ATom: Nucleation Mode Aerosol Size Spectrometer Calibration and Performance Data

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Documentation Revision Date: 2018-09-18

Data Set Version: 1

Summary

This dataset provides extensive calibration and in-flight performance data for two nucleation mode aerosol size spectrometer (NMASS) instruments utilized in the NASA Atmospheric Tomography Mission (ATom). Each NMASS has five condensation particle counters (CPCs) that detect particles above a different minimum size, determined by the maximum vapor supersaturation encountered by the particles. Operated in parallel, the CPCs provide continuous concentrations of particles in different cumulative size classes between 3 and 60 nm. Knowing the response function of each CPC, numerical inversion techniques were applied to recover size distributions from the continuous concentrations. Data provided include: NMASS counting efficiencies and diameters of calibration aerosols, inverted particle size distributions; comparisons of NMASS and Scanning Mobility Particle Sizer (SMPS) results; and performance at flows, temperatures, and pressures measured by both NMASSs and comparison with Ultra-High Sensitivity Aerosol Spectrometer (UHSAS) concentrations collected on board the NASA DC-8 aircraft during an ATom flight in February 2017.

Laboratory calibrations with a range of particle sizes and compositions show repeatability of the response function of the instrument to within 5-8% and no sensitivity in sizing performance to particle composition. Particle number, surface area, and volume concentrations from the data inversion are determined to be better than 20% for typical particle size distributions.

This dataset supports the publication in Atmos. Meas. Tech. by Williamson et al. (2018), which provides the results of NMASS calibration tests.

There are 12 data files in comma-separated format (.csv) with this dataset.

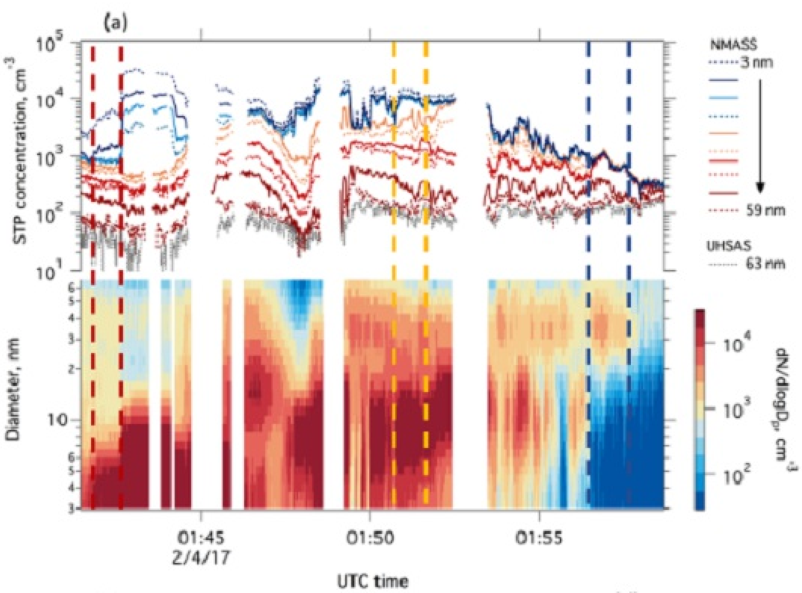

Figure 1. Example data taken on the NASA DC-8 aircraft during ATom in February 2017. The top of panel shows the STP number concentrations measured by each channel of both NMASSs, as well as the total concentration of particles from 63 to 1000 nm measured by the UHSAS. The bottom of panel shows the inverted size distribution. Figure 12 from Williamson et al. (2018).

Citation

Williamson, C.J., A. Kupc, J.C. Wilson, D.W. Gesler, J.M. Reeves, F. Erdesz, R.J. Mclaughlin, and C.A. Brock. 2018. ATom: Nucleation Mode Aerosol Size Spectrometer Calibration and Performance Data. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1607

Table of Contents

1. Data Set Overview

This dataset provides extensive calibration and in-flight performance data for two nucleation mode aerosol size spectrometer (NMASS) instruments utilized in the NASA Atmospheric Tomography Mission (ATom). Each NMASS has five condensation particle counters (CPCs) that detect particles above a different minimum size, determined by the maximum vapor supersaturation encountered by the particles. Operated in parallel, the CPCs provide continuous concentrations of particles in different cumulative size classes between 3 and 60 nm. Knowing the response function of each CPC, numerical inversion techniques were applied to recover size distributions from the continuous concentrations. Data provided include: NMASS counting efficiencies and diameters of calibration aerosols, inverted particle size distributions; comparisons of NMASS and Scanning Mobility Particle Sizer (SMPS) results; and performance at flows, temperatures, and pressures measured by both NMASSs and comparison with Ultra-High Sensitivity Aerosol Spectrometer (UHSAS) concentrations collected on board the NASA DC-8 aircraft during an ATom flight in February 2017.

