Cambustion

DMS500 MkII

Fast Particulate Analyzer

Application Note: DMS 06v03

Real-time Mode Finding and Lognormal Fitting with the DMS500 Fast Particulate Spectrometer

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Real-time Mode Finding & Lognormal Fitting with the DMS500 Fast Particulate Spectrometer

It is in the nature of a fast response multi-channel particle spectrometer that large data files containing a great deal of information are produced. This application note describes new software from Cambustion as now supplied with the DMS500 which automatically processes data into a few parameters describing the principle features of the spectrum. This

- discriminates between and separates aerosol modes
- can improve spectral resolution
- reduces spectral noise
- allows more accurate particulate mass calculation
- reduces the volume of data, allowing trends to be easily spotted and salient information to be simply extracted, easing integration with gas analysers and existing test cell facilities.

Aerosol size spectra tend to consist of certain modes (peaks), each arising from a separate physical process. For example, aerosol spectra from automotive diesel emissions tend to have a so-called *Nucleation* mode consisting of sulphate, hydrocarbon and/or water at small sizes, and an *Accumulation* mode at larger sizes consisting of soot.

Each log-normally distributed mode in an aerosol is fitted by the software to just three parameters: Number in the mode, mean size and width (geometric standard deviation, GSD) of the distribution. These parameters can then be directly weighted e.g. to give mass estimation. The new software[1,2] can either post-process DMS data files via an Excel utility, or even generate parameters in real-time from the user interface† and pass any required parameters or weightings to instrument analogue outputs for logging by existing test facilities.

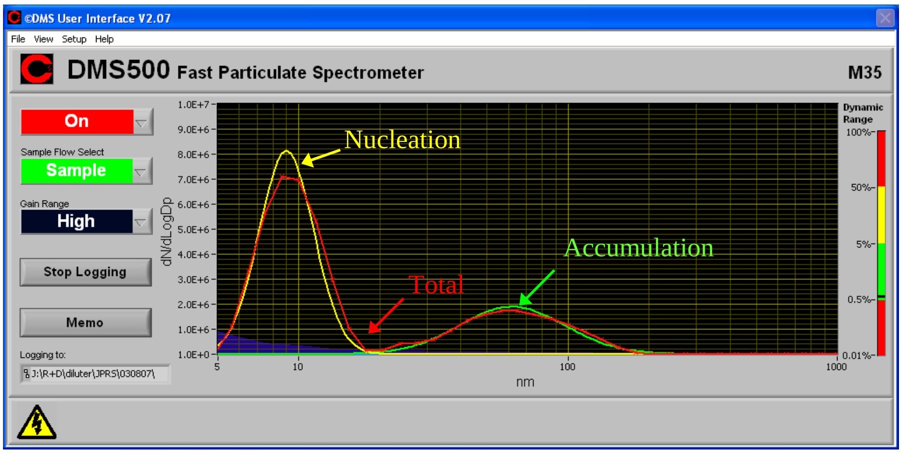

Figure 1: DMS500 v2.07 User Interface with Mode Finding

The software uses a specially written sophisticated Bayesian statistical algorithm. The algorithm considers the instrument's noise base and only returns genuine modes above this level. When used in real-time the instrument measures its own noise base and hence temporary changes in instrument noise (e.g. due to heavy environmental vibration or overdue cleaning) are automatically factored out. For mass estimation applications, this also means that spectral noise at large particle sizes does not cause a huge overestimation of mass due to the weighting used. Modes are classified into type according to size and width from information provided by a supplied *Aerosol Description File* specific to the instrument's calibration and aerosol type. The mode classification process is intelligent in the sense that

† *Sufficiently powerful PC required for real-time operation; supplied with all new DMS500 instruments*

there is no sharp size cut-off between modes and even partly overlapping modes in the real aerosol are detected and can be treated separately. This yields far more accurate number and mass than crude size cut-off methods used to distinguish between modes.

