CHAPTER 4: CLIMATOLOGY AND INTERANNUAL VARIABILITY OF OZONE AND WATER VAPOUR

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4.1 INTRODUCTION

Ozone and water vapour are radiatively active trace gases that are represented in reanalyses due to their importance for the radiative budget of the stratosphere and the resulting impacts on stratospheric temperatures, winds, and the circulation (e.g., Dee et al., 2011). However, the degree of sophistication to which ozone and water vapour fields and their variability are represented depends on the reanalysis system, which observations it assimilates, and which microphysical and chemical parameterizations it includes that affect the trace gas distributions. Since SPARC scientists are interested in using ozone and water vapour fields from reanalyses for studying climate variability and change, it is timely to assess how well these are represented by the different reanalysis systems. This chapter hence aims at **(1)** providing an overview on how ozone and water vapour are treated in the different reanalyses, **(2)** evaluating ozone and water vapour in the different reanalyses against both assimilated and independent (non-assimilated) observations, and **(3)** drawing conclusions on how the deficiencies may affect the performance of the reanalyses.

4.2 DESCRIPTION OF OZONE AND WATER VAPOUR IN REANALYSES

Ozone and water vapour in reanalyses are treated in different ways depending on the reanalysis. In the following we provide information on how the ozone and water vapour fields are represented in the different reanalyses. The information provided here expands on the information contained in Fujiwara et al. (2016) and Chapter 2, which provides an overview of the treatment of ozone (*Section* 2.2.3.2), water vapour (*Section* 2.4.3), and other variables in the reanalyses.

In most reanalyses, ozone and water vapour are prognostic variables that are affected by the assimilated observations (see Tables 4.1 and 4.2 for an overview of key aspects of these fields). The assimilated observations affecting the water vapour field typically include radiosonde humidity profiles and either radiances or retrievals from microwave and infrared sounders such as TOVS and ATOVS (see Appendix A for all acronyms used in this chapter; see also Section 2.4.2.2 in Chapter 2 for an in depth discussion of observations assimilated by the various reanalyses). These data are allowed to affect the water vapour field in the lower atmosphere, with a typical cutoff in the upper troposphere between 300 hPa and 100 hPa. Because stratospheric water vapour data are not directly assimilated, the treatment of water vapour in the stratosphere is highly variable amongst the reanalyses. For the modern reanalyses, the concentration of water vapour entering the stratosphere is typically controlled by transport and dehydration processes occurring in the forecast model, primarily in the tropical tropopause layer (TTL). Higher in the stratosphere, chemical production of water vapour through methane oxidation is parameterized in some reanalyses, while others use a simple relaxation of their modelled water vapour field to an observed climatology.

As with water vapour, the treatment of ozone is quite different from reanalysis to reanalysis. The ozone treatment in reanalyses ranges from not having an interactive field and using a climatology for radiation calculations (NCEP R1/R2), to a fully prognostic field with parameterized photochemistry (CFSR, ECMWF reanalyses), to an assimilation with an offline chemical transport model for use in the forecast model radiation calculation (JMA reanalyses).

The primary ozone observations assimilated by reanalyses are satellite UV backscatter based nadir ozone retrievals of total column ozone or broad vertically weighted averages (e.g. SBUV, TOMS/OMI data). Figures 4.1 and 4.2 give overview summaries of the assimilated total column ozone and ozone vertical profile data, respectively. However, some differences amongst the reanalysis exist in their use of particular data sets, data quality control, and filtering, and these choices potentially affect the reanalysis ozone fields. Additional observations may have been used as well, covering other spectral ranges besides the UV (namely, MW and IR) and exploiting different viewing geometries (such as limb-sounding). On one hand, the assimilation of additional data, particularly vertically resolved data, could improve the quality of the ozone reanalyses, while on the other, they can introduce sudden changes in the reanalysis timeseries that should be considered carefully when deriving long-term trends.

4.2.1 NCEP-NCAR R1 and NCEP-DOE R2

In both NCEP-NCAR R1 and NCEP-DOE R2, no ozone data were assimilated (Kalnay et al., 1996; Kanamitsu et al., 2002; Kistler et al., 2001). A climatology of ozone was used for radiation calculations.

Humidity information from satellites is not assimilated in R1 and R2 (Ebisuzaki and Zhang, 2011). In general R1 and R2 are similar in regards to their treatment of water vapour, but one major difference is that in R1 humidity is not analyzed above 300 hPa. In R2, several fixes and changes were made in the treatment of clouds, and this resulted in R2 being ~20% drier than R1 in the tropics at 300 hPa (Kanamitsu et al., 2002). Also, in R2 only relative humidity is provided as a reanalysis output. Given the focus on the upper levels here, humidity from R1 and R2 is not analyzed in this chapter. It is worth noting that between 500 and 300 hPa, R1 shows negative long-term humidity trends (Paltridge et al., 2009), although the negative trends reflect suspect radiosonde measurements at these levels and are not seen in other reanalyses or satellite data (Dessler and Davis, 2010).

4.2.2 CFSR

CFSR treats ozone as a prognostic variable that is analysed and transported by the forecast model. The CFSR forecast model uses analyzed ozone data for radiation calculations. In the forecast model, ozone chemistry is parameterized using production and loss terms generated by the NRL CHEM2D-OPP (McCormack et al., 2006). These production and loss rates are provided as monthly mean zonal means, and are a function of local ozone concentration. The rates do not include the coefficients for temperature and overhead ozone column provided by McCormack et al. (2006), nor heterogeneous chemistry, although late 20th century levels of CFCs are used indirectly because CHEM2D-OPP is based on the CHEM2D middle atmospheric photochemical transport model that includes ODS levels representative of the late twentieth century.

CFSR assimilates the version-8 SBUV profile and total column ozone (TCO) retrievals (Flynn et al., 2009) from *Nimbus-7* and SBUV/2 profile and TCO retrievals from *NOAA-9*, *-11*, *-14*, *-16*, *-17*, *-18*, and eventually *NOAA-19* (Saha et al., 2010). The ozone layers and TCO values assimilated into the

CFSR have not been adjusted to account for biases from one satellite to the next, although the use of SBUV version 8 data is expected to minimize satellite-to-satellite differences.

Despite assimilating the TCO retrievals and SBUV ozone profiles, differences were found between CFSR and SBUV(/2) ozone profile data (Saha et al., 2010). Most of the difference occurs above 10 hPa, and it was discovered that the ozone layer observational background errors in the CFSR were set too large in the upper stratosphere by a factor of between 2 (at 10 hPa) and 60 (at 0.2 hPa). Because of this, the assimilated SBUV(/2) ozone layer observations do not alter the CFSR's first guess above 10 hPa, and the model climatology is used instead.

Water vapour is treated prognostically in CFSR, and there are a number of assimilated observations that influence the analysis humidity fields in the troposphere, including GPS Radio Occultation retrievals, radiosondes, and satellite radiances. However, radiosonde humidity data is only assimilated at 250 hPa and below, and there are no specific observations to constrain humidity in the stratosphere. Stratospheric humidity in CFSR is hence primarily governed by physical processes and parameterizations in the model, including dehydration within the TTL. Since the dehydration parameterization used can lead to negative water vapour values in the vicinity of the tropopause, these are subsequently replaced by small positive values for the radiation calculations (0.1 ppmv), but the negative values are retained in the analysis. CFSR does not include a parameterization of methane oxidation.

4.2.3 ERA-40

The ERA-40 forecast model included prognostic ozone and a parameterization of photochemical sources and sinks of ozone, as described in Dethof and Hólm (2004). This parameterization of ozone production/loss rates is an updated version of the one described by Cariolle and Deque (1986, hereafter CD86). In CD86, the net ozone production rate is a function of the perturbation (relative to climatology) of the local ozone concentration, local temperature, and overhead ozone column. In addition to the CD86 formulation, the ozone parameterization in ERA-40 also includes a term representing heterogeneous chemistry that scales with the product of the local ozone concentration and square of the equivalent chlorine concentration. The coefficients of the parameterization and the climatologies vary with latitude, pressure, and month. The chlorine loading varies from year to year, between ~700 ppt in 1950 to ~3400 ppt in the 1990's. For ERA-40, the major change added to the original parameterization was the improved photochemical equilibrium ozone climatology from Fortuin and Langematz (1995).

Model-generated ozone was not used in the radiation calculations, which instead assume the climatological ozone distribution reported by Fortuin and Langematz (1995). The reason for this is due to concerns over possible degradation of the temperature analysis from ozone and temperature feedbacks, which may occur if the ozone observations are of poor quality relative to those of temperature (Dethof and Hólm, 2004).

