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Mass Measurement with the DMS500

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Why Mass Measurement from Spectral Data?

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Why mass:

- Gravimetric measurements are the basis of current legislation and historical environmental data.
- With differences in particle sizing standards (DMA mobility classification / aerodynamic sizing / DMS electrical mobility classification), particle mass is unambiguously defined.

Why from a spectral instrument:

- Improved sensitivity vs gravimetric methods
- Real-time data
- Measurement and differentiation of accumulation mode for unfiltered / partial filtered vehicles and DPF efficiency along with nucleation mode comprising the majority of mass emissions from DPF equipped vehicles.

Mass calculation from number:size data

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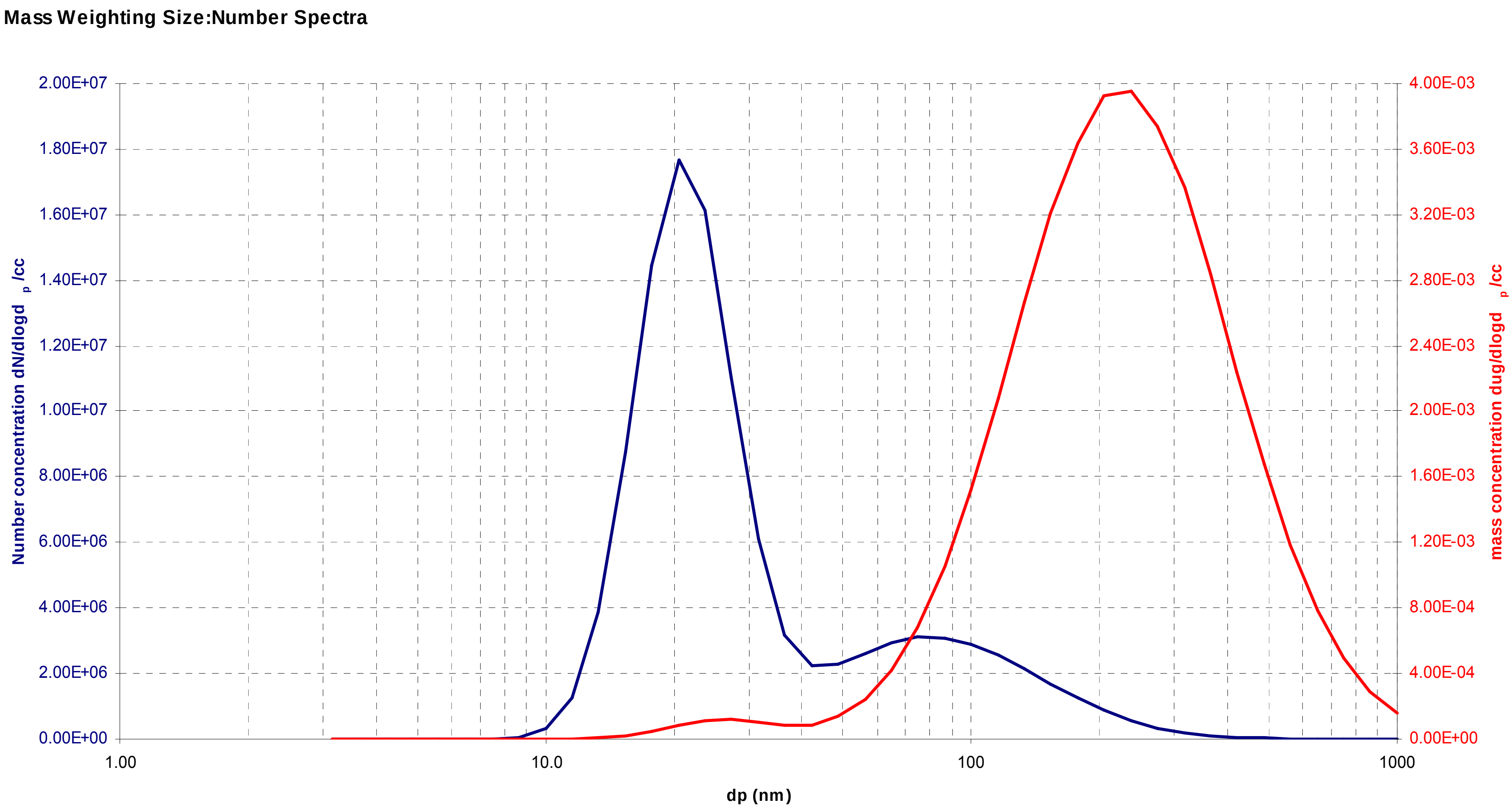
- Measurement of concentration and size allows calculation of particulate mass.



Difficulties with Mass Calculation

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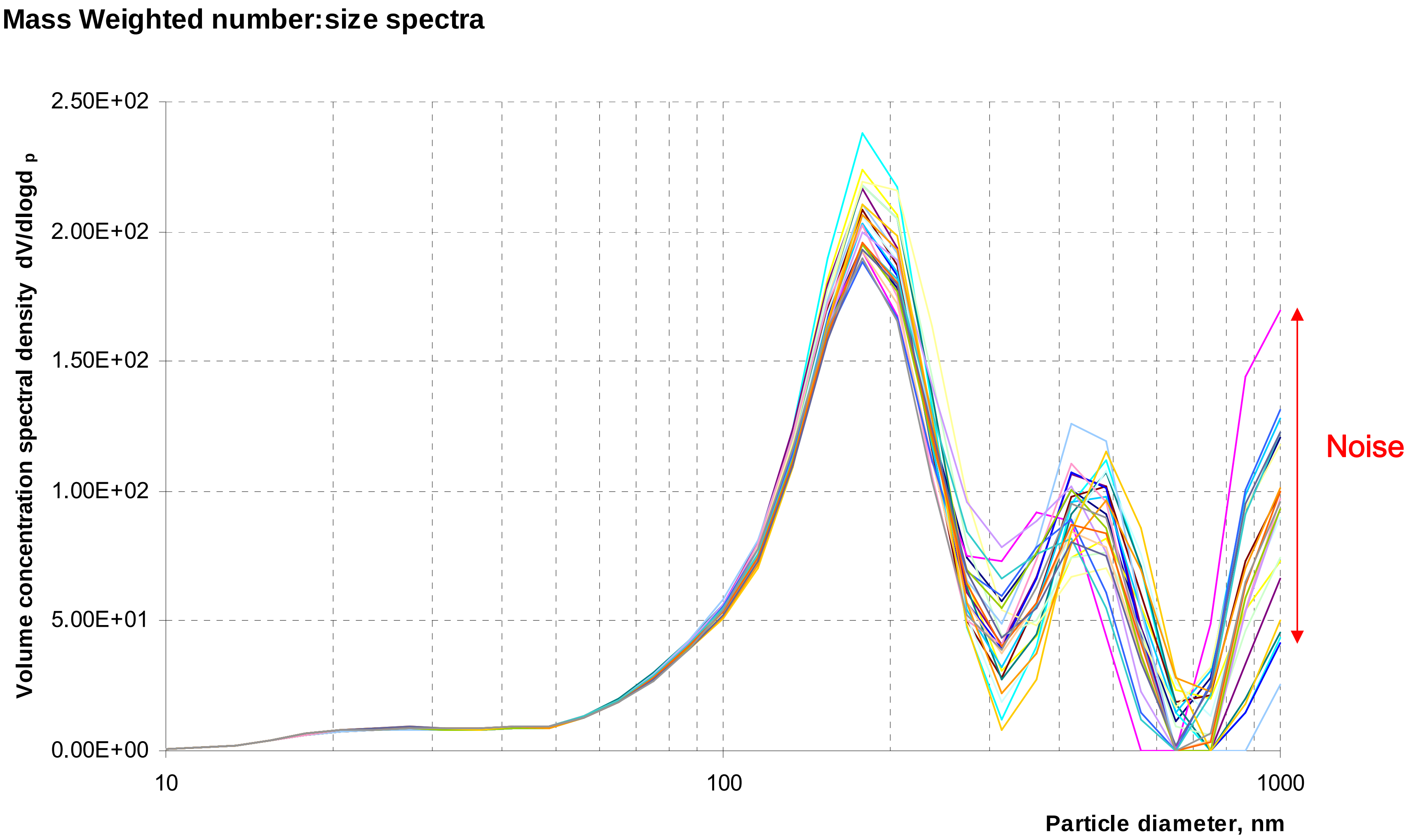
- Sensitivity to calibration
  - If mass ~ diameter^3, then 10% size error $\Rightarrow$ 30% mass error
  - solved with traceable calibration via PSL spheres
- Noise in large particle sizes amplified by mass weighting
- Effect of spectral broadening
- Particle density
  - effective density varies with particle size
  - different for nucleation & accumulation modes
  - ‘diameter’ not well defined for agglomerates

