README File for the Dataset Associated with the Research Article Titled: Evaluation of ambient ammonia measurements from a research aircraft using a closed-path QC-TILDAS spectrometer operated with active continuous passivation

Research Article Authors: Ilana B. Pollack[1], Jakob Lindaas[1], J. Robert Roscioli[2], Michael Agnese[2], Wade Permar[3], Lu Hu[3], and Emily V. Fischer[1]

Author Affiliations: [1]Department of Atmospheric Science, Colorado State University, Fort Collins, Colorado, 80523, USA; [2]Aerodyne Research Inc., Billerica, Massachusetts, 01821, USA; [3]Department of Chemistry and Biochemistry, University of Montana, Missoula, Montana 59812, USA

Citation: Pollack et al., Evaluation of ambient ammonia measurements from a research aircraft using a closed-path QC-TILDAS spectrometer operated with active continuous passivation, Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2019-11, Manuscript under review for journal Atmos. Meas. Tech.

Research Article Abstract: A closed-path quantum cascade tunable infrared laser direct absorption spectrometer (QC-TILDAS) was outfitted with an inertial inlet for filter-less separation of particles, a custom-designed aircraft inlet, a custom-built vibration isolation mounting plate, and a custom-built system for optionally adding active continuous passivation for gas-phase measurements of ammonia (NH_3) from a research aircraft. The flight-ready instrument was then deployed on the NSF/NCAR C-130 aircraft during research flights and test flights associated with the Western wildfire Experiment for Cloud chemistry, Aerosol absorption and Nitrogen (WE-CAN) field campaign. The flight-ready instrument was configured to measure large, rapid gradients in gas-phase NH_3, over a range of altitudes, in smoke (e.g., ash and particles), in the boundary layer (e.g., during turbulence and turns), in clouds, and in a hot aircraft cabin. Important design goals were to minimize motion sensitivity, maintain a reasonable detection limit, and minimize NH_3 "stickiness" on sampling surfaces to maintain fast time response in flight. The observations indicate that addition of a high frequency vibration to the laser objective in the QC-TILDAS and mounting the QC-TILDAS on a custom-designed vibration isolation plate were successful in minimizing motion sensitivity of the instrument during flight. Allan variance analyses indicate that the in-flight precision of the flight-ready instrument is 60 ppt at 1 Hz corresponding to a 3-sigma detection limit of 180 ppt. The option for active continuous passivation of the sample flow path with 1H,1H-perfluorooctylamine, a strong perfluorinated base, prevented adsorption of both water and basic species to instrument sampling surfaces. Characterization of the time response in flight and on the ground showed that adding passivant to a "clean" instrument system had little impact on the time response. In contrast, passivant addition greatly improved the time response when sampling surfaces became contaminated prior to a test flight. The observations further show that passivant addition can be a useful tool for maintaining a rapid response for in-situ NH_3 measurements over the duration of an airborne field campaign (e.g., ~2 months for WE-CAN test and research flights) since passivant addition also helps to prevent future build-up of water and basic species on instrument sampling surfaces. Therefore, we recommend the use of active continuous passivation with closed-path NH_3 instruments when rapid (> 1 Hz) collection of NH_3 is important for the scientific objective of a field campaign (e.g., measuring fluxes, sampling from aircraft or another mobile research platform). Passivant addition can be useful for maintaining optimum operation and data collection in NH_3-rich/humid environments or when contamination of sampling surfaces is likely, yet frequent cleaning

is not possible. Passivant addition may not be necessary for fast operation, even in polluted environments, if sampling surfaces can be cleaned when the time response has degraded.

Data Contacts: Ilana B. Pollack (primary), ipollack@rams.colostate.edu, 970-491-8605
Emily V. Fischer, evf@rams.colostate.edu, 970-491-8587
Jakob Lindaas,

Data Description: Airborne measurements were collected aboard the NSF/NCAR C-130 research aircraft during the Western wildfire Experiment for Cloud chemistry, Aerosol absorption and Nitrogen (WE-CAN) field campaign in summer 2018 and during 16 test-flight hours prior to the WE-CAN deployment. The aircraft conducted seventeen research flights of roughly 6-8 hour duration between 20 July and 31 August in 2018, three test flights of 2-3 hour duration between 21 September and 29 September in 2017, and two test flights on 13 July and 17 July in 2018. Research flights were conducted in the northwestern U.S. with aircraft operations based out of Boise, Idaho; test flights were conducted in the northeastern Colorado Front Range based out of the National Center for Atmospheric Research (NCAR) Research Aviation Facility (RAF) in Broomfield, Colorado. This repository contains data files associated with WE-CAN test/research flights as well as supporting ground-based experiments (e.g., performed in the laboratory at CSU and on the ground aboard the aircraft in the hangar) utilized in the analyses presented in this research article.

Format of Data Files: Data files are in ICARTT format (https://www-air.larc.nasa.gov/missions/etc/IcarttDataFormat.htm). This is common reporting method for airborne trace gas measurements from research aircraft. Files can be opened by most software (e.g., Notepad, WordPad, Excel) – anything that can read a comma delimited ASCII text file. Here, file names are formatted as WECAN-NH3_C130_YYYYMMDD_R#, where "location" represents where the data set was collected such as 1) in the LAB at CSU, 2) on the C-130 aircraft during a flight day, or 3) on ground aboard the aircraft on a ground day in the hangar at RAF, "YYYYMMDD" represents the date of collection and R# denotes final data for revision #. Ground-based and test flight data for NH_3 include flags for time periods where the instrument was performing a calibration and/or zero. Data are reported as 1Hz or 10 Hz in according with the experiment performed on a given file date. We note that each ICARTT file header contains important information regarding the data in each file such as the location the dataset was collected, any comments about the dataset collected on that date, the uncertainty, precision, and detection limit of the measurements, and data flags.

Use of this data require permission from the Data Contacts.

Funding for this work was provided by the National Science Foundation through grant number AGS- 1650786.