Chemical Agent Fate

Transport Models for Evaporating and Non-Evaporating Sessile Drops in Porous Substrates

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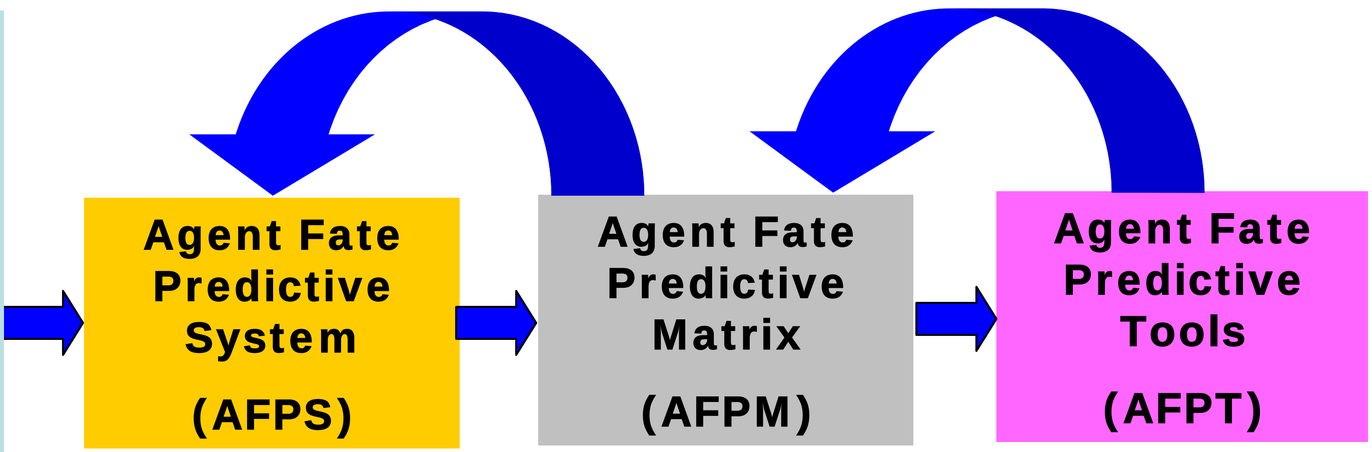
Our Mission

- To create a system that can greatly enhance the ability to predict the outcome of a chemical attack event in terms of the existing level of an agent's concentration

Agent Fate Predictive Input (AFPI)

Averaged / Instantaneous

- Wind speed
  - Turbulence
- Temperature
- RH
- Average agent droplet size and distribution
- Substrate type



Agent Fate Predictive System (AFPS)

Agent Fate Predictive Input (AFPI)

Averaged / Instantaneous

- Wind speed
  - ❖ Turbulence
- Temperature
- RH
- Average agent droplet size and distribution
- Substrate type

Surface Evaporation Module

- Sessile drops
  - ✓ Non-permeable substrates
  - ✓ Small drops/large granules
  - ➢ Permeable substrates

Substrate Module

- Liquid transport
  - ✓ Porosity
  - ✓ Saturation permeability
  - ✓ Capillary pressure [*f(s)*]
  - ➢ Phase permeability [*g(s)*]
- Evaporation model
- Vapor transport
  - ➢ Effective diffusivity
- Chemical reaction
  - ❖ Rate and mechanism
- Agent/surface interaction
  - ❖ Rate and mechanism

Experimental Module

- Finding physical properties (viscosity, density, surface tension, etc.)
- Helping to find the transport properties
  - Porosity
  - capillary pressure
  - Saturation permeability
  - Relative permeability
  - Effective diffusivity
  - Adsorption rates
  - Activation energy
  - Etc..
- Model validation

AFPS

✓ Completed
➢ On-going
❖ Planned

Agent Fate Predictive Matrix (AFPM)

Agent Fate Predictive System

(AFPS)

