Chemical Agent Fate Program (CAFP)

Development of an Evaporation Model for HD on Non-Porous Surfaces

By:

Brad Dooley
California Institute of Technology
Pasadena, California

H. K. Navaz
Kettering University
Flint, Michigan

Objectives

- To develop a **simple engineering** tool that can **predict** the evaporation rate of HD on non-porous surfaces and provide information about
  - The amount of mass being evaporated and transported by the wind
  - The amount of mass being absorbed/desorbed into a porous substrate
  - The basic behavior of a drop under the outdoor conditions

Scientific Problems to Be Addressed

- Evaporation
  - Modeling sessile drop behavior
- Validation
- Generalization
  - How to generalize our efforts to enhance prediction capability by
    - ✓ A hybrid approach
    - ✓ Imposing outdoor conditions
- Linkage to porous substrate

Evaporation Module

- A module that is mostly based on first principles and provides the following information
  - Forcing function - the evaporation rate, $\dot{m}$
    - ✓ Can be modified, improved, replaced, …
  - Topology of the droplet by solving a differential equation using the forcing function
  - Evaporated mass being added to the atmospheric air
  - Remaining mass to be transported through the porous substrate

Evaporation Module (*cont'd*) Model Development

- Forcing Function
  - Constant base area for a drop (Model A)

$$\dot{m} = 2\pi C R_s f \frac{\mu}{\ } \left(F + C_1 Re^m \quad r^n\right) \ell n\left(1 + B\right) = 2\pi C R_s \frac{\mu}{\ } \left(F + C_1 Re^m \quad r^n\right) \ell n\left(1 + B_M\right)$$

$$C = \frac{h}{R}$$

  - Shrinking base area for a drop (Model B)

$$\dot{m} = 2\pi R_s \left(1 - \quad \varphi\right) f \frac{\mu}{\ } \left(F + C_1 Re^m \quad r^n\right) \ell n\left(1 + B\right) \qquad or$$

$$\dot{m} = 2\pi R_s \left(1 - \quad \varphi\right) f \frac{\mu}{\ } \left(F + C_1 Re^m \quad r^n\right) \ell n\left(1 + B_M\right)$$

Evaporation Module (*cont'd*)
Model Development

- Interaction among drops – Group Theory
  - Model 1: $G_{evap} = \frac{1}{1+G_c}$ with $G_c = \frac{C\left(F + C_1 \quad {}^{m} \quad {}^{n}\right) \quad N^{q}\left(\frac{r}{\lambda}\right)}{}$

Where *C* and *q* can be determined experimentally. *C=3 and q=2/3*

  - Model 2:

$$G_c = \sum_{n=0}^{\infty} \frac{(-1)^n \qquad \eta_0}{\left[(n+1)\eta_0\right]}$$

$$\textit{Where} \quad \eta_0 = \qquad {}^{-1}\left(\frac{\lambda}{R}\right) \quad \textit{and} \quad 2\lambda \textit{ represents the distance between two drops}$$

$$\lambda = \frac{1}{2N^p}$$

where N is the number of drops and $p = 1\!\!\diagup\!_3$

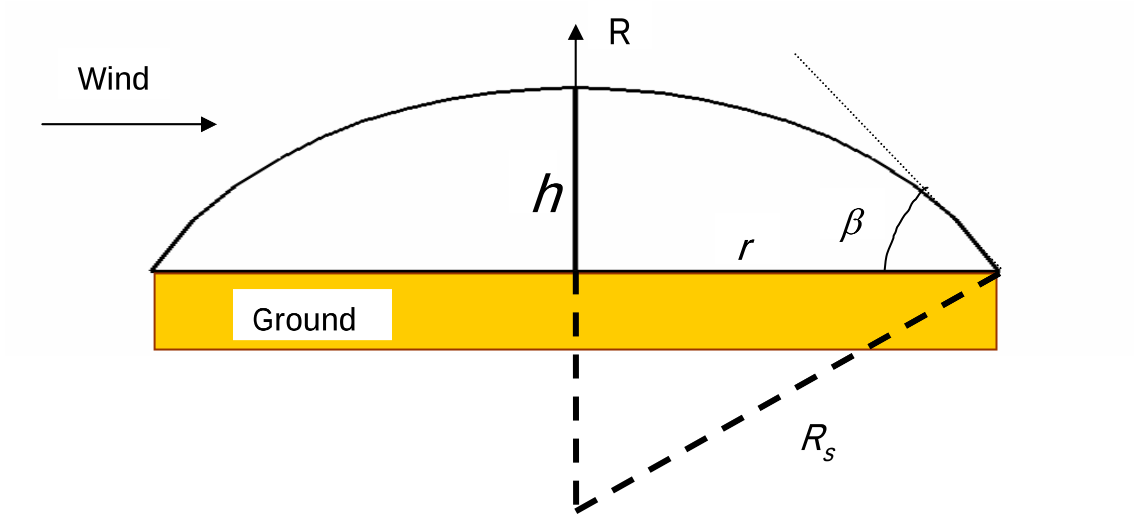
$$G_{evap} = \begin{cases} G_c^q & \textit{for } N \geq n \\ \frac{1}{q} G_c^q & \textit{for } N < n \end{cases}$$

Evaporation Module (*cont'd*) Model Development

- ($\dot{m}$ is a function of time also)
- Model A

$$\frac{dh}{dt} = \frac{-\dot{m}}{\pi \rho_\ell h^2 \left(\frac{3}{C} - 1 \right)}$$

$h/R = C$



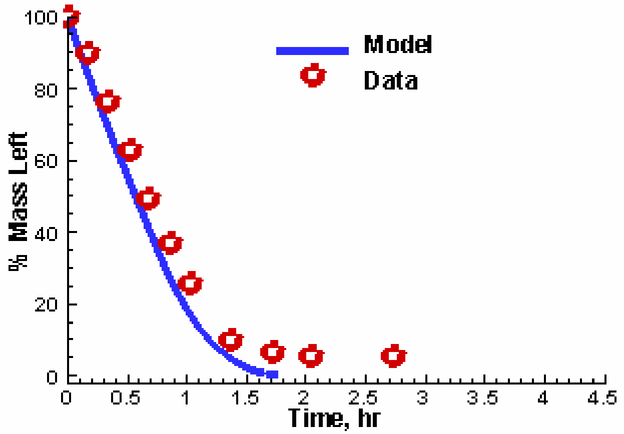
- Model B

$$\frac{dh}{dt} = \frac{-\dot{m}}{\rho_\ell \frac{\pi}{2} \left(r^2 + h^2 \right)}$$

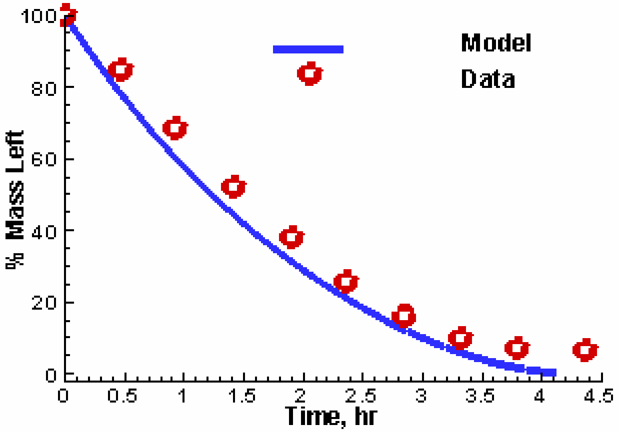
Evaporation Module (*cont'd*)
How to Predict Other Scenarios?

