

Associations between optical, physical and chemical properties of aerosols measured at ground-based networks

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1 Introduction

A large body of literature has shown that satellite-derived aerosol optical depth (AOD), typically retrieved at 550 nm wavelength, reliably correlates with mass-volume concentrations of fine mode particulate matter with aerodynamic diameter less than 2.5 μm (PM_{2.5}). Studies that have used satellite observations to generate PM_{2.5} have been instrumental for air pollution - health effects research. The associations between AOD and different chemical components of PM_{2.5} are lesser known. A handful of studies using the Multiangle Imaging SpectroRadiometer (MISR), an instrument onboard the NASA Terra satellite that provides observations of optical properties by particle type (size, shape, absorption), have provided evidence that different optical properties relate to different physical and chemical properties of particulate matter. Results have been somewhat inconsistent, showing differences depending on geographic area of analysis, optical components used, and statistical tools applied. The purpose of this analysis is to make a detailed examination of the statistical relationships between ground-level PM_{2.5} and PM_{2.5} chemical components (nitrate, sulfate, elemental carbon, organic carbon, dust) and optical measures of aerosols (e.g. aerosol optical depth, angstrom exponent).

AERONET Holben et al. (1998); Shin et al. (2018a, b, 2019)

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2 Methods

- The study encompasses the San Joaquin Valley region of central California (Figure 1). We leverage datasets available at four
10 sites - Bakersfield, Fresno, Modesto, and Visalia. At these sites there are co-located instruments from EPA’s chemical speciation network (CSN), EPA’s air quality system (AQS) and NASA’s AERONET network.

2.1 Data

- The CSN monitors are on a 1-in-3 or 1-in-6 day sampling schedule, providing $\text{PM}_{2.5}$ mass and component $\text{PM}_{2.5}$ concentrations of metals (e.g. Aluminium Al, Silicon Si, Calcium Ca, Titanium Ti, Iron Fe) obtained from X-ray fluorescence (XRF), ions
15 (nitrate NO_3^- and sulfate SO_4^{2-}) from ion chromatography, and carbons (organic OC and elemental EC) from thermal/optical analysis. To quantify dust we use the following equation Chow et al. (2015): $\text{dust} = 2.2\text{Al} + 2.49\text{Si} + 1.63\text{Ca} + 1.94\text{Ti} + 2.42\text{Fe}$

The AQS monitors provide daily concentrations of $\text{PM}_{2.5}$ mass by the EPA’s Federal Reference Method, which is the highest quality gravimetric measurement method used for regulatory purposes.

- AERONET sites are sunphotometers providing a “ground-up” measurement of aerosol optical properties at multiple wave-
20 lengths and have been used extensively to validate “top-down” satellite observations of related properties. Wavelength-specific AOD and angstrom exponents are the primary sunphotometer variables. Using quadratic log-log interpolation we calculated AOD 550 nm from AOD 440, 500, 675, 870 nm in log-log space. AOD at 550 nm is the most common wavelength retrieved from satellite instruments. A retrieval-based AERONET product, called the inversion product, provides an additional suite of aerosol properties that help distinguish size (fine, coarse effective radius), shape (asymmetry), and absorption. We excluded
25 sunphotometer and inversion variables that had a significant proportion of missing data (~90% missing). A list of the variables included in the analysis are shown in the Appendix. In a separate test we examine data from the SPARTAN site in Rehovot, Israel. The SPARTAN network provides data for $\text{PM}_{2.5}$ mass and speciation concentrations on an integrated 1 in 9 day sampling schedule, and is colocated with an AERONET site (We don’t have the speciation data for this site so we could only look at $\text{PM}_{2.5}$ for now).

