Atmospheric Carbon and Transport – America (ACT-America) Datasets: Description, Management, and Delivery

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November 22, 2022

Abstract

The ACT-America project is a NASA Earth Venture Suborbital-2 mission designed to study the transport and fluxes of greenhouse gases. The open and freely available ACT-America datasets provide airborne in-situ measurements of atmospheric carbon dioxide, methane, trace gases, aerosols, clouds, and meteorological properties, airborne remote sensing measurements of aerosol backscatter, atmospheric boundary layer height and columnar content of atmospheric carbon dioxide, tower-based measurements, and modeled atmospheric mole fractions and regional carbon fluxes of greenhouse gases over the Central and Eastern United States. We conducted 121 research flights during five campaigns in four seasons during 2016-2019 over three regions of the US (Mid-Atlantic, Midwest and South) using two NASA research aircraft (B-200 and C-130). We performed three flight patterns (fair weather, frontal crossings, and OCO-2 underflights) and collected more than 1,140 hours of airborne measurements via level-leg flights in the atmospheric boundary layer, lower, and upper free troposphere and vertical profiles spanning these altitudes. We also merged various airborne in-situ measurements onto a common standard sampling interval, which brings coherence to the data, creates geolocated data products, and makes it much easier for the users to perform holistic analysis of the ACT-America data products. Here, we report on detailed information of datasets collected, and the workflow for datasets including storage and processing of the quality controlled and quality assured harmonized observations, and their archival and formatting for users. Finally, we provide some important information on the dissemination of data products including metadata and highlights of applications of datasets for future investigations.

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Key Points:

- ACT-America provides a unique and valuable asset of high-quality measurements of atmospheric CO2, CH4, trace gases and meteorological properties.
- ACT-America data are available free and open to the public from the ORNL DAAC.
- ACT-America data provide a valuable asset to improve the accuracy and precision of regional inverse flux estimates of GHGs and beyond.

Abstract

The ACT-America project is a NASA Earth Venture Suborbital-2 mission designed to study the transport and fluxes of greenhouse gases. The open and freely available ACT-America datasets provide airborne in-situ measurements of atmospheric carbon dioxide, methane, trace gases, aerosols, clouds, and meteorological properties, airborne remote sensing measurements of aerosol backscatter, atmospheric boundary layer height and columnar content of atmospheric carbon dioxide, tower-based measurements, and modeled atmospheric mole fractions and regional carbon fluxes of greenhouse gases over the Central and Eastern United States. We conducted 121 research flights during five campaigns in four seasons during 2016-2019 over three regions of the US (Mid-Atlantic, Midwest and South) using two NASA research aircraft (B-200 and C-130). We performed three flight patterns (fair weather, frontal crossings, and OCO-2 underflights) and collected more than 1,140 hours of airborne measurements via levelleg flights in the atmospheric boundary layer, lower, and upper free troposphere and vertical profiles spanning these altitudes. We also merged various airborne in-situ measurements onto a common standard sampling interval, which brings coherence to the data, creates geolocated data products, and makes it much easier for the users to perform holistic analysis of the ACT-America data products. Here, we report on detailed information of datasets collected, and the workflow for datasets including storage and processing of the quality controlled and quality assured harmonized observations, and their archival and formatting for users. Finally, we provide some important information on the dissemination of data products including metadata and highlights of applications of datasets for future investigations.

Plain Language Summary

We describe data collected and produced by the Atmospheric Carbon and Transport - America project, including airborne and tower-based measurements of greenhouse gases (e.g., carbon dioxide and methane) and modeled atmospheric mole fractions and regional carbon fluxes of greenhouse gases over North America. In this paper, we briefly describe the data collections and archival including the instruments and methodology used to generate, manage, and distribute the data, and the significance of these new measurements for the study of the North American carbon cycle.

1 Introduction

The ACT-America (Atmospheric Carbon and Transport – America) project is a NASA Earth Venture Suborbital-2 mission designed to study the atmospheric transport and surface fluxes of greenhouse gases (GHGs), including atmospheric carbon dioxide (CO₂) and methane (CH₄), across the eastern United States. Its overarching goal is to improve the accuracy and precision of regional inverse flux estimates of GHGs (Davis et al., submitted). ACT-America aims to achieve this goal by quantifying and reducing the uncertainty in both the atmospheric transport models and the prior flux estimates used in atmospheric inversions. ACT-America conducted along-track evaluation of column CO₂ observations from the Orbiting Carbon Observatory – 2 (OCO-2) mission (Eldering et al., 2017) to better quantify regional uncertainties in atmospheric inversions. Extensive atmospheric transport and biological flux modeling complements the observational data.

This paper reports detailed information for the different types of datasets collected and produced within the ACT-America project, including their quality-assurance and quality-control

(QA/QC) procedure, the workflow for datasets including storage and processing of the harmonized observations, and their archival and formatting for users. It also provides some important information on the dissemination of data products including metadata and highlights of applications of datasets for future investigations. All the final datasets, including both observational data and results from numerical simulations (i.e., Weather Research and Forecasting model coupled to Chemistry, WRF-Chem), collected and produced by the ACT-America project have been archived and published for free and public access at the Oak Ridge National Laboratory Distributed Active Archive Center (ORNL DAAC). This paper highlights the groundwork for the access and use of ACT-America datasets.

1.1 Airborne Measurements

ACT-America flight campaigns collected in situ and lidar remote sensing measurements of GHGs, tracers and meteorological variables across a variety of continental surfaces and atmospheric conditions. Two aircraft were deployed, the NASA Langley Beechcraft B-200 King Air and the NASA Wallops C-130 Hercules. Each aircraft was instrumented with a suite of high-quality, field-tested trace gas, and meteorological instruments, listed in Table 1.

Instrument	Parameters Measured	Aircraft	Campaigns
In situ infrared Cavity Ring- Down Spectroscopy (CRDS): PICARRO G2401-m	Mole fraction of CO ₂ , CH ₄ , and CO	C-130 and B- 200	All
In situ infrared CRDS: PICARRO G2301-m	Mole fraction of CO ₂ , CH ₄ , and water vapor	C-130	All (except Summer 2016)
NOAA Programmable Flask Package whole-air samples (Sweeney et al., 2015)	Mole fractions of ~50 trace species including CO ₂ , CH ₄ , CO, nitrous oxide (N ₂ O), sulfur hexafluoride (SF ₆), select halocarbons, hydrocarbons, and sulfur-containing species, and isotopic ratios of CO ₂ and CH ₄	C-130 and B- 200	All
Continuous Ozone (O ₃) monitor (2B Technologies Model 205)	Volume fraction of O ₃	C-130 and B- 200	All
Multi-functional Fiber Laser Lidar (MFLL; Dobler et al., 2013), a Laser Absorption Spectrometer	CO ₂ column density, range to the surface, and surface reflectance	C-130	All (except Summer 2019)
Cloud Physics Lidar (CPL; Vaughan et al., 2010)	Atmospheric layers, cloud height and fractional cover, and	C-130	All (except Summer 2019)

Table 1: Overview of instruments deployed on ACT-America flight campaigns.

	atmospheric boundary layer (ABL) depth		
Compact Atmospheric Multi- Species Spectrometer (CAMS- 2; Weibring et al., 2020)	Volume fraction of Ethane (C ₂ H ₆)	B-200	All (limited data during 1st Campaign)
Quantum Cascade Laser Spectrometer (QCLS; Kostinek et al., 2019)	Mole fraction of C ₂ H ₆ , N ₂ O, CO, CH ₄ , CO ₂	C-130	Fall 2017; Summer 2019
ASCENDS CarbonHawk Experiment Simulator (ACES; Obland et al., 2015)	CO ₂ column density	C-130	All (except Summer 2019)
High Altitude Lidar Observatory (HALO; Nehrir et al., 2018)	CH ₄ column density, aerosol properties, atmospheric layers, cloud cover and fraction, and ABL depth	C-130	Summer 2019
Meteorological instrument suite (Honeywell PPT2 pressure transducer, Rosemount de-iced total air temperature probe, and Edgetech Vigilant 137 hygrometer with 3-stage TEC chilled mirror)	Horizontal winds, total and static atmospheric temperature, dew- point temperature, atmospheric pressure	C-130 and B- 200	All
GPS/INS units (Honeywell H- 764 on C-130 and Applanix Model 510 V5 on B-200)	Aircraft latitude, longitude, altitude, ground speed, etc.	C-130 and B- 200	All

Each of the two aircraft also included a suite of instruments to capture navigational data (see "GPS/INS units" in Table 1), which were incorporated into related ACT-America airborne measurements to provide geospatial context for instrumented sampling (Yang et al., 2018).