Laboratory calibrations with a range of particle sizes and compositions show repeatability of the response function of the instrument to within 5-8% and no sensitivity in sizing performance to particle composition. Particle number, surface area, and volume concentrations from the data inversion are determined to be better than 20% for typical particle size distributions.

Project: Atmospheric Tomography Mission (ATom)

The Atmospheric Tomography Mission (ATom) is a NASA Earth Venture Suborbital-2 mission. It will study the impact of human-produced air pollution on greenhouse gases and on chemically reactive gases in the atmosphere. ATom deploys an extensive gas and aerosol payload on the NASA DC-8 aircraft for systematic, global-scale sampling of the atmosphere, profiling continuously from 0.2 to 12 km altitude. Flights will occur in each of 4 seasons over a 4-year period.

Related Publication:

This dataset supports the publication in Atmos. Meas. Tech. by Williamson et al. (2018), which provides the results of NMASS calibration tests.

Williamson, C., Kupc, A., Wilson, J., Gesler, D. W., Reeves, J. M., Erdesz, F., McLaughlin, R., and Brock, C. A. 2018. Fast time response measurements of particle size distributions in the 30-60 nm size range with the nucleation mode aerosol size spectrometer, Atmos. Meas. Tech., 11, 3491-3509, https://doi.org/10.5194/amt-11-3491-2018

Acknowledgements:

This research was funded by NASA grant number NNH15AB12I.

2. Data Characteristics

Spatial Coverage: These data are mostly laboratory-derived; the spatial and temporal coverage reflect the ATom-1 and ATom-2 flights. Flights begin in California, fly north to the western Arctic, south to the South Pacific, east to the southern Atlantic, north to Greenland, and return to California across central North America.

Spatial Resolution: NA

Temporal Coverage: Periodic flights occurred during each deployment. ATom-1 was from July 29, 2016 - August 23, 2016 and ATom-2 was from January 26, 2017 - February 21, 2017.

Temporal Resolution: NA

Study area: Bounding box for the ATom flights (All latitude and longitude given in decimal degrees)

Site	Westernmost Longitude	Easternmost Longitude	Northernmost Latitude	Southernmost Latitude
ATom -1 and 2 flights	-180	180	80.52	-65.33

Data File Information

These are calibration data for two nucleation mode aerosol size spectrometer (NMASS) instruments utilized in the NASA ATom mission.

User Notes:

- CH = spectrometer channels
- CPC = condensation particle counters
- Where appropriate for generation of the respective figure, data not applicable are represented as NA or NaN, or the data cells maybe blank.
- The Values of 0 and 1 are true values.

The file names contain **_figX** to indicate a corresponding figure in the associated publication of Williamson et al., 2018.