2.2 Statistical methods

Prior to model building we examined a cluster-based correlation heat map (Figure 2), which provides the Pearson correlations between all pairs of AERONET variables grouped by a decision tree. To avoid collinearity in the regression models, we kept the most relevant of a group of variables that had a correlation coefficient > 0.9 . We then examined and picked a subset of variables connected at the mid-tier level of the tree to construct interactions. We fit simple linear regression models separately for PM2.5 mass, sulfate, nitrate, EC, OC, and dust with AOD 550 nm as the sole predictor variable. Multiple linear regression models were again fit separately for PM2.5 mass, sulfate, nitrate, EC, OC, and dust, but with the combined AERONET sunphotometer and inversion product as predictor variables and model selection was conducted using the “all possible subset method”. This method constructs models based on all combinations from 1 to k variable models. We select the best model from the combinations based on highest R², lowest RMSE, and Mallow’s Cp statistic that is close to k+1. Model selection for the Fresno and Bakersfield sites were examined separately and in combination in a “total CA” analysis, which combined data from Fresno, Bakersfield, Modesto, Visalia, and a special DRAGON campaign in late 2012-early 2013 over the region (8 co-located sites with PM2.5 mass).

All models were cross validated (CV) with 10-fold CV, and we report the CV R² and RMSE. Models were fit in R using the leaps() library.

3 Results

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```
sum <- 1 + 41
```

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6 Examples from the official template

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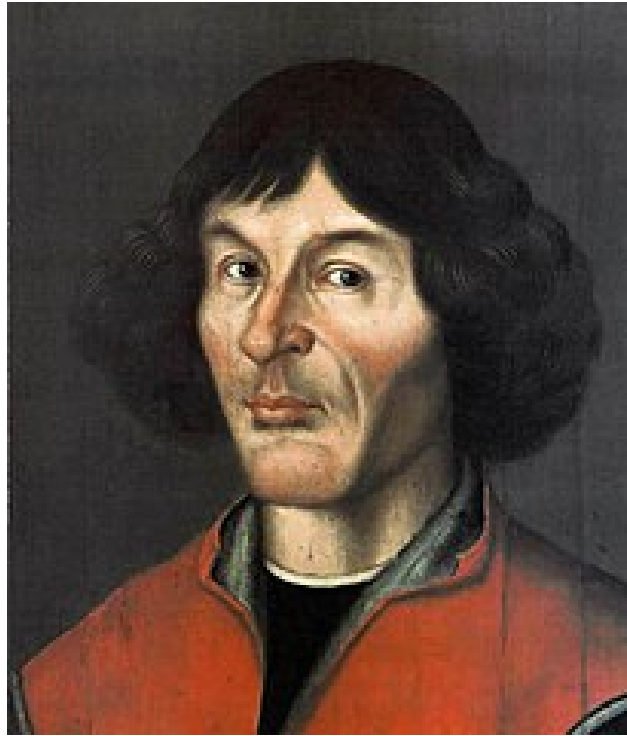


Figure 1. one column figure

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6.1.1 ONE-COLUMN FIGURES

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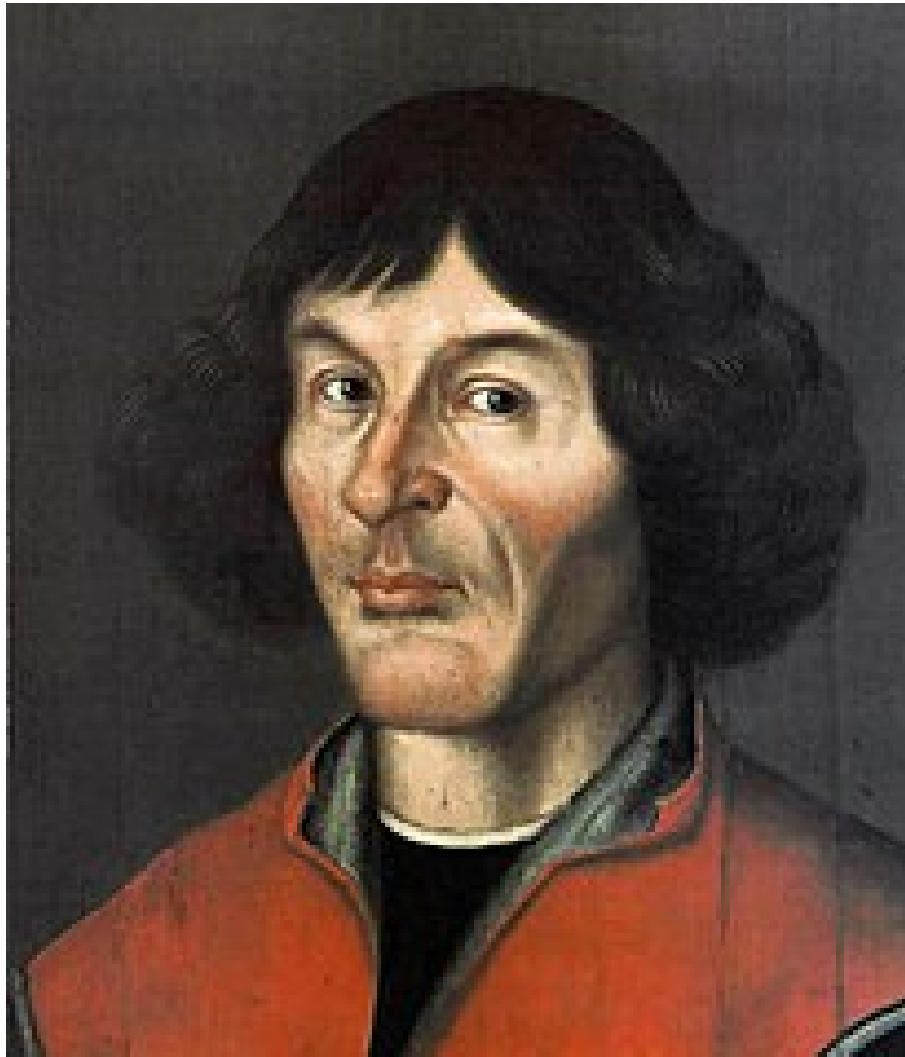


Figure 2. two column figure

Table 1. TEXT

a	b	c
1	2	3

Table Footnotes

Table 2. TEXT

a	b	c
1	2	3

Table footnotes

6.2.1 ONE-COLUMN TABLE

6.2.2 TWO-COLUMN TABLE

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6.4 EQUATIONS

6.4.1 Single-row equation

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$$1 \times 1 \cdot 1 = 42 \tag{1}$$