ERA-40 assimilated TOMS TCO and SBUV layer ozone retrievals from the end of 1978 onward (see Table 1, Dethof and Hólm, 2004; Poli, 2010). No ozonesonde measurements were assimilated, and before 1978, no ozone data were assimilated. Thus, ozone data prior to 1978 are primarily affected by the photochemical parameterization. Also, no data were assimilated during 1989-1990 because the first ERA-40 stream (1989-2002, see discussion in Chapter 2) began execution before the ozone assimilation scheme was implemented. Finally, it is worth noting that the ozone background errors were changed such that the period January 1991 to October 1996 contains different background errors than the rest of ERA-40 (Dethof and Hólm, 2004).

The water vapour field below the diagnosed tropopause in ERA-40 is largely influenced by the assimilated observations, and three main periods can be identified (Andersson et al., 2005): until 1973, ERA-40 only used the conventional in situ surface and radiosonde measurements; from 1973, satellite radiances from the VTPR (1973-1978) and the TOVS MSU, SSU, and HIRS (1978-onwards) instruments were used in addition to these data sources; from 1987 onward, 1D-Var retrievals of TCWV from SSM/I radiances were also assimilated. The radiosonde humidity measurements were generally used up to 300 hPa.

Above the diagnosed tropopause, no adjustments to the humidity field due to data assimilation were made in ERA-40. Thus, the ERA-40 stratospheric water vapour reflects TTL dehydration, transport, and methane oxidation, which was included via a simple parameterization in the stratosphere (Untch et al., 1998). The ERA-40 methane parameterization was based on a relaxation of WV to 6 ppmv at the stratopause. Several studies found that this relaxation value produced too dry of a stratopause because it was based on earlier studies during a time with lower methane levels (Uppala et al., 2005). Additionally, the ERA-40 stratospheric humidity has been shown to be too dry, due to a cold-bias in TTL temperatures related to the Brewer-Dobson circulation being too strong (Oikonomou and O'Neill, 2006).

4.2.4 ERA-INTERIM

The treatment of ozone and water vapour in ERA-INTERIM is very similar to the treatment in ERA-40, with some notable additions of new datasets that are assimilated, and an improved treatment of water vapour in the UTLS region.

As with ERA-40, total ozone from TOMS (Jan 1979–Nov 1989; Jun 1990 – Dec 1994; Jun 1996 – Dec 2001) and ozone profile information from SBUV (1979–present) are assimilated. ERA-INTERIM also assimilates TCO data from OMI (Jun 2008– Jan 2009, Mar 2009 - present) and SCIAMACHY (Jan 2003– Dec 2008), and profile data from GOME (Jan 1996– Dec 2002), MIPAS (Jan 2003– Mar 2004), and MLS (Jan-Nov 2008, Jun 2009 –present). A change in the assimilation of the SBUV data has been implemented in Jan 2008 when the assimilation of a low vertical resolution product - derived over six vertical layers (0.1-1 hPa, 1-2 hPa, 2-4 hPa, 4-8 hPa, 8-16 hPa and 16 hPa-surface) from the NOAA version 6 (v6) SBUV profiles - was replaced by that using the native 21 vertical level (v8) SBUV profiles. For Aura MLS, the version 2.2 reprocessed ozone data were used in 2008, while the assimilation from Jun 2009 onwards has relied on the near-real time product.

The ozone forecast model used in ERA-Interim is the same use in ERA-40, though the parameterization has undergone significant upgrades, especially in the regression coefficients. An account of the changes can be found in Cariolle and Teyssédre (2007).

As with ERA-40, the radiation scheme in ERA-interim does not use the prognostic ozone field. In contrast to ERA-40, the sensitivity of the temperature and wind variables to ozone data has been switched off in ERA-Interim after a preliminary assessment of the temperature and wind fields revealed unrealistic increments generated near the stratopause by 4D-Var (Dee, 2008). Without an ozone bias correction in place, 4D-Var generates large increments in temperature and horizontal wind components in an attempt to accommodate observed large local changes in ozone concentration (Dee, 2008).

An assessment of the quality of the ERA-Interim ozone reanalyses is given in (Dragani, 2011). It is shown that until December 1995 the ERA-Interim ozone analyses are in better agreement with the independent ozone observations than their ERA-40 equivalent in the upper troposphere and lower stratosphere, but slightly degraded on average in the middle stratosphere. The assimilation of GOME ozone profiles (January 1996 - December 2002) improves the agreement between the independent data and the co-located ERA-Interim analyses, exceeding that calculated for ERA-40, also in the middle stratosphere.

The ERA-Interim humidity analysis is substantially modified from that in ERA-40 due to changes in both model physics and to changes in the assimilated observations. A non-linear transformation of its control variable has been introduced to improve the Gaussianity of the humidity background errors (Andersson et al., 2005; Hólm, 2003; Hólm et al., 2002). The transformation normalizes relative humidity increments by a factor that depends on background estimates of relative humidity and vertical level. Also, a 1D-Var assimilation of rain-affected radiances was added as part of the 4D-Var outer loop (Dee et al., 2011). The ERA-Interim humidity analysis also benefits from several changes in the model physics, including changes in the convection scheme that lead to increased convective precipitation (particularly at night), a reduction of the tropical wind errors, a better phasing of precipitation events (Bechtold et al., 2004), and an improved cloud scheme.

Perhaps of most relevance for humidity in the UTLS, the revised cloud scheme contains a new parameterization that allows supersaturation with respect to ice in the cloud-free portions of grid cells with temperatures less than 250 K (Tompkins et al., 2007). The inclusion of this parameterization results in a substantial increase of relative humidity in the upper troposphere and stratospheric polar cap when compared with ERA-40 (Dee et al., 2011). However, as with ERA-40, no adjustments due to data assimilation are applied in the stratosphere (above the diagnosed tropopause). Also, methane oxidation in the stratosphere is included via a parameterization similar to the one used in ERA-40 but with a relaxation value of 6.8 ppmv at the stratopause based on the analysis of the UARS data presented by Randel et al (1998).

As with ERA-40, ERA-interim humidity is affected by the assimilation of radiosonde humidity measurement, TCWV retrievals from SSM/I, and radiances from the TOVS MSU, SSU, and HIRS instruments. Additional humidity information included in ERA-Interim comes from AIRS all-sky radiances and bending angles from GPSRO data.

4.2.5 JRA-25 AND JRA-55

In the JRA-25 and JRA-55 systems, ozone observations were not assimilated directly (Kobayashi et al., 2015; Onogi et al., 2007). Instead, the daily three-dimensional ozone fields were separately produced in advance and provided to the JRA forecast model (i.e., to the radiation scheme). Before 1978 in JRA-55, the daily ozone fields were time-interpolated based on a monthly mean climatology for 1980-1984. After 1979, ozone fields were provided by an offline chemistry climate model (MRI-CCM1, *Shibata et al.*, 2005) that assimilated satellite TCO observations. In the chemistry climate model, a nudging scheme was employed to assimilate total column ozone retrievals from TOMS on Nimbus-7 and other satellites for the period 1979–2004 and from the Ozone Monitoring Instrument on Aura thereafter. There were some differences in the ozone field preparation between the JRA-25 and JRA-55 due to the use of different versions of MRI-CCM1. For JRA-25, nudging to the climatological ozone vertical profile was also conducted, to account for a known bias in the MRI-CCM1 tropospheric ozone that leads to stratospheric ozone bias when total ozone nudging is conducted; this procedure led to reasonable ozone-layer peak values in the final ozone product. On the other hand, for the JRA-55, with a somewhat updated MRI-CCM1, this vertical-profile nudging was not conducted; this resulted in improved peak values in the vertical ozone profiles and a clear reproduction of the ozone QBO signature.

As with the other modern reanalyses, JRA-25 and JRA-55 assimilated radiosonde humidity measurements, and satellite radiances that can impact the humidity field. In the case of JRA-25, the logarithm of specific humidity is assimilated (Onogi et al., 2007). Stratospheric humidity in JRA-25 is dry-biased, and generally decreasing with time, in part due to the lack of a parameterization of methane oxidation (Onogi et al., 2007). In JRA-25, a constant value of 2.5 ppmv is used in the stratosphere in the forecast model radiation calculations (Onogi et al., 2007). There is evidence of a discontinuity at the start of 1991 between the two major processing streams of JRA-25. A jump of +0.7 ppmv and +0.9 ppmv at 150 hPa and 100 hPa, respectively, was identified by Onogi et al. (2007).

