Droplet Reaction and Evaporation of Agents Model

(DREAM)

Applied to HD on glass, DEM on glass and MS on glass

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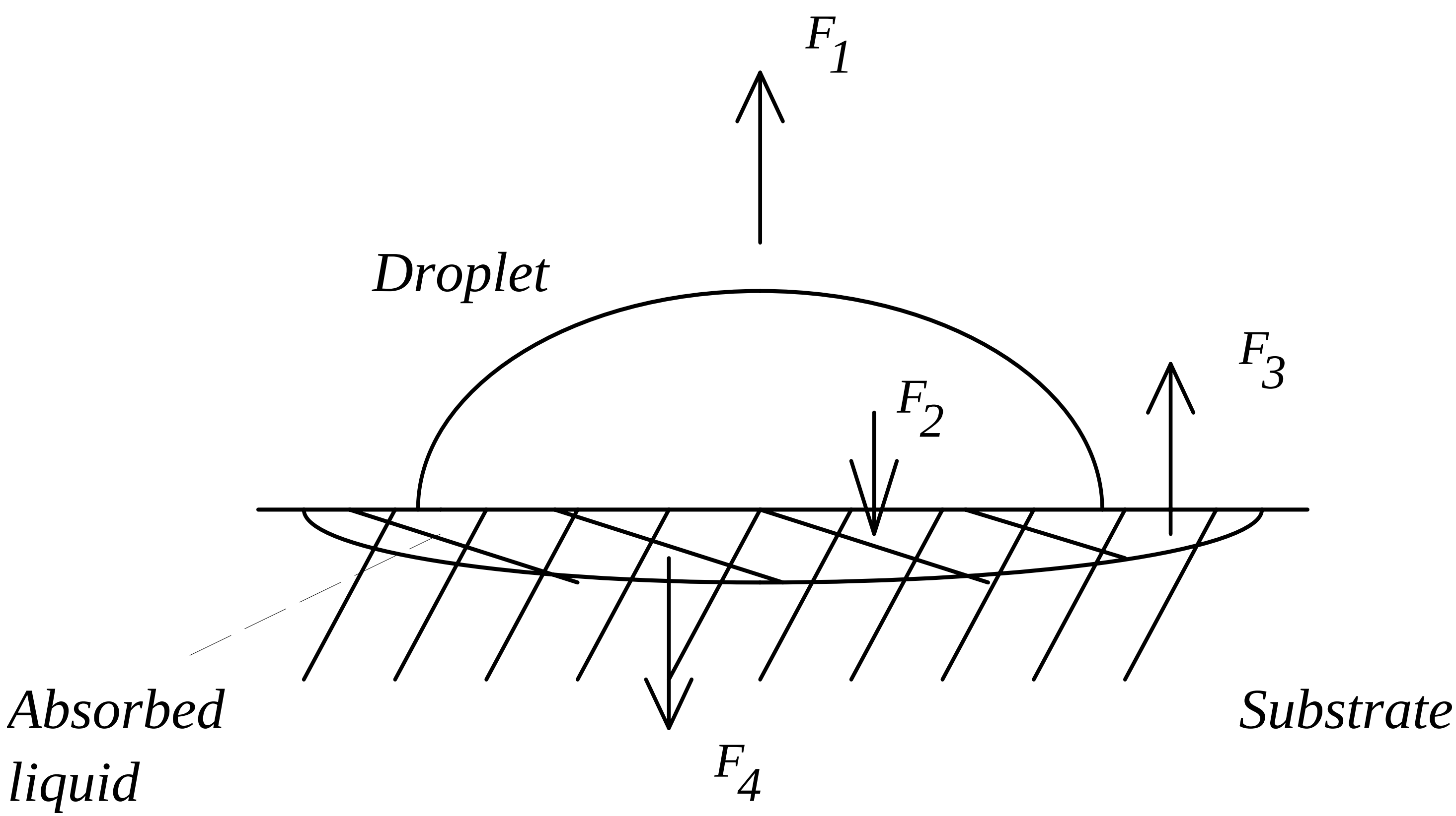
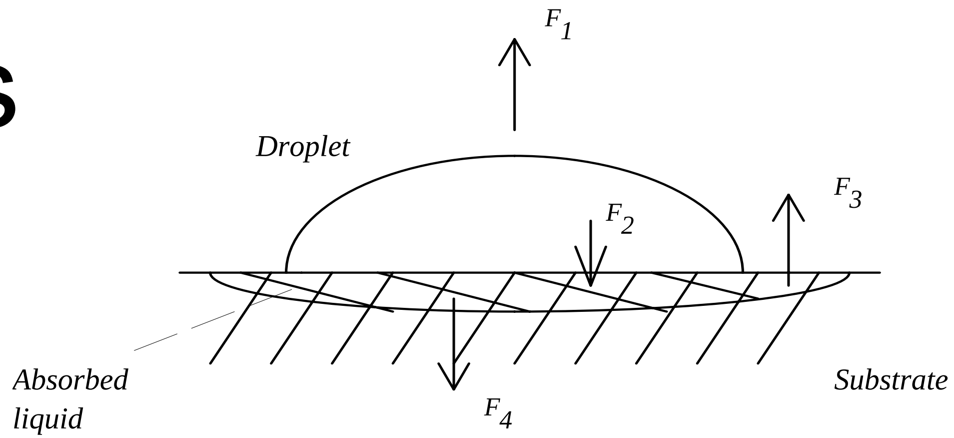
Outline

- Introduction
- Model
  - Sessile drop model
- Data
  - Dutch wind tunnel (HD, DEM and MS on Glass)
  - Czech wind tunnel (HD on Glass)
  - ECBC wind tunnel (HD on Glass)
- Fitting the model to the data

4 Transport rates



Develop in steps

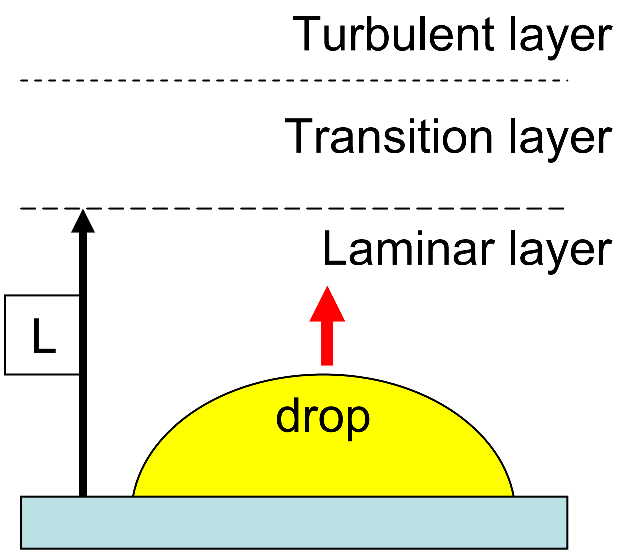


HD on Glass
MS on Glass
DEM on Glass

	Sessile Drop	Absorbed Drop
Neat Agent	Drops spread fast (seconds)	Drops absorb fast (minutes)
Thickened Agent	Drops spread slow (ten minutes)	Drops absorb slow (hours)

Add reactivity when significant chemical reactions are found

Sessile drop (F1)



- Drop mass over time

  $$m(T) = m(0) - \int_0^T \dot{m}(t)\, d\,t$$

- Fick's law

  $$d\,m(t) / d\,t = D\,A(t)\,(C_{skin} - C_{bulk}) / L$$

- Raoult's law (ideal mixtures)

  $$P_{agent\ in\ mixture} = \text{Mol fraction}_{agent\ in\ drop} \times P_{pure\ agent}$$
  $$C_{agent} = P_{agent}\ \text{Mol weight}_{agent} / (RT)$$

- Reactivity (implemented but not yet tested)

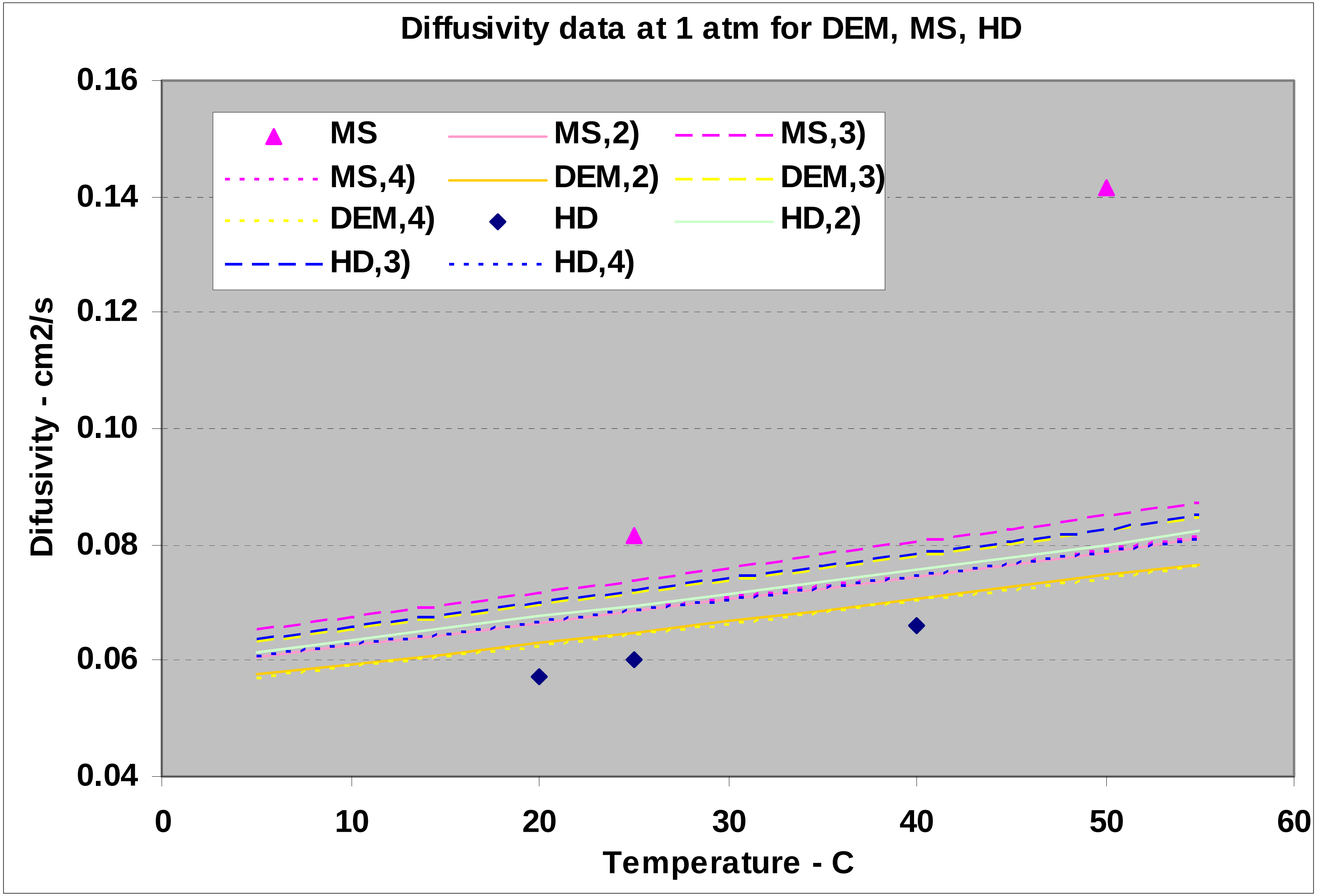
  $$d[X]/d[t] = A_e\, e^{(-E/RT)}\, [X]^x\, [Y]^y$$

