Report on the first SPARC OCTAV-UTLS meeting, Boulder, CO, USA, 18-20 July 2017

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Dates:
18 - 20 July 2017

Organisers:
Gloria L. Manney (NorthWest research Assióciates, USA and New Mexico Institute of mining and Technology, USA), Irina Petropavlovskikh (NOAA, CIRES, USA), and Peter Hoor (University of Mainz, Germany)

Host Institution:
NorthWest Research Associates, USA

Number Of Participants: **~20**

Sponsors:

Activity Webpage:
https://www.octav-utls.net

More than 20 scientists from over 15 institutions gathered for the first meeting of the emerging SPARC activity OCTAV-UTLS (Observed Composition Trends And Variability in the Upper Troposphere and Lower Stratosphere) on 18-20 July 2017 in Boulder, CO. The meeting was organized by the Co-leads of the initiative, Gloria L Manney, Irina Petropavlovskikh, and Peter Hoor, and was graciously hosted by NorthWest Research Associates (many thanks to local organizers Janet Biggs, Andy Frahm, and Joan Alexander). The activity emerged from the GAW/NDACC/SPARC UTLS observation meeting in Geneva in May 2016, which emphasized open questions from the SPARC data initiative (Hegglin *et al.,* 2016). The focus of the OCTAV-UTLS activity is on improving the quantitative understanding of composition trends and long term dynamical changes in the UTLS; understanding dynamical changes such as trends in STE and the BDC will help quantify trends in ozone, water vapour, and other species. Achieving these goals requires a detailed characterization of existing measurements in the context of the large dynamical variability in the UTLS, which introduces confounding variability and uncertainty in assessing long term changes in observations.

The first meeting was intended to bring together experts from different observational communities and on meteorological data analysis to discuss the quality and sampling characteristics (spatial and temporal coverage and resolution) and the representativeness of these observations. The activity will initially focus on the trace gases with the largest radiative impact, first ozone and then water vapour. Thus, the discussion on the first day centred around available ozone measurements in the UTLS, with discussion of water vapour measurements on the third day. Discussion on the second day focused on analysis tools to be used in OCTAV-UTLS to account for dynamical variations, including the capabilities and possible extensions of the software package JETPAC (JEt and Tropopause Products for Analysis and Characterization; Manney *et al.,* 2011) that will provide a common framework for analysing the composition data sets.

Tuesday morning saw a series of overview talks about the necessity for, goals of, and activities related to OCTAV-UTLS. **Michaela Hegglin** summarized the Geneva GAW/NDACC/

SPARC UTLS observations workshop (Hegglin *et al.*, 2016), emphasizing the importance of reducing uncertainty in UTLS trace gas observations to improving climate predictions. Following this, **Peter Hoor** summarized the activity proposal, the major goals of the activity and the planned methods. **Irina Petropavlovskikh** reported insights from the SPARC activity LOTUS (**http://igaco-o3.fmi.fi/LOTUS/**), which she also co-leads. The primary goal of LOTUS is to reduce the uncertainty in ozone trend estimates from existing data in the stratosphere.

