Using Probability Distribution Functions for Satellite Validation

David J. Lary and Leslie Lait

***Abstract*—Probability distribution functions (PDFs) can be used to assist in the validation of trace gas retrievals made by satellites. A major advantage of this approach is that large statistical samples are used that do not require correlative measurements to be co-located in space and time. Examples are shown from the launch of UARS through to the present. This approach is also useful to evaluate the consistency among Aura instruments as well as their agreement with other datasets. A key feature of this work is putting the observations of Aura in their long-term historical context via statistical comparisons with previous datasets collected over more than a decade. To validate the Aura data, we use data from a variety of platforms including solar occultation (Canadian ACE) and limb sounder satellite instruments, ozonesondes (WOUDC), lidar (NDSC), and aircraft instruments (AVE, PAVE, and MOZAIC). The width of the trace gas PDFs can be used to accurately estimate the atmospheric spatial variability (or representativeness uncertainty) of trace gases as a function of time and location. This statistical analysis is also being used as preparation for full Kalman filter chemical assimilations. The analysis is presented online at http://www.PDFCentral.info.**

***Index Terms*—Chemical data assimilation, probability distribution functions (PDFs), representativeness uncertainty, spatial variability.**

I. Introduction

SATELLITE evaluation and validation are necessary, but sampling issues often make practical application problematic. In the traditional approach to validation we require coincidence in space and time. This is a strong constraint which dramatically reduces the statistical sample sizes we can deal with. The definition of "coincident" observations varies, but such measurements are often separated in time by days and in space by distances on the order of 1000 km or more. While the approach is suitable for a quick comparison to establish that the observations are at least the correct order of magnitude, establishing instrument accuracy or precision through such comparisons is difficult because of the limited number of coincidences and the contribution of real atmospheric variability. Furthermore, issues of representativeness arise because the validation exercises are typically limited geographically. It is therefore useful to augment the traditional approach to validation with the use of probability distribution functions (PDFs) of trace gases over an extended period for a given spatial domain. In this study, we choose to consider an entire month of data and to specify the spatial domain in terms of Lagrangian flow-tracking coordinates. The analysis starts with the launch of UARS and continues up to the present.

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The authors are with the Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, GEST, University of Maryland Baltimore County, Baltimore, MD 20771 USA (e-mail: David.Lary@umbc.edu).

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It is worth noting that PDFs have been used in a variety of tracer studies. These range from considering dispersing tropospheric pollutant plumes in the planetary boundary layer [1]–[6], running water channels [7] and clouds [8], pollutant emission rates [9] to tracer transport and stratospheric O_3, CH_4, N_2O, CO, CO_2, and PV [10]–[25] tracer age and transit time [17], [26], [27] and estimation of representativeness uncertainty in chemical data assimilation [28]. Using PDFs for validation has been found useful by the Aura instrument teams, for example [29].

Not only does a PDF characterize the tracer distribution, its shape tells us about mixing barriers, how complete the mixing is, and chemical processes such as ozone depletion [15], [16], [23], [24]. For example, a narrow peak in the concentration PDF indicates that the air is well mixed and significant variability generating processes have not recently occurred (e.g., long range transport). A multimodal distribution indicates air of different origins (e.g., polar and midlatitude). In general, broad peaks indicate recent variability generating processes such as photochemistry or transport (horizontal or vertical). Chemical processes such as ozone depletion will lead to an asymmetric broadening of the PDF toward low ozone values. Good examples of these different cases are shown for POAM observations of ozone by Strahan *et al.* [23].

Measurement imprecision is one the factors that affects the widths of the PDFs, and precision of the measurements is certainly a parameter that needs validation. In many cases this is difficult because atmospheric variability swamps the effects of measurement imprecision. The PDF plots of the type described here might also help to reduce the atmospheric variability by indicating locations and conditions where it is minimized. Comparisons between measurements under these conditions could then be used to produce upper limits on measurement imprecision.