The treatment of water vapor in JRA-55 is similar to that in JRA-25. JRA-55 also does not contain a parameterization of methane oxidation. However, JRA-55 sets the vertical correlations of humidity background errors to zero above 5 hPa (50 hPa in JRA-25) to prevent spurious analysis increments at higher levels, and uses an annual mean climatology derived from HALOE and UARS MLS measurements made during 1991–1997 in the stratosphere for radiation calculations. One major change in JRA-55 was the introduction of an improved radiation scheme that greatly reduced the lower stratospheric negative temperature bias that was present in JRA-25 (Kobayashi et al., 2015, see also Ch 2.2.2 for a description of the radiative transfer models in JMA reanalyses), and it is expected that this will have a significant impact on the JRA-55 stratospheric humidity.

Stratospheric water vapour above 100 hPa is not provided from these two reanalyses and consequently not evaluated in this chapter.

4.2.6 MERRA

Ozone in MERRA is a prognostic variable, subject to assimilation, transport by assimilated winds (more precisely, the odd-oxygen family is the transported species) and parameterized chemistry. The MERRA GCM uses a simple chemistry scheme that applies monthly zonal mean ozone production rates and loss frequencies derived from a 2-dimensional chemistry model (Stajner et al., 2008). The ozone data assimilated in the reanalysis are partial columns and total ozone (defined as the sum of layer values in a profile) from a series of SBUV instruments (Flynn et al., 2009) on various NOAA platforms as depicted in Figures 4.1 and 4.2. Version 8 of the SBUV retrievals (Flynn, 2007) is used but, prior to assimilation, the native 21 vertical layers are combined into 12, each 5 km deep. All other data, including radiance observations, are explicitly prevented from impacting the analysis ozone directly. Since SBUV sensors measure backscatter solar ultraviolet radiation only daytime observations are available. In particular, the wintertime ozone in the Polar Regions is poorly constrained by observations. We note that early NOAA satellites experienced orbital drifts resulting in a loss of daylight coverage in time. For example, the equatorial crossing time for NOAA-11 drifted from about 2PM in 1989 to 5PM five years later, leading to a very limited SBUV coverage in 1994: in the middle part of the year ozone observations were unavailable south of 30°S. Similarly, the orbital drift of the NOAA-17 satellite impacted the quality of the MERRA ozone product in 2012 before observations from the NOAA-19 SBUV were introduced in 2013. With the exceptions delineated above and occasional short temporal gaps, SBUV provides a good coverage of the sunlit atmosphere.

The background error standard deviations for ozone are specified as about 4 % of the mean ozone at a given model level globally. The horizontal background error correlation lengths vary from ~400 km in the troposphere to ~800 km at the model top. Assimilated ozone fields are fed into the radiation scheme in the GCM and are used in the radiative transfer model for radiance assimilation.

Water vapour is also a prognostic assimilated variable in MERRA, however unlike ozone, the moisture fields in the stratosphere are relaxed to a 2-D monthly climatology derived from water vapour observation record from the Halogen Occultation Experiment and the Microwave Limb Sounder on EOS Aura (e.g., Rienecker et al., 2011 and references therein) with a relaxation time of 3 days. Water vapour above the tropopause does not undergo physically meaningful variations on longer timescales.

In particular, no attempt was made to account for methane oxidation or trends in stratospheric methane concentrations in the model.

MERRA assimilates specific humidity measurements from radiosondes up to 300 hPa and marine surface observations. Moisture fields are affected by microwave radiance data from SSM/I and AMSU-B/MHS, 6 μm infrared radiances from HIRS, GOES Sounder, AIRS and assimilated rain rates from TMI and SSM/I instruments.

The background error statistics for water vapour were derived using the National Meteorological Center method and applied using a recursive filters methodology (Wu et al., 2002). The moisture control variable is pseudo-relative humidity (Dee and Da Silva, 2003)

4.2.7 MERRA-2

The key differences between the treatment of ozone in MERRA and MERRA-2 are in the observing system and the background error covariances. Between January 1980 and September 2004 MERRA-2 assimilates version 8.6 retrieved SBUV (Bhartia et al., 2013) partial columns given on a 21-layer vertical grid and total ozone computed as the sum of individual layer values. Compared to the version 8 retrievals (used in MERRA), the version 8.6 algorithm uses upgraded ozone cross-sections and an improved cloud height climatology, resulting in a better agreement with independent ozone data and suitable for constructing long-term climatologies (Frith et al., 2014; McPeters et al., 2013).

Starting in October 2004 the SBUV data are turned off in MERRA-2 and replaced by the total ozone product from the Ozone Monitoring Instrument (OMI, Levelt et al., 2006) and stratospheric profiles from the Microwave Limb Sounder (MLS, Waters et al., 2006), both onboard NASA's EOS Aura satellite. The OMI data are total column ozone retrievals from collection 3 data, version-8.5 retrieval algorithm extensively evaluated by McPeters et al. (2008). The assimilation algorithm makes use of OMI's efficiency factors (averaging kernels) in order to account for a low sensitivity of these measurements to the lower troposphere in the presence of clouds (Wargan et al., 2015). The MLS data are from version 2.2 between October 2004 and May 2015 and version 4.2 (Livesey et al., 2016) afterwards.

When using the MERRA-2 ozone product one should be aware that the reanalysis record falls into the two distinct periods: the SBUV period (1980 – September 2004) and EOS Aura period (from October 2004 onward). Generally, a better quality analysis is expected in the latter period owing to higher vertical resolution of MLS profiles compared to SBUV and the availability of MLS observations at day and night.

The ozone background error variance in MERRA-2 model follows Wargan et al. (2015). At each grid point the background error standard deviation is set proportional to the background ozone at that point and time. This approach introduces a flow-dependence into the assumed background errors and allows an accurate representation of shallow structures in the ozone fields, especially in the upper troposphere and lower stratosphere. As in MERRA, the assimilated ozone is a radiatively active tracer in the GCM and it is fed into the radiative transfer model used for assimilation of radiance data.

A preliminary evaluation of the MERRA-2 ozone product is summarized in Bosilovich et al. (2015). A comprehensive product description and validation, including comparisons with MERRA is in preparation (Wargan et al., in preparation).

The treatment of stratospheric water vapour in the MERRA-2 GCM is similar to MERRA, with a 3-day relaxation to a 12-month climatology. The main innovation is the introduction of additional global constraint that ensures the conservation of the dry mass of the atmosphere and rescales the water vapour tendency by removing the globally integrated mean from the analysis increment (Takacs et al., 2016).

In addition to the moisture data used in MERRA, MERRA-2 assimilates GPS radio occultation data and radiances from the following infrared sensors introduced in recent years: IASI, CrIS and SEVIRI. These observations (e.g., IR radiances) are not highly sensitive to stratospheric water vapour, so stratospheric water vapour is not intentionally assimilated by these observations, although the observations could have some small impact on stratospheric water vapour values.

The changes introduced in the MERRA-2 observing system relative to MERRA are described in more detail in Bosilovich et al. (2015) and McCarty et al. (in preparation). The moisture control variable in the MERRA-2 assimilation scheme is based on a normalization of the pseudo-relative humidity by the background error standard deviation. The background error covariances used in MERRA-2 have been significantly retuned since MERRA (Bosilovich et al., 2015).

4.3 OBSERVATIONAL DATASETS USED FOR EVALUATION

In this section we provide a short description of the different observational datasets used in this chapter to evaluate the ozone and water vapour fields in reanalyses. Main focus of the evaluations thereby is on how well the reanalyses capture climatological mean quantities and interannual variability in these trace gases. In addition, the representation of physical features such as the ozone hole and the QBO are evaluated.

4.3.1 SBUV AND TOMS/OMI TOTAL COLUMN OZONE

Two datasets are used to evaluate the total column ozone in the reanalyses. The first is the SBUV Merged Ozone Data Set (Frith et al., 2014). The second is a combination of TOMS and Aura OMI OMTO3d total ozone observations (Bhartia and Wellemeyer, 2002). All data were processed using the TOMS version 8.6 algorithm. Because SBUV and TOMS (and for some reanalyses OMI) data are assimilated by most of the reanalyses, the comparisons to these datasets are not independent.

4.3.2 SPARC DATA INITIATIVE LIMB SATELLITE OBSERVATIONS

The SPARC Data Initiative (*SPARC Report No. 8*, in preparation, and references therein; *Hegglin et al.*, in preparation) offers monthly mean zonal mean climatologies of ozone (Neu et al., 2014; Tegtmeier et al., 2013) and water vapour (Hegglin et al., 2013) from an international suite of satellite limb sounders for use in this chapter. The zonal monthly mean climatologies have undergone a comprehensive quality assessment and are suitable for climatological comparisons of the vertical distribution and interannual variability of these constituents in the reanalyses on monthly to multi-annual timescales. We here only use a subset of the instrumental records available as specified in the respective evaluation sections.