Later the discussions turned to available ozone measurements from aircraft, satellite, lidar, and ozonesonde platforms. Aircraft data from both commercial airliners and dedicated science missions will be used within OCTAV-UTLS. Commercial airliners fly regularly and thus provide broader data coverage and statistics over long time periods. However, the measurements are generally limited to a narrow range of altitudes with quasi-horizontal flight tracks. **Valerie Thouret** and **Andreas Petzold** reported on the data available from the IAGOS project (**http://iagos.sedoo.fr/**), which includes IAGOS-core and IAGOS-CARIBIC. Within IAGOS-core, water vapour and ozone data are available since 1994. It thus allows derivation of trends; this database is growing by about 5 million data points each year. Based on this data set, **Yann Cohen** presented climatologies and trends of ozone and carbon-monoxide in different parts of the UTLS (vertically and regionally). In contrast, IAGOS-CARIBIC operates about four times a month with the goal of obtaining a more comprehensive picture of the chemical composition of the UTLS. **Andreas Zahn** gave an overview of the ozone measurements available since 2005 and how these data can be used for both climatological and process-oriented studies. Data from dedicated UTLS science missions mainly focus on specific processes. Although such missions are limited in time and to certain regions, large consistent data sets produced by combining these data have become available in recent years. Andreas Zahn also presented corresponding ozone measurements from recent HALO campaigns: TACTS covered the midlatitude UTLS over Europe in August/September 2012 and PGS the polar/sub-vortex UTLS in winter 2015/2016. Peter Hoor presented data from the SPURT mission covering the midlatitude UTLS over Europe in the early 2000's over two years. **Laura Pan** discussed the major results from the START08 campaign, which had flight tracks covering large parts of the central US and Canada. Soundings and lidar observations constitute point-source measurements, but with very fine vertical resolution and numerous stations providing many decades of measurements. **Bryan Johnson** gave an overview of ozone sonde measurements, presenting analyses of ozone sonde data showing large day-to-day variability and the annual cycle captured in the multi-decadal climatology over Boulder and other NOAA, NDACC and SHADOZ ozone sonde stations. Some of these data are available since 1971 and profiles typically extend up to an altitude of about 35 km. On behalf of **Herman G.J. Smit** he also talked about homogenization of ozone sonde data and evaluation of instrumental and processing errors as a function of altitude, which is necessary for long time trend analysis. Finally, **Irina Petropavlovskikh** showed examples of the Boulder ozone sonde data in relation to dynamical features that affect the vertical profiles of ozone (see, e.g., Figure 4). She showed the relationships of UTLS ozone variability to dynamical features such as jets and multiple tropopauses. **Thierry Leblanc** then introduced available lidar measurements from various networks (e.g., NDACC, TOLnet). He noted that accuracy and precision of ozone measurements can vary significantly in the UTLS, but also showed examples demonstrating how lidar measurements can be used to analyse air masses affected by stratosphere-troposphere exchange (STE).

The data sets with largest spatial coverage but the least horizontal and vertical resolution in the UTLS come from satellites. Initially, it is planned to incorporate six data sets in the analysis, all introduced by representatives of the respective instrument teams. All presentations focused on merits and drawbacks of satellite measurements in the UTLS and recent retrieval improvements. **Adam Bourassa** discussed the approximately 14-year data record from OSIRIS, followed by **Kaley Walker** , who described ACE-FTS UTLS measurement characteristics and highlighted some recent papers using those. MIPAS UTLS measurement characteristics for the record from 2004 to 2012 were shown by **Gabriele Stiller**. The approximately 12-year MLS dataset and the OMPS-LP were described by **Luis Millán** and by **Natalya Kramarova**, respectively. **Robert Damadeo** discussed the measurements from the suite of SAGE instruments (SAGE I, II, III) covering over 20 years. The vertical resolution

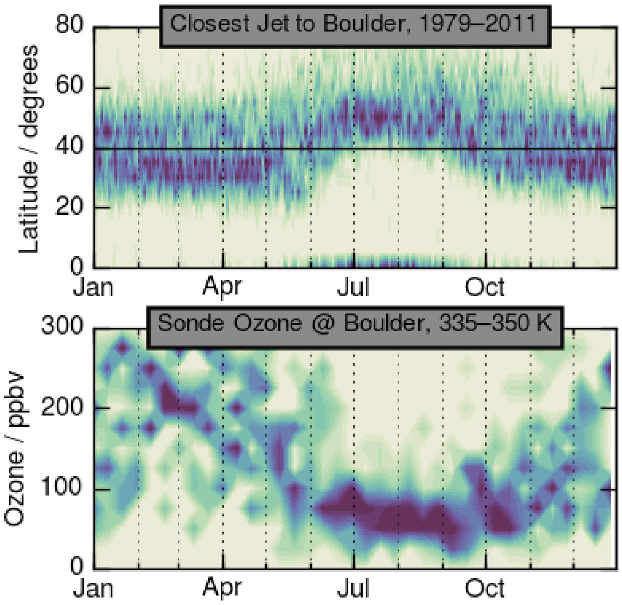

***Figure 4:** (Top) Climatological (1979–2011) frequency distribution of the closest jet to Boulder from JETPAC analysis. (Bottom) Climatological frequency distribution of ozone sonde observations in the 335–350 K isentropic layer (near the level of the subtropical jet). The subtropical jet is usually equatorward of Boulder in winter, and poleward of it in summer (during the North American monsoon), consistent with high ozone values (largely stratospheric air) in winter and low values in summer (largely tropospheric air).*