Figure 1: Flight paths of the B-200 (blue) and C-130 (red) aircraft during the five ACT-America field campaigns spanning four seasons. Measurements from aircraft were complemented with measurements of greenhouse gases from communications towers (black diamonds), deployed to complement the NOAA/GML Global Greenhouse Reference Network

(<u>https://www.esrl.noaa.gov/gmd/ccgg/ggrn.php</u>). Panel (f) shows the spiral up/down behavior of the C-130 aircraft to acquire vertical profiles on July 20, 2019 during a flight near Caldwell, Idaho.

Flight Campaign	Date	Number of Research Flights	Hours of Observations	Number of Level Legs	Number of Atmospheric Profiles
Summer 2016	Jul. 15 to Aug. 28 2016	26	263.1	150	270
Winter 2017	Jan. 30 to Mar. 10 2017	27	215.6	120	220
Fall 2017	Oct. 3 to Nov. 13 2017	23	228.5	100	295
Spring 2018	Apr. 12 to May 20 2018	26	231.4	120	334
Summer 2019	Jun. 17 to Jul. 27 2019	19	202.1	80	244

Table 2: Overview of ACT-America flight campaigns and sampling intensity in each campaign.

The ACT-America mission conducted flights in all Northern Hemisphere seasons through five campaigns (Figure 1) in order to sample the seasonal variations in greenhouse gas fluxes and

atmospheric conditions. Flights were coordinated in a way that both aircraft, C-130 and B-200, generally flew on the same day. Flights included a range of typical weather conditions including high-pressure fair-weather conditions, and the passage of mid-latitude cyclones. Furthermore, several research flights were conducted in each season to sample atmospheric CO₂ distributions along roughly 500 km along the track of OCO-2 passes (denoted as OCO-2 underflight). All flight patterns included long level legs in the atmospheric boundary layer (ABL), and lower and upper free troposphere (FT). Each OCO-2 underflight included four atmospheric level legs. Frontal flights typically crossed a front along one line at multiple altitudes. Fair weather flights via a box pattern surveyed atmospheric conditions across relatively homogeneous air masses in and around high-pressure systems. Vertical profiles were included within all flight plans, which were also used to determine ABL depths (Pal, 2019). Flights targeted midday, well-mixed boundary layer conditions and were typically conducted between 11 and 17 Local Solar Time. Flights usually included both aircraft flying in a coordinated pattern, and encompassed regions of a few hundred to one thousand kilometers in extent guided by detailed weather forecasting and nowcasting products. During the five campaigns, a total of 121 research flights, more than 1,140 hours of observations, 570 level legs, and 1,363 vertical profiles were conducted using the two aircraft (Table 2 and Figure 2). A flight catalogue is available at https://actamerica.ornl.gov/campaigns.html (Pal & Davis, 2020) with information documenting the scientific objectives of each flight, the weather conditions and GHG environment, instrument status, flight paths, and quicklooks of the measurements. These observations represent a unique and unprecedented contribution to the understanding of North American terrestrial carbon fluxes

and their intersection with atmospheric transport.



Figure 2: Sampling intensity of the B-200 and C-130 aircraft during the five ACT-America field campaigns. Color table in the upper panel indicates hours of observations for each 2 km levels. The aircraft sampled air masses from 0 to 10 km altitude (top panel) and in a variety of weather conditions (bottom panel) in the Mid-Atlantic (MA), Midwest (MW), and South regions of the United States. Three different flight patterns (frontal, fair-weather and OCO-2 underpass research flights) conducted during the field campaigns (lower panel).

1.2 Tower-based GHG measurements

Data were also collected on a network of instrumented communications towers within the ACT-America sampling domain. 11 towers were deployed to complement the routine long-term tower measurements of the NOAA/GML Global Greenhouse Reference Network (Figure 1) (Andrews et al., 2014). Tower-based instruments measured carbon dioxide and methane mole fractions representing ABL samples. Tower platforms utilized Picarro G2301 CRDS for continuous CO₂ and CH₄ measurements. Tower-based measurements began in early 2015 and continued through 2019. Data from 11 towers are provided, although not all towers have data from all years. Complete tower location, elevation, instrument height, and date/time information are available in Miles et al., 2018 and Miles et al., 2020. Calibration and uncertainty

quantification procedures used for tower-based GHG measurements can be found in Table S1. These measurements are an essential input to long-term diagnoses of the continental carbon balance and inverse flux estimates (e.g., Peters et al., 2007; Hu et al., 2019;). The aircraft flights are spatially rich and designed to complement the temporally rich but spatially sparse tower network. Daily, automated data transfer to Pennsylvania State University allowed for remote monitoring of instrument status and flight planning.

2 Airborne and Tower Data Processing and Management

The ACT-America data management lifecycle involves efforts from many investigators, including the individual instrument teams, data managers at the NASA Langley Research Center (LaRC) field data repository, and staff at the NASA-sponsored ORNL DAAC. The team worked together to develop a detailed data management plan before any data were collected, and continued to communicate regularly throughout the data collection, curation, archival, and publication process.

2.1 Data Calibration and QA/QC

During the field campaigns, the individual instrument teams collected data and performed quick QA/QC checks and processing using initial calibrations to produce preliminary (field) data. These preliminary data were used for flight planning, assessing instrument operations, and determining progress in achieving the overall project sampling strategy. After the completion of each campaign, the instrument teams performed their full data processing (e.g., applying final calibrations and measurement synchronization) and more rigorous QA/QC process to generate publication-quality data. A summary of the calibration and QA/QC procedures used by the major instruments and measurements of ACT-America is provided in Text S1. Data may be revised even after this point; For example, as instrument issues are revealed through additional analysis, as new trace gas calibration scales are adopted, or because the processing depends on final data from another instrument team. The ORNL DAAC has the capability to capture the detailed download statistics information and to contact and notify users about the corrections and data revisions.

2.2 Data Management at the LaRC Field Data Repository

The goal of the field data repository is to facilitate data exchange within the science team so that they can efficiently generate publication-quality data products. The ACT-America field data repository was operated by the Suborbital Science Data for Atmospheric Composition (SSD-AC) group at NASA LaRC (<u>https://www-air.larc.nasa.gov/missions/ACT-America/</u>).

During the campaign periods, the field data repository served several important functions, including hosting the preliminary/quick-look data, providing secure data access for science team members and collaborators, and ensuring that data adhered to standard file naming and format conventions to improve data usability. Files in the International Consortium for Atmospheric Research on Transport and Transformation (ICARTT; Aknan et al., 2013) format were additionally checked against the format standards, particularly that the sampling time stamp is monotonically increasing, no overlaps exist between sampling time intervals, and the data codes for missing data and limits of detection are properly used. During the course of the project, there were 5,552 preliminary and 6,579 publication-quality data files submitted to the field data repository, including data revisions (e.g., Davis et al., 2018; Pal, 2019; Pal et al., 2020). Preliminary data typically went through multiple revisions. The publication-quality data is

nominally submitted within six months of the end of each field campaign, though some data was subsequently revised (e.g., due to improved calibration and/or processing methods). The publication-quality data were released to the public and transferred to ORNL DAAC for long-term preservation and public distribution. The field data repository will remain open to accept future data updates.

