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## **Organic Aerosol Component (OACOMP) Value-Added Product**

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## **Acronyms and Abbreviations**

ACSM	aerosol chemical speciation monitor
AMS	aerosol mass spectrometer
AMU	atomic mass unit
BBOA	biomass burning organic aerosol
BNL	Brookhaven National Laboratory
CE	collection efficiencies
DMF	Data Management Facility
HR-AMS	high-resolution aerosol mass spectrometer
LOOA	less-oxidized organic aerosol
MOOA	more-oxidized organic aerosol
MAOS	Mobile Aerosol Observing System
NR	non-refractory
OA	organic aerosol
OACOMP	Organic Aerosol Component (value-added product)
PMF	positive matrix factorization
PNNL	Pacific Northwest National Laboratory
POA	primary organic aerosol
QA/QC	quality assurance/quality control
RIE	relative ionization efficiencies
SGP	Southern Great Plains
SNR	signal-to-noise ratio
SOA	secondary organic aerosol
VAP	value-added product
XDC	External Data Center

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## 1.0 Introduction

Organic aerosol (OA, i.e., the organic fraction of particles) accounts for 10–90% of the fine aerosol mass globally and is a key determinant of aerosol radiative forcing. But atmospheric OA is poorly characterized and its life cycle insufficiently represented in models. As a result, current models are unable to simulate OA concentrations and properties accurately. This deficiency represents a large source of uncertainty in quantification of aerosol effects and prediction of future climate change.

Evaluation and development of aerosol models require data products generated from field observations. Real-time, quantitative data acquired with aerosol mass spectrometers (AMS) (Canagaratna et al. 2007) are critical to this need. The AMS determines size-resolved concentrations of non-refractory (NR) species in submicrometer particles (PM<sub>1</sub>) with fast time resolution suitable for both ground-based and aircraft deployments. The high-resolution AMS (HR-AMS), which is equipped with a high mass resolution time-of-flight mass spectrometer, can be used to determine the elemental composition and oxidation degrees of OA (DeCarlo et al. 2006).

AMS instruments have been frequently used in DOE-supported field campaigns for characterizing aerosol composition and elucidating aerosol sources and processes. In addition, three aerosol chemical speciation monitors (ACSM) [Ng et al. 2011b] manufactured by Aerodyne Research were recently added to the ARM Climate Research Facility long-term monitoring sites (e.g., Southern Great Plains [SGP]) and the Mobile Aerosol Observing System (MAOS) for short-term (one year or less) deployments. The ACSM is a “mini” version of the AMS developed for continuous, low-maintenance operation. The ACSM measures mass concentrations and chemical composition for NR sub-micron aerosol particles, similar to the AMS. The reported detection limits for organic matter (OM), sulfate (SO<sub>4</sub>), nitrate (NO<sub>3</sub>), ammonium (NH<sub>4</sub>), and chloride (Cl) are 0.3, 0.4, 0.2, 0.5, and 0.2  $\mu\text{g m}^{-3}$  respectively [Ng et al., 2011b]. While the typical time resolution of AMS measurements is 2–5 minutes at fixed sites and 30 seconds or less on mobile-platforms (e.g., aircraft), the sampling interval of ACSM is generally 30 minutes.

Both the AMS and ACSM routinely report the concentrations of inorganic species (i.e., ammonium, sulfate, nitrate, and chloride) and total OM. Significantly improved returns in their aerosol chemistry data can be achieved via the development of a value-added product (VAP) of deriving OA components, called Organic Aerosol Components (OACOMP). OACOMP is primarily based on multivariate analysis of the measured organic mass spectral matrix. The key outputs of OACOMP are the concentration time series and the mass spectra of OA factors that are associated with distinct sources, formation and evolution processes, and physicochemical properties.

OACOMP is expected to be extremely useful for addressing the life cycle and properties of atmospheric OA, as many studies have already shown [e.g., Zhang et al. 2011]. Since the sum of all the OA factors adds up to ~100% of the total OA mass, the concentration results are particularly useful for (1) closure studies on aerosol optical and cloud condensation properties and (2) evaluating model predictions of sources and processes (e.g., primary emissions, secondary formation, biomass burning) that contribute to total OM. Estimates of the organic components in the atmosphere will help improve the representation of OAs in models that will subsequently reduce the uncertainties associated aerosol direct and indirect forcing in climate models. The long-term deployment of the ACSM instrument and the associated

OACOMP VAP provides unique data sets that will quantify seasonal and multi-year variations in aerosol composition, in contrast to field campaign data that are usually collected over a period of a few weeks.

