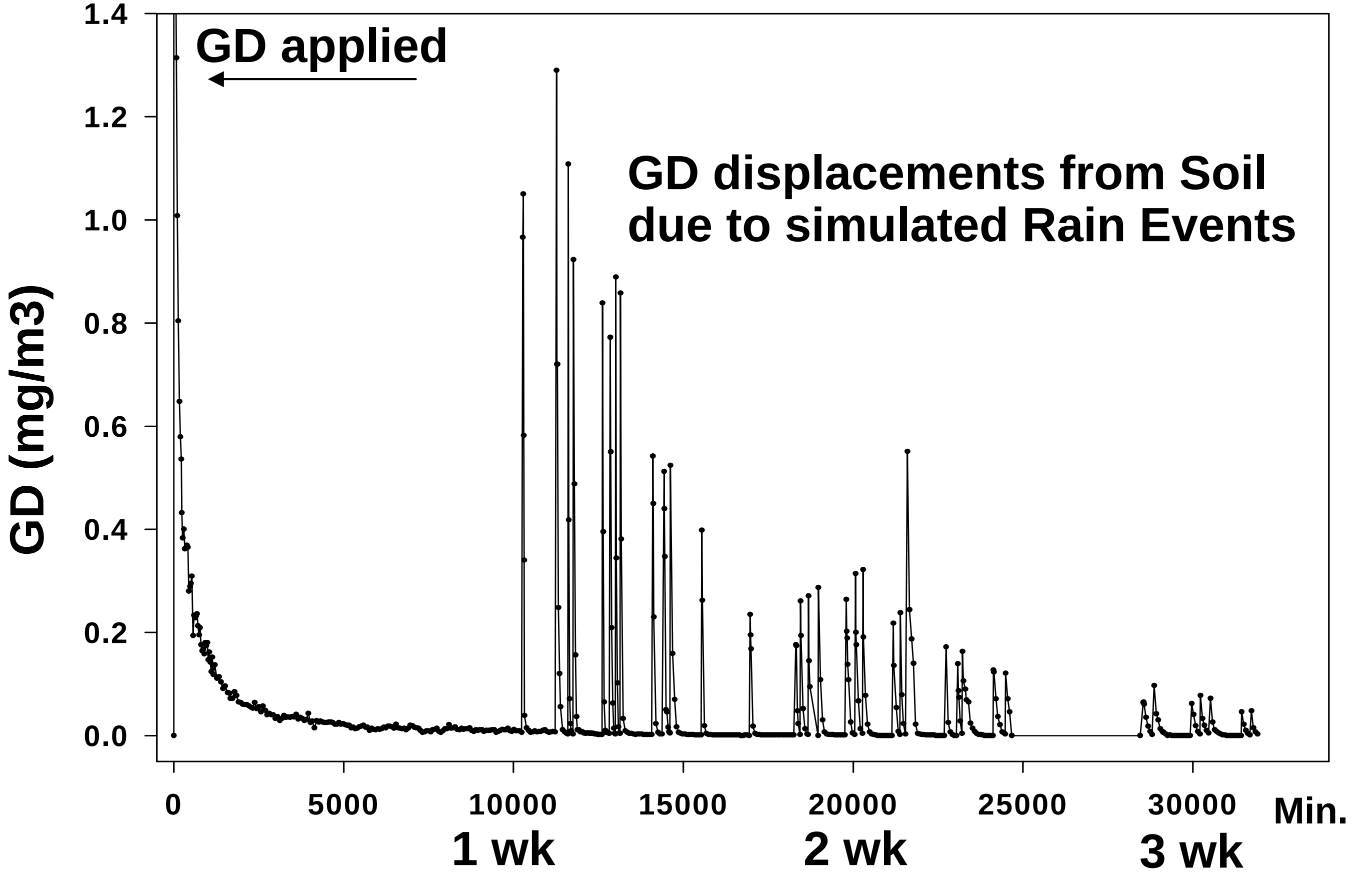


Atmospheric concentrations of GD above the soil surface: Monitored until undetectable (Time 0). Very light simulated rain events sufficient to just moisten the soil surface were applied. Rain events displacement of GD from the soil into the atmosphere above the soil. Successive displacement reactions occurred over the course of days in Response to very light simulated rain events.