Another major function of the SSD-AC group was to generate merged products, which combined all in situ measurement data onto a common time base (see Section 3). During the project, SSD-AC has created 15 revisions of certain preliminary merged products and 5 revisions for the publication quality data. These revisions were done to reflect the observational data revisions. The merged products will continue to be updated as future data revisions are uploaded.

In situ ACT-America data products are reported in ICARTT v1.1 format (Aknan et al., 2013), while lidar remote sensing data products are largely in HDF5 (Hierarchical Data Format 5) format. The ICARTT file format contains critical metadata including the investigator, variable names and descriptions, estimated measurement uncertainty, missing data and limit of detection flags, a brief instrument description, flight date, and version number, most recent data revision date, and revision history.

2.3 Data Management and Publication at the ORNL DAAC

The ORNL DAAC is one of twelve NASA Earth Observing System Data and Information System (EOSDIS) data centers, which provide open access to data from NASA's Earth Science Missions (see <u>https://earthdata.nasa.gov/about/daacs</u>). Upon receipt of the ACT-America data, the ORNL DAAC evaluated the data for completeness and structure, and created Climate and Forecasting (CF, <u>https://cfconventions.org</u>) compliant netCDF (Network Common Data Form) files from the ICARTT source data. In addition to being more broadly standardscompliant, self-describing, and consistent with interoperability best practices (see <u>https://daac.ornl.gov/datamanagement</u>), providing these netCDF files allow data users to take advantage of the numerous tools and open-source libraries that have been developed for netCDF data. These tools include the Thematic Real-time Environmental Distributed Data Services (THREDDS; <u>https://daac.ornl.gov/cgi-bin/service_dataset_lister.pl?svc_id=4</u>), which provides access and subsetting capabilities for netCDF data via programmatic and graphical interfaces.

ACT-America used an ICARTT-style file naming convention for all data products following the pattern: ACTAMERICA-instrument_platformID_YYYYMMDD_R#_L#.ext, where platformID = 'B200' or 'C130', 'merge', or 'Ground-'+ ground site name. YYYYMMDD = flight date in UTC time, R# = revision number (higher number indicates a more recent revision), L# = optional launch number (some B-200 flights had more than one sortie or launch), ext = file extension with either '.nc'/'.nc4' for NetCDF or '.ict' for ICARTT. For example, ACTAMERICA-Ozone_B200_20160726_R1_L2.nc is the netCDF file that contains the revision 1 of measurements made by the ozone instrument onboard the B-200 aircraft during its 2nd launch on July 26th, 2016.

Data files were grouped into a number of data products for publication at the ORNL DAAC, with each data product typically contains measurements from one instrument or a set of related instruments at a specific processing level (e.g., original or processed dataset). The ORNL DAAC also prepared comprehensive NASA-compliant metadata and a detailed user guide to accompany each ACT-America data product. Each user guide includes the following information: data citation, overview and description, spatial and temporal coverage and

resolution, number of data files, file formats and standards, file naming conventions, data dictionary including all measured parameters, units, and description, data application and derivation, quality assessment and uncertainty information, detailed data acquisition and methods section, data access instructions, and references.

Upon publication at the ORNL DAAC, a formal citation, including the authors, title, and date of publication, and a unique Digital Object Identifier (DOI) was issued for each data product. The data citation and DOI provide a convenient and traceable identity for each specific dataset that can be cited in the scholarly literature and linked to subsequent research efforts and products. In order to increase the visibility and maximize scientific impact of NASA data products, the ORNL DAAC provides searchable metadata to a variety of relevant data catalogues, advertises the data online through email, news, and the DAAC website, and provides user support services. All available datasets from the ACT-America project are listed at the ORNL DAAC at https://daac.ornl.gov/actamerica.

Throughout the ACT-America project, data files were revised, recalibrated, and updated, as necessary. Close communication, and automated monitoring of data availability, were essential for keeping the LaRC data repository and the holdings at ORNL DAAC in sync. The ORNL DAAC data publication system captures the revision history of all published datasets and has the capability of notifying the users about the changes occurred in each revision. The data files in each revision are also preserved in the data system so users can always access data of a particular revision.

3 Merged Airborne in situ Data Products

The airborne measurements from the ACT-America campaign were recorded on different native sampling time intervals ranging from milliseconds (e.g., 10 Hz for MFLL measurements) to tens of seconds (e.g., 5s temporal resolution for GHG measurements, Campbell et al., 2020). Additionally, instrument teams are responsible for reporting only their own data, without any of the navigational or meteorological parameters essential to its interpretation. Merging these various data files to a common standard sampling interval brings coherence to the data, creates geolocated data products, and makes it much easier for the data users to perform holistic analysis of the ACT-America data products. The ACT-America merged data products are generated at 1-second, 5-second, 60-second, and time intervals corresponding to flask sample fill times.

Merged data files in ICARTT format were prepared by LaRC through a weighted average based on the overlap between the measurement and merge time intervals as described in Chen et al. (2018). The merge files are updated to reflect revisions of any observational datasets. For each individual research flight, four key in situ observations collected by multiple instruments were merged: (1) navigational data, (2) GHG and trace gas mole fractions, (3) meteorological variables, and (4) flask samples. For the B-200, which needed refueling to cover long flight distances, the first and second sorties (L1 and L2, respectively) were also merged into a single file. In contrast, the C-130 endurance was long enough so that such sortie-merging was not required. It should be noted though that the flask samples were made at a certain interval during the flight hours (typically, 30 minutes) while all other in-situ measurements were made continuously from the time of take off to landing.

During the conversion of the merged data products from ICARTT format to netCDF format at the ORNL DAAC, the flight metadata flags (Davis et al., 2018) were added. The flight

metadata flags provide information such as the type of aircraft maneuver underway (e.g., profile versus level leg), whether or not the data are within the ABL, and the location of the data with respect to its synoptic environment (cold sector vs. warm sector of a mid-latitude weather system). These flags enable users to readily partition the data for analyses. In future, we will add surface influence functions that use an atmospheric transport reanalysis to provide a quantitative connection between the airborne data and regions upwind whose fluxes impact those airborne observations. The file header for an example C-130 5-second merged file with all meteorological variables, trace gases, navigations, and flight metadata flags can be found in Table S1.

Lidar remote sensing measurements, e.g., range-resolved backscatter from airborne lidar instruments, are not included in the merge data products because of their nature of data collection (i.e., range-resolved profiles of aerosol backscatter and extinction properties) and being incongruent to merge with in situ observations. However, in the future, parameters derived from remote sensing measurements, including atmospheric aerosol layers, ABL depths, and GHGs column density, which are currently being published as separate datasets, will be included in the merged data.

4 Modeling Data Products and Management

ACT-America brings together flux and transport models to generate simulated CO_2 and CH_4 mole fractions complementary to mission observations (Zhou et al., 2019; Feng et al., 2020) and inverse modeling systems needed to infer regional carbon fluxes using atmospheric carbon observations. The Penn State regional inversion and ensemble modeling system (Lauvaux et al., 2012; Diaz et al., 2018; Diaz et al., 2019; Feng et al., 2019a; Feng et al., 2019b; Butler et al., 2020; Barkley et al., 2019b) is the centerpiece of the analysis system. This modeling system requires inputs from carbon surface flux models and analyses, and atmospheric carbon boundary conditions, some provided by members of the ACT science team and some from other research community products (Feng et al., 2019b; Zhou et al., 2019). The reference WRF-Chem simulation is based on CO_2 inputs from the NOAA CarbonTracker Inversion system (Jacobson et al., 2020). Ensembles of all components (surface fluxes, boundary conditions, atmospheric transport realizations) are employed for the purpose of component-specific uncertainty quantification (Feng et al., 2019a; Feng et al., 2019b).