Variables

- **Atmospheric**
  - Wind speed
  - Wind turbulence intensity
  - Temperature
  - Relative Humidity (RH)
- **Agent**
  - Type
  - Average drop size or size distribution
  - Average number of drops per unit surface area
- **Substrate**
  - Type
    - ❑ Chemical composition
    - ❑ Properties (porosity, Saturation permeability, relative permeability, capillary pressure, agent's effective diffusion coefficient)

Function (s) [Information Needed]

- The amount of agent present (Instantaneous/Averaged/Targeted time)

Limitations

- Thousands of experiments and/or simulations are needed to sufficiently create a good system
- Stiff set
- Maintenance
- Updating

Agent Fate Predictive Tools (AFPT) – On Going

Agent Fate Predictive Matrix

(AFPM)

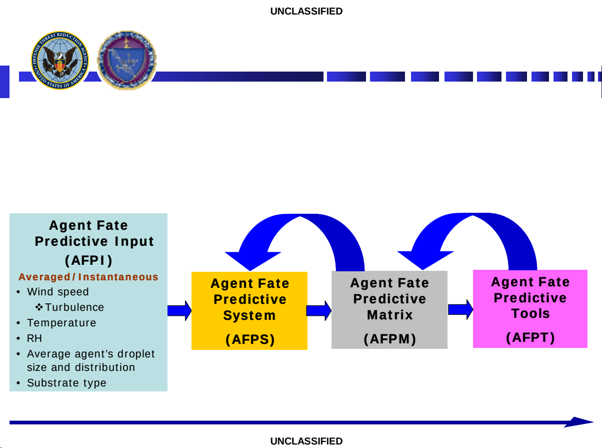
Limitations Overcome

- Thousands of experiments and/or simulations are needed to sufficiently create a good system
- Stiff set
- Maintenance
- Updating

Tools

- **Artificial Neural Network (ANN)** is a computer program that is capable of learning patterns or relationships via training examples (Taken from AFPM). It resembles biological neural nets in two ways:
  - ❖ Knowledge is acquired by the network through a learning or training process
  - ❖ Knowledge is stored via inter-neuron connection strengths (weights)
- Can asymptotically find the minimum number of required input from the AFPM
- Can be updated for new data (as they may become available), by a simple re-training process

Surface Evaporation Module



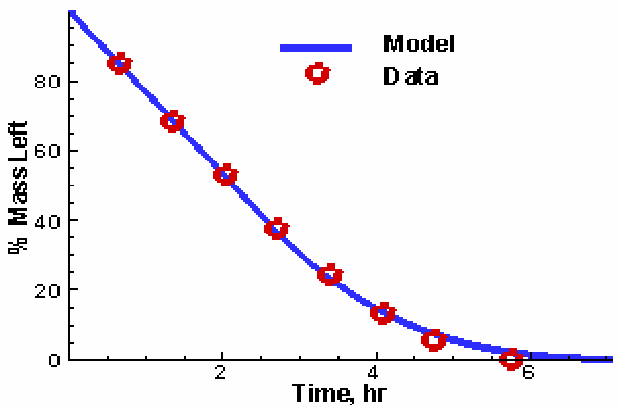
- Model developed
- Model validated with wind tunnel data
- Model validated with outdoor data
- Model and experiments showed that the percentage of mass left is a general function of temperature and non-dimensional time regardless of the drop size. Length scale: $\left(\frac{V}{r^2}\right)^{-1}$, Time scale: $tu^*\left(\frac{V}{r^2}\right)^{-1}$
- Model was used as a pilot methodology to verify the robustness of our overall approach (AFPI, AFPS, AFPM, and AFPT)

References:

