



AGENTFATE

Environmental Fate Of Chemical Warfare Agents: Agent Fate Modeling

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15 November 2004

Report Documentation Page

Form Approved
OMB No. 0704-0188

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1. REPORT DATE 15 NOV 2004	2. REPORT TYPE N/A	3. DATES COVERED -	
4. TITLE AND SUBTITLE Environmental Fate Of Chemical Warfare Agents: Agent Fate Modeling		5a. CONTRACT NUMBER	
		5b. GRANT NUMBER	
		5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)		5d. PROJECT NUMBER	
		5e. TASK NUMBER	
		5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) AFRL/HEPC-CBD		8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)	
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release, distribution unlimited			
13. SUPPLEMENTARY NOTES See also ADM001849, 2004 Scientific Conference on Chemical and Biological Defense Research. Held in Hunt Valley, Maryland on 15-17 November 2004 . , The original document contains color images.			
14. ABSTRACT			
15. SUBJECT TERMS			
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified	UU
			18. NUMBER OF PAGES 15
			19a. NAME OF RESPONSIBLE PERSON



Program Objectives/Payoffs



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)



Agent Fate Modeling

Improve prediction of CWA secondary evaporation and liquid contact & pickup

CWA Hazard Prediction Model



Release

Initial Vapor

Liquid Drops

Vapor from Falling Drops

Evaporation

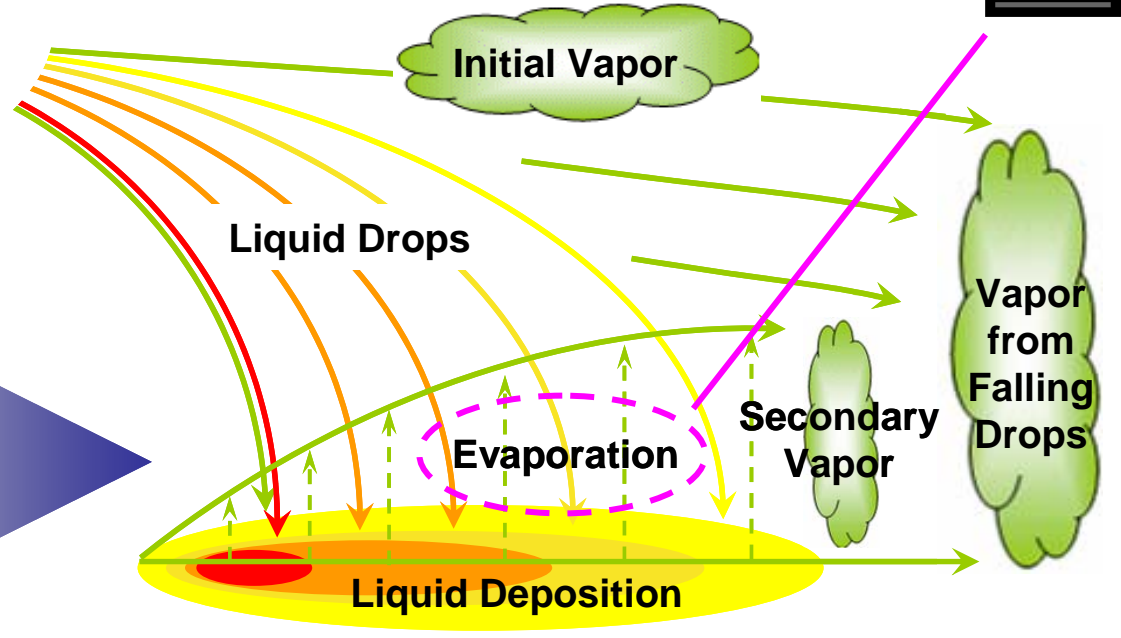
Secondary Vapor

Wind

Liquid Deposition

- Hazard**
- Challenge
 - threat
 - dissemination
 - evaporation
 - T&D
 - Toxicity
 - Exposure
 - Protection
 - Risk

Larger Droplets Smaller Droplets





Model Development Approach



Concurrently Pursuing Wide Range of Modeling Approaches
Semi-Empirical Model Is Contractual Requirement

How Data Is Used	Data used to define response		Data used to understand response	
Model Type	Empirical (fit to data)	Semi-empirical (theory with empiricism)		Theoretical (first principles)
Model Type Examples	Regression Chinn	PR2515	Roberts	STP 386 VLSTRACK FOA

