MetaData File provided: June 2015
Latest Revision : 09-August-2018

Data Set Description:

PI: Kimberly Strong
University of Toronto, Department of Physics
Toronto, Ontario, Canada

Instrument: Fourier Transform Infrared Spectrometer (FTIR)

Site(s): University of Toronto (Toronto Atmospheric Observatory - TAO)
NDACC Station Toronto
43.66 N, 79.40 W, 174 m above sea level

Measurement Quantities: Vertical Total Column Abundances above Toronto (0-120 km)
in units of [molecules/cm^2]
Vertical profiles above Toronto (0-120 km)
in units of [molecules/cm^2]

Contact Information:

Name: Kimberly Strong
Address: University of Toronto
Department of Physics
60 St. George Street
Toronto, Ontario
Canada
Phone: +001-416-946-3217
FAX: +001-416-978-8905
Email: strong@atmosp.physics.utoronto.ca
WEB: http://www.atmosp.physics.utoronto.ca/people/strong/strong.html
http://www.atmosp.physics.utoronto.ca/TAO/

Reference Articles:

E. Lutsch, E. Dammers, S. Conway, and K. Strong. Long-range Transport of NH3, CO, HCN and C2H6 from the 2014 Canadian Wildfires. Geophys. Res. Lett., 43, 8286–8297, doi:10.1002/2016GL070114, 2016.

C.H. Whaley, K. Strong, D.B.A. Jones, T.W. Walker, Z. Jiang, D.K. Henze, M. Cooke, C.A. McLinden, M. Pommier, R.L. Mittermeier, and P.F. Fogal. Improvements to our understanding of urban ozone air pollution: Sources of Toronto-area ozone during poor air quality events. Submitted to J. Geophys. Research, 2015.

C.H. Whaley, PhD thesis, Improvements to our Understanding of Toronto-Area Atmospheric omposition, University of Toronto, 2014.

D. Griffin, K. A. Walker, J. E. Franklin, M. Parrington, C. Whaley, J. Hopper, J. R. Drummond, P. I. Palmer, K. Strong, T. J. Duck, I. Abboud, P. F. Bernath, C. Clerbaux, P.-F. Coheur, K. R. Curry, L. Dan, E. Hyer, J. Kliever, G. Lesins, A. Saha, K. Tereszchuk, M. Maurice, and D. Weaver. Investigation of CO, C2H6 and aerosols in a boreal fire plume over Eastern Canada during BORTAS 2011 using ground- and satellite-based observations, and model simulations. Atmos. Chem. Phys., 13, 10227-10241, 2013.

C. Whaley, K. Strong, C. Adams, A.E. Bourassa, W.H. Daffer, D.A. Degenstein, H. Fast, P.F. Fogal, G.L. Manney, R.L. Mittermeier, B. Pavlovic, and A. Wiacek. Using FTIR measurements of stratospheric composition to identify mid-latitude polar vortex intrusions over Toronto. J. Geophys. Res. Atmos., 118 (2), 12766-12783, 2013.

K. Strong, O. Colebatch, S. Conway, P.F. Fogal, D. Griffin, D.B.A. Jones, Z. Mariani, J. Mendonca, M. Semelhago, I. Stanevich, C. Viatte, K.A. Walker, D. Weaver, C. Whaley, R. Lindenmaier, H. Fast, R. Mittermeier, J.R. Drummond, J. Franklin, J.G. Giroux, and J.C. Lin. Probing Atmospheric Composition over Canada using Ground-based FTIR Spectroscopy. Optical Society of America Fourier Transform Spectroscopy (OSA-FTS) Meeting, Arlington, Virginia, USA, 23-27 June 2013. In Imaging and Applied Optics (Optical Society of America, Washington, DC, 2013), FTh2C.1. (invited)

J.R. Taylor, D. Wunch, C. Midwinter, A. Wiacek, J.R. Drummond, and K. Strong, An Extended Intercomparison of Simultaneous Ground-Based Fourier Transform Spectrometer Measurements at the Toronto Atmospheric Observatory. J. Quant. Spectrosc. Radiat. Transfer, 109 (12-13), 2244-2260, 2008.

J. R. Taylor, PhD thesis, Instrument Characterization of a Fourier Transform Spectrometer at the Toronto Atmospheric Observatory, University of Toronto, 2008.

A. Wiacek and K. Strong. Effects of Vertical Grid Discretization in Infrared Transmission Modeling. J. Quant. Spectrosc. Radiat. Transfer, 109, 2463-2490, 2008.

A. Wiacek, J.R. Taylor, K. Strong, R. Saari, T. Kerzenmacher, N.B. Jones and D.W.T Griffith. Ground-Based Solar Absorption FTIR Spectroscopy: Characterization of Retrievals and First Results from a Novel Optical Design Instrument at a New NDACC Complementary Station. J. Atmos. Oceanic Technology, 24 (3), 432-448, 2007.