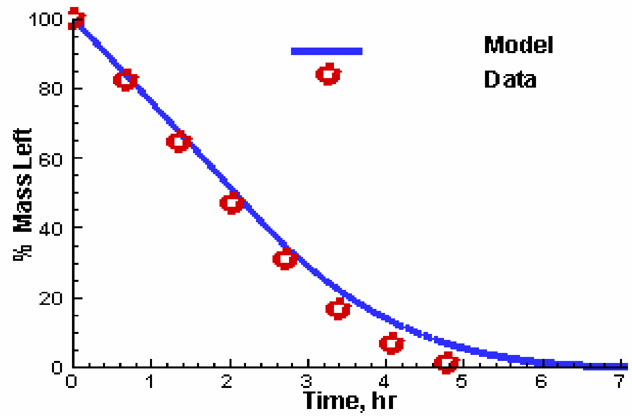
Navaz, H. K., Chan, E., and N. Kehtarnavaz, “A Comprehensive Study of HD Sessile Droplet Evaporation on Impermeable, Non-Reacting Substrates,” Presentation at the CBD November 2006, Hunt Valley, MD.,
To be submitted to the *Journal of Hazardous Materials*.

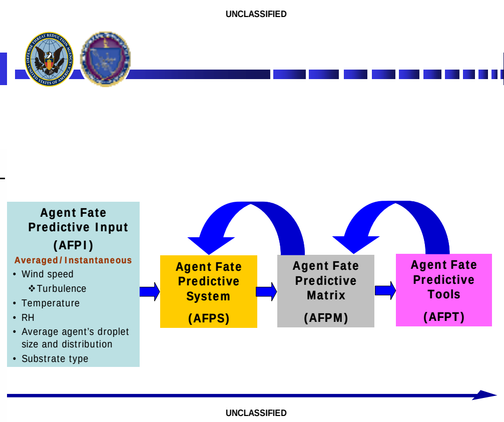
Model Development and Validation with Laboratory Data

HD on Glass, Wind Velocity = 3.66 m/s, Drop Size = 1 µL
Air Temperature = 15°C, m=1.200mg

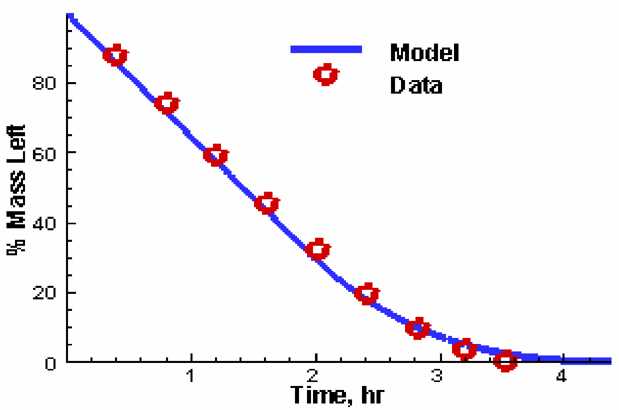


HD on Glass, Wind Velocity = 3.66 m/s, Drop Size = 1 µL
Air Temperature = 15°C, m=1.264 mg