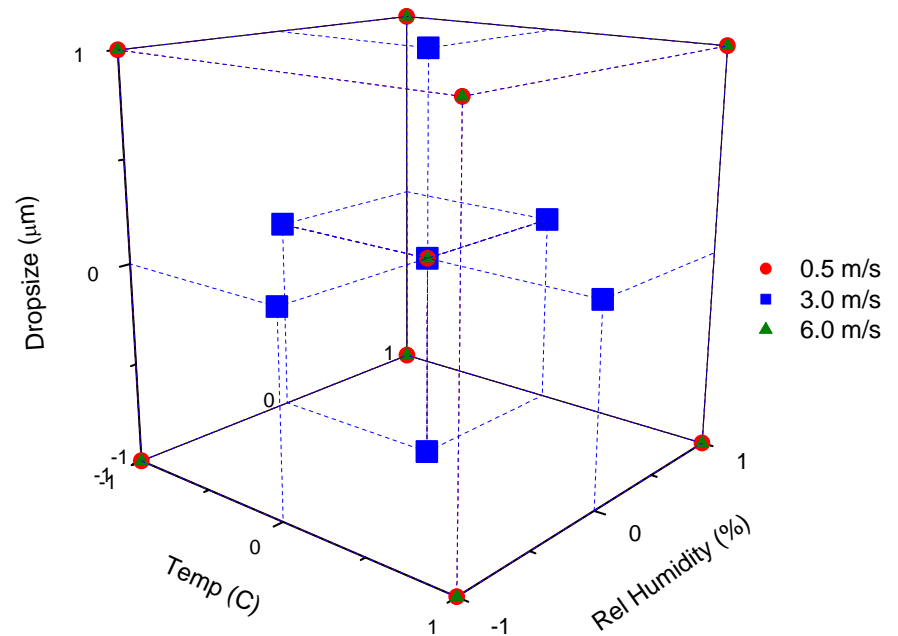


Agent Fate Data Needs



- Major factors
 - Agent, substrate, temperature, wind speed, humidity, droplet size
- 3 classical agents
- Substrates: asphalt, concrete, grass, sand, soil
- 3 factor levels for environmental conditions
 - Curvilinear effects
 - Based on operational data
- Full factorial matrix > 10,000 experiments
 - Experimental design trims to about 1300 experiments
 - Additional investigations to further reduce test matrix

Need comprehensive high quality data





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)**



State Of Data At End Of Program



Program Provides Comprehensive Data Set For 3 Classical Agents

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	✓	✓	✓	✓	✓
	≤ 15	✓	✓	✓	✓	✓
	≤ 30	✓	✓	✓	✓	✓
	> 30	✓	✓	✓	✓	✓
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	✓	✓	✓	✓	✓
	≤ 30	✓	✓	✓	✓	✓
	> 30	✓	✓	✓	✓	✓
F	≤ 0	✓	✓	✓	✓	✓
	≤ 15	✓	✓	✓	✓	✓
	≤ 30	✓	✓	✓	✓	✓
	> 30	✓	✓	✓	✓	✓

✓ Data added via Agent Fate Program



Agent Fate Testing



Multiple levels of agent fate test data needed for model development

Wind Tunnel Tests



- Controlled environment
- Factor effects on evaporation
- Primary source of model development data
- Limited scrutiny on agent/substrate interaction effects

