Overview of approaches for data merging

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CONTENTS

1 Introduction

This overview discusses different approaches to data merging from different measurement sources. In general, merging is applied when the data from one source do not have sufficient coverage (in space or/and in time). Depending on application, different approaches have been used. This overview paper summarizes these approaches applied to experimental data, which are grouped into sections according to merging type. The data assimilation as a merging approach is not considered in this paper.

2 Merging in altitude

Combination of measurements from different sources covering different altitude regions is often used when coverage of a large vertical range is desired. Such combination, which we refer to in this overview to as merging in altitude, differs from traditional averaging of profiles. In the traditional averaging – computing mean, weighted mean or median – the profiles are assumed to represent the same statistical ensemble, i.e. they are not biased with respect to each other and have the same vertical resolution. Merging in altitude discussed in this section uses each dataset in its optimal altitude range. This is a common approach in creating ozone climatologies (e.g., McPeters and Labow, 2012; McPeters et al., 2007; Sofieva et al., 2014b). Ozonesonde profiles have superior quality in the troposphere and the lower stratosphere, while satellite data have a very good quality in the stratosphere combined with uniform and global coverage - which is of high importance for creating climatologies – but have poorer quality in the upper troposphere and the lower stratosphere (UTLS). The merging method used for creating the ozone climatology from ozone soundings (in the troposphere and the UTLS) and satellite measurements (in the stratosphere) is very simple: first ozone climatologies are created separately for ozone soundings and satellite measurements, and then a linear transition from the ozone climatology at lower altitudes to the satellite climatology at upper altitudes is applied. As a result, the lower part of the profiles follows exactly the ozonesonde climatology, the upper part follows the satellite climatology, and a linear combination of ozone and satellite climatologies is used in the transition zone. For the LLM (Labow-Logan-McPeters) climatology (McPeters et al., 2007), this transition zone is z*=10-18 km pressure altitudes[1] for blending ozonesonde and SAGE II climatologies, and z*=20-28 km for blending ozonesonde and MLS/UARS data (at high latitudes in winter when SAGE II data are not available). In the newer ML climatology (McPeters and Labow, 2012), the transition from ozonesonde to MLS/Aura climatology is performed at z*=8-16 km for low and mid latitudes (40°N-40°S) and using the pressure altitude range z*=13-21 km in other latitude zones.

The merging in altitude used in the tropopause-related ozone climatology TpO3 (Sofieva et al., 2014b) is similar to that used in LLM and ML climatologies. The difference is that at altitudes where both ozonesonde and satellite data exist (from the tropopause height to 28 km), the climatologies are first merged with the weights proportional to number of measurements:

[1] Pressure altitude is defined as $z^* = 16 \cdot \log_{10}(1013/P)$, where *P* is pressure in hPa.

$$\bar{\rho} = \frac{N_{so}\bar{\rho}_{so} + N_{SA}\bar{\rho}_{SA}}{N_{so} + N_{SA}}, \qquad (1)$$

where $\bar{\rho}_{so}$ and $\bar{\rho}_{SA}$ are mean ozone profiles calculated using ozonesonde and SAGE-II data, respectively, and N_{so}, N_{SA} are the corresponding number of ozonesonde and SAGE-II measurements. The estimate $\bar{\rho}$ presents the mean over all measurements. Note that the averaging by Eq.(1) is equivalent to the weighted mean with the weights inversely proportional to the squared standard error of the mean: since many accurate measurements are averaged, uncertainty variances of $\bar{\rho}_{so}$ and $\bar{\rho}_{SA}$ are approximately $\frac{\sigma^2_{nat}}{N_{so}}$ and $\frac{\sigma^2_{nat}}{N_{SA}}$, respectively ($\sigma^2_{nat}$ is climatologic ozone variability in latitude zones). The climatological profiles in the full vertical range are constructed with the approach similar to McPeters and Labow (2012) and McPeters et al. (2007): the ozonesonde climatology is used below the tropopause, a merged climatology $\bar{\rho}$ from the tropopause to 28 km, with a smooth transition to SAGE-II data over the altitude range 20-28 km. The merging approach used for constructing TpO3 climatologic profiles is illustrated in Figure 1.

