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ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols, Version 2

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Documentation Revision Date: 2022-07-25

Dataset Version: 2.0

Summary

This dataset provides information on greenhouse gases and human-produced air pollution, including atmospheric concentrations of carbon dioxide (CO_2), methane (CH_4), tropospheric ozone (O_3), and black carbon (BC) aerosols, collected during airborne campaigns conducted by NASA's Atmospheric Tomography (ATom) mission. This dataset includes merged data from all instruments plus additional data such as numbered profiles and distance flown. Merged data products have been created for seven different aggregation intervals (1 second, 10 seconds, and 5 instrument-specific intervals). In the case of data obtained over longer time intervals (e.g., flask data), the merge files provide (weighted) averages to match the sampling intervals. This comprehensive dataset will be used to improve the representation of chemically reactive gases and short-lived climate forcers in global models of atmospheric chemistry and climate.

ATom deployed an extensive gas and aerosol payload on the NASA DC-8 aircraft for a systematic, global-scale sampling of the atmosphere, profiling continuously from 0.2–12 km altitude. Flights occurred in each of the four seasons from 2016 to 2018. Flights originate from the Armstrong Flight Research Center in Palmdale, California, fly north to the western Arctic, south to the South Pacific, east to the Atlantic, north to Greenland, and return to California across central North America. ATom established a single, contiguous, global-scale dataset. Profiles of the reactive gases will also provide critical information for the validation of satellite data, particularly in remote areas where in situ data is lacking. Complete aircraft flight information including, but not limited to, latitude, longitude, and altitude are also provided. This data release provides results from all instruments on all four ATom flight campaigns.

This is Version 2 of this dataset. All previously released data were updated to the latest available versions. For details, see Section 8. Dataset Revisions.

This dataset includes 28 data files in netCDF (*.nc) format. Files are organized by merge type (based on sampling interval) and airborne campaign (i.e., Atom-1, 2, 3, or 4).
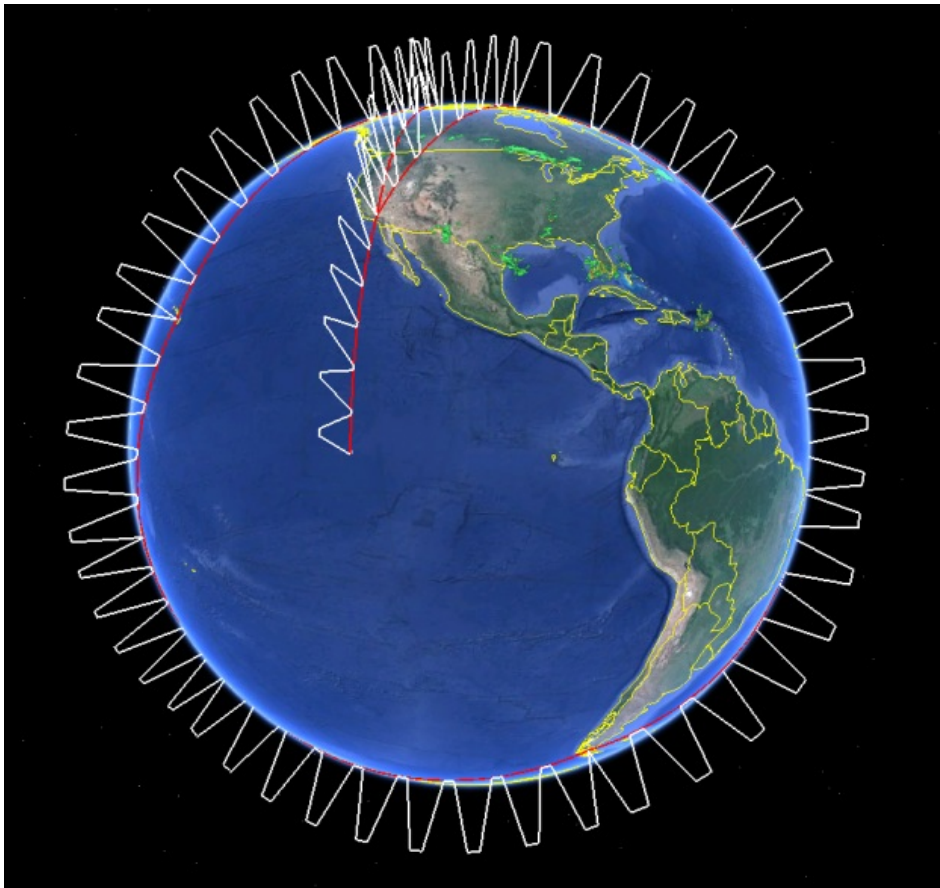
Figure 1. Generalized overview of ATom flights. During each of the four campaigns, ATom flights originated from California, flew south over the Pacific Ocean, then north to the western Arctic, southwest to New Zealand, east to Chile and the Atlantic Ocean, north to Greenland, and returned to California across North America. The aircraft continuously profiled the atmosphere from 0.2 to 12 km altitude.