The observational multi-instrument mean (MIM) for ozone during the time period 2005-2010 is derived using the SPARC Data Initiative zonal monthly mean climatologies from ACE-FTS, Aura-MLS, GOMOS, MIPAS, OSIRIS, SCIAMACHY, and SMR. These instruments all cover the 6 years from 2005-2010 and show inter-instrument differences that lie generally between ±5% from the MIM throughout the stratosphere. Differences from the MIM in the lower mesosphere and tropical lower stratosphere are somewhat higher (±10%) (Tegtmeier et al., 2013). The evaluation of the ozone QBO signal for 2005-2010 is based on the instruments OSIRIS, GOMOS and Aura-MLS, which show the most consistent QBO signal among each other (Tegtmeier et al., 2013).

The observational MIM for water vapour during the time period 2005-2010 is derived using the SPARC Data Initiative zonal monthly mean climatologies from Aura-MLS, MIPAS, ACE-FTS, and

SCIAMACHY. These instruments all cover the 6 years from 2005-2010 and show inter-instrument differences that lie generally between ±5% from the MIM throughout the stratosphere. Differences from the MIM in the tropical upper troposphere increase to ±20% (Hegglin et al., 2013).

4.3.3 AURA MLS SATELLITE DATA

The evolution of ozone in the different reanalyses is compared with that from Aura MLS retrievals in section 4.4.6. Aura MLS measures millimeter- and submillimeter-wavelength thermal emission from the limb of Earth's atmosphere. Detailed information on the measurement technique and the Aura MLS instrument is given by Waters et al. (2006). Vertical profiles are measured every 165 km along the suborbital track and have a horizontal resolution of ~200—500 km along-track and a footprint of 3—9 km across-track. Here we use version 4.2 (hereafter v4) MLS ozone measurements from September 2004 through December 2013. The quality of the MLS v4 data is described by Livesey et al. (2016). Vertical resolution of MLS ozone is about 3 km, and single-profile precision varies with height from approximately 0.03 ppmv at 100 hPa to 0.2 ppmv at 1 hPa. The v4 MLS data are quality-screened as recommended by Livesey et al. (2016). V4 stratospheric (pressures less than 100 hPa) ozone values are within ~2% of those in version 2.2 (v2), which is the version assimilated in MERRA-2 (until 31 May 2015, after which v4.2 data are used) and ERA-Interim. At pressures greater than 100 hPa, v4 MLS ozone shows high and low biases with respect to v2 at alternating levels, indicating improvement of vertical oscillations seen in v2 (Livesey et al., 2016).

4.3.4 SWOOSH MERGED LIMB SATELLITE DATA RECORD

The Stratospheric Water and Ozone Satellite Homogenized (SWOOSH) database is a monthly-mean record of vertically resolved ozone and water vapor data from a subset of limb profiling satellite instruments operating since the 1980’s (Davis et al., 2016). SWOOSH includes individual satellite source data from the SAGE-II, SAGE-III, UARS MLS, UARS HALOE, and Aura MLS, as well as a merged data product. A key aspect of the merged product is that the source records are homogenized to account for inter-satellite biases and to minimize artificial jumps in the record. The homogenization process involves adjusting the satellite data records to a “reference” satellite using coincident observations during time periods of instrument overlap. SWOOSH data are used in this chapter for timeseries evaluations that start prior to the Aura MLS record (i.e., pre-2004).

4.4 OZONE AND WATER VAPOUR EVALUATIONS

4.4.1 MULTI-ANNUAL MEAN COMPARISONS

4.4.1.1 TOTAL COLUMN OZONE SEASONAL CYCLE

In this section, SBUV and TOMS/OMI total column ozone (TCO) data are compared to the reanalyses over the climatological period 1981-2010. Figure 4.3 shows the seasonal cycle in total column ozone as a function of latitude and month from the observations and reanalyses. To first order, all of the reanalyses reproduce the major features of the seasonal and latitudinal distribution of TCO. This is not surprising, given that most reanalyses assimilate TCO data from these satellites, as discussed in section 4.2. As such, it should be stressed that the comparisons here do not represent independent verification of ozone in reanalyses, but that it rather reflects a test of the internal consistency of the data assimilation system.

Although the reanalysis TCO fields look quite similar, there are some widespread biases that are revealed by considering the differences between reanalyses and observations, as in Figure 4.4. First, the agreement between the two observational TCO datasets are ± ~6 DU (~ 2 – 3%), with TOMS/OMI generally having larger values in the tropics and lower values at high latitudes, compared with SBUV. The reanalyses generally exhibit slightly larger differences with the TCO datasets than the difference between the two TCO datasets. In some cases, a given reanalysis agrees better with one or the other TCO data sets (cf. Figure 4.5). This is likely caused by the fact that a given reanalyses assimilates that particular dataset. For example, MERRA shows extremely close agreement with SBUV, which it assimilates.

Note that ERA-40 shows substantially larger TCO values than the TCO datasets, particularly at higher latitudes, compared to the TCO data. Contributing to the large differences is the fact that ERA-40 is only available until August 2002, and thus the ozone climatology shown in Figures 4.4 and 4.5 are not derived for the same period covered by the other reanalyses and observations. Including more years with larger average ozone depletion (2003-2010) will lead to a negative sampling bias in the observational reference chosen.

However, it must be mentioned that for reanalyses that only/mainly assimilate UV-based retrievals, the high latitudes remain largely unconstrained in the winter hemisphere. The impact of these observations may also be limited depending on the filtering choices. For example, data filtering based on low solar elevation angles (less than 10º and 6º, respectively) is applied to the TOMS and SBUV observations in both ERA-40 and ERA-Interim. This is likely to further limit the observation impact on the resulting ozone field at higher latitudes. For the ERA products, the high latitude ozone fields essentially reflect transport and the ozone parameterization scheme. Dethof and Hólm (2004) showed that the ERA ozone model produces too large ozone values at high latitudes (differences from 20 DU, in the summer hemisphere, to 50 DU, in the winter hemisphere).

4.4.1.2 VERTICAL CROSS-SECTIONS

In this section, we compare zonal mean multi-annual mean cross sections of ozone and water vapour between the different reanalyses and an observational mean derived from data obtained from the SPARC Data Initiative. We here compare the time period 2005-2010 using two different sets of instruments as detailed in *Section 4.3.2*. This shorter time period has been chosen so to avoid sampling issues, which could be introduced by changing availability of instruments (changing the mix of sampling patterns) or trends in the constituents (like the strong negative trend caused by ozone depletion from the 1970s to the mid 1990s).

4.4.1.2.1 Ozone

Figure 4.6 shows the multi-annual zonal mean ozone for each reanalysis along with the SPARC Data Initiative MIM. The reanalyses all capture the general distribution of ozone well. They all have a global maximum in ozone volume mixing ratio in the tropical middle stratosphere, and their ozone isopleths follow the tropopause latitudinal structure in the first few kilometers above the tropopause. As seen in this figure, the overall structure in the absolute values is best reproduced by MERRA-2. Somewhat higher values in the maximum (>10 ppmv) than seen in the observations are produced by CFSR, JRA-25, and MERRA.

Figure 4.7 shows the relative differences between each reanalysis (R_i) and the MIM ((R_i-MIM)/MIM*100) in order to more clearly show subtle differences in the ozone distribution among the different reanalyses. The agreement is best for MERRA-2, with values well within ±5% throughout the middle and upper stratosphere, followed by MERRA and CFSR. ERA-Interim shows relatively good agreement as well with biases smaller than ±5% in the middle stratosphere, however increasing differences to the MIM in the upper stratosphere (with a low bias >10%). All reanalyses show larger biases than ±10% in the lowermost stratosphere (below 100 hPa). JRA-55 shows large improvements over JRA-25, with the latter exhibiting a strong positive bias (greater than 20% from the MIM) throughout the lower and middle stratosphere, and a strong negative bias (>20%) in the upper stratosphere. JRA-55 still shows a negative bias (greater than 10%) in the upper stratosphere, but is a clear improvement over JRA-25. It is worth noting that the diurnal cycle in ozone has not explicitly been accounted for in the observational MIM, potentially contributing to the differences seen between the reanalyses and the observations in the upper stratosphere and lower mesosphere.