of ozone in the UTLS from most of these instruments is roughly 1-2 km, but 2-3 km for MLS; uncertainties generally increase in the UTLS, but many studies have demonstrated that the measurements are still valuable there, and their broad coverage complements the observations from balloons, lidar, and aircraft.

The second day was intended to discuss common strategies and metrics for data analysis to account for variability induced by dynamical processes to get better statistics for trends. The uncertainties of a data point generally arise from uncertainties related 1) to the measurement technique or data retrievals/processing and 2) uncertainties related to the coordinate system used to interpret the data. The first uncertainty is inherent in the retrieved data, and must thus be accounted for but cannot be mitigated. However, by choosing appropriate coordinate systems based on the geophysical flow in the atmosphere and/or its thermodynamic state, dynamically-driven uncertainties can be significantly reduced.

To guarantee consistent treatment of the UTLS dynamics, the JETPAC tools will be used for all observations. JETPAC can use meteorological data from numerous reanalysis data sets to map the observations in geophysical coordinate systems, based on equivalent latitude, jet locations (e.g., subtropical or "polar" jet) and/or tropopause locations (both lapse rate and PV-based). Current and planned features of JETPAC were presented by **Gloria Manney** and **Luis Millán** in several talks; Figure 4 shows an example using JETPAC products to help interpret ozone sonde measurements at Boulder. New features may include Hadley cell coordinates (discussed by **Mark Olsen**) and additional tropopause definitions (e.g., based on isentropic PV gradients). Mark Olsen also showed how dynamical features such as QBO, ENSO affect the ozone mixing ratios using a jet-coordinate view derived from JETPAC. JETPAC was developed for satellite data, and has been extended to handle aircraft and profile (i.e., sonde and lidar) data. **Daniel Kunkel** addressed approaches for pre-processing aircraft data, which have much higher temporal and spatial resolution than the reanalysis data to be used for coordinate mapping. A similar discussion was led by **Thierry Leblanc** regarding the vertical resolution of lidar measurements. Additional discussions of methods to account for dynamical variability included tracer correlation studies (led by Peter Hoor), and using column ozone to identify STE in the extratropics (led by Mark Olsen). **Gloria Manney** also presented results from the SPARC Reanalysis Intercomparison Project that are pertinent to the selection of reanalyses to use for OCTAV-UTLS.

It was decided that ozone will be analysed in the first phase of OCTAV to define metrics and develop methods. Two test periods have been identified for the first consistent, comprehensive analyses of ozone data from all platforms, 2011-2013 and 2001-2003. JETPAC will be used as the central tool for comparison, and MERRA-2 as the initial reanalysis data set (though ERA-Interim and, eventually, ERA5 will also be used).

On day three the discussion turned to UTLS water vapour measurements. Water vapour is planned to be the focus after the development of methods for ozone since it is affected by microphysics in addition to dynamics. **Michaela Hegglin** showed climatologies from satellite measurements and their uncertainties. She pointed out that water vapour trends in the UTLS are very difficult to determine with rising tropospheric temperatures, and that there is a large discrepancy between satellite measurements and chemistry

