ATom: Volatile Organic Compounds (VOCs) from the TOGA instrument, Version 2

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Documentation Revision Date: 2021-11-29

Dataset Version: 2

Summary

This dataset provides concentrations of volatile organic compounds (VOCs) measured by the Trace Organic Gas Analyzer (TOGA) during the four ATom campaigns. These data are relevant to the impact of human-produced air pollution on greenhouse gases and on chemically reactive gases in the atmosphere. Specific data were obtained for radical precursors, tracers of anthropogenic and biogenic activities, tracers of urban and biomass combustion emissions, products of oxidative processing, precursors to aerosol formation, and compounds important for aerosol modification and transformation. TOGA measures a wide range of VOCs with high sensitivity (ppt or lower), frequency (2-minutes), accuracy (often 15% or better), and precision (<3%).

This is Version 2 of this dataset. This version contains updated data files from the ATom-4 campaign. No changes were made to files from the other ATom campaigns. For additional details see Section 8. Dataset Revisions.

There are 47 data files in ICARTT (*.ict) format included in this dataset.

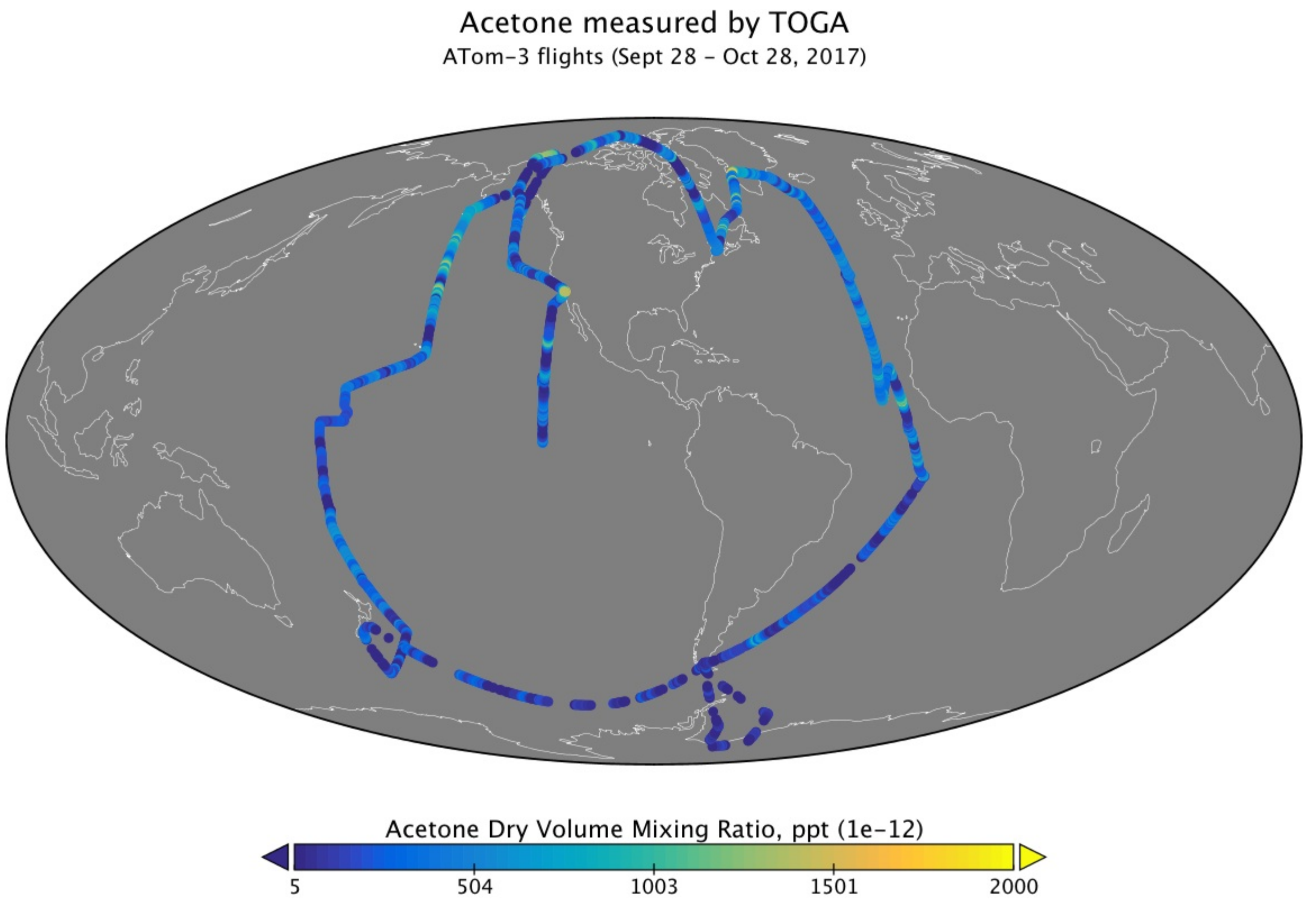

Figure 1. Measurements of atmospheric acetone concentration from samples collected by the Trace Organic Gas Analyzer (TOGA) during ATom-3 flights in 2017.