- Validate Model
- Create a matrix for the entire possible domain of operation
- Fill the matrix using the analytical model
- Use neural network curve-fit
- Create a simple engineering equation for application

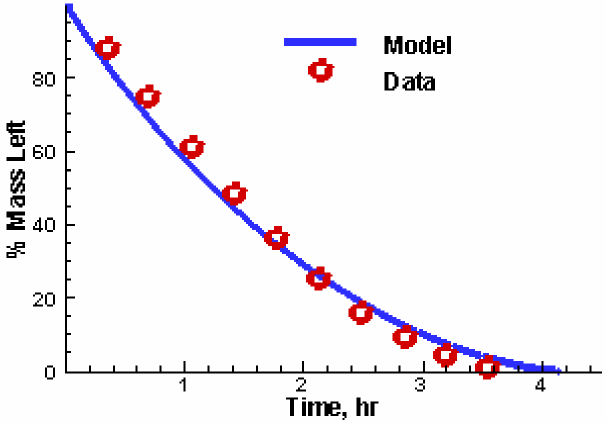
Evaporation Module (*cont'd*) Validation



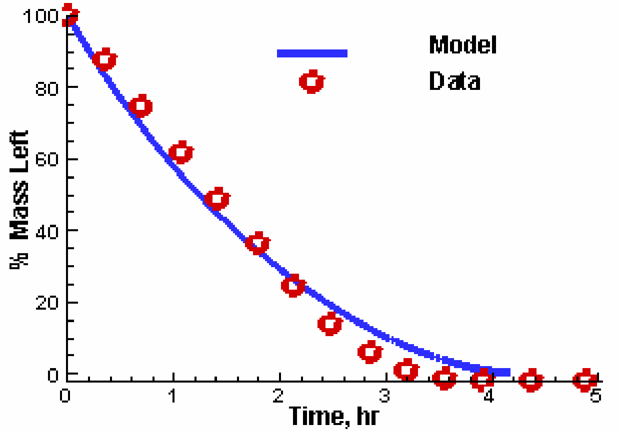
HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 1 μL
Air Temperature = 35°C, m=1.180 mg



HD on Glass, Wind Velocity = 0.26 m/s, Drop Size = 1 μL
Air Temperature = 35°C, m=1.184 mg

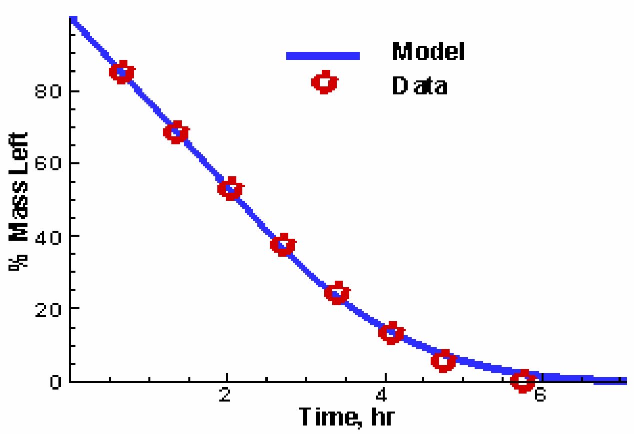


HD on Glass, Wind Velocity = 0.26 m/s, Drop Size = 1 μL
Air Temperature = 35°C, m=1.192 mg

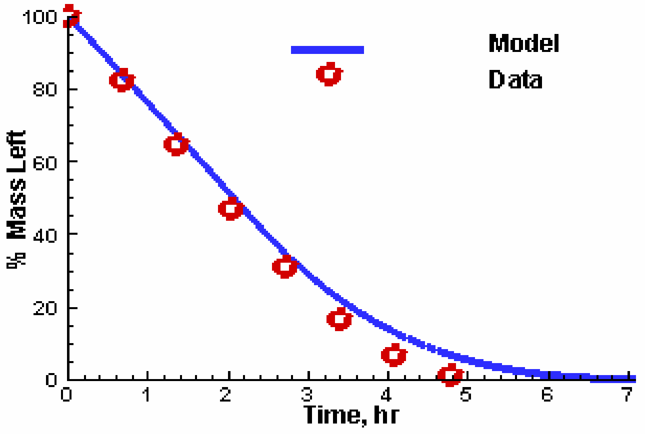


HD on Glass, Wind Velocity =0.26 m/s, Drop Size = 1 μL
Air Temperature = 35°C, m=1.204 mg

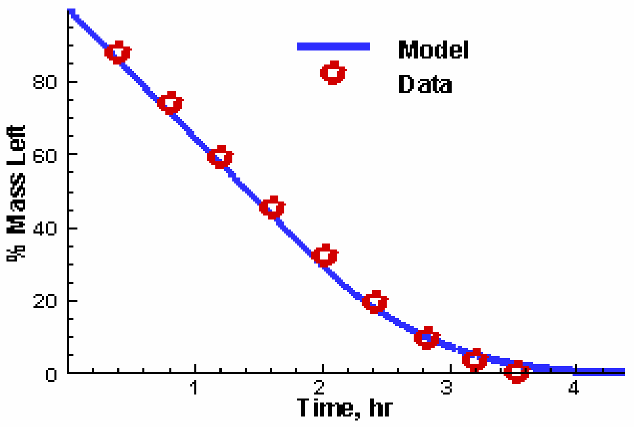
Evaporation Module (*cont'd*)
HD on Non-Porous Surface



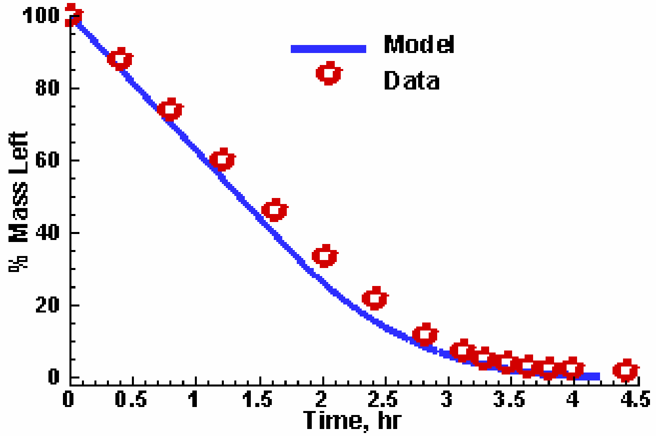
HD on Glass, Wind Velocity = 3.66 m/s, Drop Size = 1 μL
Air Temperature = 15°C, m=1.200mg



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

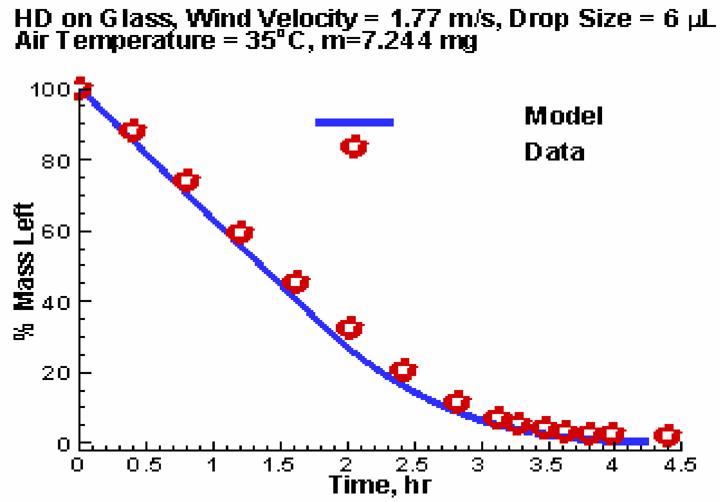


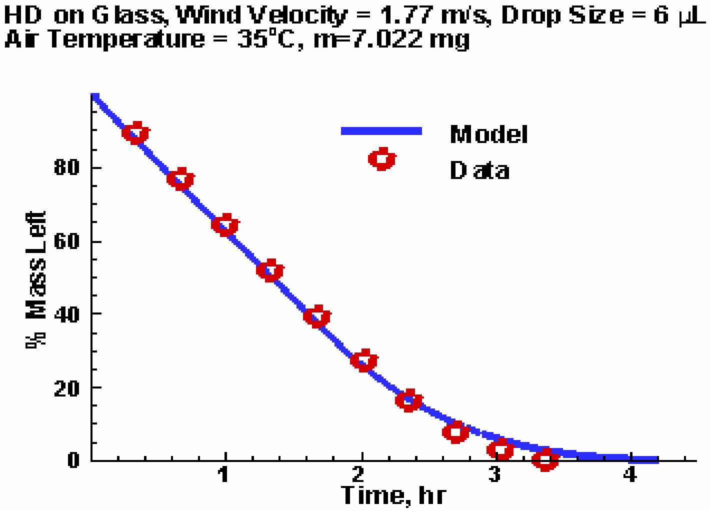
HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 6 μL
Air Temperature = 35°C, m=6.884 mg

