ATom: L2 In Situ Peroxyacetyl Nitrate (PAN) Measurements from Georgia Tech CIMS

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Documentation Revision Date: 2019-09-05

Dataset Version: 1

Summary

This dataset provides measurements of two important components of photochemical smog - peroxyacetyl nitrate (PAN) and peroxyl propionyl nitrate (PPN)- measured by the Georgia Tech Chemical Ionization Mass Spectrometer (GT-CIMS) during airborne campaigns conducted by NASA's Atmospheric Tomography (ATom) mission. The GT-CIMS measures reactive nitrogen species in the lower atmosphere. ATom deploys 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 4 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 establishes a single, contiguous, global-scale dataset. 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.

This dataset includes 21 files in comma-delimited text (ICARTT) format, with one file per flight date during the ATom-2 and ATom-3 campaigns only.

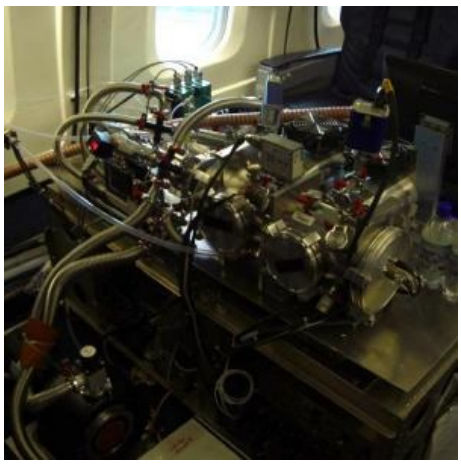

Figure 1. The Georgia Tech Chemical Ionization Mass Spectrometer (CIMS).

Citation

Huey, L.G., J.B. Nowak, D. Tanner, and S. Kim. 2019. ATom: L2 In Situ Peroxyacetyl Nitrate (PAN) Measurements from Georgia Tech CIMS. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1715

Table of Contents

1. Dataset Overview

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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

ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols. Data from all ATom instruments and all four flight campaigns, including aircraft location and navigation data, merged to several different time bases: https://doi.org/10.3334/ORNLDAAC/1581

ATom Flight Track and Navigational Data. Flight path (location and altitude) data for each of the four campaigns provided in KML and csv format: https://doi.org/10.3334/ORNLDAAC/1613

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. Note that GT-CIMS data are available for the ATom 2 & 3 campaigns only.

Table 1. Flight campaign schedule

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: 2.5 seconds

Data File Information

This dataset includes 21 files in comma-delimited text (ICARTT) format, with one file per flight date during the ATom-2 and ATom-3 campaigns. Some flight dates are missing for ATom-2. Data files conform to the ICARTT File Format Standards V1.1.

File names are structured as GTCIMSPANS_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 Variables

Missing data are indicated by -9999.

Table 2. Variables in the data files *GTCIMSPANS_DC8_YYYYMMDD_R#.ict*

Name	Units	Description
UTC_start	seconds	Start time of sample in seconds since UTC midnight on day of takeoff
UTC_stop	seconds	Stop time of sample in seconds since UTC midnight on day of takeoff
UTC_mid	seconds	Mid time of sample in seconds since UTC midnight on day of takeoff
PAN_GTCIMS	pptv	peroxyacetyl nitrate (PAN) mixing ratio in air in parts-per-trillion-by-volume
PPN_GTCIMS	pptv	peroxyl propionyl nitrate (PPN) mixing ratio in air in parts-per-trillion-by-volume

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 occur 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

Measurement Uncertainty as estimated by the authors:

PAN_GTCIMS = 20%

PPN_GTCIMS = 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 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.

Georgia Tech Chemical Ionization Mass Spectrometer (GT-CIMS)

The GT-CIMS instrument consists of a low pressure ion molecule reactor (IMR) coupled to a quadrupole mass filter by an actively pumped collisional dissociation chamber (CDC) and an octopole ion guide. The vacuum system is a 100 mm outer diameter stainless steel chamber evacuated with two small turbo pumps. The mass filter is a set of 9.5 mm diameter quadrupole rods housed in the main vacuum chamber. The CDC is a short 80 mm diameter chamber that houses an octopole ion guide and is evacuated with a hybrid molecular drag pump. The IMR is evacuated with a scroll pump that also serves as the backing pump for the mass spectrometer. More information is provided in Huey (2007).

Peroxyacyl nitrates (PANs) play an important role in tropospheric chemistry and are indicators of photochemical smog. They are toxic to the environment and can damage plants, irritate human eyes, and lead to genetic mutation.

6. Data Access

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

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Contact for Data Center Access Information:

- E-mail: uso@daac.ornl.gov
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7. References

Huey, L. G. (2007), Measurement of trace atmospheric species by chemical ionization mass spectrometry: Speciation of reactive nitrogen and future directions, Mass Spectrom Rev., 26, 166-184. https://doi.org/10.1002/mas.20118