ATom: Measurements from Particle Analysis By Laser Mass Spectrometry (PALMS)

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Documentation Revision Date: 2022-01-03

Dataset Version: 1

Summary

This dataset contains single-particle aerosol composition as measured by the Particle Analysis by Laser Mass Spectrometry (PALMS) instrument during the four ATom campaigns from 2016-2018. Single aerosol particles are classified into several particle types, including: mixed sulfate/organic nitrate, biomass burning, elemental carbon, mineral/metallic, meteoric material, alkali salt, sea salt, heavy oil combustion, and others. Particle types are reported as raw number fractions and as absolute mass concentrations. PALMS measures aerosol composition for particles from diameter ~100 to 5000 nm, with most of the particle data in the size range ~150 to 3000 nm. Also included are absolute aerosol concentrations measured by a modified Laser Aerosol Spectrometer (LAS). Integrated number, surface area, and volume concentrations from LAS are reported over multiple size ranges.

There are 278 data files included in this dataset,186 data files in ICARTT (*.ict) format and 92 files NetCDF (*.nc) format.

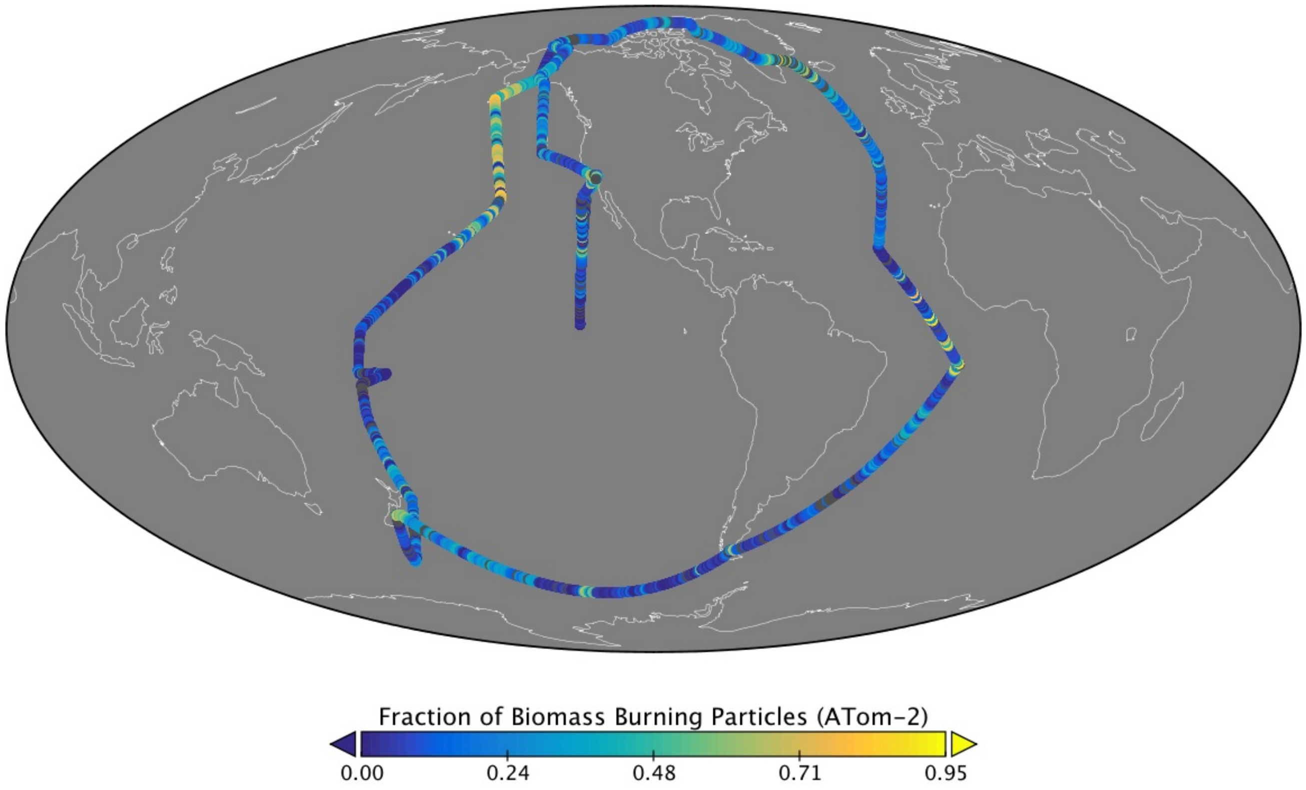

Figure 1. Fraction of aerosol particles attributed to biomass burning detected by PALMS on ATom-2 flights from 2017-01-26 to 2017-02-21.