Citation

Table of Contents

1. Dataset Overview

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critical information for the validation of satellite data, particularly in remote areas where in situ data is lacking. Complete aircraft flight information including, but not limited to, latitude, longitude, and altitude are also provided. This data release provides results from all instruments on all four ATom flight campaigns.

This is Version 2 of this dataset. All previously released data were updated to the latest available versions. For details, see Section 8. Dataset Revisions.

Project: Atmospheric Tomography Mission

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, J. Bent, H. Bian, B.C. Biggs, D.R. Blake, N. Blake, I. Bourgeois, C.A. Brock, W.H. Brune, J.W. Budney, T.P. Bui, A. Butler, P. Campuzano-Jost, C.S. Chang, M. Chin, R. Commane, G. Correa, J.D. Crounse, P. D. Cullis, B.C. Daube, D.A. Day, J.M. Dean-Day, J.E. Dibb, J.P. DiGangi, G.S. Diskin, M. Dollner, J.W. Elkins, F. Erdesz, A.M. Fiore, C.M. Flynn, K.D. Froyd, D.W. Gesler, S.R. Hall, T.F. Hanisco, R.A. Hannun, A.J. Hills, E.J. Hintsa, A. Hoffman, R.S. Hornbrook, L.G. Huey, S. Hughes, J.L. Jimenez, B.J. Johnson, J.M. Katich, R.F. Keeling, M.J. Kim, A. Kupc, L.R. Lait, J.-F. Lamarque, J. Liu, K. McKain, R.J. Mclaughlin, S. Meinardi, D.O. Miller, S.A. Montzka, F.L. Moore, E.J. Morgan, D.M. Murphy, L.T. Murray, B.A. Nault, J.A. Neuman, P.A. Newman, J.M. Nicely, X. Pan, W. Paplawsky, J. Peischl, M.J. Prather, D.J. Price, E.A. Ray, J.M. Reeves, M. Richardson, A.W. Rollins, K.H. Rosenlof, T.B. Ryerson, E. Scheuer, G.P. Schill, J.C. Schroder, J.P. Schwarz, J.M. St.Clair, S.D. Steenrod, B.B. Stephens, S.A. Strode, C. Sweeney, D. Tanner, A.P. Teng, A.B. Thames, C.R. Thompson, K. Ullmann, P.R. Veres, N. Vieznor, N.L. Wagner, A. Watt, R. Weber, B. Weinzierl, P.O. Wennberg, C.J. Williamson, J.C. Wilson, G.M. Wolfe, C.T. Woods, and L.H. Zeng. 2018. ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1581

- Version 1.5 of the current dataset. Now superseded and available only upon request.

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 format

HIAPER Pole-to-Pole Observations (HIPPO) of Carbon Cycle and Greenhouse Gases Study (2009-2011). Data available at https://www.eol.ucar.edu/field_projects/hippo

- HIPPO project homepage. HIPPO measured cross sections of atmospheric concentrations approximately pole-to-pole, from the surface to the tropopause, five times during different seasons over a three-year period. A comprehensive suite of atmospheric trace gases pertinent to understanding the Carbon Cycle was measured.

Acknowledgments

Table 1. The ATom team would like to thank the following individuals for their contributions to the success of the ATom Mission.

Contributor	Affiliation
Science Team	
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A. Webster	NASA Armstrong Flight Research Center and BAERI
B. Wehr	NASA Armstrong Flight Research Center
R. Williams	NASA Armstrong Flight Research Center
J. Wilson	NASA Armstrong Flight Research Center and Jacobs Technology, Inc.

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: Native resolution ranges from <1–2 seconds, depending on instrument and flight. Merge files present the data from different instruments averaged to various time bases, including 10-seconds and 1-second.

