Cost-effective real-time sensing of speciated fine particulate matter air pollution

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Program: FY21 R&TD Topics **Strategic Focus Area: Atmospheric composition and dynamics**

Objectives

The objective of this research is to explore a novel approach for cost-effective, real-time monitoring of speciated ambient fine particulate matter (PM). Partitioning airborne PM into chemical constituents is essential for source attribution, development of targeted regulatory controls, and assessment of health effects. Collecting particles on filter media and subsequent chemical analyses are costly and take many months. Reducing the costs, operational demands, and latencies associated with these data would be transformative not only for the responsible regulatory agencies but also for NASA, whose satellite-based particulate mapping instruments require surface measurements to convert retrieved aerosol parameters into PM data products.

Background

The primary innovations are: (1) using a comprehensive suite of ground-based, state-of-the-art optical scattering, absorption, and particle size measurements, gas-phase data, and meteorological information as real-time compositional PM predictors; and (2) training machine learning (ML) algorithms to transform daily-averaged measurements from a wide array of real-time sensors into PM speciation estimates (using co-located filter-based data collected over 24-hour integration periods as "truth") and ranking which variables are the most effective predictors.

Approach and Results

Real-time particle, trace gas, and meteorological data will train machine learning algorithms for estimating speciated PM2.5 concentrations, leveraging the following equipment installed (or to be installed) on the roof of JPL building 301 (Fig. 1):

Installed: ***Filter samplers:*** The AirPhoton SS5i-PM2.5 and the Aerosol Mass and Optical Depth (AMOD) collect PM on Teflon filters for subsequent chemical analysis. The SS5i is installed but operations were delayed due to COVID and a filter cartridge leak problem that has been now resolved; operations will begin in October 2021. AMOD operations began in May 2021. ***Optical particle counters (OPCs):*** The GRIMM EDM 164 classifies particles into 31 size bins from 0.25 µm-32 µm. The PurpleAir-II (PA) is a low-cost OPC that measures particle counts in 6 size bins from 0.3-10 µm. Both have been operating since November 2020, and each provides estimates of total PM2.5 mass concentrations. The PA has been compared with other PAs installed by JPL's Technical Facilities Management (TFM) Group, and raw data have been calibrated against the GRIMM (Fig. 2). ***Weather station:*** A Davis Vantage Pro weather station has been operating since March 2021 (Fig. 3), and provides temperature, RH, dew point, barometric pressure, solar radiation, rainfall, and wind speed/direction. ***Aethalometer:*** A multi-wavelength AethLabs MA350 black/brown carbon monitor has been operating since March 2021 (Fig. 4) and characterizes light-absorbing carbonaceous particles.

To be installed in early FY22 (delayed due to COVID): ***Submicron particle size distribution sensor:*** Caltech procured a scanning electrical mobility spectrometer (SEMS, Fig. 1) to provide particle number size distributions in the 10-500 nm size range. The bare instrument (without its final casing) was delivered by Aerosol Dynamics, Inc. to Caltech in September 2021. Tests are being run to challenge the instrument with ambient air (Fig. 5) and with known aerosols of varying sizes. Specifications for an air-conditioned case are being identified. ***Multi-wavelength polarimetric polar nephelometer:*** A custom nephelometer was purchased from AirPhoton to measure polarized aerosol scattering at 3 visible wavelengths and 6 scattering angles from 26º to 154º. The instrument (Fig. 1) will be used to retrieve aerosol extinction, size, shape, and complex refractive index. ***SO_2 and NO_2 sensors:*** An Ecotech SO_2 monitor and a 2B NO_2 absorbance monitor were loaned to JPL by the California Air Resources Board (CARB). Recently, Ambilabs LLC agreed to loan JPL a set of lower cost AQMesh SO_2 and NO_2 sensors. The AQMesh sensors will be co-located in 306-231A with the CARB instruments (which require air conditioning) for calibration, and then the AQMesh instruments will be installed on the roof of 301. Due to the pandemic, most data collection will occur FY22. ML algorithms will determine which parameters are most effective at predicting speciated PM. The ML code was written in R. Extreme gradient boosting models were trained using co-located sunphotometer aerosol measurements and EPA chemical speciation data in California. Shapely Additive Explanations ranked the predictor variables in the fitted models, providing a testbed to integrate the R&TD datasets in FY22.

Significance/Benefits to JPL and NASA

This work is aligned with the JPL Earth Science and Technology Directorate's focus on increasing our understanding of air quality, enabling better monitoring, improving our understanding of air quality events that impact human and ecosystem health, using JPL's unique expertise to benefit the nation and planet Earth, and aligning JPL research and missions with the Decadal Survey. The B301 air quality facility is within the planned Multi-Angle Imager for Aerosols (MAIA) target area over Los Angeles, and is currently observed weekly by the Multi-angle Imaging SpectroRadiometer (MISR). This R&TD work will open the door for follow-on proposals (e.g., ROSES) to evaluate using this technique with these or other satellite instruments for speciated PM mapping. A deployable, cost-effective sensor package would enable training the satellite PM retrievals with greater spatial coverage than would otherwise be possible. Discussions have been held with JPL's TFM Group regarding use of the B301 facility to calibrate their suite of PurpleAirs, which is used to assess air quality impacts on clean room operations.