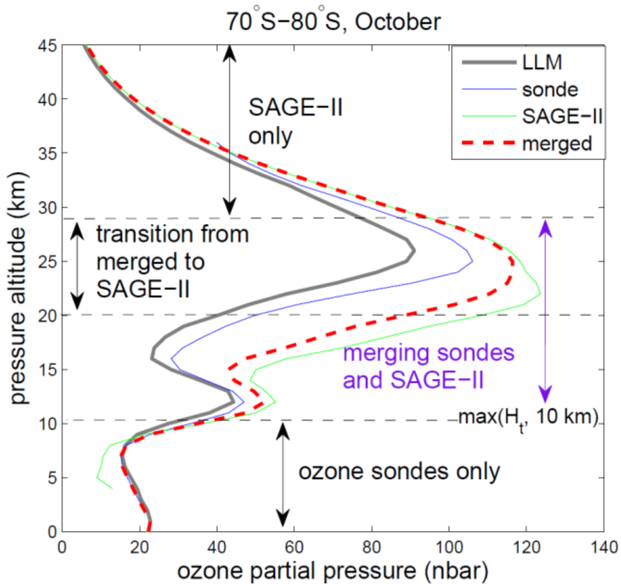

Figure 1. Illustration of climatology merging, adapted from: Illustration of merging sonde and SAGE-II data in (Sofieva et al., 2014b) **based on data in October at 70°S-80° S, for profiles with the tropopause heights 9-10 km. Altitude ranges for merging sonde and SAGE-II data and for linear transition to SAGE-II data are highlighted.**

In the retrieval algorithm from satellite measurements, often the information about air density and temperature profiles is needed. If the temperature profiles are not retrieved, they are taken from an external source. Often they are used from a meteorological model (e.g., ECMWF) and then extended, if needed, with another model (e.g., MSIS) at upper altitudes. For such blending of instantaneous profiles, the hydrostatic equation should be satisfied. For such purpose, usually an iterative procedure is applied to the temperature profiles to be merged, in order to ensure validity of the hydrostatic equation for the resulting merged atmospheric profiles.

3 Notes on ensemble estimates

When several estimates of an atmospheric parameter are available, the mean of these estimates (or a weighted mean, or the median) can be used as a reference. We will call this "ensemble estimate", in analogy with the ensemble estimates used in model simulations (e.g., Galmarini et al., 2004). The ensemble estimate can decrease a random component of the uncertainties associated with the individual measurements, provided they are non-correlated. However, it should be noted that an ensemble estimate is not necessary the estimate with the best accuracy. For example, the uncertainty of a weighted mean of the data $\bar{x} = \sum_{i=1}^{N} \alpha_i x_i$ computed with the weights inversely proportional to individual uncertainties σ_i (representing a random uncertainty component), $\alpha_i = \frac{1/\sigma_i^2}{\sum 1/\sigma_i^2}$, can be estimated as:

$$\sigma_w^2 = \frac{1}{\sum_{i=1}^{N} 1/\sigma_i^2} \cdot \frac{1}{(N-1)} \sum_{i=1}^{N} \frac{(x_i - \bar{x})^2}{\sigma_i^2}. \qquad (2)$$

The first factor in (2), $\frac{1}{\sum_{i=1}^{N} 1/\sigma_i^2} = \sigma_{wmean}^2$, is the uncertainty of the weighted mean provided the uncertainties σ_i are the only source of variations in the atmospheric parameter x. The second factor in Eq. (2) takes into account variability between x_i. This indicates that it is better to avoid averaging data with large differences, especially if an ensemble is small.

It should be noted that the comparison of data from different sources is very useful for confidence of the observed atmospheric phenomena and for assessment of the systematic uncertainty in measured atmospheric parameters.

4 Merging for trend analyses

In order to follow the evolution of middle atmosphere composition and thermal structure, long-term global measurements are needed. Ground-based and in-situ instruments have long-term data records, but they are localized in space. Satellite data provide good spatial coverage, but the duration of their data records is usually limited. Therefore, for detection of climate change on global scale, merging of data from different instruments is needed.

Merging data from different instruments is a challenging task. First, even for the same-type instruments on different platforms, mutual biases and drifts can exist due to different or/and changing sampling during instrument lifetime, in addition to instrument degradation effects (e.g., a series of SBUV(/2) and SSU/MSU/AMSU instruments). The changes in sampling pattern can affect also the resulting time series when different instruments are merged.

