

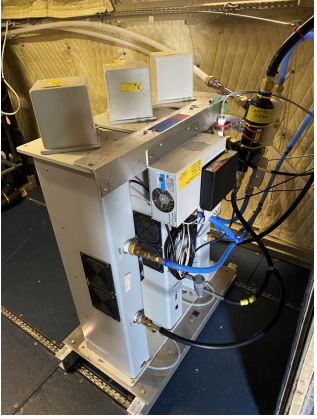
Improving uncertainty reporting for particle scattering measurements

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Scattering Coefficient Measurement and the Integrating Nephelometer



The measurement of particle light scattering coefficient is essential to characterize the aerosol particle's direct effect on the Earth radiative budget. It also plays a vital role to validate remote sensing observations and assess model simulations. Since scattering coefficient is a strong function of the particle size and abundance, the measurements have been used to improve application of aerosol optical depth observations in air quality monitoring and assessment. The TSI 3563 integrating Nephelometer has been extensively used to measure the particle scattering coefficient during field campaigns and in routine ground-based network.

Aerosol Direct Radiative Effect and its Impact on Climate Change

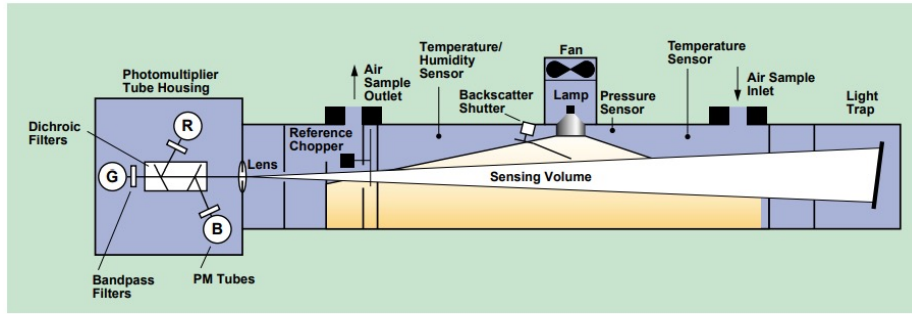


Aerosol particles cool the planet ... directly

- Aerosol particles scatter and absorb solar radiation causing a direct radiative forcing
- The radiative forcing is a strong function of aerosol particle mass, size, shape, and number concentrations, which are highly variable in space and time
- Aerosols that scatter have a cooling effect while absorbing aerosols have a warming effect. The current model estimates show a net cooling effect but with substantial uncertainty

TSI 3-Wavelengths Integrating Nephelometer

Aerosol particles are drawn into the measurement chamber through the air sample inlet and illuminated by a nearly Lambertian light source which is from a halogen lamp and an optical pipe (not shown) with an opal glass diffuser. The apertures, lens, and light trap are used to integrate the scattered light over an angular range of 7° to 170 degrees from the forward direction.



Model 3563 includes three wavelengths and a backscatter shutter, useful features for climate and air-quality studies.

Taken from: https://gml.noaa.gov/aero/instrumentation/neph_desc.html

Three photomultiplier tubes (PMT) then measure the scattered light at blue, green, and red wavelengths. The detected light signal includes the light scattered by aerosol, the walls of the measurement chamber, and the air/gas, aerosol particle absorption, and electronic noise inherent in the detectors. The particle scattering coefficient can be derived from the measurement of scattered light normalized by the proxy (or reference) of lamp incident light. The reference chopper controls three operation modes for detection of scattered light, attenuated direct lamp intensity, and PMT dark current.

Basic Measurement Principle

- Beer-Lambert law: $\frac{I}{I_0} = e^{(-\sigma_{ext}x)}$ where: I = attenuated light intensity after distance x; I₀ = incident light intensity, σ_{ext} = extinction coefficient; x = distance of light path
- $\sigma_{sp} = \sigma_{ext} - \sigma_{ap} - \sigma_{rg} - \sigma_{ag}$ where: σ_{sp} = particle total scattering coefficient; σ_{ap} = particle absorption coefficient; σ_{rp} = gas Rayleigh scattering coefficient, and σ_{ag} = gas absorption coefficient. **σ_{ap} and σ_{ag} are assumed to be negligible for common sampling conditions**
- Data Model: $\sigma_{sp}^i = B_s - W - \sigma_{rg}$ where: σ_{sp}^i = instrument particle scattering coefficient (integrated from 7° to 170 degrees); B_s = scattered light derived from the corrected and normalized PMT signal and instrument calibration; W = chamber wall scattering; σ_{rg} = gas Rayleigh scattering derived from measurement of particle-free air