Agent Application: 80 µl neat GD dropped onto soil surface using gas tight syringe (applied from 1 inch above soil surface). Approximate droplet size 3.6 µl .

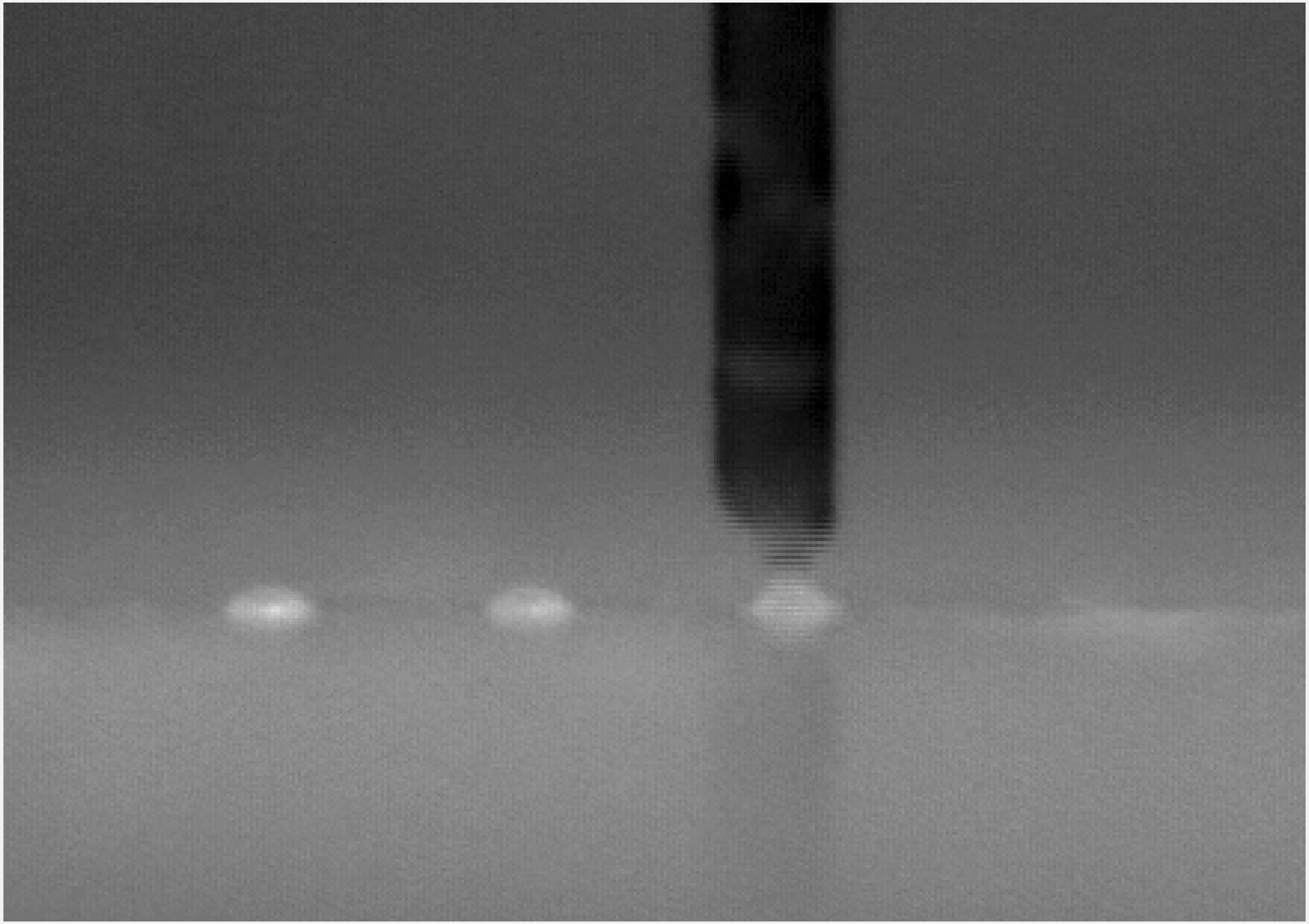
Rain Event: Moisture from the Synthetic Rain Generator, (1.6 ml distilled water/event).