For trend analyses, the datasets selected for data merging should be stable (expected to be stable). The stability is usually obtained by different calibration techniques applied to Level 1 data or it is inherent by the measurement principle (e.g., solar and stellar occultation instruments).

The datasets to be merged should have an overlapping period, in order to estimate biases or make a continuous time series of the deseasonalized anomalies. The merging methods, which have been used so far, have several different approaches to

1) Making the datasets compatible (this is the main step in merging)
2) Creating the dataset in the overlapping periods
3) Uncertainty characterization

Below we describe the methods that have been applied to creating of long-term datasets: ozone, stratospheric temperature and stratospheric aerosols.

4.1 Making the datasets compatible

There are three approaches for making the datasets compatible with each other:

1) Calibration at Level 1
2) Removal of biases between the instruments (correction offsets/factors)
3) Using the deseasonalized anomalies
4) Using a chemistry-transport model as a transfer function.

4.1.1 Calibration at Level 1b

For the same instruments operated on different satellite, a careful calibration of Level 1 data can allow achieving a compatible dataset. Such approach is used in creating the datasets based on SBUV(/2) v 8.6 measurements: the Merged Ozone Dataset (MOD, Frith et al., 2014; McPeters et al., 2013) and the Merged Cohesive ozone dataset (Tummon et al., 2015).

4.1.2 Removal of biases between the instruments

In this approach, the bias between the instruments is estimated using the overlapping period. If the overlapping period is as short as a few years (as e.g. between SAGE II and Envisat ozone sensors), the bias is considered as only latitude and altitude dependent, without season/time dependence.

Two approaches have been used for the bias correction. In the first approach, the bias is estimated using collocated data, and individual profiles are shifted using an average bias profile. This approach has been applied in creating the merged SAGE II – GOMOS dataset (Kyrölä et al., 2013): GOMOS data are taken as a reference, and the offsets are applied separately to SAGE II sunset and sunrise data, which exhibit different biases with respect to GOMOS data. A similar approach is applied in the GOME-type Total Ozone dataset (GTO, Coldewey-Egbers et al., 2015): the biases of monthly mean data are estimated using common daily gridded data only in order to minimize the differences in spatial and temporal sampling. It should be noted that the biases estimated using the collocated data can differ from biases in due to sampling patterns (Sofieva et al., 2014a).

In the second approach, the biases between monthly zonal mean values are estimated. In this case, the estimated bias partially takes into account the sampling of the datasets. This approach is used in creating the GOZCARDS dataset (Froidevaux et al., 2015), merged SAGE II-OSIRIS aerosol dataset (Rieger et al., 2015)

If the overlapping period is sufficiently long, a time-dependent bias correction can be applied. For example, in creating the GTO dataset based on GOME, GOME-II and SCIAMACHY total ozone column data, monthly zonal mean correction factors have been applied (Coldewey-Egbers et al., 2015). The uncertainty associated with the bias correction is usually added to the resulting time series (see Section 4.3 for more details).

4.1.3 Merging using deseasonalized anomalies

For creating a long-term data record and for trend analysis, the merging of deseasonalized anomalies from two or more instruments is often exploited. This method is used in the IPCC report and WMO ozone assessment (e.g., IPCC, 2013; WMO, 2014), and also in numerous separate analyses in detection of climate changes in ozone (Bourassa et al., 2014; Randel and Thompson, 2011; Sioris et al., 2014), stratospheric temperature (Randel et al., 2009; Seidel et al., 2011; Thompson et al., 2012), water vapor (Jones et al., 2009). In this approach, the seasonal cycle is removed from the individual time series (usually from the time series of monthly zonal mean values). By this operation, the biases due to different sampling patterns (including the difference in local time) and instrumental additive biases are automatically removed. In ozone studies, anomalies are often presented in relative values. While assessing the trends using deseasonalized anomalies, there is no need to fit the seasonal variations with harmonic functions (the seasonal variations do not necessary allows a simple expansion into a few harmonics).

Two or more time series of deseasonalized anomalies from individual instruments can be merged into one long-term climate data record by normalizing/shifting them to a seasonal cycle by a reference instrument at some period (for example, an overlapping period). The application of the deseasonalized anomalies to the SAGE II and OSIRIS datasets is illustrated in Figure 2.