## **2.0 Procedure**

The overall procedure of how OACOMP is generated is given in Figure 1. As part of the first step, the instrument mentor performs manual quality assurance/quality control (QA/QC) of the raw data every month that produces the A1 product stored in the ARM Data Management Facility (DMF). The second step produces the B1 product that is a netCDF file containing the original time series of aerosol composition, QA information, and other ancillary data needed to derive the OA components. The third step is the primary code that uses the mass spectra from the ACSM and a multivariate analysis technique to produce a time series of OA components and quality flags. This output is saved as a netCDF file, and a series of plots are routinely produced to help the developer determine whether the VAP is functioning properly. More detailed information on each of these steps is given in the following sections.

### **2.1 Step 1: Initial Quality Assurance of ACSM data**

1. The first step of initial quality assurance is to check the data diagnostics. The “Basic Diagnostics” tools (an Igor software window used by ACSM) provide access to the time series of all of the parameters recorded along with the raw mass spectral data by the ACSM’s data acquisition system. The diagnostics and tuning plots display many groups of parameters. These can be accessed using the data acquisition tools called “Value Explorer”. The diagnostics plots contain the time series of the following: “New Start”, “Inlet Pressure”, “Vaporizer temperature”, etc. The instrument mentor carefully examines each diagnostics plot, and problem data points, such as very low (<550 C) vaporizer temperatures, are marked and removed.
2. The second step is to apply corrections to the data and report the time series data matrices. This is one of most important aspects of data analysis and is approached by inputting careful instrument calibration results to ACSM “Review Batch”. The input for this step includes the species being analyzed (called spec name), the nitrate response factor (called masscalib\_nitrate), the relative ionization efficiencies (RIE), and the collection efficiencies (CE).
3. The last step for initial quality assurance uses “PMF Exporting tools” to prepare the positive matrix factorization (PMF) matrices. There are six steps included in the process:
  - a. initialize the matrices
  - b. after generating the error matrix, examine the error matrix and make sure the result is reasonable
  - c. down-weight weak variables to increase the error-to-signal ratio
  - d. examine the results of step 3 using a signal-to-noise ratio (SNR) graph
  - e. down-weight m/z 44 related m/z’s (which include m/z 44, 16, 17)



f. export the matrices.

For the down-weighting, as part of Step 3, a mean/median error ratio analysis is performed that calculates the mean error ratio

$$R\_mean_a = \frac{1}{N} \sum_t \frac{X_{t,a}}{E_{t,a}}$$

and the corresponding median error ratio  $R\_median_a$ . If  $R\_mean_a < 0.2$  or  $R\_median_a < 0.0$ , we call this a “bad m/z” and set  $X_{t,a} = X_{t,a}/20$  and  $E_{t,a} = mean_{t,a}(E_{t,a})$ . This forces the PMF to put very little signal in the mass spectrum for these species, which is essentially equivalent to removing them from the PMF altogether.