Table 1. Data files and descriptions

File name	Description

NMASS_diameter_d50_detection_fig3.csv	Calculated diameters using n-butanol (butanol), Fluorinet 43 (FC-43), and diethylene glycol (diethglycol) as the working fluids
NMASS_ efficiency_uncertainty_fig5.csv	Counting efficiency of the two NMASSes in the settings used for the ATom mission. The calibration was done using particles generated by ozonolysis of limonene. In the variable names below, NM**X** refers to NMASS 1 and NMASS 2, and cpc**Y** refers to CPCs 1-5
NMASS1_diameter_efficiency_uncert_amsul_fig6.csv	Counting efficiency and uncertainties of NMASS 1 using atomized ammonium sulphate (amsul) particles
NMASS1-2_efficiency_lim_amsul_dos_fig7.csv	NMASS 1, CPCs 4 and 5, and NMASS 2 CPC 5 particle diameter and counting efficiencies and uncertainties for limonene (lim) ozonolysis products, atomized ammonium sulphate (amsul), and dioctyl sebacate (dos)
NMASS2_cpc5_calibration_ct_efficiency_fig8.csv	Counting efficiency and particle diameters for three calibrations for NMASS 2 CPC 5
SMPS_NMASS_inversions_particle_size_fig10.csv	Inverted particle size distributions from NMASS and Scanning Mobility Particle Sizer (SMPS)
NMass_flow_temp_pressure_fig11.csv	CPC flows, CPC temperatures, and instrument pressures measured by both NMASSes (NMx) over the total course of an ATom flight
NMASS1-2_UHSAS_STP_particle_conc_fig12a.csv	The data are the STP number concentrations (particles per cc) measured by each channel of both NMASS 1 and 2, as well as the total concentration of particles from 63-1000 nm measured by the UHSAS used to constrain the inversion and the ambient pressure. The data used were from the NASA DC-8 aircraft during the ATom campaign in February 2017
NMASS1-2_inverted_1minute_diam_fig12lowpanel_logd.csv	Inverted size distributions (dN/dlogDp cm^-3) by corresponding time and diameters (nm). The data used for the inversion were from the NASA DC-8 aircraft during ATom in February 2017
cpc_conc_dma_diameter_150_figS3.csv	CPC concentration at each Differential Mobility Analyzer (DMA) diameter, particle diameters selected by a DMA and uncertainties
inversion_diameter_lognormal_figS2.csv	Inversion diameter, size distributions, and fitted size distributions

Table 2. Variables in the file *NMASS_diameter_d50_detection_fig3.csv*

Column	Units/format	Description
deltaT	k	Temperature difference between CPC saturator and condenser for theoretical calculations
particle_diam_butanol	nm	Calculated activation diameter using butanol as the working fluid
particle_diam_diethglycol	nm	Calculated activation diameter using diethylene glycol as the working fluid
particle_diam_fc43	nm	Calculated activation diameter using Fluorinert FC-43 as the working fluid
deltaT_d50	k	Temperature difference between CPC saturator and condenser for measured points
d50	nm	Diameter at which the CPC counts 50% of the particles

Table 3. Variables in the file *NMASS_efficiency_uncertainty_fig5.csv*

Note that cpcY represents CPCs where Y is 1-5.

Column	Units/format	Description
NMX_diam_particles	nm	Diameter of particles being measured in the calibration of NMASS 1 and NMASS2
NMX_uncert_diam	nm	Uncertainty of the particle diameter, NMASS 1 and NMASS2
NMX_cpcY_efficiency	ratio	Efficiency with which NMASS 1 and NMASS 2 CPCs 1-5 count particles of the given diameter.
NMX_cpcY_efficiency_uncert	ratio	Uncertainties of the counting efficiency data above for CPCs 1-5, NMASS 1 and NMASS 2
fit_diam_cpc_efficiency		Diameter correlated to the fitted CPC efficiency
NMX_cpcY_fit		Fitted efficiency for NMASS 1 and NMASS 2, CPCs 1-5

Table 4. Variables in the file *NMASS1_diameter_efficiency_uncert_amsul_fig6.csv*

Columns	Unit/formats	Description
diam_particle	nm	Diameter of particles being measured in the calibration
diam_uncert	nm	Uncertainty of the particle diameter
cpcx_efficiency	ratio	Efficiency with which CPC x counts particles of the given diameter where cpcx= CPCs 1-5

cpcx_efficiency_uncer	ratio	Uncertainty of the efficiency data above for each CPC, 1-5

Table 5. Variables in the file *NMASS1-2_efficiency_lim_amsul_dos_fig7.csv*

User note: Figure 7 in Williamson et al. 2018 shows data for NMASS 1, channel 3. This data file includes data for NMASS 1 and 2 but only includes data for channels 4 and 5.

