Deliverable D3.4: Standardization and data submission protocol for coarse mode particle number size distribution measurements

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Work package no	**WP3**
Deliverable no.	**D3.4**
Lead beneficiary	**TROPOS**
Deliverable type	☑ R (Document, report) ☐ DEC (Websites, patent fillings, videos, etc.) ☐ OTHER: please specify
Dissemination level	☑ PU (public) ☐ CO (confidential, only for members of the Consortium, incl Commission)
Estimated delivery date	**Month 12**
Actual delivery date	**15.07.2016**
Version	**1**
Comments	This deliverable focuses mainly on the data submission format. The final standardization for the quality assurance is postponed to D3.19, since further investigations have to be done first.

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Standardization and data submission protocol for coarse mode particle number size distribution measurements

There is a need for a standardized data submission protocol for particle number size distribution determined with aerodynamic or optical particle size spectrometers. The provisional data submission format is shown in Part I of this deliverable.

The results of the voluntary ACTRIS intercomparison workshop for aerodynamic and optical particle size spectrometers in September 2014 showed larges discrepancies between such instruments. There is a need to understand the uncertainties and limitation of this kind of particle size spectrometers. Furthermore, it should be the goal to develop a standardized method to calibrate the particle number concentration in the size range from 0.3 to 5 µm volume equivalent diameter. The actual status of the work is described in Part II of this deliverable.

The current D3.4 contains however only recommendations for data submission, but not yet for the measurements QA. Presently, only the status of investigations is given and the standardization is of the QA procedures are the on-going work. There will be a further deliverable handling the QU standardization and the uncertainties of the measurements.

D3.19: Quality assurance procedures and uncertainties for measurements of coarse mode particle number size distributions using aerodynamic and optical particle size spectrometers in long-term observation programs.

Part I: Data submission protocol

Common template for APSS and OPSS:
This template is a first step towards collecting data for in-situ number size distribution measurements of coarse mode particle collected at ground stations. It therefore covers both instrument types commonly used for this purpose, aerodynamic and optical particle size spectrometers, even though the differences in measurement principle cause a systematic deviation and a higher uncertainty as compared to the mobility particle size spectrometer. The metadata included allows distinguishing instrument type and measurement principle. Development of Standard Operating Procedures (SOPs) for these instruments may result in a separation into different templates in the future.

Definition of "Particle Number Size Distribution":
In WDCA templates, a "particle number size distribution" is defined as particle number concentration normalised by the logarithmic particle diameter interval (decadal logarithm) for which the concentration was measured, meaning d*N*/d log D_p.

Reference pressure and temperature for flows:
A regular submission or level 2 file contains the data referenced to standard conditions of temperature and pressure (273.15 K, 1013.25 hPa).

Number of size bins reported:
If necessary, please adapt the template to the number of size bins of your instrument. This will involve changes in header lines 1, 10, 11, 12, 19ff, and 266.

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Size bin diameters:
The diameters stated for each size bin are the geometric mean of lower and upper bin limit.

Spacing and position of size bins:
There are currently no SOPs for the different OPSS. For the APSS, recommendations are given in Pfeifer et al (2016). In the absence of a detailed instrument calibration by the user, the calibration, meaning number of size bins and their lower and upper limits, provided by the instrument manufacturer should be used. In case an independent calibration is available, it should be used instead.

Pfeifer, S., T. Müller, K. Weinhold, N. Zikova, S. Santos, A. Marinoni, O. F. Bischof, C. Kykal, L. Ries, F. Meinhardt, P. Aalto, N. Mihalopoulos and A. Wiedensohler (2016). Intercomparison of 15 Aerodynamic Particle Size Spectrometers (APS 3321): Uncertainties in Particle Sizing and Number Size Distribution. AMT 9, 1545–1551.

Assumptions on particle refractive index or particle density:
In terms of converting primary measurements to the definition of the volume equivalent particle diameters, the following has to be considered:

OPSS:
In case compact (spherical) particles and a realistic complex refractive index can be assumed, the particle number size distribution can be converted from optical to the volume equivalent diameter definition, using as Mie-model. In case of strongly non-spherical particles, it is suggested to keep the optical diameter definition. For OPSS, which are calibrated with a polydisperse aerosol, consisting of non-spherical particles, no conversion can be done. The refractive index of the particles used during calibration and the conversation should be documented in the "Comment" metadata item.

