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ATom: Data Stream for Modeling the Reactivity of ATom Air Parcels, 2016-2018

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Dataset Version: 1

Summary

This dataset provides Modeling Data Stream (MDS) and Reactivity Data Stream (RDS) products for each of the four ATom campaigns conducted from 2016 to 2018. MDS files contain the atmospheric constituents needed to model the RDS of the air parcels along ATom flight paths. The MDS is a continuous data stream (every 10 seconds) of the atmospheric content of these key chemical species derived from the in-situ measurements collected along ATom flight paths (as reported in the comprehensive related dataset ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols). Values for chemical species measured by multiple instruments were selected from the instrument with better coverage and/or greater precision. Missing values were filled using interpolation for short gaps. For long gaps owing to instrument failure, values were estimated using multiple linear regressions from comparable parallel flights from other ATom campaigns. All species were flagged for instrument source and values were flagged for gap-filling status. In combination, MDS and RDS provide, in essence, a photochemical climatology for each air parcel along ATom flight paths containing the reactive species that control the loss of methane and the production and loss of ozone.

There are 8 data files in ICARTT (*.ict) format and 2 data files in netCDF format (*.nc) included in this dataset. Also included are two companion files in comma-separated values (*.csv) format.

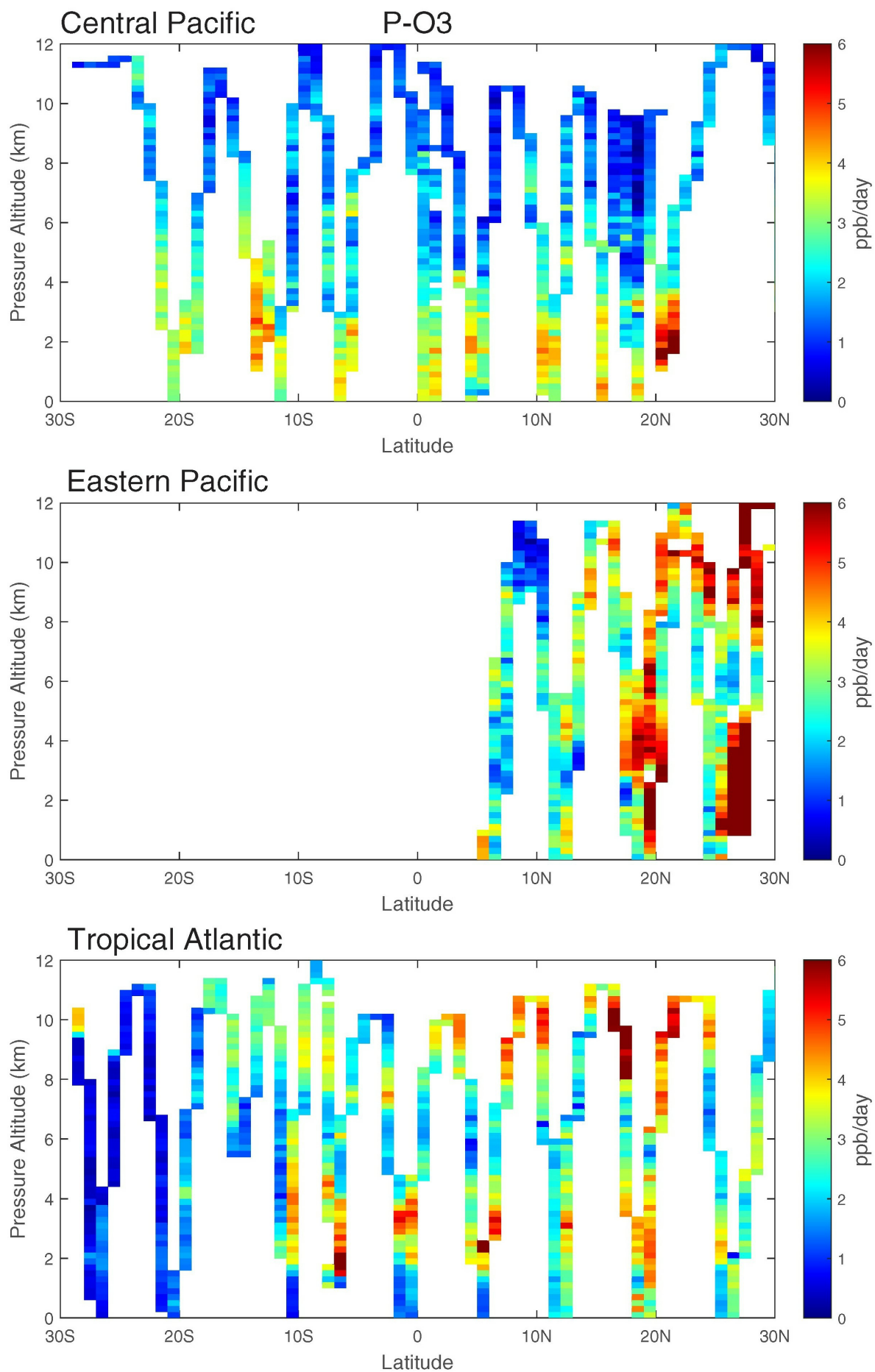


Figure 1. Curtain plots for production of ozone from the ATom-1 campaign in the Central Pacific (top), Eastern Pacific (middle), and Atlantic (bottom). The 10 s air parcels are averaged into 10-degree latitude and 200 m altitude bins. Reactivities, such as P-O3, are calculated for each 10 s air parcel from the Modeling Data Stream (MDS), Version 2, using the UC Irvine chemistry-transport model (CTM) with HNO₄ and PAN damped by thermal decomposition. Source: Guo et al. (2021)