A. Flow-Tracking Coordinates

Because a major component of the variability of trace gases is due to atmospheric transport it makes sense to use a coordinate system that "follows" the large scale flow pattern to perform our analyses [80]. In this study Lagrangian flow-tracking coordinates are used.

Under adiabatic conditions air parcels move along isentropic surfaces (surfaces of constant potential temperature, $\boldsymbol{\theta}$) [81]–[84]. So when considering tracer fields $\boldsymbol{\theta}$ is a suitable vertical coordinate. References [85]–[88] have shown the value

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of isentropic maps of Ertel's potential vorticity (PV) for visualising large scale dynamical processes. PV plays a central role in large scale dynamics where it behaves as an approximate material tracer [87].

As a result, PV can be used as the horizontal spatial coordinate instead of latitude and longitude [89]–[96]. PV is sufficiently monotonic in latitude on an isentropic surface to act as a useful replacement coordinate for both latitude and longitude, reducing the tracer field from three dimensions to two. These ideas have already led to interesting studies correlating PV and chemical tracers such as N_2O and O_3 [93], [97]–[101]. A key result of these studies is that PV and ozone mixing ratios are correlated on isentropic surfaces in the lower stratosphere, as was first pointed out by Danielsen [83].

Since the absolute values of PV depend strongly upon height and the meteorological condition, it is useful to normalize PV and use equivalent PV latitude (ϕ_e) as the horizontal coordinate instead of PV itself. ϕ_e is calculated by considering the area enclosed within a given PV contour on a given θ surface. The ϕ_e assigned to every point on this PV contour is the latitude of a latitude circle which encloses the same area as that PV contour. Therefore, for every level in the atmosphere ϕ_e has the same range of values, $-90°$ to $90°$. This provides a vortex-tracking, and indeed a flow-tracking, stratospheric coordinate system. In this study we have used UKMO meteorological analyses.

B. Analyses Grid

The analyses grid used here is cast in equivalent PV latitude ($\phi_{\rm el}$), potential temperature (θ) coordinates. With 30 latitudes between 85°S and 85°N, and 21 logarithmically spaced isentropic surfaces between the earth's surface and 2500 K. As the potential temperature at the surface changes with time we use a fixed number of isentropic levels between the current potential temperature of the surface and 315 K. Above 315 K, the levels remain fixed with time. The fixed isentropic levels correspond to the UARS surfaces spaced at 6 per decade in pressure (cf. the UARS reference atmosphere levels [102] of 315, 340, 375, 420, 465, 520, 585, 655, 740, 840, 960, 1100, 1300, 1500, 1700, 1900, 2100, 2300, and 2500 K).

The grid resolution was carefully chosen to ensure that there is usually a statistically significant number of observations per analysis grid cell over the entire time period from the launch of UARS in 1991 up to the present. This allows meaningful representativeness uncertainty statistics to be calculated based on the observations alone. When using equivalent PV latitude ($\phi_{\rm el}$), potential temperature (θ) coordinates for tracer studies short periods of less than a week are usually used since equivalent PV latitude is essentially a nonlinear rescaling of PV that depends on the PV gradient and is mostly independent of the large-scale average PV on the theta surface. For longer time-scales the PV-tracer correlations are not independent of the large-scale average PV. In addition there is interannual variability in the large-scale average PV. However, in this study we are using regions in equivalent PV latitude-theta space to split the atmosphere up in order to do intercomparisons between instruments where we will generally have significant sample sizes, i.e., greater than around 100 data points. We could equally well have used latitude and pressure or altitude to do this, but have found the comparison to be cleaner when we use an equivalent PV latitude - theta space [96].

II. Constituent Datasets Used

In this study we used observations from 33 different ozone instruments and aircraft campaigns, many of which were not available for the entire period. A full listing is given in Table I together with references.