Effect of mass weighting on noise



Effect of Spectral Broadening

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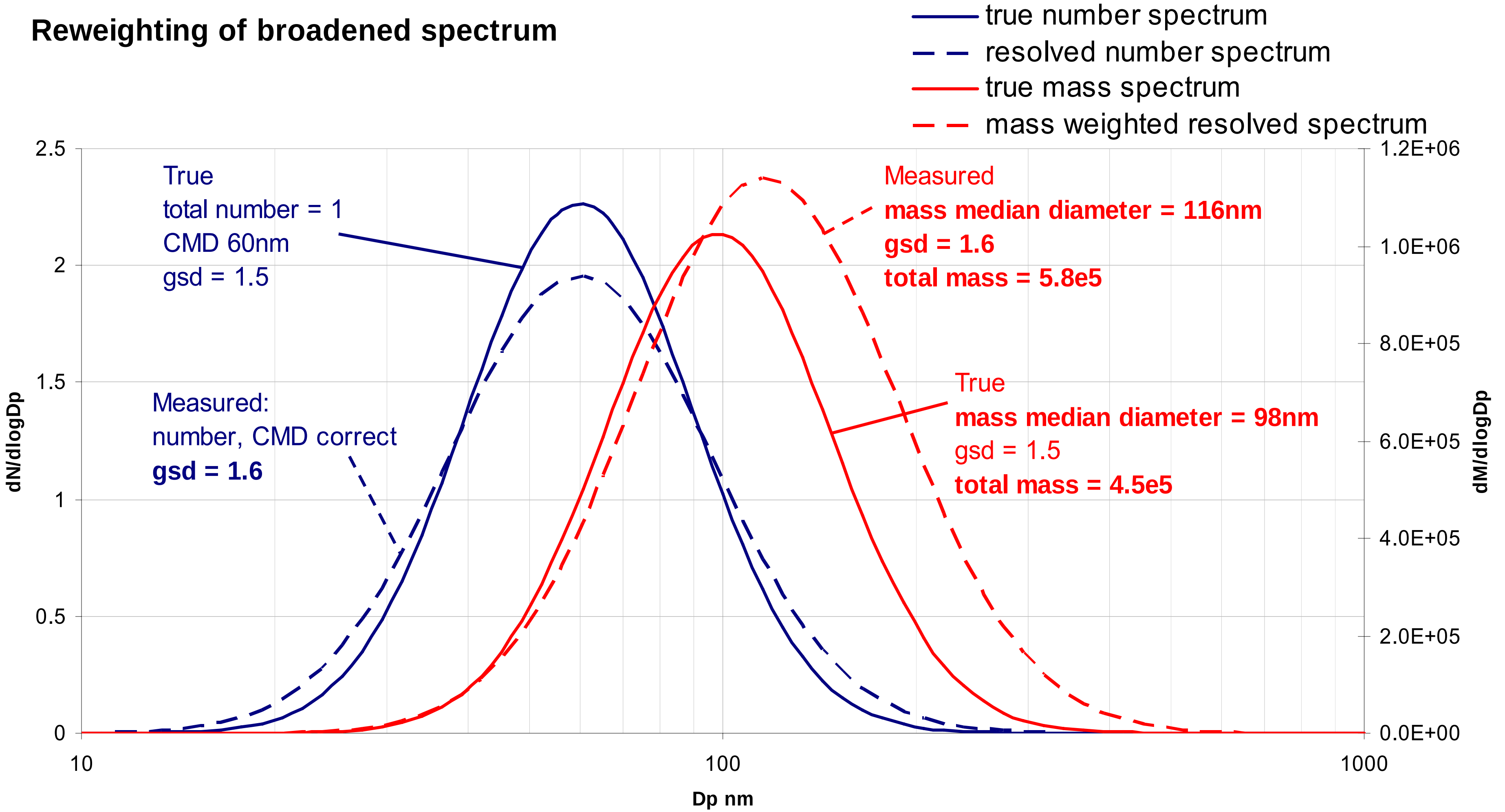

Variable Particle Density

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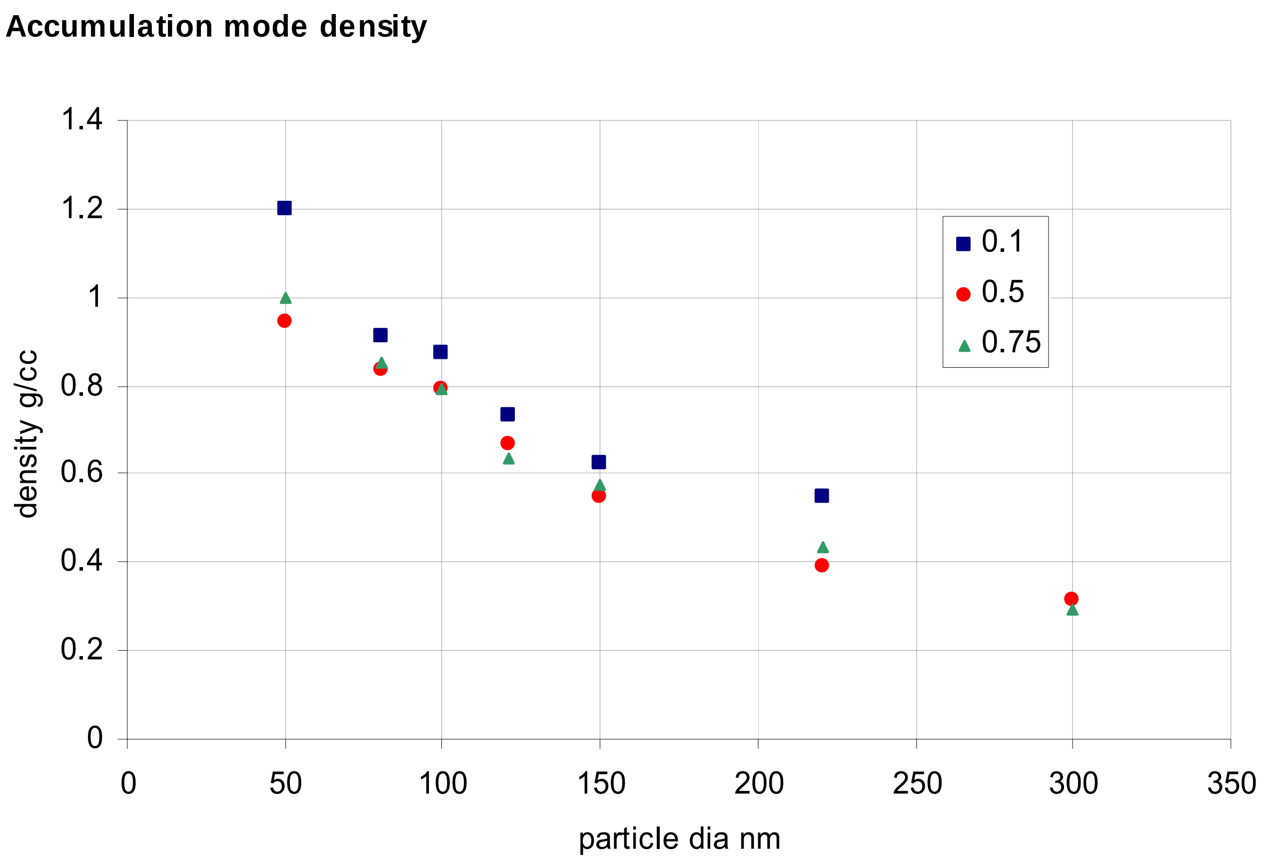
- Nucleation mode & accumulation obviously different.
- Accumulation variation demonstrated by various studies (DMA/APM, DMA/ELPI etc)
- for example, APM data (Park, Kittelson, McMurray):



[†] Environ Sci. Technology **37** 577–583 (2003)

Solution: Lognormal mode identification

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- DMS normally produces up to 41 channels of size data
- Mode identification software can reduce this to just 6 for engine aerosol:

Nucleation			Accumulation		
GMD	GSD	N/cc	GMD	GSD	conc

$$df = \frac{1}{\sqrt{2\pi}\log\sigma_g}\exp\left[-\frac{(\log CMD - \log D_p)^2}{2\log^2\sigma_g}\right]d\log D_p$$

- The nucleation and accumulation modes can then be considered separately. Factoring in air mass flow (and λ) gives total mass
- Software identifies if a mode is ‘real’ relative to the noise base of the instrument, and if not discard it
- Reduces noise related error in mass estimation, especially in ‘tail’ of accumulation mode
- Removes cross sensitivity introduced by crude size cut-off methods
- Improves spectral resolution

Lognormal Algorithm

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Bayes' Theorem:

$$\text{Posterior Probability} \propto \text{Prior Probability} \times \text{Likelihood}$$

$$P(\mathbf{w}|\mathbf{J}) \propto P(\mathbf{w}) \times P(\mathbf{J}|\mathbf{w})$$

- Prior: Assumptions about size and width of aerosol modes, gives *soft* limits on fit
- Likelihood: Probability of the data (**J**, ring currents) given some lognormal parameters (**w**).
- Posterior: The fit criterion, to be maximised

To fit:

1. Guess set of parameters and generate lognormal spectrum
2. Get ring currents for spectrum from transfer function
3. Compare these with measured ring currents, calculate likelihood (next slide)
4. Calculate Posterior from Likelihood and preset Prior
5. Iterate 1→4 to maximise Posterior