Outdoor Trials



- "Ground truth"
- Correct wind tunnel model
- Validate field model

Lab Experiments



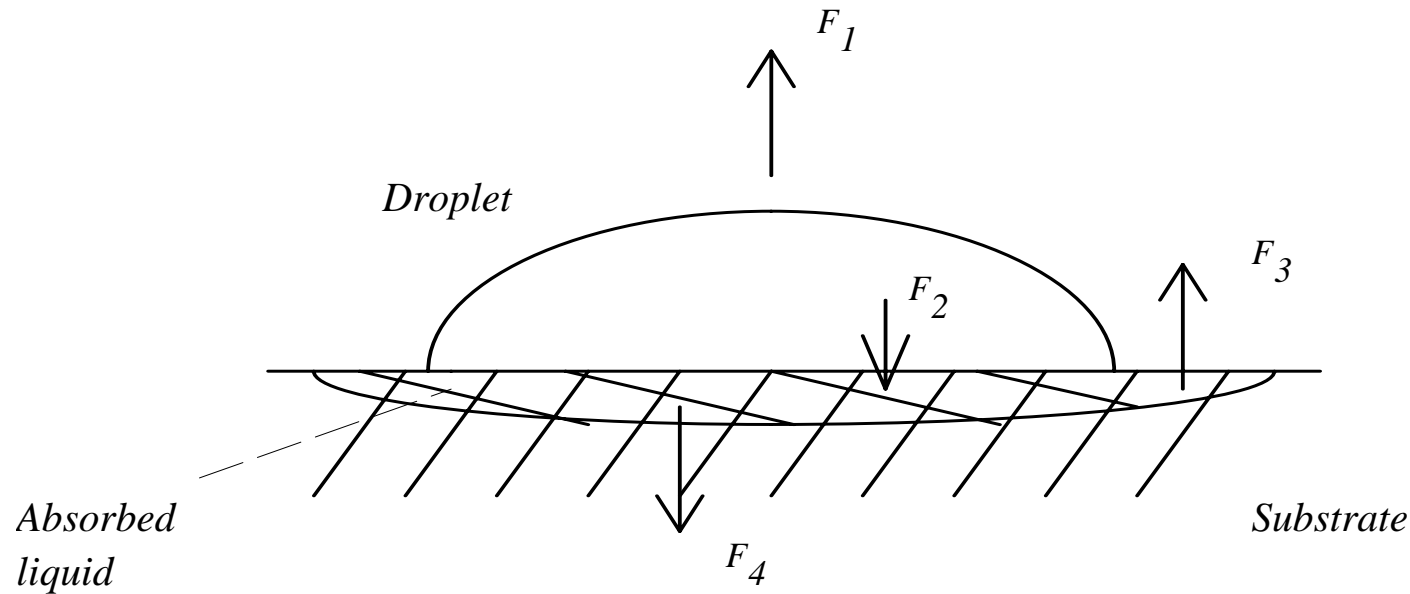
- Agent/substrate interaction
- ID substrate parameters affecting evaporation
- Expands WT model to surfaces beyond those tested



