ATom: Ultrafine Aerosol Characteristics and Formation, Lower Stratosphere, 2016-2018

Get Data

Documentation Revision Date: 2022-12-29

Dataset Version: 1

Summary

This dataset consists of (a) selected aerosol and gas-phase observations made on all four deployments of NASA Atmospheric Tomography Mission (ATom), (b) thermodynamic properties related to aerosol formation derived from these measurements, (c) 48-h back trajectories for ATom-4 observations, and (d) output from the Model of Aerosols and Ions in the Atmosphere (MAIA). ATom observations, thermodynamics, and back trajectories were inputs for MAIA model runs. MAIA runs focused on data from ATom-4 deployment, and output includes aerosol formation rates, and ultrafine particle size distributions and number concentrations in the lowermost stratosphere (LMS). ATom 1-4 deployments included all four seasons from 2016 to 2018. This investigation sought to understand how new particle formation (NPF) can occur in the LMS, factors influencing the amount of NPF, and other potential sources of ultrafine aerosols in this region of the atmosphere. The data are provided in comma-separated value (CSV) format.

This dataset includes a total of 283 files in comma-separated value (CSV) format: 4 files holding ATom observations, one for each ATom deployment; 1 file holding thermodynamic data from four ATom deployments; 64 files holding back trajectory input data; and 214 files with MAIA model output.

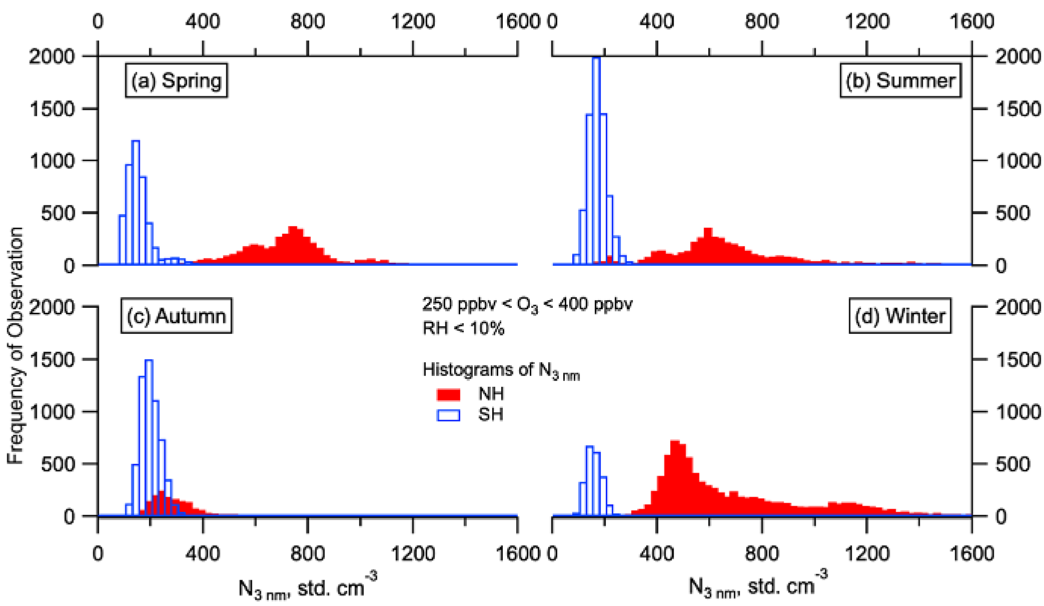

Figure 1. Histograms of the total number of aerosols between 3 and 4500 nm in the LMS (ozone 250-400 ppbv, altitude > 8 km) for the SH and NH) for all ATom deployments (a-d), by season. Modified from fig. 2 of Williamson et al. (2021).

Citation

Williamson, C.J., A. Kupc, A.W. Rollins, J. Kazil, K.D. Froyd, E.A. Ray, D.M. Murphy, G.P. Schill, J. Peischl, C.R. Thompson, I. Bourgeois, T.B. Ryerson, G.S. Diskin, J.P. DiGangi, D.R. Blake, T.P. Bui, M. Dollner, B.B. Weinzierl, and C.A. Brock. 2021. ATom: Ultrafine Aerosol Characteristics and Formation, Lower Stratosphere, 2016-2018. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1868