Likelihood Calculation

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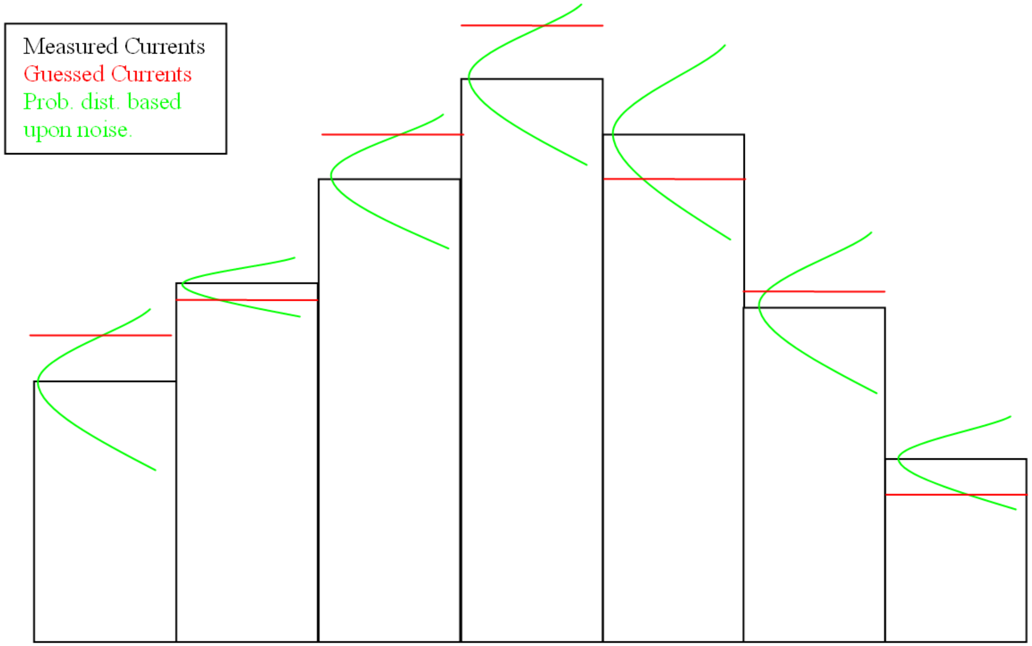
- Noise on electrometer rings measured during zero — gives expected standard deviation (σ) of guessed currents (i) from measured currents (j)
- Likelihood per ring:

$$P(j \mid i,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(j-i)^2}{2\sigma^2} \right)$$

- Assume independent probabilities, ∴ total Likelihood for 22 rings:

$$P(\mathbf{J} \mid \mathbf{w}) = \prod_{k=1}^{22} \frac{1}{\sigma_k\sqrt{2\pi}} \exp\left[-\frac{(j_k - i_k(\mathbf{w}))^2}{2\sigma_k^2} \right]$$



Example Diesel Engine Prior

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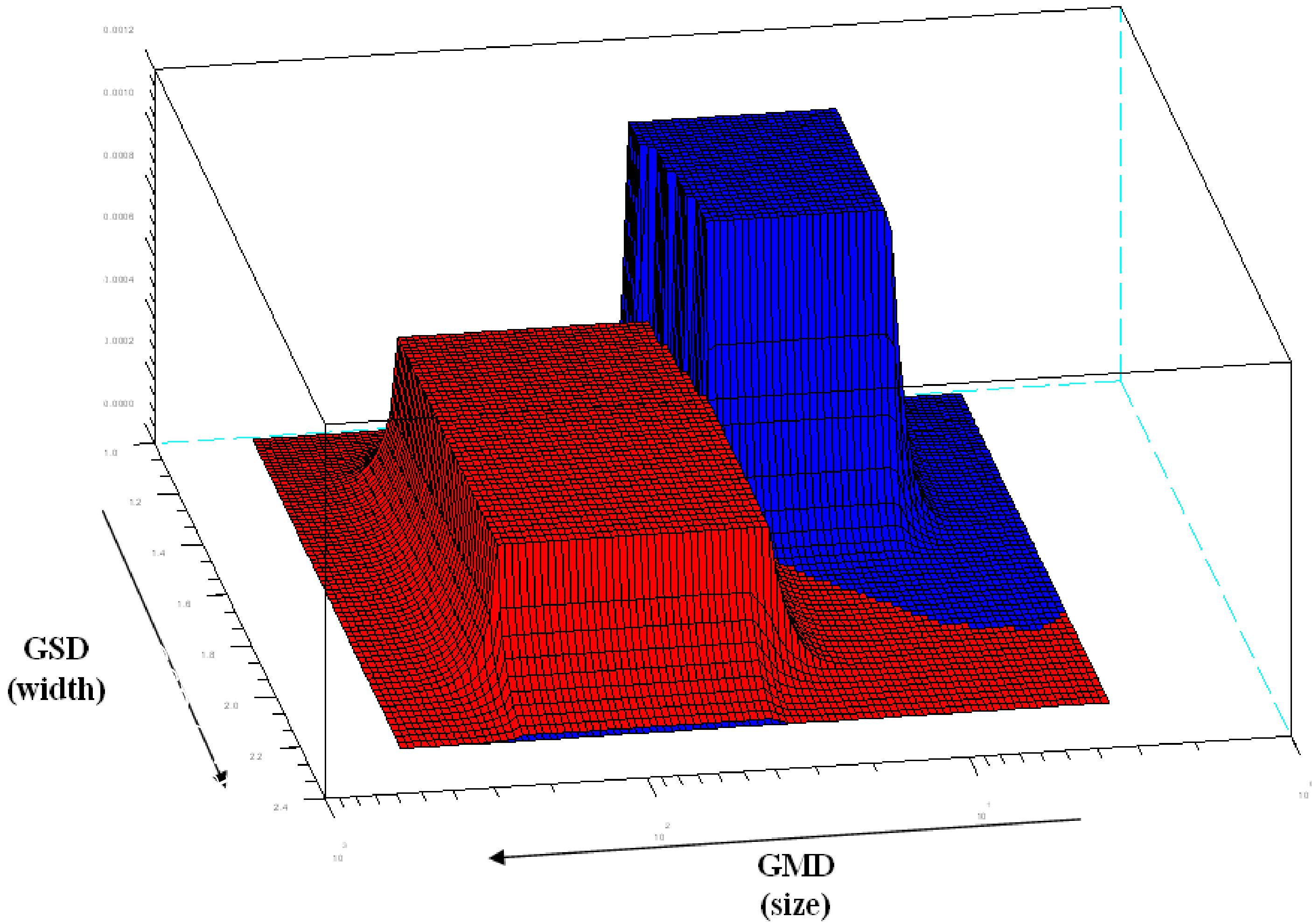

Accumulation Nucleation

How many modes?

- Let $P(H_m|\mathbf{J})$ be the probability that there are truly *m* Lognormal modes, given the measured ring currents **J.** Then by Bayes' theorem:

$$P(H_m \mid \mathbf{J}) \propto P(H_m)P(\mathbf{J} \mid H_m)$$

$$\text{Marginalisation rule}: P(X \mid I) = \int_{-\infty}^{\infty} P(X, Y \mid I)\mathrm{d}Y$$

$$\Rightarrow P(\mathbf{J} \mid H_m) = \int \cdots \int P(\mathbf{J}, \mathbf{w} \mid H_m)\mathrm{d}^m\mathbf{w} \qquad (1)$$

$$\text{Product Rule}: P(Y, X \mid I) = P(Y \mid X, I)P(X \mid I)$$

$$\Rightarrow P(\mathbf{J}, \mathbf{w} \mid H_m) = P(\mathbf{J} \mid \mathbf{w}, H_m)P(\mathbf{w} \mid H_m) \qquad (2)$$

- We assume that the prior probability of *m* modes, P(H_m), is uniform
- Equation (2) is now just the product of our original likelihood and prior, but now evaluated for a specific number of lognormals, i.e. the product of the likelihood of the overall spectrum and all the individual priors.
- (2) is substituted into (1) and evaluated. This takes considerable PC power in real-time!

Automatic mode identification on NEDC

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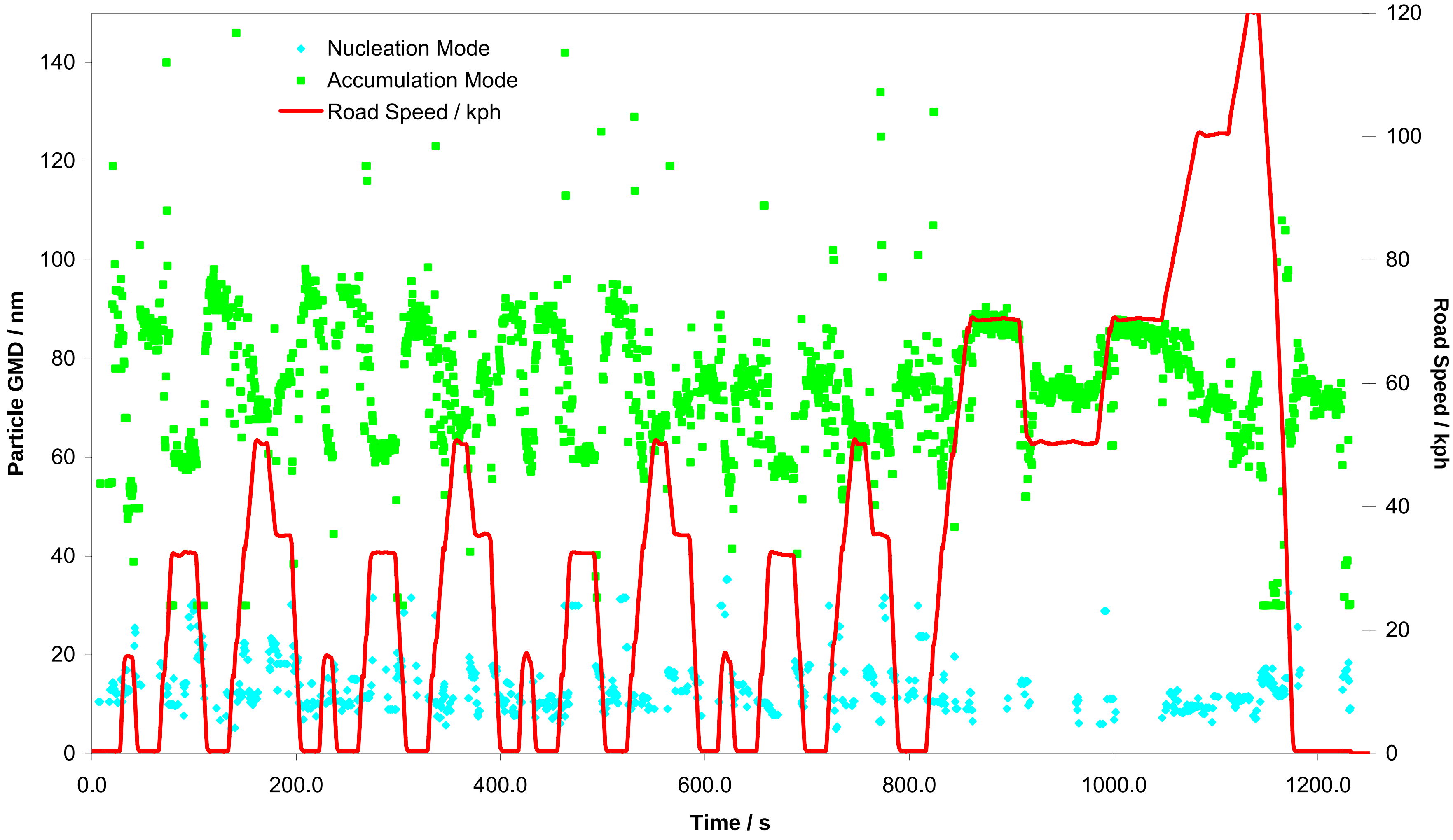

