EOS Aura Science Team Meeting 30 August – 1 September, 2016 – Rotterdam, The Netherlands Poster Abstracts

Stratospheric Ozone Loss Over the US in Summer: Recent Advances in Observations of Temperatures, Convective Injection of Condensed Phase Water, and Analyses of Volcanic Injections That are Used to Inform Model Calculations of Catalytic Mechanisms that Control the Response of O3

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In the context of changes to the structure of the Earth's climate resulting from the release of infrared active gases, most notably CO 2 and CH 4 from fossil fuel extraction, distribution and combustion, consequences to stratospheric ozone over the US in summer are considered. Key advances in observations directly related to the catalytic loss of ozone in the lower stratosphere include: Analysis of high resolution temperature observations over the central US in July and August from both SEAC 4 RS in situ observations and radio occultation (RO) observations, inclusion of gravity wave observations from both SEAC 4 RS and RO measurements, climatology of NEXRAD weather radar mapping of the 3D convective injection of condensed phase water over the central US in summer, analysis of the impact on ozone in the lower stratosphere over the US in summer using the AER 2D model calculations of the key rate limiting radicals and rate limiting catalytic loss rates as a function of water vapor, temperature and sulfate loading in the lower stratosphere, analysis of the impact on ozone in summer over the US under conditions of volcanic injection, overt sulfate addition for solar radiation management, and/or convective injection of water vapor, and analysis of the dynamic range in halogen emission from volcanic eruptions from the geologic record. Emphasis in the analysis is placed specifically on the geographic region over the Great Plains of the US in summer because of the confluence of temperatures and water vapor concentrations that initiate the heterogeneous catalytic conversion of inorganic chlorine, primarily HCl and ClONO 2, to free radical form, ClO. The ClO radical in turn engages gas phase catalytic cycles that remove ozone via the photochemical reaction mechanisms virtually identical to the catalytic photochemical processes that remove ozone over the Arctic each year in late spring. Extensive in situ observations, in the lower stratosphere of the Arctic, of the principal reaction networks that establish the relationship between observed ozone loss and the threshold in temperature, water vapor and sulfate loading is used to establish the photochemical coordinate system required to analyze ozone loss in the lower stratosphere globally. Analysis is also presented of observed ozone loss resulting from the eruption of Mt. Pinatubo that tests the photochemical structure of large ozone loss at mid-latitude for the range in sulfate loading that accompanies a volcanic eruption.

Cloud-top pressure retrieval from OMI ultraviolet measurements using the optimal estimation approach

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Cloud-top pressure is needed for ozone profile retrieval from OMI measurements. The SAO OMI ozone profile retrieval algorithm is updated to simultaneously derive cloud-top pressure using a wavelength range closely next to the ozone fitting window (270-330 nm) from Rotational Raman scattering (RRS) (345-355 nm) and O2-O2 absorption at 360 nm. The inversion procedure in this algorithm is based on the optimal estimation technique. The forward model calculates reflectance, Ring filling in and their Jacobians w.r.t. various parameters at the top of atmosphere using a RRS look-up table (LUT). The table was created based on inelastic rotational Raman scattering code LIDORT-RRS Version 2.3. We first perform direct analysis of retrieval sensitivity and retrieval error. Retrieval sensitivities show that for lower cloud O2-O2 provides higher sensitivity than RRS even for smaller cloud fractions. RRS provides good sensitivities and show less dependency on pressure and surface albedo. In the implementation for OMI, we typically use the fitting windows of 345-366 nm in UV-2 and co-added two UV-2 pixels to match the UV-1 spatial resolution. The OE-RRS retrievals are ~100 hPa higher than the operational OMCLDRR product likely because of the different RRS-LUTs and "soft" calibrations. OE-O4 retrievals agree well with OMCLDO2 product in pattern with expected lower pressures likely due to the wavelength dependent photon penetration depth.

Glyoxal measured from space as proxy for isoprene emission: chemical mechanism, constraints from aircraft observations, and relationship to formaldehyde

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Glyoxal (CHOCHO) and formaldehyde (HCHO) are short lived products of volatile organic compound (VOC) oxidation. Both species are detectable from space from instruments that measure backscattered sunlight, including the Ozone Monitoring Instrument (OMI). Isoprene, emitted by terrestrial vegetation, is the largest source of nonmethane VOCs (NMVOCs), and drives large enhancements of CHOCHO and HCHO in the continental planetary boundary layer. Satellite observations of HCHO have been widely used to estimate isoprene emission, but there are uncertainties related to the HCHO yield from isoprene oxidation, and the role of other NMVOCs as HCHO precursors. CHOCHO observations from space could provide a complementary constraint. We have used CHOCHO and HCHO aircraft observations over the Southeast United States from the Summer 2013 Southeast Nexus (SENEX) campaign, interpreted with the GEOS-Chem chemical transport model, to test understanding of the CHOCHO yield from isoprene oxidation, and its dependence on nitrogen oxide radicals. We investigate the combined value of HCHO-CHOCHO pair measured from space to inform isoprene emissions and chemistry.

