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Scanning Mobility Particle Sizer (SMPS)-Aerodynamic Particle Sizer (APS) Merged Size Distribution (mergedsmpsaps) Value-Added Product Report

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Acronyms and Abbreviations

AOS	Aerosol Observing System
APS	aerodynamic particle sizer
ARM	Atmospheric Radiation Measurement
CPC	condensation particle counter
DMA	differential mobility analyzer
DQR	Data Quality Report
QA	quality assurance
QC	quality control
netCDF	Network Common Data Form,
SGP	Southern Great Plains
SMPS	scanning mobility particle sizer
UTC	Coordinated Universal Time
VAP	value-added product

Contents

Figures

Tables

1.0 Introduction

Aerosol particles influence the Earth's radiation balance directly by absorbing and scattering light and indirectly by influencing cloud formation, properties, and lifetimes. Measurements of aerosol particle optical properties, mass loading, size distributions, microphysical properties, cloud formation properties, and chemical composition are important for understanding the aerosol life cycle and for validating earth system models that predict these quantities. The Atmospheric Radiation Measurement (ARM) user facility's Aerosol Observing System (AOS) is a highly instrumented platform designed to house instruments that measure many of these aerosol properties in situ. Currently, ARM operates at least four different instruments that measure a portion of the ambient aerosol size distribution. Most users are interested in the entire size distribution or a portion of the size distribution that extends across the measurement range of multiple instruments. However, merging these distributions is not trivial as the instruments employ different measurement principals and, in most cases, report data as a function of different representations of the aerosol diameter.

The scanning mobility particle sizer (SMPS) measures submicron particle size distributions by charging particles to their equilibrium distribution with an aerosol neutralizer, selecting a narrow size cut of particles according to their electric mobility diameter with a differential mobility analyzer (DMA), and then counting the particles with a condensation particle counter (CPC). The SMPS is mature, robust, commercial technology and is often thought of as a "gold standard" for measuring submicron aerosol particle size distributions. The SMPS instrument deployed in ARM's AOS measures particles with mobility diameter from 10.6 to 514 nm. The aerodynamic particle sizer (APS) measures sub- and super-micron particle size distributions by accelerating particles through an expansion nozzle and measuring the particle time of flight between two downstream laser beams. The particle time of flight is then converted to an aerodynamic diameter, with larger particles taking longer to transit the known distance between the laser beams. The APS instrument deployed in the AOS measures particles with aerodynamic diameters between 523 and 20,536 nm. Combining these measurements is desirable because the combined data covers most of the atmospherically relevant particle size range. It is important to note that the SMPS-measured mobility diameter and the APS-measured aerodynamic diameter are not equivalent and must be converted to a common diameter to merge the two size distributions.

This value-added product (VAP) merges size distributions measured by the SMPS and APS instruments using the method outlined by Beddows et al. (2010). The VAP iteratively shifts the APS diameter (within constraints) until a minimum residual is obtained between the SMPS and APS particle counts in the region where their measurements overlap. The APS aerodynamic diameter is then converted to a mobility diameter based on the effective density needed to perform this diameter shift. APS data are then re-binned into the native SMPS bin structure so that constant dlogDp is maintained across the entire size distribution. The VAP also calculates integrated number, surface area, and volume concentrations across the entire size distribution. Data are averaged to a 1-hour time resolution to improve signal at low particle counts and improve the VAP performance.

This VAP is for scientists who need a representation of the aerosol size distribution from approximately 10-20,000 nm mobility diameter. These data can be used for calculating aerosol scattering, estimating the impact of aerosol on cloud, calculating aerosol mass loading, and verifying aerosol-related quantities in models.

2.0 Algorithm and Methodology

The algorithm reproduces the processing described in Beddows et al. (2010), with some modifications described below. Note that the first APS bin with a 4-bin-per-decade spacing is removed from the data and not used in the algorithm or reported in the output data.