5 $A = \pi r^2$ (2)

$$x = \frac{2b \pm \sqrt{b^2 - 4ac}}{2c}. \tag{3}$$

6.4.2 Multiline equation

$$3 + 5 = 8 \tag{4}$$

$$3 + 5 = 8 \tag{5}$$

10 $3 + 5 = 8$ (6)

6.5 MATRICES

$$\begin{matrix} x & y & z \end{matrix}$$

$$\begin{matrix} x & y & z \end{matrix}$$

$$\begin{matrix} x & y & z \end{matrix}$$

6.6 ALGORITHM

If you want to use algorithms, you can either enable the required packages in the header (the default, see `algorithms: true`), or make sure yourself that the `LaTeX` packages `algorithms` and `algorithmicx` are installed so that `algorithm.sty` respectively `algorithmic.sty` can be loaded by the Copernicus template. Copernicus staff will remove all undesirable packages from your LaTeX source code, so please stick to using the header option, which only adds the two acceptable packages.

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20 For formulas embedded in the text, please use `\chem{ }`, e.g. $A \rightarrow B$.

The reaction environment creates labels including the letter R, i.e. (R1), (R2), etc.


```
i ← 10
if i ≥ 5 then
  i ← i − 1
else
  if i ≤ 3 then
    i ← i + 2
  end if
end if
```

- `\rightarrow` should be used for normal (one-way) chemical reactions
- `\rightleftharpoons` should be used for equilibria
- `\leftrightarrow` should be used for resonance structures



5



6.8 PHYSICAL UNITS

10 Please use `\unit{}` (allows to save the `math/$` environment) and apply the exponential notation, for example 3.14 km h^{-1} (using LaTeX mode: `\(3.14\,, \unit{...} \)`) or 0.872 ms^{-1} (using only `\unit{0.872\,, m\,, s^{-1}}`).

7 Conclusions

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Code and data availability. use this to add a statement when having data sets and software code available

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10 needs to be added in front of appendix figures `\appendixtables` needs to be added in front of appendix tables

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Author contributions. M. Franklin conducted analyses and wrote the manuscript. M. Sorek-Hamer conducted analyses and reviewed the manuscript. O. Kalashnikova and D. Diner conceptualized the study. D. Diner edited the manuscript.

Competing interests. The authors declare no competing interests.

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