Real-time Implementation

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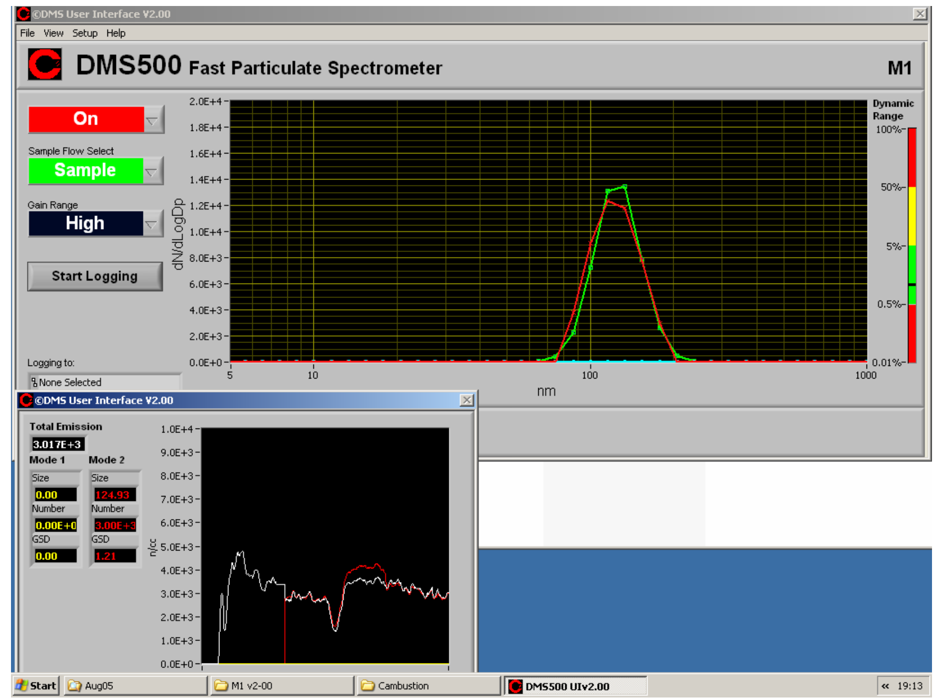
- Integrated into instrument interface
- Modes displayed in real-time along with conventional spectrum
- Summary parameters (size, concentration, σ_g) logged and available as analogue output signals
- Mass calculated and displayed, logged or available as analogue output.



Lognormal Data Processing: Reduced Noise

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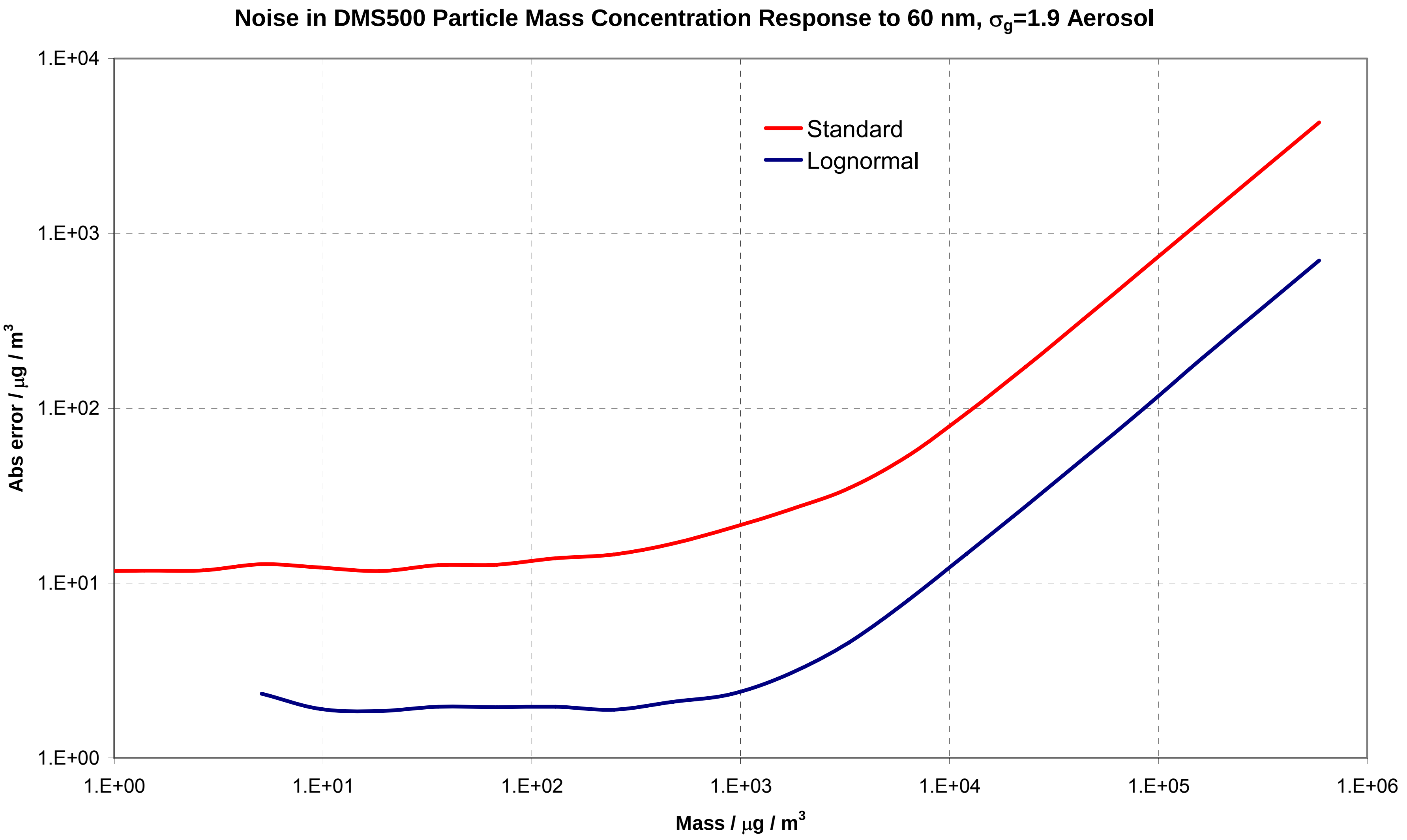

Lognormal Data Processing: Better Resolution

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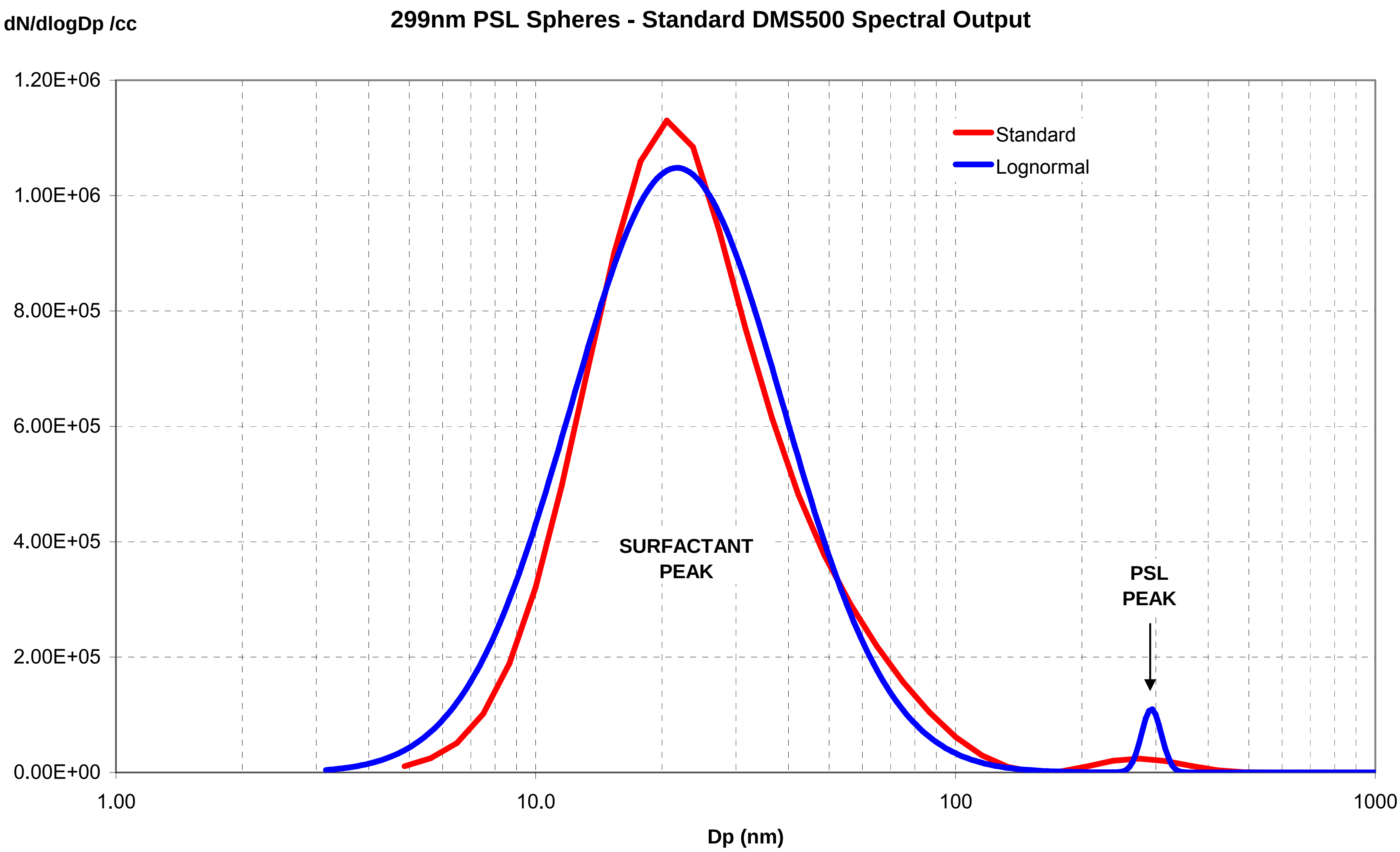

