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to consider the entire set of kinetics, photochemical, and thermodynamic parameters every three review cycles. Nevertheless, each release of the evaluation contains not only the new evaluations, but also recommendations for every process that has been considered in the past. In this way, the tables for each release constitute a complete set of recommendations.

JPL 15-10 Details

In so far as possible, all recommendations are based on the results from published laboratory studies and are not adjusted to specifically fit observations of atmospheric chemical composition. In order to provide recommendations that are as up-to-date as possible, preprints and written private communications are accepted, but only when the Panel is convinced that they will soon appear in the peer-reviewed literature. For each chemical reaction, the Panel considers whether the data are consistent with reaction rate theory and discrepancies are noted. A major use of theory is to interpolate and extrapolate data for three-body reactions when the laboratory measurements do not cover the entire range of atmospheric temperatures and pressures. In some cases where no experimental data are available, the Panel may provide estimates of rate constant parameters based on thermochemical information, published theoretical studies, or on analogous reactions for which data are available. The thermodynamics section makes an even more extensive use of theory, reflecting the developing maturity of theoretical methods for computing thermochemical parameters such as enthalpies.

The layout of JPL 15-10 has been revised and improved from that of previous evaluations to include with each note the full citations for the references cited within that note. In addition, complete bibliographies appear at the end of each major section of the evaluation, as does a Master Bibliography for the entire document. Hyperlinks have been added to the master tables in the Photochemistry, Henry's Law, and Thermochemistry sections to facilitate improved document navigation.

Availability

The evaluation can be downloaded from **http://jpldataeval.jpl.nasa.gov** in pdf format. A sign-up for email notifications of news and updates is also available from this website. For more information, please contact this article's authors.

The 2015 S-RIP workshop and 11th SPARC data assimilation workshop

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The 2015 SPARC Reanalysis Intercomparison Project (S-RIP) workshop and the 11th SPARC Data Assimilation (SPARC DA) workshop were held together at the Université Pierre et Marie Curie in Paris, France, from 12-16 October 2015. Days one and two were dedicated to discussion on the progress of S-RIP, days four and five were dedicated to scientific presentations and discussion related to SPARC DA activities, and on day three a joint session between both activities was held. The 2015 S-RIP workshop was the second one since the 2013 S-RIP planning meeting, while the 11th SPARC-DA workshop was one of a regular series (see **www.sparc-climate.org/activities/data-assimilation**) that started in 2002. As in 2014, the two activities shared the same location and week for workshops because of their close scientific link. Thirty-seven participants attended either both or one of the workshops.

The S-RIP workshop

The main goal of S-RIP is to produce a SPARC report on the intercomparison of reanalyses (with