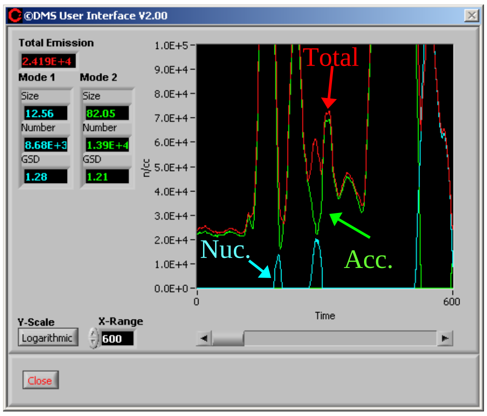

Figure 2: DMS500 v2.00 User Interface Total Concentration Window

The separation of nucleation and accumulation modes allows the nucleation particle concentration to be ignored, thereby allowing PMP comparable number measurements without the use of a hardware volatile particle remover[3]. It is also possible to use separate calibrations for each mode, thereby allowing more accurate sizing of agglomerates which charge slightly differently to spherical aerosols.

In addition to automotive application, used of an unconstrained Aerosol Description File allows lognormal parameterisation of any aerosol. For example, a Polystyrene Latex (PSL) calibration aerosol is shown in Figure 3. The aerosol is produced by nebulising an aqueous suspension of PSL spheres, then drying and electrically neutralising. An additional large unwanted peak is formed from impurities and surfactant chemicals when the water is removed. Figure 4 shows an extract from a DMS data file after a bimodal lognormal fit.

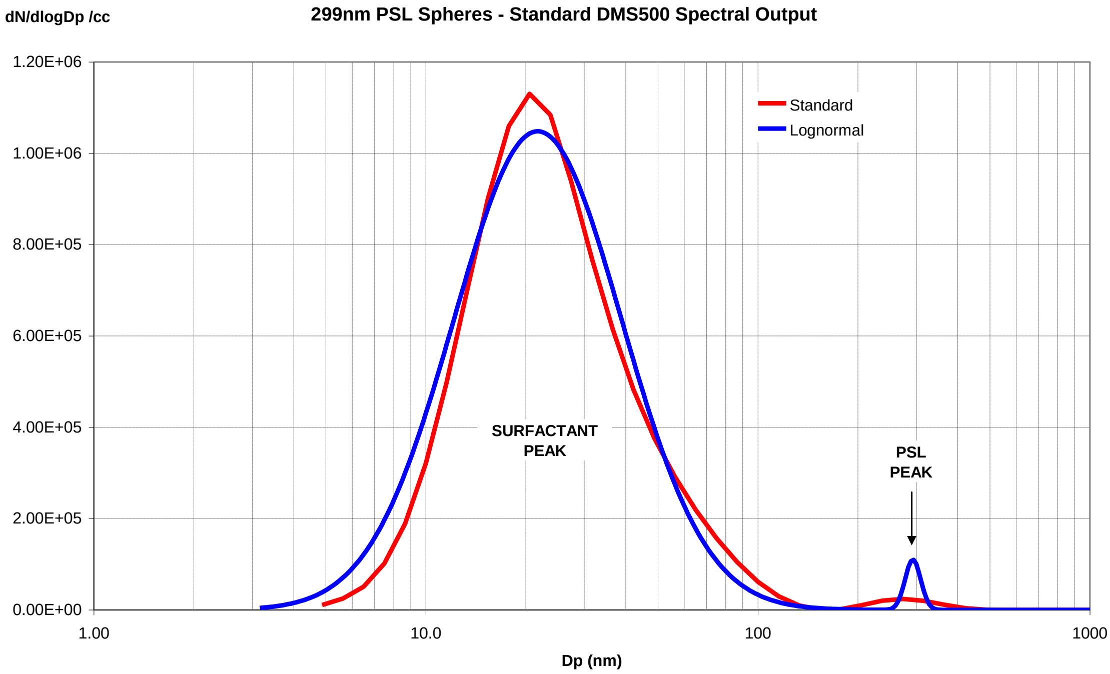

Figure 3: 299nm Polystyrene Latex Aerosol measured with DMS500, inc. large surfactant peak