Toward a reanalysis of MLS Stratospheric Chemical Observations

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MLS stratospheric chemical data will be assimilated by the Belgian Assimilation System for Chemical ObsErvations (BASCOE). This concerns the following species: O3, HNO3, HCl, H2O, N2O, ClO and CO. To prepare this reanalysis, several BASCOE experiments with different configurations have been performed covering the year 2008. In particular, the use of the averaging kernels in the assimilated results will be evaluated. We will also discuss the different PSC parameterization implemented in the model and how they perform against MLS. Early results of the reanalysis will also be presented.

Nitrogen dioxide from OMI: Air-mass factors, a-priori model profiles and stratospheric NO2 assimilation results

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In Europe, a new, community best-effort algorithm for the retrieval of NO2 columns has been developed by a consortium of institutes including IUP Bremen, BIRA-IASB, Max Planck Institute for Chemistry, and KNMI. This algorithm will be used to generate long time series of nitrogen dioxide from the sensors GOME, SCIAMACHY, GOME-2 and OMI. Major parts of this algorithm will also be used to generate the NO2 products of TROPOMI (Sentinel-5P). In our contribution we will focus on the modelling and radiative transfer aspects and separation between stratosphere and troposphere, which are needed to convert the DOAS slant columns into tropospheric vertical columns. The topics are:

- A-priori profiles from high-resolution global chemistry modelling with the TM5 model.

- Estimates of the stratospheric NO2 column by assimilating the observations in TM5.

- Air-mass factors.
- Improved cloud treatment and use of observations over snow/ice covered terrain.
- Error modelling.

The Co-location of Aqua/MODIS observations and GEOS5 Assimilated Data onto the Aura/OMI Pixel: A New Suite of OMI Data Products for the Science Community

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The OMI science team has begun releasing several new "co-located" OMI products to the science community through the Goddard Earth Sciences (GES) Data and Information Services Center (DISC). Two of these products, a merged cloud product (OMMYDCLD) and an aerosol support product (OMMYDAGDEO), co-locate Aqua/MODIS geophysical information onto OMI pixel. Aura/OMI and Aqua/MODIS both fly in the NASA A-train, a constellation of sun synchronous, earth-observing satellites that follow the same orbital track and provide near-coincident observations of the earth-atmosphere system. Three other products interpolate assimilated data fields from the Goddard Earth Observing System Model (GEOS5) and Data Assimilation System (DAS). These new products aim to support future OMI research and algorithm development. This paper will discuss the geophysical, sampling and computational issues involved in the design of these products.

Summertime free tropospheric PAN over the U.S. as observed by TES and simulated by GEOS-Chem

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We present an analysis of Tropospheric Emission Spectrometer (TES) peroxyactyl nitrate (PAN) and co-located carbon monoxide (CO) observations over North America during summer 2005 to 2010. We segregate and examine the abundance of PAN relative to CO in TES observations located within smoke plumes or in close proximity to active fires. Though CO is enhanced in retrievals impacted by smoke, we find no systematic difference in the PAN when all successful PAN retrievals are segregated by the presence of smoke in the atmospheric column. Retrievals located near active fires (within 0.2°) display a strong positive relationship between PAN and CO, but we are not able to establish a systematic relationship by region or ecosystem. We compare the PAN enhancement relative to CO in smoke-impacted samples and samples located near active fires. A large fraction of the enhancement ratios calculated from the TES data are larger than pseudo-emission factors for PAN derived from prior aircraft observations. We compare the TES PAN data to a series of GEOS-Chem simulations. We find that the Fischer et al. [2014] simulation appears to systematically underestimate the contribution of fires to elevated PAN during summer months over western North America, and overestimate the amount of PAN observed by TES over the southeastern U.S. We find improved model agreement over the southeastern U.S. by reducing NOx emissions in this region and making a series of updates to the treatment of isoprene oxidation chemistry.