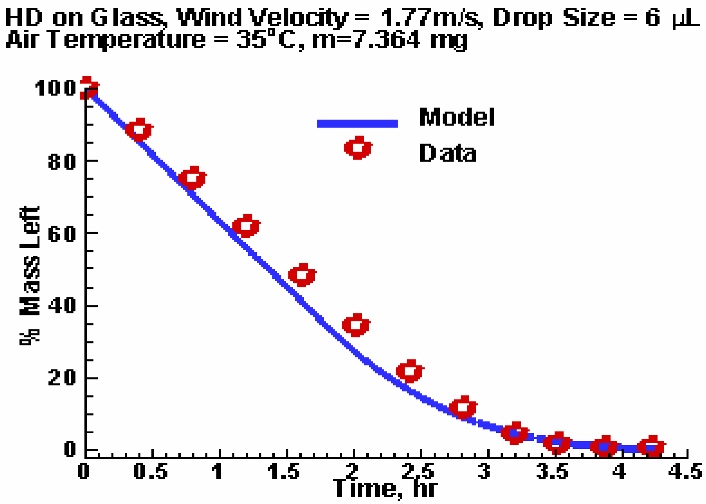


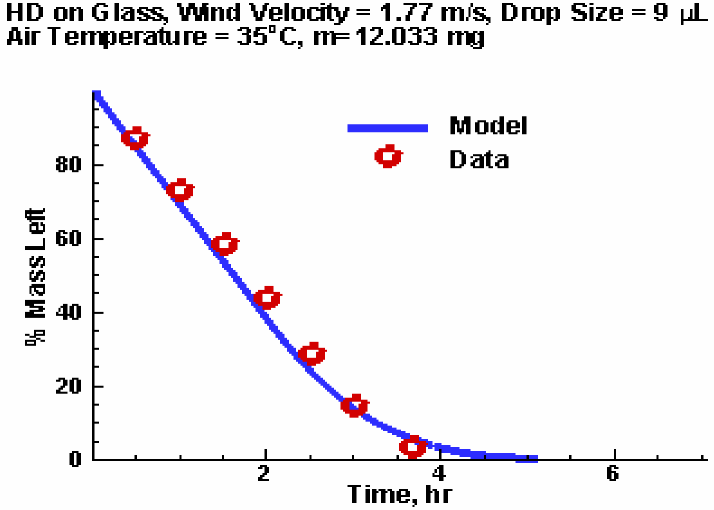
HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 6 μL
Air Temperature = 35°C, m=7.000mg

Evaporation Module (*cont'd*)
HD on Non-Porous Surface


HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 6 μL
Air Temperature = 35°C, m=7.244 mg

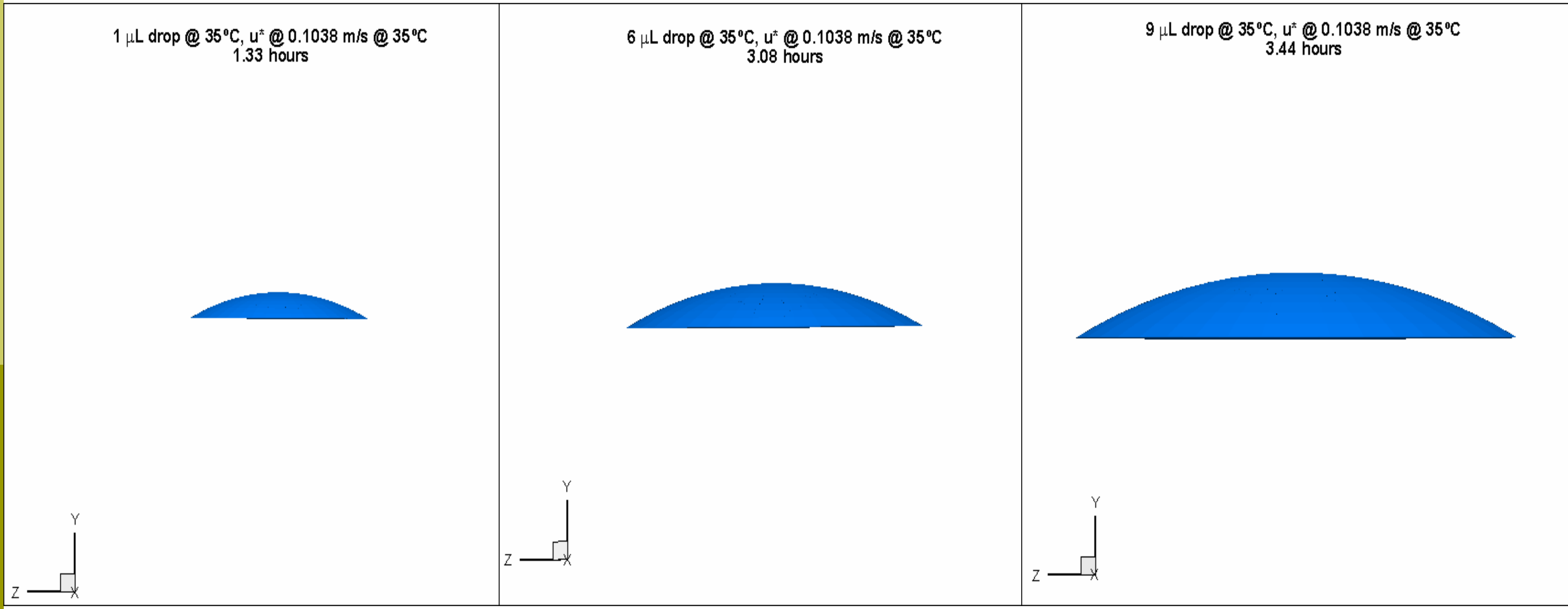

HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 6 μL
Air Temperature = 35°C, m=7.022 mg


HD on Glass, Wind Velocity = 1.77m/s, Drop Size = 6 μL
Air Temperature = 35°C, m=7.364 mg


HD on Glass, Wind Velocity = 1.77 m/s, Drop Size = 9 μL
Air Temperature = 35°C, m= 12.033 mg

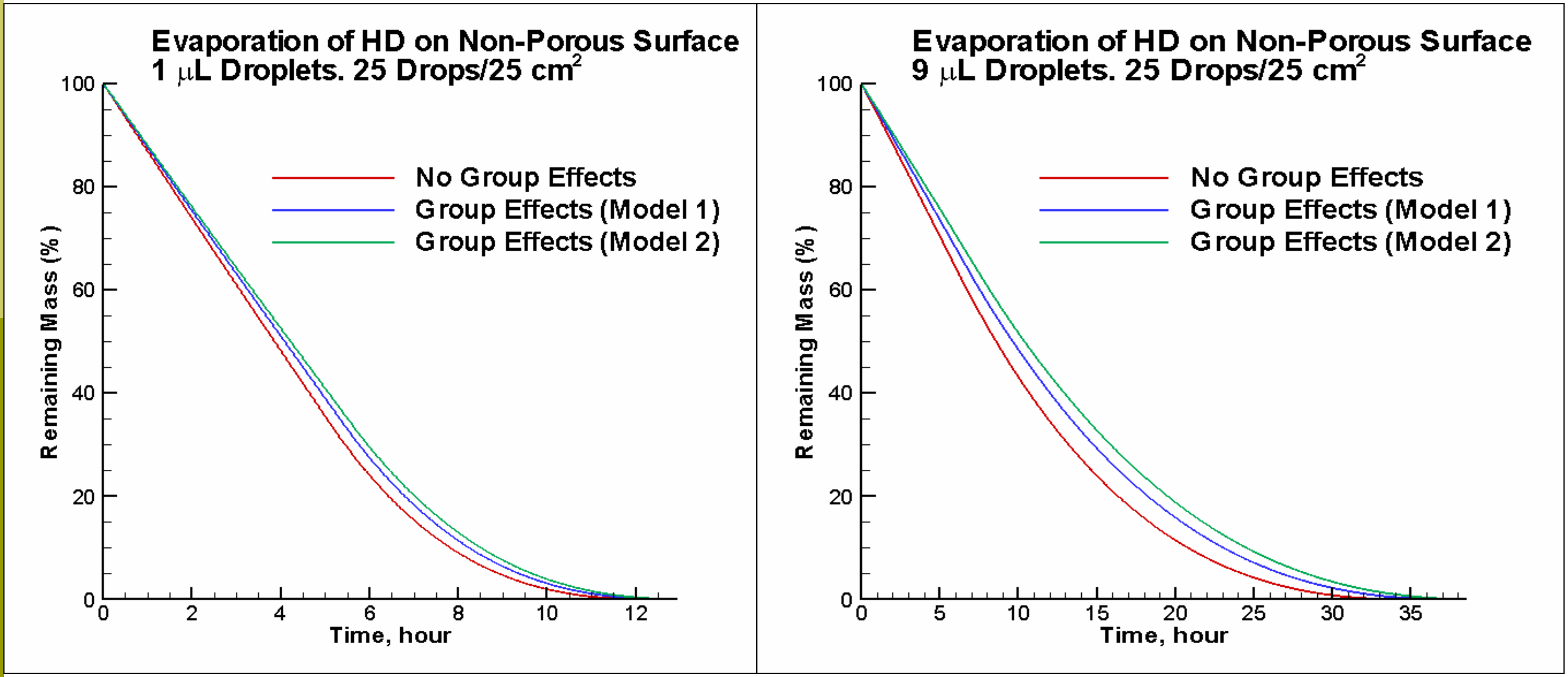
Evaporation Module (*cont'd*) - HD on Non-Porous Surface - *Droplet Topology*

- Sample animated droplet topology



Evaporation Module (*cont'd*)
HD on a Non-Porous Surface – *Group Theory*

- There are two group models embedded in the code
  - Negligible for small sparse drops
  - More significant for larger and denser drops

