10

Section 10 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 η_{1d}) and hourly fine mass ($PM_{2.5,1h}$) suitable for website uploading and sharing.

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

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

The above information is combined using the Matlab program PM25_condensing_v2.m

INPUT: The merging files have the following shape:

Neph: **Neph[instr #]_[start date]_[end date]_[site code]_hourly.csv**
AOD: **AOD_[start date]_[end date]_[site code]_hourly.csv**
$PM_{2.5}$ (phys and chem): **PM25_[start date]_[end date]_[site code].csv**

Start and end dates have the format yyyymmdd

For example, here is the data for Mammoth Cave (USMC):

Neph_20140619_to_20140715_Mammoth_USMC_hourly.csv
AOD_20140101_20141231_Mammoth_USMC_hourly
PM25_20140607_20140712_Mammoth_USMC.csv

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

[Stetson] gsnider/SPARTAN/K_constant_empirical/PM25_condensing_v2.m
or
[Stetson] gsnider/SPARTAN/neph_condensing/PM25_condensing_v2.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**

The MATLAB program PM25_condensing_v2.m keeps track of the start and end dates of the desired files, but requires frequent updates since any new Neph, AOD, or $PM_{2.5}$ file requires a new date range before generating.

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

Data generated with PM25_condensing_v2.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	η

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 κ-Kohler theory values (in PM25_condensing_v2.m)

Details of κ-Kohler method are in section 9, reconstructed fine mass (RCFM). While combining chemical and physical data together, the κ-Kohler values for mass (κ_m) and volume are calculated (κ_v). The latter (κ_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 1: κ-Kohler theory for specific species, defined for volume and mass RH growth

Material	$\kappa_{v,i}$	Density (ρ_i/ρ_{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 κ_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 κ_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.

