# *Agent Fate Predictive Modeling*

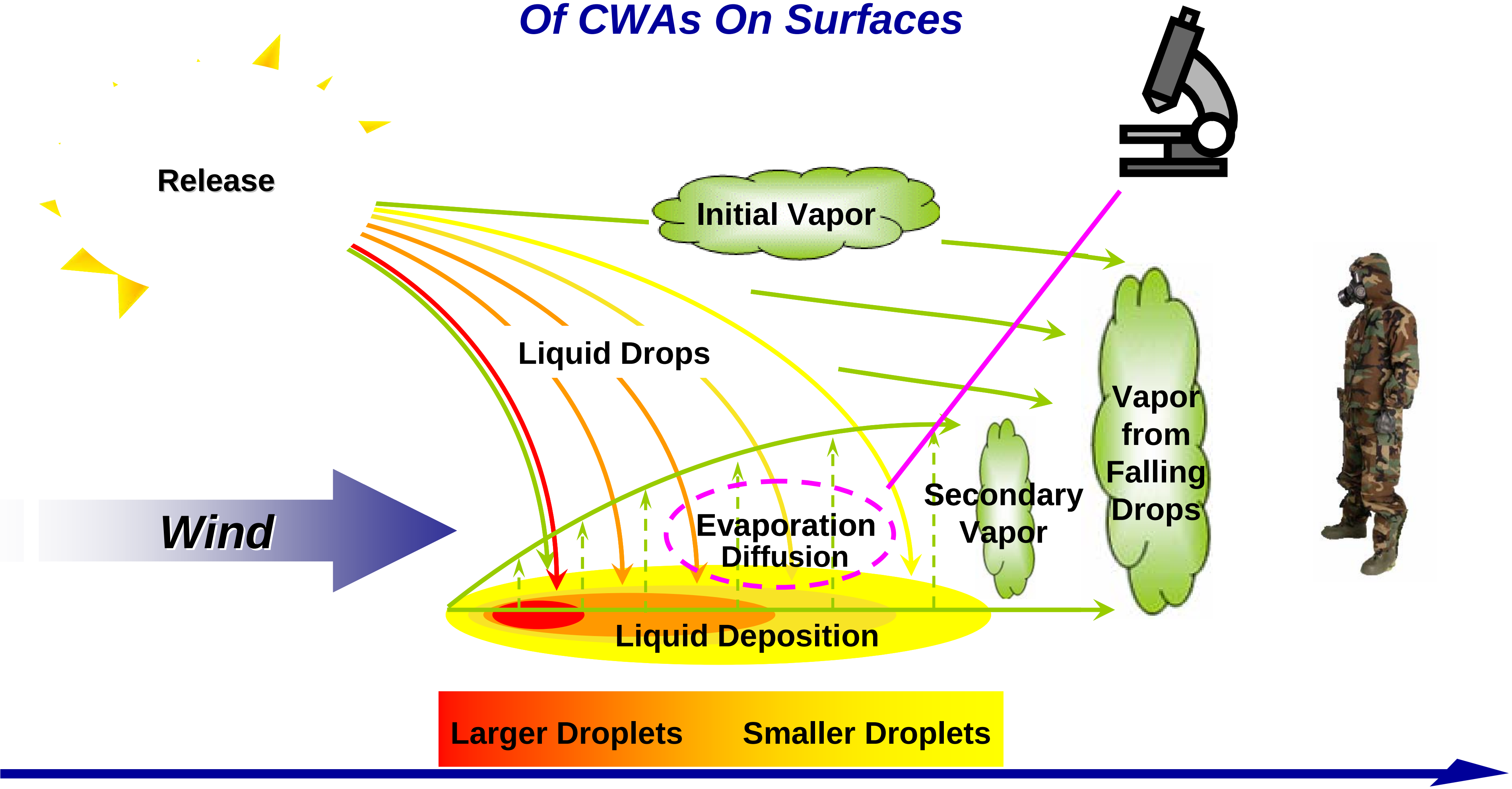
*William Kilpatrick*
*Air Force Research Laboratory*
*Wright-Patterson AFB, OH*