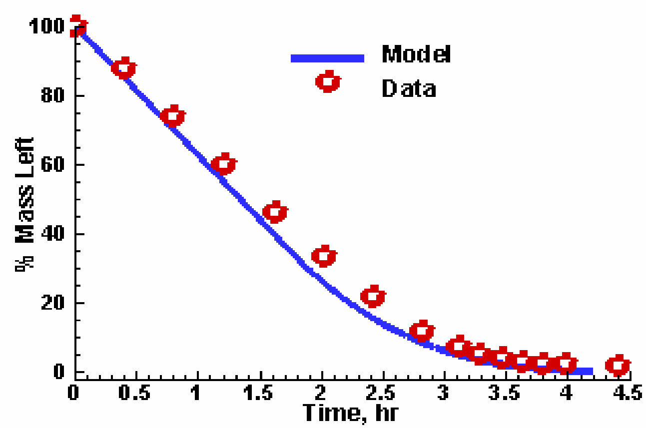




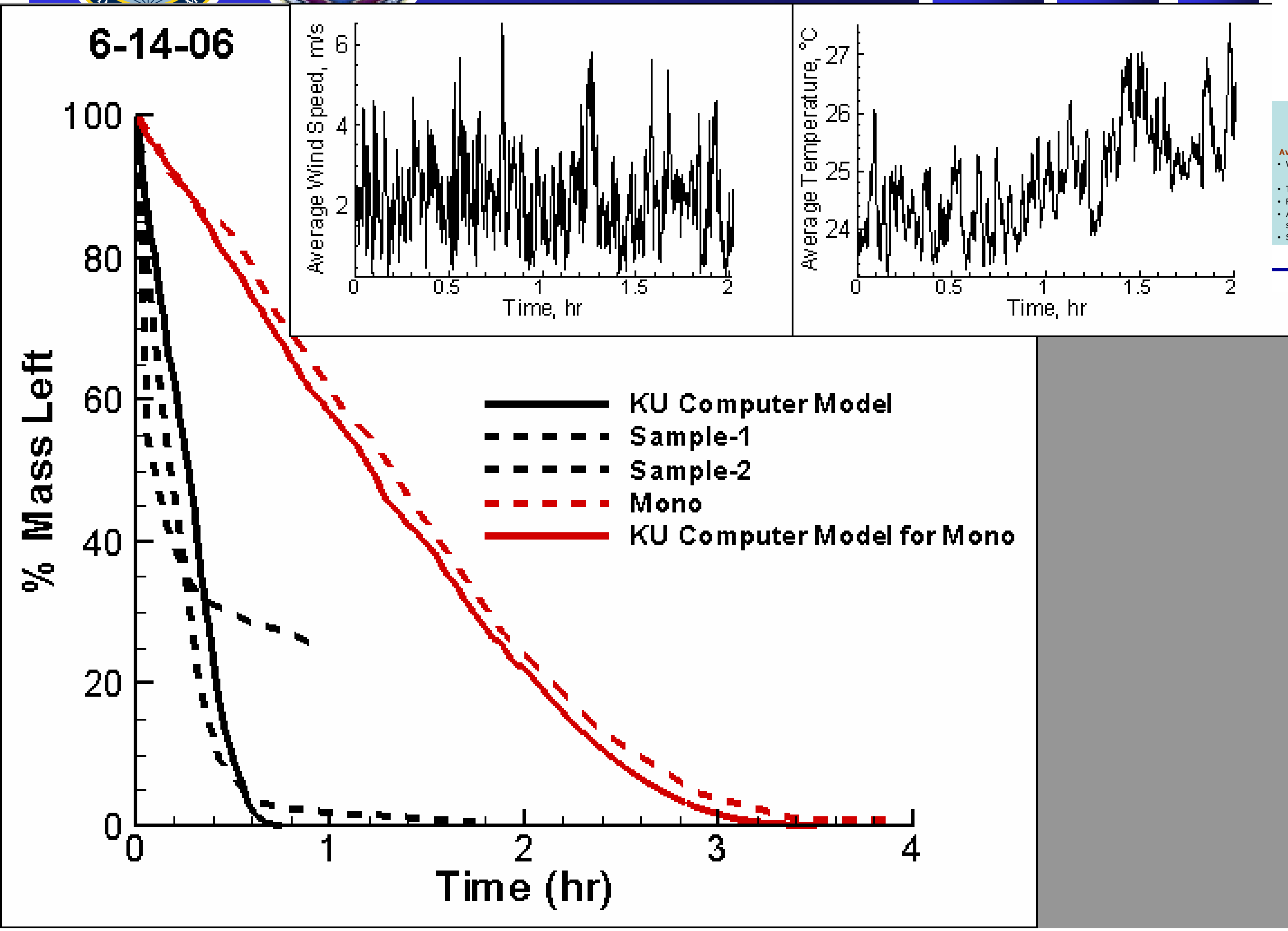
HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 6 µL
Air Temperature = 35°C, m=6.884 mg