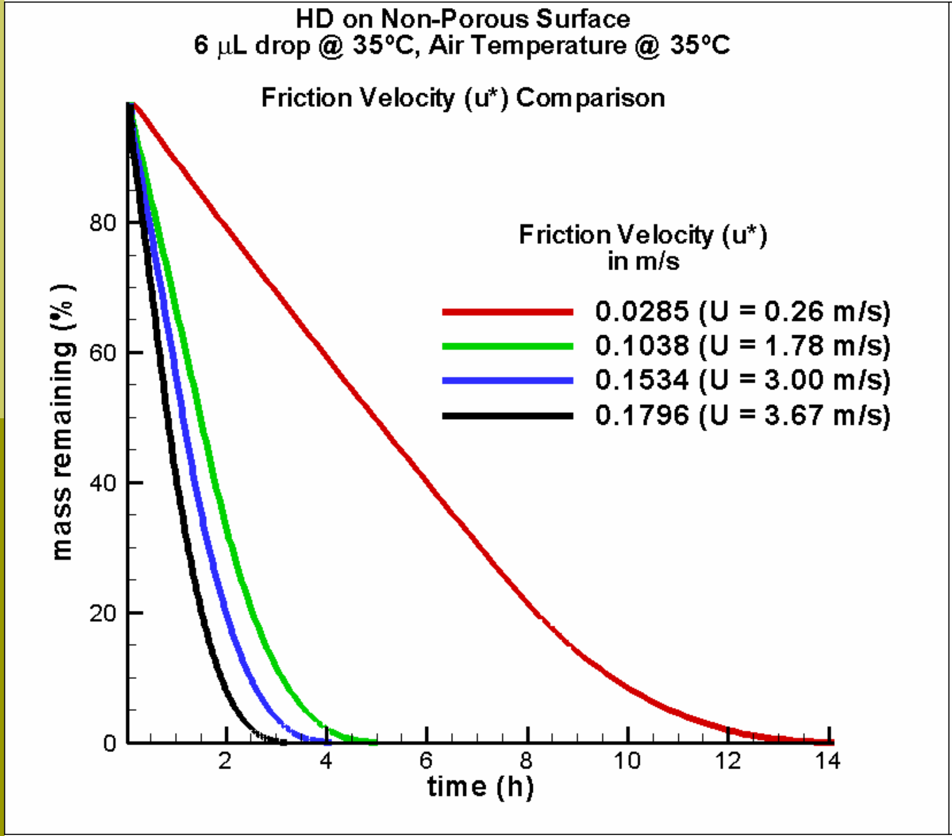


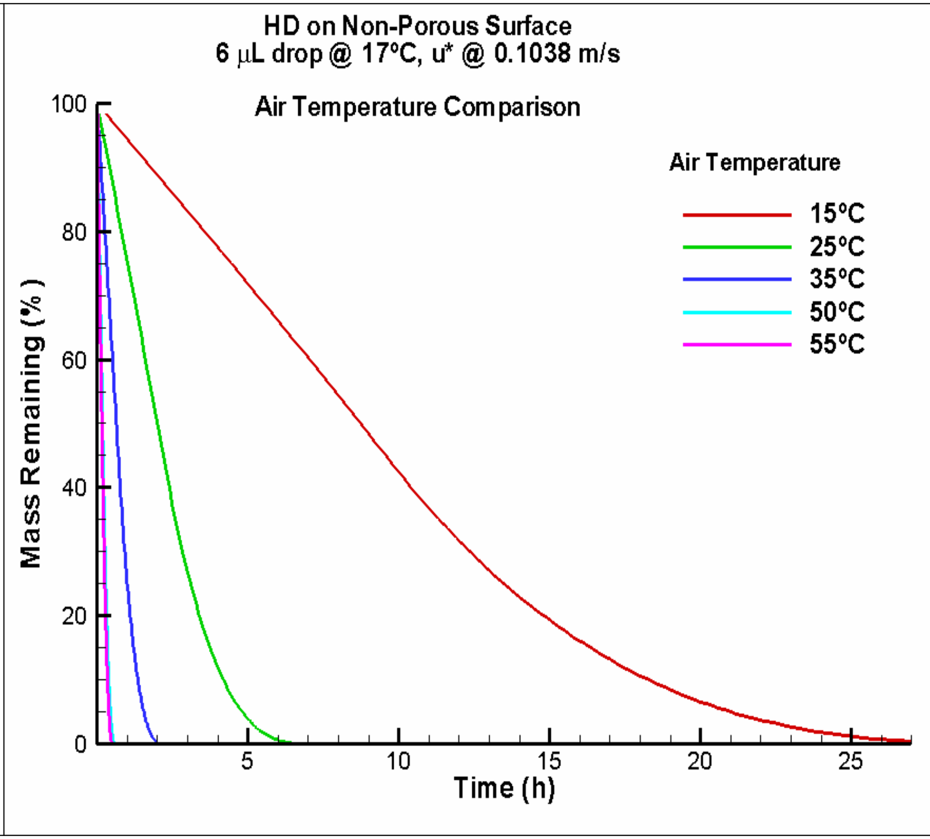
Evaporation Module (*cont'd*)
Model Generalization

			C																								
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
			T_{air}=15°C					T_{air}=25°C					T_{air}=35°C					T_{air}=50°C					T_{air}=55°C				
			T_{drop} (°C), mean value					T_{drop} (°C), mean value					T_{drop} (°C), mean value					T_{drop} (°C), mean value					T_{drop} (°C), mean value				
		u*(m/s)	17	25	35	50	55	17	25	35	50	55	17	25	35	50	55	17	25	35	50	55	17	25	35	50	55
Droplet Volume= 1μL	Number of drops per $1m^2$= 3600	0.0285																									
		0.1038																									
		0.1796																									
		0.1534																									
	Number of drops per $1m^2$= 6400	0.0285																									
		0.1038																									
		0.1796																									
		0.1534																									
	Number of drops per $1m^2$= 10000	0.0285															Expeiment												
		0.1038	Experiment												Experiment												
		0.1796	Experiment																		Experiment						
		0.1534							Experiment																		
Droplet Volume= 6μL	Number of drops per $1m^2$= 3600	0.0285																									
		0.1038													Experiment												
		0.1796																									
		0.1534																									
	Number of drops per $1m^2$= 6400	0.0285													Experiment												
		0.1038	Experiment												Experiment						Experiment						
		0.1796																									
		0.1534													Experiment												
	Number of drops per $1m^2$= 10000	0.0285																									
		0.1038													Experiment												
		0.1796																									
		0.1534																									
Droplet Volume= 9μL	Number of drops per $1m^2$= 3600	0.0285																									
		0.1038													Experiment												
		0.1796																									
		0.1534	Experiment																			Experiment					Experiment
	Number of drops per $1m^2$= 6400	0.0285																									
		0.1038																									
		0.1796																									
		0.1534																									
	Number of drops per $1m^2$= 10000	0.0285																									
		0.1038																									
		0.1796																									
		0.1534																									

Evaporation Module (*cont'd*) HD on a Non-Porous Surface – Parametric Studies

- Effect of Velocity and Air Temperature on Evaporation





Evaporation Module *(cont'd)* Model Generalization

- All the scenarios presented in the matrix will be connected by two methods:
  - Classical curve-fit
    - ✓ To have a simple engineering tool
  - Neural network
    - ✓ To have a more sophisticated tool with prediction capabilities

Evaporation Module (*cont'd*)
Model Generalization

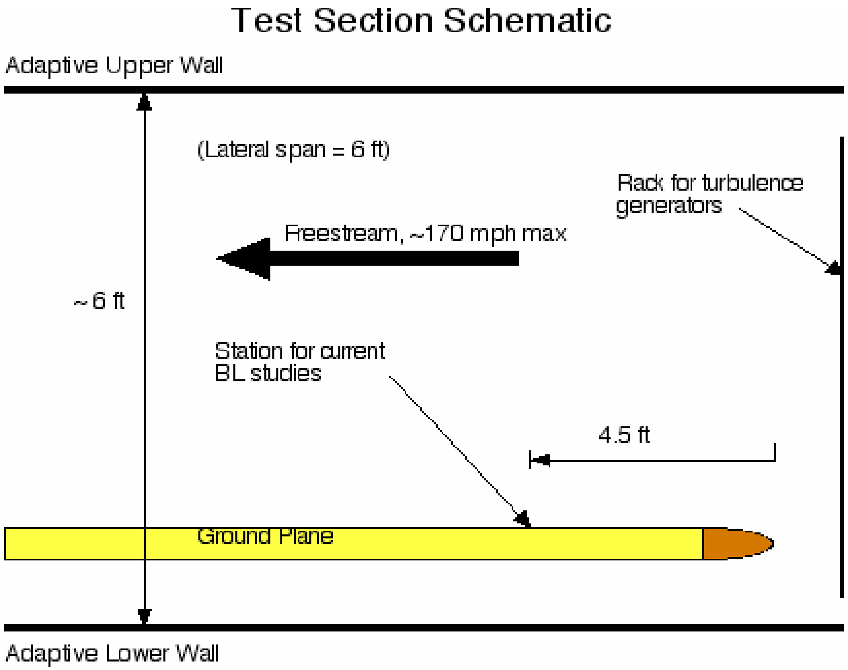
Caltech Work: Overview

- Motivating hypothesis (Navaz): The relevant velocity scale for fluid evaporation rate is not the freestream speed (U_∞), but the "friction velocity"

$$u_\tau = \sqrt{\tau_w / \rho}$$

- Variation of τ_w (and thus friction velocity) for given free stream speed demonstrated
- Simple case of drop evaporation rate evaluated experimentally
- Variation in evaporation rate with friction velocity observed
- Future experiments