D. Wunch, J.R. Taylor, D. Fu, P.F. Bernath, J.R. Drummond, C. Midwinter, K. Strong, and K.A. Walker. Simultaneous Ground-Based Observations of O3, HCl, N2O, and CH4 over Toronto, Canada by Three Fourier Transform Spectrometers with Different Resolutions. Atmos. Chem. Phys. (MANTRA Special Issue), 7, 1275-1292, 2007.

J.R. Taylor, K. Strong, C.A. McLinden, D.A. Degenstein, and C.S. Haley. Comparison of OSIRIS tratospheric O3 and NO2 measurements with ground-based Fourier Transform Spectrometer measurements at the Toronto Atmospheric Observatory. Can. J. Phys, 85, 1301-1316, 2007.

A. Wiacek, N.B. Jones, K. Strong, J.R. Taylor, R.L. Mittermeier, and H. Fast. First Detection of Meso-Thermospheric Nitric Oxide (NO) by Ground-Based FTIR Solar Absorption Spectroscopy. Geophys. Res. Lett., 33 (3), L03811, doi:10.1029/2005GL024897, 2006.

A. Wiacek, PhD Thesis, First Trace Gas Measurements Using Fourier Transform Infrared Solar Absorption Spectroscopy at the University of Toronto Atmospheric Observatory. University of Toronto, 2006.

See also, e.g., for ACE validation papers:
http://www.atmosp.physics.utoronto.ca/TAO/Publications.html
and
http://www.atmosp.physics.utoronto.ca/people/strong/papers.html

Instrument Description:
An ABB Bomem DA8 Fourier Transform Infrared (FTIR) spectrometer has been operated at the University of Toronto Atmospheric Observator (TAO) on a continous basis since May 2002 (following installation in October 2001), with a solar tracker manufactured by Aim Controls. The FTS is operated in solar absorption geometry at its maximum optical path difference of 250 cm corresponding to a spectral resolution of 0.004 cm-1. The DA8 is equipped with both InSb and MCT detectors and a KBr beamsplitter. Combined, these resources cover the mid-infrared from about 650 to 6600 cm-1. The optical filters used are those recommended by the NDACC Infrared Working Group and are listed in the table below. Filter 7 is not standard and was acquired to enable near IR measurements. There are significant coverage gaps in F6 measurements in 2002-2003. No data were recorded in Aug-Sep 2004 and Dec 2006-Jan 2007 due to a suntracker failure. Also no data were recorded in Mar-Jun 2009 due to an alignment issue.

NDACC filter	approx. range in cm-1	before June 2003	after June 2003
Filter 1	4000 to 4300	routine	routine
Filter 2	2900 to 3500	routine	routine
Filter 3	2400 to 3100	routine	routine
Filter 4	2000 to 2700	routine	routine
Filter 5	1800 to 2200	not available	routine
Filter 6	650 to 1350	routine	routine
Filter 7	5800 to 6600	not available	not available

Algorithm Description:
November 2017 (data version 002):

Vertical profiles of volume mixing ratios of trace gases are derived using the Optimal Estimation Method, as implemented in SFIT4 (SFIT4:V0.9.4.4 with full error analysis) and distributed through https://wiki.ucar.edu/display/sfit4/Infrared+Working+Group+Retrieval+Code%2C+SFIT. Vertical profiles of volume mixing ratios are weighted by the airmasses in each retrieval layerand integrated to give the total or partial columns in molecules/cm^2. We report total columns and profiles.

The retrieval results reported here use the Signal-to-Noise-Ratio (SNR) calculated from the spectrum for each target gas to define the measurement noise covariance matrix, with the a priori covariance matrix S_a adjusted to optimize the retrievals.

The microwindows and interfering species follow the NDACC IRWG recomendations.

Spectra used in the retrievals were recorded at 250 cm maximum optical path difference (OPD), except for filter 6 measurements, which are recorded at 200 cm OPD. Prior to 2006, filter 6 measurements were made at both 200 cm and 250 cm OPD.

An optimized quality criterion has been applied using a threshold for the ratio of the spectral RMS residual (goodness of fit) and degrees-of-freedom for signal (DOFS). The thresholds were determined by a trade-off curve of the number of filtered measurements for the entire time series versus the RMS/DOFS ratio. The threshold was selcted as the elbow of the trade-off curve, where the absolute second derivative is maximum. The threshold values are listed below:

C2H6: 4.75 %-rms/dofs
CH4 : 3.25 %-rms/dofs
CO : 3.00 %-rms/dofs (for QA4ECV CO data product)
HCL : 2.95 %-rms/dofs
HCN : 1.40 %-rms/dofs
HF : 4.50 %-rms/dofs
HNO3: 4.00 %-rms/dofs
N2O : 1.20 %-rms/dofs
O3 : 2.60 %-rms/dofs

In addition, a few random outliers were removed based on a qualitative assessment of the residuals.

