Capabilities, Limitations Information
Gaps for Aerosols & AQ

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Factors Affecting the AOD-PM Relationship

Aerosol vertical profile:

- AOD is a remote-sensing optical measurement for the entire atmospheric column, whereas PM2.5 is an in-situ measurements of mass at the surface. \( \rightarrow \) **PM2.5 depends on aerosol vertical profile (including PBL or mixed layer height), while AOD corresponds to total aerosol amount in the atmospheric column**

Relative humidity (or water vapor):

- AOD value increases with the increase of RH, whereas PM2.5 usually refers to the aerosol dry mass \( \rightarrow \) **AOD corresponds to RH but PM2.5 does not**

Aerosol composition and particle size:

- Different aerosol species and size have different mass extinction efficiency \( \rightarrow \) even under dry conditions, **mass-to-extinction conversion depends on aerosol composition and particle size**
On hourly scale, AOD-PM2.5 are not well correlated for most of the time.

At all the four locations in multiple years, we found that only 13-22% days the daytime AOD and PM2.5 are correlated with $R \geq 0.7$, but 30-57% days when daytime AOD and PM2.5 are negatively correlated with $R < 0$. 
But on day-to-day basis, the variations of AOD and PM2.5 are mostly in-sync: Examples of hourly variations within a month.

Day-to-day co-variations of PM2.5 and AOD are driven mostly by the synoptic-scale meteorology. Geostationary observations increase the number of daily observations compared to the LEO satellite observation.
AOD varies more closely with column water vapor than with PM2.5 over the US – example at GSFC site

Daily correlation coefficients between AOD and PM2.5 in 2012, GSFC

- Total available days: 207
  - 16% (33): $R \geq 0.7$
  - 42% (86): $R < 0.0$

Daily correlation coefficients between AOD and column water vapor in 2012, GSFC

- Total available days: 220
  - 52% (114): $R \geq 0.7$
  - 20% (45): $R < 0.0$
However, the AOD-PM2.5 ratio changes with seasons; for the same PM2.5, AOD is higher in the summer and lower in the winter.
Inferring PM via Data Assimilation

- **Using data assimilation to infer PM concentrations from satellite data**
  - Multi-spectral AOD
  - (Polarized) reflectances
  - Lidar attenuated backscatter, extinction (HSRL)

- **State estimations vs emission estimation? Which? Both.**

- **Goals:**
  - Prediction: air-quality forecasts
  - Analysis: gridded Level 4 products
Aerosol Data Assimilation

- Several algorithms:
  - 3D & 4D variational, ensembled-based, hybrid variational/ensemble

- Even when PM data is not assimilated as an observable, each of these systems can produce PM gridded fields
  - Quality depends on model parameterizations, in particular PBL, transport and aerosol processes, details of chemical processes for secondary aerosols, etc
  - Aerosol optical properties
  - Emissions are critical

- Global or regional, take your pick (resolution vs. domain)
Challenges of Aerosol Data Assimilation

- **State representation:**
  - Multiple 3D concentrations
    - Mass
    - Number (modal schemes)
    - Bin sizes (sectional schemes)
  - Number of tracers: tens to hundreds

- **Emissions:**
  - Dynamic: dust, marine, biogenic aerosols
  - Remotely sensed: biomass burning
  - Inventories: anthropogenic

- **Observation operators**
  - Intrinsic aerosol optical properties needed for remotely sensed data:
    - Mass extinction coefficient, single scattering albedo, phase matrix
  - These are often poorly known but assumed to be known due to identifiability issues:

\[
\tau = \beta \cdot M
\]
Aerosol Observables

- **Aerosol Optical Depth (AOD)** is the most commonly available observable
  - Vertically integrated mass weighted by extinction coefficient, summed over multiple species: low observability
  - Multi-spectral AOD measurements

- **Radiance Assimilation:**
  - Vector scattering calculations needed for UV-VIS measurements are not cheap
  - Surface BRDF/BPDF characterization is a challenge

- **Surface PM 2.5**
  - Single level
  - Often plagued by representativeness

- **Lidars provide vertical profiles**
  - Spatially coverage is poor (pencil thin)
  - Attenuated backscatter again requires optical assumptions which are not directly measured
  - HSRL makes a more direct measurement of aerosol extinction
    - Ground base and airborne demonstrations
    - Being considered by NASA’s ACCP Decadal mission
Current (NRT)

AEROSOL PROGRAM OF RECORD
Aerosol Observing System

AERONET
- Ground-based Sun photometers globally distributed
- Direct measurements of multi-spectral Aerosol Optical Depth
- AERONET measurements are considered the reference observation and are generally used to perform validation