Citation

Guo, H., C.M. Flynn, M.J. Prather, S.A. Strode, S.D. Steenrod, L. Emmons, F. Lacey, J.-F. Lamarque, A.M. Fiore, G. Correa, L.T. Murray, G.M. Wolfe, J.M. St.Clair, M.J. Kim, J.D. Crouse, G.S. Diskin, J.P. DiGangi, B.C. Daube, R. Commane, K. McKain, J. Peischl, T.B. Ryerson, C.R. Thompson, T.F. Hanisco, D.R. Blake, N. Blake, E.C. Apel, R.S. Hornbrook, J.W. Elkins, E.J. Hints, F.L. Moore, and S.C. Wofsy. 2022. ATom: Data Stream for Modeling the Reactivity of ATom Air Parcels, 2016-2018. ORNL DAAC, Oak Ridge, Tennessee, USA. <https://doi.org/10.3334/ORNLDAAC/1877>

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1. Dataset Overview

This dataset provides Modeling Data Stream (MDS) and Reactivity Data Stream (RDS) products for each of the four ATom campaigns conducted from 2016 to 2018. MDS files contain the atmospheric constituents needed to model the RDS of the air parcels along ATom flight paths. The MDS is a continuous data stream (every 10 seconds) of the atmospheric content of these key chemical species derived from the in-situ measurements collected along ATom flight paths (as reported in the comprehensive related dataset ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols). Values for chemical species measured by multiple instruments were selected from the instrument with better coverage and/or greater precision. Missing values were filled using interpolation for short gaps. For long gaps owing to instrument failure, values were estimated using multiple linear regressions from comparable parallel flights from other ATom campaigns. All species were flagged for instrument source and values were flagged for gap-filling status. In combination, MDS and RDS provide, in essence, a photochemical climatology for each air parcel along ATom flight paths containing the reactive species that control the loss of methane and the production and loss of ozone.