Citation

Froyd, K.D., D.M. Murphy, G.P. Schill, and C.A. Brock. 2021. ATom: Measurements from Particle Analysis By Laser Mass Spectrometry (PALMS). ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1733

Table of Contents

1. Dataset Overview

This dataset contains single-particle aerosol composition as measured by the Particle Analysis by Laser Mass Spectrometry (PALMS) instrument during the four ATom campaigns from 2016–2018. Single aerosol particles are classified into several particle types, including mixed sulfate/organic nitrate, biomass burning, elemental carbon, mineral/metallic, meteoric material, alkali salt, sea salt, heavy oil combustion, and others. Particle types are reported as raw number fractions and as absolute mass concentrations. PALMS measures aerosol composition for particles from diameter ~100 to 5,000 nm, with most of the particle data in the size range ~150 to 3,000 nm. Also included are absolute aerosol concentrations measured by a modified Laser Aerosol Spectrometer (LAS). Integrated number, surface area, and volume concentrations from LAS are reported over multiple size ranges.

Project: Atmospheric Tomography Mission (ATom)

The Atmospheric Tomography Mission (ATom) was a NASA Earth Venture Suborbital-2 mission. It studied 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. Flights occurred in each of four seasons over a 4-year period.

Related Data:

Wofsy, S.C., S. Afshar, H.M. Allen, E.C. Apel, E.C. Asher, B. Barletta, 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

- Data from all ATom instruments and all four flight campaigns, including aircraft location and navigation data, merged to several different time bases.

Wofsy, S.C., and ATom Science Team. 2018. ATom: Aircraft Flight Track and Navigational Data. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1613

- Flightpath (location and altitude) data for each of the four campaigns provided in KML and CSV formats.

2. Data Characteristics

Spatial Coverage: Global. Flights circumnavigate the globe, primarily over the oceans

Spatial Resolution: Point measurements

Temporal Coverage: Periodic flights occurred during each campaign

Deployment	Date Range
ATom-1	July 29 - August 23, 2016
ATom-2	January 26 - February 21, 2017
ATom-3	September 28 - October 28, 2017
ATom-4	April 24 - May 21, 2018

Temporal Resolution: LASaerosol: 10 s; PALMS, PALMS-Chem-Mass, and PALMS-PartType-Mass: 1 s; PALMS-Neg-Particle-Spectra and PALMS-Pos-Particle-Spectra: <1 s

Data File Information

There are 278 data files included in this dataset,186 data files in ICARTT (*.ict) format and 92 files NetCDF (*.nc) format. Files in ICARTT format conform to the ICARTT File Format Standards V1.1 and files in NetCDF format conform to CF Conventions. The file names are named **FileType**_DC8_**YYYYMMDD_R#**.ict, where **FileType** is the type of data (Table 2), **YYYYMMDD** is the start date (in UTC time) of the flight, and **R#** is the file version or revision number.

Table 2. File types and descriptions.

File Type	Number of Files	Format	Description
LASaerosol	48	ICARTT	Number, surface, and volume concentrations of dry aerosol particles measured by a commercial TSI model 3340.
PALMS	46	ICARTT	Aerosol number fractions of various particle types
PALMS-Chem-Mass	46	ICARTT	Aerosol mass concentrations in non-refractory particles
PALMS-Neg-Particle-Spectra	46	NetCDF	PALMS negative ion single-particle spectra
PALMS-PartType-Mass	46	ICARTT	Aerosol mass concentrations of various particle types
PALMS-Pos-Particle-Spectra	46	NetCDF	PALMS negative ion single-particle spectra

Data File Details

Table 3. Variable names and descriptions for LASaerosol files. "STP" is the standard temperature and pressure.