MODIS Instruments on AQUA and TERRA satellites
- TERRA (20 years) and AQUA (18 years) may last until 2023
- Temporal resolution: Daily coverage of the globe
- Spatial Resolution: 250m, 500m, 1000m depending on bands
- Several AOD algorithms available:
  - Dark target
  - Deep Blue
  - MAIAC

https://aeronet.gsfc.nasa.gov/
https://modis.gsfc.nasa.gov/
Aerosol Obs System: LEO Satellites

- **VIIRS onboard Suomi-NPP satellite:**
  - Launched in 2011
  - Temporal resolution: **Daily coverage of the globe**
  - Spatial Resolution: ~750m for aerosol retrieval
  - Several algorithms:
    - NOAA/NESDIS/STAR algorithm
    - NASA Deep Blue algorithm

- **TROPOMI onboard SENTINEL-5P**
  - Launched in 2017
  - Temporal resolution: **Daily coverage of the globe**
  - Spatial Resolution: ~7km
  - Spatial resolution is a challenge: cloud contamination
  - Reflectance measurements over the UV-SWIR spectral range

https://ncc.nesdis.noaa.gov/VIIRS/

http://www.tropomi.eu/
Aerosol Obs System: GEO satellites

- **Advanced Baseline Imager (ABI) onboard GOES satellites**
  - GOES-R or 16 launched in 2016
  - GOES-S or 17 launched in 2018
  - ABI has 16 spectral bands vs. 5 on the legacy GOES Imager
  - Spatial resolution: 500m to 2km
  - New products with higher accuracy and higher spatial resolution
  - Faster scan rate compared to the legacy GOES imager
    - Full disc image every 10 min (default mode)
    - More frequent observations (higher temporal resolution)
  - Several Algorithms:
    - NOAA Algorithm
    - NASA Dark Target (MODIS heritage)
Aerosol Obs System: GEO Satellites

- Advanced Himawari Imager (AHI) over ASIA on HIMAWARI satellite
  - Himawari-8 launched in 2014
  - AHI has 16 spectral bands
  - Spatial resolution: 500m to 2km
  - Temporal resolution:
    - Full disc image every 10 min
  - Several algorithms:
    - JAXA algorithm
    - NASA Dark Target (MODIS heritage)
    - Yonsei aerosol algorithm
    - etc

AHI RGB image
Emerging

AEROSOL PROGRAM OF RECORD
Geostationary (Virtual) Constellation

International constellation with a strong focus on air quality with TEMPO (U.S.), Sentinel-4 (Europe) and GEMS (Asia) → hourly but regional coverage

- **TEMPO**
  - UV/Vis spectrometer
  - Launch planned for 2022
  - Spatial resolution: 2 x 4.5 km²

- **Sentinel-4**
  - UV/Vis/NIR spectrometer
  - Launch planned for 2023
  - Spatial resolution: 8 x 8 km²

- **GEMS**
  - UV/Vis spectrometer
  - Launched on Feb 2020
  - Spatial resolution: 3.5 x 8 km² (over Seoul for aerosols)

- **METEOSAT 3rd generation**
  - Launch planned in 2021, 2025, 2029, 2032
  - Multipurpose VIS/IR radiometer with a spatial resolution from 500m to 2km
MAIA’s primary objective is to link exposure to different types of PM—mixtures of particles of various sizes, shapes, and compositions—with human health.

Globally distributed observations of major cities will provide large sample sizes to conduct statistically robust epidemiological studies.

Secondary targets will also be observed to enable other types of aerosol and cloud investigations.
Aerosol Obs System: LEO Satellites

- **OCI and MAPs on PACE**
  - Launch planned in Fall 2022
  - A spectrometer and a pair of multi-wavelength, multi-angle polarimeters that will measure aerosol characterization from UV to SWIR. UV channels allows retrieval of aerosol absorption
  - Global coverage every two days
  - Spatial resolution: 1 km

- **3MI on METOP-SG**
  - Launch planned in 2023
  - Multi-viewing Multi-channel Multi-polarisation Imager
  - Spatial resolution: 4km at nadir

- **EarthCARE**
  - Launch planned 2022
  - Lidar and a Multi-Spectral Imager (MSI)
  - Vertical profiles of aerosol extinction

- **ACCP**
  - Date planned: 2029
  - Polarimeter and a lidar
Scientific Machine Learning

Forward simulations
Advancing scientific discovery & engineering innovation

Optimization & inverse problems
Advancing estimation, design & control

Uncertainty quantification
Towards Predictive Science

Scientific machine learning
Towards Predictive Data Science

6 decades of Computational Science &...
Concluding Remarks

- To date, data-driven (supervised) ML algorithms has shown skill deriving PM from space observations + local ancillary information

- PM from models/DA systems at specific locations are plagued by errors of representativeness – even if models are perfect
  - Estimation at different scales

- For those regions that are well served by ground monitors, machine learning/statistical methods can be used to customize analysis and forecasts to specific stations
  - What else can we do when ground monitors are not available?
  - Universal MOS that do not depend on location? Doubtful, mainly because of emission uncertainties