We also present a series of simulations varying the amount of biomass burning NOx emissions that are immediately partitioned to PAN, and we find that the model continues to be unable to reproduce TES PAN observations over many regions/years with active wildfires.

Discrete Wavelength Techniques for OMI Total Ozone Retrieval in TOMS V9

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In the UV, most satellite total ozone algorithms use measurements between 310-340 nm because wavelengths in this spectral range are sensitive to the total column. In the TOMS V9 algorithm we apply a discrete wavelength technique on the shorter end of this range to measure ozone absorption where the cross-section is greater. At the longer end of this region, differential and direct fitting algorithms derive total ozone from fine ozone band structure where ozone sensitivity is reduced, and therefore these methods may be more sensitive to detector noise. We demonstrate that while discrete wavelength algorithms are generally less affected by detector noise, it is possible to reduce noise further by averaging high resolution OMI measurements over bands several nanometers in width. This approach enhances the signal-to- noise ratio (SNR) for total ozone at large SZA and can benefit determinations of tropospheric ozone where SNR is critical. The discrete wavelength approach in TOMS V9 is also uniquely applicable to lower spectral resolution UV sensors such as PACE and EPIC. A hybrid approach, of collecting data at high and low spectral resolution in separate wavelength regions simultaneously, is an option for detectors with programmable co-adding capability. We also describe some of the key differences between TOMS V9 and the previous version of the algorithm such as a new correction for cloud effects. Reasons and methods for anchoring the OMI TOMS ozone calibration to 312.5 nm using limb profiles from MLS are also described.

Aura TES Ozone (v007) Validation Comparisons, 2004-2015

Robert Herman (JPL; robert.l.herman@jpl.nasa.gov), Pranjit Saha, Susan Kulawik, Ming Luo, Vivienne Payne, Kevin Bowman, Bryan Johnson

We will present twelve years of comparisons of Aura TES level 2 ozone retrievals with ground truth (ozonesonde measurements) for 2004 through 2015. Ozonesondes come from the WOUDC database and also NOAA coordinated launches. The satellite data is Aura TES R14, hereafter referred to as Version 7 or v007. Year-by-year statistics of TES ozone compared to ozonesondes will be presented. The ranges for quality flags such as radiance residual rms will also be discussed.

Evaluation of UTLS carbon monoxide simulations in GMI and GEOS-Chem chemical transport models using Aura MLS observations

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This study evaluates the distribution and variation of carbon monoxide (CO) in the upper troposphere and lower stratosphere (UTLS) during 2004–2012 as simulated by two chemical transport models, using the latest version of Aura Microwave Limb Sounder (MLS) observations. The simulated spatial distributions, temporal variations and vertical transport of CO in the UTLS region are compared with those observed by MLS. We also investigate the impact of surface emissions and deep convection on CO concentrations in the UTLS over different regions, using both model simulations and MLS observations. Global Modeling Initiative (GMI) and GEOS-Chem simulations of UTLS CO both show similar spatial distributions to observations. The global mean CO values simulated by both models agree with MLS observations at 215hPa and 147 hPa, but are significantly underestimated by more than 40% at 100 hPa. In addition, the models underestimate the peak CO values by up to 70% at 100 hPa, 60% at 147 hPa, and 40% at 215hPa, with GEOS-Chem generally simulating more CO at 100 hPa and less CO at 215hPa than GMI. The simulated vertical transport of CO shows better agreement with MLS in the tropics and the SH subtropics than the NH subtropics. The two models exhibit emissionconvection-CO relationships similar to those observed by MLS over the tropics and some regions with enhanced UTLS CO.

Seasonal variation of tropospheric bromine monoxide over the Rann of Kutch salt marsh seen from space

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The Rann of Kutch (India/Pakistan) is one of the largest salt deserts in the world. Being a so-called 'seasonal salt marsh', it is regularly flooded during the Indian Summer Monsoon. We present 10 years of bromine monoxide (BrO) satellite observations by the Ozone Monitoring Instrument (OMI) over the Great and Little Rann of Kutch. OMI spectra were analysed using Differential Optical Absorption Spectroscopy (DOAS) and revealed recurring high BrO VCDs up to 1.4×10^{14} molec/cm² during April/May, but no significantly enhanced column densities during the monsoon season (June–September). In the following winter months, the BrO VCDs are again slightly enhanced while the salty surface dries up. We investigate a possible correlation of enhanced reactive bromine concentrations with different meteorological parameters and find a strong relationship between incident UV radiation and the total BrO abundance. In contrast, the second Global Ozone Monitoring Instrument (GOME-2) shows about four times lower BrO VCDs over the Rann of Kutch than found by OMI and no clear seasonal