All reanalyses (except JRA-55) indicate a positive bias in the Southern hemisphere lower stratosphere, which may be attributable to their inability to simulate Antarctic ozone depletion accurately due to data filtering and its impact at high latitudes, as discussed in *Section 4.4.1.1*. CSFR and ERA-Interim reanalyses exhibit a dipole feature in the biases (with a high bias at around 100 hPa located below a low bias located around 10 hPa), which may be a reflection of the assimilated total column and SBUV observations not carrying the vertical information of the ozone hole vertical location. A notable feature in the MERRA differences is the high bias of larger than 10% at Southern high latitudes that extends throughout the stratosphere.

4.4.1.2.2 Water vapour

Figures 4.8 and 4.9 show the multi-annual zonal mean comparison of water vapour and the relative differences between each reanalysis and the MIM ((R_i-MIM)/MIM*100), respectively. In contrast to ozone, the reanalyses do not consistently capture the distribution of water vapour. Only ERA-Interim, MERRA, and MERRA-2 show a water vapour field that is close to the observations. They resolve the distinct minimum in water vapour mixing ratios just above the tropical tropopause, another minimum in the Southern hemisphere lower stratosphere at high latitudes, and increasing values towards higher altitudes. MERRA and MERRA-2, which have water vapour distributions extending up to the lower mesosphere, exhibit the typical maximum in the upper stratosphere (e.g., Hegglin et al., 2013), however somewhat underestimate the mixing ratios that are larger than 7 ppmv in the observations. It should be noted that much of MERRA and MERRA-2 behaviour is likely a reflection of the climatology and 3-day relaxation they use.

CFSR is much too dry throughout the stratosphere and does not capture the typical isopleth structure of this trace gas. This is due to the fact that CFSR is not assimilating water vapour nor having a methane oxidation parameterization in the model in the stratosphere (see Sect. 4.2.2). JRA-25 and JRA-55 both do not have stratospheric water vapour fields. All reanalysis are biased high compared to the observations at pressures above 100 hPa (see also Jiang et al., 2015), although it has to be noted that the measurement uncertainty of limb-satellite sounders increases in this altitude region, providing an observational reference that is not well defined (Hegglin et al., 2013). Several studies in particular have shown that Aura MLS is dry biased around 200 hPa (Hegglin et al., 2013; Davis et al., 2016; Vömel et al., 2007).

4.4.1.3 SEASONAL MEAN VERTICAL PROFILES

4.4.1.3.1 Ozone

Figure 4.10 shows vertical profiles of ozone for January and July (2005-2010 average) at three different latitudes (10°N, 40°N, and 80°S) for the reanalyses and the SPARC Data Initiative MIM. In addition, the relative differences of the reanalyses to the MIM are shown. These vertical profiles reveal coarse seasonal information to expand on the annual zonal mean evaluations presented in Sect. 4.4.1.2. In general, the monthly vertical profile plots reinforce the behaviour seen in the previous section.

For ozone, the vertical profiles highlight that most reanalyses resolve the vertical distribution reasonably well, although the agreement varies somewhat with month. MERRA-2, MERRA, and CSFR show the best agreement with observations through most of the middle stratosphere, except for MERRA in July in the Southern polar region where it shows too large values. A clear outlier for ozone is JRA-25, which generally places the ozone maximum too low and has too little ozone above the maximum. JRA-55 and ERA-Interim also underestimate the ozone values in the upper stratosphere by between 10 and 20%, but they are not as strongly biased as JRA-25 (with differences of >20%). All reanalyses show larger differences from the MIM at altitudes below 100 hPa.

4.4.1.3.2 Water vapour

For water vapour, the evaluation shown in Figure 4.11 reveals good agreement between ERA-Interim and the observations above 100 hPa at all latitudes, and for MERRA and MERRA-2 particularly at 10°N and 40°N. CSFR does not exhibit a realistic water vapour distribution with values much too low in comparison with the observations. Again, all reanalyses show strongly increasing relative differences for altitudes below 100 hPa. This discrepancy may be partially due to problems with the water vapour observations at these altitudes (Hegglin et al., 2013), but may also indicate a too moist tropical upper troposphere and/or too much mixing of these air masses into the extratropical lowermost stratosphere. This issue will have to be investigated in more detail and using other observational references in Chapters 7 (exUTLS) and 8 (TTL) of the SRIP report.

4.4.1.4 SEASONAL CYCLE

Figures 4.12 and 4.13 show seasonal cycles of ozone and water vapour at different pressure levels and hence allow for the exploration of the monthly evolution of the trace gases in the reanalyses in more detail. We focus here on the Southern high-latitudes (60°S-80°S), the tropics (20°S-20°N), and the Northern mid-latitudes (40°N-60°N). These comparisons are made over the 2005-2010 time period using the SPARC Data Initiative MIM, as it is the time during which a number of independent satellite estimates are available. As such, ERA-40 is not included in the analysis because it ends in 2002.

4.4.1.4.1 Ozone

The best agreement in the ozone seasonal cycle between the SPARC Data Initiative observations and the reanalyses is obtained in the Northern hemisphere midlatitudes, where the seasonal cycles have a simple sinusoidal structure (Figure 4.12). At altitudes below 50 hPa, a maximum is prevalent during spring and a minimum during autumn. At 10 hPa, the seasonal cycle is shifted, with a maximum in summer and a minimum in winter. At 1 hPa, the seasonal cycle is opposite to that at 10 hPa, with a maximum in winter and a minimum in summer. Most of the reanalyses show a fairly accurate evolution of ozone at all these levels, except for JRA-25. This reanalysis exhibits too low values at 1 hPa, and a seasonal cycle with a bi-modal structure more similar to the tropics at 10 hPa. All reanalyses underestimate absolute values of ozone and also show somewhat too small seasonal cycle amplitudes at 250 hPa. The seasonal cycle for JRA-55 at 50 hPa shows a somewhat too slow decay of ozone values towards the autumn when compared to both the observational MIM and the other reanalyses.

In the tropics, the seasonal cycles of ozone are also fairly well reproduced by the reanalyses. However, exceptions at 250 hPa are JRA-55 and ERA-Interim which do not resolve the right structure of the seasonal cycle and are biased high. At this level, there is a documented problem with the assimilation of Aura MLS ozone data in ERA-Interim. When MLS v2.2 data are assimilated the analysis departures from sondes are as large as 20% at high latitudes, and up to 40% in the tropics (Lefever et al., 2015). At 50 hPa, JRA-25 and JRA-55 are biased high, although they both capture the structure of the seasonality correctly. At 10 hPa, JRA-55 is biased low, but has a realistic seasonal cycle. At 1 hPa, JRA-25 is biased low and has essentially no seasonal cycle variability.

In the Southern Hemisphere high latitudes, the seasonal cycles have a more complex structure due to the influence of the severe Antarctic ozone depletion and a different influence from the Brewer-Dobson circulation (which is weaker in the Southern than in the Northern Hemisphere). At 1 hPa, the reanalyses show good agreement with the MIM, except for ERA-Interim and JRA-25, which both exhibit too low absolute values. At 10 hPa, MERRA and JRA-25 are outliers, as they do not contain the strong minimum in the cycle found towards the late autumn and early winter months. At 50 hPa and 100 hPa, MERRA and JRA-25 compare better, but still underestimate the dip in the ozone cycle that appears at these levels in spring. At 250 hPa, all reanalyses underestimate the absolute values, however, with MERRA exhibiting the best agreement with the amplitude in the seasonal cycle. It is notable that MERRA-2 exhibits the closest agreement with the observations at all levels except for 250 hPa. This is expected because in this period MERRA-2 assimilates v2.2 MLS which doesn't extend that far down.

4.4.1.4.2 Water vapour

Figure 4.13 shows seasonal cycles of water vapour. More generally, water vapour exhibits much less pronounced seasonal cycles in the stratosphere than ozone. Note CFSR shows wrong amplitudes and phases of the seasonal cycle in water vapour at all levels from 100 hPa upwards. However, it is practically identical to ERA-Interim at 250 hPa, both with values around 100% higher than those shown by the observations. This result is similar that of Jiang et al. (2015), who found that reanalyses in general showed substantially more WV than Aura MLS observations.

The 100 hPa level is one of the most important levels for stratospheric water vapour studies, as it is near the level where the entry value of water vapour is set in the tropics, and is near the peak of the radiative forcing kernel for water vapour in the extratropics. At this level, ERA-Interim is the best performing reanalysis in terms of amplitude and phase of the seasonal cycle in the extratropics of the Northern and Southern hemisphere. In the tropics, ERA-Interim, MERRA, MERRA-2, and JRA-55 all exhibit seasonal cycles close to that of the SPARC Data Initiative MIM. JRA-25 and CSFR (as mentioned above) are underestimating the absolute values and also the amplitude of the seasonal cycle, and JRA-55 has extremely large values in the extratropics.