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 a 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 Publication

Guo, H., C. M. Flynn, M. J. Prather, S. A. Strode, S. D. Steenrod, L. Emmons, F. Lacey, J.-F. Lamarque, A. M. Fiore, G. Correa, L. T. Murray, G. M. Wolfe, J. M. St. Clair, M. Kim, J. Crouse, G. Diskin, J. DiGangi, B. C. Daube, R. Commane, K. McKain, J. Peischl, T. B. Ryerson, C. Thompson, T. F. Hanisco, D. Blake, N. J. Blake, E. C. Apel, R. S. Hornbrook, J. W. Elkins, E. J. Hints, F. L. Moore, and S. Wofsy. 2021. Heterogeneity and Chemical Reactivity of the Remote Troposphere defined by Aircraft Measurements. *Atmospheric Chemistry and Physics*, 21, 13729–13746. <https://doi.org/10.5194/acp-21-13729-2021>.

Related Datasets

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>

- Flight path (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

Campaign	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: 10 seconds

Data File Information

There are 8 data files in ICARTT (*.ict) format and 2 data files in netCDF format (*.nc) included in this dataset. The data files conform to the [ICARTT File Format Standards V1.1](#) or [CF Conventions](#). Also included are two companion files in comma-separated values (*.csv) format. There is one ICARTT file for each of the four ATom campaigns and each data type. The ICARTT files are named **XXX_DC8_YYYYMMDD_R#.ict**, where **XXX** is the type of data ("MDS" or "RDS"), **YYYYMMDD** is the start date (in UTC time) of the flight, and **R #** is the file version or revision number.

Table 1. File names and descriptions.

File Name	Description
Data Files	
ATom_MDS.nc	Aggregated data from the four files named MDS_DC8_YYYYMMDD_R#.ict
ATom_RDS.nc	Aggregated data from the four files named RDS_DC8_YYYYMMDD_R#.ict
MDS_DC8_YYYYMMDD_R#.ict	Contains the Modeling Data Stream (MDS) data, a continuous data stream of atmospheric constituents needed to model the RDS of the air parcels along flight paths
RDS_DC8_YYYYMMDD_R#.ict	Contains the Reactivity Data Stream (RDS) data, that uses the MDS data to calculate the reactivities of the air parcels
Companion Files	
ATom_MDS_ICARTT_data_dictionary.csv	Contains the data dictionary for the four files named MDS_DC8_YYYYMMDD_R#.ict
ATom_MDS_NetCDF_data_dictionary.csv	Contains the data dictionary for the file ATom_MDS.nc

Data File Details

Missing data are indicated by -99999.

The data dictionaries for the four files named MDS_DC8_YYYYMMDD_R#.ict and the file ATom_MDS.nc are contained in the two companion files (Table 1), whereas the data dictionaries for the four files named RDS_DC8_YYYYMMDD_R#.ict the file ATom_RDS.nc are provided in Tables 2 and 3, respectively.

Table 2. Variable names and descriptions in data files named RDS_DC8_YYYYMMDD_R#.ict.

Variable	Units	Description
ATom_parcel	Numeric	Unique number for each air parcel
Start_UTC	Seconds	Start time in seconds since 0000 UTC
Stop_UTC	Seconds	Stop time in seconds since 0000 UTC
Latitude	Decimal degrees	Latitude
Longitude	Decimal degrees	Longitude
Pressure	mb	Pressure
O3_Pmean	ppb/day	O3 production reactivity mean over 5 days per parcel
O3_Pstd	ppb/day	O3 production reactivity standard deviation over 5 days per parcel
O3_Lmean	ppb/day	O3 loss reactivity mean over 5 days per parcel
O3_Lstd	ppb/day	O3 loss reactivity standard deviation over 5 days per parcel
CH4_Lmean	ppb/day	CH4 reactivity mean over 5 days per parcel
CH4_Lstd	ppb/day	CH4 reactivity standard deviation over 5 days per parcel
J_O1Dmean	1e-5/s/day	O1D J-value mean over 5 days per parcel
J_O1Dstd	1e-5/s/day	O1D J-value standard deviation over 5 days per parcel
J_NO2mean	1e-5/s/day	NO2 J-value mean over 5 days per parcel
J_NO2std	1e-5/s/day	NO2 J-value standard deviation over 5 days per parcel

Table 3. Variable names and descriptions for the file ATom_RDS.nc.