The goal of model data management for ACT-America is to facilitate the use of model data within the ACT-America team and by broader communities. To achieve this goal, we followed lessons learned (Wei et al., 2014) from past research projects, i.e., the Multi-scale Synthesis and Terrestrial Model Intercomparison project (MsTMIP) (Huntzinger et al., 2013), to apply management practices for ACT-America model data products. Specifically, we ensured appropriate resources for model data planning, preparation, and management; established close collaboration between data experts and science researchers; produced model data and metadata in proper formats and standards; provided detailed data documentation, including the model data provenance; and provided an on-demand approach to distribute data. Selected model data products are published through the ORNL DAAC (see https://daac.ornl.gov/actamerica), to ensure long-term preservation of key model data produced by ACT-America.

The model data management team at the ORNL DAAC set up a high-throughput, accesscontrolled, easy-to-use online data portal that enables ACT-America researchers to upload, browse, and download model data. The underlying infrastructure of this data portal leverages the File Transfer Protocol Secure (FTPS) and a modern cloud-based file sharing platform (Dropbox). This portal also provides an easy-to-use Web user interface that allows ACT-America researchers to browse model data products and choose different mechanisms to access them.

The CF-compatible netCDF format was chosen for ACT-America model data products to increase usability and interoperability. The THREDDS data server provided by the ORNL DAAC allows data to be accessed through standard Web API (i.e., Open-source Project for a Network Data Access Protocol; OPeNDAP) in an on-demand manner. Users can choose to subset and access data in a region or temporal range of interest, instead of downloading the entire data files.

For model data, besides the fundamental characteristics (e.g., spatial extent, temporal extent, and variable names), one additional key metadata is their provenance, including version of the transport model used, boundary conditions and prior fluxes used in a particular simulation, and major model parameters. The data management team at the ORNL DAAC worked with modeling scientists to document such provenance metadata for every single simulation output to be shared with other researchers. To ensure the traceability of model outputs, the input data (e.g., boundary conditions and prior fluxes), if specifically created for ACT-America and not publicly available from another source, are also stored and managed through the ACT-America model data portal. For example, the "ACT-America: Gridded Ensembles of Surface Biogenic Carbon Fluxes" dataset (Zhou et al., 2019) is one key dataset used as prior fluxes for the ACT-America project through the model online data portal and published through the ORNL DAAC to facilitate public use as well.

5 Applications of ACT-America Data

The airborne measurements of atmospheric carbon dioxide, methane, trace gases and meteorological properties alongside the continuous tower-based GHGs measurements over the Central and Eastern United States provide a valuable asset to improve the accuracy and precision of regional inverse flux estimates of GHGs. This asset has a wide range of applications, including but not limited to, quantifying and reducing uncertainties in simulated atmospheric transport of GHGs; quantifying and reducing uncertainties in a priori CH_4 and CO_2 flux estimates, especially CH_4 emissions and biogenic CO_2 fluxes; and evaluating the ability of the OCO-2 to observe spatial variations in tropospheric CO_2 (Davis et al., submitted).

Various studies have leveraged ACT-America measurements to improve our understanding and modeling of regional flux estimates of GHGs. For example, Pal et al. (2020) analyzed the airborne 5-second merged in situ measurements (Davis, et al., 2018) in frontal passages collected by the ACT-America summer 2016 campaign to understand how GHG distributions change vertically and horizontally during a synoptic event. The observational analyses presented define new metrics involving horizontal and vertical GHG contrasts across fronts during summer which will be used to evaluate simulations of GHG transport. In another study (Barkley et al., 2019a), CH₄ and C₂H₆ observations (Davis, et al., 2018; DiGangi et al., 2018) from the ACT-America campaigns were used to adjust oil/gas and animal agriculture emissions across the south-central U.S. such that modeled CH₄ and C₂H₆ enhancements match the observed plume. Successful modeling from this study raises the possibility of using trace gas measurements along frontal crossings to solve for emissions in other large regions of the United States. Using a similar modelling technique, a large discrepancy between N₂O emission inventories and top-down derived agricultural Midwest emissions (Eckl et al., 2020). Baier et al. (2020) analyzed the multispecies measurements in flasks (Sweeney et al., 2015) sampled during the wintertime ACT-America campaign for background characterization and source apportionment of regional anthropogenic CO₂ and CH₄ fluxes. In this study, oil and natural gas influence was broadly observed throughout the entire observational domain. These whole-air flask samples illuminated significant wintertime regional CO₂ and CH₄ sources or sinks during ACT-America and provide additional information for informing regional inverse modeling efforts. ACT-America data were compared to global CO₂ simulations to quantify uncertainties in the global simulations (Chen et al., 2019).

Rigorous investigation on exploring the feature of the observed CO₂ using flux and transport models is underway, such as using ACT-America airborne data to evaluate OCO-2 Model Intercomparison Project (MIP) V9 estimated CO₂ fluxes; evaluating the skill of ten global CO₂ inversion models from the OCO-2 MIP using 148 airborne vertical profiles of CO₂ for frontal cases from the ACT-America Summer 2016 campaign (Gaudet et al., *in review*); high resolution modeling to explain the elevated CO₂ band observed along the frontal boundary shown in Pal et al. (2020) (Samaddar et al., 2020), using ACT-America airborne data to evaluate the newly developed CO₂ transport in an NCAR state-of-art global model MPAS (Zheng et al., 2020); using CO₂ observations from ACT-America, NOAA towers, and Ameriflux to evaluate Carnegie-Ames-Stanford Approach (CASA) models; using flask Carbonyl Sulfide measurements to disentangle the CO₂ sources; and evaluating of OCO-2 XCO₂ variability at local and synoptic scales using ACT-America lidar and in situ observations (Bell et al., 2020).

6 Accessibility of ACT-America Data

NASA promotes the full and open sharing of Earth Science data with the research and applications communities, private industry, academia, and the general public (details at <u>https://earthdata.nasa.gov/earth-observation-data/data-use-policy</u>). Data from ACT-America are available free and open to the public from the ORNL DAAC, which is a CoreTrustSeal Certified Repository (<u>https://www.coretrustseal.org/</u>) and adheres to the FAIR data principles (<u>https://www.forcel1.org/group/fairgroup/fairprinciples</u>). A free NASA Earthdata Login account is required to access ACT-America data. Users are required to obtain an account at <u>https://urs.earthdata.nasa.gov/</u>. By establishing an account, users can be notified of changes or updates to the data. To better support the carbon cycle modeling research, ACT-America airborne CO₂ observations are also integrated into the NOAA/GML Observation Package (ObsPack) data products (Masarie et al., 2014). ObsPack brings together direct atmospheric greenhouse gas measurements derived from one or more national or university laboratories.

The Airborne Data Visualizer (available at: <u>https://actamerica.ornl.gov/visualize/</u>) (ORNL DAAC, 2020) was developed to enhance the understanding and accessibility of data collected for the ACT-America mission. It runs on a server maintained by the ORNL DAAC and takes advantage of the rich metadata packaged with the instrument measurements in the netCDF files to create an informative interface for exploration of the data.