III. Historical Context

The number of observational datasets available is very dependent on the constituent. Ozone has the longest time record and widest array of observation platforms. It is of interest to see how the observations made by Aura fit into this decade and a half of observations made since the launch of UARS by satellite, aircraft, lidars and sondes. To do this we have constructed a complete set of PDFs of all the instruments listed above that have measured ozone at any time from the launch of the NASA UARS in October 1991 up until the present.[1]

Fig. 1(a) shows an example of histograms of ozone observations using data during the January of all years from the launch of UARS in September 1991 until the present in the Lagrangian region $455\ K < \theta < 585\ K, 43° < \phi_{\rm el} < 55°$. For this Lagrangian region observations from 13 different platforms were available including EOS Aura MLS in green, NASA aircraft campaigns in red, and a few observations from ACE in black. To put the observation histograms in context it is valuable to know exactly where the observations were located within the Lagrangian region and the associated temperatures, this can sometimes help explain any differences that may exist. Fig. 1(b)–(e) show histograms of the associated equivalent PV latitudes ($\phi_{\rm el}$), temperatures, pressures (in megabits) and altitudes (in kilometers).

This example was chosen as there is reasonable agreement between all the sensors within the envelope observed by the aircraft campaigns (including the Aura Validation Experiment, AVE). It is clear that there is natural variability in this Lagrangian region over the month of January. Experience has shown that a helpful measure is how well the median values line up. It is interesting to note that there is good agreement (with the exception of CLAES which we shall examine further) in the median ozone volume mixing ratio (VMR) between instruments that made observations in 2004, such as MLS Aura and AVE aircraft, and others such as ILAS and MLS UARS which were from earlier years. Another use of this view of the data is that it allows us to use the data to examine the variability we expect in a constituent as a function of time and location.

It should also be noted that distributions with only a few measurements are not statistically converged (i.e., if more observations were available the shape of the histograms would change), these were only included for the sake of completeness. This is particularly so in the case of 2004 and 2005 when we would like to compare ACE and Aura, but the data volume from ACE is much smaller than that from Aura.

[1]These PDFs are available online at PDFCentral (gest.umbc.edu/PDFCentral/) and put the Aura data into a historical context.