Semi-Empirical Evaporation Model



Droplet-based physics model with empirical fit to data



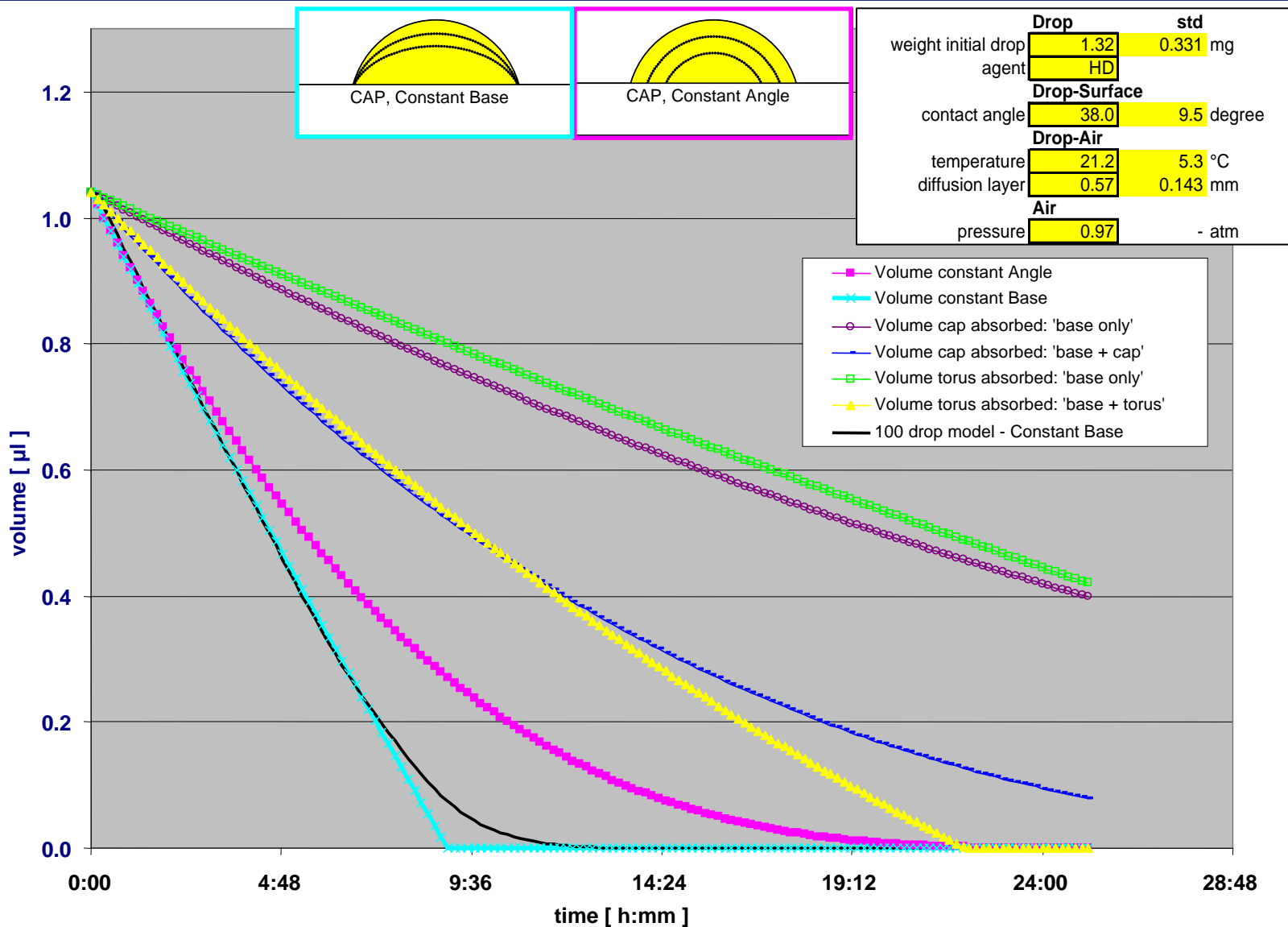
- F_1 = mass transfer - primary evaporation
- F_2 = mass transfer - absorption
- F_3 = mass transfer - desorption
- F_4 = mass transfer - decomposition

Approach:

- Droplet-based evaporation
- Segregate mass transfer into constituent components
- Add key physico-chemical processes
- Calibrate unknown model parameters to empirical data
- Limited model inputs with extensibility