Name	Units	Description

Start_LAS	Seconds	Start time in seconds since 0000 UTC
End_LAS	Seconds	End time in seconds since 0000 UTC
N_LAS	std cm^{-3}	Integrated number concentration, approx.0.1 to 4.8 um dry diameter
S_LAS	std um^{2} cm^{-3}	Integrated surface area concentration, approx.0.1 to 4.8 um dry diameter
V_LAS	std um^{3} cm^{-3}	Integrated volume concentration, approx. 0.1 to 4.8 um dry diameter
Nacc_LAS	std cm^{-3}	Integrated number concentration, approx. 0.1 to 0.9 um dry diameter
Sacc_LAS	std um^{2} cm^{-3}	Integrated surface area concentration, approx. 0.1 to 0.9 um dry diameter
Vacc_LAS	std um^{3} cm^{-3}	Integrated volume concentration, approx. 0.1 to 0.9 um dry diameter
Ncoarse_LAS	std cm^{-3}	Integrated number concentration, approx. 0.9 to 4.8 um dry diameter
Scoarse_LAS	std um^{2} cm^{-3}	Integrated surface area concentration, approx. 0.9 to 4.8 um dry diameter
Vcoarse_LAS	std um^{3} cm^{-3}	Integrated volume concentration, approx. 0.9 to 4.8 um dry diameter

Table 4. Variable names and descriptions for PALMS files.

Name	Units	Description
PALMSstartTime	Seconds	Start time in seconds since 0000 UTC
SulfOrgNitFrac_PALMS	Number fraction	Mixed sulfate-organic-nitrate particles
BioBurnFrac_PALMS	Number fraction	Biomass burning particles
SootFrac_PALMS	Number fraction	Elemental carbon particles
MineralFrac_PALMS	Number fraction	Mineral/metallic particles
MeteoricFrac_PALMS	Number fraction	Particles with meteoric material
AlkaliSaltFrac_PALMS	Number fraction	Alkali salt particles
SeaSaltFrac_PALMS	Number fraction	Sea salt particles
OilCombFrac_PALMS	Number fraction	Particles from heavy oil combustion
UnclassFrac_PALMS	Number fraction	Unclassified particles
OrgSulfMF_PALMS	Mass fraction	Organic-to-sulfate mass fraction
IEPOXmf_PALMS	Mass fraction	Fraction of submicron aerosol mass attributed to IEPOX sulfate
GASmf_PALMS	Mass fraction	Fraction of submicron aerosol mass attributed to glycolic acid sulfate
SulfNeut_PALMS	Molar Ratio	Degree of sulfate neutralization as NH4+:SO42-
Npos_PALMS	Count	Number of particles positive ion spectra used
NNeg_PALMS	Count	Number of negative ion spectra used
NAcid_PALMS	Count	Number of spectra used for SulfNeut data product

Table 5. Variable names and descriptions for PALMS-Chem-Mass files.

Name	Units	Description
StartTimeChem_PALMS	Seconds	Start time in seconds since 0000 UTC
OrgMass_PALMS	ug stdm^{-3}	Mass concentration of organic material in non-refractory particles
SulfateMass_PALMS	ug stdm^{-3}	Mass concentration of sulfate in non-refractory particles
BromineMass_PALMS	ug stdm^{-3}	Mass concentration of bromine in non-refractory particles
IodineMass_PALMS	ug stdm^{-3}	Mass concentration of iodine in non-refractory particles
IEPOXsulfMass_PALMS	ug stdm^{-3}	Mass concentration of IEPOX sulfate ester in non-refractory particles
GASMass_PALMS	ug stdm^{-3}	Mass concentration of glycolic acid sulfate in non-refractory particles

Table 6. Variable names and descriptions for PALMS-Neg-Particle-Spectra and PALMS-Pos-Particle-Spectra files.