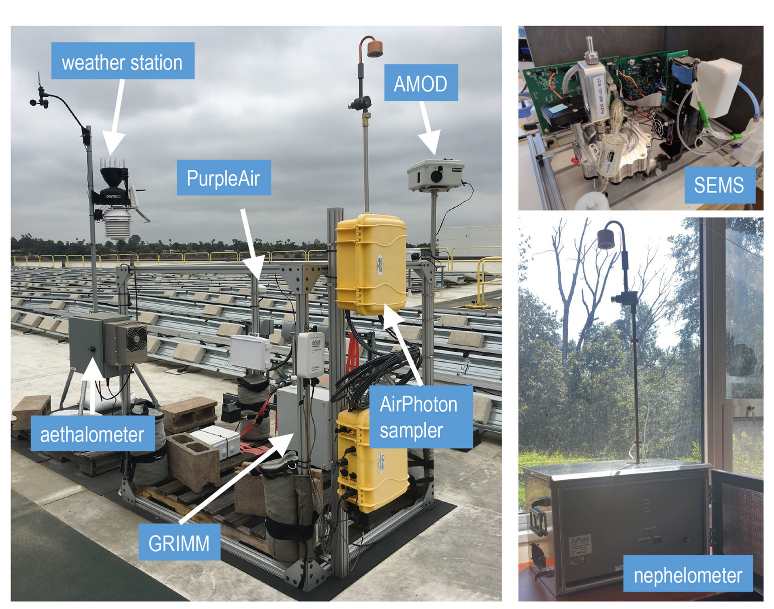
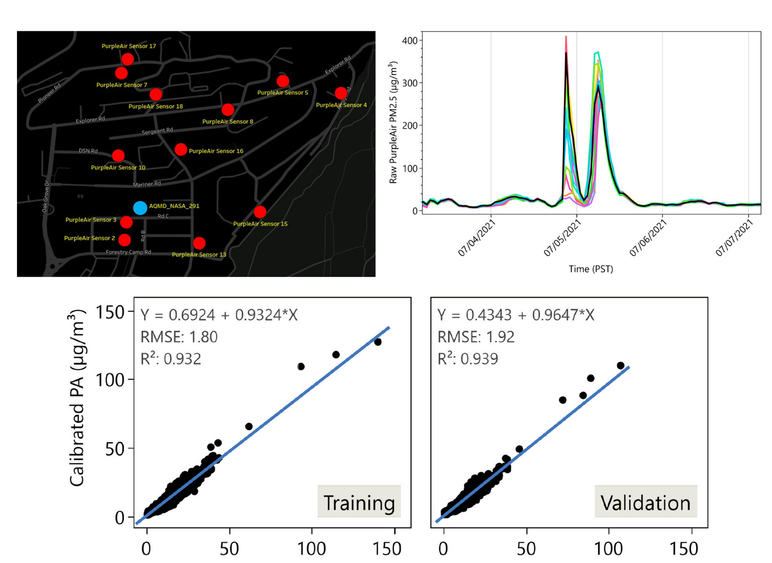


Figure 1. Left: Instruments installed on the roof of JPL building 301. Upper right: Photograph of the SEMS, without enclosure. Lower right: Photograph of the nephelometer.



$$PM_{2.5,calibrated} = a_0 + a_1 PM_{2.5,raw} + a_2 PM^2_{2.5,raw} + a_3 T + a_4 RH$$

Figure 2. Top left: In addition to the PurpleAir sensor on the roof of B301 (blue dot), JPL's TFM Group installed several PA sensors around the Lab (red dots). Top right: Under normal conditions, the PA sensors yield very similar concentrations. During PM peaks caused by July 4 fireworks, greater variability among the sensors is observed. Bottom: PurpleAir (PA) PM2.5 measurements were plotted against co-located GRIMM data and fitted to a regression model to correct the raw PA data for biases, using raw PA data, temperature (T), and relative humidity (RH) as independent variables. The model calibrates the PA data with R^2 >0.90 and ~1.9 µg/m³ mass concentration error.