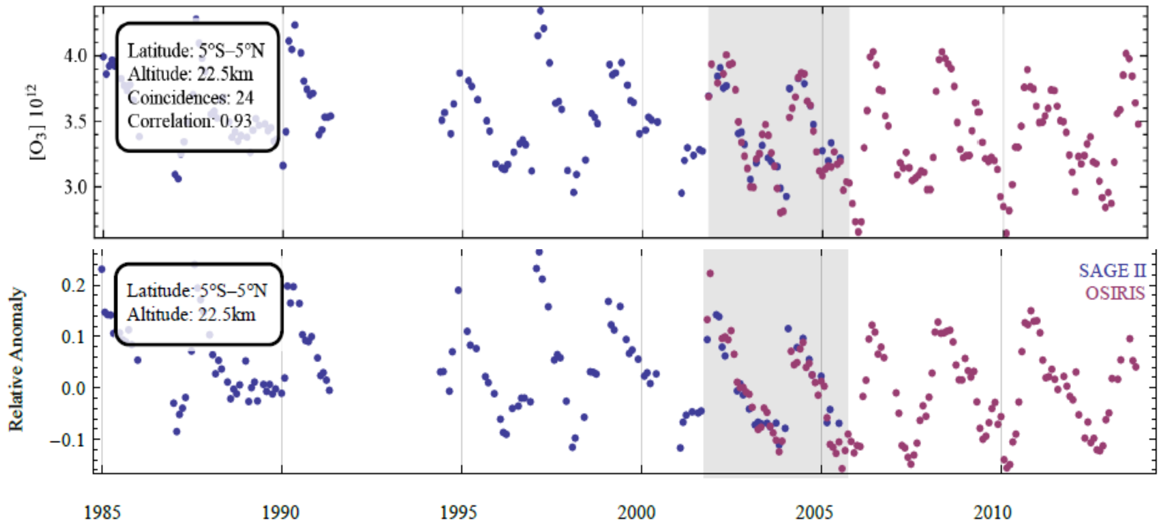

Figure 2. Adapted from (Bourassa et al., 2014)**. Top: time series of monthly average ozone number density at 22.5 km at latitudes 5°N-5°S; bottom: deseasonalized ozone anomalies for this location.**

A potential pitfall in this approach is changing sampling pattern over instrument life time. This requires a special consideration. By comparison of de-seasonalized anomalies from different instruments, like it is done in WMO ozone assessment using the de-seasonalized anomalies from the Ozone_cci limb instruments (WMO, 2014), it becomes possible to detect anomalous records from individual instruments and estimate uncertainties in the evaluated trends (Harris et al., 2015; WMO, 2014).

4.1.4 Merging using a model as a transfer function

Hegglin et al. (2014) proposed to use a chemistry-transport model nudged to the observed meteorology as a transfer function for merging the datasets from different instruments.

The authors have applied the proposed method for merging the stratospheric water vapor profiles from SAGE II, HALOE, MIPAS, ACE-FTS, SCIAMACHY and MLS/Aura. They have used the simulations with the chemistry-transport model CMAM30 nudged to the meteorological parameters (but not water vapor) from ERA-Interim reanalysis.

In this approach, relative biases and drifts to CMAM30 are calculated for each instrument avoiding the periods where the instruments and the ERA-Interim data have known problems. Using CMAM30 as a transfer function, each instrument monthly zonal mean record is then adjusted relative to Aura-MLS. The applied data merging is illustrated in Figure 3.

As noted by the authors, there is a potential pitfall in this approach in that long-term changes in the merged data set could be influenced by the long-term trend in the model. A special care should be taken in order to avoid this. In addition, models might not reproduce satisfactorily the atmospheric variability, thus introducing an additional uncertainty into a merged dataset. For the application discussed in Hegglin et al. (2014) all these aspects are discussed and taken into account.

Using a model as a transfer function might be also an approach for merging datasets that do not have overlapping periods.

4.2 Dataset in the overlapping period

After bias correction, there are two approaches for using the data in the overlapping periods

1) Using an average of individual datasets (or weighted mean) in the overlapping period

2) Using only one instrument at a time.

Both approaches have been widely used in creating the merged datasets, without a clear preference for one of these methods.

