ATom: Measurements from the Quantum Cascade Laser System (QCLS), Version 2

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Documentation Revision Date: 2021-09-23

Dataset Version: 2

Summary

This dataset provides atmospheric concentrations of CO2, CH4, CO, and N2O measured by the Harvard Quantum Cascade Laser System (QCLS) instruments during airborne campaigns conducted by NASA's Atmospheric Tomography (ATom) mission. The QCLS (DUAL and CO2) instrument package contains two separate optical assemblies and calibration systems, and a common data system and power supply. The QCLS DUAL instrument simultaneously measures CO, CH4, and N2O concentrations, in situ, using two thermoelectrically cooled pulsed-quantum cascade lasers light sources, a multiple pass absorption cell, and two liquid nitrogen-cooled solid-state detectors. The QCLS CO2 instrument measures CO2 concentrations in situ using a thermoelectrically cooled pulsed-quantum cascade laser light source, gas cells, and liquid nitrogen cooled solid-state detectors. The CO2 mixing ratio of air flowing through the sample gas cell is determined by measuring absorption from a single infrared transition line at 4.32 microns relative to a reference gas of known concentration.

This is Version 2 of this dataset. For additional details see Section 8. Dataset Revisions.

There are 94 data files in ICARTT (*.ict) format included in this dataset.

Figure 1. The Harvard QCLS (DUAL and CO2) instrument package contains two optical assemblies and calibration systems and a common data system and power supply.

Citation

Commane, R., J.W. Budney, Y. Gonzalez ramos, M. Sargent, S.C. Wofsy, and B.C. Daube. 2021. ATom: Measurements from the Quantum Cascade Laser System (QCLS), Version 2. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1932

Table of Contents

1. Dataset Overview

This dataset provides atmospheric concentrations of CO2, CH_4, CO, and N_2O measured by the Harvard Quantum Cascade Laser System (QCLS) instruments during airborne campaigns conducted by NASA's Atmospheric Tomography (ATom) mission. The QCLS (DUAL and CO_2) instrument package contains two separate optical assemblies and calibration systems, and a common data system and power supply. The QCLS DUAL instrument simultaneously measures CO, CH_4, and N_2O concentrations, in situ, using two thermoelectrically cooled pulsed-quantum cascade lasers light sources, a multiple pass absorption cell, and two liquid nitrogen-cooled solid-state detectors. The QCLS CO_2 instrument measures CO_2 concentrations in situ using a thermoelectrically cooled pulsed-quantum cascade laser light source, gas cells, and liquid nitrogen cooled solid-state detectors. The CO_2 mixing ratio of air flowing through the sample gas cell is determined by measuring absorption from a single infrared transition line at 4.32 microns relative to a reference gas of known concentration.

This is Version 2 of this dataset. For additional 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 Publication

Gonzalez, Y., R. Commane, E. Manninen, B.C. Daube, L.D. Schiferl, J.B. McManus, K. McKain, E.J. Hintsa, J.W. Elkins, S.A. Montzka, C. Sweeney, F. Moore, J.L. Jimenez, P. Campuzano Jost, T.B. Ryerson, I. Bourgeois, J. Peischl, C.R. Thompson, E. Ray, P.O. Wennberg, J. Crounse, M. Kim, H.M. Allen, P.A. Newman, B.B. Stephens, E.C. Apel, R.S. Hornbrook, B.A. Nault, E. Morgan, and S.C. Wofsy. 2021. Impact of stratospheric air and surface emissions on tropospheric nitrous oxide during ATom. Atmospheric Chemistry and Physics 21:11113–11132. https://doi.org/10.5194/acp-21-11113-2021

Related Datasets

Commane, R., J.W. Budney, Y. Gonzalez Ramos, M. Sargent, S.C. Wofsy, and B.C. Daube. 2020. ATom: Measurements from the Quantum Cascade Laser System (QCLS). ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1747

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

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 the four ATom 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 ATom campaigns provided in KML and CSV format.

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

Temporal Resolution: 1 second

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

Data File Information

There are 94 data files in ICARTT (*.ict) format included in this dataset. Data files conform to the ICARTT File Format Standards V1.1.

Fourty-seven data files are named- QCLS-CH4-CO-N2O_DC8_**YYYYMMDD_R#**.ict and 47 data files are named QCLS-CO2_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.

File Name	Description
QCLS-CH4-CO-N2O_DC8_YYYYMMDD_R#.ict	Dry air molar mixing ratios for CH_4, CO, and N_2O
QCLS-CO2_DC8_YYYYMMDD_R#.ict	Dry air molar mixing ratios for CO_2

Data File Details

Missing data values are represented by -99999.

Table 2. Variables names and descriptions for data files named QCLS-CH4-CO-N2O_DC8_YYYYMMDD_R#.ict.