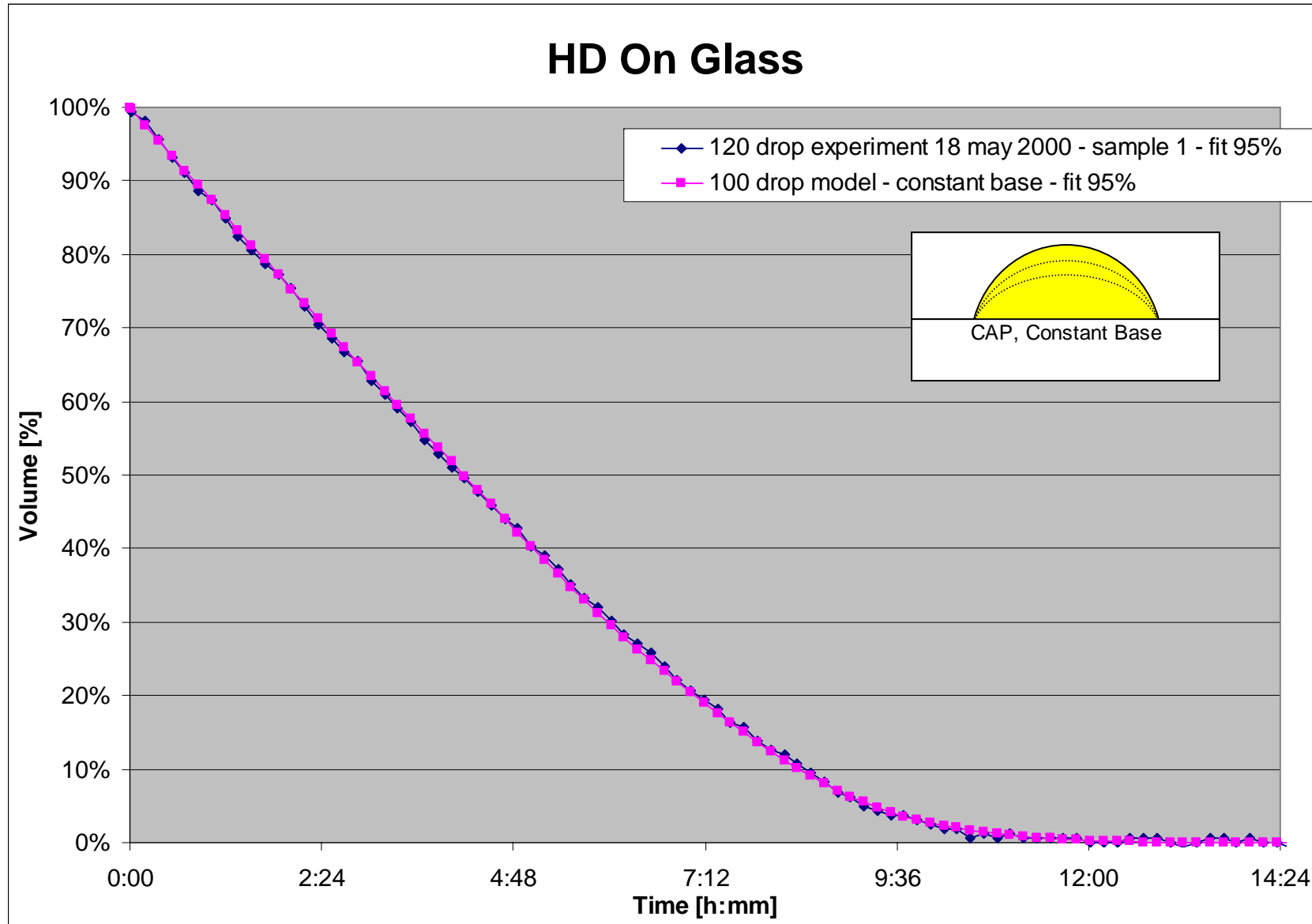


Non-Porous Surface Evaporation Model



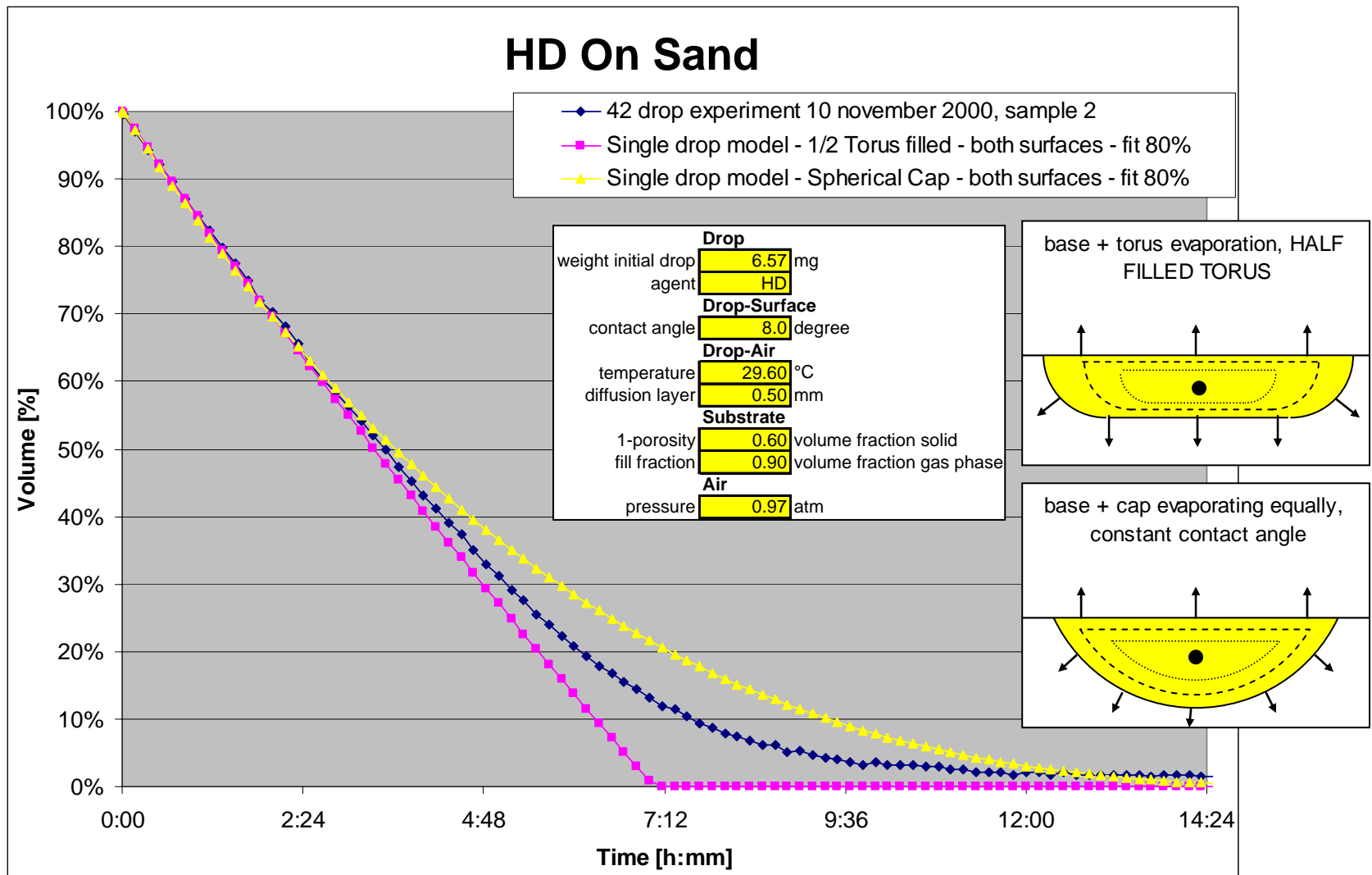


Non-Porous Surface Evaporation Model Example





Porous Surface Evaporation Model





Wind Tunnel Model To Field Model