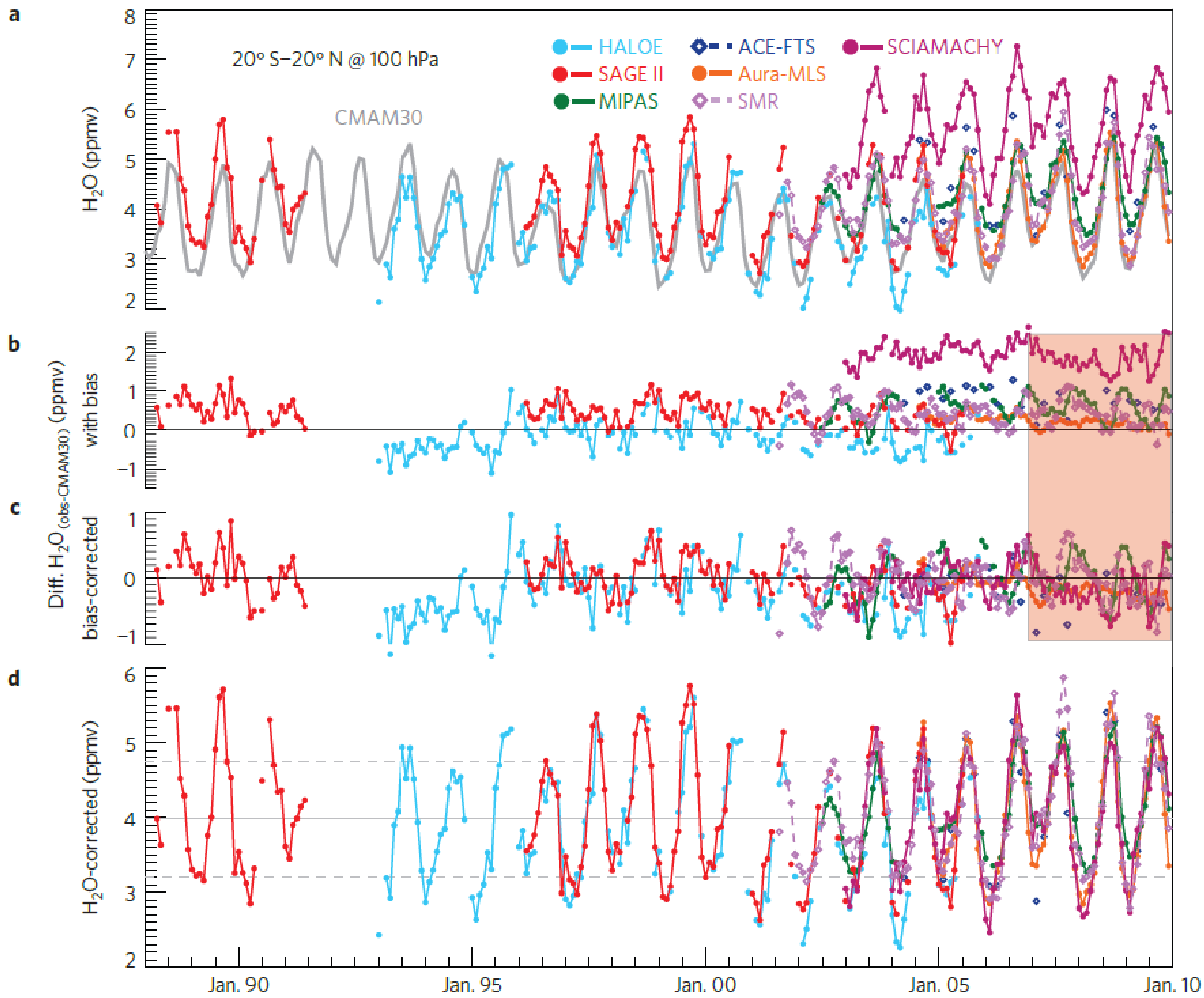

Figure 3 Illustration of data merging from Hegglin et al. (2014)**: Time series of monthly zonal mean water vapor at 100 hPa averaged over 20S–20N for 1988–2010. (a) Absolute mixing ratios from different instruments (colors) and CMAM30 (grey). (b–d): Differences (b), bias-corrected differences between observations and CMAM30 (c), and bias-corrected absolute mixing ratios from observations (d). Grey solid and dashed horizontal lines in d indicate mean and 1σ (standard deviation) of the observational record averaged over the whole time period. The red box encompasses months excluded from the relative-bias determination owing to identified problems in ERA-Interim.**

4.3 Uncertainty characterization for merged datasets

The uncertainty of averaged data is usually characterized by the standard error of the mean. If a bias correction is applied to one or more datasets, the associated uncertainty is added to the error budget (e.g., Kyrölä et al., 2013). The uncertainty associated with the bias correction is usually small, since biases are estimated using large data samples.