Column	Units/format	Description
particle_diam_dos	nm	Diameter of dioctyl sebocate (dos) particles
particle_diam_uncert_dos	nm	Dos particle diameter uncertainty
NM1_ch4_dos	ratio	Counting efficiency of NMASS 1 CH 4 dos particles
NM1_ch5_dos	ratio	Counting efficiency of NMASS 1 CH 5 dos particles
NM2_ch5_dos	ratio	Counting efficiency of NMASS 2 CH 5 dos particles
NM1_ch4_dos_uncert	ratio	Uncertainty of the efficiency with which NMASS 1 CH 4 counts dos particles of the given diameter
NM1_ch5_dos_uncert	ratio	Uncertainty of the efficiency with which NMASS 1 CH 5 counts dos particles of the given diameter
NM2_ch5_dos_uncert	ratio	Uncertainty of the efficiency with which NMASS 2 CH 5 counts dos particles of the given diameter
particle_diam_amsul	nm	Diameter of ammonium sulphate (amsul) particles
particle_diam_amsul_uncert	nm	Amsul particle diameter uncertainty
NM1_ch4_amsul	ratio	Counting efficiency of NMASS 1 CH 4 amsul particles
NM1_ch5_amsul	ratio	Counting efficiency of NMASS 1 CH 5 amsul particles
NM2_ch5_amsul	ratio	Counting efficiency of NMASS 2 CH 5 amsul particles
NM1_ch4_amsul_uncert	ratio	Uncertainty of the efficiency with which NMASS 1 CH 4 counts amsul particles of the given diameter
NM1_ch5_amsul_uncert	ratio	Uncertainty of the efficiency with which NMASS 1 CH 5 counts amsul particles of the given diameter
NM2_ch5_amsul_uncert	ratio	Uncertainty of the efficiency with which NMASS 2 CH 5 counts amsul particles of the given diameter
particle_diam_lim	nm	Diameter of limonene (lim) particles
particle_diam_lim_uncert	nm	Lim particle diameter uncertainty
NM1_ch4_lim	ratio	Counting efficiency of NMASS 1 CH 4 lim particles
NM1_ch5_lim	ratio	Counting efficiency of NMASS 1 CH 5 lim particles
NM2_ch5_ lim	ratio	Counting efficiency of NMASS 2 CH 4 lim particles
NM1_ch4_ lim_uncert	ratio	Uncertainty of the efficiency with which NMASS 1 CH 4 counts lim particles of the given diameter
NM1_ch5_lim_uncert	ratio	Uncertainty of the efficiency with which NMASS 1 CH 5 counts lim particles of the given diameter
NM2_ch5_lim_uncert	ratio	Uncertainty of the efficiency with which NMASS 2 CH 5 counts lim particles of the given diameter

Table 6. Variables in the file *NMASS2_cpc5_calibration_ct_efficiency_fig8.csv*

Column	Units/format	Description
particle_diam_cal1	nm	Diameter of particles being measured in the first calibration
cpc5_1	ratio	Counting efficiency of NMASS 2 CPC 5 for calibration 1
particle_diam_cal2	nm	Diameter of particles being measured in the second calibration
cpc5_2	ratio	Counting efficiency of NMASS 2 CPC 5 for calibration 2
particle_diam_cal3	nm	Diameter of particles being measured in the third calibration
cpc5_3	ratio	Counting efficiency of NMASS 2 CPC 5 for calibration 3
particle_diam_fit	nm	Diameter for fits to calibrations
count_efficiency_fit_1	ratio	Fitted counting efficiency for the first calibration
count_efficiency_fit_2	ratio	Fitted counting efficiency for the second calibration
count_efficiency_fit_3	ratio	Fitted counting efficiency for the third calibration
count_efficiency_fit_all	ratio	Fitted counting efficiency for all calibrations

Table 7. Variables in the file *SMPS_NMASS_inversions_particle_size_fig10.csv*

Column	Units/format	Description
NM_inv_diam	nm	Diameter for NMASS inversion
SMPS_inv_diam	nm	Diameter for SMPS inversion
size_distribution_NM_a	nm	dN/dlogD for first NMASS inversion
size_distribution_SMPS_a	nm	dN/dlogD for NMASS inversion a
size_distribution_NM_b_all	nm	dN/dlogD NMASS inversion b with NM2ch5 counting efficiency fitted to all calibrations
size_distribution_NM_b_1	nm	dN/dlogD NMASS inversion b with NM2ch5 counting efficiency fitted to first calibration
size_distribution_NM_b_2	nm	dN/dlogD NMASS inversion b with NM2ch5 counting efficiency fitted to second calibration
size_distribution_NM_b_3	nm	dN/dlogD NMASS inversion b with NM2ch5 counting efficiency fitted to third calibration
size_distribution_SMPS_b	nm	dN/dlogD for SMPS inversion

Table 8. Variables in the file *NMass_flow_temp_pressure_fig11.csv*

Column	Units/format	Description
ambient_pressure	hPa	Ambient pressure
time	UTC	Time
NMx_deltaT_meas_cpcy	k	Measured temperature difference for NMx where x is NMASS 1 and NMASS 2 and cpcy is CPC 1-5
NMx_Pdn	hPa	Internal pressure of NMASS 1 and also provided for MNASS 2
NMx_Qtot	cc/min	Total flow on NMASS 1 and also provided for MNASS 2

Table 9. Variables in the file *NMASS1-2_UHSAS_STP_particle_conc_fig12a.csv* (see Figure 1).