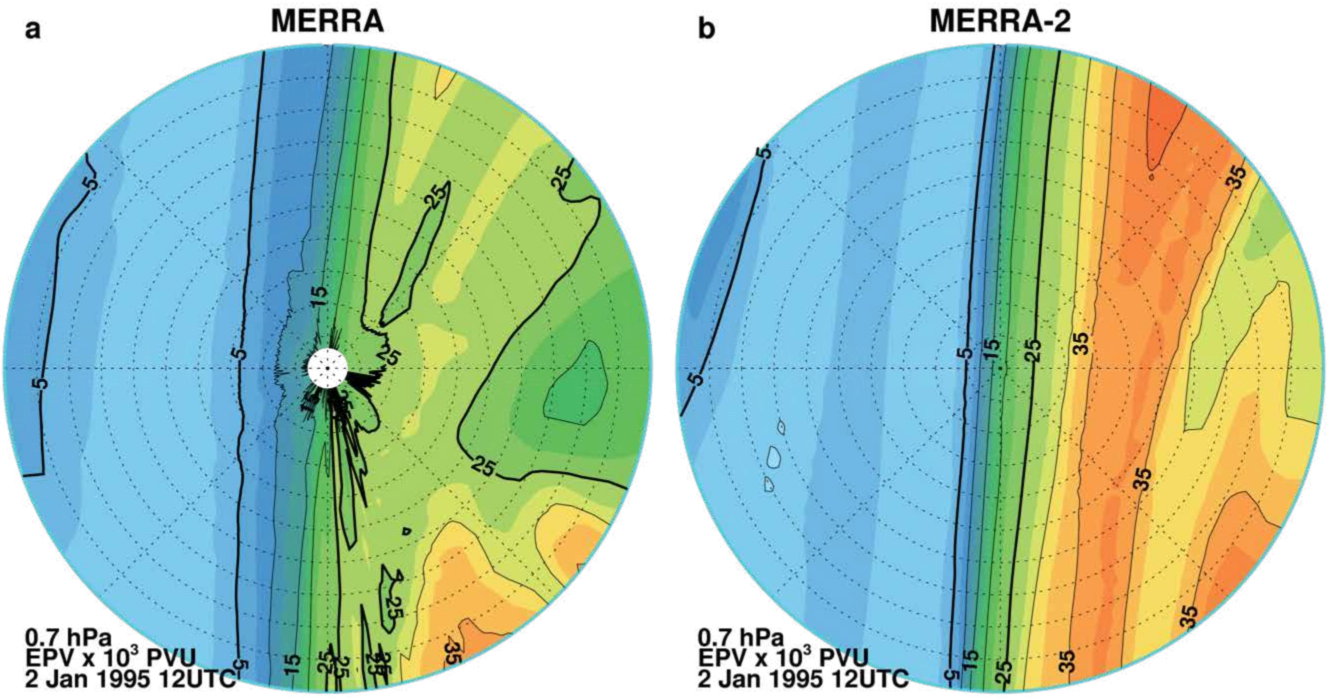

Figure 3: EPV at 0.7hPa on 2 January 1995 at 12UTC from (a) MERRA and (b) MERRA-2.

an interim report being produced in 2016 and the final full report in 2018), holding workshops annually between 2013 and 2018. As at the 2014 workshop, we discussed progress and current issues facing each chapter of the report, with one of the chapter leads (see **http://s-rip.ees.hokudai.ac.jp/report/structure.html**) reporting on the current status of each chapter. Rapporteurs were assigned for each chapter and they made brief summary presentations at the end of the workshop.

During the workshop, three major points were discussed. The first was the replacement of **David Tan**, who stepped down as S-RIP co-lead in July 2015 upon his departure from ECMWF. The workshop participants agreed that the collaborative link between reanalysis centres and SPARC data users has been successfully established during the past two years and that it is currently not critical to have a co-lead from one of the reanalysis centres; instead, it is more important to strengthen the scientific coordination of the project toward the goal of completing the 2018 report. After the workshop, two new co-leads, **Gloria Manney** and **Lesley Gray**, were confirmed with concurrence from the S-RIP working group members and chapter co-leads. **Masatomo Fujiwara** remains as co-lead. The second discussion point was the S-RIP interim report, consisting of Chapters 1-4, which will be published in 2016. **Jonathon Wright** agreed to be one of the editors of the interim report along with the S-RIP co-leads. The third discussion point focused on the consideration of an S-RIP special issue. Jonathon also agreed to take the lead on researching and organizing a special issue and we have subsequently negotiated with Atmospheric Chemistry and Physics to have a special issue on "The SPARC Reanalysis Intercomparison Project (S-RIP)" **www.atmos-chem-phys.net/special_issue829.html**), which was launched in January 2016. **Peter Haynes**, **Gabriele Stiller**, and **William Lahoz** kindly agreed to be the editors of this special issue.

S-RIP/SPARC-DA joint session on reanalyses

The joint session day started with four presentations about recent updates from reanalysis centres. **Larry Coy** discussed the NASA MERRA-2 reanalysis released in 2015. MERRA-2 has improved ozone as compared to MERRA thanks to the use of the latest SBUV/2 Version 8.6, Aura Microwave Limb Sounder (MLS), and Aura Ozone Monitoring Instrument (OMI). Model upgrades also improved the representation of the Quasi-Biennial Oscillation (QBO). A new cube-sphere grid led to a better representation of cross-polar flow (see **Figure 3**). From 2004 onwards, MLS temperature profiles have been assimilated improving the representation of the