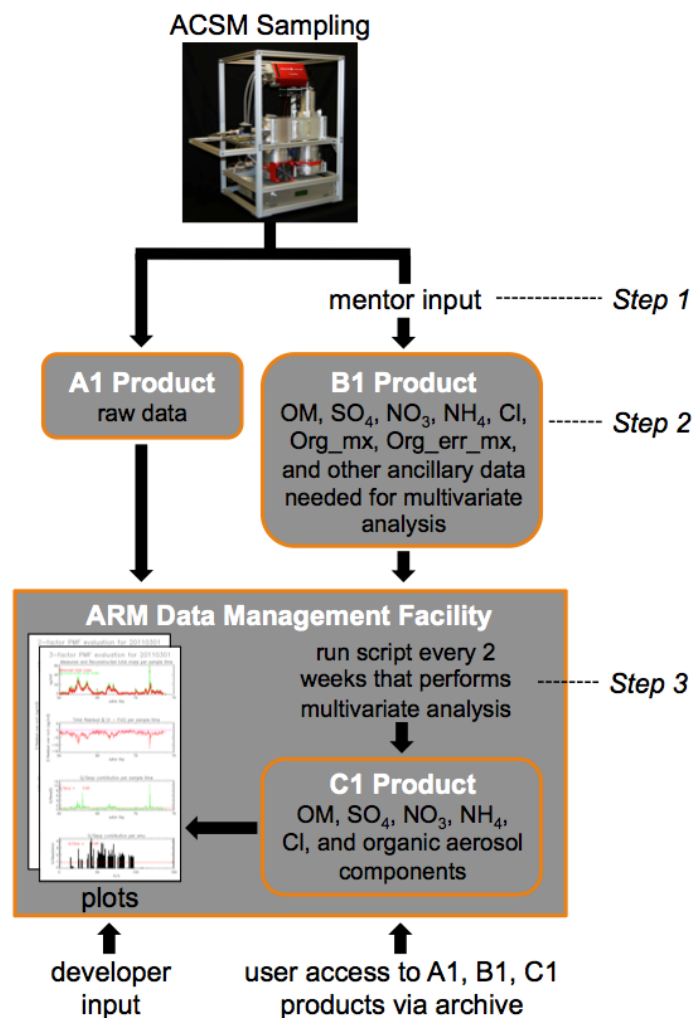
With the above three steps, the ACSM data with initial quality assurance are generated and ready for further analysis.

## 2.2 Step 2: B1 Product

Once per month, the instrument mentor performs quality control on the raw ACSM data, which include the time series of mass concentrations for the variables total organics, ammonium, sulfate, nitrate, and chloride. Two additional variables are added: the organic mass spectral matrix and organic mass spectral error matrix, which are indexed by time and atomic mass units (AMUs). The mentor packages these data up and ships it to the External Data Center (XDC) at Brookhaven National Laboratory (BNL).

Once at the XDC, the QCed data is unpackaged and split into daily files. These daily files are then transferred via File Transfer Protocol (FTP) to the DMF at Pacific Northwest National Laboratory (PNNL), where they are automatically processed by the ingest software. The ingest software takes the QCed data and produces daily netCDF files, which are then stored at the archive where they are made available to the user community.

At this time, the XDC to DMF process is semi-automated; however, the procedure is nearly ready to be fully automated.



**Figure 1.** Flowchart of the steps needed to derive OACOMP from ACSM data. Additional details of each step are given in the text.

## 2.3 Step 3: Determination of Organic Aerosol Components

### 2.3.1 Preprocessing

The input ACSM data are fairly noisy, so we take a series of preprocessing steps to remove spikes in the data, down-weight noisy samples, and fix other problem areas before we run the PMF analysis. In the following steps, the letter  $X$  stands for the org\_mx data matrix, the letter  $E$  stands for the org\_mx\_err error matrix, and the  $t$  and  $a$  represent the indices for time and species (m/z).

1. Zeros detected in the input error matrix are replaced with the maximum error value in that matrix.
2. Large spikes are removed from both org\_mx and org\_mx\_error matrices. If

$$\frac{X_{t,a}}{(X_{t-1,a} + X_{t+1,a})} > 3$$

we replace  $X_{t,a}$  with an average of the two bracketing points. The exact same process is applied to the `org_mx_err` matrix.

### **2.3.2 2PMF Calculations**

A PMF code is used to compute the OA components that require a sufficiently long time window to obtain reasonable results. The following steps are performed:

1. Run the PMF code for 2 and 3 factors, using `fpeak = 0.0`, and a fifteen-day rolling window centered on each day of analysis. Thus, 15 PMFs are produced that contain time series output that covers each day.
2.  $F[P][a]$  is mass spec matrix for factor P,  $G[t][P]$  is time series matrix for factor P. We normalize F and G such that  $\sum_a F_{P,a} = 1$  for each factor P. The normalization factor for G is the inverse of the normalization factor for F, as  $\mathbf{X} \sim \mathbf{GF}$ .