cycle is observed. One reason for this finding might be the earlier local overpass time of GOME-2 compared to OMI (around 9:30 vs. 13:30 LT), as the ambient conditions significantly differ for both satellite instruments at the time of the measurements. Further possible reasons are discussed and mainly attributed to instrumental issues. OMI additionally confirms the presence of enhanced BrO concentrations over the Dead Sea valley (Israel/Jordan), as suggested by former ground-based observations. The measurements indicate that the Rann of Kutch salt marsh is probably one of the strongest natural point sources of reactive bromine compounds outside the polar regions and is therefore supposed to have an significant impact on local and regional ozone chemistry.

The Importance of Data Preservation of Aura Mission Data Sets

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The Aura mission was launched in July 2004, and has been in orbit and delivering data for the past 12 years. Eventually the mission will end and before the science teams disband. It is imperative to think now about preserving the pertinent data, metadata, ancillary information, documentation and software used in creating the many Aura data sets. This information is valuable for future scientists in understanding what went into creating the Aura data. Waiting until years after can result in loss of data and documentation as experienced by data from the Nimbus project. ESDIS assigned the GES DISC the task of preservation of data at its archive. This presentation provides an overview of the successfully completed data preservation of the HIRDLS science data, and the current status of preserving MLS, and what needs to be done for OMI.

Remotely-sensed total-column OMI and Pandora observations over terrestrial and marine environments and their use for estimating surface nitrogen dioxide

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The Pandora spectrometer, an instrument that uses a direct-sun approach to column measurements of trace gases, has performed well in a range of polluted regimes in North America, Europe, and Asia. Pandora shows promise for (1) satellite validation of current (OMI and GOME) and future (TROPOMI and TEMPO) missions and (2) long-term observations of ground-truth ozone (O3) and nitrogen dioxide (NO2 - an O3 precursor) column amounts that are important for monitoring the earth system. We report the first comparisons of a collocated Pandora, in situ surface, and OMI observations in two regions: (1) the industrialized South African Highveld and (2) the Eastern US coast in the Northern Atlantic Ocean. We contrast the performance of the remote-sensing

instruments, satellite and ground, in each terrestrial and marine environment. The terrestrial ground-based measurements were made during January-March 2011 at the Welgegund atmospheric station of North-West University Potchefstroom, ~ 100 km south-west of the Johannesburg-Pretoria conurbation. The marine ship-based surface measurements were completed during July-August 2014 in the North Atlantic as part of the Deposition of Atmospheric Nitrogen to Coastal Ecosystems (DANCE) campaign, ~ 100 km east of the mid-Atlantic United States. Both locations have no local pollution source, but are influenced by terrestrial air masses from regional pollution sources. Comparisons of coincidental, quality-controlled OMI and Pandora total column O3 and NO2 measurements show statistically significant correlation in both environments. For NO2, the difference between the two instruments is $\sim 20\%$, which is comparable to previous studies under similar conditions. Using the novel Knepp-Kollonige method, we derive surface NO2 values from OMI and Pandora column measurements and compare to the land and sea in situ NO2. The planetary boundary layer (PBL) height, a key variable in converting the column NO2 amount to a surface value, was not measured directly at each location and a co-located Atmospheric InfraRed Sounder (AIRS) product, planetary boundary layer top, was used. The AIRS-estimated PBL height agreed within 10% of radiosonde-derived values (launched at the Irene weather station, 150 km northeast of Welgegund). Absolute differences between Pandora-estimated surface NO2 and the in situ measurements were best at the terrestrial site (~0.5ppbv), while detecting clean marine air proved difficult for both OMI and Pandora with differences greater than 1ppby. These observations highlight the impact air pollution can have on downwind terrestrial and marine locations as well as provide evaluation of satellite- and groundbased remote sensors in both environments.