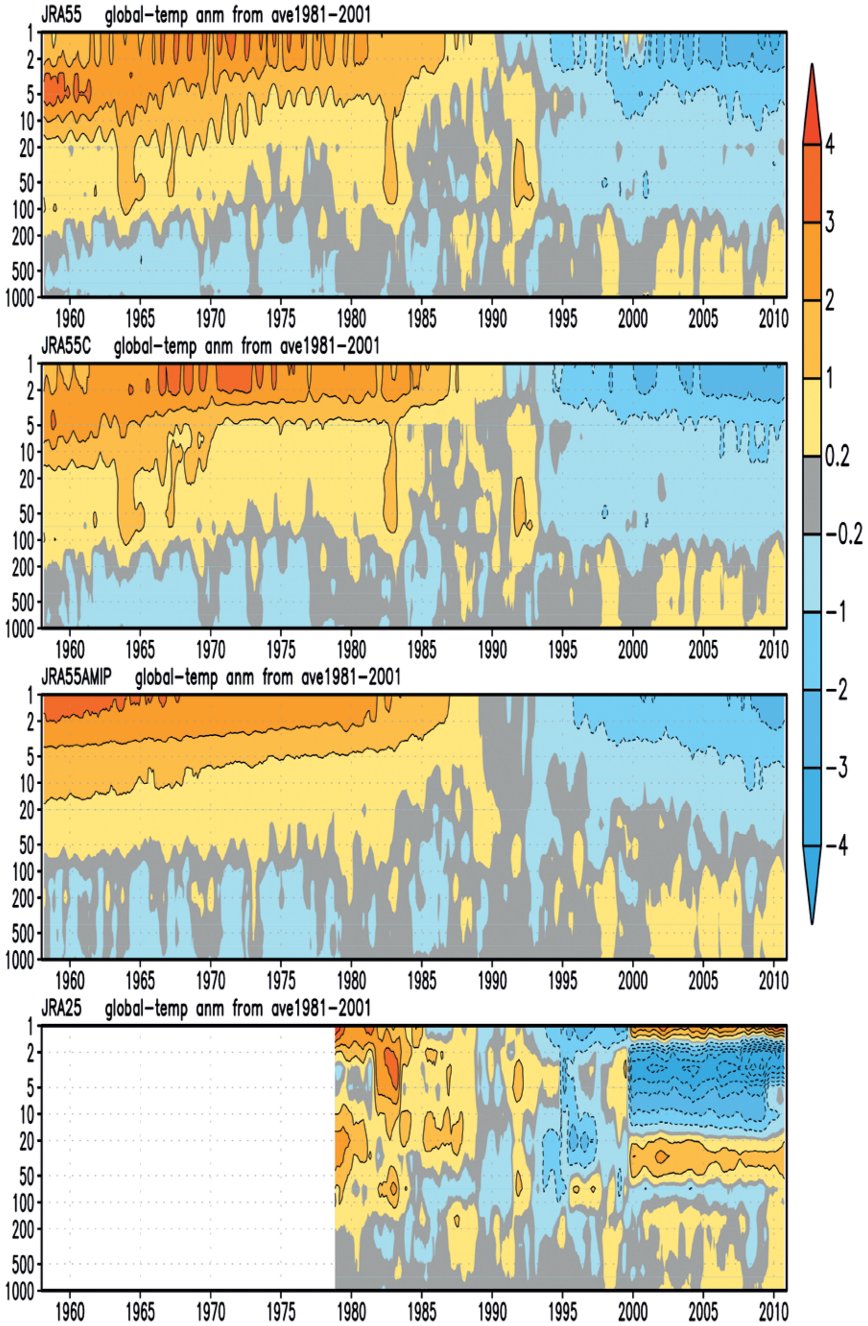

Figure 4: Global mean temperature anomalies (5-month running mean anomalies, anomalies mean climatology 1980-2001) for JRA-55 (top), JRA-55c (second from top), JRA-55AMIP (third from top) and JRA-25 (bottom).

upper stratosphere. New CRTM-based SSU assimilation also significantly impacted stratospheric temperatures, particularly in the 1980s and early 1990s. Additional information about MERRA-2 and access to the data can be found here: **http://gmao.gsfc.nasa.gov/reanalysis/MERRA-2**.