Instrument Calibration by CO₂ and Particle-free Air

- The manufacturer's outlined instrument calibration procedure is to establish a linear relationship between the instrument scattering coefficient, B_s, and the PMT signal corrected for dark current and normalized by the lamp intensity, as well as to characterize the magnitude of chamber wall scattering
- The slope and intercept is determined by measuring scattering by CO₂ gas and particle-free air samples, which have independently known scattering coefficients

$$Slope = \frac{\sigma_{k,CO_2} - \sigma_{k,air}}{\sigma_{m,CO_2} - \sigma_{m,air}}, Offset = Slope \cdot \sigma_{m,air}$$

Where: σ_{k,CO_2} and $\sigma_{k,air}$ are known Rayleigh scattering coefficients for CO₂ gas and particle-free air; σ_{m,CO_2} and $\sigma_{m,air}$ are measured scattering coefficients

- The instrument calibration is not a direct calibration for particle scattering coefficient measurements, as there is no particle calibration standard**
- $\sigma_{m,air}$ is monitored routinely during field operation using an in-inline particle filter. This is to assess instrument noise as well as detect and compensate any drift in the instrument signal

Truncation Correction for σ_{sp}^i to estimate σ_{sp}

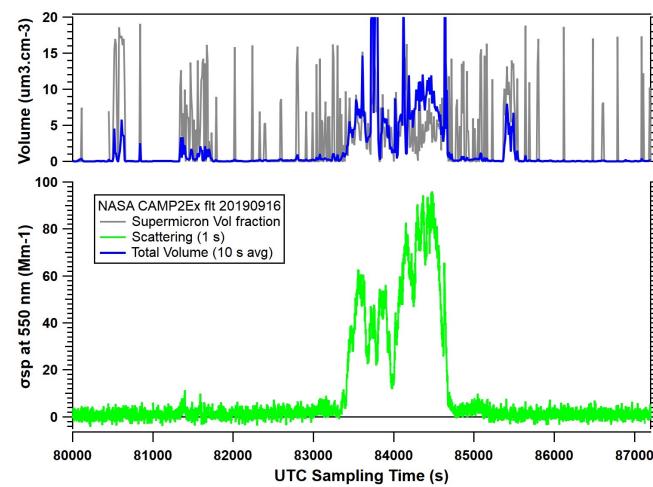
- As the instrument calibration is based on gas Rayleigh scattering, correction of σ_{sp}^i is necessary to estimate σ_{sp} . This reflects the phase function difference between gas Rayleigh scattering and particle Mie Scattering
- The widely used correction factor was developed by Anderson and Ogren (1998): $c = a + b\alpha$; where α is Angstrom exponent, a proxy of particle population size; offset a and slope b were estimated through Mie-scattering model calculations
- The correction factor is a strong function of particle population size and is intended for measurement of scattering by submicron particles

Uncertainty Budget

Uncertainty Source	Uncertainty Type	Estimated Magnitude
Instrument Noise	Random	1 – 3 Mm ⁻¹ for 1 s data
Calibration by particle-free air and CO ₂	Systematic	3 - 5% (WMO SOP)
Truncation correction	Systematic (Best available estimate)	10% for PM1, 20 - 50% for > PM1 (WMO SOP), sampling condition dependent

- Instrument noise is estimated using photon-counting statistics
- The calibration uncertainty is largely due to the uncertainties associated with known CO₂ and air scattering coefficients

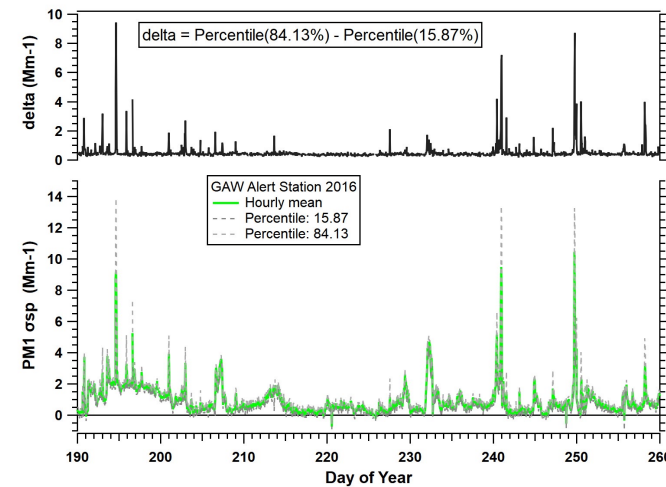
Use Case 1: CAMP²Ex Airborne Observation Uncertainty Reporting