APSS:
In case a realistic particle density and dynamic shape factor can be assumed, the particle number size distribution can be converted from aerodynamic to the volume equivalent diameter definition.
The following equation should be used:

$$D_{\mathrm{P,Ve}} = D_{\mathrm{P,Ae}} \sqrt{\frac{\rho_0}{\rho_\mathrm{P}} \chi}$$

The particle density and dynamic shape factor used during calibration and conversion should be documented in the "Comment" metadata item.

Percentiles quantifying atmospheric variability:
In order to quantify the atmospheric variability over the hourly averaging period, regularly reported data usually contain the 15.87 and 84.13 percentiles for the averaging period in addition to the arithmetic mean. Please use interpolation if the percentiles do not match exactly by any data points in the averaging period.

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Flags commonly used with this format:

Flag	Data Valid (V) / Invalid (I)	Description	Comment
000	V	Valid measurement	
110	V	Episode data checked and accepted by data originator.	Used for valid data higher or lower than the 2 sigma range at the station.
185	V	Possible local contamination indicated by wind direction or velocity	
186	V	Possible local contamination indicated by single scattering albedo	
187	V	Possible local contamination indicated by occurrence of new particles.	Used in a setting where new particle formation indicates contamination)
459	I	Extreme value, unspecified error	Unexplained extreme values, technical problem suspected.
499	V	Inconsistent with another unspecified measurement.	For example, peak not seen by other co-located aerosol instruments.
559	V	Unspecified contamination or local influence, but considered valid	
640	V	Instrument internal relative humidity above 40%.	Used to signal possible hygroscopic growth of aerosol particles.
651	V	Agricultural activity nearby	
652	V	Construction / activity nearby.	Includes disturbance by other lab activity.
662	V	Too high sampling flow, data considered valid.	E.g., aerosol flow rate out of range but considered valid.
676	V	Station inside cloud	
677	I	Icing or hoar frost in the intake.	
699	I	Mechanical problem, unspecified reason.	E.g. problems with flow, leaks.
980	I	Missing due to calibration or zero/span check	
999	I	Missing measurement, unspecified reason	

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The template itself is a living electronic document that doesn't lend itself to be included in a document formatted for printing. The most current version of the template is always available at the website of the WMO Global Atmosphere Watch (GAW) World Data Centre for Aerosol (WDCA) collaborating with ACTRIS.

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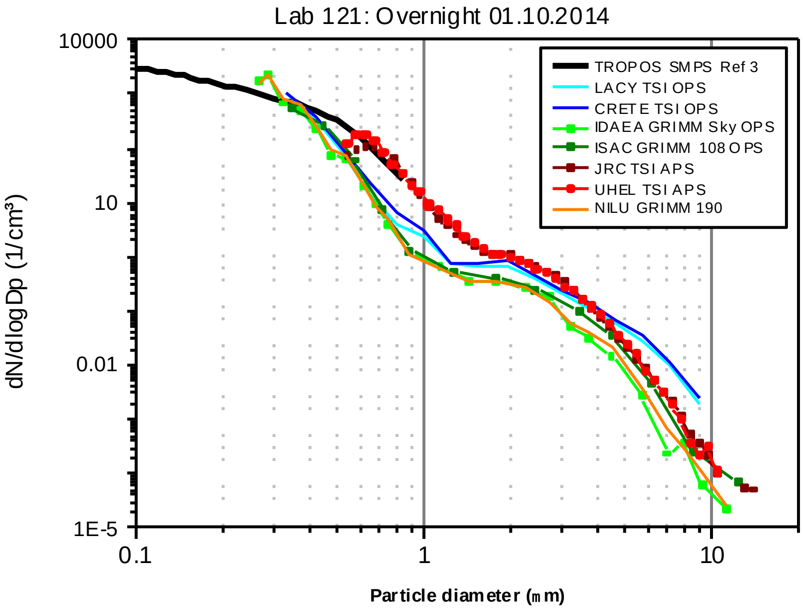
Part II: Standardized Quality Assurance of aerodynamic and optical particle size spectrometers

During the voluntary ACTRIS intercomparison workshop for aerodynamic and optical particle size spectrometers, the following mismatch between the different instruments was determined.