Hans Hersbach presented the ERA5 reanalysis, successor of ERA-Interim, which ECMWF has started to produce (completion in 2016). Among the different improvements in model, observations, and data assimilation techniques, an update to the semi-Lagrangian scheme allows a significant improvement in the forecast of sudden stratospheric warming (SSW) events. The configuration of the call of the radiation scheme has been upgraded, reducing the temperature bias of 3-5°K in the upper stratosphere. ERA5 analyses will be provided hourly.

Craig Long provided updated information on NOAA reanalyses. NCEP-1 and NCEP-2 are still running, as is CFSR, but with the system having changed to CFSv2 from April 2011. Version 2c of the NOAA–CIRES 20th Century Reanalysis (20CR), covering the period 1851-2011, is now available, while at NOAA CPC a reanalysis using only conventional data (*i.e.* surface and radiosonde observations only; similar to JRA-55C) is being developed for the period from the 1940s to present. Finally, he presented the NOAA's future plans, including the Next Generation

Global Prediction System (NGGPS), which unifies the short-term weather forecast system, 2-to-6-week forecast system, and climate forecast system; and the NCEP/EMC Unified Global Coupled Modeling System (UGCMS) which will be used to make a fully coupled reanalysis (1979-present) and attendant model reforecasts.

Chiaki Kobayashi presented the JRA-55C reanalysis that assimilates only conventional surface and upper air observations, with no use of satellite observations, using the same data assimilation system as the JRA-55 (Kobayashi *et al*., 2014). The reanalysis covers the period 1972-2012 and can be downloaded at: **http://rda.ucar.edu/datasets/ds628.2**. JRA-55C aims to produce a more homogeneous dataset unaffected by changes in historical satellite observing systems. The dataset is intended for studies of climate change or multi-decadal variability. The climatological properties deduced from the early results of the JRA-55C are similar to those of the JRA-55 in the troposphere and lower stratosphere, except for high southern latitudes. On the basis of forecast skill, the quality of the JRA-55C is inferior to that of JRA-55, however JRA-55C has better temporal homogeneity. **Figure 4** provides an example of JRA-55C compared to other JRA products.

Yayoi Harada discussed the extraordinary features of planetary wave propagation during boreal winter 2013/2014, with predominance of zonal wavenumber-2. Since 1958, the starting year of JRA-55, the boreal winters of 2008/2009 and 2013/2014 have been the only winters when the ratio of the wavenumber-2 contribution to the sum of wavenumber-1 and wave number-2 were greater than 75% (Harada *et al*., 2010). She concluded that the mechanisms related to the features in winter 2013/2014 can be summarized as follows: (1) there was remarkable blocking activity over the North Pacific basin modulated by La niña-like SST conditions that excited wavenumber-2 in the upper troposphere; and (2) upward wave-packet propagations over western Russia influenced the expansion and continuation of the Aleutian