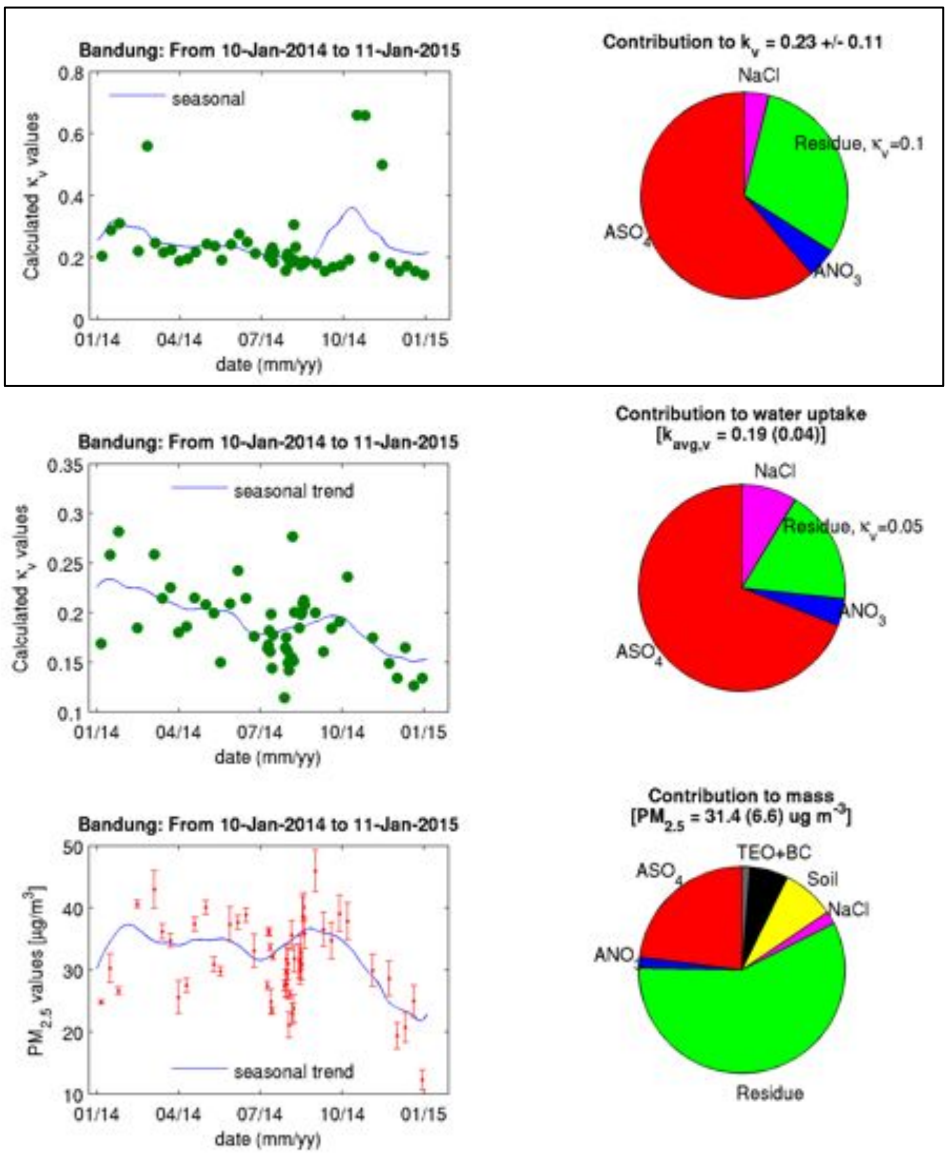

Figure 1: Top, outlined: Unfiltered (unscreened) κ_v values at Bandung site, Bottom: four panels of data, including filtered κ_v values (and $PM_{2.5}$ mass trends), resulting in a lower mean value.

Merging species κ_v results

The components of $\kappa_{v,tot}$ are obtained by linear combinations of mass measurements m_i, assumed densities ρ_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):

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

Table 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 0.18(0.09), 60 nm**	2008
California coast[2]	Various	**0.2 – 0.4, 150-250 nm**	

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

Mass fractions, per component can sometimes lead to suspecious results such that $\boldsymbol{\kappa_{v,tot}}$ > 0.6. The residue composition (associated with organics) is defined as in **section 9** 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 preweighed 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 bad values (possible reasons: too-high IC/ICP/EBC results, or too low PM)