# Overview

- What Is Agent Fate?
- History of Agent Fate Modeling
- Agent Fate DTO Predictive Modeling
- Post-DTO Agent Fate Modeling
- Transitioning Agent Fate Modeling S&T
- Summary

# What Is Agent Fate?

***Measuring and Predicting The Physico-Chemical Processes Of CWAs On Surfaces***



# History of Agent Fate Modeling

- Sutton (1933) - PR 1102
  - 1st theoretical investigation in light of turbulence theory (i.e., wind velocity & temperature gradients) on smooth surfaces
- Pasquill (1942) – PR 2335
  - First indepth treatment of aerodynamic effect on evaporation
  - Introduced molecular diffusivity in lieu of air viscosity in Sutton’s model to describe vapor transport based on momentum exchange
- Calder (1947) – PTP33
  - Theoretical treatment on problem of eddy diffusion and evaporation
  - Used lab data to establish laws of turbulent flow
- Monaghan & McPherson (1971) – STP 386
  - 2-D atmospheric diffusion model calibrated to Canadian Prairie Grass
- NUSSE (1979)
  - Used STP 386 prairie grass methodology with correction factors for sand and HD

# History of Agent Fate Modeling

- Chinn (1981)
  - Empirical model based on volatility, drop size, wind velocity, & agent purity
- D2PUFF/D2PC (1987) [DoD model for industrial chemical hazards]
  - 2-D atmospheric diffusion model with semi-empirical correction for transition to rough surfaces
  - Used in CSEPP
- VLSTRACK (1992) [DoD model for passive defense applications]
  - Engineering evaporation model for mass transfer (i.e., non-dimensional parameters)
  - Key evaporation parameters calibrated to evaporation data (surface evaporation, absorption rate, desorption rate)
- Roberts (1994) [Integrated into HPAC version 4.0]
  - Physics model of evaporation from sand and concrete surfaces
- SCIPUFF/HPAC (1996) [DoD model for counter-force applications]
  - Lagrangian transport and diffusion model; turbulence diffusion based on second-order closure theory

# History of Agent Fate Modeling Lessons Learned

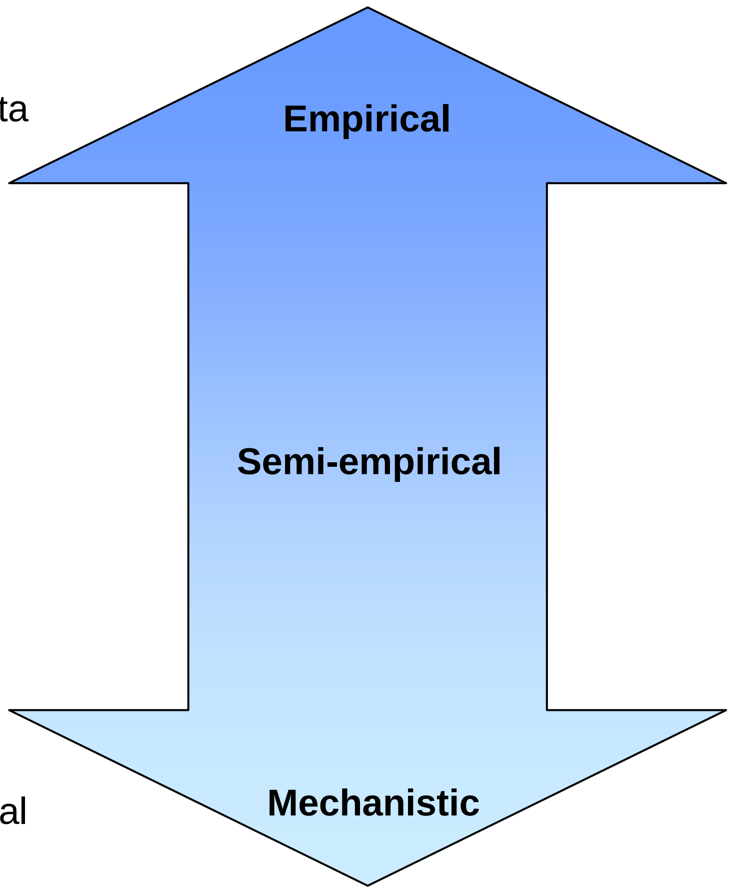
- Mix of empirical and physics-based modeling
- Similar physics (2-D diffusion, dimensionless mass and energy parameters)
- Porous substrate modeling empirically driven or simple physical representations
- No explicit agent-surface interaction chemistry
- *Model accuracy, fidelity, and confidence limited by empirical data*