Data File Information

This dataset includes 28 data files in netCDF (*.nc) format. Files are organized by merge type (based on aggregation interval; Table 3) and flight campaign (ATom-1, 2, 3, or 4). The netCDF files are structured as GeoTrajectory, where the observations for a flight segment are connected along a one-dimensional track in space, with time increasing monotonically along the track.

The files are named according to their merge type and flight date as MER-TYPE_DC8_ATom-N.nc, where

- MER-TYPE = merge type (Table 3)
- ATom-N = flight campaign, either ATom-1, 2, 3, or 4

Table 3. Merge Types. Instrument acronyms are listed in Table 5.

Merge Type	Averaging Interval	Description
MER-1HZ	1 second	Merge of measurement data at 1-second intervals across all instruments
MER-MED	25 seconds	Data merged to MEDUSA sampling interval
MER-PFP	Between 5–40 minutes	Data merged to PFP sampling interval
MER-SAGA-AERO	Between 8–25 minutes	Data merged to SAGA-AERO sampling interval
MER-TOGA	120 seconds	Data merged to TOGA sampling interval, from 1-second merge file
MER-WAS	Between 120–200 seconds	Data merged to WAS sampling interval
MER10	10 seconds	Merge of measurement data at 10-second intervals across all instruments

Data File Details

There are over 450 individual variables measured by the 25 instruments onboard the NASA DC-8. A list of all data variables is provided in the companion file ALLNAMES.txt and in the header information of the netCDF files.

Table 4. Companion files that are included in this dataset.

File Name	Description
ALLNAMES.txt	A list of all data variables included in the merge files
ATom_merge.pdf	A PDF copy of this user guide
ATom_merging_Rcode_20210804.pdf	R code used to create ATom merge ICARTT files The ORNL DAAC subsequently converted the ICARTT files to the provided netCDF format.

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 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 instrument. 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.
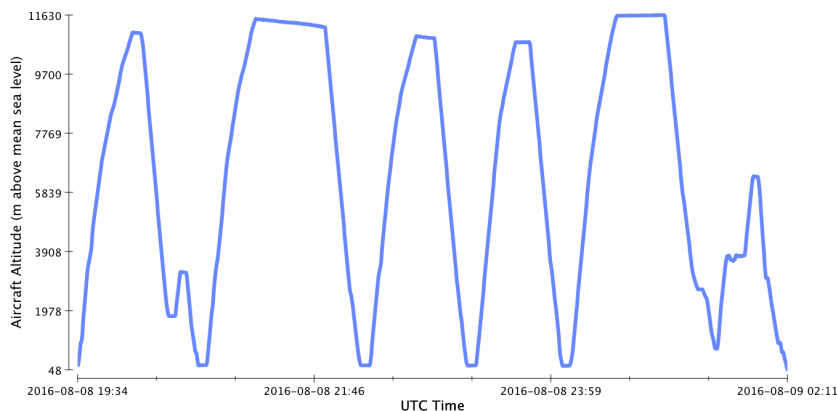

Figure 2. ATom flights continuously sampled atmospheric profiles. In this flight from Pago Pago, American Samoa to Christchurch, New Zealand, on August 8, 2016, the aircraft sampled 12 vertical profiles from about 50 to 11,000 meters above mean sea level. ATom measures more than 100 distinct chemical, aerosol, radiative, and physical parameters. Fast instrument sampling rates provide spatially resolved, simultaneous, and contiguous observational data, providing a nearly complete chemical description of each air parcel.

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.

Table 5. Instruments on board the NASA DC-8 for ATom campaigns, their measurements, and associated variable groups in netCDF data files. Additional information about each instrument and the DC-8 platform is available at https://espo.nasa.gov/atom/instruments.