(Different Priors used to those for Diesel Engines!)

Density Function - SMPS

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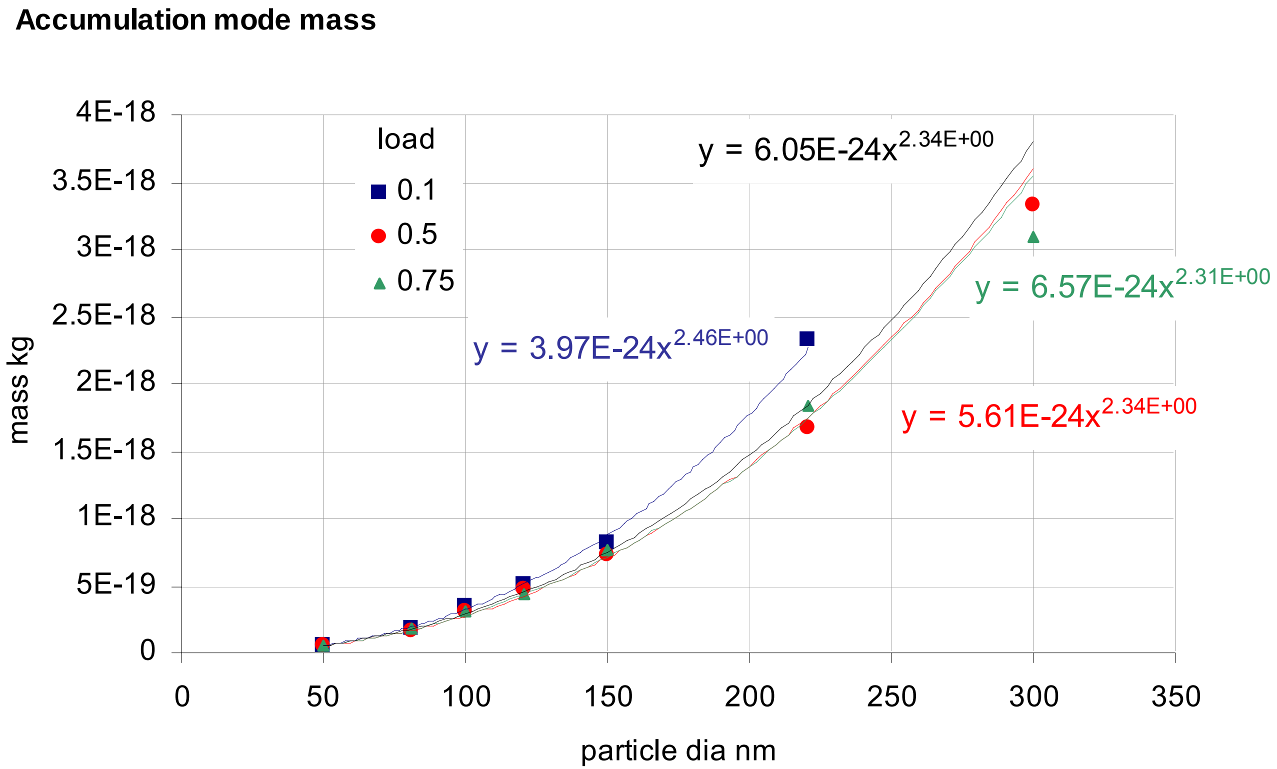
- Based upon work by Park, Cao, Kittleson and McMurry†
- Related DMA diameter to mass for heavy duty diesel via an effective density by cutting with Aerosol Particle Mass Analyser (APM)
- Recently shown to also apply to light duty diesel‡

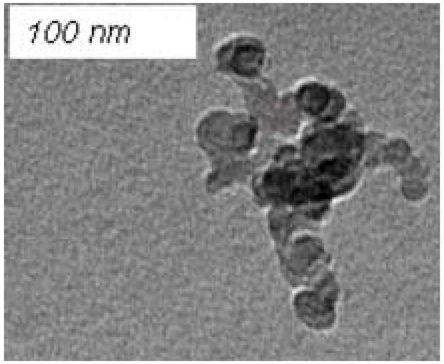


† Environ Sci. Technology **37** 577–583 (2003)

‡ J.S. Olfert *et al.* in preparation

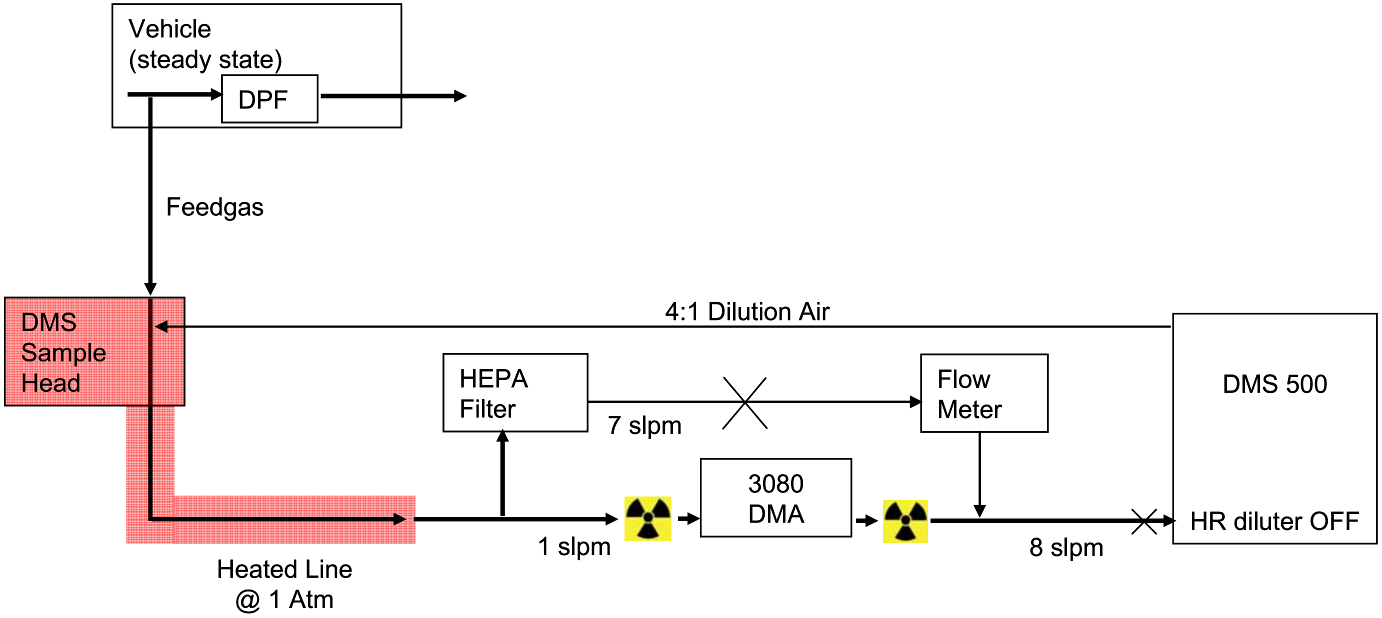
Accumulation Mode Size

What size is this?