Citation

Apel, E.C., E.C. Asher, A.J. Hills, and R.S. Hornbrook. 2021. ATom: Volatile Organic Compounds (VOCs) from the TOGA instrument, Version 2. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1936

Table of Contents

1. Dataset Overview

This dataset provides concentrations of volatile organic compounds (VOCs) measured by the Trace Organic Gas Analyzer (TOGA) during the four ATom campaigns. Specific data were obtained for radical precursors, tracers of anthropogenic and biogenic activities, tracers of urban and biomass combustion emissions, products of oxidative processing, precursors to aerosol formation, and compounds important for aerosol modification and transformation. TOGA measures a wide range of VOCs with high sensitivity (ppt or lower), frequency (2-minutes), accuracy (often 15% or better), and precision (<3%).

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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 Datasets

Apel, E.C., E.C. Asher, A.J. Hills, and R.S. Hornbrook. 2019. ATom: L2 Volatile Organic Compounds (VOCs) from the Trace Organic Gas Analyzer (TOGA). ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1749

- Version 1 of this dataset. Now superseded and available only upon request.

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, 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.L. Wagner, A. Watt, R. Weber, B.B. Weinzierl, P.O. Wennberg, C.J. Williamson, J.C. Wilson, G.M. Wolfe, C.T. Woods, L.H. Zeng, and N. Vieznor. 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

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: 120 seconds (35-second integrated sampling time for each measurement)

Data File Information

There are 47 data files in ICARTT (*.ict) format included in this dataset that contain concentrations of volatile organic compounds (VOCs). Data files conform to the ICARTT File Format Standards V1.1. Files are named TOGA_DC8_**YYYYMMDD_R#**.ict where **YYYYMMDD** is the start date (in UTC time) of the flight and **R#** is the file version or revision number.

Data File Details

No data values are indicated by -999, and data values below the detection limit are indicated by -888.

Table 1. Variable names and descriptions.

Name	Units	Description
Time_Start	seconds	Start time in seconds since 0000 UTC

Time_Stop	seconds	End time in seconds since 0000 UTC
CFC11_TOGA	ppt	CFC-11 gas dry volume mixing ratio
CFC113_TOGA	ppt	CFC-113 gas dry volume mixing ratio
CH3Cl_TOGA	ppt	Methyl chloride gas dry volume mixing ratio
CH2Cl2_TOGA	ppt	Dichloromethane gas dry volume mixing ratio
CHCl3_TOGA	ppt	Chloroform gas dry volume mixing ratio
C2Cl4_TOGA	ppt	Tetrachloroethene gas dry volume mixing ratio
ClBenzene_TOGA	ppt	Chlorobenzene gas dry volume mixing ratio
CHBrCl2_TOGA	ppt	Bromodichloromethane gas dry volume mixing ratio
CHBr2Cl_TOGA	ppt	Dibromochloromethane gas dry volume mixing ratio
CH3Br_TOGA	ppt	Methyl bromide gas dry volume mixing ratio
CH2Br2_TOGA	ppt	Dibromomethane gas dry volume mixing ratio
CHBr3_TOGA	ppt	Bromoform gas dry volume mixing ratio
CH2ClI_TOGA	ppt	Chloroiodomethane gas dry volume mixing ratio
CH2BrI_TOGA	ppt	Bromoiodomethane gas dry volume mixing ratio
CH3I_TOGA	ppt	Methyl iodide gas dry volume mixing ratio
CH2I2_TOGA	ppt	Diiodomethane gas dry volume mixing ratio
Propane_TOGA	ppt	Propane gas dry volume mixing ratio
iButane_TOGA	ppt	Isobutane gas dry volume mixing ratio
nButane_TOGA	ppt	n-Butane gas dry volume mixing ratio
iPentane_TOGA	ppt	Isopentane gas dry volume mixing ratio
nPentane_TOGA	ppt	n-Pentane gas dry volume mixing ratio
x2MePentane_TOGA	ppt	2-Methylpentane gas dry volume mixing ratio
x3MePentane_TOGA	ppt	3-Methylpentane gas dry volume mixing ratio
nHexane_TOGA	ppt	n-Hexane gas dry volume mixing ratio
x224TrimePentane_TOGA	ppt	2,2,4-Trimethylpentane gas dry volume mixing ratio
nHeptane_TOGA	ppt	n-Heptane gas dry volume mixing ratio
iButene1Butene_TOGA	ppt	Isobutene + 1-Butene gas dry volume mixing ratio
Isoprene_TOGA	ppt	Isoprene gas dry volume mixing ratio
Benzene_TOGA	ppt	Benzene gas dry volume mixing ratio
Toluene_TOGA	ppt	Toluene gas dry volume mixing ratio
EthBenzene_TOGA	ppt	Ethylbenzene gas dry volume mixing ratio
mpXylene_TOGA	ppt	m-Xylene + p-Xylene gas dry volume mixing ratio
oXylene_TOGA	ppt	o-Xylene gas dry volume mixing ratio
aPinene_TOGA	ppt	alpha-Pinene gas dry volume mixing ratio
Tricyclene_TOGA	ppt	Tricyclene gas dry volume mixing ratio
Camphene_TOGA	ppt	Camphene gas dry volume mixing ratio
bPineneMyrcene_TOGA	ppt	beta-Pinene + Myrcene gas dry volume mixing ratio
LimoneneD3Carene_TOGA	ppt	Limonene + D3-Carene gas dry volume mixing ratio
CH2O_TOGA	ppt	Formaldehyde gas dry volume mixing ratio
CH3CHO_TOGA	ppt	Acetaldehyde gas dry volume mixing ratio
Propanal_TOGA	ppt	Propanal gas dry volume mixing ratio
Butanal_TOGA	ppt	Butanal gas dry volume mixing ratio
Acrolein_TOGA	ppt	Acrolein gas dry volume mixing ratio
MAC_TOGA	ppt	Methacrolein gas dry volume mixing ratio
Acetone_TOGA	ppt	Acetone gas dry volume mixing ratio
MEK_TOGA	ppt	Methyl ethyl ketone gas dry volume mixing ratio
MVK_TOGA	ppt	Methyl vinyl ketone gas dry volume mixing ratio
CH3OH_TOGA	ppt	Methanol gas dry volume mixing ratio
C2H5OH_TOGA	ppt	Ethanol gas dry volume mixing ratio