In the Southern hemisphere high latitudes, MERRA and MERRA-2 perform best in comparison with the observation at 1 hPa, although a slight low bias as mentioned in Sect. 4.4.1.2.2. At 50 and 100 hPa, ERA-Interim shows the best agreement with the phase and also amplitude of the seasonal cycle in the observations, although its mean values are somewhat lower showing better agreement with MERRA and MERRA-2.

In the tropics and also the Northern hemisphere mid-latitudes, MERRA and MERRA-2 generally perform slightly better than ERA-Interim in terms of phase and amplitude in the middle and upper stratosphere (levels between 50 and 1 hPa). At 250 hPa in turn, JRA-25 and JRA-55 are closer to the observational values than the other reanalyses for the tropics.

4.4.2 INTERANNUAL VARIABILITY

In this section, we use interannual variability to test the physical consistency of each reanalysis' ozone and water vapour timeseries. Absolute values and anomalies are shown. Anomalies are calculated for each reanalysis by subtracting the multiyear monthly mean from ist monthly mean values. The anomalies are a good indicator for how well physical processes (e.g., transport, dehydration, etc) in reanalyses are represented.

4.4.2.1 Ozone

Figure 4.14 shows the interannual variability of ozone at different pressure levels and latitude bands (Southern high latitudes at 50 hPa, tropics at 10 hPa, and Northern mid-latitudes at 100 hPa). At all levels, MERRA-2 is the best performing reanalysis in terms of both absolute values and the structure in its interannual variability when compared with the SPARC Data Initiative observations, highlighting the benefit of the assimilation of vertical limb observations. MERRA-2 exhibits clear improvements over MERRA, which tends to underestimate interannual variability at 100 hPa in the Northern mid-latitudes and at 10 hPa in the tropics.

JRA-55 also shows a clear improvement over JRA-25 at all levels, at least in terms of the amplitude and structure of interannual variability.

ERA-Interim, while generally agreeing with the observations on the mean ozone values, shows too large amplitudes in the interannual variability. In particular, it overestimates the positive anomalies after 2007 in the Northern mid-latitudes at 100 hPa, and also at Southern hemisphere high latitudes at 50 hPa. Finally, CSFR is possibly the worst performing reanalysis in terms of reproducing the right interannual variability in the different regions of the atmosphere.

4.4.2.2 Water vapour

Figure 4.15 shows the interannual variability of water vapour at different pressure levels and latitude bands (Southern high latitudes and tropics at 100 hPa, and Northern mid-latitudes at 250 hPa) in comparison with SPARC Data Initiative mean observations.

In the tropics at 100 hPa, the level that is often referred to for testing stratospheric water vapour entry values against observations, all but one reanalyses follow the water vapour anomalies surprisingly well despite mostly underestimating its amplitude (by around ±0.3 ppmv), which is also reflected in the reanalyses underestimating the mean values (by around 1 ppmv). An exception to this is CSFR, which does not show any clear interannual variability and which has water vapour values that go down to 0 ppmv. Only in 2009, CSFR seems to obtain some information on water vapour at these levels, increasing its values to above those of other reanalysis and hence greatly improving its performance.

In the Southern hemisphere high-latitudes, interannual variability is very weak. The best performing reanalysis here is ERA-Interim, which resolves a weak two-year oscillation. MERRA and MERRA-2 also perform relatively well. Both JRA-25 and JRA-55 show rather erratic behaviour when compared to the observations, and CSFR shows some irregularities in the evolution of the water vapour.

In the Northern hemisphere mid-latitudes, interannual variability in the observations is also weak, but shows a pronounced spike after 2009. The reanalyses all follow the ups and downs extremely well, even CFSR, which at this level is constraint by observations (see Sect. 4.2.2).

4.4.3 OZONE TIMESERIES IN EQUIVALENT-LATITUDE

Equivalent latitude is commonly used as a vortex-centred coordinate in stratospheric studies (e.g., Butchart and Remsberg, 1986 and references therein; Manney et al., 1999), and is also useful (though interpretation becomes more complicated, e.g., Manney et al., 2011; Pan et al., 2012) as a geophysically-based coordinate in the UTLS (e.g., Hegglin et al., 2006; Santee et al., 2011). Equivalent latitude is defined as the latitude that would encompass the same area between it and the pole as a given potential vorticity (PV) contour. The figures below compare time series of v4 MLS ozone (Section 4.3.2.3) for late 2004 through 2013 with the MERRA, MERRA-2, ERA-Interim, CFSR, and JRA-55 reanalyses, in the middle (Figure 4.16) and lower (Figure 4.17) stratosphere and the UTLS (Figure 4.18). Aura MLS ozone is interpolated to isentropic surfaces using temperatures from MERRA; EqL/time series are then produced using a weighted average of MLS data in EqL and time, with data additionally weighted by measurement precision (e.g., Manney et al., 2007; Manney et al., 1999).

At the stratospheric levels (Figure 4.16, 4.17) MERRA-2 matches MLS more closely over the full period than do the other reanalyses. This is expected since MERRA-2 assimilates MLS stratospheric ozone profiles (v2 for the period shown here) and OMI column ozone beginning in October 2004 (in fact, at 850K, a suggestion of poorer agreement can be seen in September 2004). ERA-Interim also shows very close agreement with MLS at stratospheric levels in the period (2008, and mid-2009 through present) when it assimilates v2 MLS ozone.

The biases seen in the reanalyses that do not assimilate MLS and OMI ozone vary in magnitude and sign, not only between the reanalyses, but also with altitude and latitude. MERRA shows an overall high bias at 850K (Figure 4.16), with largest biases in the Antarctic winter. ERA-Interim and CFSR show small low biases with respect to MLS at 850K in the tropics, whereas JRA-55 shows a large low bias in this region. JRA-55 biases increase strongly with altitude, becoming even larger in the upper stratosphere (not shown), suggesting that column ozone alone is not sufficient to constrain the CTM used in the offline calculation close to observations. Each of the reanalyses except MERRA-2 shows a quasi-biennial pattern in the tropical differences from MLS, indicating deficiencies in the model/DAS representation of the QBO (see Chapter 9) that are much improved in MERRA-2.

At 520K (Figure 4.17), MERRA-2 and ERA-Interim agree very closely with MLS during the period when MLS data are assimilated. This is especially apparent in the Antarctic winter and spring, where other assimilated ozone products (e.g., SBUV2, TOMS) do not provide measurements in darkness, where simplified chemical parameterizations do not adequately represent heterogeneous loss processes, and where the improved vertical resolution of MLS (compared to SBUV2) more adequately constrains the vertically-limited structure of the ozone hole. High biases in the Arctic winter in MERRA and CFSR may also be partially related to inadequate representation of ozone chemistry and lack of measurements, though the predominant importance of the latter is suggested by their appearance even in years with minimal chemical ozone loss.

In the UTLS (e.g., 350K, Figure 4.18), significant biases are present in all reanalyses in middle and high latitudes (poleward of the tropopause, thus in the lowermost stratosphere), but are relatively small. MERRA-2 biases are slightly smaller than those in the other reanalyses, and the biases in ERA-Interim change character noticeably at the beginning of 2008 when MLS and OMI ozone are first assimilated. Seasonally varying biases just poleward of the tropopause are pervasive in the reanalyses, suggesting variations in the ability of the DAS to capture quasi-isentropic stratosphere-troposphere exchange (STE) processes; such STE processes will be explored further in Chapter 7.

4.4.4 OZONE QBO SIGNAL

The Quasi-Biennial Oscillation (QBO) of the tropical zonal wind is one of the dominant influences on the interannual variability of equatorial ozone through variations in transport and chemistry. The QBO signal in tropical ozone has a double peaked structure with maxima in the lower (50-20 hPa) and middle/upper (10-2 hPa) stratosphere (Hasebe, 1994; Zawodny and Mccormick, 1991). Below 15 hPa, ozone is mainly under dynamical control and the QBO signal results from the transport of ozone by the QBO-induced residual circulation. Above 15 hPa, ozone is under photochemical control and the QBO signal is understood to arise from QBO-induced temperature variations (Ling and London, 1986; Zawodny and Mccormick, 1991) together with QBO-induced variability in the transport of NO_y (Chipperfield et al., 1994). A realistic characterization of the altitude-time QBO structure is an important aspect of the physical consistency of ozone data sets.

Figure 4.19 shows altitude-time sections of deseasonalized ozone anomalies from 2005 to 2010 from the SPARC Data Initiative satellite observations and from the reanalysis data sets. The combined ozone measurements from the limb-viewing satellite instruments display a downward propagating QBO ozone signal with a shift in the phase around 15 hPa. All of the reanalyses exhibit some degree of quasi-biennial variability, however differences exist regarding the phase, amplitude, vertical extent and downward propagation of the signal.