One can clearly see that the optical particle size spectrometers are lower in concentration compared to the aerosol dynamic particle size spectrometers. It can however not be determined which particle number size distributions are more correct, since no concentration standard was available for particle in the size range 0.3 to 5.0 µm.

The aim of the actual investigations is to understand these discrepancies and to develop an ACTRIS standard for particle number concentration for the above given size range. The present status is that we investigated the particle number concentration of the TSI-OPSS and the TSI-APSS by feeding monodisperse, spherical Latex-particles into the instruments. So far, we compared the total particle number concentration measured by a Condensation Particle Counter (CPC) and the candidate instruments for Latex particles in the size range from 0.6 to 2.0 µm, assuming that the CPC has no sampling losses in this size range.

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<u>Results:</u>

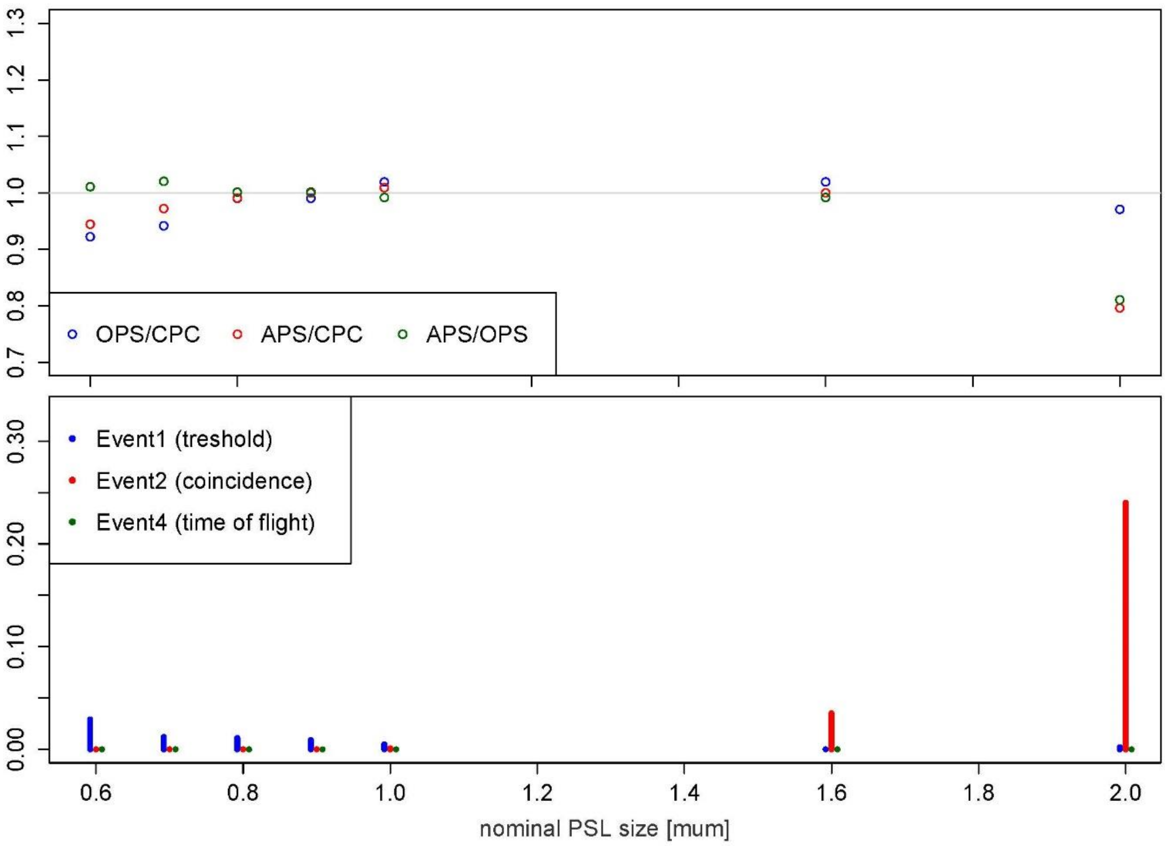

Figure 1: The upper part of the plot shows the counting efficiency of the APSS and OPSS against the CPC. Generally, for the size range from 0.6 to 1.0 µm an acceptable efficiency of 100 +/- 10% was determined for all instruments. Only for 2.0 µm, the counting efficiency was lower. The lower part of the plot explain the reason for the APSS, coincidence was the problem.