Acetone and Hydrogen Cyanide from Aura-TES

Susan S. Kulawik (BAERI and NASA Ames; Susan.S.Kulawik@nasa.gov), Vivienne H. Payne, Emily Fischer, Dejian Fu

We explore two new chemical tracers from the Tropospheric Emission Spectrometer (Aura-TES): acetone and HCN, both of which show sensitivity in the upper troposphere. Acetone has both biogenic and combustion sources, and is a major precursor of PAN and a major controller of the oxidative capacity of the upper troposphere. HCN is a unique species in that it is a combustion byproduct with no biogenic sources, and can be used to trace the combustion influence of TES observations. We show HCN for a major fire in Indonesia in 2006, for South America/Southern Atlantic/Africa over different seasons, and North America, where there is validation data during the ARCTAS campaign. Residuals of Aura-TES in the acetone band, a proxy for acetone, will be also shown as well. We indirectly validate the new products using aircraft field measurements, the GEOS-Chem model, and comparisons to TES methanol, PAN, and carbon monoxide. A major error source for quantitative use of the new products is uncertainty in the plume height, since TES sensitivity varies by altitude. A method of post-processing is used to

accurately estimate the volume mixing ratio given the actual plume height and plume thickness.

Using Microwave Limb Sounder observations and the Match technique to assess the validity of analysis winds and heating rates.

Nathaniel Livesey (JPL; Nathaniel.J.Livesey@jpl.nasa.gov), Michelle Santee, Gloria Manney

The long-standing "Match" technique uses Lagrangian trajectories to identify cases where the composition of an airmass is observed on two or more occasions. This approach accounts for the impact of advection on the airmass, enabling observed changes in airmass composition to be ascribed to chemical or microphysical processes, or to irreversible mixing. The Match technique was pioneered with ozonesonde observations, and used to quantify chemical destruction of Arctic stratospheric ozone. The technique has previously been applied to the far denser ozone observations from the Microwave Limb Sounder (MLS) instrument on NASA's Aura satellite, launched in 2004, and used to quantify both Arctic and Antarctic ozone loss for multiple years. We extend that prior work to MLS observations of other trace gases, including nitrous oxide and methyl chloride, both long-lived trace gases, and water vapor, which behaves as a long-lived trace gas in most circumstances. In the absence of chemical or microphysical processes, observed changes in the abundance of these species in matched airmasses can be indicative of irreversible mixing and/or of errors in the trajectory calculations used to identify matched observations. Accordingly, this technique can provide insights into the accuracy of analysis fields used to drive the trajectories. We present preliminary results from such an analysis, focused on the winds and heating rates in the recently released MERRA-2 analysis dataset.

Aura CO and Ozone profiles retrieved from combined TES and MLS measurements: algorithm, data and applications

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The co-located TES nadir and MLS limb tangent measurements are optimally combined to retrieved Aura CO and Ozone profiles. Compared to the two standalone retrievals by the instrument teams, these new Aura joint retrievals improve the profile resolution and sensitive ranges in the upper troposphere and lower stratosphere. For example, the degree of freedom for signal (DOFS) between surface and 50hPa for TES alone is < 2, and for the combined CO profiles is 2-4. The Aura CO version 1 product including the retrieval characteristic data has been released to the public. We briefly describe the algorithm and the data validation using in-situ data for CO. This product has been used

to study complex chemical-transport processes related to pollutants emitted from the fires in the tropical region. We will present examples of Aura CO data applications, including evaluations of the key parameters describing the pollutant transport mechanisms in the NASA GISS composition-climate model. The prototyping for Aura O3 profile retrieval is in progress. We will present some preliminary results.

OMI, emissions inventories, and detection of missing sources

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Our understanding of the impacts of air pollution on health and the environment, and our ability to predict future levels, are limited by our knowledge of its sources. Here, a global, OMI-derived SO2 emissions inventory that is independent of "bottom-up" inventories is presented. While it is generally consistent with these conventional databases, since this new approach is able to detect sources (in addition to quantifying their emissions), many anthropogenic sources were identified that are evidently missing from conventional inventories. The methodology, inventory highlights, and applications to OMI NO2 and other pollutants are will be discussed.

OMI Ozone and the Transition to NPP OMPS

Richard McPeters (NASA GSFC; Richard.D.McPeters@nasa.gov), David Haffner, Gordon Labow

OMI mapping of total column ozone continued the record started with Nimbus 7 TOMS and Earth Probe TOMS. The OMPS (Ozone Mapper Profiler Suite) nadir mapper on Suomi NPP will now be used to further extend the record of ozone mapping. A version 9 algorithm has been applied to the ten year plus record of OMI ozone observations. This processing incorporates the Brion/Daumont/Malicet ozone cross sections in an optimal estimation algorithm. Bias relative to NOAA 19 SBUV/2 total column ozone is less than half a percent. Agreement with the version 2 processing of ozone for the OMPS nadir mapper is also better than half a percent. By using OMPS ozone to extend the OMI mapper data record, we will have a consistent record of spatial variation of ozone for years to come. In particular this will enable accurate mapping of the ozone hole each year to verify the recovery.