- DMS Calibrated with PSL Spheres
- Compare SMPS (mobility) sizing with DMS (electrical mobility) sizing for Diesel Agglomerates

Test apparatus



DMA:DMS Diameter Relationship – Diesel Agglomerates

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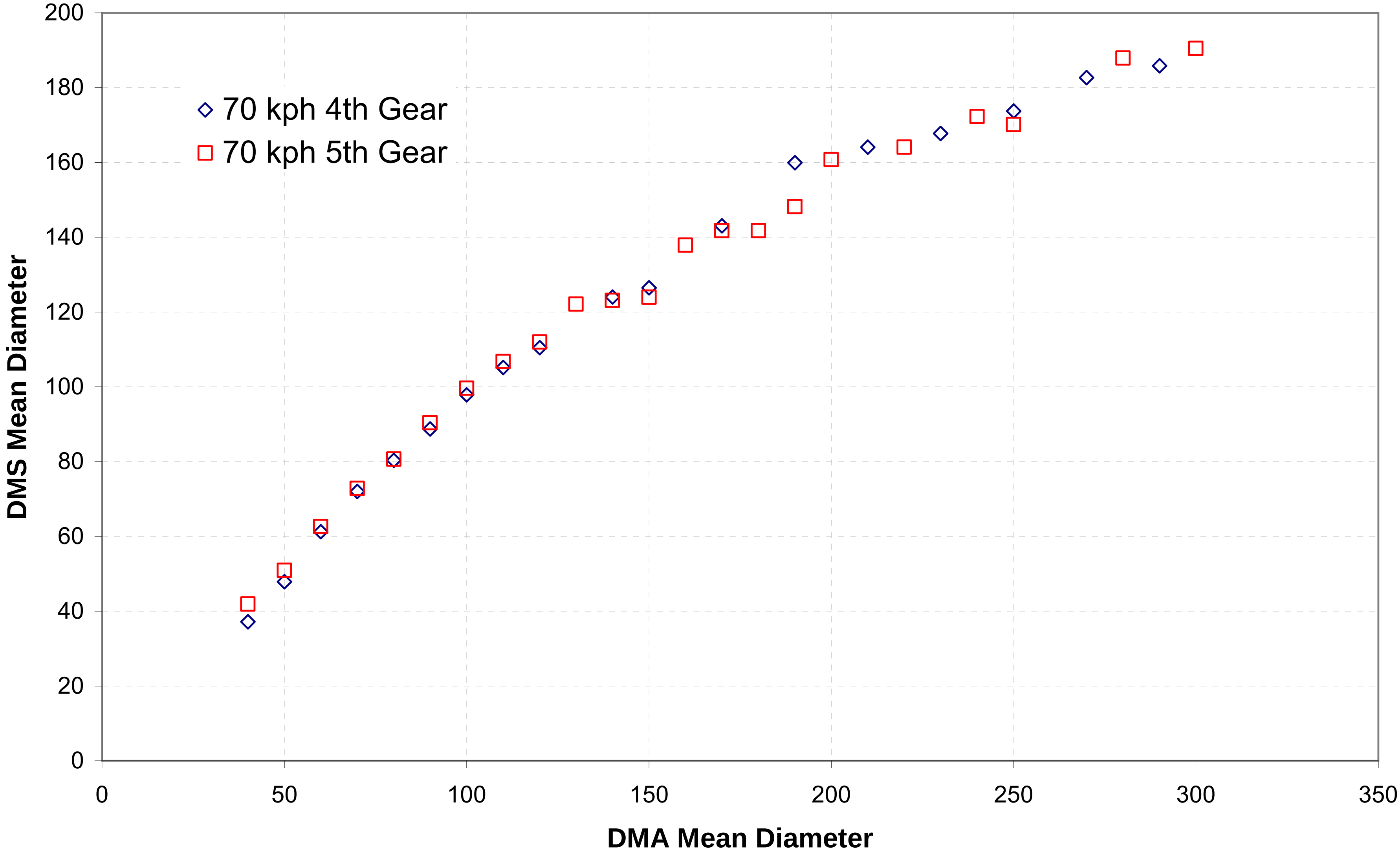
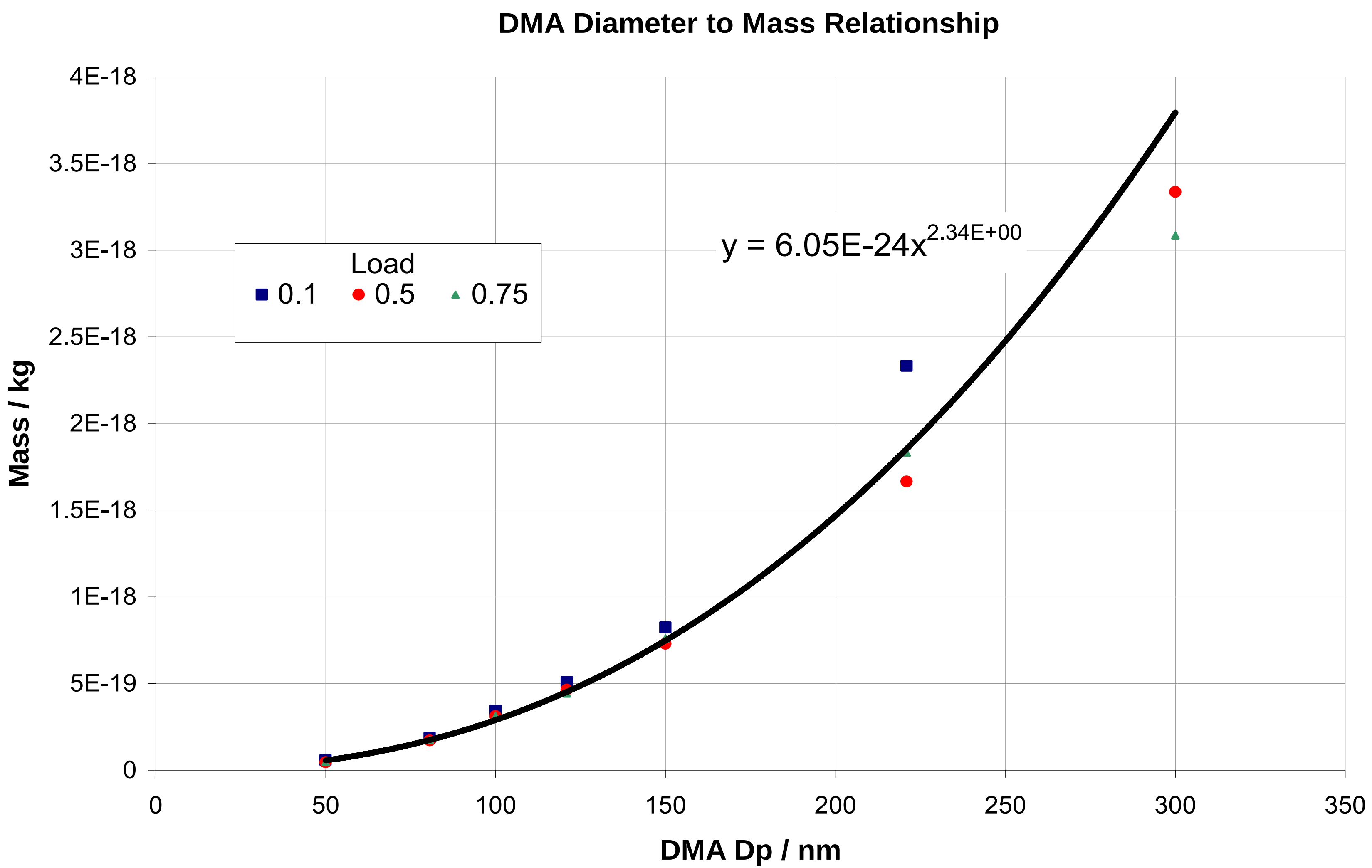


New DMS Mass Weighting Rule



New DMS Mass Weighting Rule

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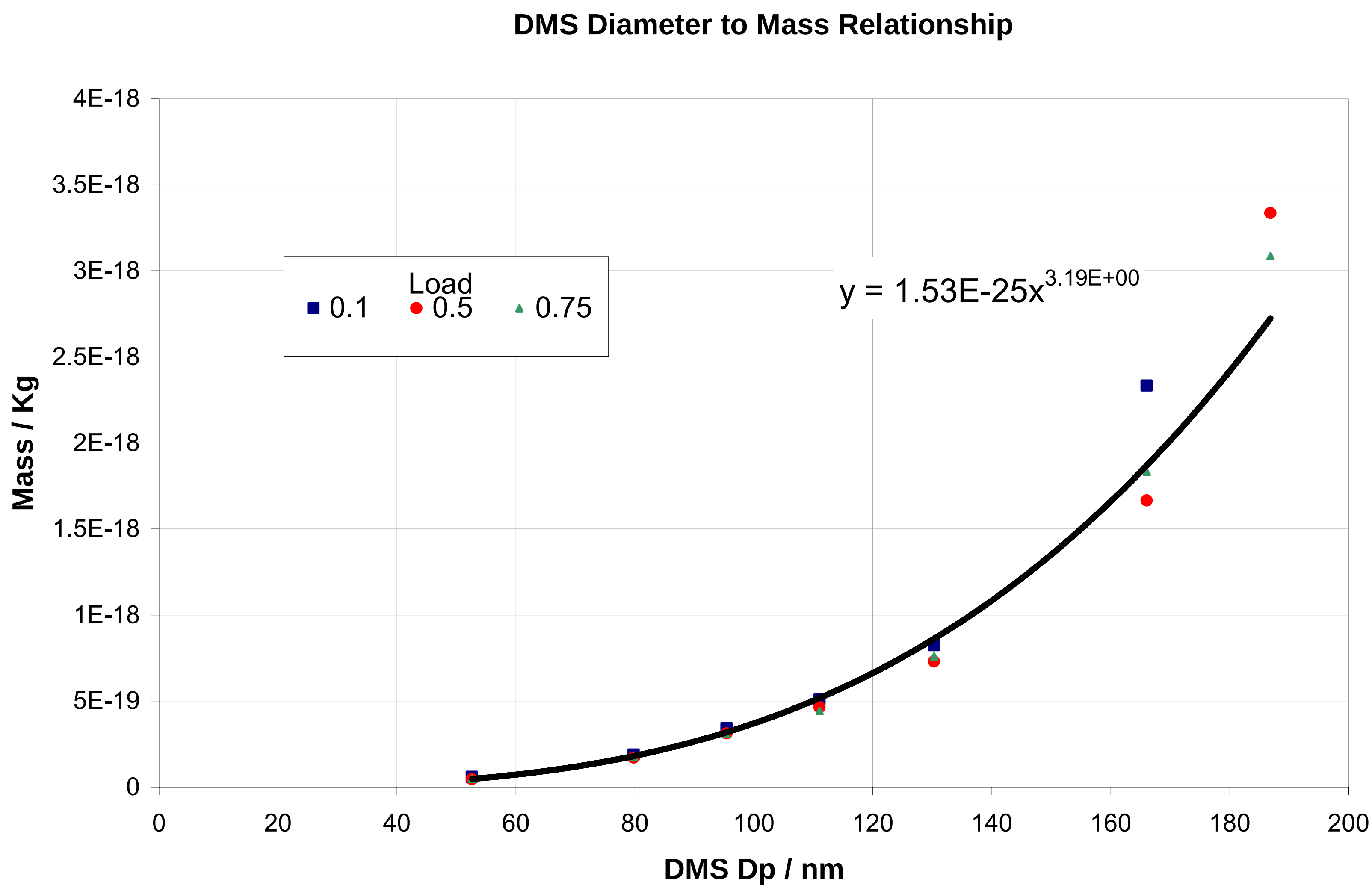