Table of Contents

1. Dataset Overview

This dataset consists of (a) selected aerosol and gas-phase observations made on NASA Atmospheric Tomography Mission (ATom) campaigns 1-4, (b) thermodynamic properties related to aerosol formation derived from these measurements, (c) 48-h back trajectories for Atom 4 observations, and (d) output from the Model of Aerosols and Ions in the Atmosphere (MAIA). Atom observations, thermodynamics, and back trajectories were inputs for MAIA model runs. MAIA runs focused on data from Atom 4 campaign, and output includes aerosol formation rates, and ultrafine particle size distributions and number concentrations in the lowermost stratosphere (LMS). ATom 1-4 deployments included all four seasons from 2016 to 2018. This investigation sought to understand how new particle formation (NPF) can occur in the LMS, factors influencing the amount of NPF, and other potential sources of ultrafine aerosols in this region of the atmosphere

Project: Atmospheric Tomography Mission

The Atmospheric Tomography Mission (ATom) is a NASA Earth Venture Suborbital-2 mission to study the impact of human-produced air pollution on greenhouse gases and on chemically reactive gases in the atmosphere. ATom deployed 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. Around-the-world flights were conducted in each of four seasons between 2016 and 2018.

Related Dataset:

Wofsy, S.C., et al. 2021. ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols, Version 2. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1925

Related Publications:

Williamson, C.J., A. Kupc, A. Rollins, J. Kazil, K.D. Froyd, E.A. Ray, D.M. Murphy, G.P. Schill, J. Peischl, C. Thompson, I. Bourgeois, T.B. Ryerson, G.S. Diskin, J.P. DiGangi, D.R. Blake, T.P. V. Bui, M. Dollner, B. Weinzierl, and C.A. Brock. 2021. Large hemispheric difference in nucleation mode aerosol concentrations in the lowermost stratosphere at mid- and high latitudes. Atmospheric Chemistry and Physics 21:9065–9088. https://doi.org/10.5194/acp-21-9065-2021

Brock, C.A., C. Williamson, A. Kupc, K.D. Froyd, F. Erdesz, N. Wagner, M. Richardson, J.P. Schwarz, R.-S. Gao, J.M. Katich, P. Campuzano-Jost, B.A. Nault, J.C. Schroder, J.L. Jimenez, B. Weinzierl, M. Dollner, T. Bui, and D.M. Murphy. 2019. Aerosol size distributions during the Atmospheric Tomography Mission (ATom): methods, uncertainties, and data products. Atmospheric Measurement Techniques 12:3081–3099. https://doi.org/10.5194/amt-12-3081-2019

Acknowledgments

This work was supported by the National Aeronautics and Space Administration's Earth Venture program through awards NNX15AJ23G and NNH15AB12I and by NOAA's Health of the Atmosphere and Atmospheric Chemistry, Carbon Cycle, and Climate programs.

2. Data Characteristics

Study Areas: Global

Spatial Resolution: Point measurements

Temporal Coverage: 2016-07-29 to 2018-05-21

Temporal Resolution: 1 second

Study Areas: Latitude and longitude are provided in decimal degrees.

Site	Northernmost Latitude	Southernmost Latitude	Easternmost Longitude	Westernmost Longitude
Global	80	-80	180	-180

Data File Information

This dataset includes a total of 283 files in comma-separated value (CSV) format: 4 files with ATom observations, one for each ATom deployment; 1 file with thermodynamic data from four ATom deployments; 64 files with back trajectory input data; and 214 files with MAIA model output. The files are described below.

Table 1. File names and descriptions

File names	Descriptions	Data Sources
ATom**X**_Observations.csv	Observations from the ATom flights, where ATomX is ATom 1, 2, 3, or 4. There are four files.	Wofsy et al. (2018). Selected variables at 1 second resolution.
ATomThermodynamics.csv	Thermodynamic data calculated for ATom 1, 2, 3, and 4. There is one file.	Derived from Wofsy et al. (2018) observations.
MAIAinput_**YYYYMMDD**_R**A**_trajectory**BB**_length**CCC**.csv	Back trajectory data at 0.25-degree resolution for ATom-4 observation in lowermost stratosphere. These data were input to the MAIA model. There are 64 files.	National Center for Environmental Prediction (NCEP, 2015) global forecast system (GFS) meteorology. NCEP provided temperature, relative humidity, and pressure along the trajectories for the MAIA runs.