Column	Units/format	Description
time		Time
NMx_conc_cpcy	particle per cc	STP concentration in NMASS 1 and NMASS 2 CPCs 1-5 (10 columns of data)
UHSAS_bin0		Particle size distributions by the UHSAS

*The efficiency of each NMASS CPC is taken as the ratio of the standard temperature and pressure (STP, taken as 273.16 K and 1013 hPa) concentration measured in the NMASS to that measured in the reference CPC. The concentration of the NMASS and reference CPCs is calculated as the number of pulses counted by the instrument per unit of time divided by the flow rate, corrected for dead time. This concentration is corrected for pressure and temperature to get the STP concentration.

Table 10. Description of data file *NMASS1-2_inverted_1minute_diam_fig12lowpanel_logd.csv*

Inverted size distributions (dN/dlogDp cm^-3) by corresponding time and diameters (nm) (see Figure 1). Columns are diameters ranging from 2.6 to 5335 nm and rows are time. Gaps in the data are where the aircraft flew through clouds, which can cause artifacts--NMASS data were removed and values set to -9999.

diameter	2.67375	3.0	**...**	5334.8398
time				
3569015770	-9999	49.6239		0
3569015771	-9999	103.4474		0
3569015772	-9999	1960.461		0
3569015773	-9999	6244.644		0
...				
3569018594	-9999	26.56958199		0
3569018595	-9999	13.7481308		0
3569018596	-9999	13.91835117		0

Table 11. Variables in the file *NMASS_inverted_av_size_distr_1min_fig12.csv*

Column	Units/format	Description

final_diam_20170203	nm	Diameter for inverted data
size_distribution_mean_0141	cm^-3	Mean dN/dlogD for minute of 0141
size_distribution_mean_0156	cm^-3	Mean dN/dlogD for minute of 0156
size_distribution_mean_0150	cm^-3	Mean dN/dlogD for minute of 0150

Table 12. Variables in the file *cpc_conc_dma_diameter_150_figS3.csv*

These data are from a TSI 3776 CPC used as a reference instrument.

Column	Units/format	Description
cpc_avg_conc_PSL_150	cm^-3	CPC concentration for 150nm PSL at each DMA diameter
cpc_avg_unc_150	cm^-3	Uncertainty on CPC concentration
dma_diam_avg_PSL_150	nm	Diameter of particles selected by DMA
dma_diam_unc_psl_150	nm	Uncertainty on DMA diameter
fit_cpc_avg_conc_PSL_150	cm^-3	Fit to CPC concentrations
fitX_cpc_avg_conc_PSL_150	nm	Diameter for fitted CPC concentrations

Table 13. Variables in the file *inversion_diameter_lognormal_figS2.csv*

Column	Units/format	Description
inv_diam	nm	Diameter of inversion
lognormal_size_dist_case1	cm^-3	Size distribution for case 1, dn/dlogdp
lognormal_size_dist_case2	cm^-3	Size distribution for case 2, dn/dlogdp
lognormal_size_dist_case3	cm^-3	Size distribution for case 3, dn/dlogdp
lognormal_size_dist_case4	cm^-3	Size distribution for case 4, dn/dlogdp
lognormal_size_dist_case5	cm^-3	Size distribution for case 5, dn/dlogdp
lognormal_size_dist_case6	cm^-3	Size distribution for case 6, dn/dlogdp
lognormal_size_dist_case7	cm^-3	Size distribution for case 7, dn/dlogdp
fit_lognormal_size_dist_case3	cm^-3	Fitted size distribution for case 3, dndlogd
lognormal_SD_case8	cm^-3	Size distribution for case 8, dn/dlogdp
fit_lognormal_SD_case8	cm^-3	Fitted size distribution for case 8, dndlogd

3. Application and Derivation

The two NMASS instruments provide a high-quality, contiguous tropospheric dataset of nucleation and Aitken-mode size distributions with global coverage of the Pacific and Atlantic Ocean basins and seasonal variation. These data will be used to evaluate the dominant mechanisms of atmospheric new particle formation and the contribution of nucleated particles to the global distribution of cloud-active particles and, through model sensitivity studies, their subsequent influence on radiative forcing.

