STANDARD OPERATING PROCEDURES

Generating Time-Resolved $PM_{2.5}$

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1.0 SCOPE AND APPLICATION

This SOP describes the method of combining quality assured nephelometer data (SPARTAN SOP Nephelometer Revision 2.1) with filter average $PM_{2.5}$ mass concentrations (SPARTAN SOP Gravimetric Analysis Revision 3.0) and chemical composition information (SPARTAN SOP RCFM Revision 3.1) to produce hourly and daily estimates of $PM_{2.5}$ concentrations. The assessment of $PM_{2.5}$ hygroscopicity as described in SPARTAN SOP RCFM Revision 3.1 is site specific and time varying based on the measured chemical composition. The temporally resolved, site-specific κ-Kohler parameters for volume (κ_v) are calculated and used to refine the relationship between total nephelometer scatter and $PM_{2.5}$. Hygroscopic growth factors are used to estimate dry (RH = 35 %) hourly $PM_{2.5}$ from hourly nephelometer measurements of total scatter at 550 nm at ambient relative humidity. A cut-off of 80 % RH is applied to calculation of temporally-resolved $PM_{2.5}$, above which hygroscopic uncertainties and total water mass dominate scatter measurements.

REVISION HISTORY			
Revision No.	Change Description	Date	Authorization
2.0	General reorganization and clarification; update to classification of satellite overpass times	August 29, 2018	Crystal Weagle
2.1	Update and clarification to data validation protocol	April 9, 2020	Crystal Weagle
2.2	Update procedure to determining dry total scatter	December 19, 2023	Haihui Zhu

2.0 CALCULATION OF TIME-RESOLVED $PM_{2.5}$

2.1 Volume growth factors

The κ-Kohler parameter for the total $PM_{2.5}$ mass ($\kappa_{v,tot}$) of each filter is determined by linear combination of mass measurements (m_i,), assumed densities (ρ_i), and κ-Kohler constants for each measured chemical component ($\kappa_{v,i}$):

$$\kappa_{v,tot} = \frac{1}{V}\sum_i \frac{m_i}{\rho_i}\kappa_{v,i} \qquad (1)$$

where V is the total volume sampled over the filter. It is assumed that the relative contribution of the chemical components remains constant of the sampling period, thus the κ parameter also remains constant. The resultant volume growth factor (f_v) is a simple function of filter-specific κ-Kohler parameter and the measured ambient relative humidity (RH):

$$f_v(\mathrm{RH}) = 1 + \kappa_{\mathrm{v,tot}} \frac{\mathrm{RH}}{100 - \mathrm{RH}} \tag{2}$$

2.2 Determining dry total scatter and $PM_{2.5}$

Nephelometer scatter measurements are available at three wavelengths (457 nm, 520 nm, and 634 nm). We use green light (520 nm) scattering at ambient condition and the volume growth factor to estimate dry total scatter:

$$b_{sp,\text{dry-1h}} = \frac{b_{sp,\mathrm{1h}}(RH)}{f_v(\mathrm{RH})} \tag{3}$$

Changes in dry scatter are proportional to changes in $PM_{2.5}$ mass as,

$$b_{sp,\mathrm{dry}} = \alpha PM_{2.5,dry} \tag{4}$$

where α ($m^2\ g^{-1}$) is the mass scattering efficiency and is a function of aerosol size distribution, effective radius, and dry chemical composition. For the determination of time-resolved $PM_{2.5}$ concentrations from integrated filter samples, composition, density, and size distribution are treated as constant over the sampling period such that α is approximately equal to the average over sampling period ($< \alpha >$). Under this assumption, the predicted mass changes in low humidity (35 % RH) are proportional to water-free (0 % RH) scatter:

$$\mathrm{PM}_{2.5,\text{dry-1h}} = < \mathrm{PM}_{2.5,\mathrm{dry}} > \frac{b_{sp,\text{dry-1h}}}{< b_{sp,\mathrm{dry}} >} \tag{5}$$

where the < > indicates the average $PM_{2.5}$ concentration measured on the PTFE® filters over the sampling period, which is typically 9 days. The explicit compensation for aerosol water is then:

$$PM_{2.5,dry-1h} = \frac{< PM_{2.5,dry} >}{< \frac{b_{sp}(RH)}{f_v(RH)} >} \cdot \frac{b_{sp-1h}(RH)}{f_v(\mathrm{RH})} \tag{6}$$

3.0 DATA VALIDATION

- The mass fraction of chemical components can lead to $\kappa_{v,tot}$ values > 0.6. When this occurs, the value is flagged as suspicious and investigated for potential erroneous measurements such as very low $PM_{2.5}$ mass or high value obtained from IC or ICP-MS analysis.
- To account for transient meteorological events a derivative-based screening protocol is applied to screen hourly scatter values where the change is greater than $\pm$ 50 Mm^{-1} $hour^{-1}$ in low $PM_{2.5}$ environments and $\pm$ 250 Mm^{-1} $hour^{-1}$ in high $PM_{2.5}$ environments. Values exceeding the threshold are not used to estimate hourly $PM_{2.5}$.
- Under the circumstance that a filter-specific κ-Kohler parameter is not available (e.g. all chemical analysis is not complete), a default value of 0.2 is used in Eq. 2 until a filter-specific value is available.
- Under the circumstance that a nephelometer is operating without coincident filter sampling, dry scatter is estimated with Eq. 4 using the site average mass scattering efficiency. The resulting time-resolved $PM_{2.5}$ is considered preliminary and should not be used for research purposes.
- When the hourly-averaged ambient relative humidity, as recorded by the nephelometer, exceeds 80 % the $PM_{2.5}$ is not estimated as hygroscopic uncertainties increase, and water mass dominates the scatter measurement.

This SOP corresponds to data version 1.1 of the Time Resolved $PM_{2.5}$.