MTBE_TOGA	ppt	Methyl tert-butyl ether gas dry volume mixing ratio
DMS_TOGA	ppt	Dimethyl sulfide gas dry volume mixing ratio
HCN_TOGA	ppt	Hydrogen cyanide gas dry volume mixing ratio
CH3CN_TOGA	ppt	Acetonitrile gas dry volume mixing ratio
EthONO2_TOGA	ppt	Ethyl nitrate gas dry volume mixing ratio
iPropONO2_TOGA	ppt	Isopropyl nitrate gas dry volume mixing ratio

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

Table 2. Uncertainties of individual chemical species.

Species	Uncertainty
CH2Cl2	15%
CHCl3	15%
C2Cl4	15%
ClBenzene	15%
CHBrCl2	20%
CHBr2Cl	15%
CH2Br2	15%
CHBr3	30%
CH2ClI	20%
CH2BrI	30%
CH3I	50%
CH2I2	40%
Propane	30%
iButane	15%
nButane	15%
iPentane	15%
nPentane	15%
x2MePentane	15%
x3MePentane	15%
nHexane	15%
x224TrimePentane	15%
nHeptane	30%
iButene1Butene	20%

Isoprene	15%
Benzene	15%
Toluene	15%
EthBenzene	20%
mpXylene	20%
oXylene	20%
aPinene	30%
Tricyclene	50%
Camphene	30%
bPineneMyrcene	30%
LimoneneD3Carene	30%
CH2O	40%
CH3CHO	20%
Propanal	20%
Butanal	30%
Acrolein	30%

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 greenhouse gasses and ozone-depleting substances 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 Community Climate Models (CCM). ATom also differentiates between hypotheses for the formation and growth of aerosols over the remote oceans.

Trace Organic Gas Analyzer

The Trace Organic Gas Analyzer (TOGA) measures volatile organic compounds (VOCs). Specific data were obtained for radical precursors, tracers of anthropogenic and biogenic activities, tracers of urban and biomass combustion emissions, products of oxidative processing, precursors to aerosol formation, and compounds important for aerosol modification and transformation. TOGA measures a wide range of VOCs with high sensitivity (ppt or lower), frequency (2-minutes), accuracy (often 15% or better), and precision (<3%). Over 50 species were routinely measured throughout the full altitude range. The major components of the instrument are the inlet, cryogenic pre-concentrator, gas chromatograph, mass spectrometer detector, zero air/calibration system, and the control/data acquisition system. All processes and data acquisition are computer-controlled. For additional information, see Apel et al. (2010), Apel et al. (2015), and the ESPO TOGA Instrument page.

6. Data Access

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

ATom: Volatile Organic Compounds (VOCs) from the TOGA instrument, Version 2

Contact for Data Center Access Information:

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

7. References

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8. Dataset Revisions

Version	Release Date	Description
2.0	2021-11-29	Updated files for the ATom-4 campaign (2018-04-24 to 2018-05-21). Files from the other ATom campaigns were not changed.
1.0	2019-12-30	Initial release of 47 data files from the four ATom campaigns. Now superseded and available only upon request.