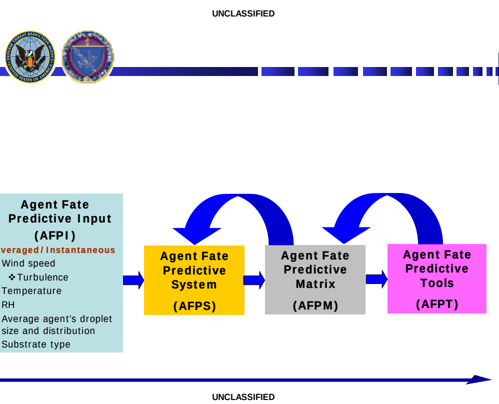


HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 6 µL
Air Temperature = 35°C, m=7.000mg

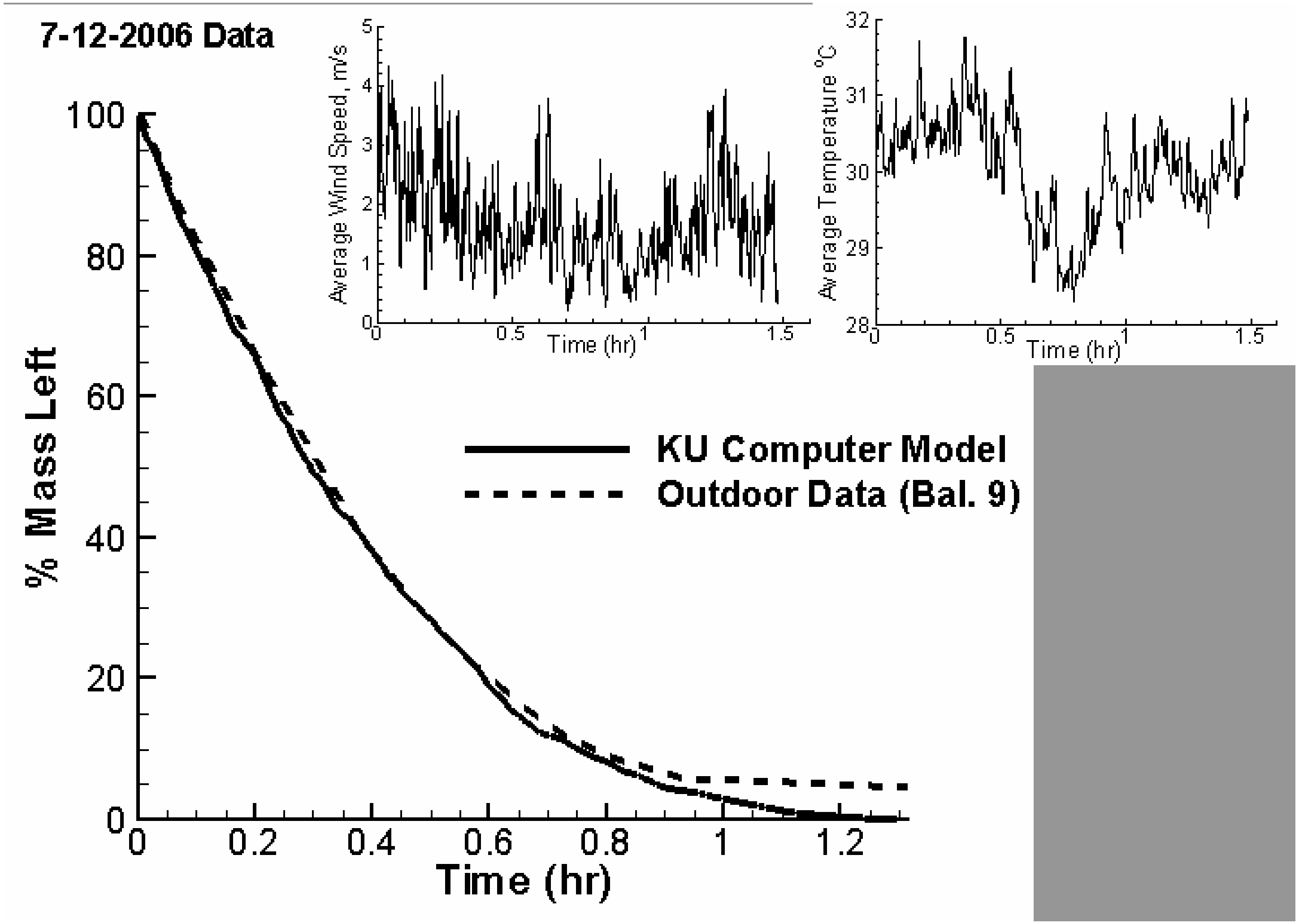