Variable Name	Units	Description
START_UTC	seconds	Start time in seconds since 0000 UTC
CH4_QCLS	ppb	Dry air molar mass mixing ratio of methane (CH_4) in parts per billion
N2O_QCLS	ppb	Dry air molar mass mixing ratio of nitrous oxide (N_2O) in parts per billion
CO_QCLS	ppb	Dry air molar mass mixing ratio of carbon monoxide (CO) in parts per billion

Table 3. Variables names and descriptions for data files named QCLS-CO2_DC8_YYYYMMDD_R#.ict.

Variable Name	Units	Description
START_UTC	seconds	Start time in seconds since 0000 UTC
CO_2_QCLS	ppm	Carbon dioxide (CO_2) dry air molar 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 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

Table 4. Uncertainties for QCLS variables.

Name	Accuracy	Precision
CH4_QCLS	1 ppb	0.5 ppb
N2O_QCLS	0.2 ppb	0.1 ppb
CO_QCLS	3.5 ppb	0.15 ppb
CO2_QCLS	0.1 ppb	0.02 ppb

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.

Quantum Cascade Laser System

The Harvard QCLS (DUAL and CO_2) instrument package contains two separate optical assemblies and calibration systems and a common data system and power supply. The two systems are mounted in a single standard HIAPER rack. For CO_2 a reference gas was run every 15 mins with low and high span calibrations every 30 mins. In-flight calibrations for QCLS had two schemes:

1. For Atom-1 and 2, blanks were run every 15 mins and calibrations were conducted every 30 mins.
2. For Atom-3 and 4, blanks were run and calibrations were conducted every 30 mins.

The Harvard QCL DUAL instrument simultaneously measured CO, CH_4, and N_2O concentrations in situ using two thermoelectrically cooled pulsed-quantum cascade lasers (QCL) light sources, a multiple pass absorption cell, and two liquid nitrogen-cooled solid-state detectors. These components were mounted on a temperature-stabilized, vibrationally isolated optical bench with a heated cover. The sample air was preconditioned using a Nafion drier (to remove water vapor) and was reduced in pressure to 60 mbar using a Teflon diaphragm pump. The trace gas mixing ratios of air flowing through the multiple pass absorption cell was determined by measuring absorption from their infrared transition lines at 4.59 microns for CO and 7.87 microns for CH_4 and N_2O using molecular line parameters from the HITRAN database.

The Harvard QCL CO_2 instrument measured CO_2 concentrations in situ using a thermoelectrically cooled pulsed-quantum cascade laser (QCL) light source, gas cells, and liquid nitrogen cooled solid-state detectors. These components were stabilized along the detection axis, vibrationally isolated, and housed in a temperature-controlled pressure vessel. Sample air entered a rear-facing inlet, was preconditioned using a Nafion drier (to remove water vapor), then was reduced in pressure to 60 mbar using a Teflon diaphragm pump. A second water trap, using dry ice, reduced the sample air dewpoint to less than -70C prior to detection. The CO_2 mixing ratio of air flowing through the sample gas cell was determined by measuring absorption from a single infrared transition line at 4.32 microns relative to a reference gas of known concentration.

Additional information can be found on the ESPO QCLS Instrument page.

6. Data Access

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

ATom: Measurements from the Quantum Cascade Laser System (QCLS), Version 2

Contact for Data Center Access Information:

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

7. References

Gonzalez, Y., R. Commane, E. Manninen, B.C. Daube, L.D. Schiferl, J.B. McManus, K. McKain, E.J. Hintsa, J.W. Elkins, S.A. Montzka, C. Sweeney, F. Moore, J.L. Jimenez, P. Campuzano Jost, T.B. Ryerson, I. Bourgeois, J. Peischl, C.R. Thompson, E. Ray, P.O. Wennberg, J. Crounse, M. Kim, H.M. Allen, P.A. Newman, B.B. Stephens, E.C. Apel, R.S. Hornbrook, B.A. Nault, E. Morgan, and S.C. Wofsy. 2021. Impact of stratospheric air and surface emissions on tropospheric nitrous oxide during ATom. Atmospheric Chemistry and Physics 21:11113–11132. https://doi.org/10.5194/acp-21-11113-2021

8. Dataset Revisions

Version	Release Date	Description
2.0	2021-09-23	• Initial release of QCLS-CH4-CO-N2O_DC8_YYYYMMDD_R#.ict files from the ATom-4 campaign. ◦ Files named QCLS-CH4-CO-N2O_DC8_YYYYMMDD_R#.ict files for the first three ATom campaigns were updated to latest version. ◦ Files named QCLS-CO2_DC8_YYYYMMDD_R#.ict have not changed.
1.0	2020-04-14	• Initial release of 82 ICARTT files. Now superseded and available only upon request. ◦ Published 35 files named QCLS-CH4-CO-N2O_DC8_YYYYMMDD_R#.ict for the first three ATom campaigns ◦ Published 47 files named QCLS-CO2_DC8_YYYYMMDD_R#.ict for the four ATom campaigns.