Mass Estimation from DMS500

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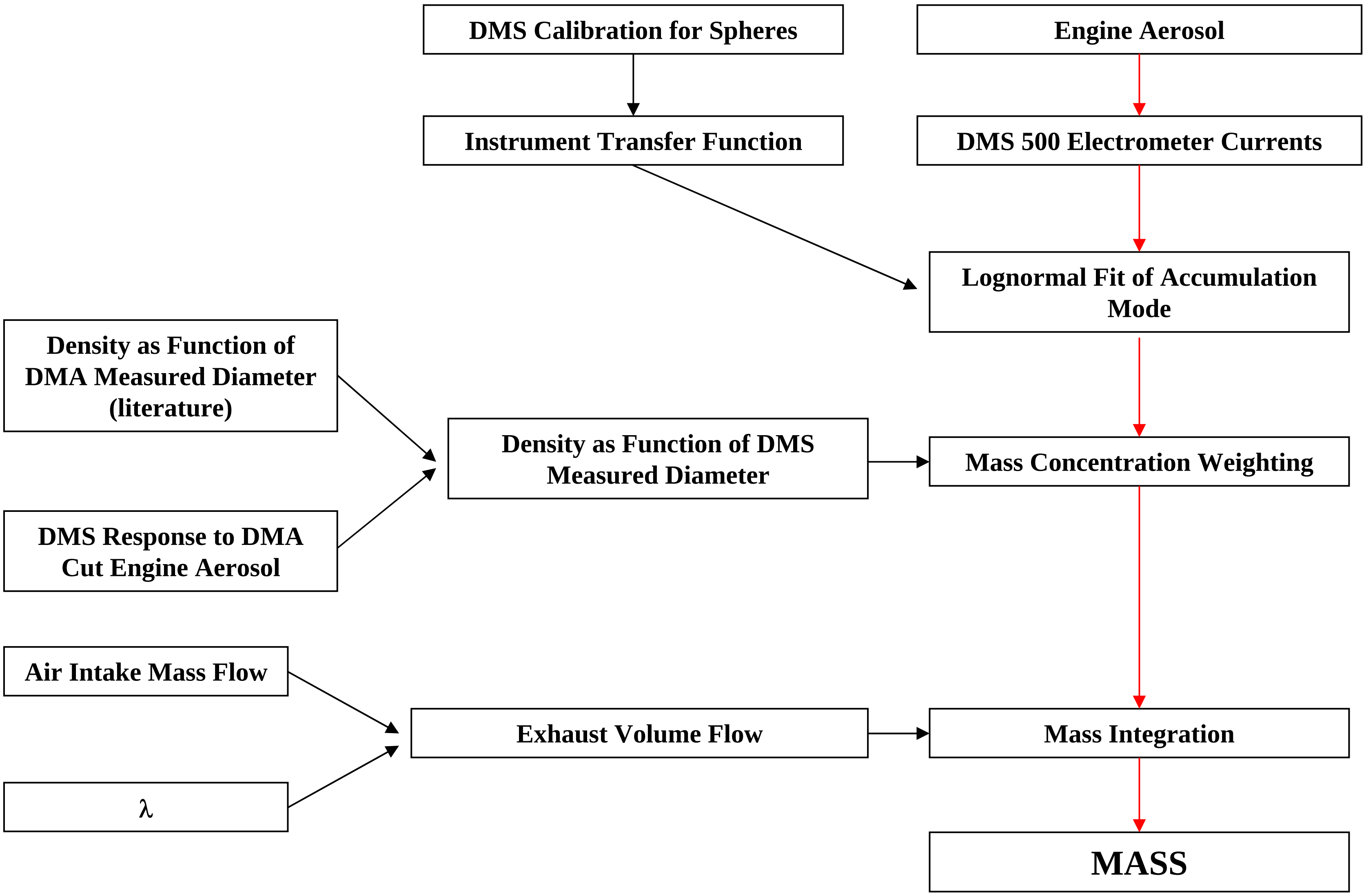

Summary – DMS500 Mass Calculation

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- Lognormal mode identification
  - reduces large particle noise by data redundancy
  - discriminates between nucleation & accumulation modes to calculate soot mass, or apply different density laws.
  - takes into account spectral blurring in instrument to correctly resolve mode widths.
  - reduces amount of data to be handled by users
  - allows nucleation mode to be measured and ignored at will, from one test.
- Mass weighting of particulate modes
  - mass : diameter relationship derived from DMA literature, but modified due to different charge : drag ratio sizing basis.

Validating Mass Measurements

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- Correlation is very easy to demonstrate:
  - most instruments (not CPC!) are linear with increasing concentration, so just test at a variety of concentrations with similar aerosols
  - even easier, test over different periods of emission.
- Neither of these give useful validation
  - must ensure a variety of particle sizes in validation data set
  - data presented here covers peaks between about 60nm and 140nm mobility diameter for different steady state conditions.
  - confidence improved by agreement with a priori calculation, rather than just a posterior correlation

DPF Mass Correlation Validation

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- Production vehicle (2.2l common rail) with DPF on chassis rolls and 2.0l common rail engine with prototype calibration on engine dyno.
- Measurements taken both by DPF weighing and filter paper measurement.
- Steady state test points selected for validation over maximum particulate size range.
- NEDC cycle mass for real application validation
- DMS500 sample drawn from pre-DPF flow via built-in dilution system and heated line.
- Mass flow calculated from intake MAF and exhaust lambda logged to DMS500 auxiliary analogue inputs.

Test Points

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- NEDCs (sometimes inc EUDCs), warm and cold start
- 100 kph (5th gear), 70 (4th/5th), 32 (2nd) cruises
- 1500 rpm @ 190, 650, 700 nm
- Fixed speed/load points on engine dyno

- DPF weighings (DMS primary + secondary dilution, heated line)
- Filter Paper in CVS Tunnel (DMS secondary dilution)

DMS500 Built-in 2 Stage Dilution

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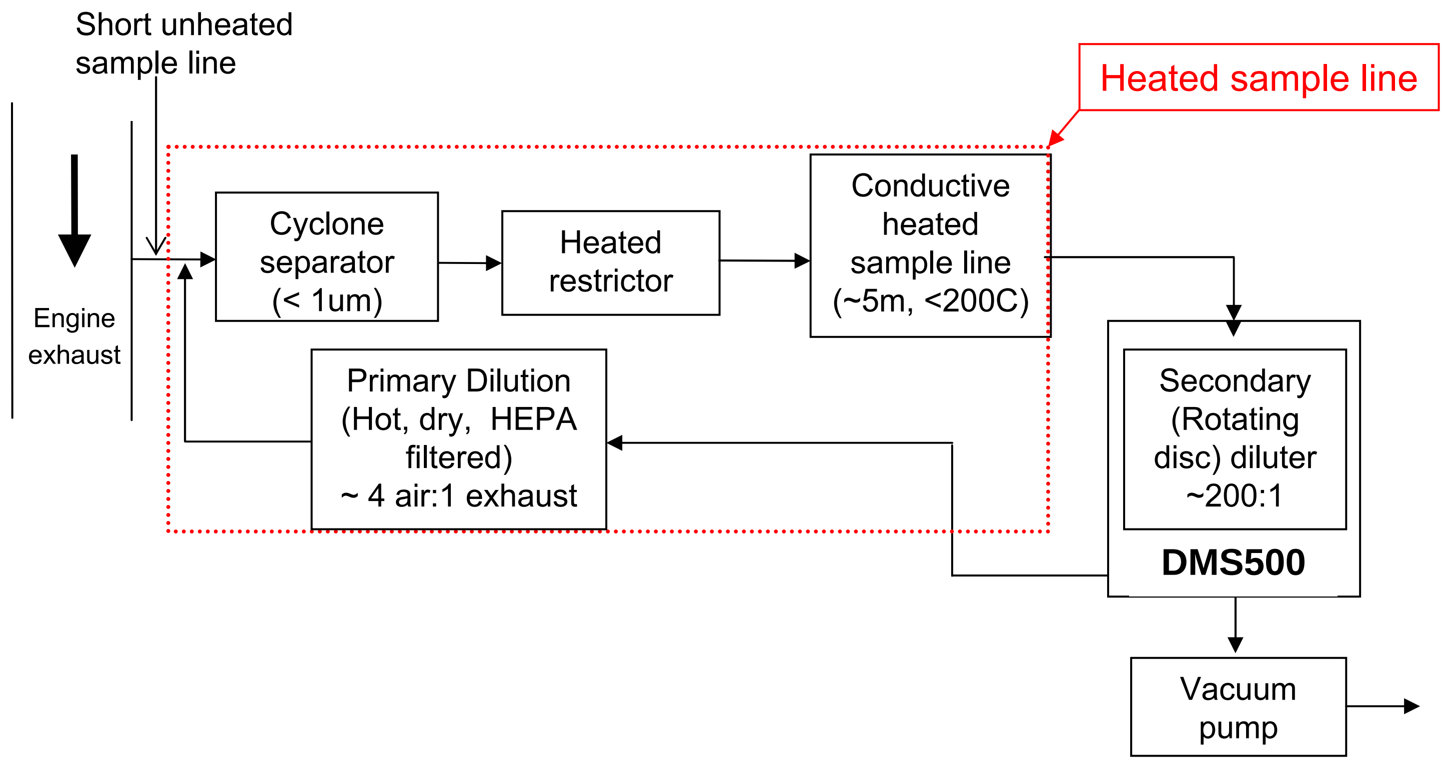