Instrument	Full Name	Investigator	Type	Measurements	Variable Group in netCDF Files
AMP	In Situ Measurements of Aerosol Microphysical Properties	Charles Brock	Spectrometer (in situ)	Aerosol Size Distribution	NAerosol, SDAerosol
AO2	NCAR Airborne Oxygen Instrument	Britton Stephens		O_2, CO_2	AO2
ATHOS	Airborne Tropospheric Hydrogen Oxides Sensor	William H. Brune	Fluorescence	OH, Naphthalene, HO_2, NO	ATHOS-HOx, ATHOS-OHI, ATHOS-OHR
CAFS	Charged-coupled device Actinic Flux Spectroradiometers	Samuel R. Hall	Spectrometer (in situ)	Spectrally resolved actinic flux and photolysis frequencies typically calculated for the following species: O_3, NO_2, NO_3, CH_2O, HONO, HNO_3, N_2O_5, HNO_4, PAN, H_2O_2, CH_3OOH, CH_3ONO_2, $CH_3CH_2ONO_2$, CH_3CHO, CH_3CH_2CHO, CHOCHO, CH_3COCHO, 3-Butanedione, Methacrolein, MVK, $(CH_3)_2CO$, MEK, Br_2, BrO, BrNO, $BrNO_2$, $BrONO$, $BrONO_2$, BrCl, HOBr, $CHBr_3$, Cl_2, ClO, $ClNO_2$, ClONO, $ClONO_2$	CAFS-JV
CAPS Vienna	Cloud Aerosol and Precipitation Spectrometer (University of Vienna)	Bernadett Weinzierl		Aerosol, Particle size distribution, Cloud Liquid Water Content	Cloudindicator, NCoarseAerosol

CIT-CIMS	Chemical Ionization Mass Spectrometer (California Institute of Technology)	Paul Wennberg	Chemical Ionization Mass Spectrometer	HNO3, H2O2, CH3OOH, HCN, PAA, PNA, SO2	CIT-H2O2, CIT-HCN, CIT-HNO3, CIT-MHP, CIT-PAA, CIT-PNA, CIT-SO2
DLH	Diode Laser Hygrometer	Glenn S. Diskin	Laser absorption	H2O	DLH-H2O
GT-CIMS	Chemical Ionization Mass Spectrometer (Georgia Tech)	L. Greg Huey	Chemical Ionization Mass Spectrometer	HNO3, SO2, HNO4, HCl, Br2, BrO, PAN	GTCIMSPANS
HR-AMS	Aircraft High-Resolution Time-of-Flight Aerosol Mass Spectrometer (University of Colorado, Boulder)	Jose-Luis Jimenez	Spectrometer (in situ)	Organic Aerosol, NH4, NO3, SO4, NR-Cl, Br-, Iodine, seasalt, MSA, ClO4, pRONO2	AMS, AMSSD
ISAF	In Situ Airborne Formaldehyde	Glenn M. Wolfe	Fluorescence	CH2O	ISAF-H2CO
LIF-SO2	Laser Induced Fluorescence - Sulfur Dioxide	Andrew Rollins	Fluorescence	SO2	SO2-LIF
Medusa	Medusa Whole Air Sampler	Britton Stephens	Whole Air Sampling	O2, CO2, N2, Argon, CO2 isotopes	MEDUSA MEDUSA-Kernel
MMS	Meteorological Measurement System	T. Paul Bui		3D Wind, Turbulence, Temperature, Position, Velocities, Attitudes, True-Airspeed, Potential Temperature	MMS
NOAA Picarro	NOAA Picarro	Kathryn McKain	Spectrometer (in situ)	CO2, CH4, CO	NOAA-Picarro
NOAA ToF CIMS	NOAA Iodide Ion Time-of-Flight Chemical Ionization Mass Spectrometer	J. Andy Neuman	Chemical Ionization Mass Spectrometer	HCOOH, ClNO2, N2O5, BrO, Cl2, BrCN, BrCl, C2H4O3S	NOAACIMS-BrCN, NOAACIMS-BrCl, NOAACIMS-BrO, NOAACIMS-C2H4O3S, NOAACIMS-Cl2, NOAACIMS-ClNO2, NOAACIMS-HCOOH, NOAACIMS-N2O5
NOyO3	NOAA Nitrogen Oxides and Ozone	Thomas B Ryerson	Chemiluminescence	NO, NO2, NOy, O3	NOyO3-NO, NOyO3-NO2, NOyO3-NOy, NOyO3-O3
PALMS	Particle Analysis By Laser Mass Spectrometry	Gregory Schill	Spectrometer (in situ)	Particle Composition, Aerosol	PALMS, PALMS-PartType-Mass, PALMS-Chem-Mass
PANTHER	PAN and Trace Hydrohalocarbon ExpeRiment	James W. Elkins	Gas chromatography	(CH3)2CO, PAN, H2, CH4, CO, N2O, SF6, CFCl3, CF2Cl2, Halon-1211	GCECD, GCMSD
PFP	Programmable Flask Package Whole Air Sampler	Stephen (Steve) Montzka	Whole Air Sampling	N2O, SF6, H2, CS2, OCS, CO2, CH4, CO, CFCs, HCFCs, HFCs, Solvents, Methyl Halides, Hydrocarbons, Perfluorocarbons	PFP