### **2.3.3 OACOMP Calculations**

1. Read in all 15 PMF files that span any part of each target day.
2. Because the factors can swap around (i.e., factor 1 may be more-oxidized organic aerosol [MOOOA] one run and less-oxidized organic aerosol [LOOOA] run the next), we have to identify each factor from each input PMF run with its physical process. So we loop over all 15 input PMFs and do the following:
  - a. First, see if there is any biomass burning. For each factor in the 3-factor PMF, calculate the ratio of the mass spec ( $F[P][a]$ ) for AMU 60 to the sum over all AMUs. If this ratio is  $> 0.008$  for some factor P, we know we have biomass burning, and we identify the biomass burning (BBOA) factor as the one with the largest such ratio. If there is biomass burning, we use the 3-factor PMFs for all additional calculations. If not, then use the 2-factor PMFs (and set the BBOA variables on output to zero).
  - b. To assign the two non-biomass factors, for each PMF run do a correlation for each non-biomass factor P' for each time series  $G[t][P']$  with the time series  $G0[t][P]$  from the previous PMF. The P' that correlates best with the previous P is identified as belonging to the same process.
3. We then average the 15 values for  $G[t][P]$  and the 15 values for  $F[P][a]$ , using the correct P for each run and for each process.
4. We then look at the averaged  $F[P][a44]$  for AMU 44. Whichever P has the largest mass spec value for AMU 44 is assigned the MOOA component, and the other one is the LOOA component.

### **2.3.4 QC the Output**

Flags are assigned to each data point to indicate the quality of the data. The following tests will flag the output data as "bad":

Bit 1: OACOMP unable to be performed, data filled with missing (this usually means that all the PMFs in the rolling 15-day window were either missing or failed some other test).

Bit 2: The output data value is below the "valid\_min" threshold (currently 0.0 for all output fields).

Bit 3: The output data value is above the "valid\_max" threshold (currently 300.0). (The purpose of valid\_min and valid\_max is to find processing bugs [which will often return nonsense data] more than it is to identify reasonable scientific values. Thus, these thresholds are very loose, and no data in our current test runs fail these tests.)

Bit 4: Three or fewer valid PMF runs were used for the day in question. This usually means there was a gap in ACSM data, but it could also indicate a lot of PMFs failing one of the tests below.

The following tests flag the data as "indeterminate", which means it can probably still be used, but the user should be aware of the following conditions:

Bit 5: Fewer than 15 valid PMF runs were used in our final averaging. This could mean a minor gap in the data, or it could mean some PMFs failed one of the tests below.

Bit 6: At least one PMF in our fifteen-day rolling window had at least one factor with the AMU 44 mass\_spec fraction greater than 0.3. Qi has indicated that this does not make physical sense, but sometimes the mathematics of the PMF return mass\_specs like this. Any PMF with this condition will not be used in our final average, so you will always see bit 5 set when bit 6 is set.

Bit 7: At least one PMF in our fifteen-day rolling window had a ratio of AMU 43 to AMU 44  $< 0.01$  or  $> 10$ . This has not happened in our initial test run, so it is possible that these limits should be tightened. Again, any such PMF would not be used in the final average.

Bit 8: Comparison of the sum of the time series factors with the ACSM total\_organics field. If the ratio of  $|ts\_factor\_sum/total\_organics| > 1.4$  or  $< 0.7$ , and the total\_organics is  $> 1.0 \mu\text{g m}^3$ , we set this bit.

Bit 9: If total\_organics is  $< 1.0 \mu\text{g m}^3$ , we cannot do a reasonable comparison with the sum of time series factors, because our ratio blows up. So we set this bit instead to indicate we cannot compare our calculations with total\_organics.

Bit 10: This simply indicates that there was no biomass burning for this day, so the BBOA fields are all set to 0.0 by definition. This is obviously not an error or problem, but is included to simply identify when it happened.

For the PMF tests (bits 6 and 7), all the values mass\_spec and time\_series values for all factors for a given day will have this condition set for the whole day, since they represent conditions of the whole analysis. Any PMF that failed this condition would not be used in the final averages, so if bits 6 or 7 are set you will always see bit 5 (and maybe bit 4) set as well. Bits 8 and 9 will be set on a time sample by sample basis, since they are tests on the final time series data.

### 3.0 Input Data

OACOMP requires only data from the ACSM instrument, and it uses the B1 data product. The B1 data product is available from the filename "sgpaosacsmcalC1.b1.yyymmdd.xxxxxx.cdf," where

- sgp stands for the Southern Great Plains site
- aos stands for the aerosol observing system
- acsm is the instrument
- yyyy is the year
- mm is the month
- dd is the day
- xxxxxx is the initial start time of the data.

