# SOP #11

## Combining AOD, Light Scatter, and $PM_{2.5}$ into Daily $PM_{2.5}$/AOD Ratios

**General summary:** In this section we outline the process of merging hourly aerosol optical depth values ($AOD_{1h}$), 550nm (green) aerosol scatter ($b_{sp,1h}$), and 9-day average fine aerosol concentrations ($PM_{2.5,9d}$) into one file. The merged data is the transformed into satellite $PM_{2.5,24h}/AOD_{10\text{-}14h}$ ratios (defined as $\eta_{1d}$) and hourly fine mass ($PM_{2.5,1h}$) suitable for website uploading and sharing.

| REVISION HISTORY | | | |
|---|---|---|---|
| Revision No. | Change Description | Date | Authorization |
| 2.0 | Update of scripts used to perform hourly $PM_{2.5}$ estimates and etta calculations | July 15, 2018 | Paul Bissonnette |

**Processing $PM_{2.5}$, scatter, and AOD data:**

For step 10 to work, we must have quality assurance from Nephelometer (**SOP #5**), AOD (**SOP #4**), $PM_{2.5}$ physical data (**SOP #3**), and $PM_{2.5}$ chemical data (**SOP #7, 8**) from a given site.

The above information is combined using the Matlab program **PM25_Daily.m**

**INPUT**: The merging files have the following shape:

Neph: **Neph[PM Size]_[site code]_hourly.csv**

AOD: **AOD_[site code]_hourly.csv**

$PM_{2.5}$ (phys. and chem.): **PM25_Speciation_[site code].csv**

**OUTPUT**: The above are merged via the data condensing routine located at:

[Stetson] data1/paulb/HEI_Codes/PM25_Daily.m

The output file (one per site) has the format:

[Stetson] gsnider/SPARTAN/neph_condensing/

[Site name_code]/PM25/**PMhourly_[start date]_[end date]_[site code].csv**

Because Excel corrupts the break points of the generated .csv file, DO NOT OPEN WITH EXCEL before uploading to website (Spartan-network.org)

**Data generated with PM25_Daily.m:**

| **Col 1** | **Col 2** | **Col 3** | **Col 4** | **Col 5** | **Col 6** | **Col 7** | **Col 8** | **Col 9** | **Col 10** | **Col 11** | **Col 12** | **Col 13** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| DateTime | Temp_C | RH | fRH | Bsp_550nm | AOD_550nm | PM_filter | BC | NH4 | Nitrate | Sulfate | PM_h | $\eta$ |

The data columns come from a combination of hourly nephelometer data, hourly* AOD data, and 9-day physical and chemical filter data.

Physical filter information:

1. Black carbon (surface reflectance)
2. Total deposited mass (pre- and post-weighed on microbalance)

Chemical information:

1. Anion concentrations (seven total)
2. Cation concentrations (six total)
3. Trace metal concentrations (24 total)

**Calculating and filtering $\kappa$-Kohler theory values (in PM25_Daily.m)**

Details of $\kappa$-Kohler method are in SOP #10, reconstructed fine mass (RCFM). While combining chemical and physical data together, the $\kappa$-Kohler values for mass ($\kappa_m$) and volume are calculated ($\kappa_v$). The latter ($\kappa_v$) is used to estimate growth factors for local aerosol populations in a given location.

The figure below is an example of a .png automatically generated by running the condensing program. It is found in the folder/template as follows:

[**Stetson**]: gsnider/SPARTAN/K_constant_empirical/[Sitename_code]_kappa_timeline.png

Table 10.1: κ-Kohler theory for specific species, defined for volume and mass RH growth

| Material | $\kappa_{v,i}$ | Density ($\rho_i/\rho_{H2O}$) | $\kappa_{m,i}$ | Ref. |
|---|---|---|---|---|
| **Soil/sand/dust** | 0 | 2.5 | 0 | |
| **BC** | 0 | 2 | 0 | |
| **Mixed OM** | 0.05* | 1.35 | 0.037 | B |
| **$ANO_3$** | 0.67 | 1.72 | 0.39 | A |
| **$ASO_4$** | 0.56 | 1.77 | 0.32 | A |
| **Sea salt** | 1.2 | 2.17 | 0.55 | A |