GD on Dry Composite Soil



- GD displacement into air remains ≥0.05 mg/m3 (IDLH) after 35 Rain Events
- Light simulated Rain Events were applied after GD conc. in air ≤0.005 mg/m3
- GD persists much longer in complex soil (e.g., sand + clay + humus)

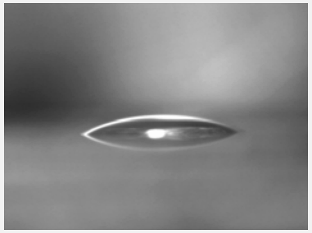
1 nL droplets on a Teflon surface



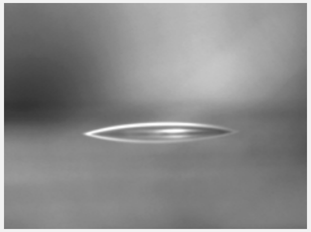
Optical Results

Agent Drop on Non-Absorbent, Non-Reactive Surface

$t = t_0$



$t > t_0$



$t >> t_0$

Evaporation Sequence

Concrete

Cut-away

- **Agent absorbs rapidly**
- **Spreads deep into substrate**
- **Follows aggregate**
- **Varies with concrete type**

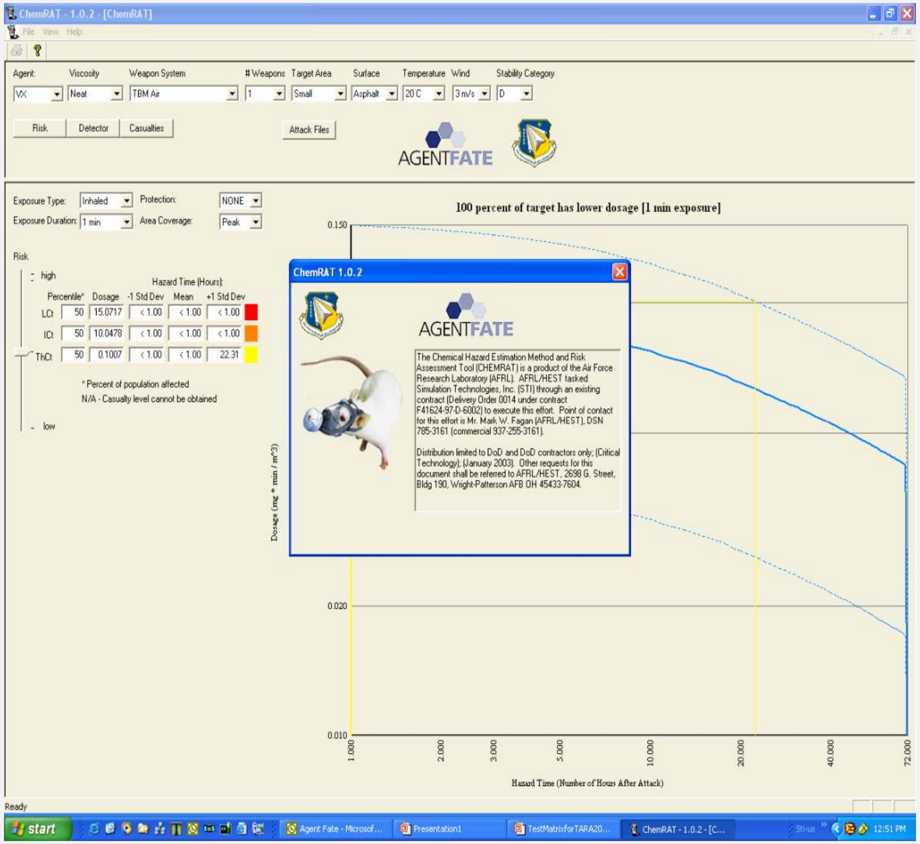
Asphalt

Cut-away

- **Agent absorbs rapidly**
- **Spreads wide over substrate**
- **Creates tar-like solvate**