MAIAoutput_**YYYYMMDD**traj_**EEE_FFFF**pptSO2_**GG**_00E_4s.csv	Model output from the MAIA model. The MAIA runs were exclusively for ATom-4. There are 214 files.	Previous data products are inputs for MAIA model.

Data File Details

<u>ATom observations</u>:

The file naming convention is *ATom**X**_Observations.csv* (e.g, ATom1_Observations.csv), where X = the ATom deployment 1, 2, 3, or 4.

Table 2. Variables in the file **ATomX_Observations.csv.** Instrumentation used in collecting these data are described in Williamson et al. (2021).

Variable	**Units/format**	**Description**
ATom_number		Indication of the ATom deployment 1 = ATom-1: July-August 2016 2 = ATom-2: January-February 2017 3 = ATom-3: September-October 2017 4 = ATom-4: May-June 2018
Bio_burn_mass_palms ;	mg m^{-3}	Mass of particles classified by the PALMS instrument as biomass burning
final_diam	µm	Geometric mean of each diameter bin of the measured size distribution
final_dlogd	µm	Geometric width of each diameter bin of the measured size distribution
g_alt	km	Altitude
g_latitude	degrees north	Latitude
g_longitude	degrees east	Longitude
h2o_dlh	ppbv	Water vapor concentration
nm2_conc1	cm^{-3} *	NM_conc = particle concentration, std. cm-3 *
nm2_conc2	cm^{-3}	Particle concentration, std. cm-3
nm2_conc3	cm^{-3}	Particle concentration, std. cm-3
nm2_conc4	cm^{-3}	Particle concentration, std. cm-3
nm2_conc5	cm^{-3}	Particle concentration, std. cm-3
nm2_counts1	s^{-1}	Instrument counts for individual particles
nm2_counts2	s^{-1}	Instrument counts for individual particles
nm2_counts3	s^{-1}	Instrument counts for individual particles
nm2_counts4	s^{-1}	Instrument counts for individual particles
nm2_counts5	s^{-1}	Instrument counts for individual particles
n_accum_amp	std. cm^{-3}	Accumulation mode: number concentration of 60-1000 nm particles
n_aitken_amp	std. cm^{-3}	Aitken mode: number concentration of 12-60 nm particles
n_coarse_amp	std. cm^{-3}	Coarse mode: number concentration of 1000-4500 nm particles
n_nucl_amp	std. cm^{-3}	Nucleation mode: number concentration of 3-12 nm particles
o3_cl	ppbv	Concentration of ozone
pot	K	Potential temperature
pw	hPa	Pressure
Rhw_dlh	%	Relative humidity over supersaturated water
so2_lif	pptv	Concentration of sulfur dioxide
s_accum_amp	um^2 std. cm^{-3}	Accumulation mode: surface area of 60-1000 nm particles
s_aitken_amp	um^2 std. cm^{-3}	Aitken mode: surface area of 12-60 nm particles
s_coarse_amp	um^2 std. cm^{-3}	Coarse mode: surface area of nm particles
s_nucl_amp	um^2 std. cm^{-3}	Nucleation mode: surface area of 3-12 nm particles
time_utc	UTC	Date and time of measurement
tw	K	Ambient temperature

*Std. = All data provided at standard temperature and pressure: 1013 hPa and 0 Celsius.

Thermodynamics data:

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

Variable	Units/format	Description
time_utc	UTC	Date and time of measurement
nucleation_barrier_max	unitless	Calculated barrier to nucleation
neg_binary_psat	pptv	Saturation vapor pressure for negative ion cluster (parts per trillion volume)
g_latitude	degrees north	Latitude of measurement location
g_longitude	degrees east	Longitude of measurement location
g_alt	km	Altitude
atom_number		Indication of the ATom deployment: 1=ATom-1: July-August 2016 2=ATom-2: January-February 2017 3=ATom-3: September-October 2017 4=ATom-4: May-June 2018

Back trajectory files:

The file naming convention is *MAIAinput_**YYYYMMDD**_R**A**_trajectory**BB**_length**CCC**.csv* (e.g., MAIAinput_20180427_R0_trajectory10_length194.csv), where

- **YYYYMMDD** is the start date of the trajectory.
- **A** is the version number of the back trajectory. All files are R0.
- **BB** is the trajectory number for the specified day's flight.
- **CCC** is the length of trajectory.

Table 4. Variables in the back trajectory files.