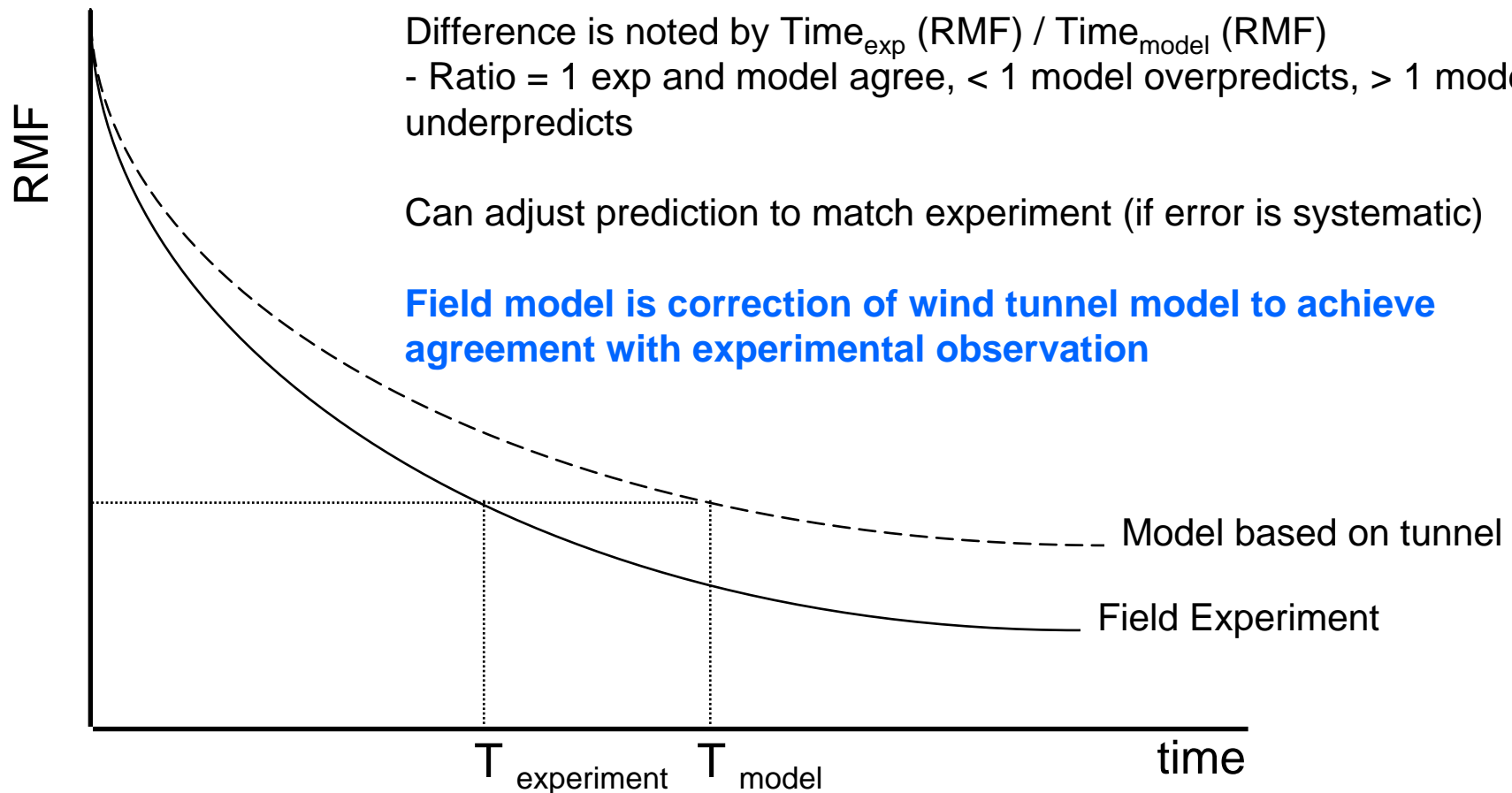


Field trials contain effects not accounted for in wind tunnel model so when you plug field trial observation data into wind tunnel model there are differences

Difference is noted by $\text{Time}_{\text{exp}} (\text{RMF}) / \text{Time}_{\text{model}} (\text{RMF})$
- Ratio = 1 exp and model agree, < 1 model overpredicts, > 1 model underpredicts

Can adjust prediction to match experiment (if error is systematic)

Field model is correction of wind tunnel model to achieve agreement with experimental observation