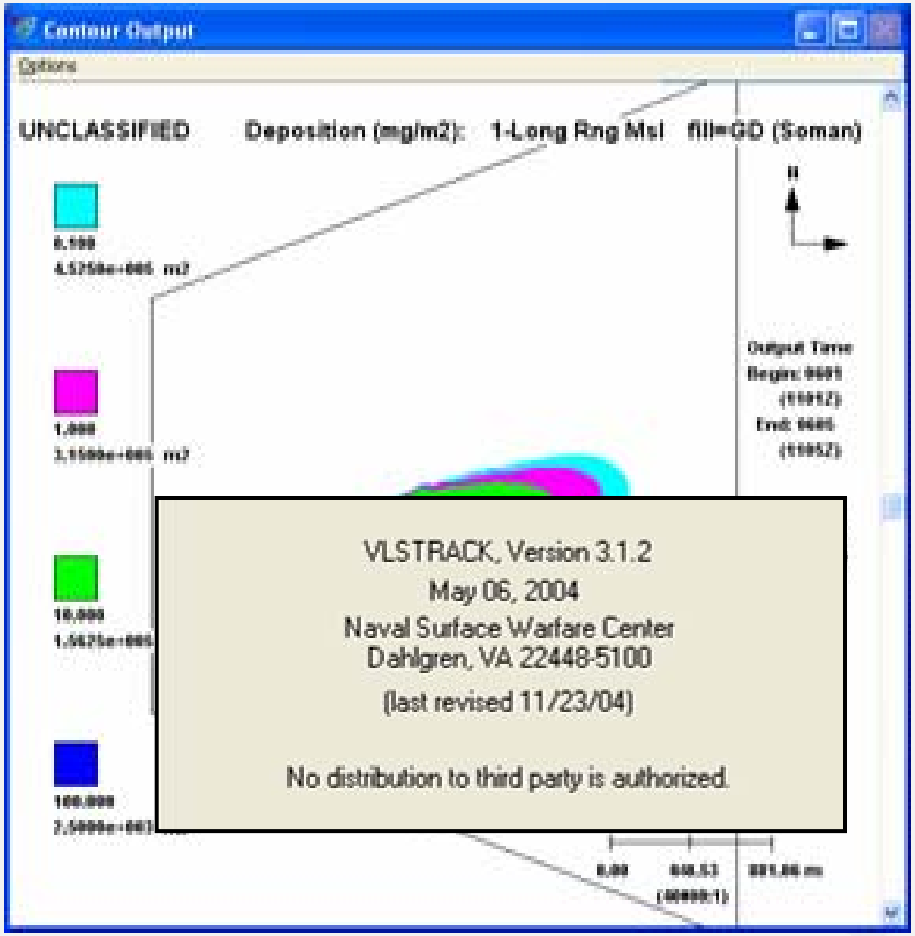
Decision Aiding Analysis & Tools
CHEMRAT

- CHEMRAT initiated by warfighter urgent need request
- Developed and fielded in 3 months
  - Ver 1.0 released in Jan 2003
  - Deployed to OIF
- Interim accredited by DATSD-CBD in April 2003
- Transitioned to JOEF in FY05
- Currently used by USAF, USN, NORTHCOM, DHS, DOE
- Ver 1.5 to be released in 1st quarter FY06
  - Updated data from Agent Fate Program



Decision Aiding Analysis & Tools VLSTRACK Update

- VLSTRACK updated to version 3.1.2
  - Released June 2004
- Updated with Agent Fate Program data
- VLSTRACK is integration test bed for transition of Agent Fate evaporation models to JEM
- New contact hazard and liquid pickup model being added



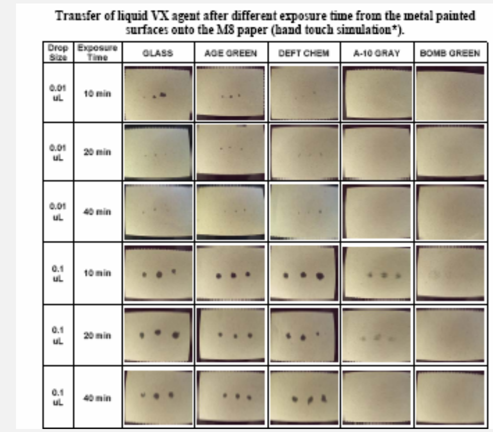
Decision Aiding Analysis & Tools AFMAN 10-2602 Table Updates

