



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 2.0) with filter average PM_{2.5} mass concentrations (SPARTAN SOP Gravimetric Analysis Revision 3.0) and chemical composition information (SPARTAN SOP RCFM Revision 3.0) 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 3.0 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

2.0 CALCULATION OF TIME-RESOLVED PM_{2.5}

2.1 Volume growth factors

The κ-Kohler parameter for the total PM_{2.5} mass (κ_{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 (κ_{v,i}):

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

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):

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

2.2 Determining dry total scatter and PM_{2.5}

Nephelometer scatter measurements at three wavelengths (457 nm, 520 nm, and 634 nm) are averaged into hourly intervals and converted to 550 nm via a fitted angstrom exponent. The volume growth factor is then used to estimate dry total scatter:

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

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

$$b_{sp,\text{dry}} = \alpha PM_{2.5,\text{dry}} \quad (4)$$

where α (m² 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 ($\langle \alpha \rangle$). Under this assumption, the predicted mass changes in low humidity (35 % RH) are proportional to water-free (0 % RH) scatter:

$$PM_{2.5,\text{dry-1h}} = \langle PM_{2.5,\text{dry}} \rangle \frac{b_{sp,\text{dry-1h}}}{\langle b_{sp,\text{dry}} \rangle} \quad (5)$$

where the $\langle \rangle$ 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:

$$PM_{2.5,\text{dry-1h}} = \frac{\langle PM_{2.5,\text{dry}} \rangle}{\langle \frac{b_{sp}(\text{RH})}{f_v(\text{RH})} \rangle} \cdot \frac{b_{sp-1h}(\text{RH})}{f_v(\text{RH})} \quad (6)$$

4.0 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.
- 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.
- When a long-term η value is less than $20 \mu\text{g m}^{-3}$ or exceeds $250 \mu\text{g m}^{-3}$, the data is investigated for potential erroneous measurements such as very high scatter, or very low $PM_{2.5}$ that could be effecting the average.