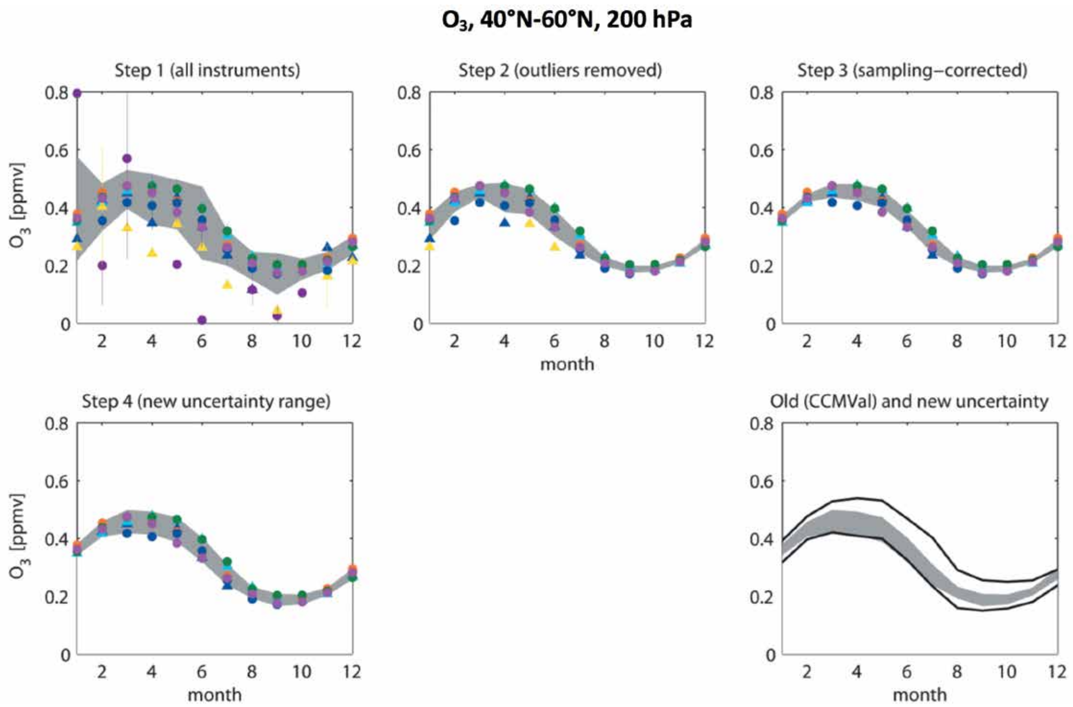

Figure 5: Ozone seasonal cycle diagnostic for 40-60°N at 200hPa. Upper left (step 1): 2005-2010 multi-annual mean values of all available instruments (each colour denotes a different instrument). The uncertainty range (grey shading) is calculated as the 1-sigma standard deviation over all instruments' multi-annual mean values. Upper centre (step 2): all data points outside the 1-sigma standard deviation from step 1 are removed and the uncertainty range recalculated. Upper right (step 3): all data points impacted by a sampling bias estimated to be larger than 10% are removed and the uncertainty range is recalculated. Lower left (step 4): as step 3, except that the uncertainty range is recalculated now taking not only the inter-instrument but also the inter-annual spread into account. This increases the uncertainty range, but is important in order to produce an uncertainty that free-running models can be compared against. Lower right: comparison between CCMVal range (black lines) and SPARC-DI multi-instruments range (grey shading).

High, which might be related to strong downward propagation over northern Canada and no occurrence of a major SSW in this winter.

Albert Hertzog (invited) presented long-duration balloon experiments in the upper troposphere/lower stratosphere (UTLS) and validation of the dynamics in various reanalyses. NCAR/NCEP and ERA-40 reanalyses had difficulties in capturing synoptic-scale variability of the poorly observed Southern Hemisphere storm track in the early 1970s. On the other hand, an excellent agreement between reanalysis fields and independent observations is found in the northern mid-latitudes. However, in the tropical tropopause region, a large and long-lasting difference is found between the balloon observations and reanalysis products. This is due to the poor resolution of equatorial waves in reanalyses as a result of missing radiosonde observations in the tropical regions, in particular over the oceans. This presentation also introduced the Strateole 2 long-duration campaign that will be carried out around the Equator from 2018-2021 (**http://tinyurl.com/strateole**).

Jingwei Liu presented an evaluation of the China Meteorological Administration (CMA) operational analysis (COA) data with two reanalysis datasets (ERA-Interim and R-2) for the period 2010-2012. For the 500hPa geopotential height field, COA data generally showed very high correlations and low root mean square errors (RMSE) compared to the other two reanalyses, however there are large inconsistencies in the tropics and over Antarctica. For relative humidity at 500hPa, COA generally showed small biases and RMSEs globally, with higher correlations with ERA-Interim compared to R-2. CMA is preparing a reanalysis dataset using their operational weather forecast model with an assimilation system in collaboration with NCAR.

Siddarth Das presented a comparison of *in situ* rocketsonde observations with different reanalyses (MERRA, ERA-40, ERA-Interim and NCEP-II). The reanalyses and observations agree well in terms of the amplitude of the annual and semi-annual oscillations, however, the reanalyses underestimate the QBO when compared to observations.

Felix Plöger compared trends of stratospheric mean age-of-air calculated with the CLaMS Lagrangian transport model driven by two different reanalyses (ERA-Interim and JRA-55). Climatologically, the age-of-air from both simulations agrees well with observations, however, in terms of decadal trends the ERA-Interim-driven simulation agrees well with observations, but not the one driven by JRA-55. By separating the contribution of residual circulation (*i.e.* slow transport) and isentropic eddy mixing (*i.e.* fast mixing), the aging by mixing in JRA-55 is negative in the Northern Hemisphere, which is not the case for ERA-Interim.