A = (Hersey et al., 2013), B = (Dusek et al., 2011),

Each printout contains four pieces of information:

1. Top left: Seasonal trend in $\kappa_v$ values, calculated by taking a 45-day forward and backward running mean (91 days total, or about three months, e.g. one season).
2. Top Right: Relative contributions to growth factor. Usually $ANO_3$ dominates, however sometimes residue is largest contributor. We assume $\kappa_{v,org}$ = 0.1. The value $\kappa_v$ above the pie chart is the mean for the entire measurement period.
3. Bottom left: Contribution to volume. This takes mass data from each major chemical species and converts to volume via density (we assume volumes are additive).
4. Bottom right: Contribution to mass is simply the contribution to total-weighed $PM_{2.5}$ mass (RCFM helps decide how to parse). The $PM_{2.5}$ mass in brackets is the mean over the total measurement period.

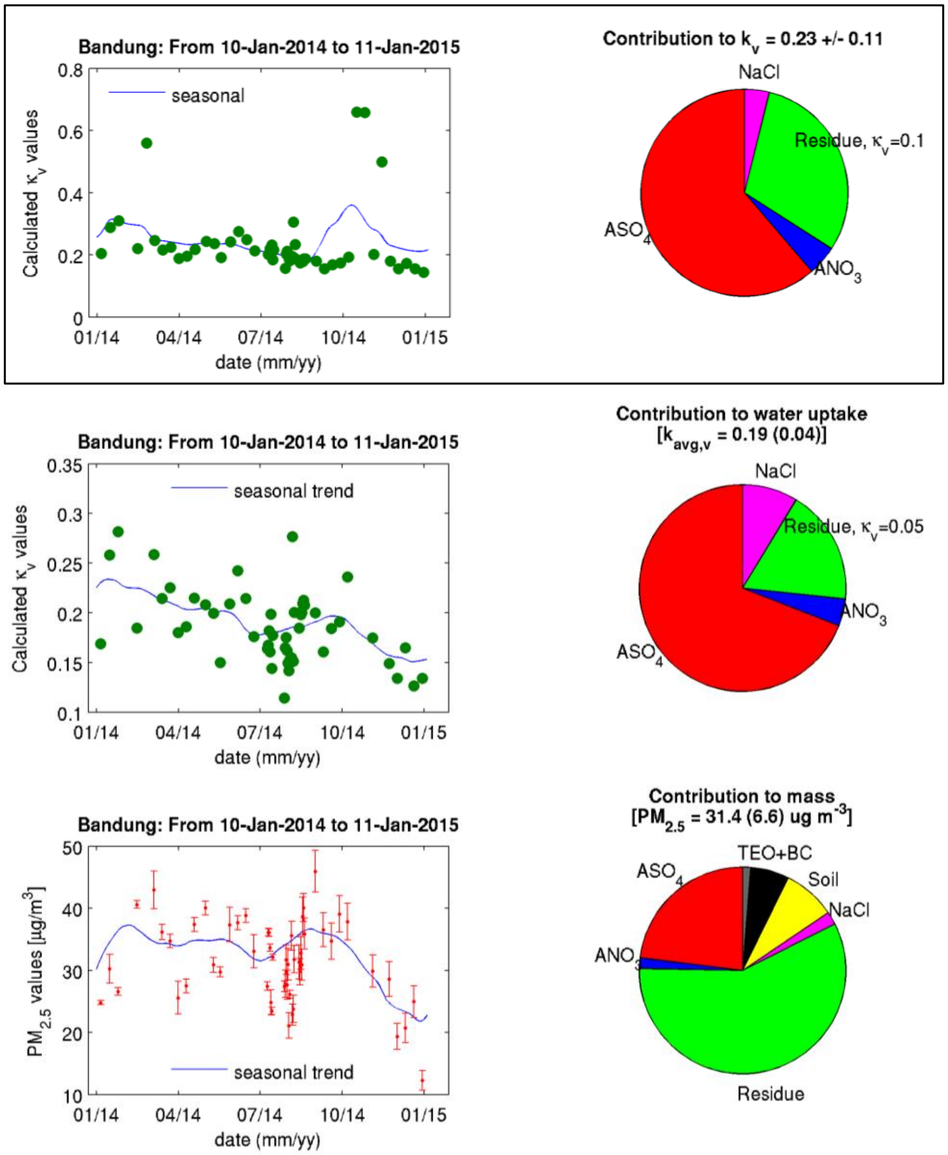


Figure 10.1: Top, outlined: Unfiltered (unscreened) $\kappa_v$ values at Bandung site, Bottom: four panels of data, including filtered $\kappa_v$ values (and $PM_{2.5}$ mass trends), resulting in a lower mean value.

## Merging species $\kappa_v$ results

The components of $\kappa_{v,tot}$ are obtained by linear combinations of mass measurements $m_i$, assumed densities $\rho_i$. Volume growth factors $\kappa_{v,i}$ are obtained from cited works.

$$\kappa_{v,tot} = \frac{1}{V}\sum_i \frac{m_i}{\rho_i}\kappa_{v,i} \qquad \text{Eq. 1}$$

Volume growth factors are a simple function of $\kappa_{v,tot}$ and percent relative humidity (0 < RH < 100):

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

Table 10.2: Mean volumetric uptake constant per SPARTAN site

| Location | Host Institute | $\kappa_{v,tot}$ (SD) | Sampling Period |
|---|---|---|---|