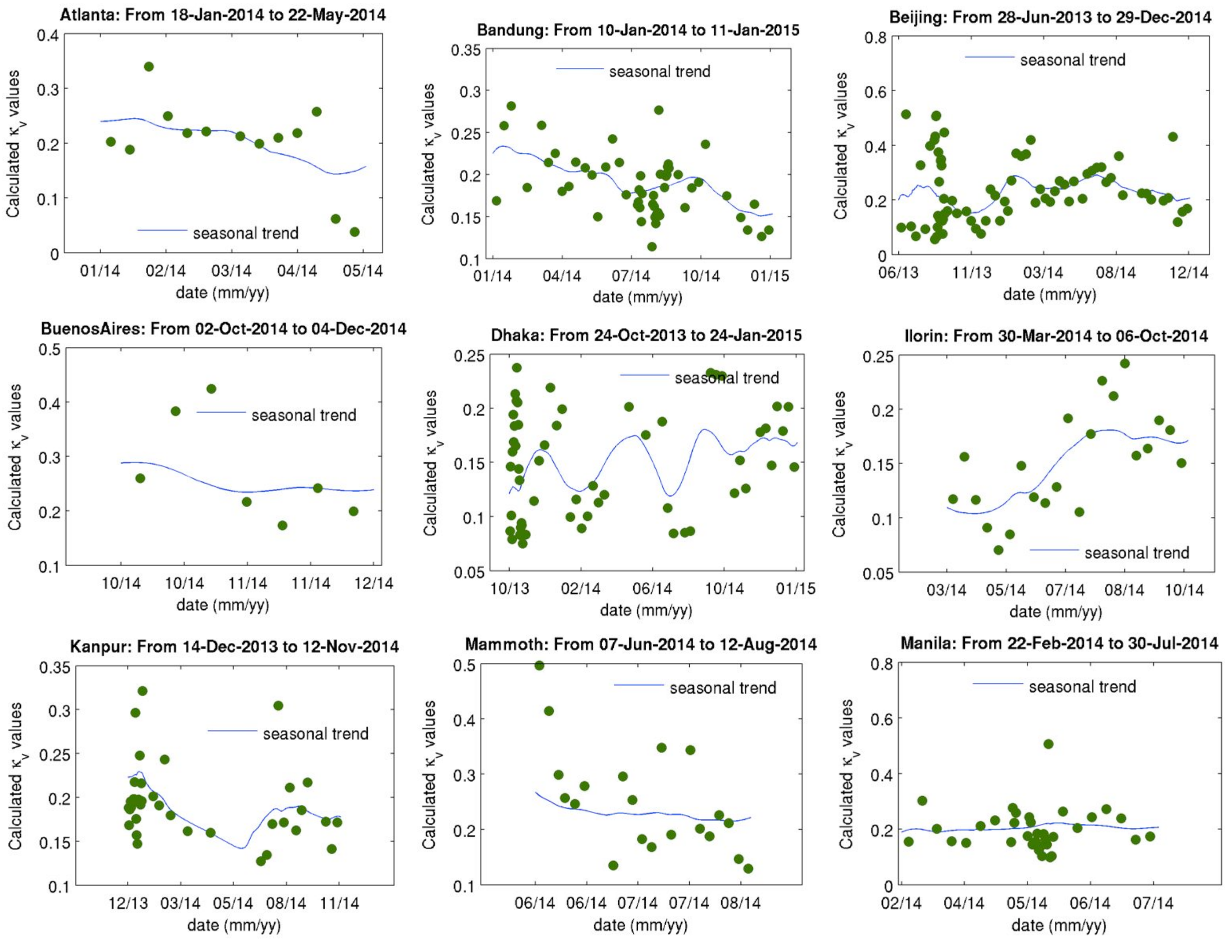

Figure 2: Seasonal trends in κ_v for nine SPARTAN sites. Suspicious growth factors (those where $\kappa_{v,tot} > 0.8$) have been checked and eliminated.

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

The seasonal κ_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 filer-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.

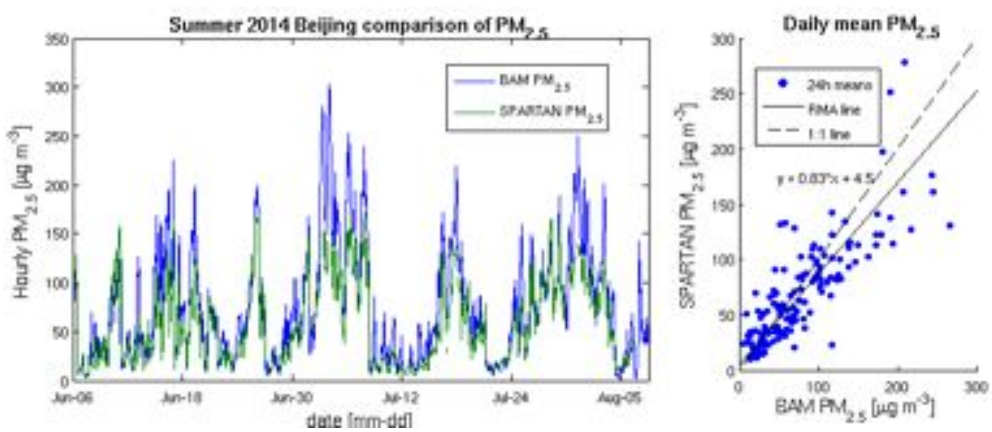

Figure 3: Reconstructed hourly $PM_{2.5}$ using the merged SPARTAN filter-nephelometer data. Plot is overlaid with a MetOne BAM-1020 at the US Beijing Embassy (15 km away). Reduced major axis (RMA) slope shows reconstructed hourly SPARTAN $PM_{2.5}$ underestimates BAM measurements by a factor 0.83 with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

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

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

The Matlab file columns 8 – 11 (BC, NH_4, Nitrate, and Sulfate) are held constant for given 9-day periods (though logged hourly as to fit file format). We do not interpolate changes in sub-composition of aerosol; by definition we assume κ_v is constant during a given 9-day sampling period.

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