To acknowledge the science teams who have created and shared data products, users should include a bibliographic citation to any data products used in publications. Proper citations, including the authors, title, publisher, and DOI, will help others find and re-use the data and also establish methods to track the impact of the ACT-America mission. The citation and DOI for each ACT-America data product are provided on each data product landing page and each data product User Guide.

7 Summary

The ACT-America study is a multi-year effort to better understand and quantify sources and sinks of major greenhouse gases. ACT-America provides a unique and valuable asset of high-quality airborne measurements of atmospheric carbon dioxide, methane, trace gases and meteorological properties over the Central and Eastern United States, along with tower-based measurements and modeled atmospheric greenhouse gases mole fractions and regional carbon fluxes. Through all five seasonal campaigns, a total of 121 research flights, more than 1,140 hours of observations, 570 level legs, and 1,363 vertical profiles were conducted using the two aircraft, i.e., C-130 and B-200. ACT-America data products, including the merged airborne insitu data, provide a valuable asset to improve the accuracy and precision of regional inverse flux estimates of GHGs and beyond. A few of research applications are highlighted in Section 5. A special issue collection reported major scientific findings (available at:

https://agupubs.onlinelibrary.wiley.com/doi/toc/10.1002/(ISSN)1944-9224.ACT-AMERICA1) and another is under development

(https://agupubs.onlinelibrary.wiley.com/hub/jgr/journal/21698996/features/call-for-papers). A full catalogue of known ACT-America publications can be found at the ORNL DAAC ACT-America website (https://actamerica.ornl.gov/publications.shtml). Better estimates of greenhouse gas transport, sources, and sinks, enabled by the detailed data collected by ACT-America, will help to reduce uncertainty in terrestrial carbon cycle models at regional to continental scales and to monitor regional carbon fluxes to support climate-change mitigation efforts.

Acknowledgements

The ACT-America project is a National Aeronautics and Space Administration (NASA) Earth Venture Suborbital 2 project funded by NASA's Earth Science Division. The ORNL DAAC is sponsored by NASA under Interagency Agreement 80GSFC19T0039. ORNL participation in ACT-America was funded by NASA under interagency agreement NNL15AA10I (Wei, Shreshta, Boyer). Other co-authors were supported by the following NASA grants: NNX15AG76G to Penn State (Davis); NNX15AJ06G (Baier, Sweeney) and NNX15AW47G (Fried) to University of Colorado-Boulder; NNX16AN17G to Clark University (Williams); NNL15AQ00B to Exelis (Dobler); 80NSSC19K0730 to Texas Tech and a Texas Tech University start up research grant (Pal); and NNX15AI97G (O'Dell) to Colorado State University.

Complementary support for tower-based measurements was provided by NASA grant NNX14AJ17G and NIST grant 70NANB15H336. NASA co-authors were supported by NASA Science Mission Directorate funding awarded in response to the Earth Venture Suborbital-2 Announcement of Opportunity NNH13ZDA001N-EVS2. Roiger was supported by DLR VO-R via the young investigator research group "Greenhouse Gases.". T. Lauvaux was supported by the French research program Make Our Planet Great Again (project CIUDAD).

The authors acknowledge NASA's Earth System Science Pathfinder Program Office, NASA's Airborne Sciences Program, NASA's Atmospheric Science Data Center, as well as the administrative and flight forecasting support from Penn State's Department of Meteorology and Atmospheric Sciences.

All ACT-America data products are open and freely available from the ORNL DAAC: <u>https://daac.ornl.gov/actamerica</u>.

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Earth and Space Science

Supporting Information for

Atmospheric Carbon and Transport – America (ACT-America) Datasets: Description, Management, and Delivery

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Contents of this file

Table S1: Meteorological, trace gases, and navigational variables in an example C-130 5-second merged file.

Introduction

This document contains supporting Information (Table S1), which provids meteorological, trace gases, and navigational variables in an example C-130 5-second merged file.

Variable name	Description	Units
Instrument: Portable Flask Packa	ge	
BENZ_MoleFraction_PFP	benzene mole fraction	ppt
C2F6_MoleFraction_PFP	hexafluorethane mole fraction	ppt
C2H2_MoleFraction_PFP	acetylene mole fraction	ppt
C2H6_MoleFraction_PFP	ethane mole fraction	ppt
C3H8_MoleFraction_PFP	propane mole fraction	ppt
CF4_MoleFraction_PFP	carbon tetrafloride mole fraction	ppt
CH2BrCl_MoleFraction_PFP	bromochloromethane mole fraction	ppt
CH3I_MoleFraction_PFP	methyl iodide mole fraction	ppt
CH4C13_MoleFraction_PFP	C-13 of CH4 mole fraction	per mil
CH4_MoleFraction_PFP	methane mole fraction	ppb
CHLF_MoleFraction_PFP	chloroform mole fraction	ppt

CO2C14_MoleFraction_PFP	C-14 of CO2 mole fraction	per mil
CO2_MoleFraction_PFP	carbon dioxide mole fraction	ppm
CO_MoleFraction_PFP	carbon monoxide mole fraction	ppb
DIBR_MoleFraction_PFP	dibromomethane mole fraction	ppt
DICL_MoleFraction_PFP	dimethyl chloride mole fraction	ppt
F113_MoleFraction_PFP	CFC113 mole fraction	ppt
F115_MoleFraction_PFP	CFC115 mole fraction	ppt
F11B_MoleFraction_PFP	F11 mole fraction	ppt
F125_MoleFraction_PFP	pentafluoroethane mole fraction	ppt
F134A_MoleFraction_PFP	Tetrafluoroethane mole fraction	ppt
F13_MoleFraction_PFP	F13 mole fraction	ppt
F143a_MoleFraction_PFP	1-1-1-trifluoroethane mole fraction	ppt
F152A_MoleFraction_PFP	1-1-difluoroethane mole fraction	ppt
F227e_MoleFraction_PFP	F227 mole fraction	ppt
F236fa_MoleFraction_PFP	F236fa mole fraction	ppt
F23_MoleFraction_PFP	fluoroform mole fraction	ppt
F32_MoleFraction_PFP	F32 mole fraction	ppt
F365m_MoleFraction_PFP	pentafluorobutane mole fraction	ppt

FC12_MoleFraction_PFP	FC12 mole fraction	ppt
H1211_MoleFraction_PFP	halon 1211 mole fraction	ppt
H1301_MoleFraction_PFP	halon 1301 mole fraction	ppt
H2402_MoleFraction_PFP	halon 2402 mole fraction	ppt
H2_MoleFraction_PFP	hydrogen mole fraction	ppb
HF133a_MoleFraction_PFP	HF133a mole fraction	ppt
HF22_MoleFraction_PFP	HF22 mole fraction	ppt
MCFA_MoleFraction_PFP	methyl chloroform mole fraction	ppt
MEBR_MoleFraction_PFP	methyl bromide mole fraction	ppt
MECL_MoleFraction_PFP	methyl chloride mole fraction	ppt
N2O_MoleFraction_PFP	nitrous oxide mole fraction	ppb
OCS_MoleFraction_PFP	carbonyl sulfide mole fraction	ppt
P218_MoleFraction_PFP	P218 mole fraction	ppt
PCE_MoleFraction_PFP	perchloroethylene mole fraction	ppt
SF6_MoleFraction_PFP	sulfur hexafloride mole fraction	ppt
SO2F2_MoleFraction_PFP	sulfuryl fluoride mole fraction	ppt
TCE_MoleFraction_PFP	trichloroethylene mole fraction	ppt
TOL_MoleFraction_PFP11	toluene mole fraction	ppt

iC4H10_MoleFraction_PFP	isoButane mole fraction	ppt	
iC5H12_MoleFraction_PFP	isoPentane mole fraction	ppt	
nC4H10_MoleFraction_PFP	neoButane mole fraction	ppt	
nC5H12_MoleFraction_PFP	neoPentane mole fraction	ppt	
nC6H14_MoleFraction_PFP	n-Hexane mole fraction	ppt	
Instrument: Picarro CRDS			
CH4_DryMoleFraction_PICARRO	Methane dry mole fraction	ppm	
CO2_DryMoleFraction_PICARRO	carbon dioxide dry mole fraction	ppm	
CO_DryMoleFraction_PICARRO	Carbon monoxide dry mole fraction	ppm	
Dewpoint_PICARRO	dew point	к	
H2O_MassMixingRatio_PICARRO	Water vapor mass mixing ratio	g kg-1	
H2O_VaporPressure_PICARRO	Derived water vapor pressure	hPa	
H2O_VolMixingRatio_PICARRO	Water vapor volume mixing ratio	percent	
RHi_PICARRO	Derived relative humidity wrt ice	percent	
RHw_PICARRO	Derived relative humidity wrt liquid water	percent	
Instrument: CAMS-2 Spectrometer			
C2H6_MixingRatio_CAMS2	C2H6 mixing ratio by volume	ppbv	
Instrument: Cloud Physics Lidar			