Bernard Legras compared the age-of-air among three reanalyses: MERRA, ERA-Interim, and JRA-55. The study concluded that significant discrepancies remain among reanalyses and observations. especially in long-term trends. The age spectrum diagnostic is a more robust test than the mean age-of-air for evaluating reanalyses, as the mean age is dependent on the tail distribution of ages, which tends to be badly represented in reanalyses.

Luis Millan talked about low column ozone events outside of the polar regions in winter/spring. These events are primarily the result of ozone variability due to dynamical processes rather than chemical processes. Satellite data of total column ozone from Aura OMI as well as vertical profiles from Aura MLS were used to develop a climatology of low ozone events and their relationships to stratosphere-troposphere exchange to evaluate their representation in reanalyses. The accuracy of their representation is being used as a metric to assess the reanalyses' ability to capture dynamically-driven ozone variability in the upper troposphere and stratosphere.

Thirteen posters were also displayed during the joint session. Titles and author names are available here: **http://events.oma.be/indico/event/6/page/4**.

The SPARC DA Workshop

Harmonization of long-term data records and bias correction in data assimilation

Susann Tegtmeier (invited) summarized the SPARC Data Initiative (DI), which aims to compare vertically-resolved trace gas climatologies derived from satellite measurements, identify outliers and provide merged data sets that will be used by the scientific community. The initiative is focusing on 25 trace gases and aerosols from 18 satellite instruments and results are being compiled in a SPARC report (SPARC, 2016). **Figure 5** illustrates the added value of the merged datasets provided by the SPARC DI activity.

Hans Hersbach (invited) presented the variational bias correction (VarBC) methods applied to satellite radiance measurements by forecast centres. These methods can be used to merge and filter outliers of different long-term data sets resulting in assimilated fields at each assimilation cycle and not on a monthly-zonal average basis. The implementation of a VarBC scheme requires a parametric form that represents the observation bias where parameters are optimized at the same time as the control variables (Dee and Uppala, 2009). From the ERA-Interim experience, ECMWF has learned that an adaptive bias correction system is required to correct time-varying instrument errors, handle major atmospheric forcing events (*e.g.*, Pinatubo), detect data drifts, and maintain optimal consistency among data sources. However, as long as models have systematic errors it is not possible to completely eliminate false climate signals in a reanalysis.

Quentin Errera presented a reanalysis of MIPAS stratospheric observations of N_2O and CH_4. The reanalysis generally agrees well with independent observations but suffers from time consistency due to discontinuities in the MIPAS observing system. The use of the averaging kernels of the observations, the filtering of outliers by a background quality check, and the use of a calibrated B-matrix using an ensemble method allow the reanalysis to almost eliminate the vertical oscillations in N_2O and CH_4 observations found in the tropical lower stratosphere.

On the added value of chemical data assimilation of upper tropospheric and stratospheric measurements

Richard Ménard (invited) examined the theoretical foundation of a method to estimate error covariances based on analysis residuals in observation space, also known as the Desroziers method. His analysis also included a method based on *a posteriori* diagnostics of variational analysis schemes. Using a mathematical analysis of convergence with a simplified regular observation network, he identified the conditions for convergence to the truth. In particular, he found that the estimation of variance parameters converges to the truth if the error