The largest deviations between the observations and reanalyses are found for JRA-25, which displays no QBO signal above 15 hPa but instead positive anomalies from 2005 to mid-2007 followed by negative anomalies after this time period. In contrast, ERA-interim shows predominantly negative anomalies in the 100 – 10 hPa range during the pre-2008 time period, followed by negative anomalies afterwards.

CFSR and MERRA show anomalies roughly consistent in amplitude and frequency with the QBO ozone signal in the satellite data. However, there is no clear downward propagation of the signal similar to what has been noted for SBUV data (McLinden et al., 2009), the only vertically resolved ozone measurements assimilated into CFSR and MERRA. In addition, the vertical structure of the anomalies is somewhat shifted, so that instead of two peaks in the lower (50-20 hPa) and middle/upper (10-2 hPa) stratosphere, only one peak around 15 hPa is detectable.

JRA-55 and MERRA-2 show the best agreement with the satellite data with a very similar phase and amplitude. JRA-55 exhibits a realistic downward propagation of the QBO signal with time, while for MERRA-2 the downward propagation is less distinct. Overall, the QBO features in MERRA-2 (including the downward propagation) are much improved in comparison to MERRA (Coy et al., 2016). Nearly all reanalysis data sets extend the QBO ozone signal below 100 hPa, which is not present in the satellite observations.

Figure 4.20 shows the differences between each reanalysis' ozone anomalies and the observational ozone anomalies for the time period 2005-2010. Additionally, each panel displays the contour lines of the reanalysis anomalies itself. The largest differences are seen for JRA-25 in the upper stratosphere and ERA-Interim in the lower stratosphere. The smallest differences to the observations are found for MERRA-2 and JRA-55. For CFSR and MERRA, differences are in the middle range and show similar structures as the QBO anomalies itself, being smaller than the observations (red shading) in case of positive anomalies and larger (blue shading) otherwise.

4.4.5 OZONE HOLE AREA

The Antarctic "ozone hole" is a region of severe ozone depletion that starts in late August to early September and which lasts until November to early December. The ozone hole is usually defined to be the area within the 220-DU contour of TCO. The average ozone hole area of six reanalyses and the TOMS/OMI observations over the 21 September – 20 October period are shown in Figure 4.21. This period is chosen to avoid the partial coverage of the TOMS/OMI data that occurs during the early part of September. For almost all years through 2002 the observations are larger than the reanalyses. This is consistent with the reanalyses generally underestimating the amount of ozone loss, resulting in a smaller area. Starting in 2003, most of the models track the observations fairly well. It should be stressed that this is not a truly independent comparison because all reanalyses except for MERRA assimilate the TOMS and/or OMI observations. However, this comparison does show the general consistency of most of the reanalyses in reproducing realistic interannual to decadal scale changes in the size of the Antarctic ozone hole.

Table 4.3 shows the mean differences and standard deviations of the reanalysis areas from TOMS/OMI. The newer reanalyses (MERRA-2, ERA-Interim, JRA-55, and NCEP-CSFR) are all within 1 million km^2 (5.2%) of the observations. These reanalyses have root-mean-square (RMS) differences from TOMS/OMI within 0.9 million km^2 (14.6%), except for MERRA-2 that shows a RMS of 2.8 million km^2 (44.5%). Overall, JRA-55 has the smallest RMS difference from TOMS/OMI, while the MERRA-2 model has the smallest mean difference from the observations.

There are a few notable outlier points in Fig 4.21 that warrant further explanation. MERRA-2 had no ozone hole in 1994, and MERRA had no ozone hole in 1993, 1994, and 2010. MERRA also had a noticeably reduced ozone hole area for 1997 and 2009. Overall, the lack of ozone hole during these years was caused by insufficient ozone observations constraining the ozone field, as ozone holes are not represented in the parameterized chemistry used in MERRA and MERRA-2. More specifically, in 1994, orbital drift of the NOAA-11 satellite (that provided the SBUV/2 TCO data assimilated by both MERRA and MERRA-2) meant that data were not taken south of ~30°S during Austral spring. Similarly, data were not taken south of ~40°S in 1993. In 1997, the MERRA ozone hole was only weakly constrained in late September because the NOAA-11 data did not extend as far south (~ 60 – 65°S). In contrast, the NOAA-14 data used by MERRA-2 extended farther south, which explains why MERRA-2 does not have the bias in the ozone hole size that MERRA does.

In 2009 and afterwards, the MERRA ozone hole was affected by orbital drift of the NOAA-17 satellite and the concomitant loss of SBUV/2 observations at high southern latitudes during Austral spring. MERRA-2 is unaffected during this time period because it assimilates Aura OMI ozone observations.

ERA-40 did not assimilate ozone data in 1989 and 1990, resulting in high ozone values, and so the hole is very small. The ERA-40 model also severely underestimates the area in 1997, most likely due to the gap in assimilated TCO data from Earthprobe TOMS data between August and December that year (NOAA-9 SBUV/2 layer data were still assimilated during this timeframe). In contrast, the ERA-Interim ozone hole area is too large in 1995. This is likely due to a lack of assimilated TCO observations in ERA-Interim during 1995, the only year for which TCO data are not assimilated by ERA-interim (see Fig 4.1).

4.4.6 LONGTERM EVOLUTION

4.4.6.1 TOTAL COLUMN OZONE TIMESERIES

In this section, we consider the time evolution of the total column ozone field in reanalyses, in comparison to several satellite data sets, including the TOMS/OMI and SBUV(2) data sets that are used as input by all of the reanalyses. Figure 4.22 shows the deseasonalized total column ozone anomaly evolution in reanalyses and two TCO data sets. There are several features of these plots that are worth noting. First, a general trend towards decreasing ozone in the high southern latitudes can be seen in all of the data sets, reflecting the Antarctic ozone hole depletion discussed in the previous section. Also, in some cases, the unique features in a given TCO data set can be seen in the reanalysis that assimilate that given data set. For example, the SBUV dataset has pronounced QBO-related anomalies in the tropics (particularly after ~1998) that are present in the reanalyses that assimilate this data set (i.e., CFSR, MERRA, and MERRA-2).

A more detailed look at the differences between the reanalyses and TCO data sets is given by Figures 4.23 and 4.24, which shows the time evolution of the differences between the reanalyses and the observations. The upper left panel of Fig. 4.23 shows the difference between the TOMS/OMI and SBUV data sets, and illustrates an apparent step change in their difference at the beginning of 2004. Because of this step change and the associated differences between the two data sets, comparisons are shown separately for each data set in Figure 4.23 (SBUV) and Figures 4.24 (TOMS/OMI). Generally, the comparison between the reanalyses and the TCO data they assimilate is better than with the data set they don’t assimilate. For example, MERRA, MERRA-2, and CFSR assimilate SBUV data. Their differences to SBUV in Figure 4.23 are in general smaller in magnitude and more homogeneous in space and time than their differences to the TOMS data in Figure 4.24. In some cases, particularly for MERRA and CFSR, the discontinuity in 2004 between TOMS/OMI and SBUV is very clear in Figure 4.24, whereas no such difference is seen with SBUV in Figure 4.23.

Similarly, the differences between TOMS/OMI and the ECMWF reanalyses are more homogeneous and generally smaller in magnitude than the differences from SBUV. Also, the period when no ozone data were assimilated by ERA-40 in 1989 and 1990 can easily be seen in both figures, and gives some sense of the importance of the assimilated TCO data in constraining the ozone field in the reanalysis.

4.4.6.2 OZONE TIMESERIES AT SELECT LEVELS

Figures 4.25 and 4.26 show the differences in the timeseries between reanalyses and the SWOOSH satellite limb profiler merged ozone data set at two different pressure levels (10 and 70 hPa). In addition to reinforcing the points made earlier in the chapter, this plot allows for the testing of the homogeneity of the ozone fields in the reanalyses that could be caused by changing observational data sets that are assimilated. The SWOOSH record is based primarily on v4.2 Aura MLS ozone starting in August 2004, so it must be stressed that the comparison with reanalyses after that time is not truly independent. However, before that time, SWOOSH does not contain any data that are assimilated by the reanalyses.

At 10 hPa, there are no large and obvious jumps in the reanalyses for the most part. CSFR, MERRA, and MERRA2 show smallest differences relative to the observations. ERA-Interim and JRA-25 show a positive bias at Southern and Northern hemisphere mid-latitudes, while JRA-55 indicates a negative bias in its ozone across the tropics. A clear signature is seen at Southern high latitudes after the Mt Pinatubo eruption, when all reanalyses show too high ozone values compared to observations.