Model Validation with Outdoor Data 2006

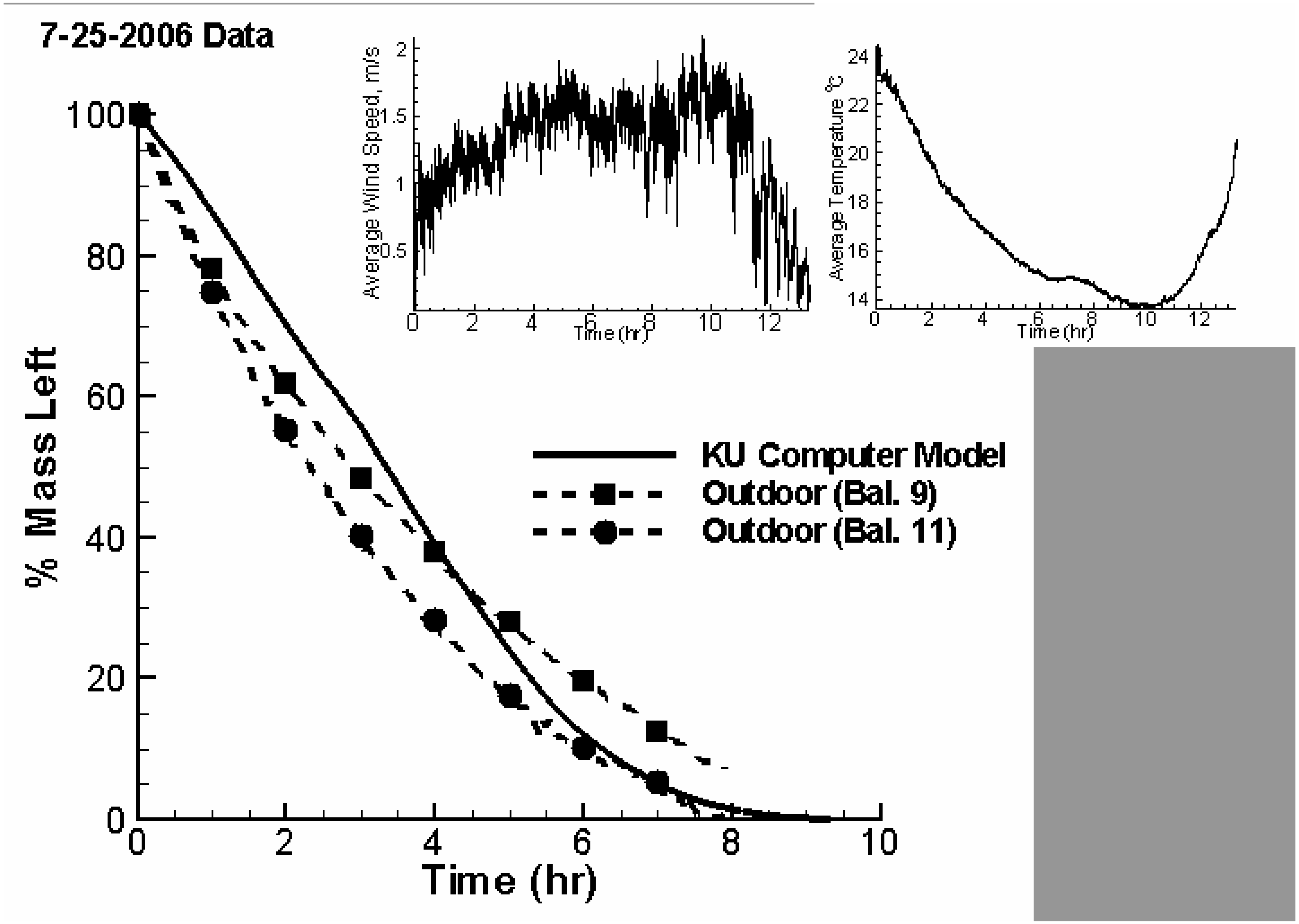




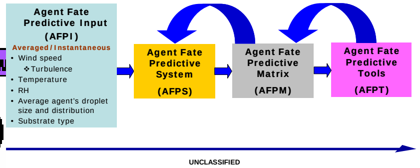
Model Validation with Outdoor Data - 2006