QCLS	Quantum Cascade Laser System	Bruce Daube	Laser absorption	CO2, CO, CH4, N2O		QCLS-CH4-CO-N2O, QCLS-CO2
SAGA	Soluble Acidic Gases and Aerosols	Jack Dibb	Ion Chromatography	Na, NH4, K, Mg, Ca+2, Cl, Br-, NO3, SO4, C2O4-2, Be-7, Pb-210, HNO3		SAGA-AERO, SAGA-MC
SP2	Single Particle Soot Photometer (NOAA)	Joshua (Shuka) Schwarz	Photometer	Black Carbon, Aerosol		SP2-BC
TOGA	Trace Organic Gas Analyzer	Eric Apel	Gas chromatography, Spectrometer (in situ)	VOCs		TOGA
UCATS	UAS Chromatograph for Atmospheric Trace Species	Brad Hall	Gas chromatography, Spectrometer (in situ)	N2O, SF6, CH4, CO, O3, H2, H2O, CHCl3, CCl4, CF2Cl2, CFCl3, CF2ClCFCl2, Halon-1211		UCATS-GC, UCATS-H2O, UCATS-O3
WAS (UCI)	Whole Air Sampler (University of California, Irvine)	Donald R. Blake	Whole Air Sampling	NMHCs, Halocarbons, Alkyl Nitrates, OCS, DMS, CS2		WAS
GEOS5		Paul Newman	Weather Analysis and Prediction Model	GEOS5 forward processing meteorological products interpolated to the flight track: winds, vorticity, humidity, temperature, simply specified tracers (CO, SO2, many aerosol types)		GEOS5
GMI		Sarah Strode	Chemistry-Transport Model	GMI full chemistry CTM hindcast: gas-phase chemistry (40 species) along 10-sec merge, interpolated to the flight track		GMI

ATom is closely linked to satellites measuring atmospheric chemical composition: (i) ATom provides unique data for validation and algorithm development for OCO-2, GOME-2, TROPOMI, GOSAT, plus those planned for geostationary orbit (TEMPO), and the TCCON network. (ii) ATom uses satellite data to extend its airborne in-situ observations to a global scale. (iii) ATom directly engages CCM groups and delivers a single, large-scale, contiguous in-situ dataset for model evaluation and improvement.

Merge File Methods

This dataset includes merged data from all instruments. A variety of merged file types have been created for each flight date. The merge files include additional data such as numbered profiles and distance flown. In the case of data obtained over longer time intervals (e.g., flask data), the merge files provide (weighted) averages of 1-second data to match the sampling intervals. The ICARTT file merge procedure was performed by the ATom team. It was executed in R language and the merge script ATom_merging_Rcode_20210804.pdf)is provided as a companion file with this dataset. The merged ICARTT files were then converted to netCDF-4 format by ORNL DAAC.

For more information, see the ATom website on the NASA Earth Science Project Office (ESPO) site at https://espo.nasa.gov/atom.

6. Data Access

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

ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols, Version 2

Contact for Data Center Access Information:

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7. References

8. Dataset Revisions

Version	Release Date	Description
2.0	2022-07-26	Table 5 of the User Guide was updated to fix errors in the Measurements column.
2.0	2021-08-26	All previously-released data were updated to the latest available versions.
1.5	2020-09-24	All previously-relbrased data were updated to the latest available versions.
1.4	2019-11-25	Initial release of MER-TOGA and MER-WAS data from ATom-4 campaign. All previously-released data were updated to the latest available versions.
1.3	2019-06-14	Initial release of MER-TOGA and MER-WAS data from ATom-3 campaign. All previously-released data were updated to the latest available versions.

Version	Release Date	Description
1.2	2019-04-05	Initial release of partial ATom-3 and Atom-4 data. Data from Atom-1 and Atom-2 were updated to the latest versions.
1.1	2018-08-23	Provides updated data from ATom-1 and ATom-2 with edits to the author list, metadata, and user guide.
1.0	2018-03-28	Initial release of data from ATom-1 and ATom-2

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