| **Atlanta** | Emory University | 0.20 (0.08) | Jan. – May 2014 |
| **Bandung** | IIT Bandung | 0.19 (0.04) | Jan. 2014 – Jan. 2015 |
| **Beijing** | Tsinghua University | 0.24 (0.12) | June 2013 – Dec. 2014 |
| **Buenos Aires** | CITEDEF | 0.27 (0.10) | Oct. – Dec. 2014 |
| **Dhaka** | Dhaka University | 0.15 (0.05) | Oct. 2013 – Nov. 2014 |
| **Ilorin** | Ilorin University | 0.15 (0.05) | March – Oct. 2014 |
| **Kanpur** | IIT Kanpur | 0.19 (0.04) | Dec 2013 – Apr. 2014 |
| **Mammoth Cave** | Mammoth Cave Nat. Park (IMPROVE) | 0.25 (0.10) | June – Aug. 2014 |
| **Manila** | Manila Observatory | 0.20 (0.08) | Feb. – July 2014 |
| **All-site Average** | - | **0.20 (0.07)** | - |
| Continental US[1] | Various | **0.16(0.07), 80 nm**<br>**0.18(0.09), 60 nm** | 2008 |
| **California coast[2]** | Various | **0.2 – 0.4,**<br>**150-250 nm** | |

[1](Padró et al., 2012), [2](Hersey et al., 2013)

Mass fractions, per component, can sometimes lead to suspicious results such that $\boldsymbol{\kappa_{v,tot}}$ > 0.6. The residue composition (associated with organics) is defined as in **SOP #10** to be **[RM] = [PM] – [IN$_{tot}$]**. The value [RM] can be negative either because $IN_{tot}$ is too large, or PM too small.

- We initially screen out negative PM values, which may occur when debris was on pre-weighed filter, change in balance calibration, or other unknown effects.
- If [$IN_{tot}$] is larger than [PM] by 10%, i.e. ([PM] - [$IN_{tot}$])/[$IN_{tot}$] < -0.1, we keep the negative value. When [RM] is more negative we manually inspect those masses to determine on a case-by-case basis.
- If mass values are $\boldsymbol{\kappa_{v,tot}}$ > 0.6 we manually inspect to verify potential erroneous measurements (possible reasons: too-high IC/ICP/EBC results, or too low PM).