The algorithm steps are:

1. Load the b-1 level data for the SMPS and the APS.
2. Average the data to 1 hour.
3. Remove the first APS bin, i.e., the bin centered on 514 nm and with a 4-bin-per-decade bin width.
4. Identify the upper and lower limit of the APS size range based on the data in the APS "diameter_aerodynamic" coordinate.
5. Calculate the mobility diameter coordinate that the merged size distribution product will use. The merged diameter coordinate uses the same bin structure as the SMPS data but extrapolates out to larger sizes. To standardize the VAP, we use a fixed diameter range. The midpoint mobility diameters range from 10.555 to 20,909.234 nm. The midpoint diameter is calculated assuming a 64-bin-per-decade bin width and beginning with a theoretical bin centered at 514 nm (Equations 1 and 2). Note that due to rounding errors in the SMPS text file, there will be slight differences in the midpoint diameters reported in the SMPS and merged size files. These bins are theoretically identical. Contact the translator for more information regarding slight differences in midpoint diameters between the SMPS and merged size distribution data.

$$Dp(n+1) = Dp(n) * 10^{\frac{1}{64}} \tag{1}$$

$$Dp(n-1) = Dp(n)/10^{\frac{1}{64}} \tag{2}$$

6. Remove APS and SMPS size distributions that are filled with zero or nan and flag the data.
7. Calculate the APS and SMPS volume-weighted size distributions.
8. Fit a spline to each SMPS size distribution.
9. Enter the minimization subroutine, which determines the effective density that best aligns the APS data with the SMPS data where their measurements overlap. Steps in the minimization routine are:

   a. Convert the APS aerodynamic diameter to a mobility diameter using Equation 3. Note that we assume a shape factor of unity.

$$D_{mob} = {D_{aero}}\Big/{\sqrt{\rho_{eff}}} \tag{3}$$

   b. Calculate the number of bins where the SMPS and the adjusted APS size ranges overlap.

      i. If the number of overlapping bins is less than three, the routine returns an artificially high residual to force larger overlap of the two size distributions.

   c. Calculate the SMPS number and volume at the adjusted APS bin centers using the SMPS spline.

   d. Calculate the residual between the SMPS number (or volume) and the APS number (or volume). The residual is calculated as follows:

$$R = \sum(SMPS_{num} - APS_{num})^2 \tag{4}$$

   e. Minimize the residual calculated in Equation 3. Two different global solvers are used to minimize the residuals; the dual_annealing and differential_evolution solver both from the scipy.optimize library. In total, four solutions of effective density are calculated; one solution for each solver in both number and volume space.

10. Determine the effective density that will be used for the final conversion of aerodynamic diameter to mobility diameter. The effective density is chosen using the following routine:

    a. The four density solutions are rounded to the nearest tenth.

    b. If three or more density solutions are equal, this density is chosen.

    c. If fewer than three solutions are equal, the mean and standard deviation of the four solutions is calculated. The chosen density is the mean, provided all four solutions are within one standard deviation of the mean.

    d. If none of these conditions are met or the chosen density is outside the range 1.5-3, the data is flagged and no merged size distribution is calculated.

11. Convert each APS aerodynamic midpoint diameter to mobility diameter using Equation 3 and the effective density chosen.
12. Fit a spline to the APS size distribution in mobility diameter space.
13. Calculate the APS number concentration at each mobility midpoint diameter that corresponds to a diameter in the merged size mobility diameter coordinate using the spline from step 12.
14. Concatenate the APS data onto the end of the SMPS size distribution data. Note that if both APS and SMPS data exist in a particular bin, the SMPS data is chosen. APS data is only used for bins with no SMPS data.
15. Calculate total number concentration, surface area, and volume for the merged size distribution.
16. Apply QA/QC flags.

It is worth noting several important points regarding the merging algorithm described above. First, the minimum effective density that can be calculated by the algorithm is approximately 1.5 g/cm^3. This is due to the restriction that the APS and SMPS have a minimum of three size bins of overlap as described in step 9.b.i. Note also that the APS data are re-binned onto the SMPS bin structure. Integrated quantities (e.g., number, surface area, and volume) are calculate for the users, but should users want to calculate quantities over custom diameter ranges, note that bin spacing is 64 bins/decade and size distributions are reported in dN/dlogDp units.

Second, due to noise in the data several local minima in the solution space exist. We empirically observed more spread in the solutions when least-squares solvers were used to minimize the residuals. Therefore, we forego least-squares solvers in favor of the two global solvers listed in 9.f, which minimized the spread of the calculated effective density. Nevertheless, the algorithm is still prone to errors when data are of poor quality due to instrument issues or when the number of particles in the region where the SMPS and APS data overlap is very small. The APS and SMPS themselves also have the largest error in the region where their measurements overlap (i.e., the upper end of the scan range for the SMPS and the lower end of the measurement range for the APS). We strongly advise VAP users to pay close attention to the QA/QC flags and not use data that is flagged as bad. In the future, we plan to use a machine learning algorithm to further filter out problematic data. Extending the measurement range of the SMPS would also improve algorithm performance and is being discussed as a potential future change.