In the following figures, 2a to 2n, particle number size distributions determined by the APSS and OPSS are plotted for rather monodisperse latex particles in the size range from 0.6 to 2.0 µm. The APSS and OPSS seem to widen the distribution significantly already for such spherical and monodisperse latex particles, although they have been calibrated with latex particles by the manufacturer.

In further investigations, we will select highly monodisperse particles from the ambient aerosol to understand the response of the instruments in term of particle number size distribution and counting efficiency for particle greater than 1.0 µm.

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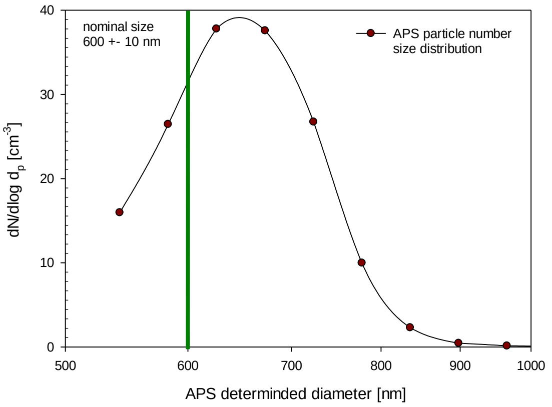

Figure 2a: APSS – 600 nm Latex particles

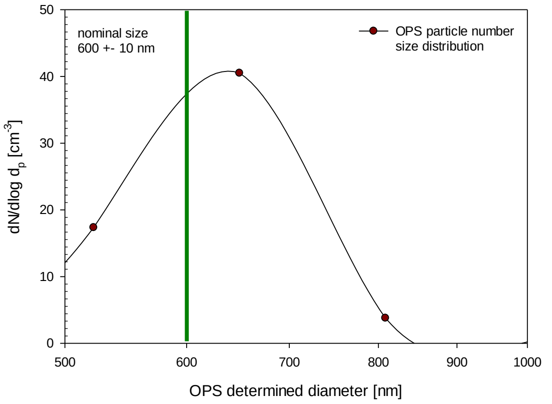

Figure 2b: OPSS – 600 nm Latex particles

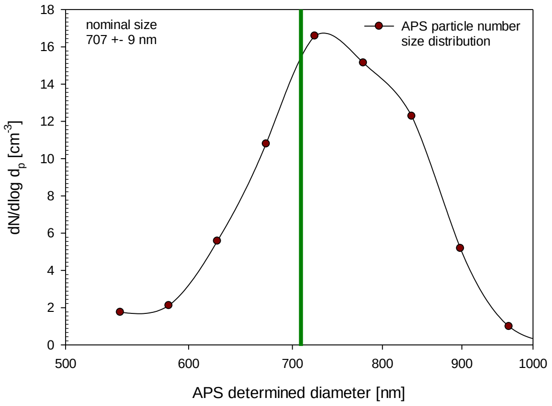

Figure 2c: APSS – 707 nm Latex particles

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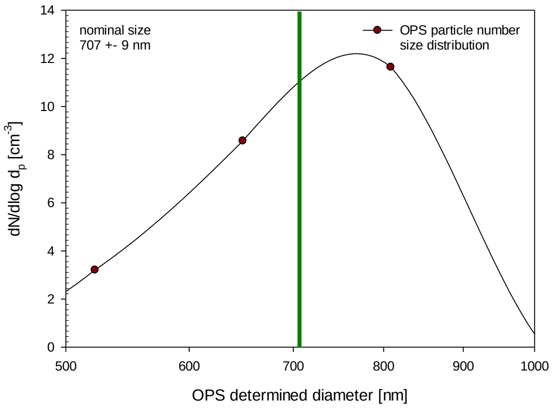