Recent developments in the operational aerosol layer height retrieval algorithm for the Sentinel-4 mission

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The Sentinel-4 mission is a part of the European Commission's Copernicus programme, the goal of which is to provide geo-information to manage environmental assets, and to observe, understand and mitigate the effects of the changing climate. The Sentinel-4/UVN instrument design is motivated by the need to monitor trace gas concentrations and aerosols in the atmosphere from a geostationary orbit. The on-board instrument is a high resolution UV-VIS-NIR (UVN) spectrometer system that provides hourly radiance measurements over Europe and northern Africa with a spatial sampling of 8 km. The main application area of Sentinel-4/UVN is air quality. One of the data products that is being developed for Sentinel-4/UVN is the Aerosol Layer Height (ALH). The goal is to determine the height of aerosol plumes with a resolution of better than 0.5 - 1 km. The ALH product thus targets aerosol layers in the free troposphere, such as desert dust, volcanic ash and biomass during plumes. KNMI is assigned with the development of the Aerosol Layer Height (ALH) algorithm. Its heritage is the ALH algorithm developed by Sanders and De Haan (ATBD, 2016) for the TROPOMI instrument on board the Sentinel-5 Precursor mission that is to be launched in June or July 2016 (tentative date). The retrieval algorithm designed so far for the aerosol height product is based on the absorption characteristics of the oxygen-A band (759-770 nm). The algorithm has heritage to the ALH algorithm developed for TROPOMI on the Sentinel 5 precursor satellite. New aspects for Sentinel-44/UVN include the higher resolution (0.116 nm compared to 0.4 for TROPOMI) and hourly observation from the geostationary orbit. The algorithm uses optimal estimation to obtain a spectral fit of the reflectance across absorption band, while assuming a single uniform layer with fixed width to represent the aerosol vertical distribution. The state vector includes amongst other elements the height of this layer and its aerosol optical thickness. We will present the development work around the ALH retrieval algorithm in the framework of the Sentinel-4/UVN instrument. The main challenges are highlighted and retrieval simulation results are provided. Also, an outlook towards application of the S4 bread board algorithm to Sentinel-5 Precursor data later this year will be discussed.

Evaluation and Scientific Uses of the TES/OMI Multispectral Ozone Product

Jessica L. Neu (JPL; jessica.l.neu@jpl.nasa.gov), Dejian Fu, Greg Osterman, Kevin Bowman, Vivienne Payne, Annmarie Eldering

We present an evaluation of the ability of jointly-retrieved ozone profiles using thermal infrared radiances from the Tropospheric Emission Spectrometer (TES) and ultraviolet radiances from the Ozone Monitoring Instrument (OMI) to capture near-surface ozone features as seen by ground station monitors, ozonesondes, and the Community Multi-scale Air Quality (CMAQ) model. We further demonstrate the scientific uses of this data

for understanding and quantifying pollution events at the regional scale and within megacities.

Chemistry Simulations using MERRA-2 Reanalysis with the GMI CTM and Replay in Support of the Atmospheric Composition Community

Luke Oman (NASA/GSFC; luke.d.oman@nasa.gov) and Susan Strahan

Simulations using reanalyzed meteorological conditions have been long used to understand causes of atmospheric composition change over the recent past. Using the new Modern-Era Retrospective analysis for Research and Applications, version 2 (MERRA-2) meteorology, chemistry simulations are being conducted to create products covering 1980-2016 for the atmospheric composition community. These simulations use the Global Modeling Initiative (GMI) chemical mechanism in two different models: the GMI Chemical Transport Model (CTM) and the GEOS-5 model developed "Replay" mode. "Replay" mode means an integration of the GEOS-5 general circulation model that is incrementally adjusted each time step toward the MERRA-2 analysis. The GMI CTM is a 1° x 1.25° simulation and the MERRA-2 GMI "Replay" simulation uses the native MERRA-2 approximately ½° horizontal resolution on the cubed sphere. The "Replay" simulations is driven by the online use of key MERRA-2 meteorological variables (i.e. U, V, T, and surface pressure) with all other variables calculated in response to those variables. A specialized set of transport diagnostics is included in both runs to better understand trace gas transport and changes over the recent past.