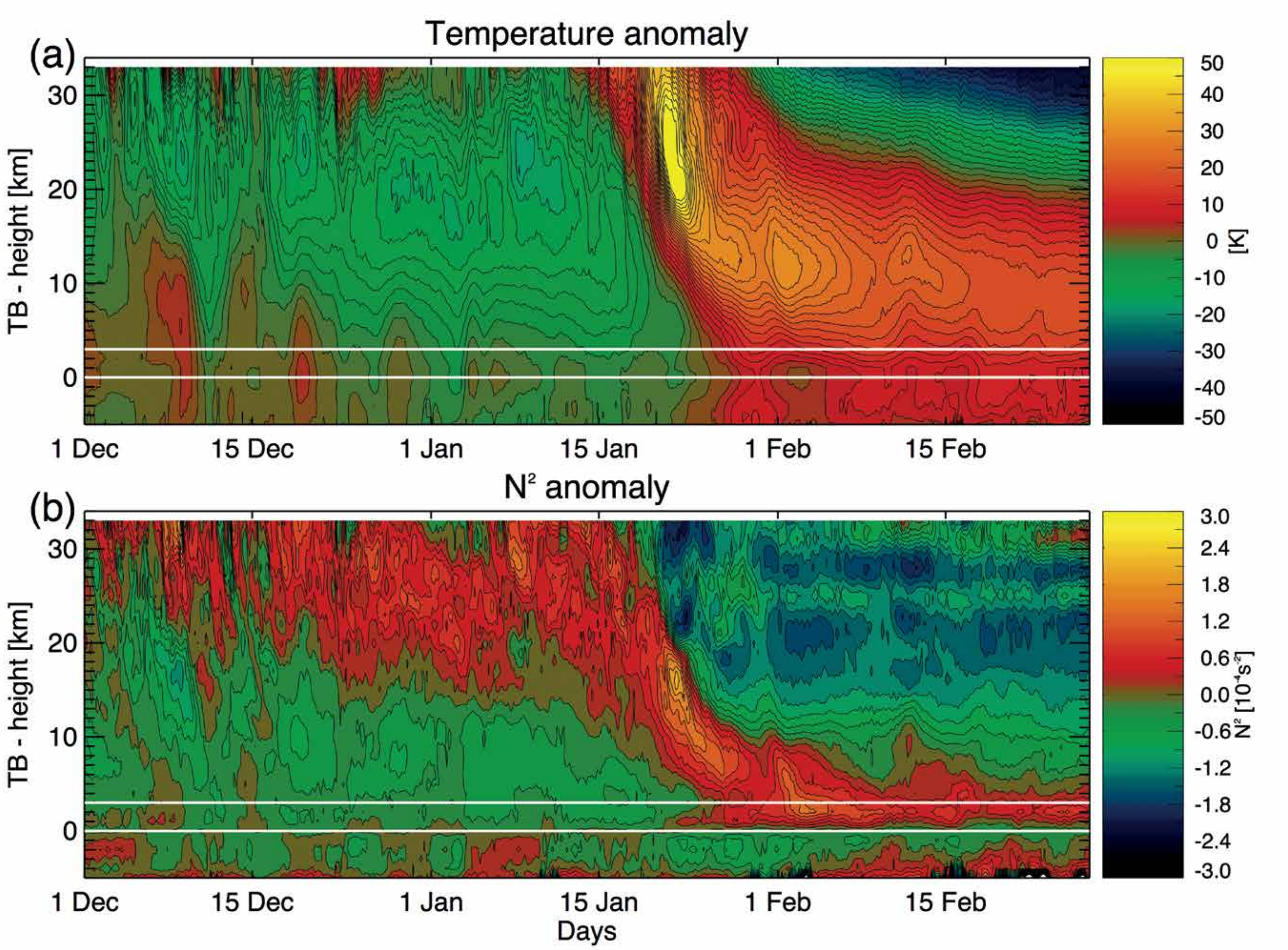

Figure 6: Temperature anomaly (top) and Brunt-Väisälä buoyancy frequency squared (N^2, bottom) zonally averaged between 75-90°N from MERRA-2 reanalysis.

correlation is specified correctly. The convergence is also much faster with the analysis increment (Desroziers) method than with the method designed for variational analysis schemes (Ménard, 2015).

Frank Baier reported on the extraction of wind information from MIPAS trace gas observations, work which is part of the European ARISE project to derive better stratospheric wind profiles. The inversion scheme is based on the SACADA assimilation model and uses adjoint advection of wind bias. MIPAS observations of HNO_3, O_3, H_2O, N_2O, and CH_4 from March 2003 were assimilated over 6-hour time windows and results were analysed with respect to species, latitude, and time. While experiments with simulated tracer and wind fields show reduced errors, comparisons with wind radio soundings over Kiruna show no bias reduction and need further investigation.