Figure 2d: OPSS – 707 nm Latex particles

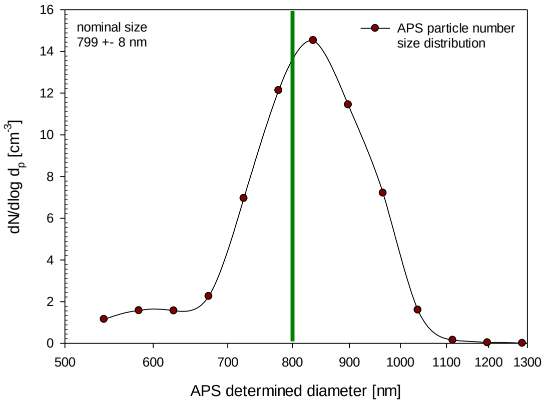

Figure 2e: APSS – 799 nm Latex particles

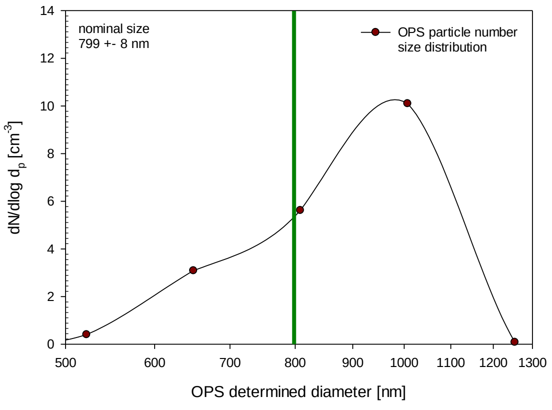

Figure 2f: OPSS – 799 nm Latex particles

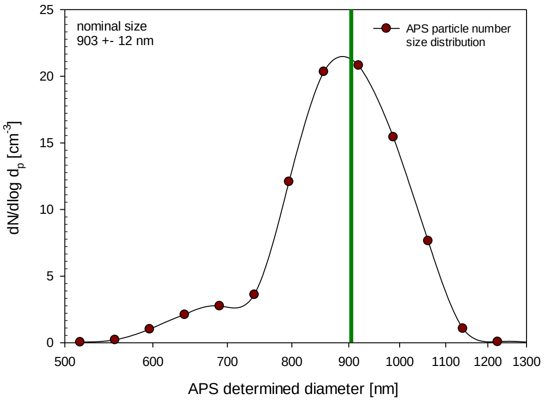

Figure 2g: APSS – 903 nm Latex particles

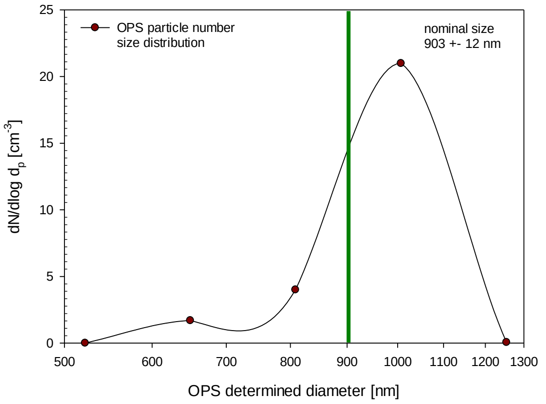

Figure 2h: OPSS – 903 nm Latex particles

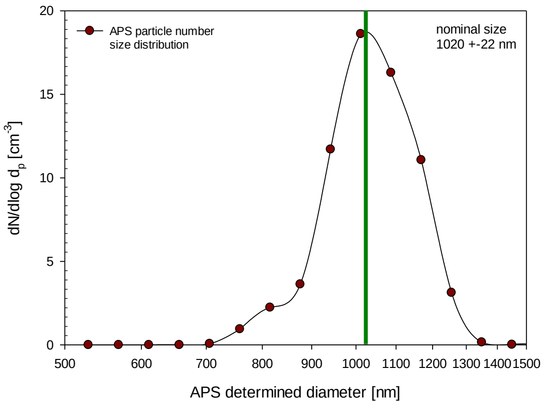

Figure 2i: APSS – 1020 nm Latex particles