TABLE I
CONSTITUENT DATASETS USED IN THIS STUDY

Instrument	Version	References	Years	Website
Aircraft				
Airborne Antarctic Ozone Experiment (AAOE)			1987	http://cloud1.arc.nasa.gov/aaoe/
Airborne Arctic Stratospheric Experiment (AASE)			1988-9	http://cloud1.arc.nasa.gov/aase/
Airborne Arctic Stratospheric Experiment II (AASE 2)			1991-2	http://cloud1.arc.nasa.gov/aase2/
Stratospheric Photochemistry Aerosols & Dynamics Experiment (SPADE)			1992	http://cloud1.arc.nasa.gov/spade/
Airborne Southern Hemisphere Ozone Experiment (ASHOE)			1994	http://cloud1.arc.nasa.gov/ashoe_maesa/
Tropical Ozone Transport Experiment (TOTE)			1995-6	
Stratospheric Tracers of Atmospheric Transport (STRAT)			1995-6	http://cloud1.arc.nasa.gov/strat/
Subsonic Aircraft: Contrail and Clouds Effects Special Study (SUCCESS)			1996	http://cloud1.arc.nasa.gov/success/
Photochemistry and Ozone Loss in the Arctic Region In Summer (POLARIS)			1997	http://cloud1.arc.nasa.gov/polaris/
Wb57 Aerosol Mission (WAM)			1998	mtp.jpl.nasa.gov/missions/wam/
The SAGE III Ozone Loss & Validation Experiment (SOLVE)			1999-2000	http://cloud1.arc.nasa.gov/solve/
The Cirrus Regional Study of Tropical Anvils & Cirrus Layers - Florida Area Cirrus Experiment (CRYSTAL-FACE)			July 2002	http://cloud1.arc.nasa.gov/crystalface/
The SAGE III Ozone Loss & Validation Experiment (SOLVE II)			January 2003	http://www.espo.nasa.gov/solveII
The Pre-Aura Validation Experiment (PREAVE)			January 2004	
The Aura Validation Experiment (AVE), San Jose			Winter 2004	http://cloud1.arc.nasa.gov/ave/
The Aura Validation Experiment (AVE), Houston			Fall 2004	http://cloud1.arc.nasa.gov/ave-houston/
Measurement of Ozone & Water vapour by Airbus In-service Aircraft (MOZAIC)		[30]	1994-present	http://www.aero.obs-mip.fr/mozaic/
Satellite and Shuttle Instruments				
Atmospheric Chemistry Experiment (ACE)	1 & 2.1	[31]–[36]	2004-present	http://www.ace.uwaterloo.ca/index.php https://databace.uwaterloo.ca/level2/
The Atmospheric Trace Molecule Experiment (ATMOS)	3	[37]	1992-4	http:/remus.jpl.nasa.gov/atmos/atmos.html
Microwave Limb Sounder (MLS) on UARS, 183 GHz & 205 GHz channels	5	[38]–[43]	1991-1999	http://mls.jpl.nasa.gov/
Microwave Limb Sounder (MLS) on NASA EOS Aura [44], [45]	01	[42]	2004-present	http://mls.jpl.nasa.gov/
Cryogenic Limb Array Etalon Spectrometer (CLAES) on NASA UARS	9	[46]–[48]	1991-1993	http://www.spasci.com/CLAES
CRyogenic Infrared Spectrometers & Telescopes for the Atmosphere (CRISTA)		[49]–[51]	1994,1997	http://www.crista.uni-wuppertal.de/
Halogen Occultation Experiment (HALOE) on NASA UARS	19	[52]–[54]	1991-present	http://haloedata.larc.nasa.gov/download/
Improved Limb Atmospheric Spectrometer (ILAS) on ADEOS		[55]–[60]	1996-7	http://www-ilas.nies.go.jp/
Improved Stratospheric and Mesospheric Sounder (ISAMS) on NASA UARS	10	[61]–[65]	1991-2	
Polar Ozone & Aerosol Measurement Experiment (POAM) II	6	[66]–[70]	1992-6	http://wvms.nrl.navy.mil/POAM/
Polar Ozone & Aerosol Measurement Experiment (POAM) III	4	[66]–[70]	1998-present	http://wvms.nrl.navy.mil/POAM/
Stratospheric Aerosol and Gas Experiment II (SAGE II)	6.2	[71], [72]	1991-present	http://www-sage2.larc.nasa.gov/
NOAA Solar Backscatter UltraViolet Instrument (SBUV/2)	8	[73]–[76]	1991-present	
Ground-based Instruments and Sondes				
Lidar and microwave observations from the Network for the Detection for Stratospheric Change (NDSC)		[77]–[79]	1991-present	ftp://ndsc.ncep.noaa.gov/
Ozone sondes from the World Ozone & Ultraviolet Radiation Data Centre (WOUDC)			1991-present	http://www.woudc.org/index_e.html