3.0 Input Data

The input data for this VAP come from the standard ARM b-1 level SMPS and APS netCDF files. The data are averaged onto a 1-hour time grid. If more than half of the average period is missing data from either instrument, the data are excluded from the VAP and a merged size distribution is not calculated. Data that are flagged as problematic in Data Quality Reports (DQRs) at the time of the VAP processing are also excluded. However, DQRs are often filed after the VAP data have been processed. In these cases, bad data may be included in the VAP. Users are encouraged to examine the DQRs for both the SMPS and APS data for the periods of interest.

The input file names are as follows:

XXXaossmpsYY.b1 and XXXaosapsYY.b1 where XXX is the is the site code and YY is the facility code. For example, sgpaosmpsE13.b1 represents SMPS data from the ARM Southern Great Plains (SGP) observatory and its E13 extended facility.

Variables retrieved from the input data streams and used by the VAP are listed in Table 1.

Table 1. Input variables used by the mergedsmpsaps VAP.

Variable name	Description and notes
aps_dN_dlogDp	Aerosol number size distribution for particles with aerodynamic diameters between 523 and 20,536 nm as measured by the APS. Units are $1/cm^3$.
aps_total_N_conc	Aerosol number concentration from the APS integrated size distribution. Units are $1/cm^3$.
smps_dN_dlogDp	Aerosol number size distribution for particles with mobility diameters between 10.6 and 514 nm as measured by the SMPS. Units are $1/cm^3$.
smps_total_N_conc	Aerosol number concentration from the SMPS integrated size distribution. Units are $1/cm^3$.

4.0 Output Data

The mergedsmpsaps VAP produces a single daily file named XXXmergedsmpsaps.YY.c1.YYYYMMDD.HHMMSS.nc where XXX is the site code, YY is the facility code, and YYYYMMDD.HHMMSS is the date and time.

Output variables unique to the mergedsmpsaps VAP are shown below in Table 2. The rest of the variable are passed through from the b-1 level files.

Table 2. Variables output by the mergedsmpsaps VAP.

Variable name	Description and notes
effective_density	Aerosol particle effective density with units g/cm^3. Calculated as described in §2.9 and §2.10.
qc_effective_density	Bit-packed quality checks for effective_density. The checks are: 1) Input smps_dN_dlogDp data have bad quality. 2) Input aps_dN_dlogDp data have bad quality. 3) Calculated effective density is less than a minimum threshold of 1.4 g/cm^3. 4) Calculated effective density is greater than a maximum threshold of 3.0 g/cm^3 The effective_density values are flagged as bad at timestamps where any of the four checks above fail. If checks 1) or 2) fail, the effective_density value is also set to missing.
effective_density_solution_strength	A flag variable that tracks the solution strength of the selected effective density. Calculated as described in §2.10.
merged_dN_dlogDp	Aerosol number size distribution for particles with merged mobility diameters between 10.6 and 20,536 nm as calculated by the VAP. Units are 1/cm^3.
qc_merged_dN_dlogDp	Bit-packed quality checks for merged_dN_dlogDp. The checks are: 1) Input smps_dN_dlogDp data have bad quality. 2) Input aps_dN_dlogDp data have bad quality. 3) The merged_total_N_conc exceeds the sum of smps_total_N_conc and aps_total_N_conc. 4) effective_density failed limit qc check (qc check 3 or 4) The merged_dN_dlogDp values are flagged as bad at timestamps where checks 1, 2, or 4 fail. If check 3) fails, the value is flagged as indeterminate. If checks 1) or 2) fail, the merged_dN_dlogDp value is set to missing.
merged_total_N_conc	Aerosol number concentration from the merged integrated size distribution. Units are 1/cm^3.
qc_merged_total_N_conc	Bit-packed quality checks for merged_total_N_conc. The checks are: 1) Input smps_dN_dlogDp data have bad quality. 2) Input aps_dN_dlogDp data have bad quality. 3) The merged_total_N_conc exceeds the sum of smps_total_N_conc and aps_total_N_conc. 4) effective_density failed limit qc check (qc check 3 or 4)