.00E+03	6.88E-01	1.60E+01	3.00E+00	1.00E+02	C:\Cambustion\M25\Bimodal_25_1.dmx				
lution Ratio	Sample Flow	**Mode 1 Conc**	**Mode 1 CMD**	**Mode 1 GSD**	**Mode 2 Conc**	**Mode 2 CMD**	**Mode 2 GSD**	4.87	5.62
1.00	7.94	**6.68E+05**	**21.52**	**1.788**	**4.10E+03**	**290.75**	**1.071**	9.88E+03	2.72E+04
1.00	7.94	**6.68E+05**	**21.61**	**1.785**	**5.00E+03**	**292.14**	**1.061**	1.02E+04	2.96E+04
1.00	7.94	**6.68E+05**	**21.65**	**1.785**	**6.87E+03**	**293.60**	**1.050**	1.05E+04	3.20E+04
1.00	7.94	**6.69E+05**	**21.66**	**1.785**	**9.39E+03**	**294.18**	**1.044**	1.08E+04	3.44E+04
1.00	7.94	**6.71E+05**	**21.66**	**1.786**	**7.03E+03**	**294.06**	**1.102**	1.12E+04	3.68E+04
1.00	7.94	**6.72E+05**	**21.67**	**1.785**	**7.90E+03**	**294.35**	**1.146**	1.08E+04	3.82E+04
1.00	7.94	**6.62E+05**	**21.69**	**1.787**	**5.09E+03**	**291.77**	**1.055**	1.29E+04	3.60E+04
1.00	7.94	**6.55E+05**	**21.75**	**1.783**	**4.82E+03**	**292.00**	**1.050**	0.00E+00	1.43E+04
1.00	7.94	**6.59E+05**	**21.75**	**1.793**	**4.77E+03**	**294.32**	**1.057**	4.78E+03	2.16E+04
1.00	7.94	6.59E+05	21.75	1.793	4.77E+03	294.32	1.057	2.39E+04	3.87E

Figure 4: DMS Data File Showing Bimodal Lognormal Parameters for 299nm PSL

Two main points are worthy of note. Firstly, the software correctly identifies both the surfactant and PSL peaks even though the former is slightly skewed and is two orders of magnitude greater in concentration than the latter. Secondly, the PSL peak is correctly identified as having a very narrow GSD (width) of ~ 1.05, which is considerably greater spectral resolution than can be offered by the traditional data processing algorithms used in any real time electrical mobility particle spectrometer currently available. Such high spectral resolution is normally associated with slow scan instruments such as the SMPS. This is possible with the new algorithm as it bypasses the normal data processing algorithm and works directly with the raw instrument response, constrained to find lognormal features.

A further effect of the lognormal fitting software is to reduce the instrument noise base, and hence increase the sensitivity. An illustration of this effect is shown in Figure 5, showing that sensitivity in terms of number concentration can be improved by up to a factor of 2.