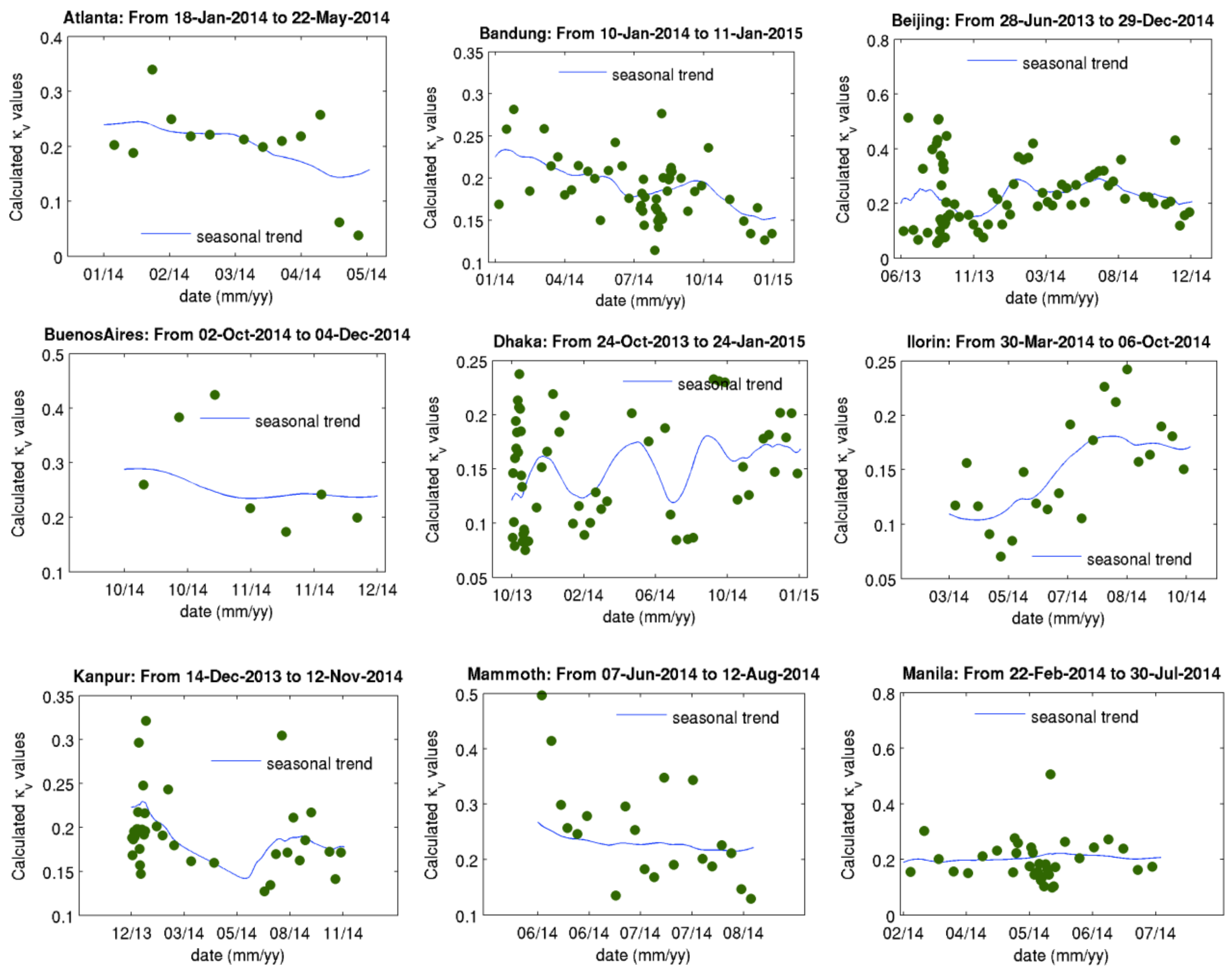


Figure 10.2: Seasonal trends in $\kappa_v$ for nine SPARTAN sites. Suspicious growth factors (those where $\kappa_{v,tot} > 0.8$) have been checked and eliminated.