MLH-AMSL_CPL	derived mixed layer height in ASL	m
GroundHeight-AMSL_CPL	derived ground height above MSL	m
Instrument: 2B Technologies Con	tinuous O3	
O3_DryMoleFraction	ozone mole fraction	ppb
Instrument: In Situ Quantum Cas	cade Laser Spectrometer (QCLS)	
C2H6_MixingRatio_QCLS	C2H6 dry mixing ratio	ppbv
Aircraft navigation and meteorol	ogical variables	
ALTP	pressure altitude	m
AircraftSunAzimuth	aircraft sun azimuth	degree
AircraftSunElevation	aircraft sun elevation	degree
CabinPressure	cabin pressure	hPa
Dewpoint_Nav	dew point	К
DifferentialPressure	differential pressure	hPa
DriftAngle	drift angle	degree
GPS_ALT	global positioning system altitude	m
GRD_SPD	ground speed	m s-1
H2O_MixingRatio_Nav	H2O mixing ratio	g kg-1
H2O_RelativeHumidity_Nav	relative humidity	percent

H2O_SatVaporPressureIce_NavH2O sat vapor pressure icehPaH2O_SatVaporPressureWater_NavH2O vapor pressure waterhPaH2O_VaporPressure_NavH2O vapor pressurehPaHDGtrue headingdegreeIASindicated air speedm s-1LATITUDElatitudedegree_northLOCAL_SUN_TIMElocal sun timehLONGITUDEindicated air speeddegree_eastMachNumbermach number1PITCHpitch angledegreePRESSUREstatic pressurehPaRolLroll angledegreeSZAsolar azimuth angledegreeSolarZenithAnglestatic pressurehPaStaticPressurestatic pressurehPaSunAzimuthsun azimuth angledegree			
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StaticPressurestatic pressurehPaSunAzimuthsun azimuthdegree	SolarZenithAngle	solar zenith angle	degree
SunAzimuth sun azimuth degree	StaticPressure	static pressure	hPa
	SunAzimuth	sun azimuth	degree

TAS	true air speed	m s-1	
TEMPERATURE	static air temperature	К	
ТНЕТА	potential temperature	К	
TRK	track angle	degree	
TotalAirTemp	total air temperature	К	
VerticalSpeed	vertical speed	m s-1	
U_WINDS	U wind direction	m s-1	
V_WINDS	V wind direction	m s-1	
Wind_Direction	wind direction	degree	
Wind_Speed	wind speed	m s-1	
Metadata flag information			
Air_flag	Warm/Cold air flag		
BL_FT_flag	ABL or free troposphere flag		
Flight_flag	Flight pattern flag		
Maneuver_flag	Maneuver flag		
Maneuver_flagQC	Maneuver flag QC		
Extracted ground elevation			

Altitude_AGL	Aircraft altitude above ground level from Google Maps API	m
GroundElevation- AMSL_GoogleMaps	ground elevation above mean sea level from Google Maps API	m

Table S1. Meteorological, trace gases, and navigational variables in an example C-130 5-second merged file.

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Earth and Space Science

Supporting Information for

Atmospheric Carbon and Transport – America (ACT-America) Datasets: Description, Management, and Delivery

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Contents of this file

Text S1: Summary of the calibration and QA/QC procedures used by the major instruments and measurements of ACT-America.

Introduction

This document contains supporting Information (Text S1), which provides a summary of the calibration and quality-assurance and quality-control (QA/QC) procedures used by the major instruments and measurements of ACT-America.

Text S1. Summary of the calibration and QA/QC procedures used by the major instruments and measurements of ACT-America.

• Airborne PICARRO GHG measurements

In situ CO_2 , CH_4 , and CO were measured via cavity ringdown spectroscopy using a PICARRO G2401-m analyzer, while H₂O(v) was measured using a similar PICARRO G2301m analyzer. Ambient air was sampled using a modified Rosemont total air temperature gas sampling probe (Buck Research Inst. LLC) sampling 12" from the fuselage to avoid the aircraft boundary layer. The flow was split, with one branch proceeding directly to the G2301-m analyzer and the other dried using a PermaPure Nafion dryer (PD-200T-24-MSS). The latter was then compressed with a diaphragm pump (Vacuubrand, Inc.) to a constant pressure of ~1070 mbar maintained using an absolute pressure proportional relief valve (Tavco, Inc.), then sampled by the G2401-m analyzer. An onboard cylinder standard was used to perform hourly in-flight single point offset calibrations of CO_2 , CH_4 , and CO. This calibration gas was introduced at the inlet with a flow greater than the total system flow so as to avoid pressure disruption. Calibration slopes of CO₂, CH₄, and CO were calculated from weekly three point ground calibrations using cylinder standards. All standards were obtained from NOAA ESRL with concentrations traceable to WMO standards (CO₂: X2007; CH₄: X2004A; CO: X2014A). H₂O(v) was calibrated between campaigns with a water source measured simultaneously by the analyzer and a NISTtraceable frost-point hygrometer (Edgetech).

• Ozone measurements

In situ O₃ was sampled with a $\frac{1}{2}$ " OD (3/8" ID) FEP tube sheathed inside a 5/8" OD (1/2" ID) stainless steel forward facing J-probe inlet. This flow was introduced into a 9" x 1.5" diameter PFA sampling manifold. Flow exiting the manifold was exhausted from the aircraft through a static exhaust port. Thus, flow through the manifold was driven by the differential between the impact pressure from the forward facing inlet and the static pressure from the exhaust, typically ~30 L/min during flight. O₃ concentrations were measured from air subsampled from the upstream side of the manifold via UV absorption using a 2B Technologies Model 205 analyzer. The air from the analyzer was then exhausted to the downstream side of the manifold to minimize pressure differentials across the analyzer. O₃ background offsets were corrected using zeros

measured hourly in flight by scrubbing incoming air with a potassium iodide cartridge. Calibration of the analyzer was performed between campaigns using a NIST-traceable UV photolysis source (Model 306, 2B Technologies).