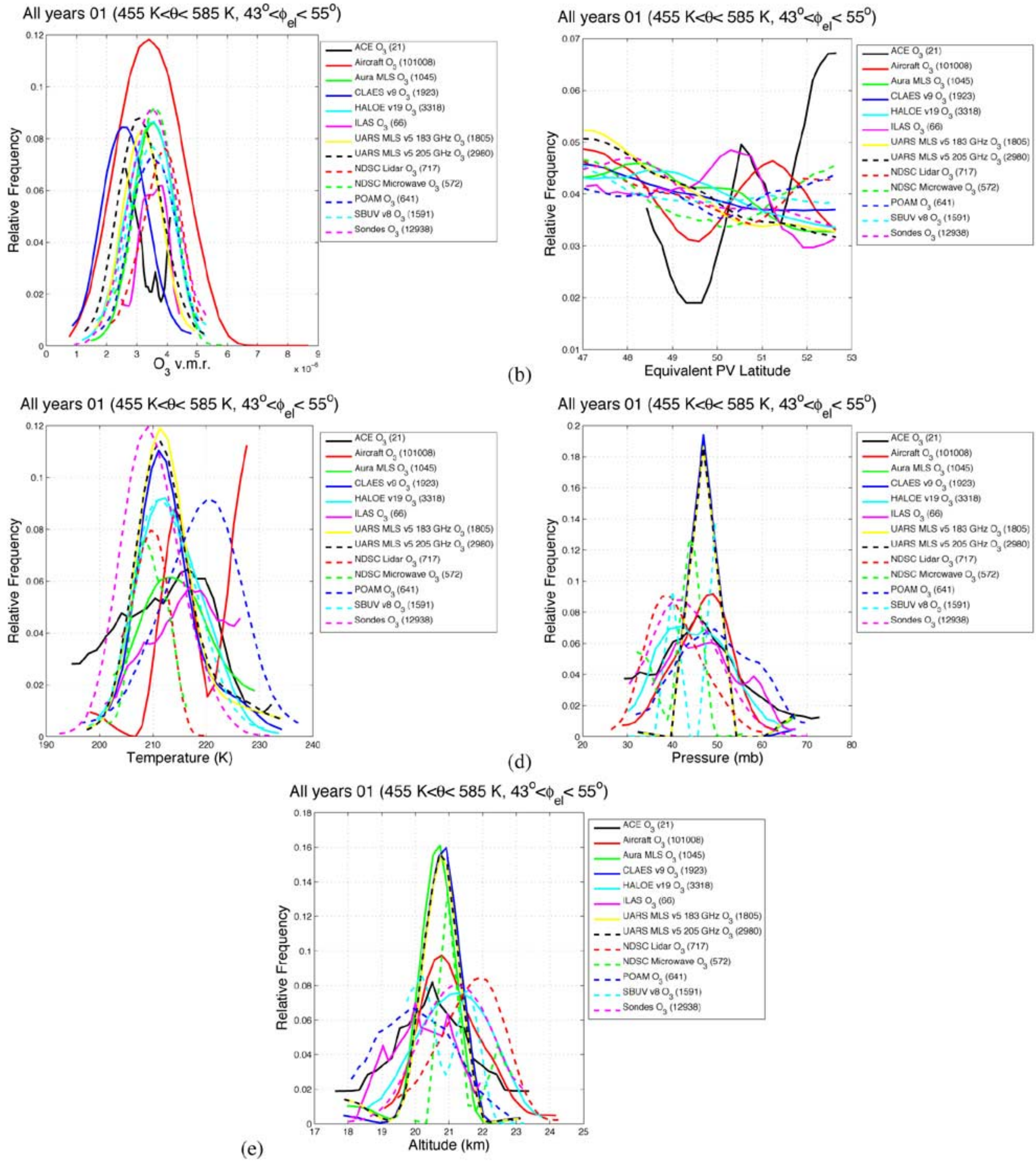

Fig. 1. (a) Example of histograms of ozone observations using data during the January of all years from the launch of UARS in September 1991 until the present in the Lagrangian region $455\ K < \theta < 585\ K, 43^\circ < \phi_{\mathrm{el}} < 55^\circ$. For this Lagrangian region observations from 13 different platforms were available including EOS Aura MLS in green, NASA aircraft campaigns in red, and a few observations from ACE in black. To put the observation histograms in context it is valuable to know exactly where the observations were located within the Lagrangian region and the associated temperatures, this can sometimes help explain any differences that may exist. (b)–(e) Histograms of the associated equivalent PV latitudes (ϕ_{el}), temperatures, pressures (in millibits) and altitudes (in kilometers).