- Reported Uncertainties for 1 s data:
 - Random uncertainty: 3 Mm⁻¹
 - Systematic Uncertainty: 30%
- Reported systematic uncertainty is mostly due to truncation correction and the best available estimate over the entire flight, not targeted to a given sampling period
- Integrated particle volume measurement shows supermicron mode contribution was highly variable and large at times
- σ_{sp} (particle scattering coefficient) can have large variability in short temporal/spatial scale; however, it may not have significant impact on data reported at 1 sec interval

Use Case 2: GAW Alert Station Uncertainty Reporting

- Per WMO SOP, submicron scattering data are reported in hourly arithmetic mean and 15.87 and 84.13 percentile values derived from 60 sec. measurements
- The percentile interval is a good measure of the dispersion of the measurement values. The dispersion is attributed to both measurement uncertainty and ambient variability
- The systematic uncertainty associated with truncation correction is estimated at ~ 10%. The random uncertainty should be negligible given the reporting time interval
- The ambient variability is evident in the large percentile interval values



Discussion

- Particle scattering coefficient measurements are reported in two different ways (i.e., percentiles vs. systematic and random uncertainties); however, both provide useful information to define the potential range of dispersion of the measurement results
- The difference in uncertainty reporting can be attributed to the difference in data reporting frequency
- Reported measurement precision is estimated using the observed instrument noise, generally consistent with the VIM definition “random measurement error”
- The percentile interval does not directly fit to the current VIM definitions, while providing useful and necessary information to many applications, e.g., model assessment. Furthermore, the measurement uncertainty can not be delineated from the reported percentile intervals. The percentile interval can be compared with an estimate of the upper limit of measurement uncertainty, consistent with “target measurement uncertainty”
- The truncation correction is derived from model simulations with idealized assumptions and later evaluated in lab and field experiments. The uncertainty associated with this correction cannot be characterized as the VIM defined “systematic measurement error” or “measurement bias” since there is no particle calibration standards for this measurement or known true value
- The uncertainty introduced by the truncation correction can be characterized as the best available estimate, which may be consistent with the VIM keyword: “target measurement uncertainty”

Future Direction – Metadata Standard Needs

- Uncertainty metadata standards are necessary to enable implementation of the R and I in F.A.I.R. principles. The use cases can contribute to the WMO-coordinated efforts to evolve the WIGOS metadata standard (WMDS), which will better document the uncertainty of observations
- The metadata standards should be based on VIM keywords and definitions with consideration of the terms broadly used in literature publications and textbooks
- The metadata standards should cover the current reporting practice, with the goal to help instrument scientists understand what and how to report the uncertainties useful to researchers at large
- Given that many atmospheric composition measurements do not have SI-traceable calibration standards, it is important to evaluate the necessity to differentiate the systematic uncertainty estimate derived from calibration or other methods, and the impact of this approach on the data use in various applications
 - Non-calibration based approaches are often the only feasible methods
 - Non-calibration based approaches may not cover all processes that can introduce systematic uncertainties
 - Most users will not have the need to investigate this level of detail if calibration was involved

Metadata Standard Requirements for Uncertainty

The use cases highlight the metadata need for standardized uncertainty reporting, which should be VIM-based and adopt terms commonly used in literature publication and textbooks. The basic metadata needs for particle scattering measurements and similar ones are summarized in the table below to solicit feedback from communities at large

Tentative Name	Associated VIM Term(s)	Tentative Description
Measurement Uncertainty	Measurement Uncertainty	A non-negative parameter characterizing the dispersion of the quantity values of a measurand, which is attributed to the measurement
Systematic Measurement Uncertainty	Measurement Bias	Estimate of the component of measurement uncertainty that remains constant or varies in a predictable manner
Random Measurement Uncertainty	measurement precision	Closeness of agreement between indications or measured quantity values obtained by replicate measurements or related to the largest change in measurement quantity value that causes no detectable indication in measurement
Total Measurement Variability		A non-negative parameter characterizing the dispersion of the quantity values of a measurand, which is attributed to the measurement and ambient variability
Measurement Uncertainty - Best Estimate		A best-estimate non-negative parameter characterizing the dispersion of the quantity values of a measurand, which is attributed to the measurement

References

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