John W. Lucas Adaptive Wall Wind Tunnel (GALCIT)


Test Section Schematic

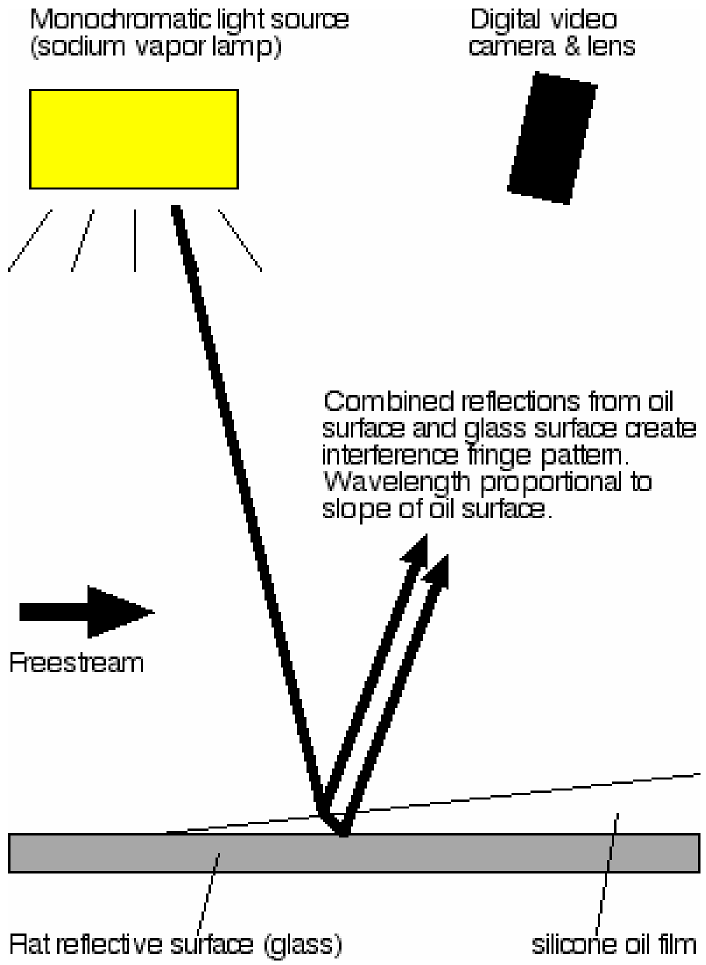
- Turbulence generators (may be) placed in rack upstream of ground plane to increase freestream turbulence level.
- Boundary layer properties examined on ground plane at specified distance from leading edge.

Free Stream Turbulence Generation

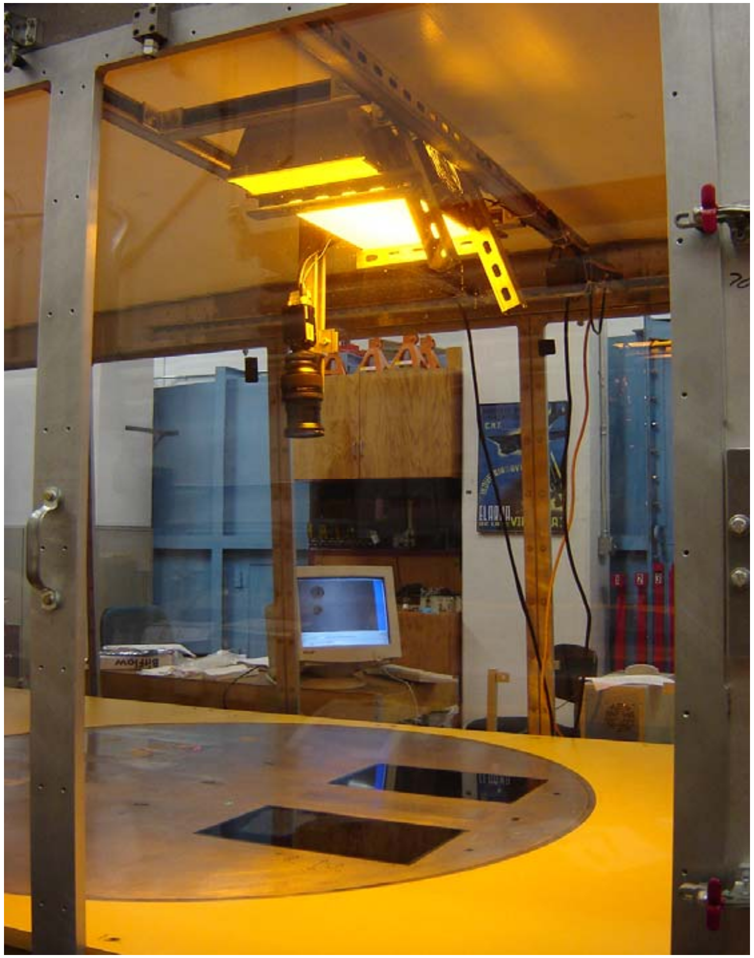
- Bungee cords stretched within frame in free stream.
- Act as turbulence generator; also vibrate quite a bit at high speeds.
- Various configurations available to “dial in” turbulence level.
- Idea: Bahram Valiferdowsi

Wall Shear Stress Measurement

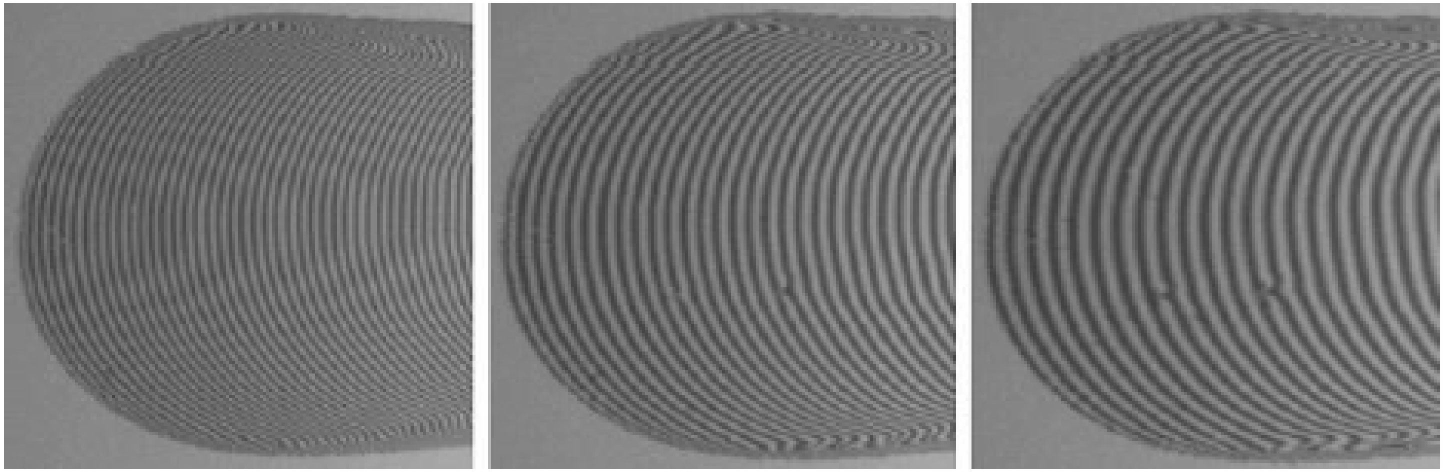
- Oil film technique used by Nagib and others.
- *Relatively* non-intrusive - camera and lamp placed in tunnel, but near test section roof.
- By observing interference fringes growing with time, wall shear stress may be calculated.