Variable name	Description and notes
	The merged_total_N_conc values are flagged as bad at timestamps where checks 1, 2, or 4 fail. If check 3) fails, the value is flagged as indeterminate. If checks 1) or 2) fail, the merged_total_N_conc value is set to missing.
merged_total_SA_conc	Aerosol surface area concentration from the merged integrated size distribution. Units are nm^2/cm^3.
qc_merged_total_SA_conc	Bit-packed quality checks for merged_total_SA_conc. The checks are: 1) Input smps_dN_dlogDp data have bad quality. 2) Input aps_dN_dlogDp data have bad quality. 3) The merged_total_N_conc exceeds the sum of smps_total_N_conc and aps_total_N_conc. 4) effective_density failed limit qc check (qc check 3 or 4) The merged_total_SA_conc values are flagged as bad at timestamps where checks 1, 2, or 4 fail. If check 3) fails, the value is flagged as indeterminate. If checks 1) or 2) fail, the merged_total_SA_conc value is set to missing.
merged_total_V_conc	Aerosol surface area concentration from the merged integrated size distribution. Units are nm^3/cm^3.
qc_merged_total_V_conc	Bit-packed quality checks for merged_total_V_conc. The checks are: 1) Input smps_dN_dlogDp data have bad quality. 2) Input aps_dN_dlogDp data have bad quality. 3) The merged_total_N_conc exceeds the sum of smps_total_N_conc and aps_total_N_conc. 4) effective_density failed limit qc check (qc check 3 or 4) The merged_total_V_conc values are flagged as bad at timestamps where checks 1, 2, or 4 fail. If check 3) fails, the value is flagged as indeterminate. If checks 1) or 2) fail, the merged_total_V_conc value is set to missing.
aps_dN_dlogDp	Aerosol number size distribution for particles with aerodynamic diameters between 523 and 20,536 nm as measured by the APS. Units are $1/cm^3$.
aps_total_N_conc	Aerosol number concentration from the APS integrated size distribution. Units are $1/cm^3$.
smps_dN_dlogDp	Aerosol number size distribution for particles with mobility diameters between 10.6 and 514 nm as measured by the SMPS. Units are $1/cm^3$.
smps_total_N_conc	Aerosol number concentration from the SMPS integrated size distribution. Units are $1/cm^3$.
DA_num_density	Effective density solution using the dual annealing number method described in 9.e. Not intended for general use.
DA_vol_density	Effective density solution using the dual annealing volume method described in 9.e. Not intended for general use.
DE_num_density	Effective density solution using the differential evolution number method described in 9.e. Not intended for general use.

Variable name	Description and notes
DE_vol_density	Effective density solution using the differential evolution volume method described in 9.e. Not intended for general use.
resid_DA_num	Residual from calculating effective density using the dual annealing number method described in 9.e. Not intended for general use.
resid_DA_vol	Residual from calculating effective density using the dual annealing volume method described in 9.e. Not intended for general use.
resid_DE_num	Residual from calculating effective density using the differential evolution number method described in 9.e. Not intended for general use.
resid_DE_vol	Residual from calculating effective density using the differential evolution volume method described in 9.e. Not intended for general use.

Figures 1 through 4 illustrate some of the algorithm variable outputs mentioned in Table 2.