Variable	Units	Description
parcel	Numeric	parcel #, a unique MDS & RDS id
UTC__R	Seconds	Second of the day in UTC time
IStrat		Location in atmosphere, 0=troposphere, 1=stratosphere
Lat__R	Degrees north	Latitude
Lng__R	Degrees east	Longitude
Pres_R	hPa	Pressure
P-O3	ppb/day	O3 production reactivity mean over 5 days per parcel
P-O3s	ppb/day	O3 production reactivity standard deviation over 5 days per parcel
L-O3	ppb/day	O3 loss reactivity mean over 5 days per parcel
L-O3s	ppb/day	O3 loss reactivity standard deviation over 5 days per parcel

L-CH4	ppb/day	CH4 reactivity mean over 5 days per parcel
L-CH4s	ppb/day	CH4 reactivity standard deviation over 5 days per parcel
J-O1D	1e-5/s	O1D J-value mean over 5 days per parcel
J-O1Ds	1e-5/s	O1D J-value standard deviation over 5 days per parcel
J-NO2	1e-3/s	NO2 J-value mean over 5 days per parcel
J-NO2s	1e-3/s	NO2 J-value standard deviation over 5 days per parcel
SolLat	Degrees	Solar latitude (deg) =lat-dec

3. Application and Derivation

ATom builds the scientific foundation for mitigation of short-lived climate forcers, in particular, methane (CH₄), tropospheric ozone (O₃), and Black Carbon aerosols (BC).

ATom Science Questions

Tier 1

- What are chemical processes that control the short-lived climate forcing agents CH₄, O₃, 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 Chemistry-Climate Models (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

Information on quality is not available.

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 Chemistry-Climate Models (CCMs). ATom also differentiates between hypotheses for the formation and growth of aerosols over the remote oceans.

Modeling Data Stream and Reactivity Data Stream

The Modeling Data Stream (MDS) provides a data stream (every 10s along ATom flight paths) that has all the key species needed to model the reactivity of the air parcels. An MDS is provided for each ATom campaign. The MDS is a continuous data stream atmospheric content of these key species derived from in situ measurements collected along ATom flight paths and reported in the comprehensive ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols product (Wofsy et al., 2018). A minimally intrusive method was used to interpolate data with gaps >10s. For large gaps due to instrument failure, values were estimated using multiple linear regressions from parallel flights from other ATom campaigns compared against pressure, noontime solar zenith angle, and latitude. Values for species measured by multiple instruments were selected from the instrument with better coverage and/or greater precision. The Reactivity Data Stream (RDS) uses the MDS to calculate the reactivities of the air parcels. In combination, MDS and RDS provide a photochemical climatology for each air parcel along ATom flight paths containing the reactive species that control the loss of methane and the production and loss of ozone. Additional information regarding the modeling approach can be found in Guo et al. (2021) and Prather et al. (2017).

6. Data Access

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

[ATom: Data Stream for Modeling the Reactivity of ATom Air Parcels, 2016-2018](#)

Contact for Data Center Access Information:

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7. References

Guo, H., C. M. Flynn, M. J. Prather, S. A. Strode, S. D. Steenrod, L. Emmons, F. Lacey, J.-F. Lamarque, A. M. Fiore, G. Correa, L. T. Murray, G. M. Wolfe, J. M. St. Clair, M. Kim, J. Crouse, G. Diskin, J. DiGangi, B. C. Daube, R. Commane, K. McKain, J. Peischl, T. B. Ryerson, C. Thompson, T. F. Hanisco, D. Blake, N. J. Blake, E. C. Apel, R. S. Hornbrook, J. W. Elkins, E. J. Hints, F. L. Moore, and S. Wofsy. 2021. Heterogeneity and Chemical Reactivity of the Remote Troposphere defined by Aircraft Measurements. *Atmospheric Chemistry and Physics* 21:13729–13746. <https://doi.org/10.5194/acp-21-13729-2021>

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