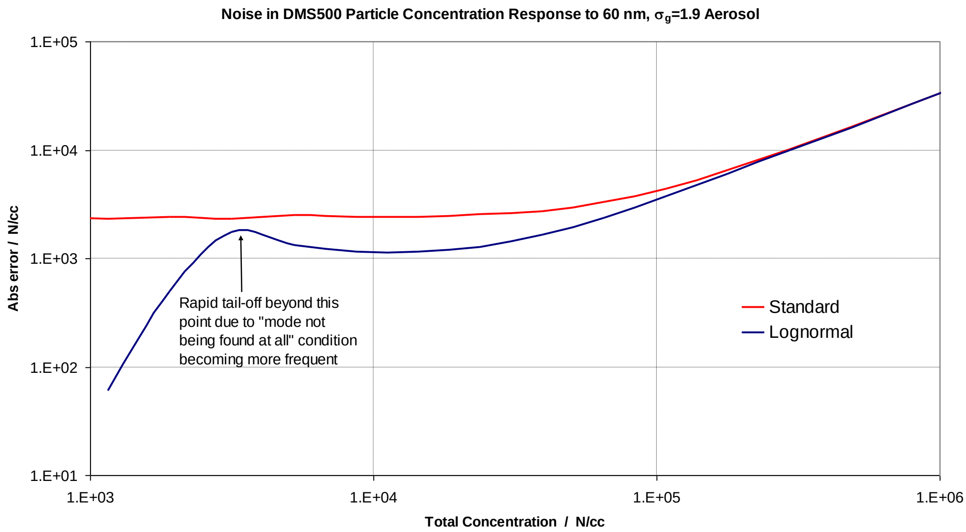

Figure 5: Standard deviation from mean concentration measurement generated by taking DMS500 response to computer simulated (non-varying) 60 nm aerosol, adding real instrument noise base, then running DMS data processing algorithms,

This application note now concentrates upon the application of this software to automotive diesel emissions, specifically to a Euro stage III diesel car. A DMS500 with heated sample line and both primary (air) and secondary (rotating disc) dilution was used to directly sample the feedgas upstream of a diesel particulate filter (DPF). The following plots show the particulate emissions over the course of an entire New European Drive Cycle (NEDC), firstly with all spectral information shown, then just the number in each of the nucleation and accumulation modes.

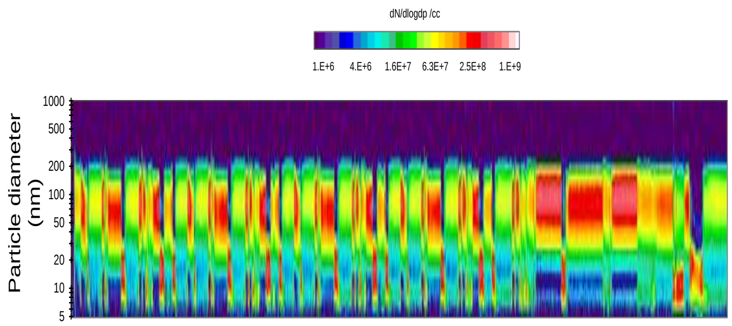

Figure 6: Contour Plot of Particle Concentration over NEDC

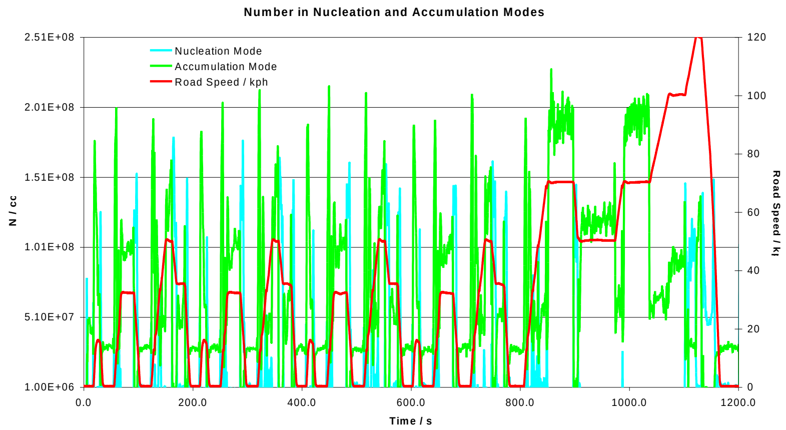

Figure 7: Nucleation and Accumulation Mode Number

The complex information in Figure 6 has been reduced to just two parameters in Figure 7.