Diffusivity, D in air

- How ‘mobile’ are the molecules in air?
  - Depends on temperature, pressure, molecular mass, molecular volume, and air properties

- Two estimation methods found
  - Fuller,Schettler,Giddings method (Lyman et al. 1982)
    - All above dependencies
    - Not suitable for phosphor components: no molecular volume data
  - Simple method (Danish EPA)
    - Eliminates molecular volume dependence

Diffusivity Data and Estimations



Vapor Concentration at skin, C_{skin}

- Get vapor concentration from vapor pressure
  - Get 'volatility' using ideal gas law: $C = P\ Mw / (R\ T)$

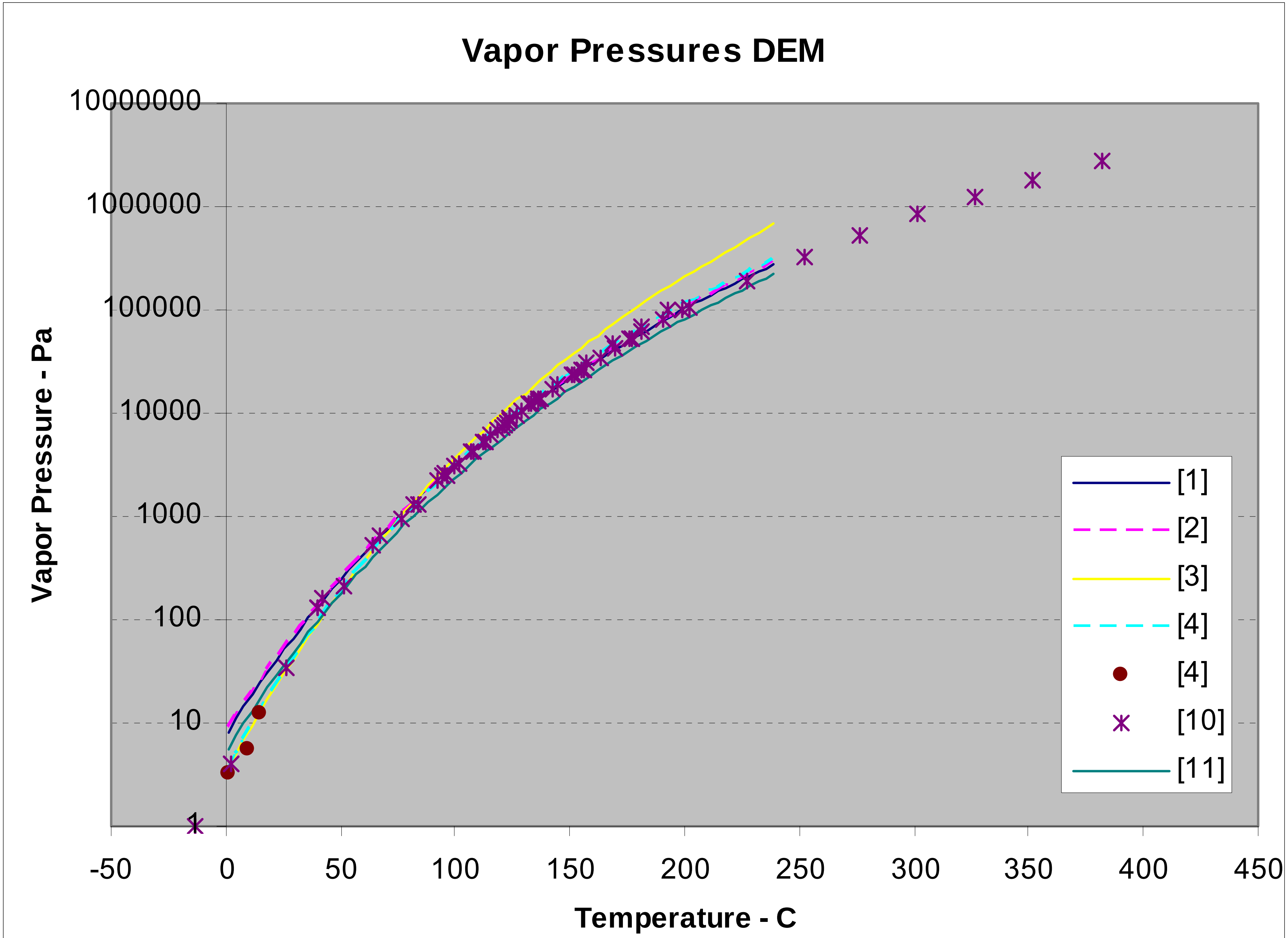
- Depends on
  - Agent
    - from data (if available)
    - or estimation methods
  - Temperature
    - Antoine equation (used for model)
      - three constants a,b,c fitted to data