Shear Stress Measurement Apparatus



Wall Shear Stress Measurements



- Numerous images taken at 10-30 sec intervals.
- Fringe spacing growth rate, ds/dt, easy to evaluate.

$$\tau_w = \frac{2n\mu}{\lambda}\frac{ds}{dt}$$

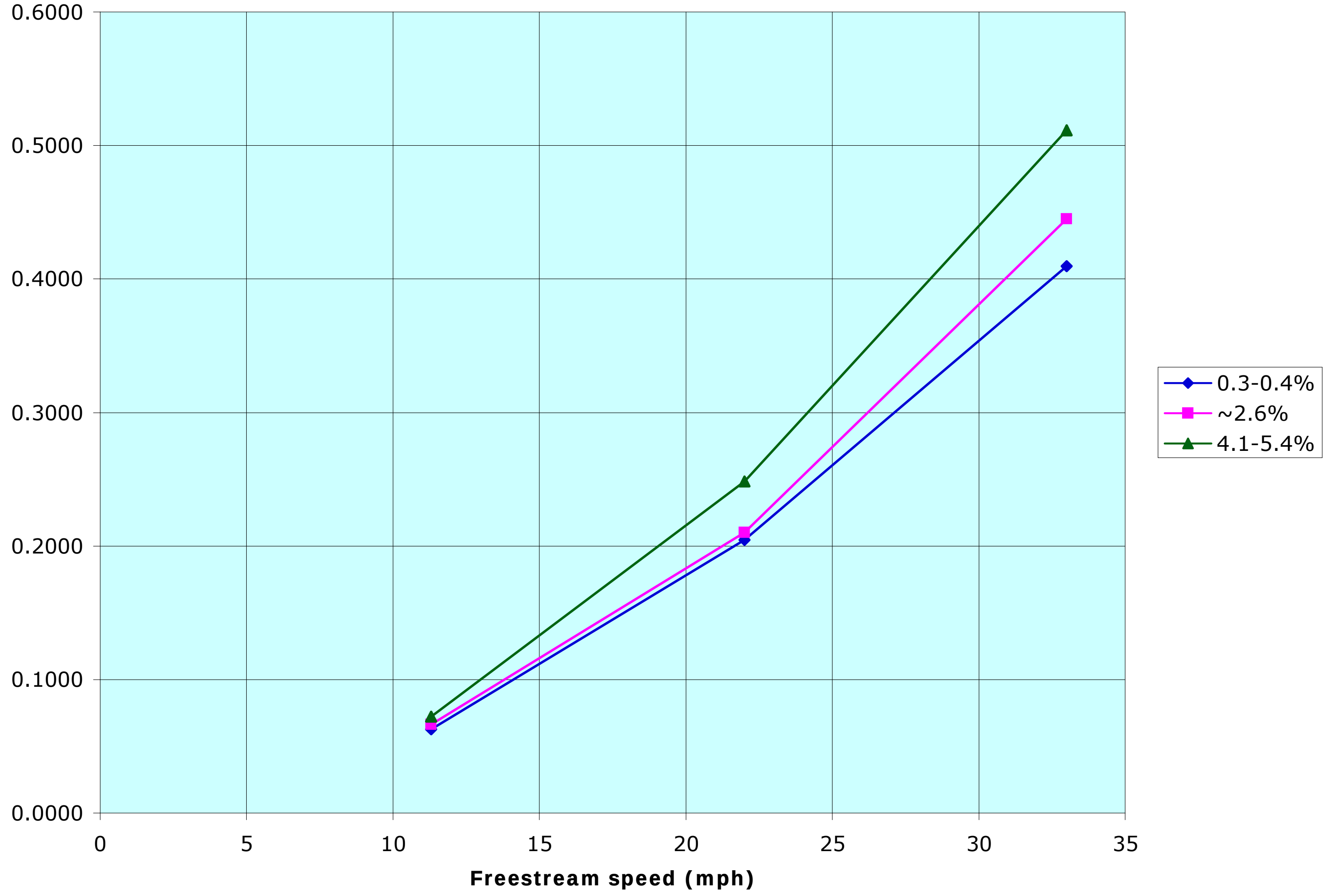
- *n* = oil index of refraction; μ = dynamic viscosity; λ = light wavelength.

Wall Shear Stress Variation with Free Stream Turbulence

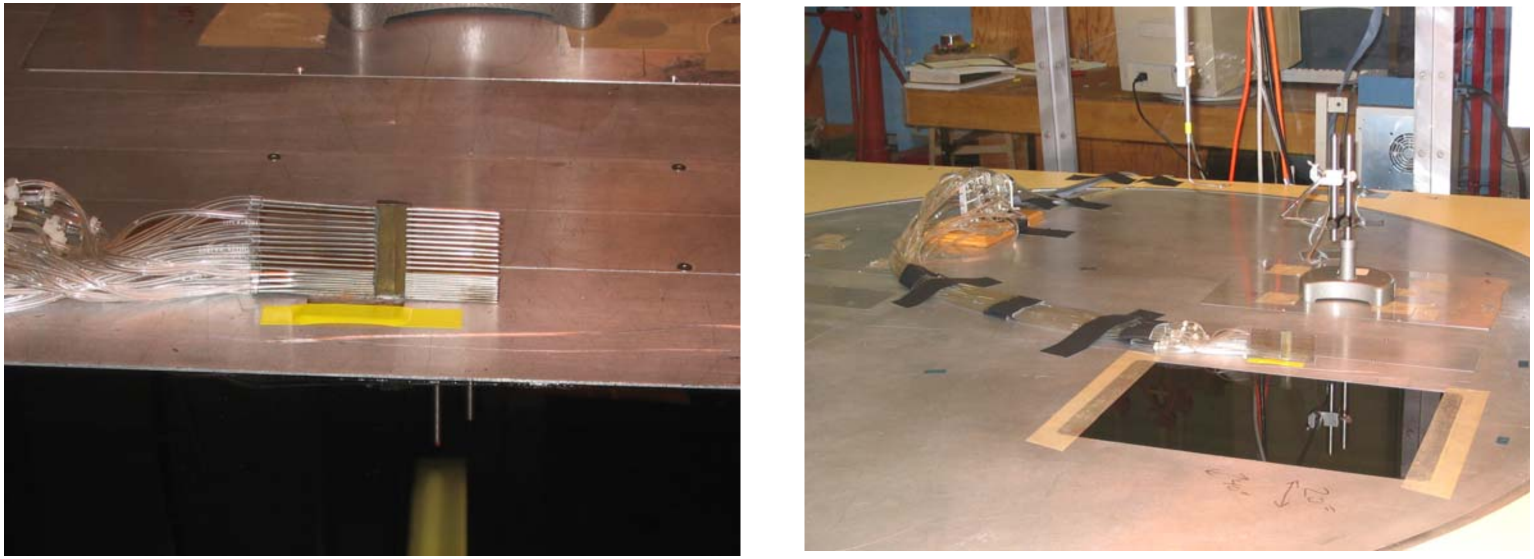
	Turbulence Level		
Speed (mph)	0.3-0.4%	~2.6%	4.1-5.4%
11.3	0.0626	0.0663	0.0723
22	0.2048	0.2102	0.2483
33	0.4096	0.4450	0.5115

- Wall shear stress (τ_w) given above in Pa.
- Notable increase in τ_w as turbulence level increases.
- Data at 1% turbulence level showed slight *decrease* in τ_w; calibration drift of pitot-static pressure transducer suspected.

Free Stream Turbulence Intensity Affecting τ_w - Plot

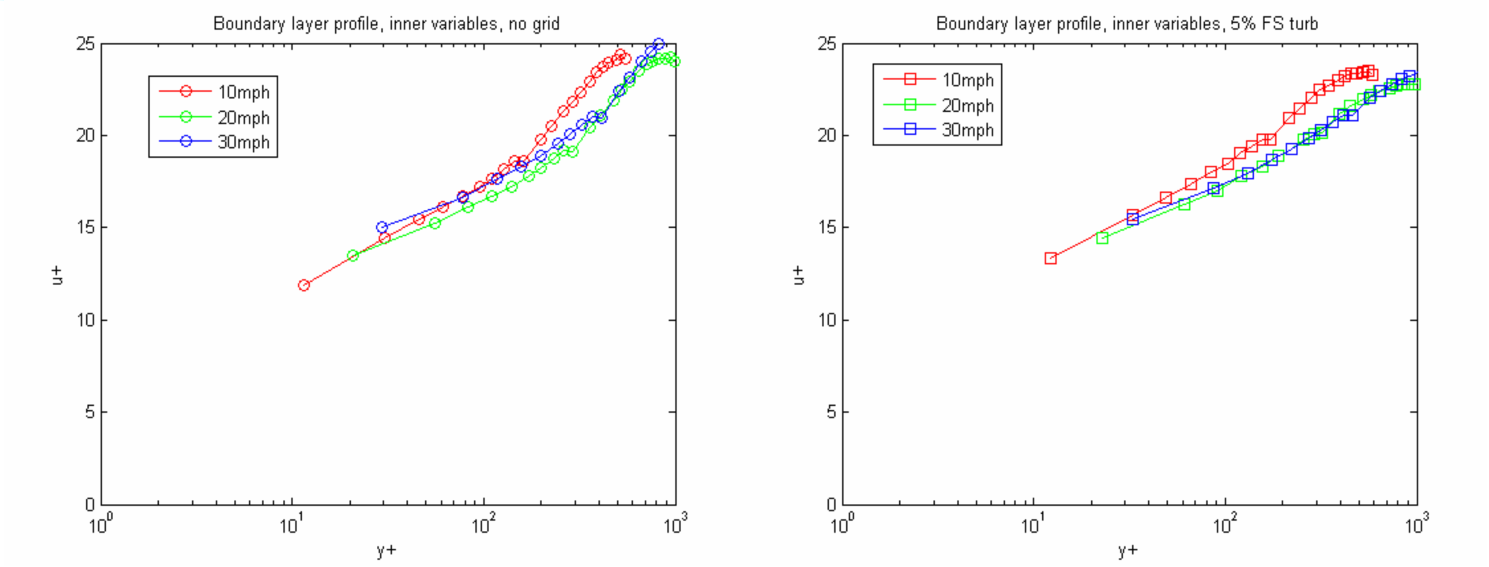


Boundary Layer Profile Measurement



- 22-element boundary layer rake used to measure dynamic pressures at select heights
- Static pressure taken from nearby pitot-static tube