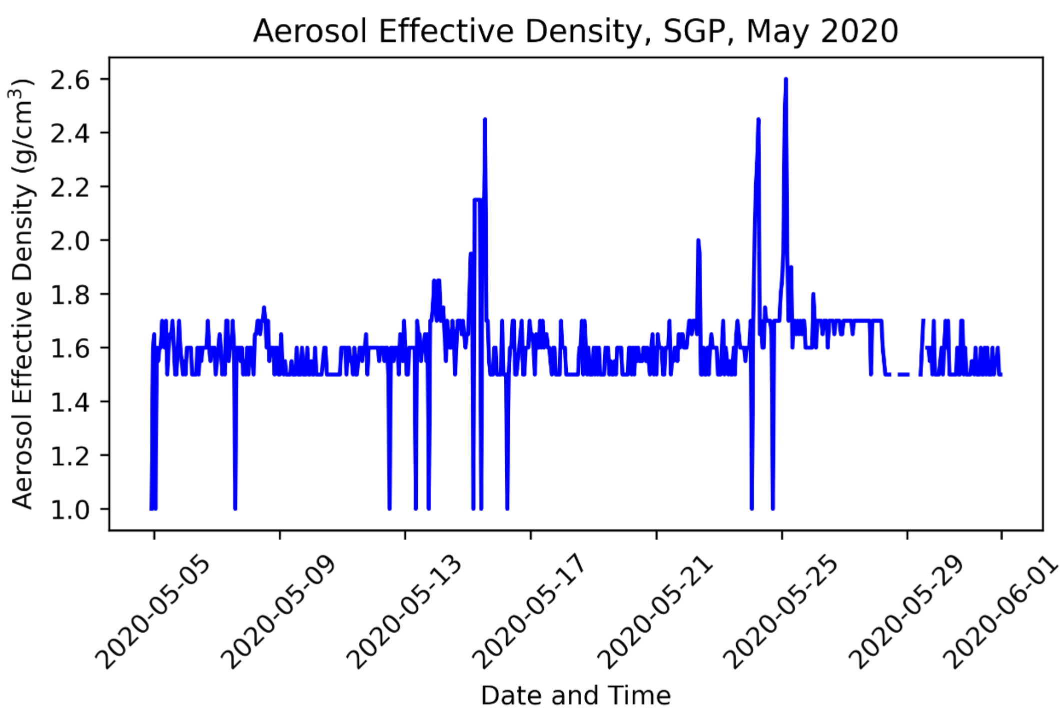

Figure 1. Aerosol effective density derived by the merged size distribution VAP algorithm.

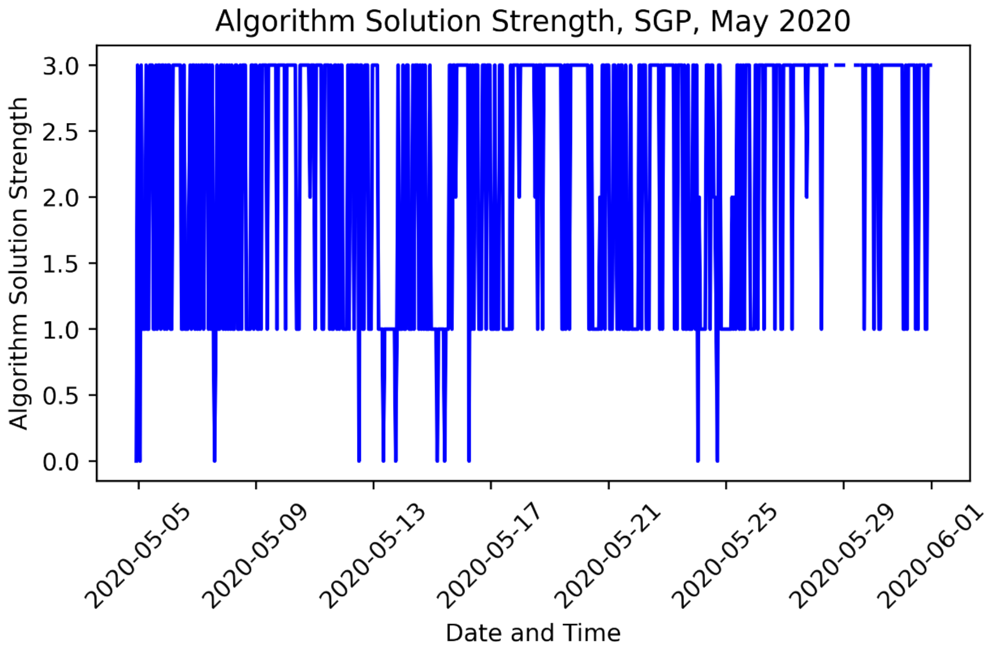

Figure 2. Algorithm solution strength for the aerosol effective density solution derived by the merged size distribution VAP algorithm. Higher solutions strength scores indicate higher confidence in the retrieved effective density and range from 0-3.