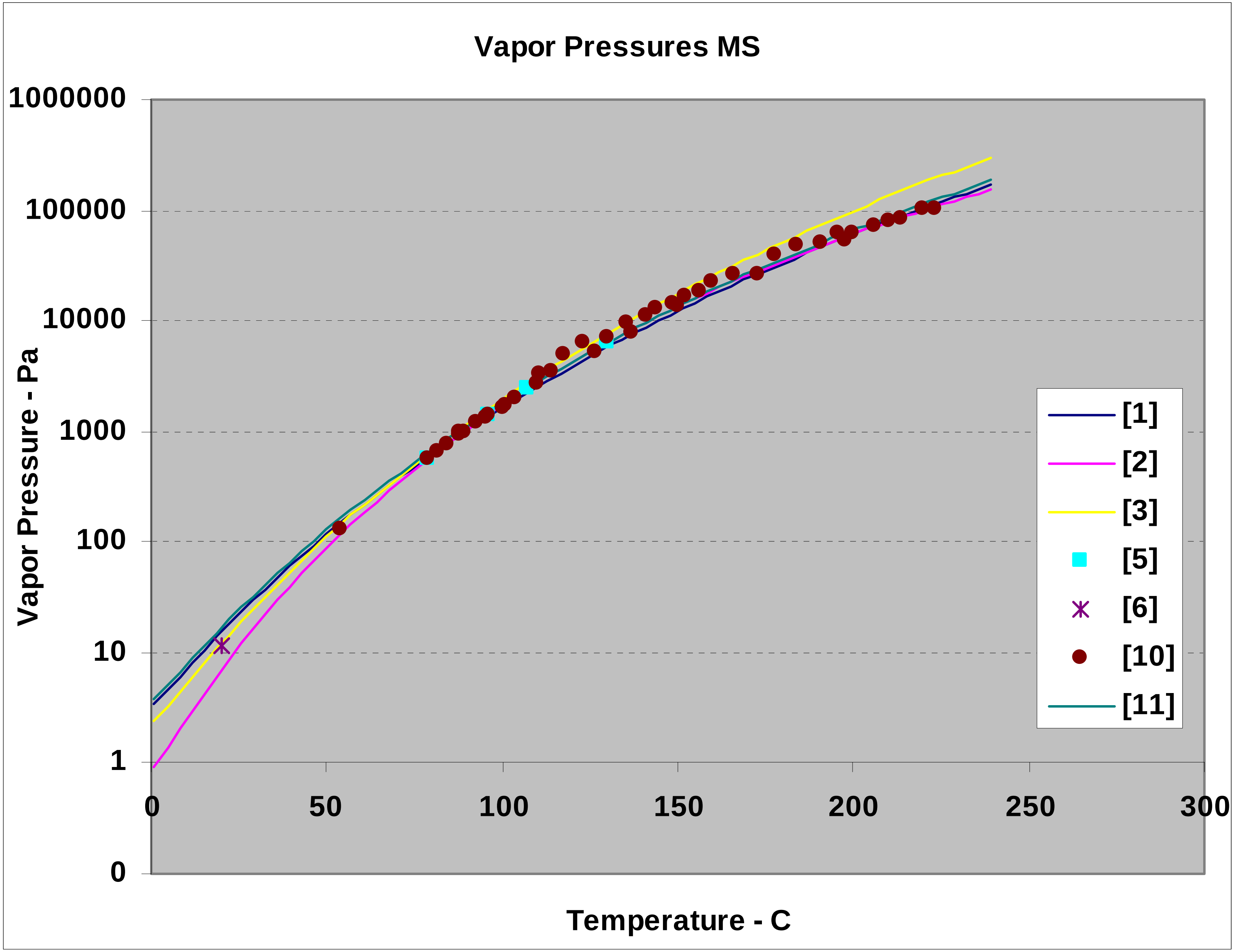
Antoine equation

$$P = 133.322 * 10^{a-b/(T+c)}$$

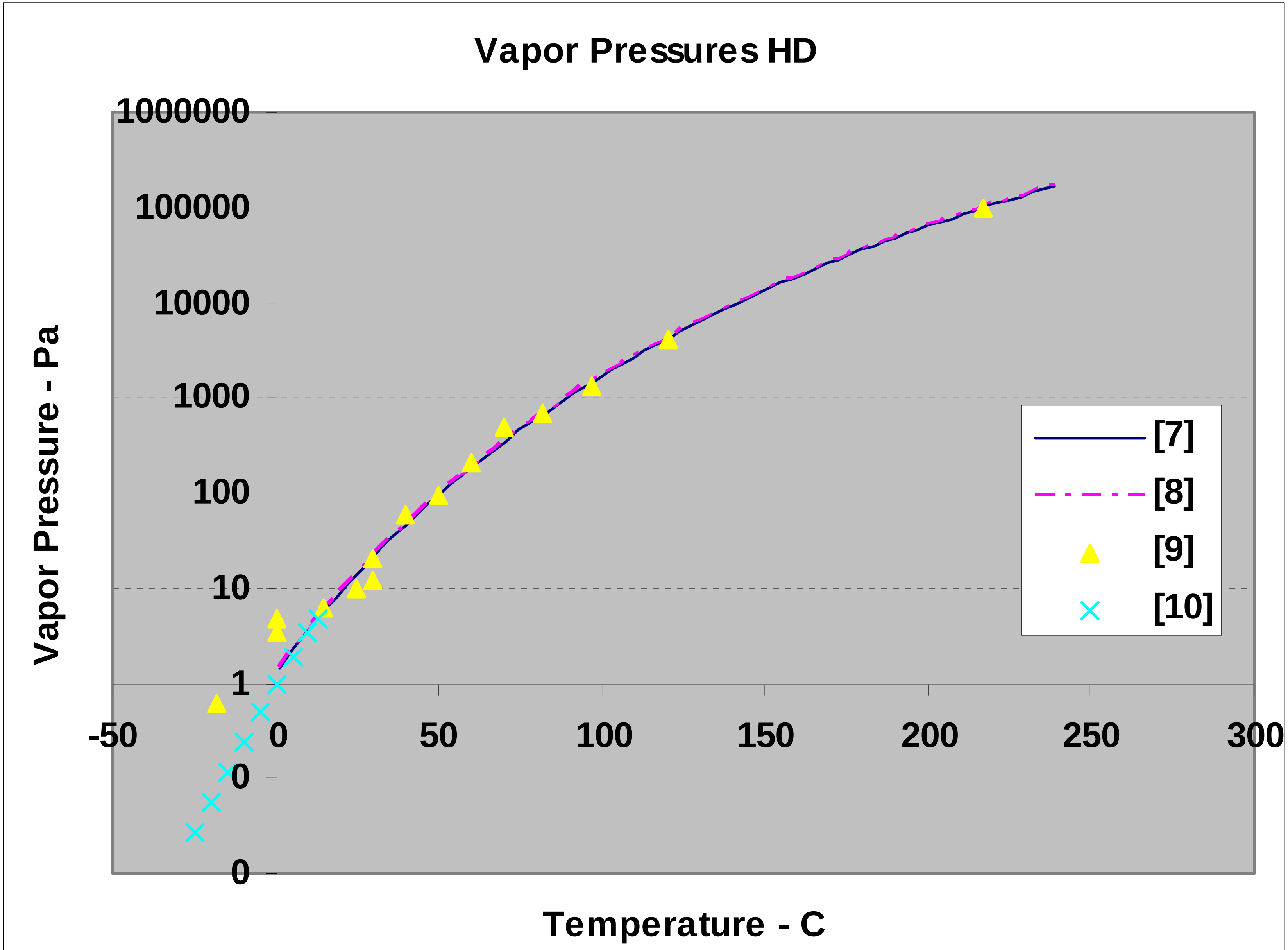
Clausius-Clapperon
Ideal gas

$$\ln \frac{p_2}{p_1} = -\frac{\Delta \overline{H}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$


Vapor Pressures DEM
Vapor Pressure - Pa
Temperature - C
10000000
1000000
100000
10000
1000
100
10
1
-50
0
50
100
150
200
250
300
350
400
450
[1]
[2]
[3]
[4]
[4]
[10]
[11]



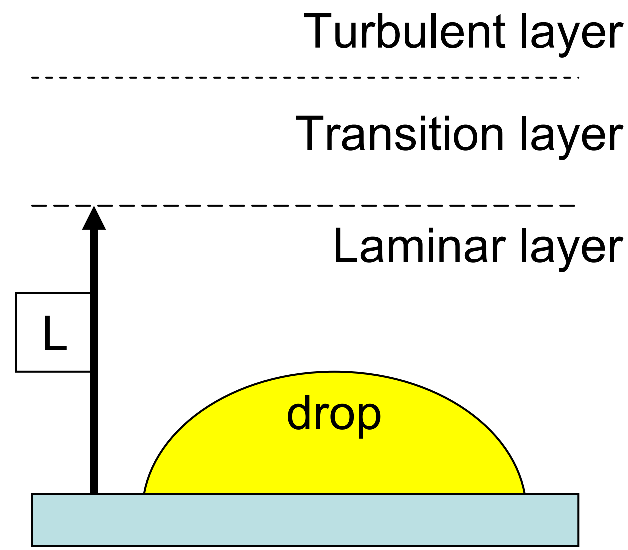
Vapor Pressures MS
Vapor Pressure - Pa
1000000
100000
10000
1000
100
10
1
0
0
50
100
150
200
250
300
Temperature - C
[1]
[2]
[3]
[5]
[6]
[10]
[11]



Vapor Pressures HD
1000000
100000
10000
1000
100
10
1
0
0
-50
0
50
100
150
200
250
300
Vapor Pressure - Pa
Temperature - C
[7]
[8]
[9]
[10]

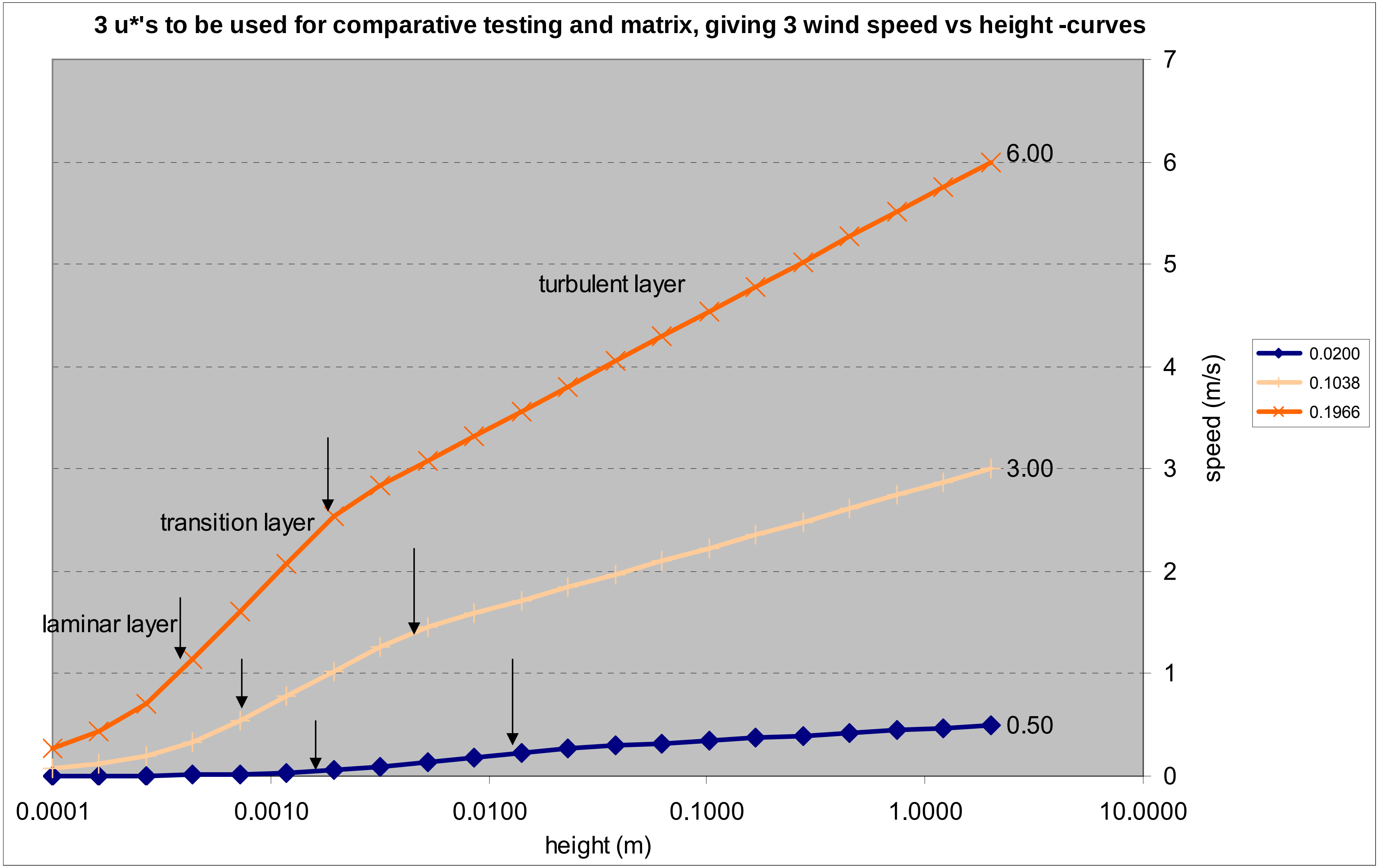
Diffusion layer thickness, L

- Depends on
  - wind speed
  - temperature (viscosity air)
  - pressure
  - on turbulence
  - drop size