Variable	Units/format	Description
Time_s	s	Time along the trajectory, starting at 0, ending at the corresponding observation at 48 h, in seconds.
p_hpa	hPa	Pressure along the trajectory
T_K	K	Temperature along the trajectory
RHw_pct	percent	Relative humidity over supersaturated water
H2O_pcm3	cm^{-3}	Water vapor concentration
air_pcm3	cm^{-3}	Volumetric number density of air
LON	degrees	Longitude of each point on the trajectory on the 0 - 360 scale
LAT	degrees	Latitude of each point on the trajectory
DOY	blank	Day of year
LST_s	s	Local solar time
UTC_s	s	Time along the trajectory in seconds before the observation point. The UTC_s values range -172800 to 0. The simulation begins at Time_s = 0 and UTC_s = -172800 s, that is, 48 hours before the observation point. The simulation ends at UTC_s = 0 and Time_s = 172800 s (= 48 h).
time_h	h	Time along trajectory in h
lon180	degrees	Longitude of each point on the trajectory on the -180 to +180 scale

MAIA output files:

The file naming convention is *MAIAoutput_**YYYYMMDD**traj_**EEE_FFFF**pptSO2_**GG**_00E_4s.csv*
(e.g., MAIAoutput_20180427traj_000_0020pptSO2_02_00E_4s.csv), where

- **YYYYMMDD** is the year month and day of the observation
- **EEE** trajectory number is the trajectory run for every 2 minutes of data
- **FFFF** is assumed starting concentration of SO_2 concentration in pptv
- **GG** is the assumed starting condensation sink in units of 1×10^{-4} s^{-1}.

Table 5. Variables in the MAIA output files.

Variable	Units/format	Description
time_s	s	Time along the trajectory starting at 0 and ending at the corresponding observation at 48 h. Refer also to the table above for this variable description
pressure_hPa	hPa	Pressure

temperature_k	K	Temperature
ionizationpcm3ps	cm^{-3} s^{-1}	Ionization rate
H2O_pcm3	cm^{-3}	Water vapor concentration
RHw_pct	percent	Relative humidity over supersaturated water
OH_pcm3	cm^{-3}	OH concentration
SO2_pcm3	cm^{-3}	SO2 concentration
H2SO4pr_pcm3ps	cm^{-3} s^{-1}	H2SO4 production rate
H2SO4_pcm3	cm^{-3}	H2SO4 concentration
ncc_nh2so4	cm^{-3}	Concentration of particles larger than the critical cluster
Nncc_pcm3	cm^{-3}	Concentration of particles larger than the critical cluster, cm^{-3}
N2_65_pcm3	cm^{-3}	Concentration of particles larger than 2.65 nm
N4_pcm3	cm^{-3}	Concentration of particles larger than 4 nm
N5_pcm3	cm^{-3}	Concentration of particles larger than 5 nm
N6_pcm3	cm^{-3}	Concentration of particles larger than 6 nm
N7_pcm3	cm^{-3}	Concentration of particles larger than 7 nm
N8_pcm3	cm^{-3}	Concentration of particles larger than 8 nm
N9_pcm3	cm^{-3}	Concentration of particles larger than 9 nm
N10_pcm3	cm^{-3}	Concentration of particles larger than 10 nm
N12_pcm3	cm^{-3}	Concentration of particles larger than 12 nm
anions_pcm3	cm^{-3}	Concentration of anions
CS_ps	s^{-1}	Aerosol condensation sink for 1 molecule H2SO4
cnr_pcm3ps	cm^{-3} s^{-1}	Charged nucleation rate
nnr_pcm3ps	cm^{-3} s^{-1}	Neutral nucleation rate
cpfr_2_65_pcm3ps	cm^{-3} s^{-1}	Charged particle formation rate at 2.65 nm
npfd_2_65_pcm3ps	cm^{-3} s^{-1}	Neutral particle formation rate at 2.65 nm
time_h	h	Time (hour)

3. Application and Derivation

In Williamson et al. (2021), the MAIA model (Lovejoy et al., 2004; Kazil and Lovejoy, 2007; Kazil et al., 2007), back trajectories, thermodynamic calculations and emissions estimates were used to understand new particle formation (NPF) in the lowermost stratosphere (LMS), factors influencing the amount of NPF, and other potential sources of ultrafine aerosol in this region. The MAIA model was run along back trajectories, initiated at the aircraft location, which were calculated using the Traj3D trajectory model (Bowman, 1993) and meteorology from the National Center for Environmental Prediction (NCEP, 2015) global forecast system (GFS).