IV. Bias Detection

In some cases, using PDFs affords clear bias detection. For example, Fig. 2 shows ozone PDFs for observations made by UARS CLAES (red line) and seven other instruments including ISAMS (red line) during the January of all years from the launch of UARS in September 1991 until the present in the Lagrangian region $1900\ K < \theta < 2300\ K, -90^\circ < \phi_{\mathrm{el}} < -79^\circ$. For this Lagrangian region observations from seven different platforms were available including EOS Aura MLS in black. There is a clear low bias of CLAES between contemporary measurements such as ISAMS (green line) and UARS MLS (navy and cyan

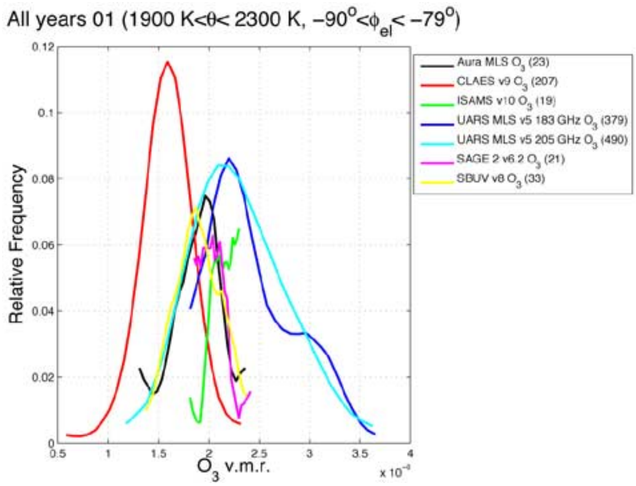

Fig. 2. Example of histograms of ozone observations using data during the January of all years from the launch of UARS in September 1991 until the present in the Lagrangian region $1900\ K < \theta < 2300\ K, -90^\circ < \phi_{\mathrm{el}} < -79^\circ$. For this Lagrangian region observations from seven different platforms were available including EOS Aura MLS in black.

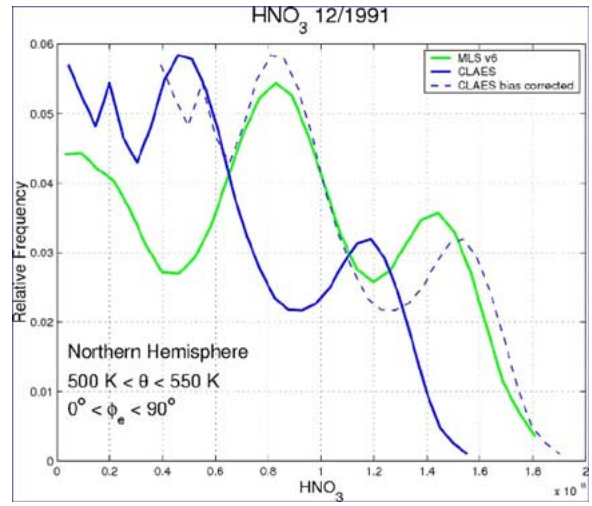

Fig. 3. HNO_3 PDFs for UARS MLS (green line) and CLAES (blue line) on the 500 K isentropic surface for December 1991. There is an obvious bias of approximately 3.5 ppbv for the primary (mid-latitude) peak at this altitude. Notice that a 3.5 ppbv shift of the CLAES curve (dashed blue line) does not bring the secondary peaks into complete coincidence, indicating that the biases are mixing ratio dependent.

lines) of around 0.75 ppmv. This is not restricted to this case but is a general feature of comparisons between CLAES and other instruments in the upper stratosphere. It is interesting that this is not true of CLAES observations in the lower stratosphere so the PDFs can be useful in examining spatially and temporally changing biases. In their overview of UARS ozone validation based primarily on intercomparisons among UARS and stratospheric aerosol and gas experiment II measurements Cunnold *et al.* [103] noted the relatively systematic, vertical structure differences between CLAES and other ozone observations.