- Empirical in semi-empirical model
  - Constant diffusion layer thickness for an experiment
  - ~ laminar layer thickness
  - order of magnitude: 1 millimeter
  - Fitted to data

Wind speed vs Height



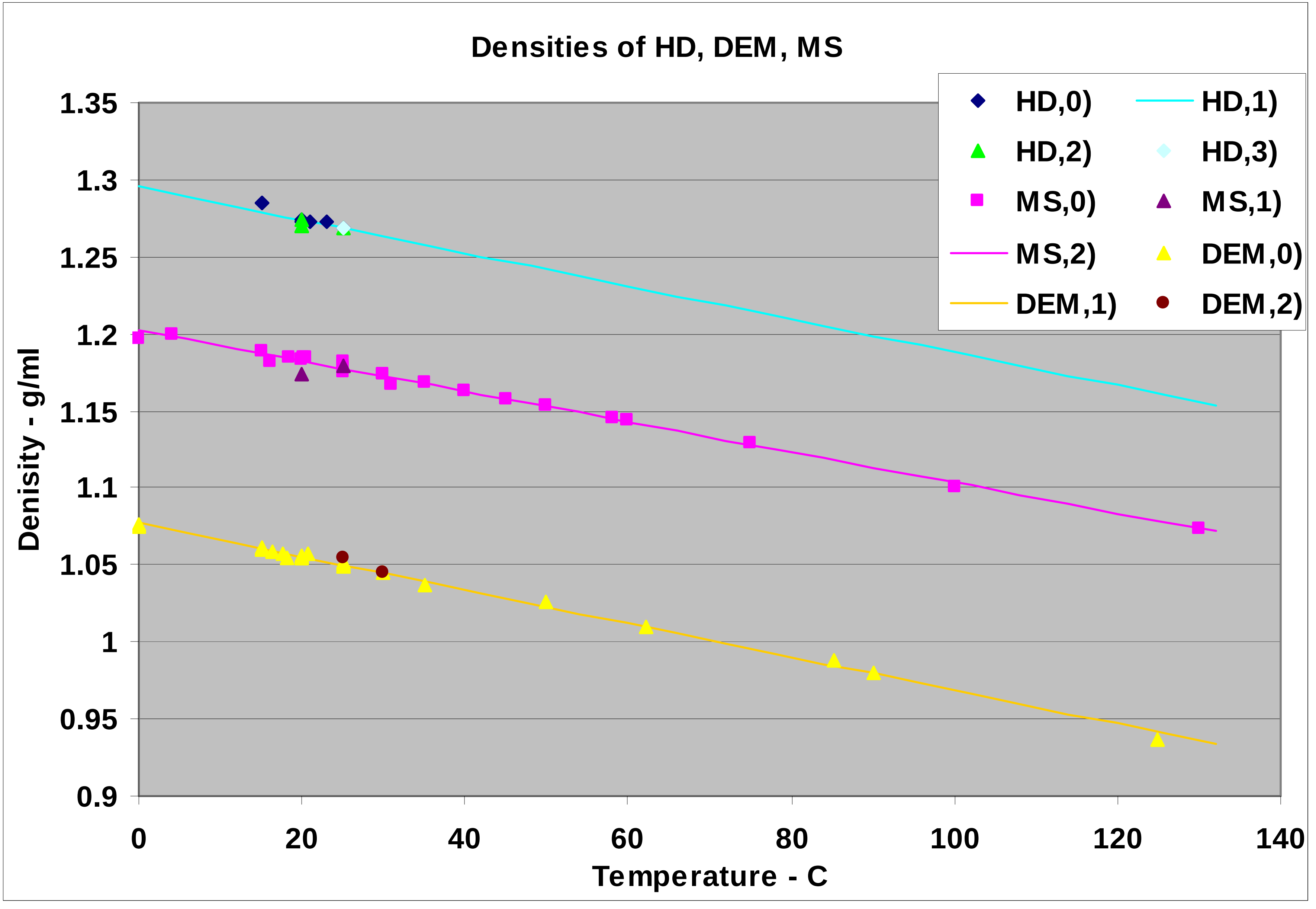
Area of evaporation, A(t)

- Volume from initial drop mass
    - Liquid density a function of agent and of drop temperature

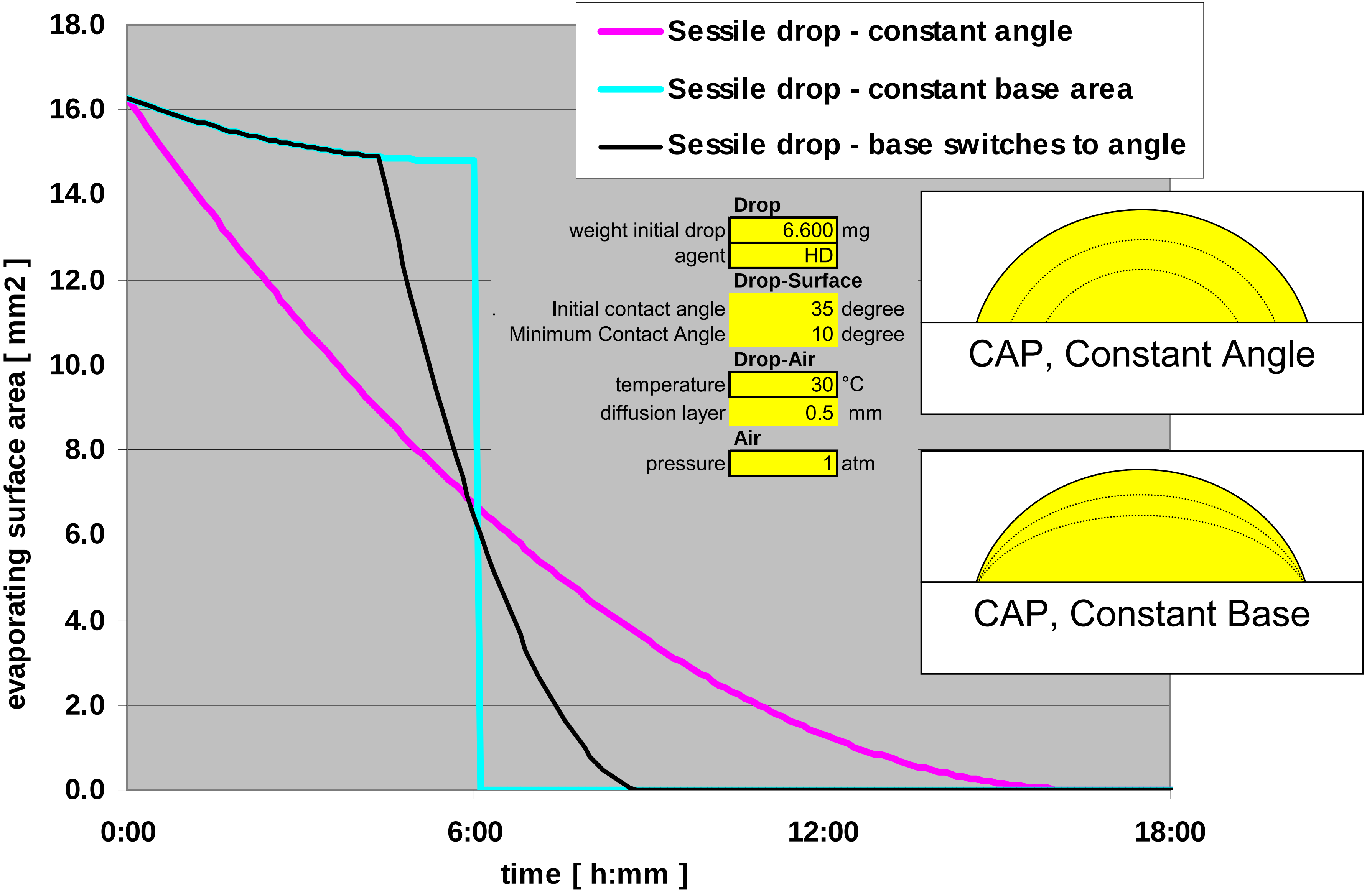
- Shape over time
  - From observed shape and time behavior of sessile drops:

    One shape (spherical cap), but two modes needed

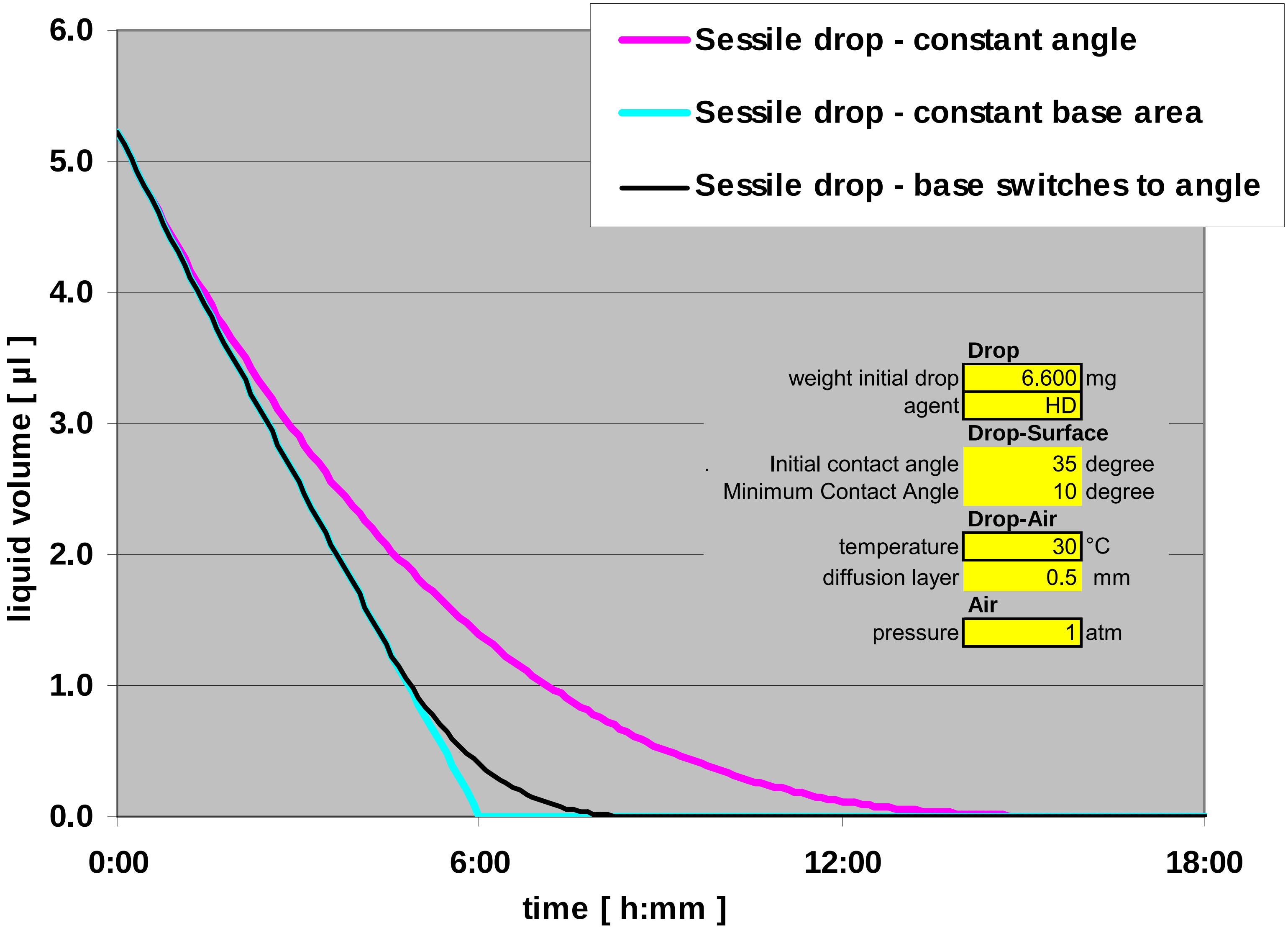
    - Constant base area mode
    - Constant contact angle mode


Densities of HD, DEM, MS
Denisity - g/ml
Temperature - C
1.35
1.3
1.25
1.2
1.15
1.1
1.05
1
0.95
0.9
0
20
40
60
80
100
120
140
HD,0)
HD,1)
HD,2)
HD,3)
MS,0)
MS,1)
MS,2)
DEM,0)
DEM,1)
DEM,2)

Area of evaporation over time



Volume of drop over time

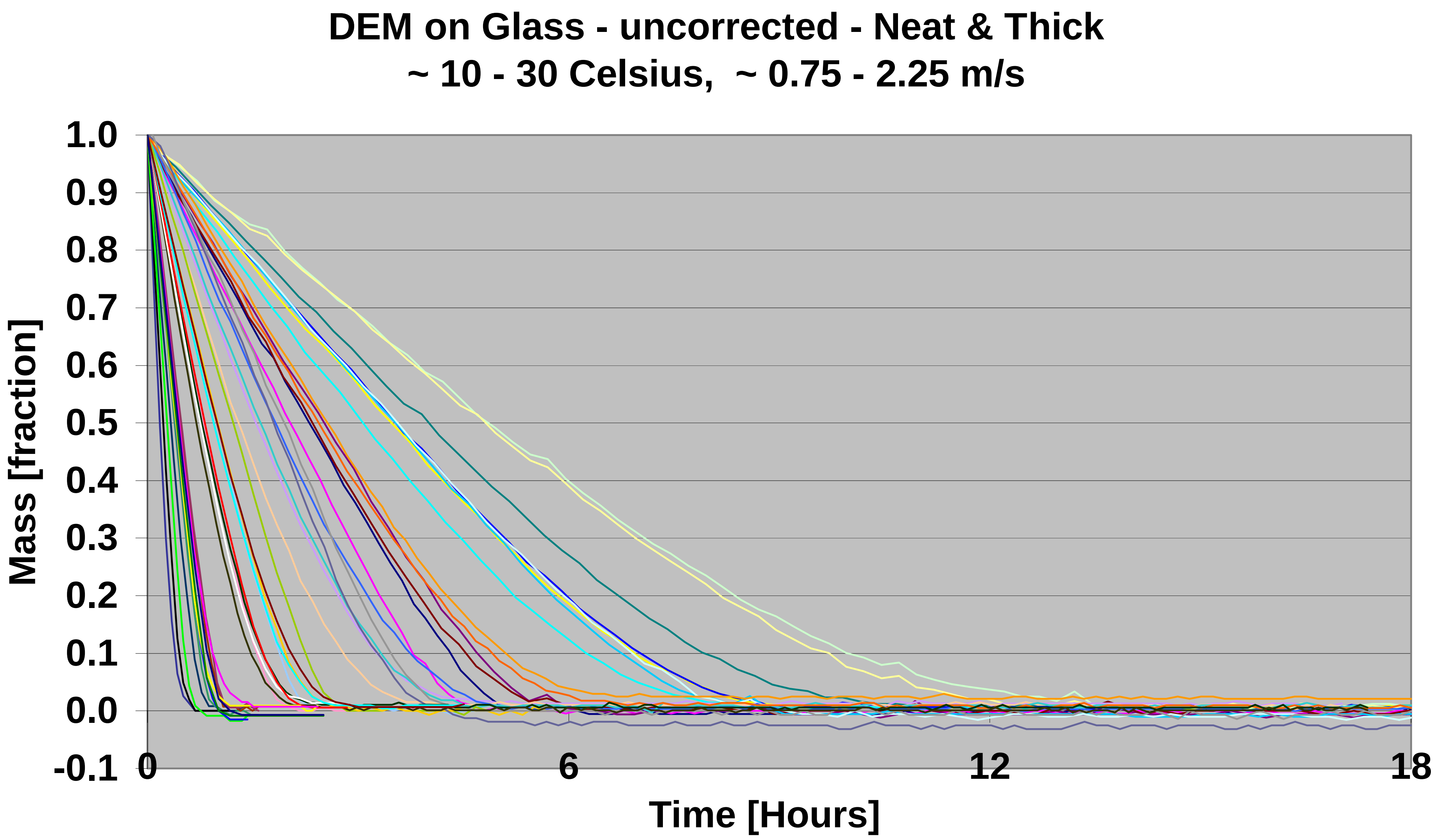


DATA

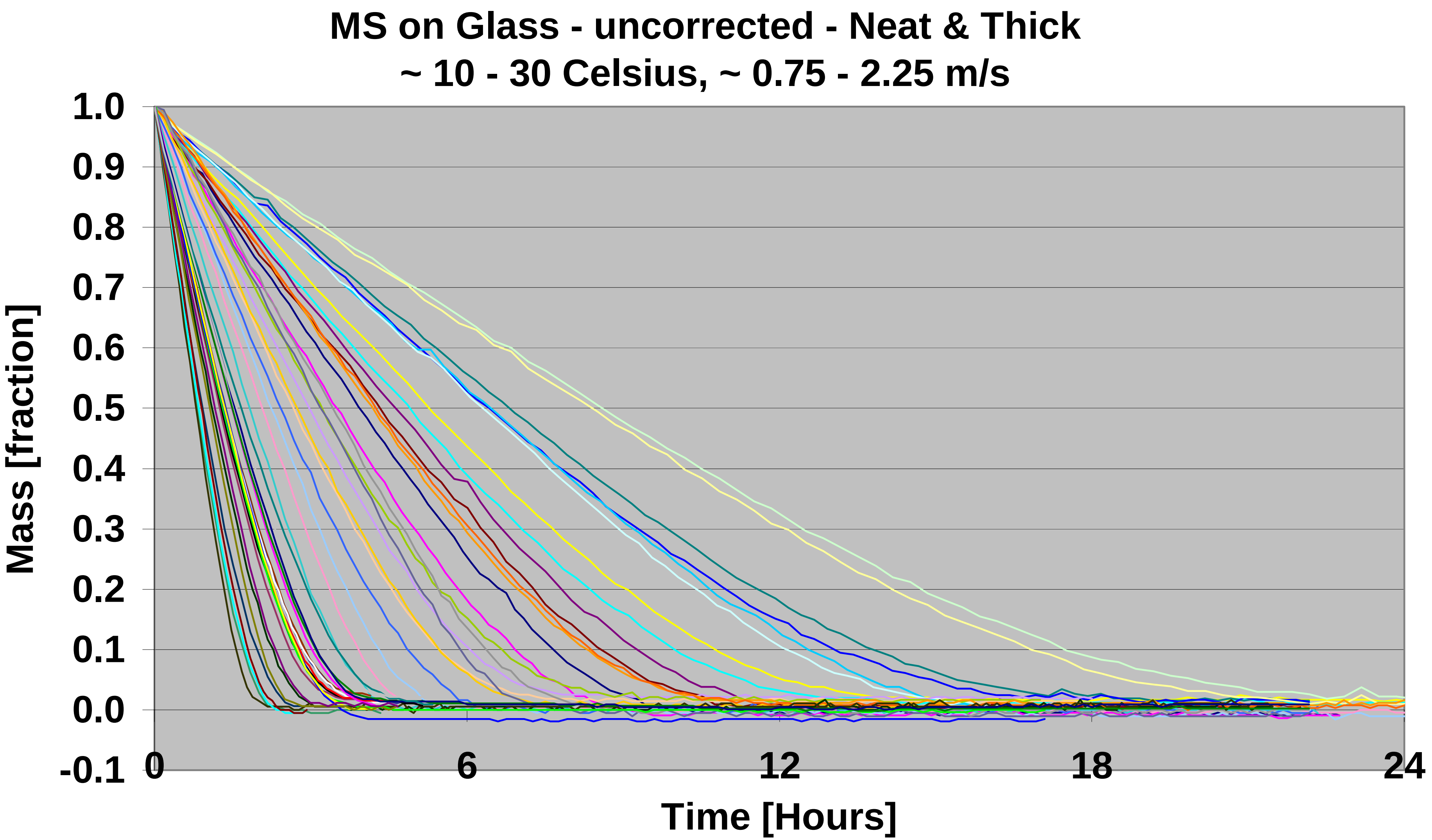
- Czech data
  - 30 mass over time curves HD on Glass
- Dutch data (neat and thick)
  - 42 mass over time curves DEM on Glass
  - 46 mass over time curves MS on Glass
  - 11 mass over time curves HD on Glass
- ECBC data
  - 5 mass over time curves HD on Glass