Ancillary Data:
October 2016 - for QA4ECV CO data product (data version 003):

Line compilation: The ATM line list (http://mark4sun.jpl.nasa.gov/toon/linelist/linelist.html) is used in the forward calculation. For interferring species, the HITRAN 2008 line list with additional pseudo-line parameters is used.

July 2015:

Line compilation: The HITRAN 2008 line list with additional pseudo-line parameters is used in the forward calculation. Details regarding the C2H6 pseudo line list can be found in Franco et al., 2015.

Physical models: Temperature and pressure profiles are derived from NCEP analyses for each day to approx. 1.0 mbar and WACCM monthly mean above.

A priori profiles of trace gas volume mixing ratios are from the WACCM v6 model, where possible and/or appropriate. HALOE climatologies, MkIV balloon flight results (http://mark4sun.jpl.nasa.gov/science.html) and "Standard Profiles" used in MIPAS retrievals (http://www.atm.ox.ac.uk/group/mipas/species) are also used as a priori information for some species when no WACCM v6 profiles are available or where their use improves the retrievals

The Instrumental Line Shape (ILS) is monitored with HBr cell spectra (and since 2016 also with an N2O cell) on a quasi-regular basis. The cell spectra are analysed with Linefit [Hase, Applied Optics, 1999].

A local weather station was installed in Oct. 2001 and records surface temperature, pressure, humidity, solar radiation, UV intensity and winds.

Expected Precision/Accuracy of Instrument:
July 2015:
The error calculations in this work are based on the methodology of Rodgers [1,2]. In addition to the measurement (Sm) errors calculated as described in those papers, random forward model parameter errors have been calculated as described by Rodgers [3] the Kb values calculated by SFIT4 and our best estimate of the uncertainties in temperature (Stemp) and solar zenith angle (Ssza). Systematic forward model errors, i.e. errors due to uncertainties in line intensity and line widths, are calculated based HITRAN 2008 errore. Interference errors, as described by Rodgers and Connor [4] have also been calculated to account for uncertainties in retrieval parameters (wavelength shift, instrument line shape, background slope and curvature, phase error) and in interfering gases simultaneously retrieved. These interference errors are included in the random uncertainty estimate. The error budget calculation is described in depth by Batchelor et al. [5]. The total error (Stotal) has been determined by adding all components in quadrature:

Stotal={(Sm^2+Stemp^2+Sint1^2+Sint2^2+Ssza^2)+Slint^2+Slwdth^2}^1/2

N.B. Smoothing error is not included in the error estimate.

The data user is referred to a careful discussion of error analysis for ground-based FTIR observations presented in:

[1] Rodgers CD. Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation. Rev Geophys 1976;14(4):609-624.

[2] Rodgers CD. Characterization and error analysis of profiles retrieved from remote sounding measurements. J Geophys Res 1990;95:5587-5595.

[3] Rodgers CD. Inverse Methods for Atmospheric Sounding: Theory and Practice. Series on Atmospheric, Oceanic and Planetary Physics, vol. 2. New Jersey: World Scientific Publishing Co Pte Ltd, 2000.

[4] Rodgers CD, Connor BJ. Intercomparison of remote sounding instruments. J Geophys Res 2003;108,

doi:10.1029/2002JD002299.

[5] Batchelor RL, Strong K, Lindenmaier R, Mittermeier RL, Fast H, Drummond JR, Fogal PF. A new Bruker IFS 125HR FTIR spectrometer for the Polar Environment Atmospheric Research Laboratory at Eureka, Canada - measurements and comparison with the existing Bomem DA8 spectrometer. J Atmos Oceanic Technol 2009; 26(7), doi:10.1175/2009JTECHA12151.

Instrument History:

October 2001: Installation

Early 2002: Additional work by Bomem to improve the alignment.

Summer 2002: Exit apertures installed on MCT and InSb detectors.

November 2002: MCT detector replaced (to improve sensitivity).

August-September 2004 and Dec 2006-Jan 2007: No data due to suntracker failure.

March-June 2009: No data were recorded due to an alignment issue.

July 2009: Bomem service visit.

April 2011: Scanning mirror motor replacement.

September 2012: Metrology laser replaced by Bomem Service engineer.

August 12, 2014: Began operations with a "Community Solar Tracker" suntracker. This uses the same mirrors as the previous Aim Controls heliostat but provides active tracking with a CCD camera rather than four photodiodes.

April 2015: DA8 electronics issues.

March-May 2015: Computer replaced.

October-November 2015: New scan motor bearing and instrument alignment.

February 2016: First N2O cell tests.

June 7, 2016: DA8 internal source mirror motor failed. Replaced July 25.