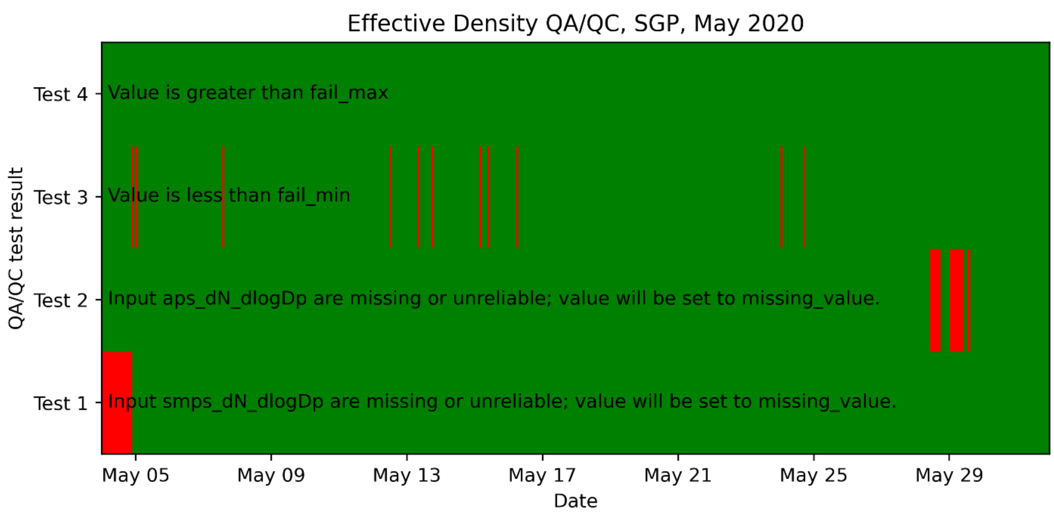

Figure 3. Results of the QA/QC tests for the effective_density variable. Red lines indicate data where the indicated QA/QC test has failed.

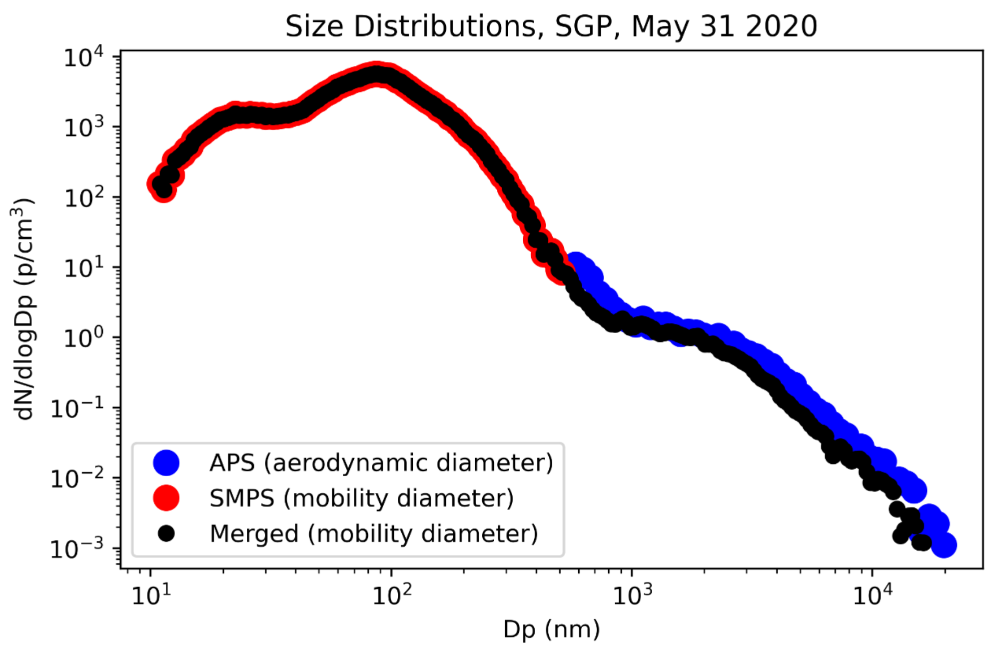

Figure 4. APS, SMPS, and merged size distributions across the entire size range covered by the merged distribution. Note that the APS size distribution is plotted as a function of aerodynamic diameter while the SMPS and merged size distributions are plotted as a function of mobility diameter.

5.0 Summary

The mergedsmpsaps VAP merges the size distribution from the ARM SMPS and APS, providing users with an aerosol size distribution from approximately 10-20,000 nm mobility diameter. Size distributions are presented in dN/dlogDp units. The merged size distribution is converted to a constant dNdlogDp spacing of 64 bins per decade. The VAP also calculates integrated number, surface area, and volume concentrations across the entire size distribution. Data are averaged to a 1-hour time resolution to improve signal at low particle counts and improve the VAP performance. The VAP produces daily netCDF files, each of which spans a 24-hour interval beginning at midnight (UTC). A several-day delay on processing is imposed to allow for input data to become fully available before the VAP is run.

This VAP is for scientists who need a representation of the aerosol size distribution across the size range measured by the SMPS and the APS instruments. These data can be used for calculating aerosol scattering, estimating the impact of aerosol on cloud, calculating aerosol mass loading, and verifying aerosol-related quantities in models.

6.0 References

Beddows, DCS, M Dall'osto, and RM Harrison. 2010. “An Enhanced Procedure for the Merging of Atmospheric Particle Size Distribution Data Measured Using Electrical Mobility and Time-of-Flight Analysers.” *Aerosol Science and Technology* 44(11): 930–938, https://doi.org/10.1080/02786826.2010.502159

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