The 2015–2016 Arctic winter: Perspectives on extremes in polar processing and meteorological variability from the 12-year record of Aura Microwave Limb Sounder measurements

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In the last decade, the Arctic lower stratosphere has seen some of the most dynamically disturbed winters, with stratospheric sudden warmings that curtailed polar processing early in the season and limited chemical ozone loss, as well as several winters marked by exceptionally cold conditions and severe chemical ozone loss. The occurrence in recent winters of different combinations of extreme meteorological conditions, and their impact on polar chemical processes, has underscored the Arctic stratosphere's sensitivity to a spectrum of dynamical variability. The Aura Microwave Limb Sounder (MLS) provides a suite of measurements enabling quantification of polar processing and chemical ozone loss. Here we use MLS observations in conjunction with meteorological analyses for a comprehensive examination of lower stratospheric polar processing during the Arctic winter of 2015–2016. An atypically large volume of persistently low temperatures

through much of the winter led to extensive polar stratospheric cloud formation, which in turn brought about an unprecedented (for the Arctic) degree of denitrification and dehydration. As a consequence of early-winter processing and an unusually large and elongated vortex with significant portions exposed to sunlight, substantial chlorine activation (enhanced abundances of ClO, depressed abundances of HCl) was evident earlier than is typical in Arctic winter. Polar processing then continued unabated until being terminated by a major final stratospheric sudden warming in early March. In this talk we will use a Lagrangian "Match"-based approach to quantify the amount of denitrification, dehydration, and chemical ozone destruction in the 2015–2016 winter, and we will place the extent of polar processing in this winter in the context of the previous 11 Arctic winters observed by Aura MLS.

The Sentinel 5 precursor cloud support product (FRESCO)

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TROPOMI on the Sentinel 5 precursor mission is a next generation OMI and SCIAMACHY. It covers the OMI wavelength range, plus two bands in the near infra-red (675-775 nm) and short wave infra-red (2305-2385 nm). Not only the spectral range has been extended, the spatial resolution is 3.5 by 7 km in nadir, and up to 9 by 14 at the edges of the swath. This has been achieved while increasing the signal to noise ration compared to OMI. Of course the combination of extended spectral coverage and smaller pixel size means that the data volume is much larger than that of OMI. The extended wavelength range allows us to retrieve additional Level 2 products: methane and carbon monoxide from the SWIR, and aerosol layer height from the NIR are new products compared to OMI. Having the oxygen A-band available also means that we can use it for cloud retrieval instead of the O2-O2 or rotational Raman scattering cloud products used on OMI. On the poster we present the cloud support product that will be used by the KNMI level 2 products derived from TROPOMI observations, including nitrogen dioxide. This cloud product is an adaptation of FRESCO for TROPOMI.

Using DISCOVER-AQ and KNMI NO2-sonde data for OMI Validation

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The DISCOVER-AQ campaign was a large-scale field experiment aimed at better linking surface and column measurements of key trace gases including NO2. The KNMI NO2-sonde participated in each of the four DISCOVER-AQ deployments. Through the use of a tethered balloon platform, the NO2-sonde was able to profile the lower portion of the boundary and capture the daytime diurnal variation of the highly dynamic vertical structure and distribution of NO2 near the surface. This tethered balloon platform also helped fill the gap between the surface and the lowest extent of the regular aircraft spirals

at each site. The focus of this work will be on the validation opportunities this unique NO2-sonde dataset can provide for OMI in combination with the broader DISCOVER-AQ data catalog. Particular attention will be given to the comparison of OMI NO2 columns using NO2-sonde and aircraft data. As the campaign progressed, so did the experimental design of the NO2-sonde. As such several important NO2-sonde developments will be highlighted.

SHADOZ (Southern Hemisphere Additional Ozonesondes) Network Report: Updates and Station Activities

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SHADOZ (Southern Hemisphere Additional Ozonesondes) has collected more than 6000 profile sets from ozonesondes and radiosondes in the tropics and subtropics since 1998. Measurements originate at 14 long-term stations; map of the stations and data are archived at http//:croc.gsfc.nasa.gov/shadoz. Through affiliation with the Network for Detection of Atmospheric Composition Change (NDACC; www.ndsc.ncep.noaa.gov) and posting of profiles to the NASA Aura Validation Data Center (AVDC) and WMO's World Ozone and UV Data Centre (woudc.org), SHADOZ data are distributed across the satellite, monitoring and modeling communities. We review recent major activities of SHADOZ, including re-activation of five SHADOZ stations: Ascension, Fiji, Irene, San Cristobal, Natal. Examples of newer data from those sites will be shown. The most significant SHADOZ activity we have recently carried out is the first major reprocessing of the 18-year ozonesonde dataset to account for changes in radiosonde and ozonesonde instrumentation and biases among stations. The reprocessing has been done following guidelines of WMO and SI2N (SPARC/Intl Ozone Commission/IGACO and NDACC). Noting that SHADOZ will turn 20 in 2018, SHADOZ prospects for the period through 2020 will be presented.