Representation of the stratosphere and mesosphere in models and analyses

Scott Osprey (invited) presented the QBO initiative (QBOi), a new SPARC activity (Anstey *et al.*, 2015; Hamilton *et al.*, 2015). The talk reviewed the performance of several CMIP5 and CCMVal-2 model simulations that reproduce observed characteristics of the QBO, showing that simulations usually do not accurately reproduce all characteristics simultaneously. To understand why models struggle to reproduce the QBO, QBOi has set up an experiment protocol that will be used to identify and distinguish the mechanisms important for accurately simulating the QBO.

François Lott (invited) presented the recent techniques used to represent non-orographic gravity waves in general circulation models, *e.g.,* the global spectral and multi-wave parameterizations. He showed how multi-wave parameterizations can be made efficient when made stochastic. He also showed how parameterized gravity waves can easily be related to their convective and frontal sources using well-understood theories. The relation with the sources render the launched wave stress very intermittent, a behaviour supported by isentropic balloon observations. He also illustrated how this intermittency is significant for the timing of the Southern Hemisphere vortex breakdown (de la Camara *et al.*, accepted).

Kris Wargan used the MERRA-2 reanalysis in combination with model simulations to study the behaviour of the polar tropopause during the 2009 major SSW. MERRA-2 shows strengthening of the polar tropopause inversion layer (TIL) during major SSW events, in agreement with previous studies (see **Figure 6**). Model simulations reveal that the primary mechanism involves an enhanced convergence of the vertical residual wind at the tropopause, but that the model underestimates the TIL's strengthening.

Yvan Orsolini examined the coupling between the stratosphere, mesosphere, and lower thermosphere (MLT) during SSWs with Elevated Stratopause (ES) events. Using the Whole Atmosphere Chemistry Climate Model (WACCM) it was shown that westward-travelling planetary waves are important to simulate the ES evolution and stratopause recovery. The impact of ES events extends well across the Equator, altering tropical wind, temperature, and ozone. After ES events, the migrating semidiurnal tides amplify due to tropical stratospheric ozone and wind anomalies (Limpasuvan *et al.*, 2016).

Valery Yudin presented an analysis of simulations from various whole atmosphere (WA) models (*i.e.* models with lids at altitudes of around 500km). WA models require further development and calibration to obtain realistic representation of wave dynamics (planetary waves, gravity waves, and tides). This presentation also highlighted two upcoming NASA thermosphere missions, ICON and GOLD, scheduled for 2017, which will provide observations of wind, temperature, and several chemical constituents at altitudes from 90-250km. These datasets will be important for space weather predictions made by NOAA and NCAR using WA models.

Sergey Skachko revisited the "model ozone deficit", the fact that many stratospheric chemistry transport models (CTM) underestimate ozone by 20-35% in the upper stratosphere/lower mesosphere (USLM). Using the CTM of the Belgian Assimilation System for Chemical ObsErvation (BASCOE), the sensitivity of the model was tested with respect to various inputs and compared to MLS ozone profiles. In particular, the ozone deficit is reduced when the photolysis rates are calculated online using ozone and temperature from the model instead of interpolating photolysis rates from a precalculated look-up table. Bias is also reduced when ERA-Interim temperature, used by the CTM, is bias-corrected in the USLM to match MLS temperature. These changes reduced the model deficit from 22 to 12%, although this deficit is still significant compared to MLS ozone observations.

Johannes Flemming studied the feedback of different representations of stratospheric ozone on temperature in the radiation scheme of the ECMWF model. The ozone representations were taken from climatologies, calculated by linearized parameterization, or calculated explicitly by solving a stratospheric chemical equation system. The different representations led to considerable differences between the temperature fields. However, temperature biases in the ECMWF model cannot be reduced just by taking into account ozone. Interestingly though, the use of prognostic ozone did not show any improvement in simulated temperature compared to the use of climatological ozone fields.

Next workshop

The next SPARC DA and S-RIP workshops will again be held jointly in 2016, this time in Victoria (BC), Canada, from 17-21 October. SPARC-DA will start the week and S-RIP will close the week with a joint session on Wednesday. More information is available on the SPARC-DA workshop page (**http://events.oma.be/indico/event/12**) and the S-RIP webpage (**http://s-rip.ees.hokudai.ac.jp/events/meeting2016**).

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