Onboard NOAA Programmable Flask Packages

NOAA Programmable Flask Packages (PFPs) were sampled in-flight and promptly returned to NOAA's Global Monitoring Laboratory in Boulder, CO for analysis of greenhouse gases, carbon isotopes, halocarbons and hydrocarbon species. A first sample aliquot was analyzed on the Measurement of Atmospheric Gases that Influence Climate Change (MAGICC) system for dry-air mole fractions of CO₂, CH₄, CO, N₂O, SF₆, and H₂ (https://www.esrl.noaa.gov/gmd/ccgg/aircraft/analysis.html). MAGICC gases were calibrated to standard scales maintained at NOAA/GML (Dlugokencky 2005; Hall 2007; Novelli 1991; Zhao and Tans 2006). A second aliquot of sample air was analyzed on a custom-built GC/MS (PR1) system for approximately 50 additional non-methane hydrocarbons, halocarbons, and other sulfur-containing compounds and reported on NOAA absolute calibration scales derived in-house from pure components and highprecision gravimetric techniques. Remaining flask sample air was transferred to the Stable Isotope Laboratory at University of Colorado-Boulder's Institute of Arctic and Alpine Research (INSTAAR) for stable isotopic measurements of carbon dioxide and methane (d¹³C-CO₂ and (d¹³C –CH₄). For these species, INSTAAR maintains standards that tie sample measurements to the local realization of the VPDB-CO₂ scale (Miller et al, 2002, Trolier et al., 1996, Vaughn et al., 2004). A subset of the ACT-America flask samples has undergone CO₂ graphitization at INSTAAR's Laboratory for AMS Radiocarbon Preparation and Research (Turnbull et al., 2009; Turnbull et al. 2007) and subsequent analysis for radiocarbon (¹⁴CO₂) by the University of California at Irvine. Flask data have undergone several quality control measures to assess analysis errors, sampling errors, or storage biases. Analysis errors in measurement systems were detected through drift in target or standard gas measurements or via abnormal initial flask pressure or humidity before during measurement of sample aliquots. Similar to Sweeney et al. (2015), flask sampling errors were identified using onboard PFP data logs used to both record flask mass flow rates and flushing times, and to ensure that the flask target storage pressures were reached for each sample. Potential contamination or leaks in sample lines were identified using indicator species such as CO, tetrafluoroethane (Freon 134a, C₂H₂F₄) and bromochlorodifluoromethane (Halon-1211, CBrClF₂), emitted from engine exhaust, onboard air-conditioners, and aircraft fire extinguishers respectively (Sweeney et al., 2015). Enhanced mole fractions of the aforementioned gases in flask samples, when unaccompanied by co-enhanced species indicative of anthropogenic emissions plumes, were flagged for potential sample contamination.

• Cloud Physics Lidar (CPL)

CPL is a multi-wavelength (355, 532 and 1064 nm) elastic backscatter lidar that enables a comprehensive analysis of radiative and optical properties of clouds and aerosols [McGill et al., 2002]. CPL data have been used for cloud properties analysis [McGill et al., 2003; McGill et al., 2004] and validation of satellite retrievals [McGill et al., 2007; Yorks et al.,

2011b; Hlavka et al., 2012]. CPL measures the total attenuated backscatter (e.g., aerosol plus Rayleigh) as a function of altitude at each wavelength. Additional cloud and aerosol properties include the particle depolarization ratio for phase discrimination, lidar ratio, extinction coefficient, optical depth, and backscatter color ratio. Final CPL data product accuracy depends upon the number of laser pulses averaged and the aerosol loading of the atmosphere.

The steps to producing calibrated CPL profiles of normalized relative backscatter (NRB) are: (1) geo-locate the raw CPL data; (2) correct for detector nonlinearity, range, and instrument artifacts; (3) normalize to laser energy; and (4) subtract solar background signal. The ancillary information included in the Level-1 data file is the navigation data from the aircraft and coincident meteorological data (i.e., temperature, pressure, relative humidity). CPL uses Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) reanalysis data for meteorological variables. The calibration method for CPL backscatter data at all three wavelengths is the Rayleigh normalization technique, which normalizes the CPL signal to the actual atmospheric signal from molecular (Rayleigh) scattering [McGill et al., 2007]. The molecular backscatter and extinction coefficients are computed using temperature and pressure from MERRA-2. No in-flight calibration is required. CPL Level-2 data products (i.e., cloud phase, backscatter and extinction coefficients, cloud optical depth, etc.), which are provided in HDF5 format, are derived using the algorithms outlined in Yorks et al. [2011a], Yorks et al. [2011b], and Hlavka et al. [2012].

The CPL QA/QC activities have three stages: (1) in-field data assessment, (2) preliminary QA/QC, and (3) final data products. First, the CPL team applies the calibration and data processing algorithms, as described above, to the raw data acquired during flight. The team produces initial data products within 24-48 hours of each flight. In-field data assessment is performed using browse image analysis (images available at the CPL website http://cpl.gsfc.data.gov). If the browse images pass the in-field QA/QC, the preliminary data products are produced using standard atmospheric profiles for calibration. Once MERRA-2 reanalysis data become available (approximately 1 month after a campaign), the CPL data is reprocessed to produce the final data products. Final data products are examined by the CPL team to assess data quality before the data is archived at the DAAC.

ABL depths have been derived from the CPL backscatter data using a wavelet algorithm (Davis et al, 2000) and quality-checked by hand. This data set is in the process of being documented and added to the ACT-America data archive.

• Multifunctional Fiber Laser Lidar (MFLL)

The Multifunctional Fiber Laser Lidar (MFLL) was developed by Harris Corporation and further advanced through significant test flights and collaboration with NASA Langley Research Center, as a testbed for the Active Sensing of CO₂ Emissions over Nights Days and Seasons (ASCENDS) Mission. MFLL uses an Intensity Modulated Continuous Wave (IMCW) measurement method which allows simultaneous transmission and reception of two or more closely spaced (50 pm) wavelengths precisely positioned on the CO₂ line at

1571.1192 nm to acquire the differential absorption over the column of air between the aircraft and the target of interest (e.g. clouds, ground) (Dobler et al. 2013; Lin et al. 2013). Systematic assessments of MFLL lidar data with certain flags are performed to assure and control the quality of MFLL data during lidar data processing. The most critical QA/QC procedures are lidar power check, aircraft attitude evaluation, and cloud determination. A constant threshold for the total power of all channels of MFLL signals is applied to ensure high enough signal-to-noise ratio (SNR) for XCO₂ retrieval. To avoid measurement errors caused by aircraft attitude variations aircraft pitch and roll angles only within \pm 5 degrees are tolerated in data processing. Furthermore, thin and thick clouds are identified based on lidar ranging capability. These clouds could reduce lidar SNR or totally block lidar returns from the ground. In these cases, partial column CO₂ retrievals are also reported.

MFLL data processing uses two basic procedures in calibrating MFLL measurements for its XCO₂ retrieval. The first one is MFLL instrument short-path measurements. This calibration compensates the wavelength-dependent throughput of the internal optics of the instrument and accounts for the differences in lidar signal path lengths within and outside the instrument. After this calibration, MFLL data and differential absorption optical depth (DAOD) measurements are further calibrated with in situ derived DAOD values obtained from aircraft spiral CO2 observations (Campbell et al. 2020). This calibration procedure not only makes remote sensing and in situ measurements consistent but also reduces the impacts of various potential error sources on XCO₂ retrievals. With these calibrations, along with QA/QC, MFLL XCO₂ retrievals reach high accuracy (0.8 ppm) and precision (0.26 ppm with 1-min integration; Campbell et al., 2020).