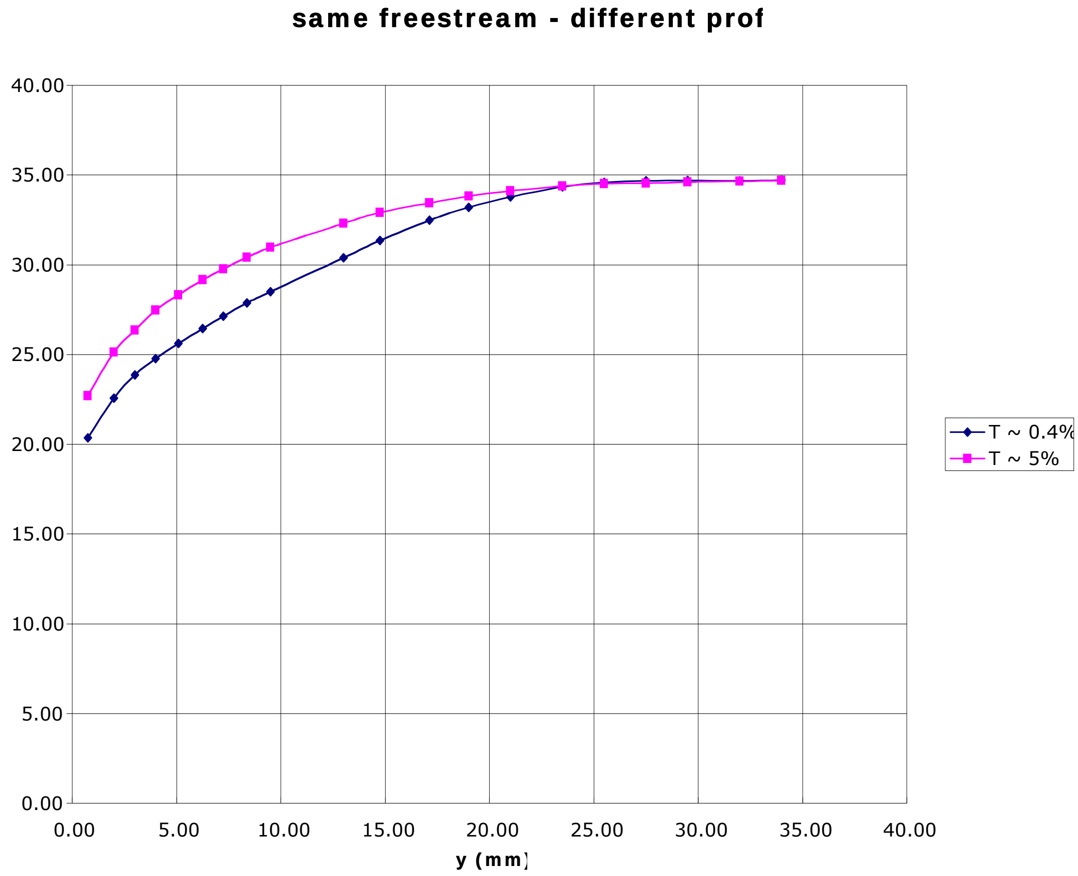
Boundary Layer Profile Comparison - ~0.4% vs. 5% free Stream Turbulence



- Both profiles follow Clauser turbulent boundary layer profile; shape changes slightly near free stream transition
- In no case is laminar sub-layer accessible ($y^+<5$).

Profile Shape Change with Free Stream Turbulence Level

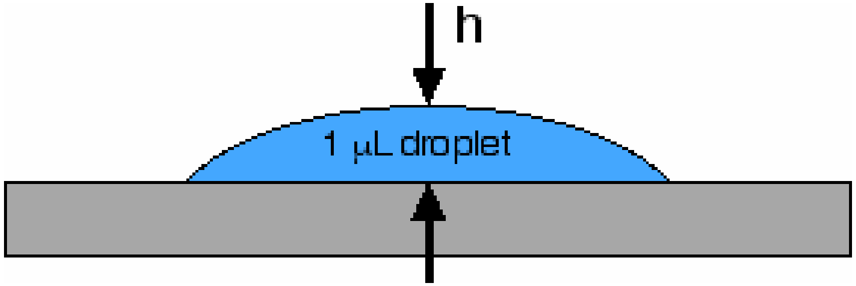
- At the same freestream speed, the shape of the boundary layer visibly varies with added freestream turbulence T.
- The higher T curve “stays high” lower, requiring a more abrupt reduction to zero.
- This agrees with the observed higher shear stress at the wall.



Critical Parameter for Evaporation: Wall Shear?

- It is hypothesized (Navaz) that evaporation rate of liquid droplets is based on the friction velocity (u_τ) rather than the free stream speed (U_∞).
- Current experiments demonstrate that for a constant U_∞, τ_w may be increased by up to 25% by imposing 5% turbulence intensity on the free stream flow.
- 25% increase in τ_w -> 12% increase in u_τ.
- Change in evaporation rate by up to 20% thus expected by model.

Relative Sizes: 1 μL Droplet and Laminar Sub-Layer

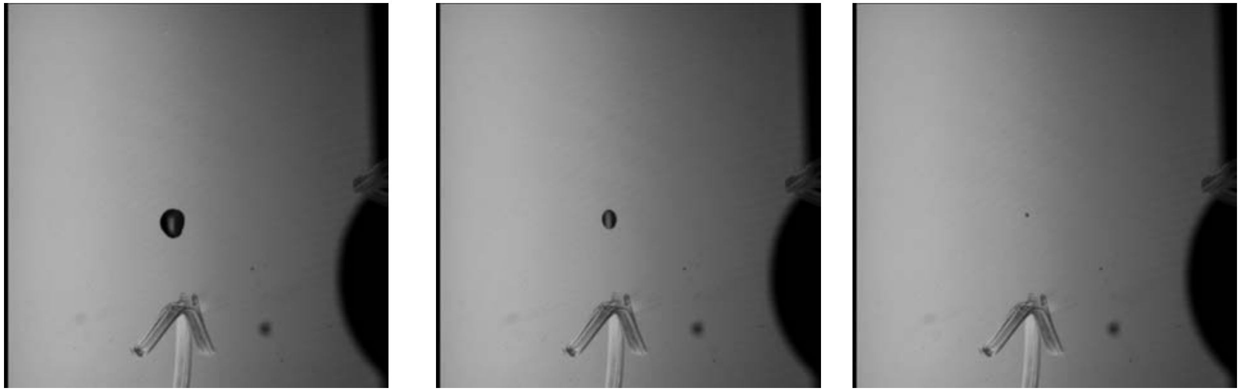


- 10 mph free stream and low turbulence level, present BL experiments
- Laminar sub-layer thickness ($y^+ = 5$) is ~ 0.3 mm
- 1 μL droplet has height *h* of ~ 0.2 mm (Navaz)
- Droplet lies entirely within laminar sub-layer, where friction velocity u_τ is the dominant flow parameter (and only velocity scale!).

Proof-of-Concept Experiment

- Evaporation rate of 2.5 ml water drop in 10 mph free stream examined at turbulence intensity levels of 0.4% and 5%.
- Droplet dispensed on glass, video camera observes evaporation.
- Ensembles for each case taken, mean evaporation time recorded.