Next, the plot has been zoomed to the extra-urban phase of the cycle:

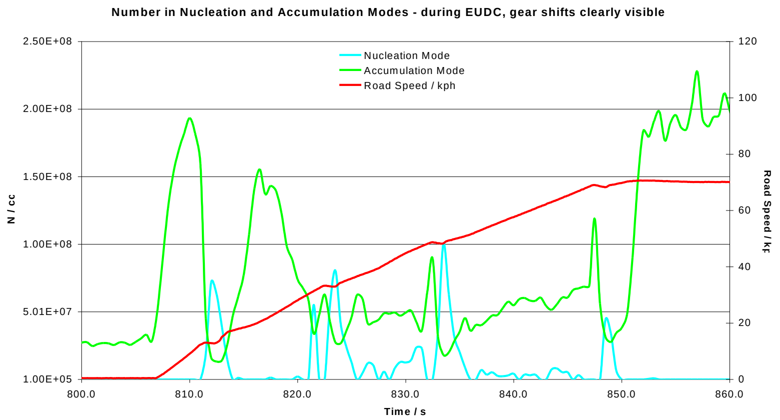

Figure 8: A Section from the Extra Urban Phase

In this plot, gearshifts can be clearly identified; when the throttle is released the accumulation mode (soot) is attenuated and the nucleation mode is boosted. Figure 9 shows a plot of the mean size of each mode:

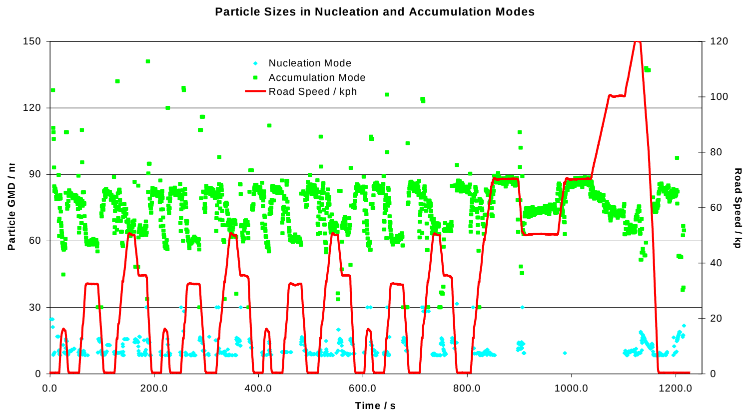

Figure 9: Mean Mode Particle Sizes over the NEDC

If not of interest, information about any mode can be ignored; for example, ignoring the nucleation mode in this case acts as a “software volatile particle remover”. The next plot shows a real-time estimation of mass passing into the DPF, based upon weighting the accumulation mode parameters (see application note DMS01 for fuller details):

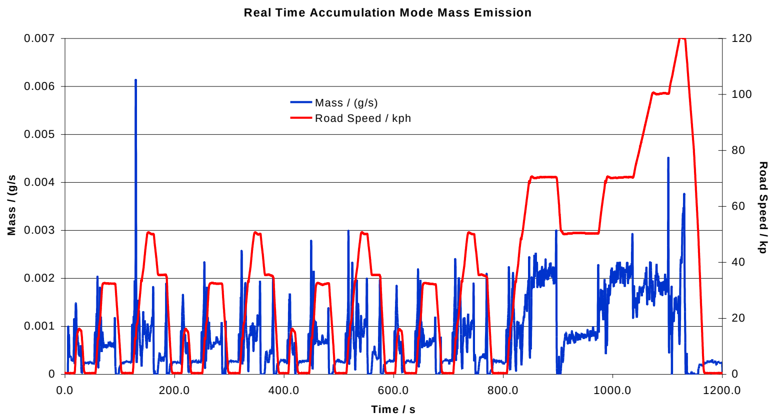

Figure 10: Mass Estimation over the NEDC

Finally, we examine the *tailpipe* (post-filter) emissions during a DPF regeneration event[4]. Under control of the ECU, the combustion conditions are from time to time adjusted to heat deposits in the DPF and burn them off. Two of Cambustion’s range of fast response gas analysers (HFR500 for hydrocarbons and the CLD500 for NO) were used to analyse the *feedgas* and complement the DMS500. Only one, nucleation type, particle mode is seen.