# Agent Fate DTO Modeling

## *Model Development Is Data Intensive Activity*

Fit To Data

Theoretical




*Key Features*

- Numerically Efficient
- Limited To Available Data
- No Physical Representation
- Requires Response Data
- Excellent Prediction

- Numerically Inefficient
- Extensible Beyond Data Space
- Physical Representation
- Requires Response and Physical Parameter Data

*Examples*

Chinn

Pasquill

Roberts

VLSTRACK

STP 386

# Empirical Model

## *Fit To Response Variable*

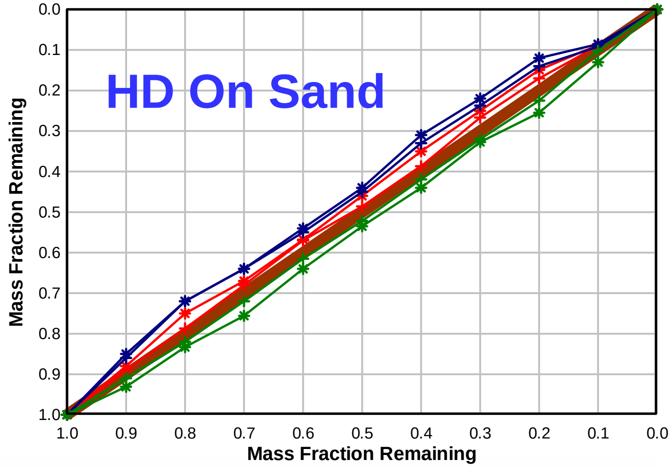
**Model Output:** Agent fraction remaining over time

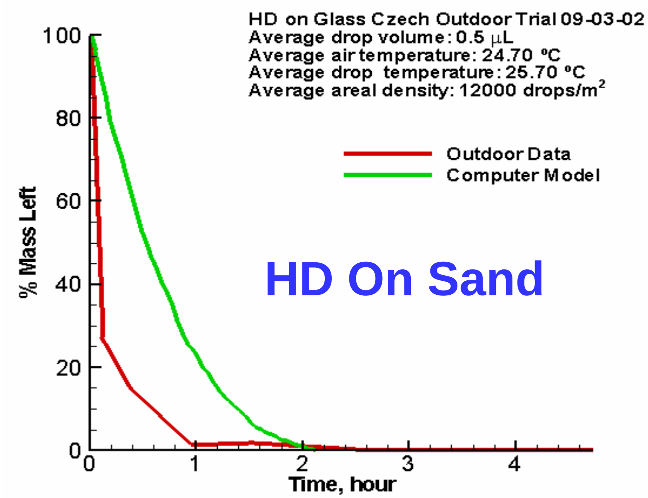
**Model Inputs:** Ground temperature, droplet, size, wind speed, humidity