Refer to Williamson et al. (2021) for additional details.

4. Quality Assessment

Accuracy and uncertainties are dependent on the instrumentation. Refer to Brock et al. (2019) for additional information.

5. Data Acquisition, Materials, and Methods

This dataset consists of aerosol and gas-phase measurements made on the ATom campaign and Model of Aerosols and Ions in the Atmosphere (MAIA) model output data.

Using in-situ, global-scale measurements of the size distribution of particles from ATom, a mode of aerosol <12 nm was observed in the lowermost stratosphere (LMS) at middle and high latitudes. This mode is substantial only in the northern hemisphere, and was observed in all four seasons. The MAIA model (Lovejoy et al., 2004; Kazil and Lovejoy, 2007; Kazil et al., 2007), was used to investigate new particle formation (NPF) in the LMS, factors influencing the amount of NPS and other potential sources of ultrafine aerosol in this region. Model inputs included back trajectories, thermodynamic calculations, and emissions estimates

The MAIA model was run along back trajectories, initiated at the aircraft location, which were calculated using the Traj3D trajectory model (Bowman, 1993) and the National Center for Environmental Prediction (NCEP, 2015) global forecast system (GFS) meteorology. NCEP provided temperature, relative humidity, and pressure along the trajectories for the MAIA runs. MAIA was initialized using condensation sinks and SO_2 concentrations estimated from ATom observations at similar latitudes and altitudes. The initial aerosol size distribution is specified as a lognormal mode with the given condensation sink. The geometric mean diameter (46 nm) and geometric standard deviation (2.8 nm) were obtained by fitting a lognormal mode to the size distribution observed at the ATom measurement locations.

Refer to Williamson et al. (2021) for additional details.

6. Data Access

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

ATom: Ultrafine Aerosol Characteristics and Formation, Lower Stratosphere, 2016-2018

Contact for Data Center Access Information:

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

7. References

Bowman, K.P. 1993. Large-scale isentropic mixing properties of the Antarctic polar vortex from analyzed winds. Journal of Geophysical Research 98:23013. https://doi.org/10.1029/93JD02599

Brock, C.A., C. Williamson, A. Kupc, K.D. Froyd, F. Erdesz, N. Wagner, M. Richardson, J.P. Schwarz, R.-S. Gao, J.M. Katich, P. Campuzano-Jost, B.A. Nault, J.C. Schroder, J.L. Jimenez, B. Weinzierl, M. Dollner, T. Bui, and D.M. Murphy. 2019. Aerosol size distributions during the Atmospheric Tomography Mission (ATom): methods, uncertainties, and data products. Atmospheric Measurement Techniques 12:3081–3099. https://doi.org/10.5194/amt-12-3081-2019

Kazil, J., and E.R. Lovejoy. 2007. A semi-analytical method for calculating rates of new sulfate aerosol formation from the gas phase. Atmospheric Chemistry and Physics 7:3447–3459. https://doi.org/10.5194/acp-7-3447-2007, 2007.

Lovejoy, E.R., J. Curtius, and K.D. Froyd. 2004. Atmospheric ion-induced nucleation of sulfuric acid and water. Journal of Geophysical Research 109:D08204. https://doi.org/10.1029/2003JD004460

NCEP: National Centers For Environmental Prediction/National Weather Service/NOAA/U.S. Department Of Commerce. 2015. NCEP GFS 0.25 Degree Global Forecast Grids Historical Archive. UCAR/NCAR - Research Data Archive. https://doi.org/10.5065/D65D8PWK

Williamson, C.J., A. Kupc, A. Rollins, J. Kazil, K.D. Froyd, E.A. Ray, D.M. Murphy, G.P. Schill, J. Peischl, C. Thompson, I. Bourgeois, T.B. Ryerson, G.S. Diskin, J.P. DiGangi, D.R. Blake, T.P. V. Bui, M. Dollner, B. Weinzierl, and C.A. Brock. 2021. Large hemispheric difference in nucleation mode aerosol concentrations in the lowermost stratosphere at mid- and high latitudes. Atmospheric Chemistry and Physics 21:9065–9088. https://doi.org/10.5194/acp-21-9065-2021

Wofsy, S.C., et al. 2018. ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1581