Convective influence on the lower stratospheric water vapor in the boreal summer Asian monsoon region

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Processes maintaining the localized maxima in lower stratospheric water vapor over the boreal summer Asian monsoon region are investigated using trajectory and cloud models that resolve the detailed cloud microphysical processes, with observation-based convection and radiation schemes. We examine the impact of convective influence along parcel trajectories on cloud formation and dehydration by tracing the trajectories through time-dependent fields of convective cloud top heights estimated from global rainfall and geostationary brightness temperatures. Parameters such as the rainfall threshold used for

identification of deep convection are derived by comparison with the CloudSat deep convective cloud top product as enhanced by colocated CALIOP measurements. The simulated water vapor field at the 100 hPa level and cloud occurrence frequencies in the tropical tropopause layer (TTL) are constrained by corresponding observations from MLS and CALIPSO, respectively. The observed maximum in the 100 hPa level water vapor field over the Asian monsoon region is only present in the simulation with convective influence, indicating the importance of convective hydration for the summertime water vapor distribution. Convection moistens the 100 hPa level over the Asian monsoon by ~1 ppmv, where ~75% of this moistening is due to convection occurring locally within the monsoon region. Convection also increases the cloud occurrence frequency in the TTL over the southern sector of the Asian monsoon anticyclone by ~20%. Parcels are convectively hydrated in the southeastern sector of the anticyclone, transported westward by the anticyclonic circulation, and dehydrated in the southwestern sector. The relative importance of extreme convective events that inject ice and water vapor near or above the tropopause will also be examined.

A Re-processed SHADOZ Dataset: Impacts of Station Bias and Agreement with Satellites

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The NASA Goddard Space Flight Center SHADOZ (Southern Hemisphere Additional Ozonesondes) project has been collecting vertical profiles of ozone and P-T-U from balloon-borne ozonesonde and radiosonde instruments since 1998. These long-term data sets (> 17 years) have become complementary analyses tools for process studies, model development, and satellite validation. Over the years methods for calibration ozonesondes for day of flight preparations have changed and evolved as laboratory studies and field campaigns increase our understanding of the measurement characteristics and uncertainties. We have completed the first major re-processing of SHADOZ data at several stations to account for changes in ozonesonde operating procedures and data processing. We use OMI and MLS ozone products to observe changes in the SHADOZ ozonesonde time series before and after reprocessing. We show that the degree to which re-processing can be done is observable in the differences with the satellite measurements. In comparisons with MLS, the re-processed time series show variable degree of improvement with height due to the choice of solution strength, biases with the radiosonde pressure sensor, and uncertainties in the ECC sensors' pump efficiency. As expected, there is little difference between the original and reprocessed data records among stations that are consistent in pre-launch preparation procedures, apply 'best practices', and are diligent in metadata reporting. This minor impact is reflected in comparisons with OMI and MLS.

PAN in the Eastern Pacific Free Troposphere: A Satellite View of the Sources, Seasonality, Interannual Variability and Timeline for Trend Detection

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Peroxyacetyl nitrate (PAN) is an important trace gas that serves to transport nitrogen oxide radicals (NOx = NO + NO2) throughout the troposphere. There is strong evidence that PAN decomposition in specific plumes of Asian origin subsiding over the eastern Pacific can lead to significant O3 enhancements. Thus quantifying the spatial and temporal variability of PAN over the eastern Pacific is an important part of understanding the O3 budget upwind of the North American airshed. We will present observations of PAN from the Tropospheric Emission Spectrometer (TES) over the eastern Pacific for April and July 2006–2010, as well as the spring-to-summer seasonal transition for 2006. We focus our analysis on July because prior work based on in situ observations has primarily addressed the transpacific transport of PAN in spring. Plumes containing elevated PAN are present almost every day in the month of July, and we show that elevated PAN observed in July has multiple sources, including fires in Siberia, anthropogenic sources in southeastern China, and re-circulated pollution from the continental U.S. Based on the variability observed in the TES PAN retrievals over this region, we predict it would be faster to detect a trend of a given magnitude in PAN using satellite observations over the eastern Pacific region rather than surface in situ observations, and that a trend of a given magnitude would be more quickly detected in summer than spring.