4. Quality Assessment

The response function of each of the CPC channels was determined, and the repeatability of the d50 of each channel was determined to be better than 5% for all but one channels, which had a repeatability of 8%. An evaluation of the propagation of all uncertainties for a range of size distributions shows that particle number, surface area, and volume concentrations within the nucleation and Aitken size range can be determined to better than 20% for typical particle size distributions. Performance may be worse for very low concentrations of particles with modes at the extreme edges of the NMASS detection range. No sensitivity in sizing performance to particle composition was found for three diverse particle compositions.

5. Data Acquisition, Materials, and Methods

Calibration Methodology (from Williamson et al., 2018)

Two nucleation mode aerosol size spectrometers (NMASS) instruments were operated in parallel with five condensation particle counters (CPCs) per instrument in the NASA Atmospheric Tomography Mission (ATom). Each CPC detects particles above a different minimum size, determined by the maximum vapor supersaturation encountered by the particles. Operated in parallel, the CPCs provide continuous concentrations of particles in different cumulative size classes between 3 and 60 nm. Knowing the response function of each CPC, numerical inversion techniques can then be applied to recover a size distribution from the continuous concentrations while taking into account the non-ideal response function of each channel. By maintaining constant downstream pressure, the instrument operates reliably over a large range of ambient pressures and during rapid changes in altitude, making it ideal for aircraft measurements. Different working fluids including n-butanol (butanol), Fluorinet 43 (FC-43), and diethylene glycol (diethglycol) were evaluated to determine the best working fluid to reduce size variations caused by uncontrolled temperature fluctuations.

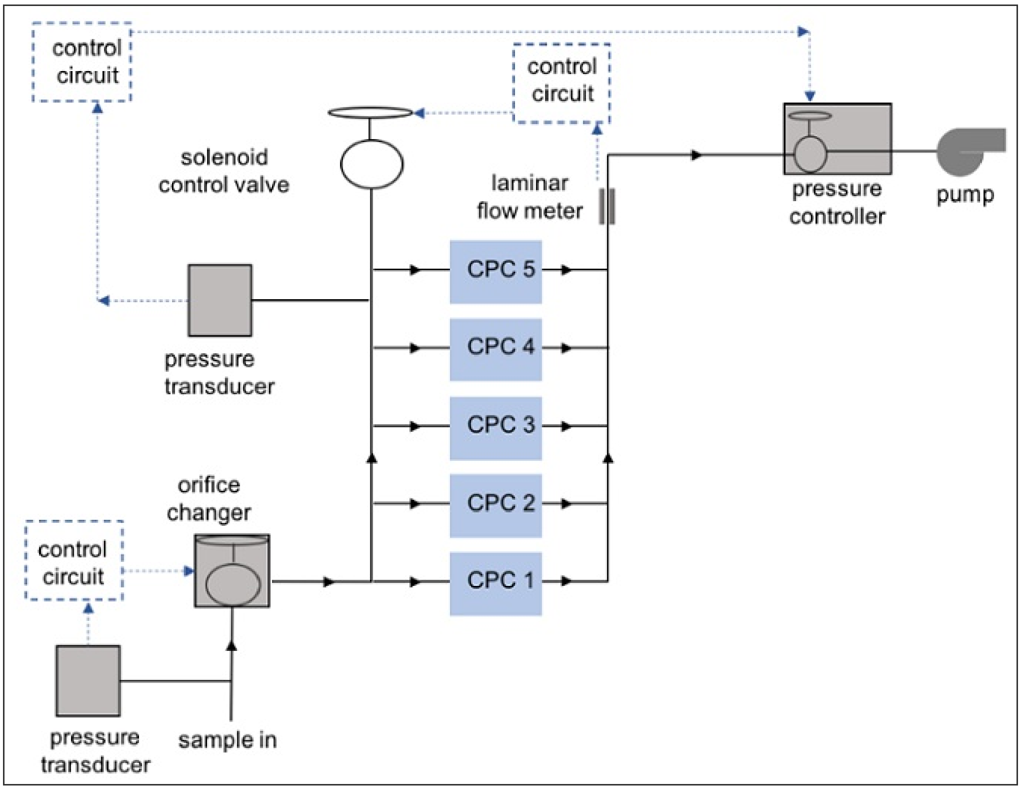

Figure 2. Schematic of the NMASS layout and flow system (Williamson et al., 2018).