**Model Type:** Exponential decay function

**Model Data:** Agent fraction remaining, droplet, size, wind speed, humidity, agent substrate

**Experimental Method:** Wind tunnel, end extraction validation to open air trials



# Theoretical Model

## *Modeling of Fundamental Physico-Chemical Mechanisms*

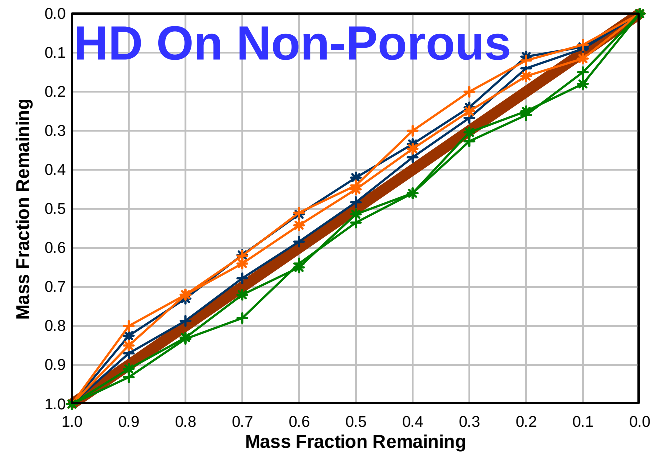
**Model Output:** Agent fraction remaining over time

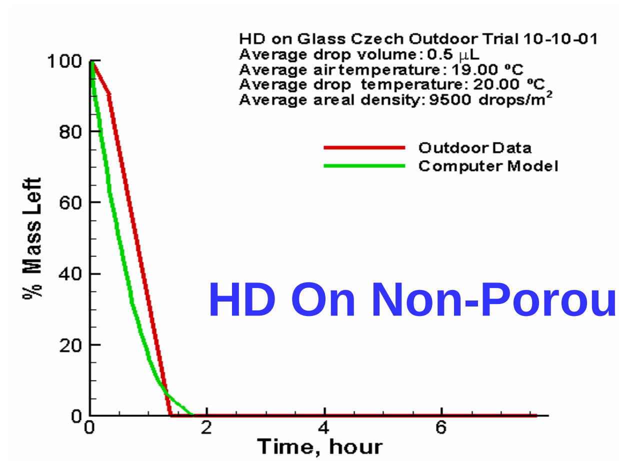
**Model Inputs:** Re, Sc, Pr, u*, height of drop, wetted area radius, contact angle, air viscosity, drop & air temperature, saturation, permeability, relative permeability, diffusion coefficient, capillary pressure, porosity, surface tension, chemical interaction params

**Model Type:** Engineering model

**Model Data:** Agent fraction remaining, droplet, size, wind speed, humidity, agent substrate, permeability data, initial wetted area size, diffusion coefficients, agent reaction data

**Experimental Method:** Wind tunnel, end extraction, various lab experiments, reaction kinetics, open air field trials for model validation



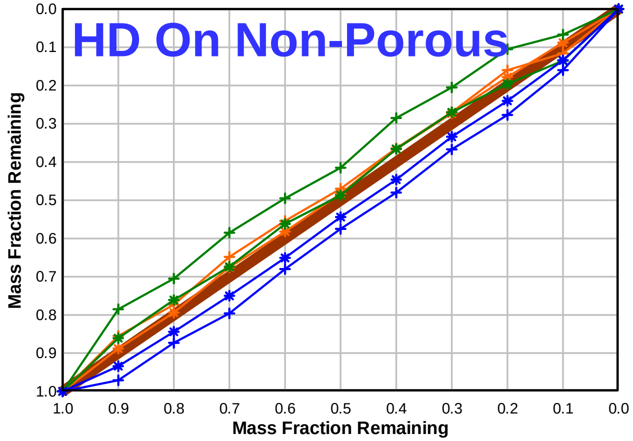



# Semi-Empirical Model

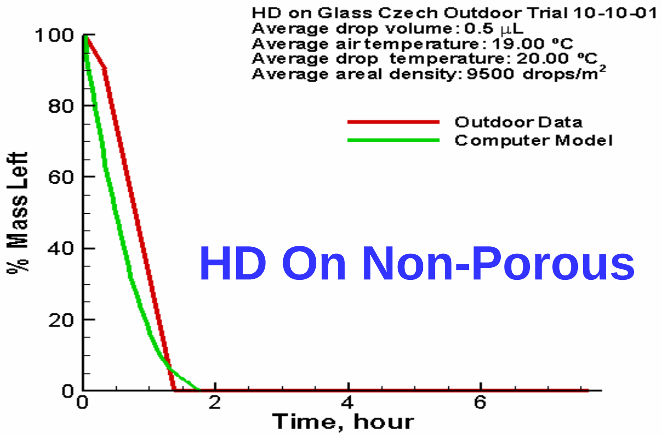
## *Physics-Based Model With Empirical Fitting*