- Much more data on the way
  - UK, Czech, Dutch and ECBC
    - Establish proper tunnels performance
    - Compare effects tunnel size (and turbulence intensity)

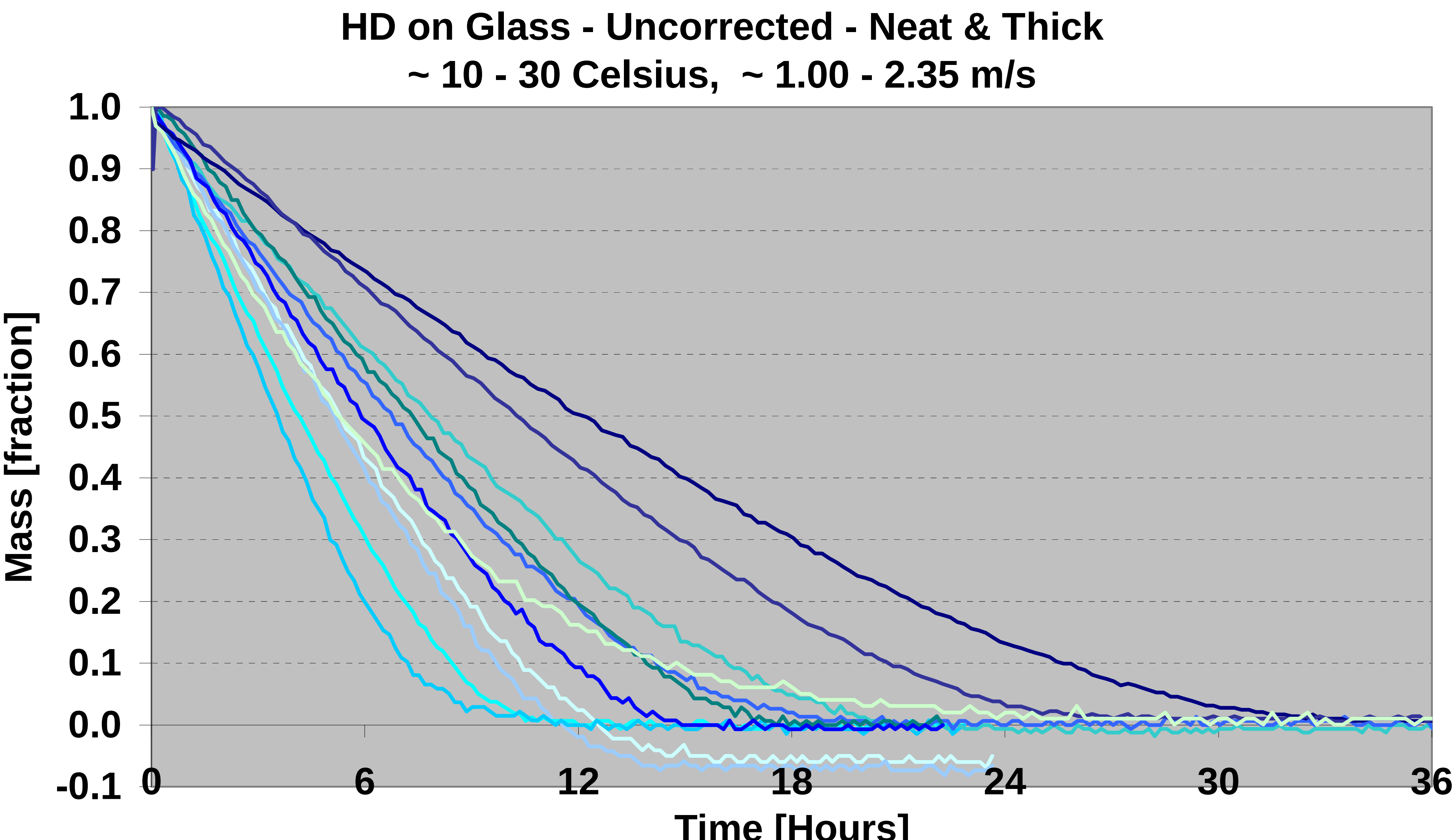
Dutch DEM data, 42 curves



Dutch MS data, 46 curves



Dutch HD data, 11 curves



Fitting the model to the data

used empirical fit functions for contact angles and ‘effective average diffusion layer thickness’

- Initial angle
- Minimum angle

assumed to depend on

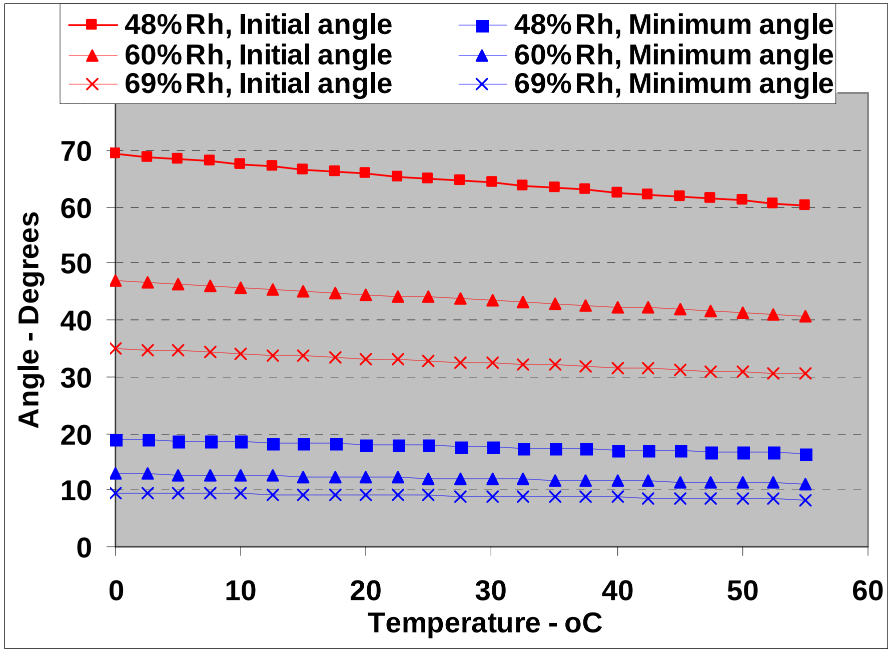
- temperature
- relative humidity

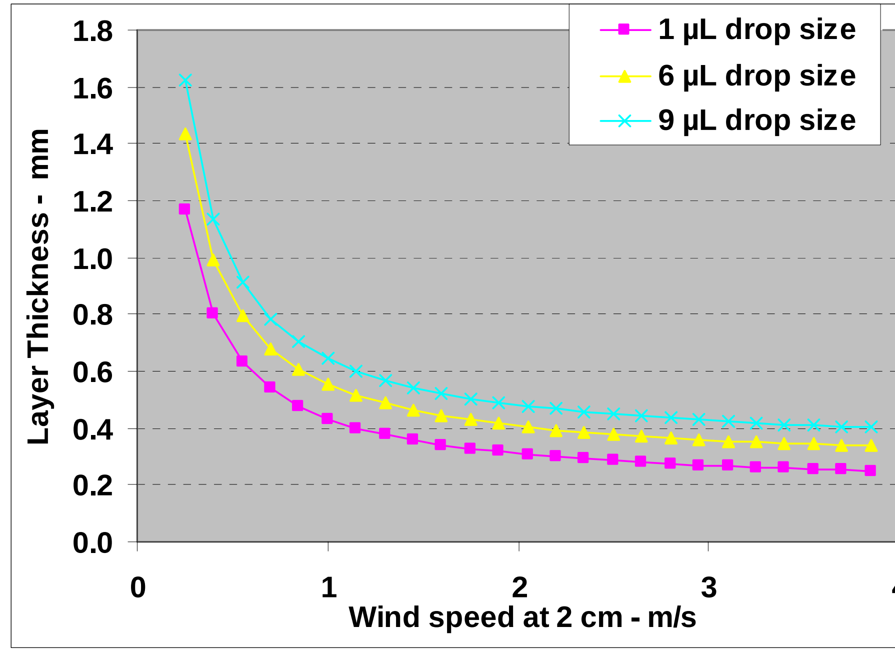
- ‘Effective average diffusion layer thickness’