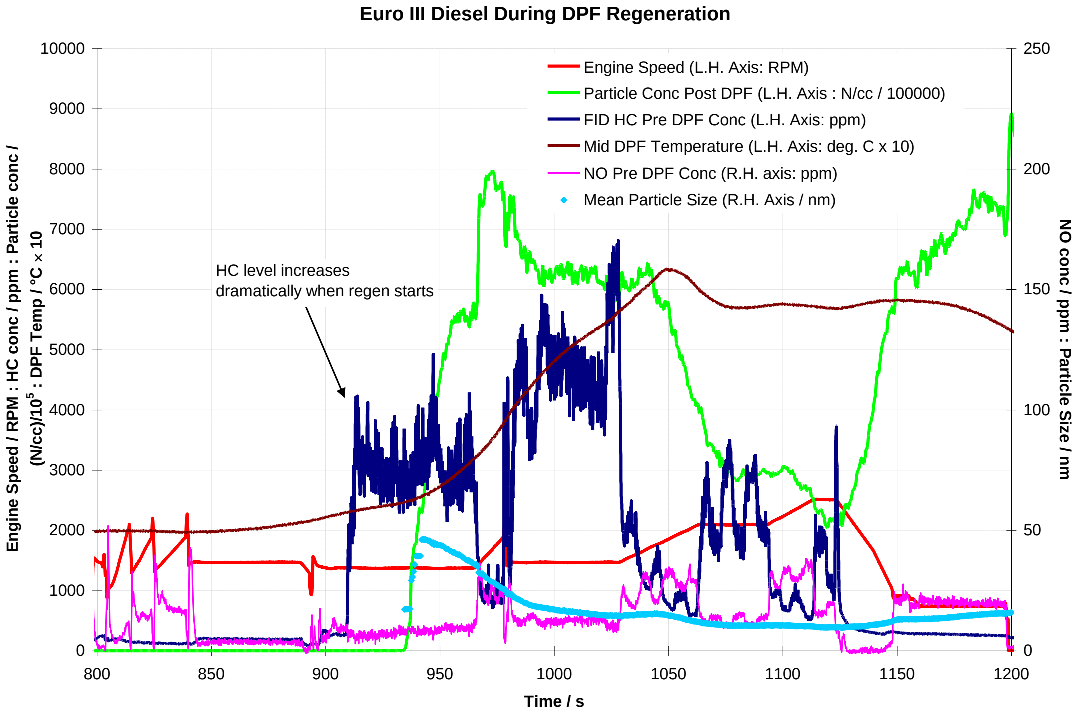

Figure 11: Diesel Particulate Filter Regeneration during NEDC

The engine made a further attempt to regenerate the DPF on the next NEDC cycle, and this time no particulate matter was seen, showing that the nucleation material seen in Figure 11 originates in the exhaust and aftertreatment system rather than from the engine.

It has been demonstrated that the new mode finding software extracts simple and meaningful information from DMS500 data, and allows quick visual analysis of trends.

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[1] *Correlation of Particle Mass Measurements with Electrical Mobility Classified Spectra*. K. Reavell, J. Symonds, *9th ETH Conference on Combustion Generated Nanoparticles,* Zurich **2005**

[2] *Diesel soot mass calculation in real-time with a differential mobility spectrometer*, J.P.R. Symonds, K. St.J. Reavell, J.S. Olfert, B.W. Campbell, S.J. Swift, *Journal of Aerosol Science*, **38** 52–68 **2007**

[3] *Calibration of Fast Electrical Mobility Spectrometers for Engine Particulate Measurement*, K. St.J. Reavell and J.P.R. Symonds, *11th ETH Conference on Combustion Generated Nanoparticles,* Zurich **2007**

[4] *Transient gas and particulate emissions measurements on a Peugeot 406 HDI diesel vehicle including a DPF regeneration event*. B. Campbell, M. Peckham, J. Symonds, J. Parkinson, A. Finch, *Society of Automotive Engineers Technical Paper* 2006-01-1079 **2006**