High-Altitude Lidar Observatory (HALO)

NASA Langley Research Center has developed the High-Altitude Lidar Observatory (HALO) system to address the observational needs of NASA's weather, climate/radiation, carbon cycle, and atmospheric composition focus areas. HALO is a modular and multifunction airborne lidar developed to measure atmospheric H₂O and CH₄ mixing ratios and aerosol, cloud, and ocean optical properties using the differential absorption lidar (DIAL) (Nehrir et al., 2017) and high spectral resolution lidar (HSRL) (Hair et al. 2008) techniques, respectively. To respond to a wide range of airborne process studies, HALO can be rapidly reconfigured to provide either, H₂O DIAL/HSRL, CH₄ DIAL/HSRL, or CH₄ DIAL/H₂O DIAL measurements using three different modular laser transmitters and a single multi-channel and multi-wavelength receiver. For the summer 2019 ACT-America campaign HALO employed the CH₄ DIAL/HSRL configuration and archived the standard suite of aerosol extensive and intensive products as described in Hair et al. 2008 as well as the mixed layer height as described in Scarino et al., 2014. HALO also measured, for the first-time, distributions of column weighted XCH₄ during this campaign and will archive those products once the development and validation effort has been completed. HALO data are sampled at 0.5-s temporal and 1.25-m vertical resolutions. The vertical resolution for the aerosol measurements is increased to 15 m in post-processing to increase the SNR of the aerosol intensive and extensive retrievals. Aerosol backscatter

and depolarization products are averaged 10 s horizontally and aerosol extinction products are averaged 60 s horizontally and 150 m vertically. The polarization and HSRL gain ratios are calculated as described in Hair et al., 2008. Operational retrievals also provide mixing ratio of non-spherical-to-spherical backscatter (Sugimoto and Lee, 2006), aerosol type (Burton et al., 2012) and aerosol mixed-layer height (Scarino et al., 2014). The raw data are quality controlled by applying a cloud screening mask to remove attenuated signals below clouds. The data are further screened when the aircraft is within 2 km of the surface or when the lidar profile does not reach within 1km of the surface. For the mixing layer height product which is the principal lidar observable for ACT-America, the retrievals are quality controlled beyond the methods described in Scarino et al. (2014) by applying a user defined and time dependent threshold on the wavelet transform. All data products are archived in an H5 file format with 10 second horizontal resolution. Future methane column products will be archived at the 0.5 second native resolution.

• Quantum Cascade Laser Spectrometer (QCLS)

Observations are referenced to calibration gas mixtures every 10 mins in flight using a two-point calibration procedure (zero and target mixing ratios) for all measured species (except H₂O). The target calibration gas mixtures (resembling mole fractions close to atmospheric ambient values) have been cross-calibrated against NOAA standards using a cavity ring-down spectrometer (Picarro G2301) and are thus traceable to WMO standards for CH4 and CO2 (WMO X2004A for CH4 – Dlugokencky et al., 2005, WMO X2007 for CO2 – Zhao and Tans, 2006). C2H6, CO and N2O are compared to NOAA flask samples traceable to WMO standards (PI: Colm Sweeney) taken during the ACT-America field campaigns. QA/QC procedures further include manual review of every flight and removal of spurious data associated with in-cavity pressure anomalies.

• Compact Atmospheric Multi-Species Spectrometer (CAMS-2) Ethane Measurements

Weibring et al. (2020) discuss comprehensive details of the 2nd generation Compact Atmospheric Multispecies Spectrometer (CAMS-2) employed in acquiring high precision 1-second ethane measurements on the B-200 airplane autonomously without an onboard operator. Ethane mixing ratios were determined by sampling ambient air through a multipass absorption cell where a mid-IR laser operating at a wavelength of 3.34 microns (2996.86 cm-1) was directed back and forth to achieve an optical pathlength of 47.6 m. At this wavelength, the laser is absorbed by a manifold of strong ethane lines and the retrieved ambient mixing ratios are determined employing the Beer-Lambert Absorption Law. To validate the direct absorption results, known calibration mixtures of ethane in air were introduced into the inlet before and after every flight, and the resulting direct absorption determinations were in agreement with the retrieved calibration values to within 6%. The final reported data employed the pre- and post-flight calibrations to correct the data. Comparisons of the continuous CAMS ethane data with time-coincident Portable Flask Package ethane data acquired on the B-200 resulted in agreement in the 4 to 5% range. Post mission exchange of ethane standards also produced agreement in this same range and given the uncertainties in the assigned standards values as well as the spectroscopic parameters, this level agreement was considered quite good. With each successive campaign, the ambient ethane performance was improved, and during 4th and 5th campaigns we routinely achieved 1-second (1 σ) ethane precisions in the 30 to 40 pptv range during flight.

• Tower-based GHG measurements

Prior to deployment, the instruments were calibrated in the laboratory using 4 NOAA-calibrated tanks. A field calibration tank was sampled daily and used to apply a zero-offset correction. Round robin tests using 3-4 NOAA-calibrated tanks were conducted every 1-2 years. NOAA flask measurements were used for comparison at the Mildred, Greenfield, and Mooresville sites. The averaging interval standard deviation and uncertainty derived from periodic flask sample to in-situ measurement comparisons are provided in the data files. Based on flask to in-situ comparisons and round robin testing presented in Richardson et al. (2017), the estimated compatibility of these measurements is approximately 0.18 ppm CO2 and 0.6 ppb CH4.

Meteorological and navigation data products C-130

Two levels of post-collection data quality control are performed. The first occurs within 24 hours of the end of the research flight, and the second within 6 months after the last research flight. These two distinct phases are often referred to as "field/preliminary" and "public/publication quality" data.

The preliminary phase of quality control is intended to capture, highlight, and remove errors in the original signal recordings obtained from the instruments, to prevent error propagation into the derived quantities which are reported in the meteorological and navigation file. Automated checks include plausible value (does the instantaneous signal make sense), plausible rate of change (are the changes between instantaneous values realistic and physically explainable), and internal consistency (are the instantaneous values sensible in relation to other measured values). Each of these processes occur within the field/preliminary phase.

The second phase of data quality control consists of further analysis that expands to an evaluation of instrument biases and long-term stability of the sensors, as well as instrument inter-comparisons with redundant sensor networks (both in situ and model comparisons, where applicable).

The instrumentation supported by NSRC is regularly calibrated by the NASA Armstrong metrology calibration laboratory or within-house by the NSRC Instrumentation Engineer. The calibration records are applied within the second phase of the data quality control process, prior to the submission of publication quality data. Additionally, for ACT-America, a set of aircraft calibration maneuvers were performed regularly throughout the mission to assess the fidelity and stability of the aircraft pitotstatic and inertial navigation system used to derive horizontal winds. These maneuvers allow for the quantification of errors in the measurement of static pressure and the true heading alignment of the inertial navigation system. Calibration factors derived from the aircraft maneuvers are applied in the second phase of quality control to aircraft true heading, aircraft static pressure, calculated wind speed, and calculated wind direction.

O B-200

Navigational and meteorological measurements obtained on board the LaRC B-200 aircraft have been carefully processed and screened to preserve their integrity and accuracy. Lab characterization, scheduled maintenance, and ground tests procedures in a static environment were performed on all instrumentation involved in making required airborne supporting measurements (Stickney et al., 1990; Edgetech Vigilant 137 Operation Manual). Navigational and meteorological measurements were also calibrated and verified using dynamic airborne flight maneuvers (Barrick et al. 1996; Haering, 1985). This was especially critical to meet the desired accuracy of horizontal winds. Reversed heading maneuvers were performed several times during each field mission to verify accurate derivation of horizontal winds. Static pressure position error and heading alignment were determined and corrections applied to wind calculations. Intercomparison flight legs between the LaRC B-200 and WFF C-130 were also conducted for additional correlative quality assurance purposes. Respective navigational parameters were verified during ground and airborne flights utilizing inertial and GPS techniques via two well documented systems. Navigational and attitude parameters from both a differential GPS (DGPS) and Applanix Pos/AVTM direct georeferencing system (DG) were recorded during all flights for redundancy and quality assurance purposes. The DGPS technique enhances the accuracy limits of GPS receivers by removing selective availability, atmospheric conditions, timing, and satellite orbit errors. The Applanix DG system integrates DGPS measurements with an inertial measurement system for added stability and accuracy (Mostafa et al. 2001).