Calibration, laboratory, and in-flight performance evaluations:

- Data from the NASA DC-8 aircraft during ATom in February 2017 were used to examine the STP (standard temperature and pressure taken as 273.16 K and 1013 hPa) number concentrations (particles per cc) measured by each channel of both NMASS 1 and 2, as well as the total concentration of particles from 63-1000 nm measured by the Ultra-High Sensitivity Aerosol Spectrometer (UHSAS) used to constrain the inversion and the ambient pressure.

- The counting efficiency of the two NMASSes were evaluated in the settings used for the ATom mission (downstream pressure at 120hPa saturator temperatures of both instruments are set to 39°C, condenser temperature of NMASS 1 are 2.6, 16.2, 21.4, 26.2 and 29.7°C and condenser temperatures of NMASS 2 are 12.2, 13.6, 20.4, 27.2 ad 30.7°C). The calibration was done using particles generated by ozonolysis of limonene.

- Laboratory studies were also used to determine the counting efficiencies of each NMASS CPC as a function of particle diameter. Aerosols used in the study were produced with three different methods: 1) limonene ozonolysis (lim), 2) atomization of ammonium sulphate (amsul), and 3) atomization of 2-diethylhexyl (dioctyl) sebacate (dos). These methods produce particles of widely differing composition that can help identify any composition-dependent sizing effects.

- The dependence of the counting efficiency with size was studied by placing a Boltzmann steady-state charge distribution on the generated particles with a Po-210 neutralizer and passing them through a nano-DMA to select particles of a single electrical mobility. The effect of composition on counting efficiency was evaluated by comparing response curves from a single channel for the three different particle compositions. Knowing the response function of each CPC, numerical inversion techniques were applied to recover a size distribution from the continuous concentrations while taking into account the non-ideal response function of each channel.

- Inverted particle size distributions from NMASS and Scanning Mobility Particle Sizer (SMPS), the standard technique for ground-based measurements of nucleation-mode particle size distributions, were examined. Aerosols were generated by atomizing ammonium sulphate, and particle sizes were selected by a DMA.

Refer to Williamson et al., 2018 for additional details.

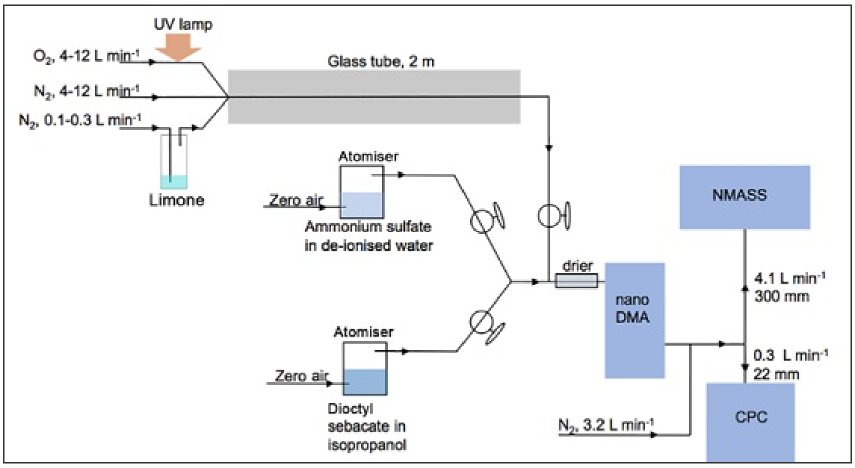

Figure 3. Diagram of the calibration set up used to characterize the NMASS counting efficiency as a function of particle diameter. The calibration includes different aerosol types such as limonene, ammonium sulfate, and dioctyl sebacate particles to test the instrument sensitivity to particle composition.

6. Data Access

These data are available through the Oak Ridge National Laboratory (ORNL) Distributed Active Archive Center (DAAC).

ATom: Nucleation Mode Aerosol Size Spectrometer Calibration and Performance Data

Contact for Data Center Access Information:

- E-mail: uso@daac.ornl.gov
- Telephone: +1 (865) 241-3952

7. References

Williamson, C., Kupc, A., Wilson, J., Gesler, D. W., Reeves, J. M., Erdesz, F., McLaughlin, R., and Brock, C. A. 2018. Fast time response measurements of particle size distributions in the 30-60nm size range with the nucleation mode aerosol size spectrometer, Atmos. Meas. Tech., 11, 3491-3509, https://doi.org/10.5194/amt-11-3491-2018