assumed to depend on

- wind speed
- drop size

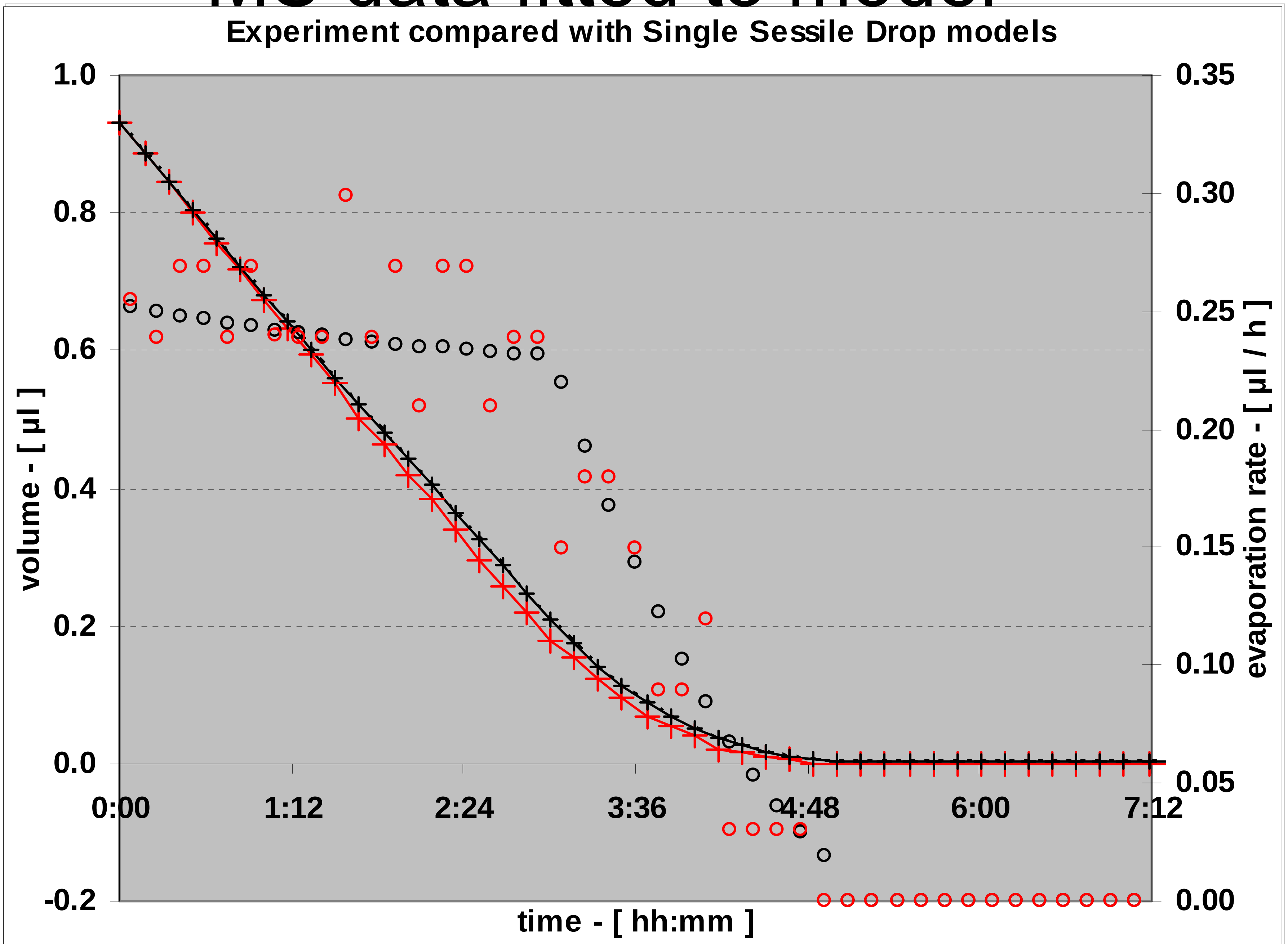
MS fit functions



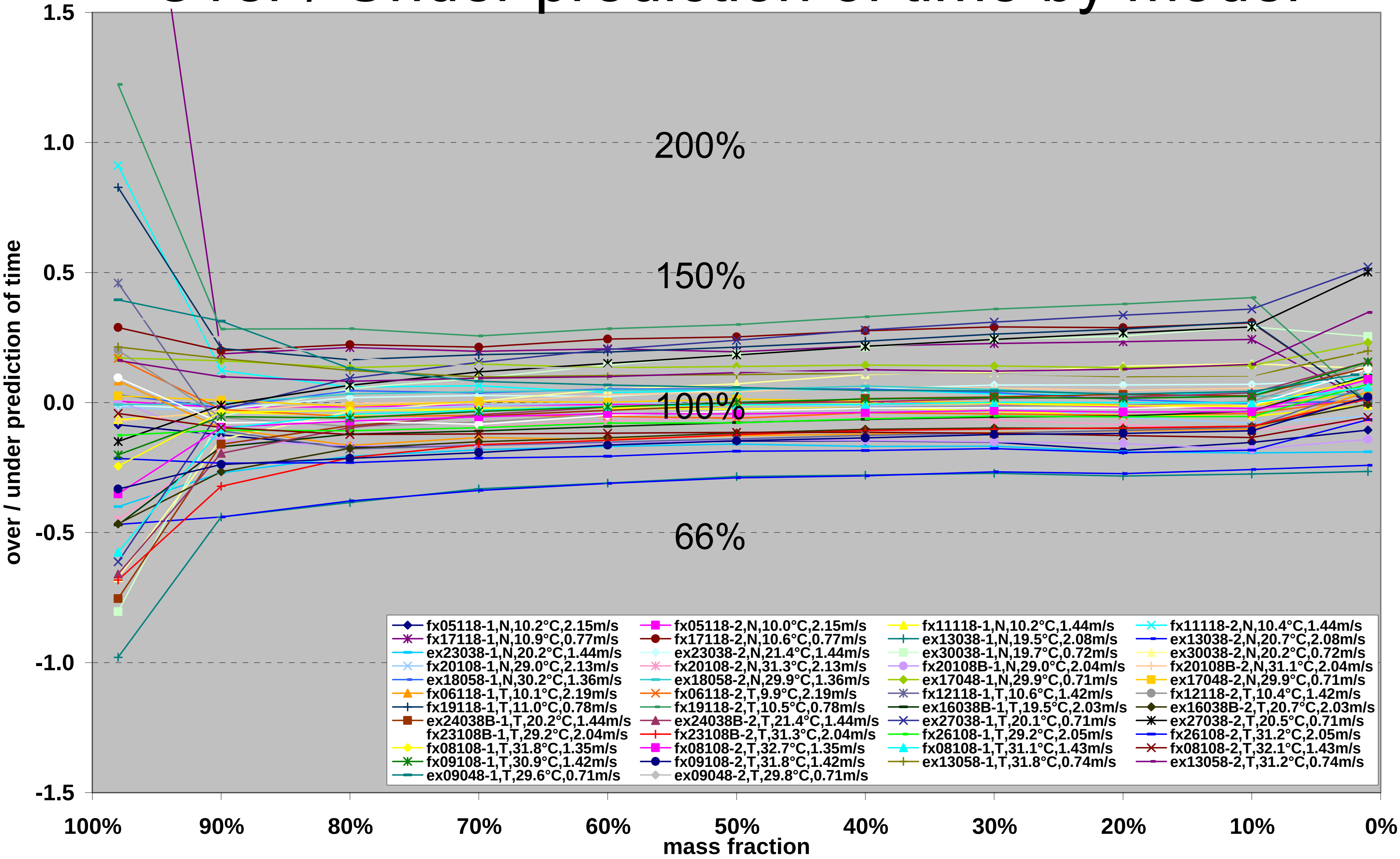


- Temperature
  - Exponential
- Relative Humidity
  - Exponential
- Wind Speed
  - Inverse with offset
- Drop Size
  - Exponential