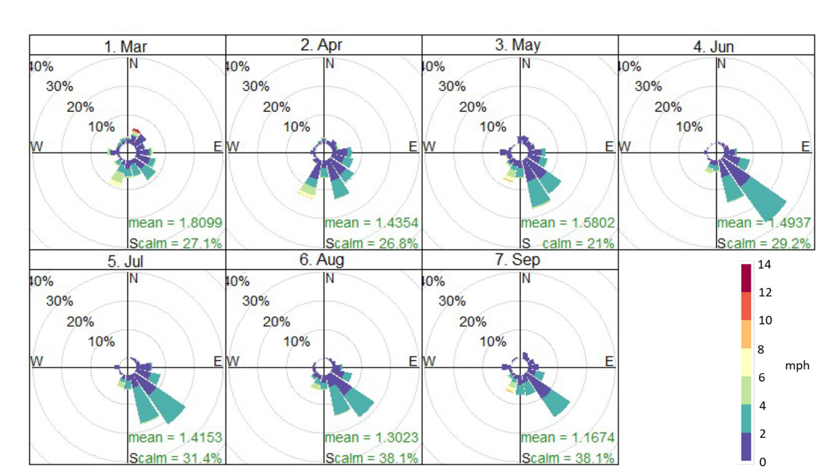


Figure 3. Wind measurements by the weather station indicate that wind mostly blows from S/SE and peaks in early afternoon around 1-2 pm.

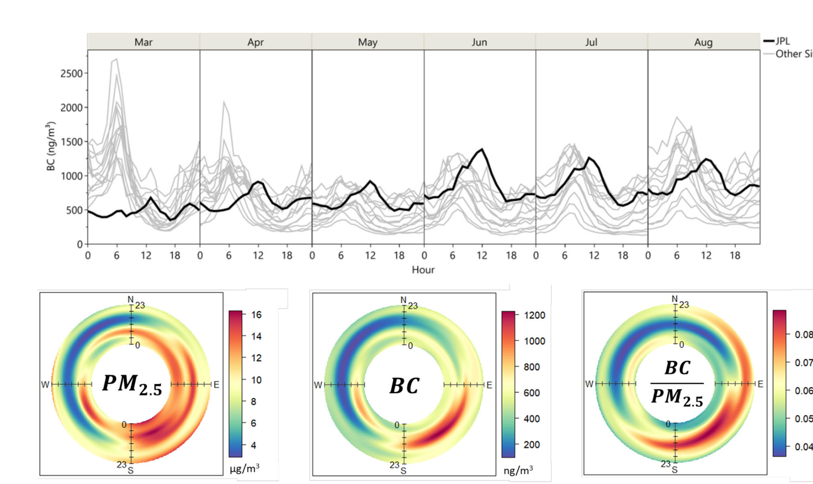


Figure 4. Top: Diurnal pattern of black carbon (BC) at JPL against other sites in the Los Angeles Basin. Most sites show a BC peak during morning rush hours. At JPL, BC peaks in mid-day, coincident with the peak of truck traffic on the nearby freeways. Bottom: These polar annulus plots show average PM2.5 and BC concentrations (and BC/PM2.5 ratio) by wind direction and hour of the day (represented by the 0-23 radial scale between the inner and outer rings). PM2.5 is impacted by winds from many directions, consistent with the regional nature of this pollutant. The midday BC peaks are mainly associated with SE winds, pointing to the intersection of the 210 and 134 freeways as a probable source.

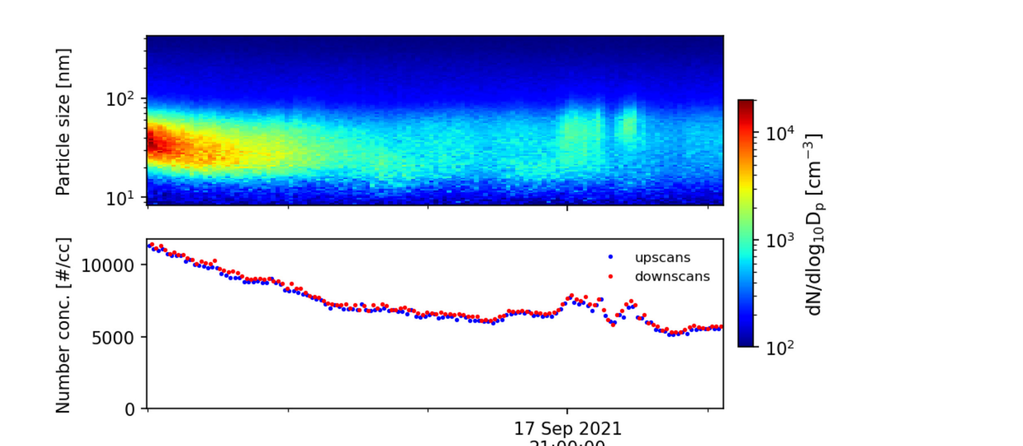


Figure 5. Time series of particle size distribution (top) and particle number concentration (bottom) in ambient air measured by the SEMS at Caltech on September 17, 2021. Each scan takes about 1 minute. For these initial unattended runs, peak voltage was limited, which limited the maximum detectable size. Laboratory tests with synthetic aerosols will be performed next to calibrate size sensitivity. The instrument is expected to detect particles up to 400 nm.

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