Name	Units	Description
AeroDiam	Microns	The aerodynamic diameter of the particle derived from the time between the timing and trigger scatter signals
Altitude	Meters	Altitude of aircraft
AreasNoID	Fraction of ions	The areas of all peaks for which no mass number was assigned
AreasNonInt	Fraction of ions	The areas of all peaks with half-mass or other non-integer peak identification

DateTime	Seconds	Start time in seconds since 0000 UTC
ExcimerND	Fraction of ions	The value of a neutral density filter in the excimer beam
FlagBioBurn	Numeric	Shows if a particle was identified by automated criteria as a biomass burning particle
FlagKRich	Numeric	Shows if a particle was identified by automated criteria as an alkali-rich particle
FlagMinMet	Numeric	Shows if a particle was identified by automated criteria as a mineral or metal particle
FlagSeaSalt	Numeric	Shows if a particle was identified by automated criteria as a sea salt particle
FlagSoot	Numeric	Shows if a particle was identified by automated criteria as a soot particle
FlagSulfOrg	Numeric	Shows if a particle was identified by automated criteria as a sulfate-organic-nitrate mixture
FlightTDay	Numeric	UTC time of measurement in seconds since 0000 UTC
JouleMtr	Relative	The time the particle was sampled in seconds since Jan 1, 1904
Latitude	Decimal degrees	Latitude
Longitude	Decimal degrees	Longitude
MassScaleA	us	A constant in an equation to convert ion arrival time to mass: time = A + B*sqrt(mass)
MassScaleB	us (D_a-1)/2	A constant in an equation to convert ion arrival time to mass: time = A + B*sqrt(mass) D_a = aerodynamic diameter
MScaleFitVariance	D_a^2	The variance when the positions of the peaks are fit to the mass scale equation using integer values for the peak positions
NumPks	1	Number of non-zero peaks in each mass spectrum
spectra	Fraction of ions	Two-dimensional array giving the area of every mass peak for every particle mass spectrum
TimingScatHt	Degree	The size of the optical pulse when the particle scattered light as it went through the first 405 nm laser beam
TotalMCPBackground	Electrons	There is a very small ion background in PALMS in the positive ion mode, mostly at m/z=12. This is the value that was subtracted to obtain TotalMCPSignal
TotalMCPSignal	Electrons	The total signal from the microchannel plate (MCP) integrated over all peaks in the mass spectrum
TrigScatHt	Relative	The size of the optical pulse when the particle scattered light

Table 7. Variable names and descriptions for PALMS-PartType-Mass.

Name	Units	Description
StartTime_PALMS	Seconds	Start time in seconds since 0000 UTC
SulfOrgNitMass_PALMS	ug $stdm^{-3}$	mass concentration of mixed sulfate-organic-nitrate particles for 0.1-4.8 um dry diameter
BioBurnMass_PALMS	ug $stdm^{-3}$	mass concentration of biomass burning particles for 0.1-4.8 um dry diameter
SootMass_PALMS	ug $stdm^{-3}$	mass concentration of elemental carbon particles for 0.1-4.8 um dry diameter
MineralMass_PALMS	ug $stdm^{-3}$	mass concentration of mineral/metallic particles for 0.1-4.8 um dry diameter
MeteoricMass_PALMS	ug $stdm^{-3}$	mass concentration of particles with meteoric material for 0.1-4.8 um dry diameter
AlkaliSaltMass_PALMS	ug $stdm^{-3}$	mass concentration of alkali salt particles for 0.1-4.8 um dry diameter
SeaSaltMass_PALMS	ug $stdm^{-3}$	mass concentration of sea salt particles for 0.1-4.8 um dry diameter
OilCombMass_PALMS	ug $stdm^{-3}$	mass concentration of particles from fuel oil combustion for 0.1-4.8 um dry diameter
UnclassMass_PALMS	ug $stdm^{-3}$	mass concentration of unclassified particles for 0.1-4.8 um dry diameter
NposMass_PALMS	Count	number of positive ion particle spectra

3. Application and Derivation

ATom builds the scientific foundation for mitigation of short-lived climate forcers, in particular, methane (CH_4), tropospheric ozone (O_3), and Black Carbon aerosols (BC).