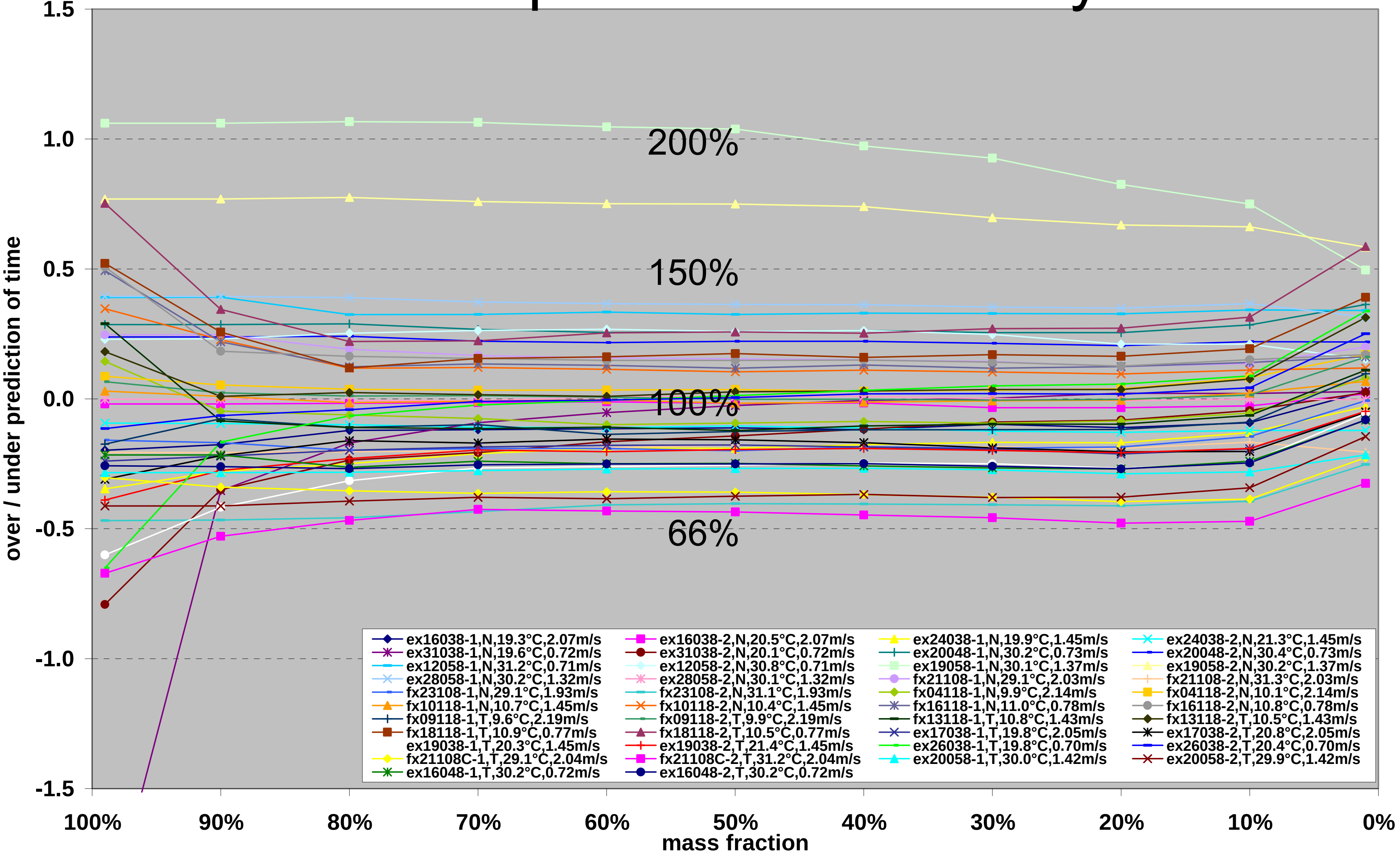
MS data fitted to model



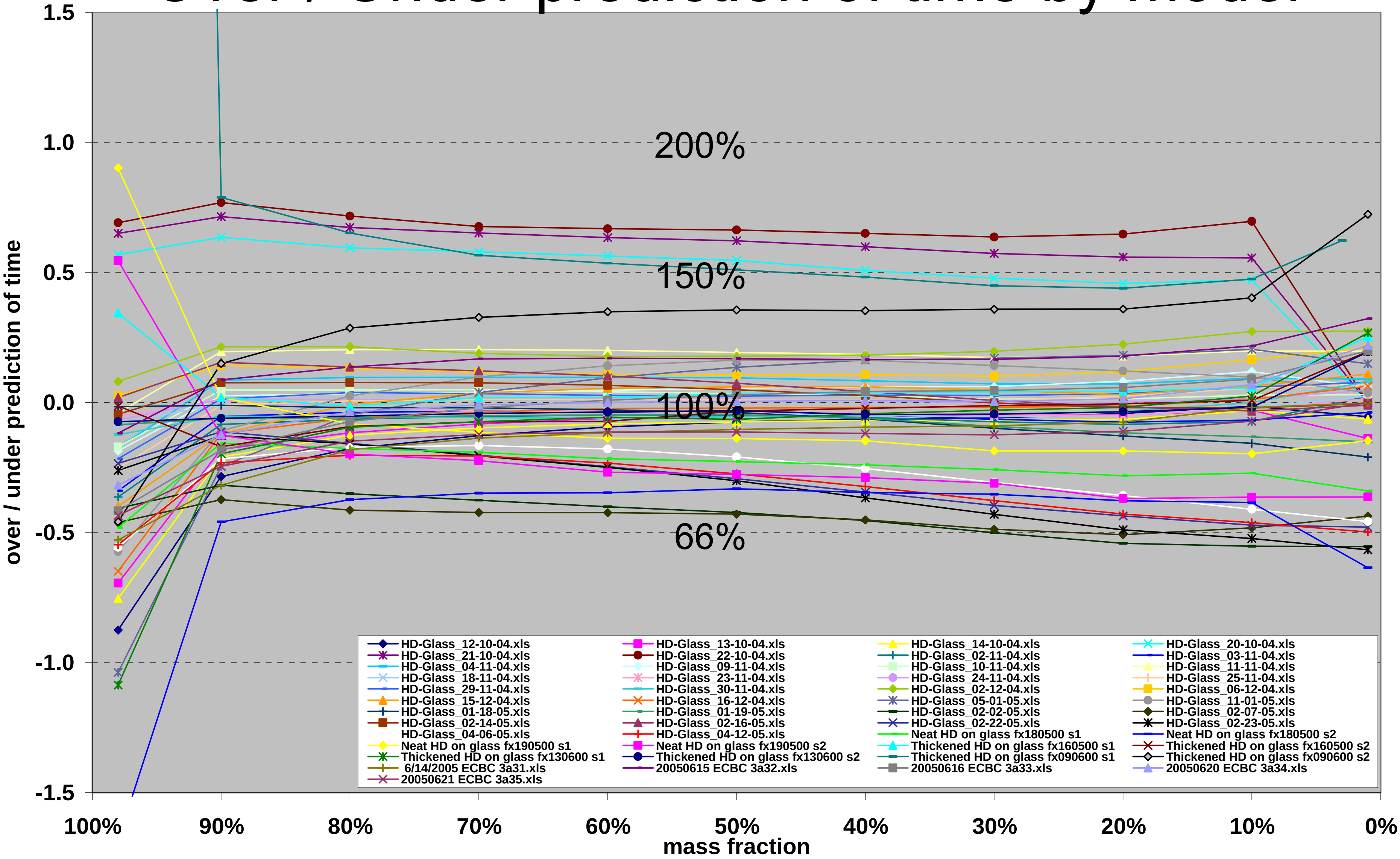
MS on Glass
Over / Under prediction of time by model



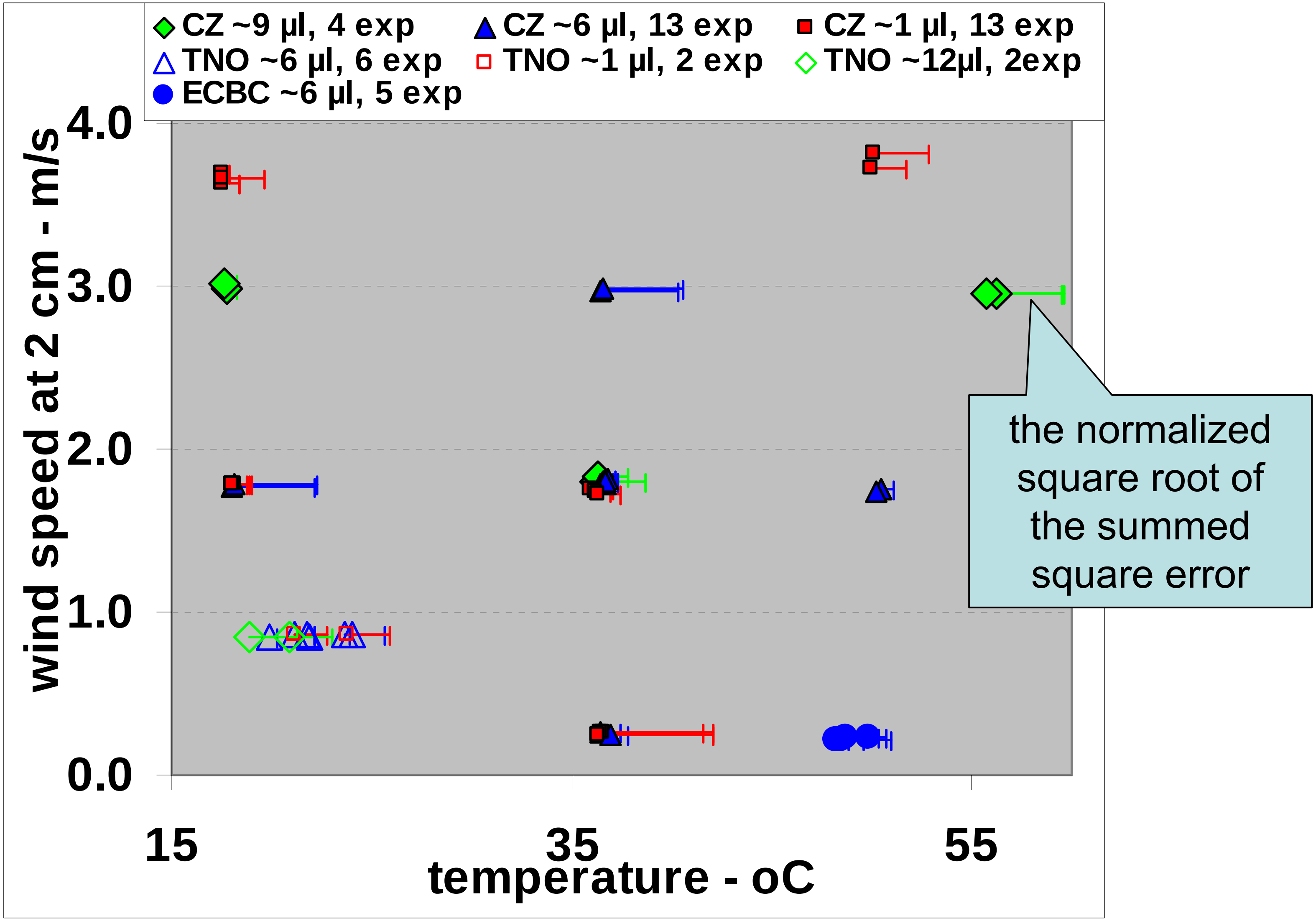
DEM on Glass
Over / Under prediction of time by model



HD on Glass
Over / Under prediction of time by model



Data space and Fit Quality's
HD on Glass



Conclusion

- Semi–Empirical Sessile Drop model
  - Fits existing data fairly well
    - Persistence times typically within 66% to 150% of experiment
  - Work in progress
    - More sessile drop data
    - Experimental Contact angle functions
    - Reactivity not tested yet

- Semi–Empirical Absorbed drop model
  - Prototype exists, Awaiting data

MS data fitted to model