Vehicle Tests: Mass Conc. over NEDC

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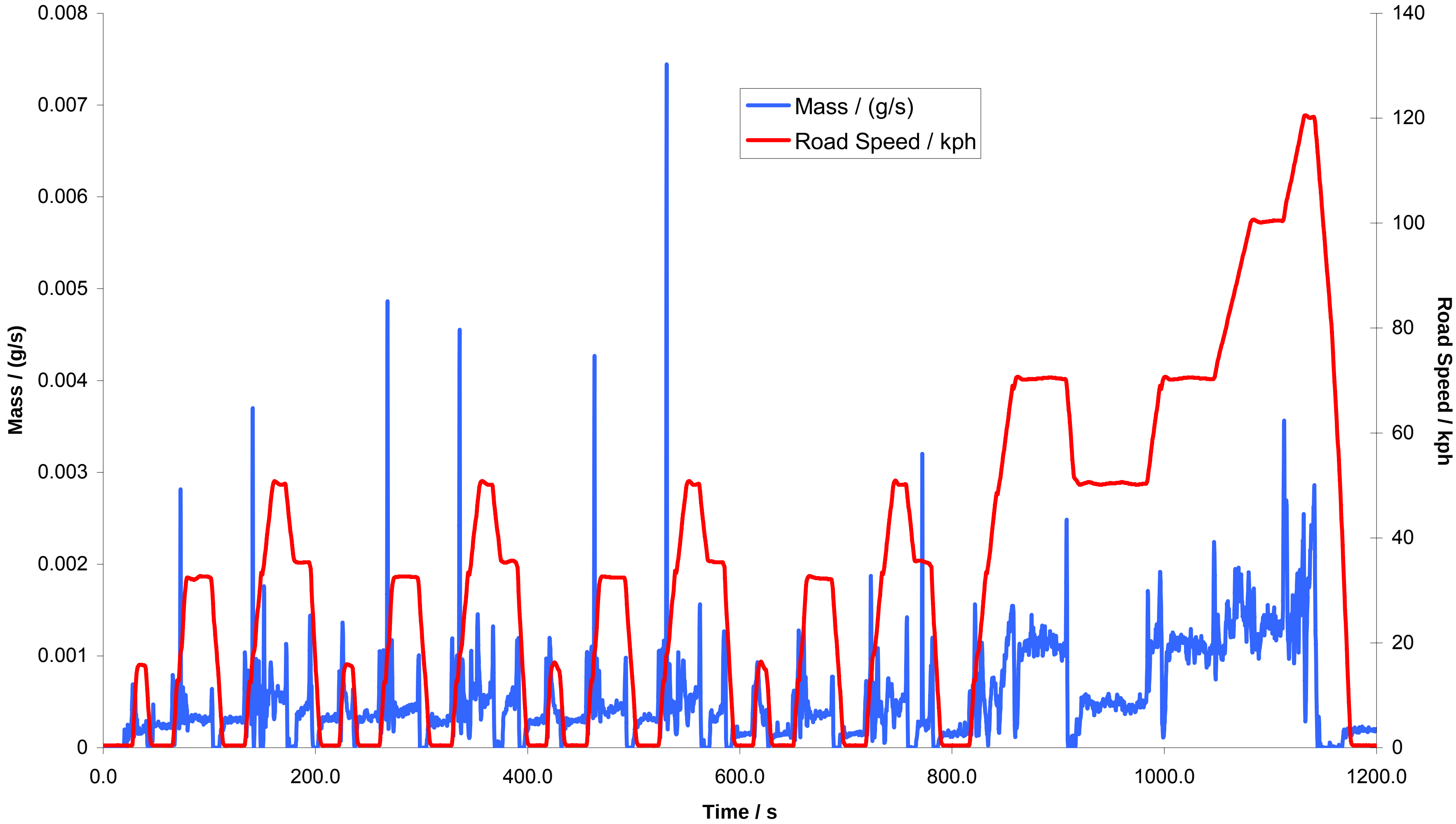

DMS Mass Test Results

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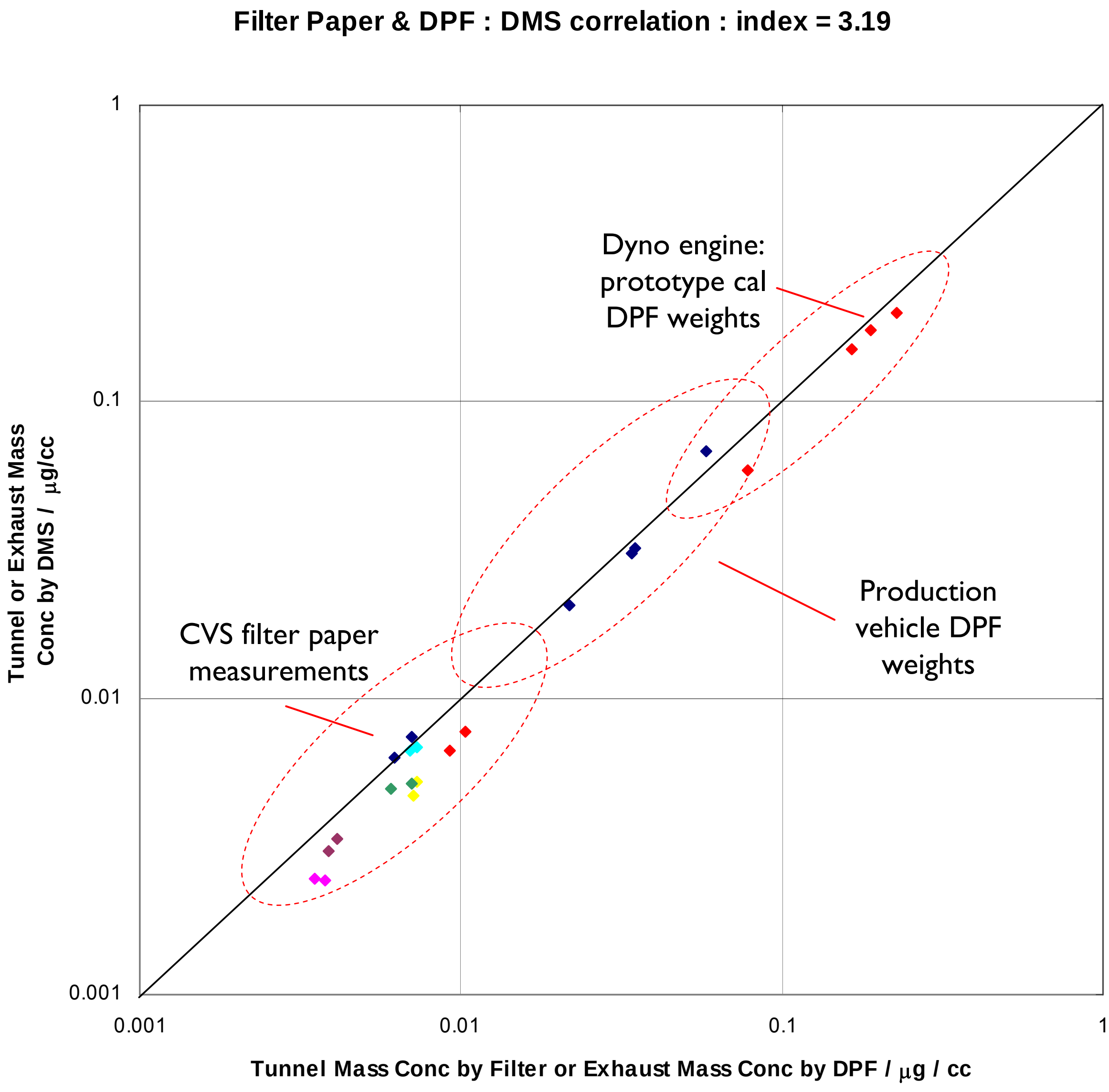

- DMS measurements within 10% of DPF mass measurement
- DMS underestimates filter paper mass: presumed due to adsorption of gas phase materials on filter.

Conclusions

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- Mass calculation from spectral data allows correlation with gravimetric measurements and standards.
- Issues with mass calculation accuracy include size calibration, large particle noise floor and variable density.
- Mode identification reduces noise floor, improves size distribution accuracy and allows discrimination between nucleation and accumulation modes
- Variable particle density model modified for DMS size response
- Mass measurement validated on two drivetrains, against DPF and filter papers weights.
- Agreement with DPF soot mass within 10%
- Approximate 10% underestimate compared with filter paper weighings: assumed due to gas phase adsorption onto filter paper.