The OACOMP VAP reads and uses the org\_mx (organic matrix array), qc\_org\_mx (QC for the organic matrix array), org\_mx\_err (organic error matrix), qc\_org\_mx\_err (QC for the organic error matrix), and total\_organics arrays from the file.

## 4.0 Output Data

The OACOMP VAP currently produces a single output file for each day, with organic aerosol components available at the same time intervals (~30-min increments) as the original ACSM data. The file names are “sgpoacomp1zhangC1.c1.yyyymmdd.xxxxxx.cdf,” where

- sgp stands for the Southern Great Plains site
- oacomp is the VAP name
- zhang is the VAP developer
- c1 is the type of data product (in this case, a derived one)
- the time variables in the filename are the same as for the B1 product.

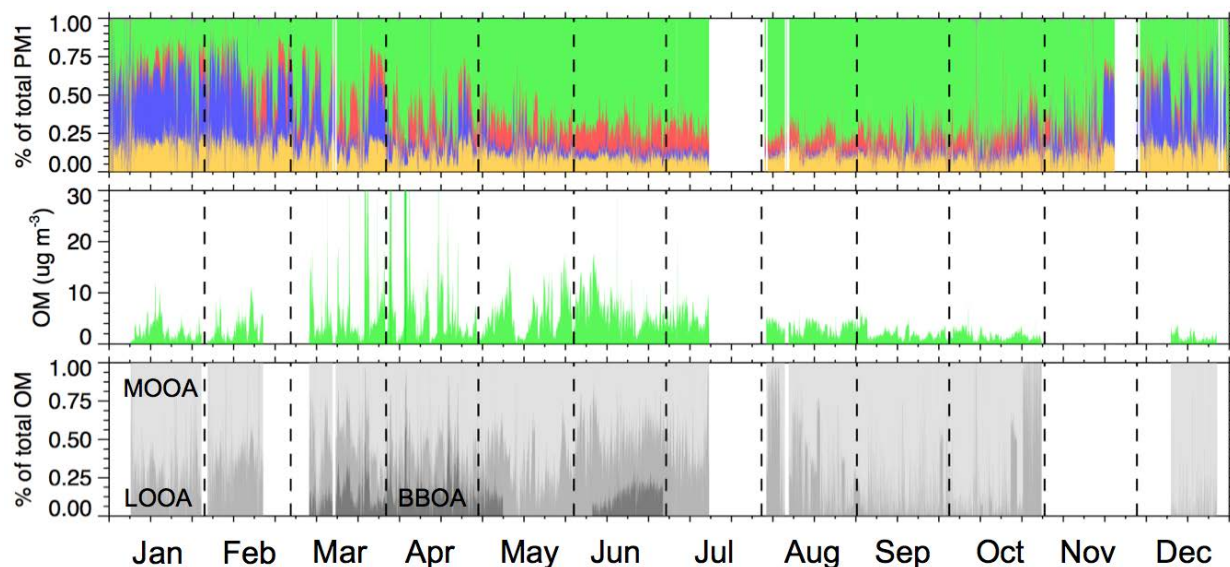
In addition to the time and location arrays in the file, the following arrays are included in the netCDF files:

- time\_series\_MOOOA: time series for more-oxidized oxygenated organic aerosol component
- qc\_time\_series\_MOOOA: quality control information for time\_series\_MOOOA
- mass\_spectrum\_MOOOA: mass spectra for more-oxidized oxygenated organic aerosol component
- qc\_mass\_spectrum\_MOOOA: quality control information for mass\_spectrum\_MOOOA
- time\_series\_LOOOA: time series for less-oxidized oxygenated organic aerosol component
- qc\_time\_series\_LOOOA: quality control information for time\_series\_LOOOA
- mass\_spectrum\_LOOOA: mass spectra for less-oxidized oxygenated organic aerosol component
- qc\_mass\_spectrum\_LOOOA: quality control information for mass\_spectrum\_LOOOA
- time\_series\_BBOA: time series for biomass burning organic aerosol component
- qc\_time\_series\_BBOA: quality control information for time\_series\_BBOA