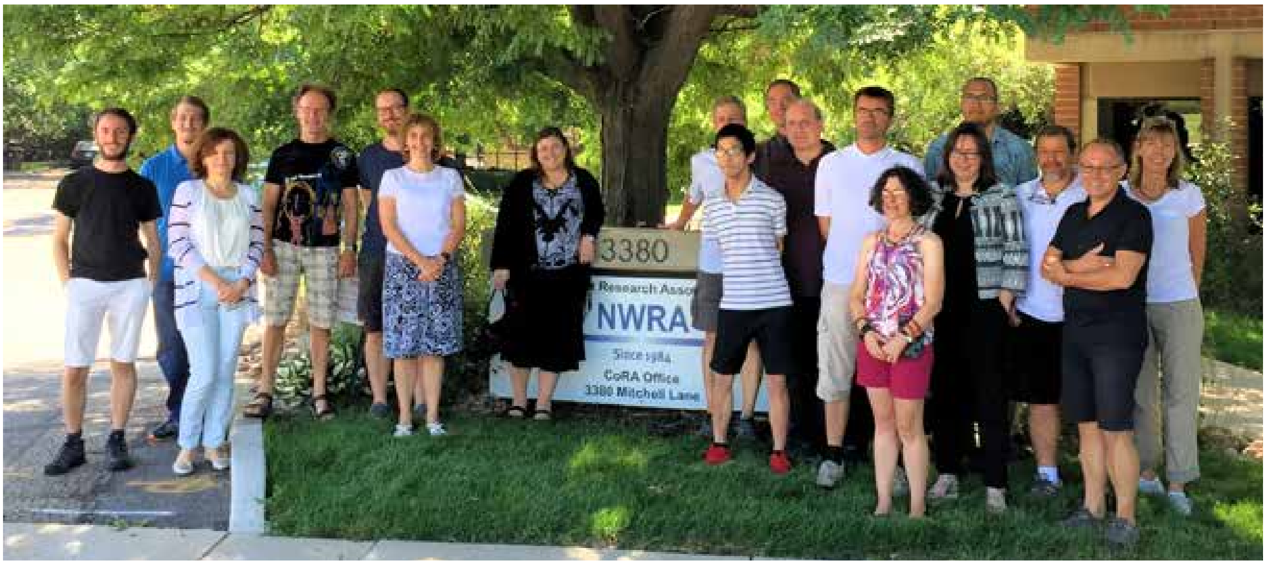

Figure 5: *Group photograph of the OCTAV-UTLS Workshop participants in front of NWRA Boulder office.*

climate and reanalysis models. The necessity of addressing uncertainties in the UTLS is demonstrated by much larger differences between models and observations as altitude decreases from the stratosphere into the UTLS. Satellite water vapour data sets from the years after 2000 have been compared in the SPARC WAVAS II activity, which was summarized by **Gabi Stiller**. She showed that the difference from frost point measurements is small between 10-100 hPa, but increases in the UTLS. Aircraft water vapour data sets were presented for commercial and UTLS specific scientific missions: **Andreas Zahn** presented the data from IAGOS-CARIBIC and **Andreas Petzold** that from IAGOS-core. On behalf of **Martina Krämer** Andreas Petzold also talked about JULIA, the Juelich database for water vapour measurements. This database includes humidity measurements from 53 field campaigns with more than 418 dedicated flights and, combined with IAGOS data since 1996, constitutes the largest airborne humidity data set. Another database from dedicated science missions is available at DLR in Germany; **Stefan Kaufmann** compared these data to water vapour from the operational ECMWF IFS model. Finally, **Holger Vömel** pointed out the necessity of further in-situ balloon measurements of water vapour for trend estimates, since accurate stratospheric water vapour measurements from balloon are scarce.

The meeting was closed with a summary discussion led by **Peter Hoor** that can be encapsulated as follows: the overall goal of OCTAV-UTLS is to account for the transport barrier induced variability in UTLS tracer observations by using different observation platforms with common reanalysis data and consistent geophysically-based analysis methods. This will allow better quantification of UTLS composition trends, and provide deeper insight into the dynamical processes affecting UTLS composition. The participants agreed to prepare data sets for the initial test periods to conform with JETPAC input standards to begin the consistent analysis. The outcomes will be discussed in a follow up meeting in Mainz, Germany in June 2018. Updates and news will be made available on **https://www.octav-utls.net**.

Acknowledgements

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References

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