Droplet Evaporation Experiment



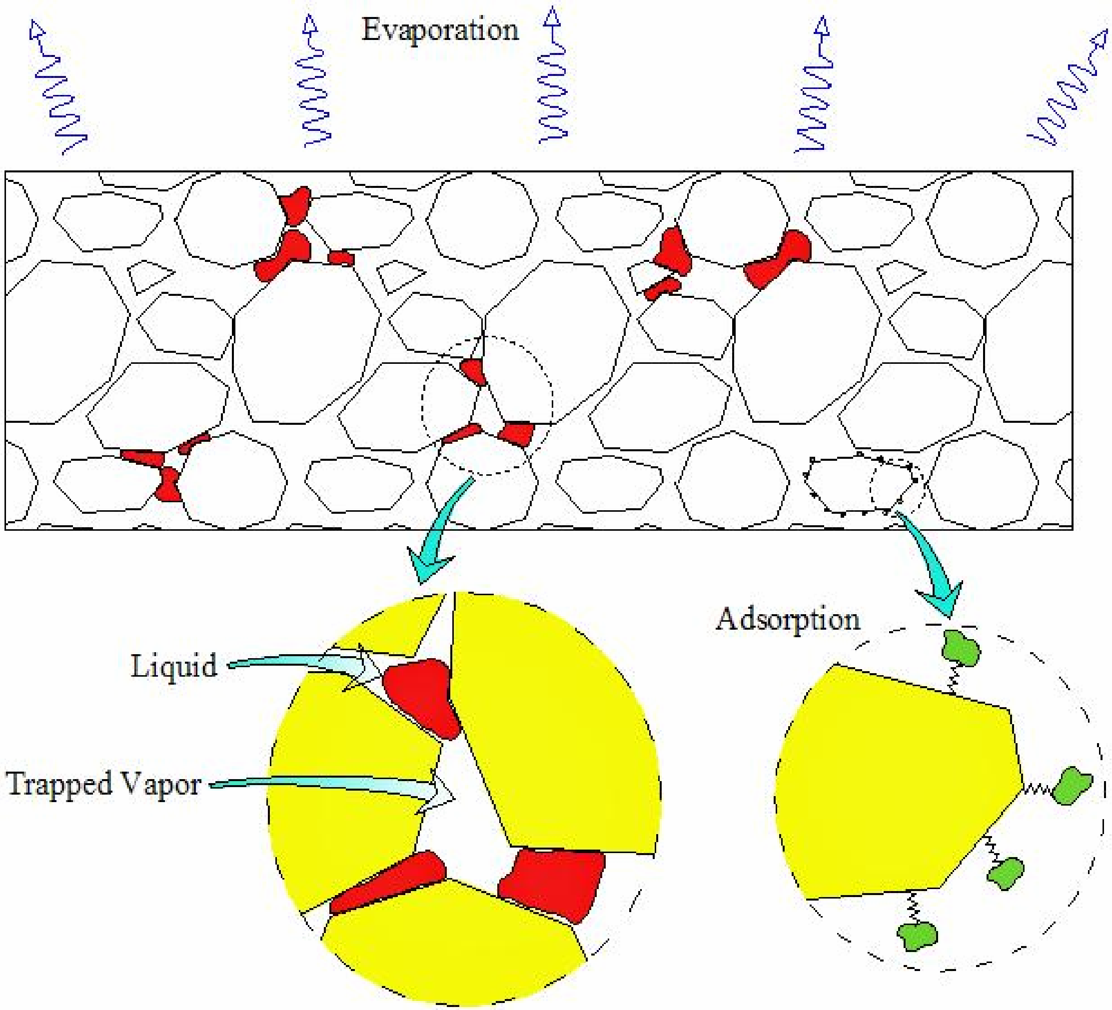
Turbulence intensity level (%)	0.4	5
Friction velocity (m/s)	0.23	0.25
Mean drop evaporation time (sec)	**900**	**850**

Upcoming Work at Caltech

- Evaporation rate measurement
  - Instantaneous rate measurement
  - More accurate optical techniques
  - Mass measurement (microbalance?)
- Still higher turbulence intensity levels
- Further collaboration/verification with numerical model of H. Navaz
- Different surfaces (concrete, etc.)

Evaporation Module
Link to the Porous Surface

- Simultaneous process present with evaporation
  - Capillary diffusion
  - Secondary evaporation
  - Vapor entrapment
  - Adsorption



Porous Media/Substrate Modeling Observations

- Liquid simulants established a finite network in a porous domain (Czech concrete)

Porous Media/Substrate Modeling Proposed Approach

- Modeling effort
  - Solve the governing equation by capillary network model (CNM)
- Verification effort
- Generating the Design of Experiment matrix
- Obtaining solution for the entire matrix
- Curve fitting
  - Classical
  - Neural Network

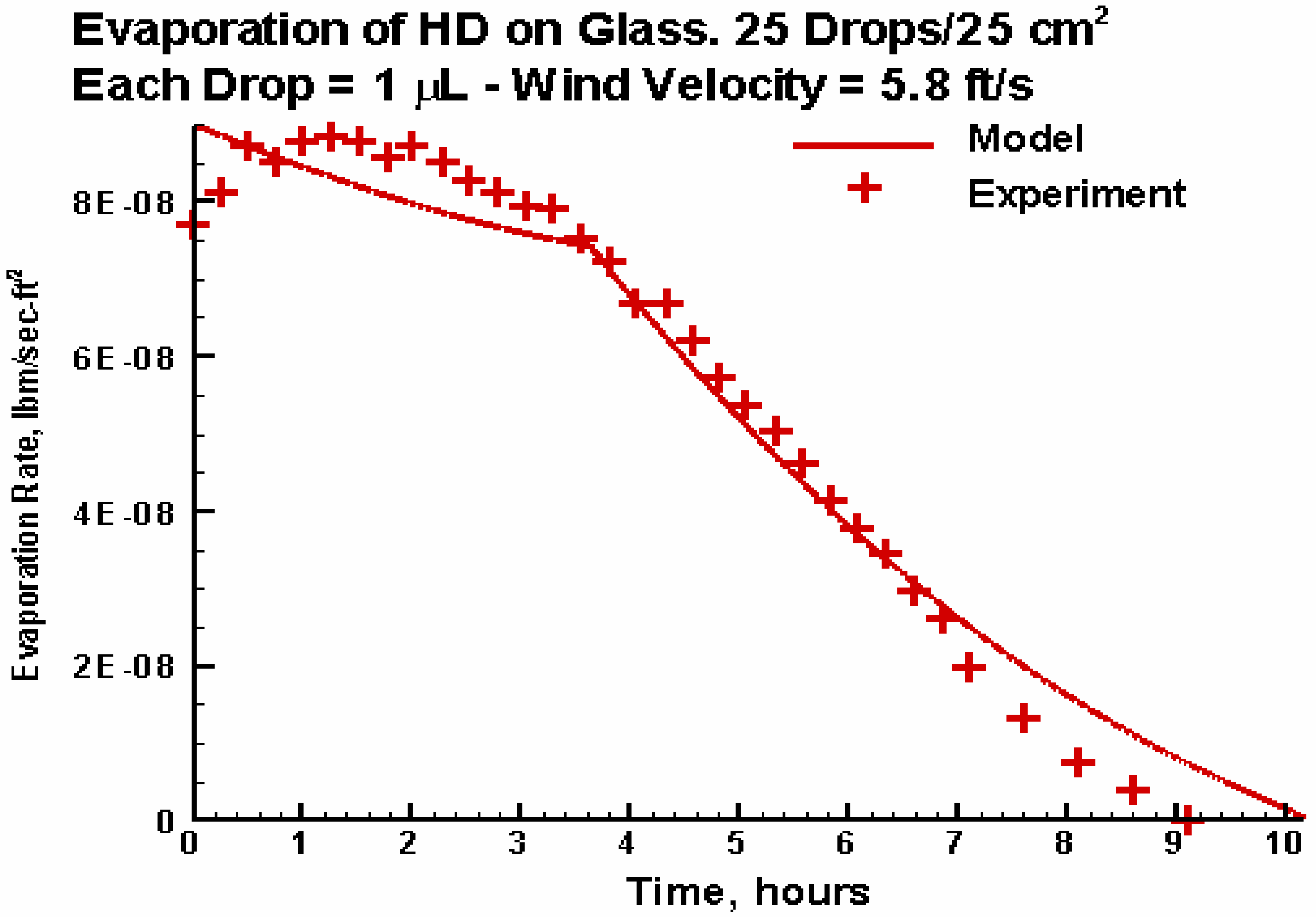
Porous Media/Substrate Modeling Adding Adsorption Model

- Add adsorption model to the porous substrate model
- Ensure robustness of the algorithm
- Validate model by
  - Conducting laboratory tests
- Verify the model
  - Laboratory
  - Outdoor

Conclusion

- Developed an evaporation model
- Verified the model with experimental data
- Extended the domain of applicability by using a hybrid analytical/experimental method
- Developed a framework for tackling a more complex problem – HD on porous substrate
- Resolving wind/turbulence/shear stress issues
- Incorporating the effects of wind turbulence intensity on evaporation

Evaporation Rate Validation



Evaporation of HD on Glass. 25 Drops/25 cm^2
Each Drop = 1 μL - Wind Velocity = 5.8 ft/s