- `mass_spectrum_BBOA`: mass spectra for biomass organic aerosol component, unnormalized
- `qc_mass_spectrum_BBOA`: quality control information for `mass_spectrum_BBOA`
- `time_series_MOOOA_std`: standard deviation of mass spectra for more-oxidized oxygenated organic aerosol component
- `mass_spectrum_MOOOA_std`: standard deviation of time series for less-oxidized oxygenated organic aerosol component
- `time_series_LOOOA_std`: standard deviation of mass spectra for less-oxidized oxygenated organic aerosol component
- `mass_spectrum_LOOOA_std`: standard deviation of time series for less-oxidized oxygenated organic aerosol component
- `time_series_BBOA_std`: standard deviation of mass spectra for biomass burning organic aerosol component
- `mass_spectrum_BBOA_std`: standard deviation of time series for biomass burning organic aerosol component
- `total_organics`: mass concentration time series of total organic
- `ammonium`: mass concentration time series of ammonium
- `sulfate`: mass concentration time series of sulfate
- `nitrate`: mass concentration time series of nitrate
- `chloride`: mass concentration time series of chloride

For a description of the quality control information, see Section 2.3.4. The time series of the ACSM data of organics, ammonium, sulfate, nitrate, and chloride are included as well for convenience.

An example of the output of the OACOMP VAP is shown in Figure 2. At the SGP site, organic aerosols are the dominant type of aerosol during the late spring, summer, and early fall. Secondary organic aerosols (LV-OOA and SV-OAA) are the largest component organic aerosols during most of the year. Biomass burning aerosols occur mostly during the late winter and spring months. Primary OAs are very small and cannot be detected by the ACSM. This is likely due to the fact that the SGP is located far from large emission sources of primary anthropogenic aerosols. The changing composition of aerosols during the year could alter the overall optical, hygroscopic, and cloud droplet nucleating properties of aerosols, which in turn influence direct and indirect radiative forcing. The data shown in Figure 2, coupled with other data at the SGP site, provide a mean of evaluating whether a climate model is predicting direct and indirect radiative forcing in the region for the right reasons.



**Figure 2.** Relative fraction of OM (green), sulfate (red), nitrate (blue), and ammonium (organ) measured by the ACSM at the SGP site from January to December 2011 (top panel), along the time series of OM (middle panel) and the relative fraction of organic aerosol components determined by the OACOMP VAP (bottom panel). LOOA, MOOA, and BBOA are less-oxidized organic aerosol, more-oxidized organic aerosol, and biomass burning organic aerosol, respectively.

## 5.0 Future Plans

The procedures developed for this VAP have also been used to determine OA components from an ACSM instrument deployed during the BNL intensive operational period (IOP) between June and August of 2011. A more sophisticated AMS instrument was deployed during the IOP so that the OA components from both systems could be directly compared. Similar OA components were derived from both systems, suggesting that the procedure developed for the ACSM is consistent with how organic components have been derived from AMS instruments over the past several years.

Nevertheless, there are two ongoing activities to ensure the quality of the OA components produced, including:

- Automation of initial data quality procedure: Currently, Step 1 (Figure 1) is not fully automated. It would be useful to automate all or part of the tasks associated with this step. The instrument mentor is currently investigating how this could be achieved, but it will likely depend on updates to the ACSM software from the manufacturer.
- Refinements to the preprocessing procedure: Modifications to the preprocessing procedures in Step 3 as described in Section 2.3 will be further tested and evaluated by the VAP developer, as more data are collected and analyzed.

To increase the value of the OACOMP to the scientific community, the following tasks are being pursued:

- Additional sites: The OACOMP VAP has only been implemented for the ACSM instrument deployed at the SGP site. ARM has a second ACSM, but it is not yet collecting data. Once the ACSM is deployed and running operationally, the OACOMP VAP can be applied to that datastream. Another ACSM instrument is part of the MAOS, and the OACOMP VAP can be run for future IOPs as needed. Currently, the ACSM as part of MAOS has been deployed during the 2012–2013 Two-Column Aerosol Project (TCAP) field campaign.
- Additional types of derived quantities: The mass spectra from the ACSM contain important information on the chemical composition and oxidation degree of the OA factors, which could be surrogates for hygroscopicity and/or volatility under certain circumstances that can also be compared with simulated values.
- Additional instrument inter-comparisons: The VAP may be further refined in the future to include comprehensive evaluation of the correlations among aerosol chemistry data from the AMS/ACSM and concurrent ARM measurements of aerosol radiative properties.

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