If several datasets are merged, the range of variation of individual climate parameters about the merged value gives an indication of systematic error/full error associated with the merged dataset. Such characterization of the uncertainties, in addition to the standard error of the mean, has been applied in GOZCARDS (Froidevaux et al., 2015) and in the merged time series of deseasonalized anomalies from the HARMOZ dataset (WMO, 2014).

A special attention requires a sampling error, which results from the instrument sampling pattern and can constitute a significant part of the total uncertainty, especially for sensors with relatively coarse sampling (Foelsche et al., 2011; Sofieva et al., 2014a; Tegtmeier et al., 2013; Toohey et al., 2013). In creating time series of stratospheric temperatures, either a diurnal correction (MSU-AMSU dataset, Mears and Wentz, 2009; Mears et al., 2011) or a full sampling bias correction (radio-occultation measurements, (Foelsche et al., 2011)) is applied based on a 4D temperature field from meteorological or chemistry-transport model. For ozone field, a similar sampling bias correction seems to be not feasible due to lack of a sufficiently good chemistry-transport model.

In the GTO dataset, the uncertainty of the monthly zonal mean data takes partially into account the sampling uncertainty, estimates of which is obtained with the CTM (Coldewey-Egbers et al., 2015). A parameterization proposed in Sofieva et al. (2014a) can be also useful for characterization of sampling uncertainty.

In several recent paper (Frith et al., 2014; Mears et al., 2011; Povey and Grainger, 2015), the use of Monte-Carlo simulations (or ensemble estimate) to characterization of the merged datasets is discussed.

5 Discussion: application to the MLT

The mesosphere and the lower thermosphere are characterized by very large variability due to photo-chemical and dynamical processes. The MLT region is strongly affected by waves (gravity, tidal, planetary), circulation and oscillation patterns (pole-to-pole circulation, QBO, SAO), as well as solar and geomagnetic influence.

Analogous to merging in the stratosphere, if the merged dataset is targeted to trend analysis, using a meteorological model for conversion to another unit (mixing ratio or number unit) or to another vertical grid (pressure, altitude) should be avoided, since trends in model temperature field can be not realistic. Furthermore, trends in number density and mixing ratio are different due to climatic changes in air density profiles (McLinden and Fioletov, 2011).

Gravity wave effects can be minimized by averaging data (zonally, monthly). Averaging can also reduce planetary wave effects.

The most relevant merging methods for creating long-term MLT datasets seem to be using deseasonalized anomalies or using a CTM as a transfer function (e.g., for taking into account diurnal variations). However, CTMs may not represent properly atmospheric tides and other variations in the MLT.

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7 Acronyms and abbreviations

AMSU	Advanced Microwave Sounding Unit
CCI	Climate Change Initiative
ECMWF	European Center for Medium-Range Weather Forecasts
ENVISAT	Environmental Satellite
GOME	Global Ozone Monitoring Experiment
GOMOS	Global Ozone Monitoring by Occultation of Stars
HALOE	Halogen Occultation Experiment
LLM climatology	ozone climatology by McPeters, Labow and Logan (McPeters et al., 2007)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
ML climatology	ozone climatology By McPeters and Labow (McPeters and Labow, 2012)
MLS	Microwave Limb Sounder
MSIS	Mass Spectrometer and Incoherent Scatter Radar
MSU	Microwave Sounding Unit
NOAA	National Oceanic and Atmospheric Administration
OSIRIS	Optical Spectrograph and Infrared Imager System
SAGE (I, II, III)	Stratospheric Aerosol and Gas Experiment
SBUV	Solar Backscatter Ultraviolet
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SMR	Sub-Millimetre Radiometer
SSU	Stratospheric Sounding Unit

UARS	Upper Atmospheric Research Satellite
UTLS	the upper troposphere and the lower stratosphere
WMO	World Meteorological Organization