**Model Output:** Agent fraction remaining over time

**Model Inputs:** Ground temperature, droplet, size, wind speed, humidity, agent properties, diffusion layer thickness, initial contact angle, plug initial surface radius and depth, pore fill fraction, transition point from liquid to vapor transport phase, activation energies, reaction kinetics, order of reactions, impurities & their diffusivity & volatility




**Model Type:** Diffusion-based physics model

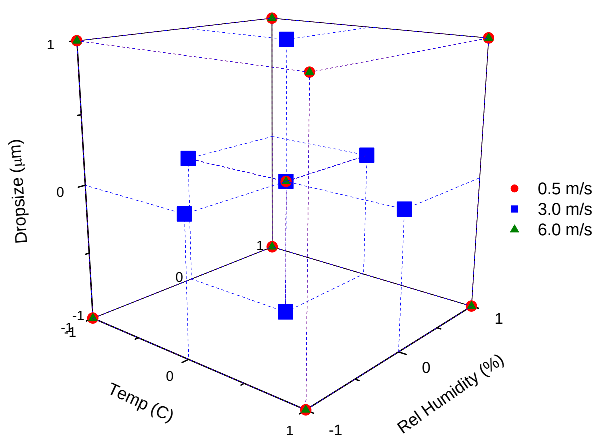



**Model Data:** Agent fraction remaining, droplet, size, wind speed, humidity, agent substrate, agent reaction data

**Experimental Method:** Wind tunnel, end extraction, various lab experiments, reaction kinetics, open air field trials for model validation

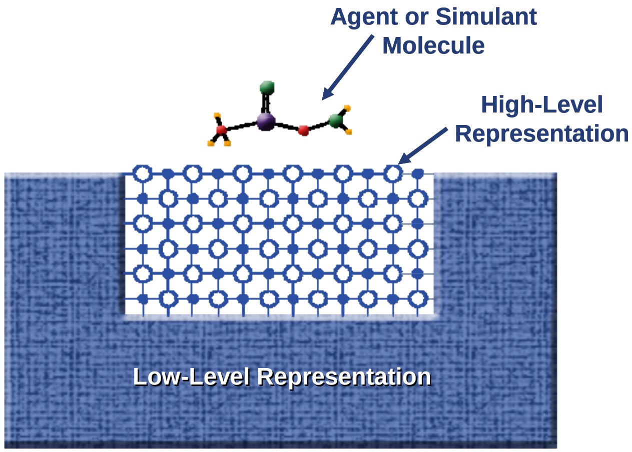
# Future of Agent Fate Modeling

## Factorial Experimentation (Historical Approach)




- Too many permutations
- Limited/no use of agents in the field
- Risk & cost associated with any agent work
- Rate of emerging threats overcomes ability to generate data in a timely manner

## Model Agent/Material Interaction (Future Approach)

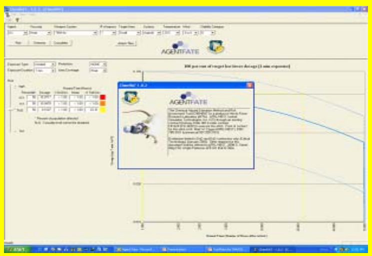


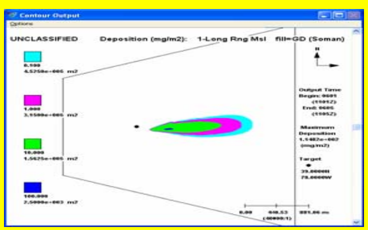

- Computational chemistry & physical modeling
- Reduces dependence on large quantity of agent-material experiments
- Better focuses experimental requirements
- Greater use of simulants to validate key physico-chemical processes