**Integrating κv results with hourly nephelometer and 9-day $PM_{2.5}$ data**

The seasonal $\kappa_v$ value is then interpolated into hourly values, $\kappa_{v,h}$, whereby it is used to estimate dry scatter 550 nm nephelometer scatter. Humidity above 80% is presently ignored (converted to NaN values). Otherwise the dry scatter is defined as:

$$b_{sp,\text{dry-1h}} = \frac{b_{sp,\text{1h}}\{\text{RH} < \text{RH}_{\text{max}}\}}{f_v(\text{RH})} \qquad \text{Eq. 3}$$

The dry scatter is then used to calculate hourly $PM_{2.5}$ via hourly dry scatter $b_{sp,\text{1h}}$, 9-day filter-measured $PM_{2.5}$, and a 9-day mean of dry scatter (Snider et al., 2015).

$$\text{PM}_{2.5,\text{dry-1h}} = <\overline{\text{PM}}_{2.5,\text{dry,9d}}> \frac{b_{sp,\text{dry-1h}}}{<b_{sp,\text{dry, 9d}}>} \qquad \text{Eq. 4}$$

Using the equation 4 we obtain reasonably accurate hourly $PM_{2.5}$ estimates, as shown below.

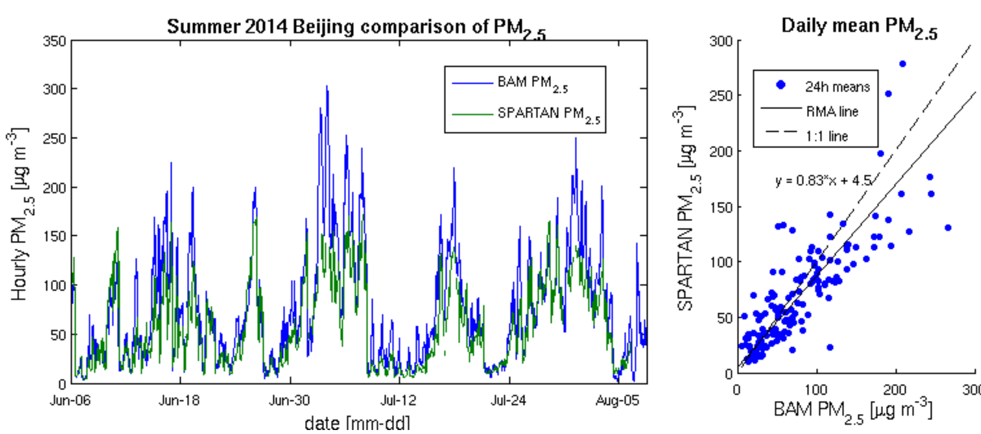


Figure 10.3: Reconstructed hourly $PM_{2.5}$ using the merged SPARTAN filter-nephelometer data. Plot is overlaid with a MetOne BAM-1020 at the US Beijing Embassy (15 km away). Reduced major axis (RMA) slope shows reconstructed hourly SPARTAN $PM_{2.5}$ underestimates BAM measurements by a factor of 0.83 with an absolute mass bias of 4.5 μg $m^{-3}$ (while measuring over a concentration range of 10 – 300 μg $m^{-3}$). Pearson correlations between SPARTAN and BAM are r = 0.80 (hourly) and 0.82 (daily). Depending on RH and gaseous ammonia concentrations, it is not uncommon to find BAM instruments reporting greater masses than gravimetric instruments (Watson et al., 1998).

Combining daily AOD (**SOP #4**, averaged over satellite-relevant hours), we take daily means of the $PM_{2.5}$ in equation 4 and obtain daily $\eta$:

$$\eta = \frac{\mathrm{PM}_{2.5,24\mathrm{h}}}{\mathrm{AOD}_{10\text{-}14\mathrm{h}}} \qquad \text{Eq. 5}$$

**References**


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Watson, J. G., Chow, J. C., Moosmuller, H., Green, M., Frank, N. and Marc, P.: Guidance for using Continuous Monitors in PM2.5 Monitoring Networks., 1998.