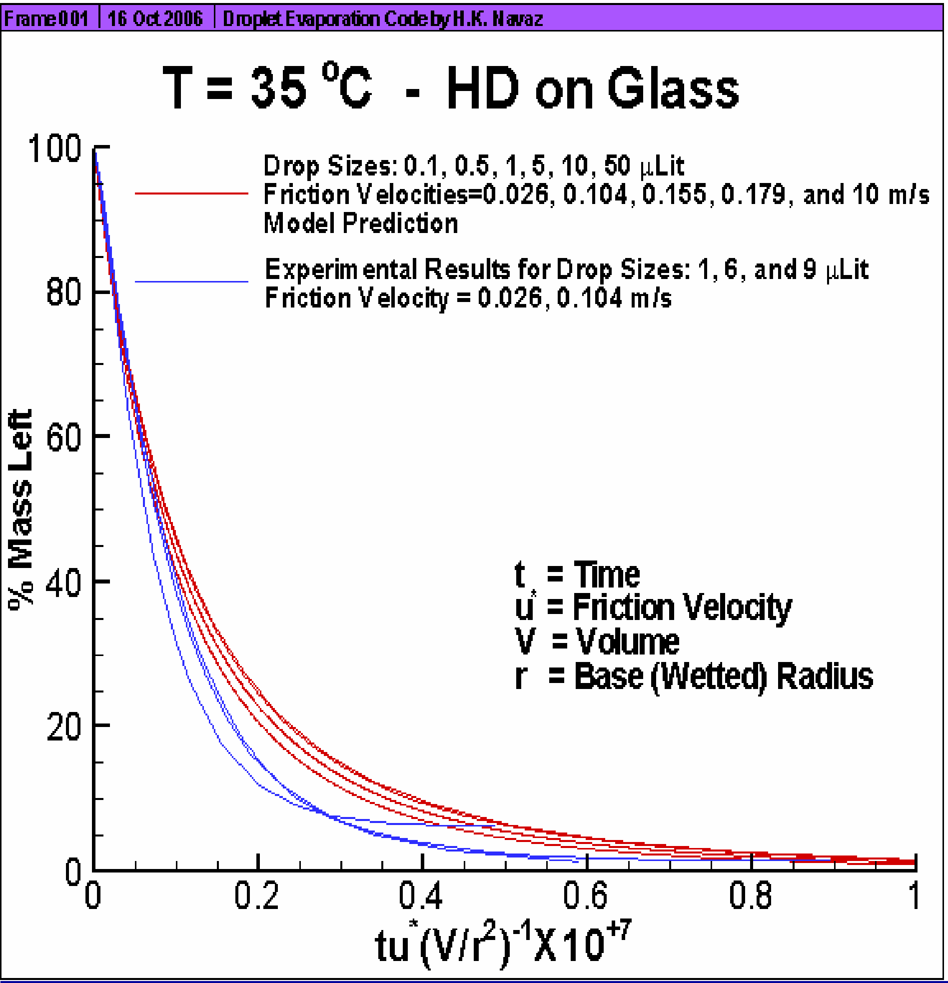


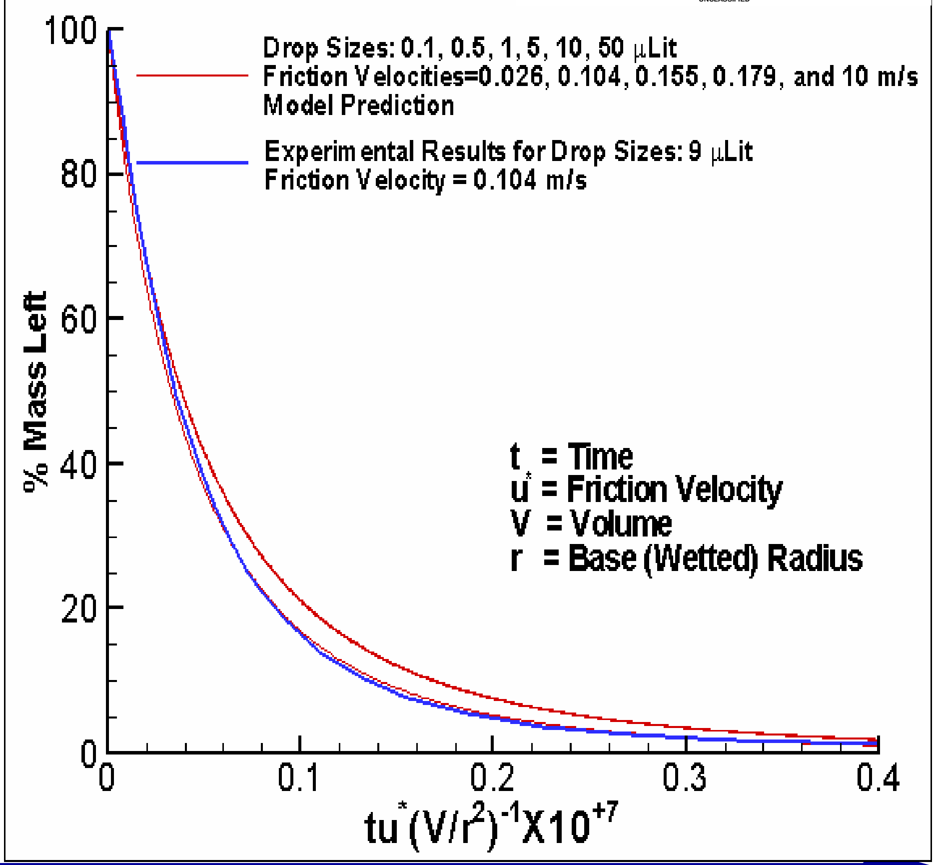
Model Validation with Outdoor Data - 2006



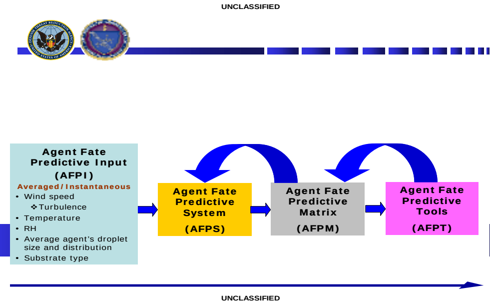
Evaporation Model Scalability







Conclusions



- Developed a robust system based on first principles and innovative methods for the Agent Fate Program
- Proved the robustness of the system by applying it to the evaporation of HD on glass
- Developed hybrid experimental and analytical methods to find the transport properties in a porous substrate
  - Capillary pressure
  - Relative permeability
- Addressed the scalability issue that assists us in developing the experimental methods
- Developed two analytical models for agent transport through a porous substrate

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