ATom Science Questions

Tier 1

- What are chemical processes that control the short-lived climate forcing agents CH_4, O_3, and BC in the atmosphere? How is the chemical reactivity of the atmosphere on a global scale affected by anthropogenic emissions? How can we improve the chemistry-climate modeling of these processes?

Tier 2

- Over large, remote regions, what are the distributions of BC and other aerosols important as short-lived climate forcers? What are the sources of

new particles? How rapidly do aerosols grow to CCN-active sizes? How well are these processes represented in models?
- What type of variability and spatial gradients occurs over remote ocean regions for greenhouse gases (GHGs) and ozone-depleting substances (ODSs)? How do the variations among air parcels help identify anthropogenic influences on photochemical reactivity, validate satellite data for these gases, and refine knowledge of sources and sinks?

Significance

ATom delivers unique data and analysis to address the Science Mission Directorate objectives of acquiring “datasets that identify and characterize important phenomena in the changing Earth system” and “measurements that address weaknesses in current Earth system models leading to improvement in modeling capabilities.” ATom will provide unprecedented challenges to the CCMs used as policy tools for climate change assessments, with comprehensive data on atmospheric chemical reactivity at global scales, and will work closely with modeling teams to translate ATom data to better, more reliable CCMs. ATom provides extraordinary validation data for remote sensing.

4. Quality Assessment

Quality assessment procedures differ by data file type. Quality flags are provided within the data files for many of the measured parameters.

5. Data Acquisition, Materials, and Methods

Project Overview

ATom makes global-scale measurements of the chemistry of the atmosphere using the NASA DC-8 aircraft. Flights span the Pacific and Atlantic Oceans, nearly pole-to-pole, in continuous profiling mode, covering remote regions that receive long-range inputs of pollution from expanding industrial economies. The payload has proven instruments for in situ measurements of reactive and long-lived gases, diagnostic chemical tracers, and aerosol size, number, and composition, plus spectrally resolved solar radiation and meteorological parameters.

Combining distributions of aerosols and reactive gases with long-lived GHGs and ODSs enables disentangling of the processes that regulate atmospheric chemistry: emissions, transport, cloud processes, and chemical transformations. ATom analyzes measurements using customized modeling tools to derive daily averaged chemical rates for key atmospheric processes and to critically evaluate CCMs. ATom also differentiates between hypotheses for the formation and growth of aerosols over the remote oceans.

Particle Analysis by Laser Mass Spectrometry

The NOAA Particle Analysis by Laser Mass Spectrometry (PALMS) instrument measures single-particle aerosol composition using UV laser ablation to generate ions that are analyzed with a time-of-flight mass spectrometer. The PALMS size range is approximately 150 nm to >3000 nm and encompasses most of the accumulation and coarse mode aerosol volume. Individual aerosol particles are classified into compositional classes. The size-dependent composition data are combined with aerosol counting instruments from Aerosol Microphysical Properties (AMP), the Langley Aerosol Research Group Experiment (LARGE), and other groups to generate quantitative, composition-resolved aerosol concentrations. Background tropospheric concentrations of climate-relevant aerosol including mineral dust, sea salt, and biomass burning particles are the primary foci for the ATom campaigns. PALMS also provides a variety of compositional tracers to identify aerosol sources, probe mixing state, track particle aging, and investigate convective transport and cloud processing. Additional information can be found in Froyd et al. (2019) and on the ESPO PALMS Instrument page.

6. Data Access

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

ATom: Measurements from Particle Analysis By Laser Mass Spectrometry (PALMS)

Contact for Data Center Access Information:

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- Telephone: +1 (865) 241-3952

7. References

Froyd, K.D., D.M. Murphy, C.A. Brock, P. Campuzano-Jost, J.E. Dibb, J.-L. Jimenez, A. Kupc, A.M. Middlebrook, G.P. Schill, K.L Thornhill, C.J. Williamson, J.C. Wilson, and L.D. Ziemba. 2019. A new method to quantify mineral dust and other aerosol species from aircraft platforms using single-particle mass spectrometry. Atmospheric Measurement Techniques 12:6209-6239. https://doi.org/10.5194/amt-12-6209-2019