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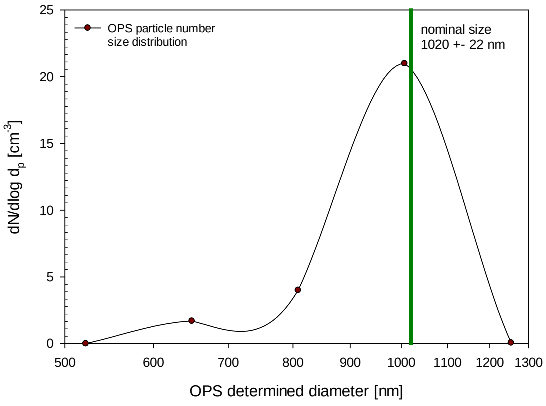

Figure 2j: OPSS – 1020 nm Latex particles

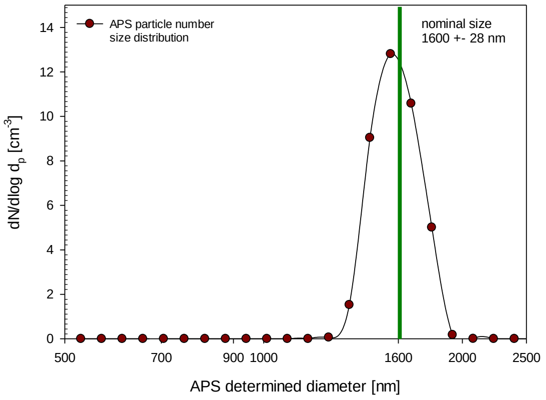

Figure 2k: APSS – 1600 nm Latex particles

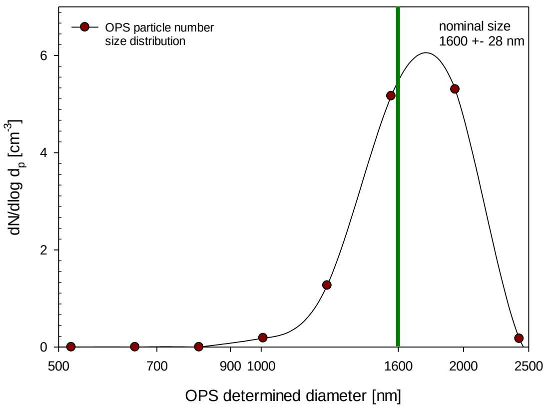

Figure 2l: OPSS – 1600 nm Latex particles

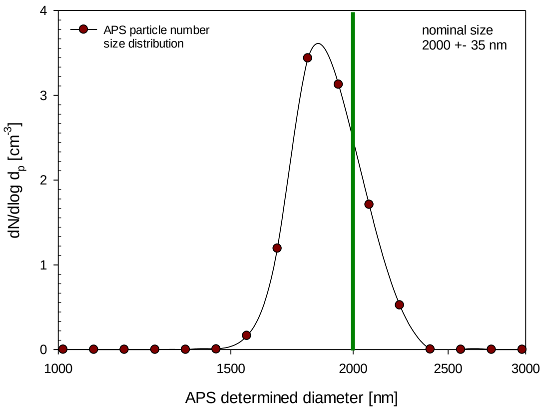

Figure 2m: APSS – 2000 nm Latex particles

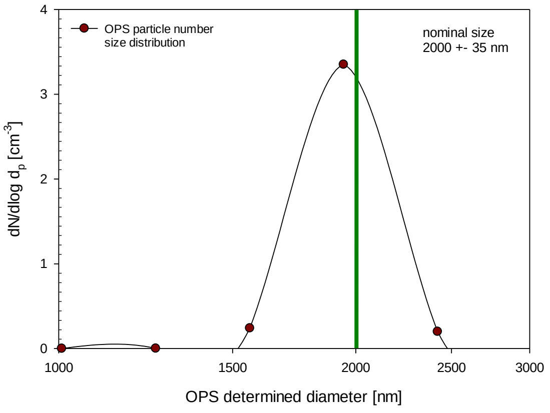

Figure 2n: OPSS – 2000 nm Latex particles

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