- USAF guidance manuals being updated with revised hazard prediction tables
  - AFMAN 10-2602
  - AFMAN 10-2517
- Estimates derived from updated VLSTRACK predictions
- Incorporates newest agent fate data
- Scheduled release in Dec 2005

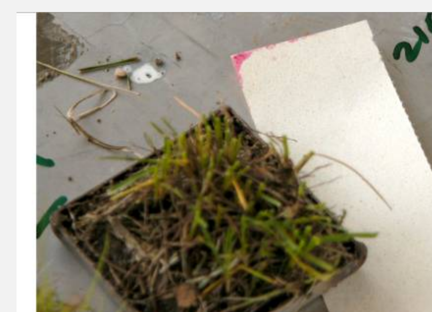
Vapor Hazard VX On Concrete ECt 16									
		Stability		PSC D	PSC F	PSC D	PSC F	PSC D	PSC F
		Wind Speed (knots)		2		6		10	
Agent	Release	Munition	Temp °C (°F)						
VX	Low Alt.	TBM	-5 (23)	0.21	0	0.0	0	0.03	0
VX	High Alt.	TBM	-5 (23)	0	0	0.0	0	0	0
VX	Low Alt.	TBM	10 (50)	24.0	16	0.49	0	0.3	0.1
VX	High Alt.	TBM	10 (50)	9	0	0	0	0.1	0.0
VX	Low Alt.	TBM	25 (77)	72	72	3.57	1.5	1.88	0.9
VX	High Alt.	TBM	25 (77)	72	20	4.6	0.43	0.6	0.22
VX	Low Alt.	TBM	50 (122)	72	72	56.19	72	45.19	22.19
VX	High Alt.	TBM	50 (122)	72	72	43.19	16	7.8	13.5

Decision Aiding Analysis
Revised C-CW CONOPS and TTPs

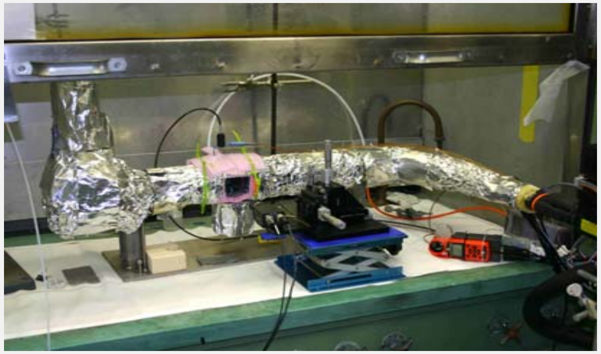
- Leveraged live agent outdoor tests to quantify and assess detection levels of:
  - CAMs
  - M-22 ACADAs
  - M-8 paper
  - M-256A kits
  - HAPSITE
  - M-279 surface sampler
- Determine droplet spread factors
- Quantify transfer of liquid agent by vehicles
- Determine effectiveness of foot/glove decon procedure


Transfer of liquid VX agent after different exposure time from the metal painted surfaces onto the M8 paper (hand touch simulation*).

Drop Size	Exposure Time	GLASS	AGE GREEN	DEFT CHEM	A-10 GRAY	BOMB GREEN
0.01 uL	10 min					
0.01 uL	20 min					
0.01 uL	40 min					
0.1 uL	10 min					
0.1 uL	20 min					
0.1 uL	40 min					



Transitioning CW Agent Fate S&T Into Products For CBDP Users



Vapor Hazard VX On Concrete ECt 16									
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		Wind Speed (knots)		2		6		10	
Agent	Release	Munition	Temp °C (°F)						
VX	Low Alt.	TBM	-5 (23)	0.21	0	0.0	0	0.03	0
VX	High Alt.	TBM	-5 (23)	0	0	0.0	0	0	0
VX	Low Alt.	TBM	10 (50)	24.0	16	0.49	0	0.3	0.1
VX	High Alt.	TBM	10 (50)	9	0	0	0	0.1	0.0
VX	Low Alt.	TBM	25 (77)	72	72	3.57	1.5	1.88	0.9
VX	High Alt.	TBM	25 (77)	72	20	4.6	0.43	0.6	0.22
VX	Low Alt.	TBM	50 (122)	72	72	56.19	72	45.19	22.19
VX	High Alt.	TBM	50 (122)	72	72	43.19	16	7.8	13.5