The homogeneity however is somewhat disrupted in MERRA-2 and ERA-Interim, when they start assimilating Aura-MLS ozone; after MLS comes online in 2004 the differences with MERRA-2 are less than 5%, but increase for ERA-Interim. The difference in behaviour may be partially explained by ERA-Interim having assimilated an older version of the MLS ozone dataset (v2.2 versus v4).

At 70 hPa, the differences between the ozone in the reanalyses and SWOOSH are becoming larger. A strong inhomogeneity in the timeseries is particularly seen after 2004, after Aura-MLS comes online, with most of the reanalyses (except CSFR and MERRA) exhibiting large positive biases when compared to the observations. Before 2004, the reanalyses differences to the observations are relatively smooth, mostly negative for CSFR, MERRA, and MERRA-2, patchy for ERA-Interim, and mostly positive for JRA-25 and JRA-55 (especially in the tropics).

4.5 SUMMARY

In this chapter the basic treatment of ozone and water vapour in reanalyses has been described, and comparisons between reanalyses and both independent and assimilated observations have been presented. Here we briefly summarize some of the key characteristics and differences of the treatment of ozone and water vapour in reanalyses that are provided in this chapter. We then summarize some of the key findings of this chapter.

While in principle the treatment of these two species by reanalyses could be quite similar, in practice most reanalyses treat these two species quite differently from one another, and their treatment varies greatly among the different reanalyses. As an example for ozone, some reanalyses don’t treat it prognostically (i.e., R1, R2), whereas others specify it as a boundary condition from an offline model (i.e., JRA-25, JRA-55), whereas others treat it as a prognostic variable with parameterized photochemical production/loss (e.g., CFSR, MERRA, ERA-Interim). As documented here, the different reanalyses also vary in the ozone observations they assimilate, with generally similar usage of observations within a given reanalysis centre, and a trend towards utilizing the newest generation of vertically resolved ozone measurements that have become available (e.g., by Aura MLS) in the last decade.

Reanalyses all assimilate humidity information in the troposphere from some combination of radiosondes and satellite radiances or retrievals of quantities such as precipitable water vapour. In the stratosphere, none of the reanalyses assimilate water vapour observations. Beyond these similarities, the treatment of water vapour in the stratosphere varies greatly among the reanalyses. For example, the specific cut-off altitude for assimilation of radiosonde varies; for some reanalyses it is a fixed pressure level and others it is the diagnosed tropopause. In some reanalysis stratospheric WV is affected by processes such as dehydration, transport, and methane oxidation, but other reanalyses either relax to a climatology (i.e., MERRA, MERRA-2) or simply contain invalid data in the stratosphere (e.g., JMA reanalyses, R1, R2). Because of the lack of assimilated data and poor representation of WV in the stratosphere, reanalysis stratospheric WV fields should not be used in scientific studies. In a number of the reanalyses a climatology or a constant value for stratospheric water vapour is used as input to the radiative transfer code in the forecast model rather than the analysed value.

Given the differences in treatment of these species amongst the different reanalyses, it is perhaps unsurprising that the comparisons between reanalyses and observations can vary quite widely. Overall, comparisons to assimilated observations show that total column ozone is mostly well re-produced by reanalyses, but there are limitations even in this field because of the lack of TCO data during polar night. The vertical distribution is weakly constrained because of the lack of assimilation of vertically resolved data, but is somewhat constrained by the ozone parameterizations used. In the overworld stratosphere, this leads to differences of ~10-50% between the reanalyses and (mostly) independent observations (at least for water vapour) from the SPARC Data Initiative. Some reanalyses do better than others, with MERRA and MERRA-2 in particular showing good agreement through much of the stratosphere. Reanalysis parameterizations of ozone have no representation of heterogeneous chemistry. This fact, combined with the lack of assimilated observations in polar night, make the use of reanalysis ozone for Antarctic ozone hole studies fraught. When observations are available, the reanalyses produce reasonable ozone holes, but often the exact timing is delayed due to a lack of observations.

Given the lack of assimilation of stratospheric water vapour data by reanalyses, for water vapour there are large differences in the agreement between reanalyses and independent observations. In particular, CFSR has an extreme dry bias, with very low values produced. On the other hand, JRA-55 has an extremely wet lower stratosphere. MERRA and MERRA-2 have reasonable values for stratospheric water vapour, but their values are a relaxation to a climatology for MLS, so the field does not represent the control of water vapour by physical processes such as dehydration and transport through the TTL. ERA-40 and ERA-I have true "prognostic" water vapour in the stratosphere, and ERA-I has surprisingly reasonable values given that its field is predominately controlled by TTL dehydration and a very crude methane oxidation parameterization.

APPENDIX A: LIST OF ACRONYMS

1D-Var: 1-dimensional variational data assimilation scheme
MIM Multi-Instrument Mean
20CR: 20th Century Reanalysis of NOAA and CIRES
AIRS: Atmospheric Infrared Sounder
Aqua: a satellite in the EOS A-Train satellite constellation
ATMS: Advanced Technology Microwave Sounder
ATOVS: Advanced TIROS Operational Vertical Sounder
Aura: a satellite in the EOS A-Train satellite constellation
CFC: chlorofluorocarbon
CFSR: Climate Forecast System Reanalysis of NCEP
CFSv2: Climate Forecast System, version 2
CHEM2D: The NRL 2-Dimensional photochemical model
CHEM2D-OPP: CHEM2D Ozone Photochemistry Parameterization
CIRES: Cooperative Institute for Research in Environmental Sciences (NOAA and University of Colorado Boulder)
CrIS: Cross-track Infrared Sounder
ECMWF: European Centre for Medium-Range Weather Forecasts
EOS: NASA's Earth Observing System
ERA-15: ECMWF 15-year reanalysis
ERA-20C: ECMWF 20th century reanalysis
ERA-40: ECMWF 40-year reanalysis
ERA5: A forthcoming reanalysis developed by ECMWF
ERA-Interim: ECMWF interim reanalysis
GFS: Global Forecast System of the NCEP
GNNS-RO: Global Navigation Satellite System Radio Occultation (see also GPS-RO)
GPS-RO: Global Positioning System Radio Occultation (see also GNSS-RO)
HIRS: High-resolution Infrared Radiation Sounder

IASI: Infrared Atmospheric Sounding Interferometer
IFS: Integrated Forecast System of the ECMWF
IR: Infrared
JCDAS: JMA Climate Data Assimilation System
JMA: Japan Meteorological Agency
JRA-25: Japanese 25-year Reanalysis
JRA-55: Japanese 55-year Reanalysis
JRA-55AMIP: Japanese 55-year Reanalysis based on AMIP-type simulations
JRA-55C: Japanese 55-year Reanalysis assimilating Conventional observations only
MERRA: Modern Era Retrospective-Analysis for Research
MIPAS: Michelson Interferometer for Passive Atmospheric Sounding
MLS: Microwave Limb Sounder
MRI-CCM1: Meteorological Research Institute (JMA) Chemistry Climate Model, version 1
MSU: Microwave Sounding Unit
MW: Microwave
NASA: National Aeronautics and Space Administration
NCAR: National Center for Atmospheric Research
NCEP: National Centers for Environmental Prediction of the NOAA
NMC: National Meteorological Center (now NCEP)
NOAA: National Oceanic and Atmospheric Administration
NRL: Naval Research Laboratory
ODS: Ozone Depleting Substance
OMI: Ozone Monitoring Instrument
QBO: quasi-biennial oscillation
R1: NCEP-NCAR Reanalysis 1
R2: NCEP-DOE Reanalysis 2
RH: Relative Humidity
RTTOV: Radiative Transfer for TOVS
SEVIRI: Spinning Enhanced Visible and InfraRed Imager
SBUV & SBUV/2: Solar Backscatter Ultraviolet Radiometer
SCIAMACHY: Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SPARC: Stratosphere-troposphere Processes And their Role in Climate
S-RIP: SPARC Reanalysis Intercomparison Project
SSM/I or SSMI: Special Sensor Microwave Imager
SSU: Stratospheric Sounding Unit
TCWV: Total Column Water Vapor
TCO: Total Column Ozone
TIROS: Television Infrared Observation Satellite
TMI: Tropical Rainfall Measuring Mission (TRMM) Microwave Imager
TOA: top of atmosphere
TOMS: Total Ozone Mapping Spectrometer
TOVS: TIROS Operational Vertical Sounder
TTL: Tropical tropopause layer
UV: Ultraviolet
VTPR: Vertical Temperature Profile Radiometer
WV: Water Vapor

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