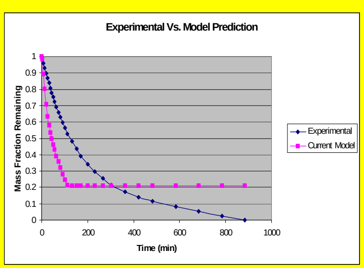
# Future of Agent Fate Modeling

- Pro's
  - Reduce live agent experimental requirement
  - Greater use of simulants
  - Independent of threat agent or material
  - More responsive to growing need of threat agent data
- Con's
  - Multiple experiments replace single response surface experiment
  - New experimental methods need to be designed
  - Still require some live agent factorial testing to validate models and key processes

# Maintain Transition Focus


**Acquisition Support**

**Decision Aids**

**CONOPS TTP**

**S&T Community**

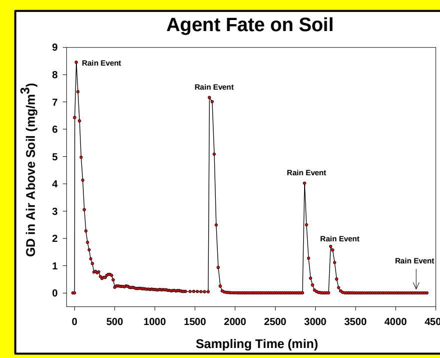
FOR EVALUATION PURPOSES ONLY

Agent: VX — Temperature Range: 15°C to 35°C

Wind Speed Range: < 6 knots — Stability Classes: Unstable (A or B)

Hazard Duration (hours):

| Munition | Exposure Time | Mild Surface: Asphalt | Mild Surface: Concrete | Mild Surface: Grass | Mild Surface: Barren | Mild Surface: Sand | Lethal Surface: Asphalt | Lethal Surface: Concrete | Lethal Surface: Grass | Lethal Surface: Barren | Lethal Surface: Sand |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 500 kg Bomb | 1h | > 72 | 11 - 12 | 8 - 9 | > 72 | > 72 | < 1 | < 1 | < 1 | < 1 | < 1 |
| | 6h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | < 1 | 2 - 3 | < 1 | < 1 |
| Ballistic Missile Lg Submunitions | 1h | > 72 | > 72 | [illegible] | > 72 | > 72 | < 1 | < 1 | < 1 | < 1 | < 1 |
| | 6h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | < 1 | 7 - 8 | < 1 | < 1 |
| Ballistic Missile Sm Submunitions | 1h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | < 1 | < 1 | < 1 | < 1 |
| | 6h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | < 1 | 10 - 11 | < 1 | < 1 |
| Ballistic Missile Central Burst | 1h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | < 1 | < 1 | < 1 | < 1 |
| | 6h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | < 1 | 5 - 6 | < 1 | < 1 |
| Ballistic Missile Line Release | 1h | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 |
| | 6h | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 | 1 - 2 |
| Cruise Missile | 1h | > 72 | 2 - 3 | [illegible] | > 72 | 4 - 5 | < 1 | < 1 | < 1 | < 1 | < 1 |
| | 6h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | 1 - 2 | < 1 | < 1 | < 1 |
| SR Ball. Missile Central Burst | 1h | > 72 | > 72 | [illegible] | > 72 | > 72 | < 1 | < 1 | < 1 | < 1 | < 1 |
| | 6h | > 72 | > 72 | > 72 | > 72 | > 72 | < 1 | < 1 | 2 - 3 | < 1 | < 1 |



# Summary

- Lessons learned provided modeling starting point
- DTO covered full spectrum of agent fate modeling
- Traditional experimental approach too unwieldy for growing need of agent fate data
- Greater emphasis on computational modeling holds promise to be more responsive and less costly
- S&T community becomes a prime user for future agent fate modeling technology