The same approach has been used for many other instrument combinations and constituents. For example, Fig. 3 shows a comparison of HNO_3 observations over the northern hemisphere from MLS and CLAES on the 500 K isentropic surface and demonstrates the use of PDFs in bias detection. When the MLS PDF (green line) is compared to CLAES (blue line), a clear bias of approximately 3.5 ppbv can be seen for the primary (midlatitude) peak. However, the two PDFs cannot be brought into coincidence by an overall shift of the CLAES curve by this amount. Indicating that the differences between the measurements cannot be described as a simple bias. These types of discrepancies become clear from an analysis of the shape of the PDF. This type of analysis will be very useful for the validation of Aura datasets using coincident ensembles [29].

Other studies have also found issues with the CLAES HNO_3 data. Kumer *et al.* [104] compared CLAES version 7 data to two ATMOS missions and found that the CLAES HNO_3 maximum VMR values were of the order of 6%–15% less than correlative for CLAES values less than or equal to 8 parts per billion by volume (ppbv). In a data modeling comparison Chipperfield *et al.* [105] found that during the model initialization chemical inconsistencies in the UARS data became evident.

It is noteworthy that in the case of both O_3 and HNO_3 the interannual variability between the datasets (not all shown here) is less than the bias often found between the instruments. The obvious example of this is CLAES in Fig. 2.

V. Conclusion

A preliminary examination of EOS Aura MLS data indicates a good agreement with the historical ozone data record since the launch of UARS in 1991. The analysis used probability distribution functions to put the Aura data in a historical context.[2] In this study we have restricted ourselves to considering PDFs in interinstrument bias detection. However, they could be used in many other ways, for example, using the shapes of the PDFs to examine mixing processes.

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[2]The analysis is presented online at http://www.PDFCentral.info.

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David J. Lary received the B.Sc. degree in physics and chemistry (first class double honors) from King's College London, London, U.K., in 1987 with the Sambrooke Exhibition Prize in Natural Science, and the Ph.D. degree in atmospheric chemistry from the Churchill College, University of Cambridge, Cambridge, U.K., in 1991. His thesis described the first chemical scheme for the ECMWF numerical weather prediction model.

He then held postdoctoral Research Assistant and Associate positions at Cambridge University until receiving a Royal Society University Research Fellowship in 1996 (also at Cambridge). From 1998 to 2000, he held a joint position at Cambridge and the University of Tel-Aviv, Tel-Aviv, Israel, as a Senior Lecturer and Alon Fellow. In 2000, the Chief Scientific Adviser to the British Prime Minister and Head of the British Office of Science and Technology, Professor Sir D. King, recommended him to be appointed as a Cambridge University Lecturer in chemical informatics. In 2001, he joined the University of Maryland Baltimore County (UMBC/GEST), Baltimore, as the first distinguished Goddard Fellow in earth science. He is currently involved with NASA Aura validation using probability distribution functions and chemical data assimilation, neural networks for accelerating atmospheric models, the use of Earth Observing data for health and policy applications, and the optimal design of Earth Observing Systems. The thread running through all the research is atmospheric chemistry and the use of observation and automation to facilitate scientific discovery.

Dr. Lary's automatic code generation software, AutoChem, has received three NASA awards and has been recommended for the NASA Software of the Year Award.

Leslie Lait received the B.A. degree in physics and mathematics from Union College, Lincoln, NE, in 1981 and the Ph.D. degree in physics from Iowa State University, Ames, in 1987. His doctoral thesis described the first applications of M. Salby's asynoptic space-time Fourier transform analysis to real satellite measurements.

After graduating from Iowa State, he spent two years as a National Research Council Fellow at NASA's Goddard Space Flight Center, Greenbelt, MD. Subsequently, he remained at Goddard, where his research has centered on applications of quasi-conservative coordinate analysis of noncoincident measurements of trace gases from satellite remote-sensing instruments and airborne *in situ* instruments. He currently provides support for field experiments for validating the EOS Aura instruments.