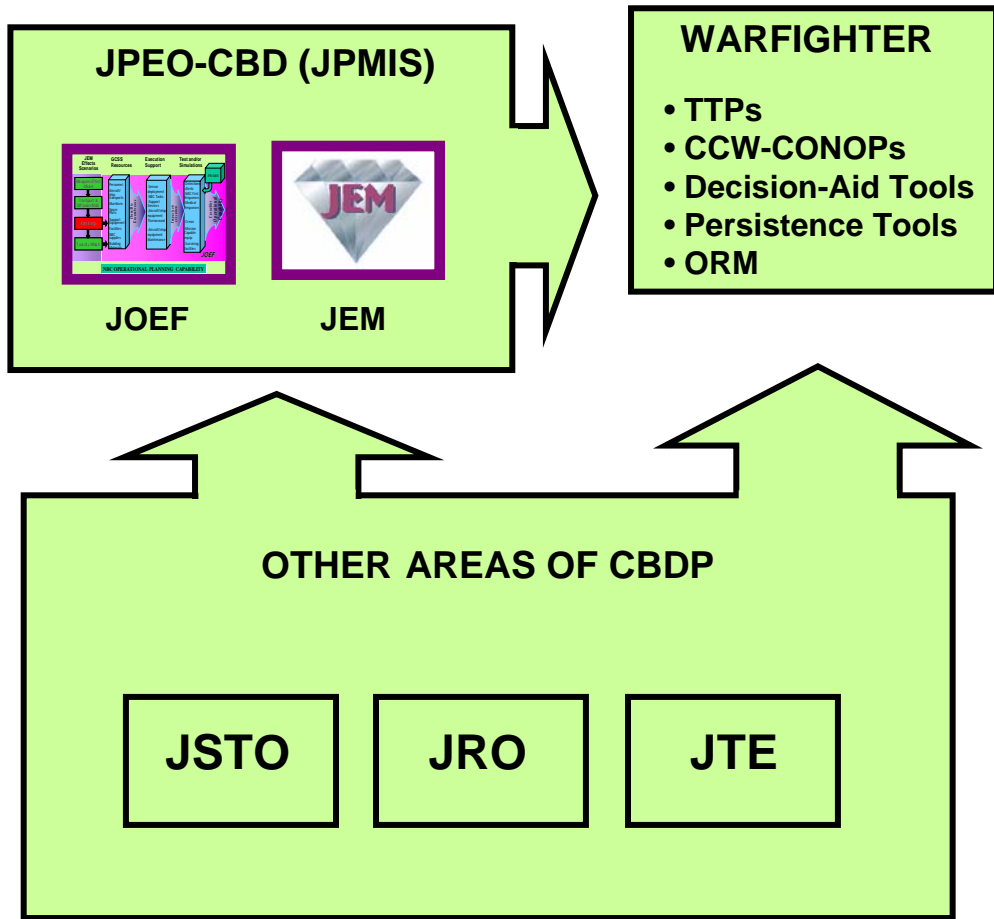
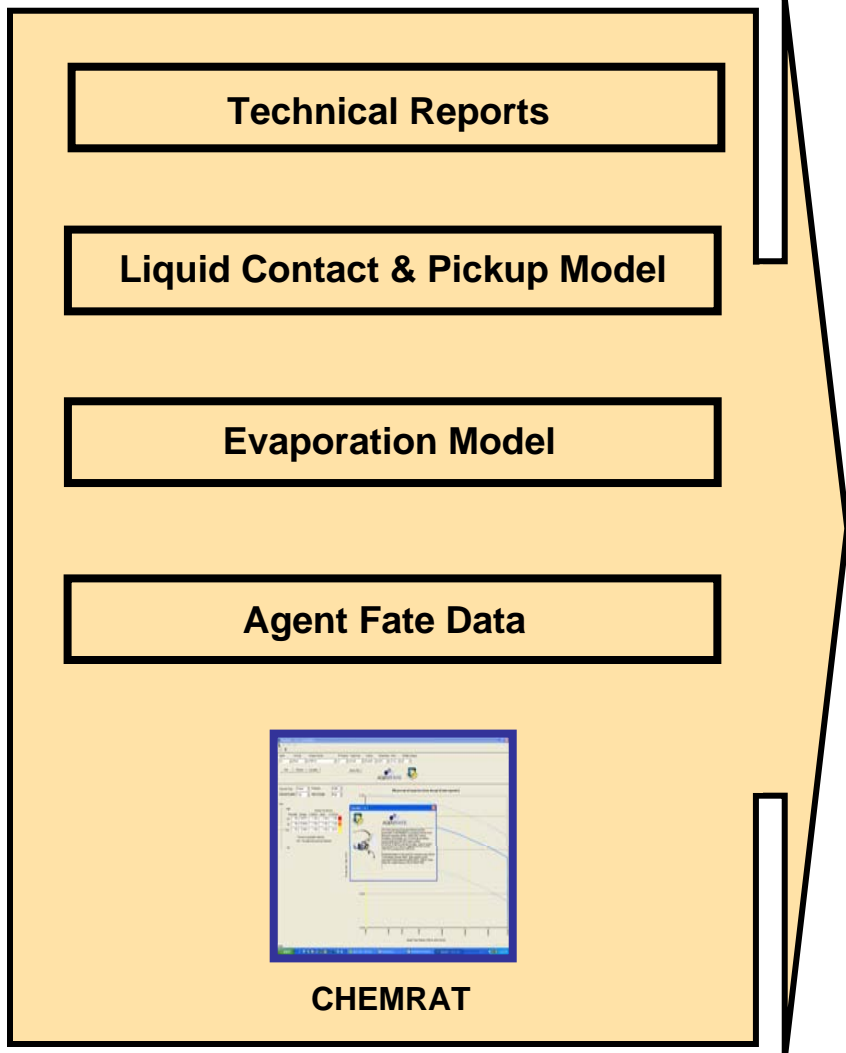




Agent Fate Technology Transition



Agent Fate Program Products





Summary



- DTO objective is to develop better persistence models
 - Improve secondary evaporation and liquid contact/pickup models
- Pursuing empirical, semi-empirical, and theoretical model development efforts
 - Semi-empirical model is contractual requirement
- Wide range of indoor/outdoor persistence testing and analytical chemistry needed to develop models
- Non-porous semi-empirical evaporation model completed
- Limited development of non-porous surface model
- Wind tunnel models must be converted to field models
- Models and data transition to CBDP and warfighter
 - Evaporation model program of record is Joint Effects Model