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Technical report

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Technical report

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Abstract

We discuss the insights that research satellite observations from the last 30 years have provided on the spatio-temporal variability of the polar middle atmosphere. Starting from the time of the NASA LIMS (Limb Infrared Monitor of the Stratosphere) and TOMS (Total Ozone Mapping Spectrometer) instruments, both launched in 1978, we show how these observations have augmented our knowledge of the polar middle atmosphere, in particular how information on ozone and tracers has augmented our knowledge of: (i) the spatial and temporal characteristics of the wintertime polar stratosphere and the summertime circulation; and (ii) the roles of chemistry and transport in determining the stratospheric ozone distribution. We address the increasing joint use of observations and models, in particular in data assimilation, in contributing to this understanding. Finally, we outline requirements to allow continuation of the wealth of information on the polar middle atmosphere provided by research satellites over the last 30 years.

Spatio-temporal variability of the polar middle atmosphere: Insights from over 30 years of research satellite observations

1 Introduction

In October 1978 the NASA LIMS (Limb Infrared Monitor of the Stratosphere; acronyms are provided in an Appendix) instrument was launched, heralding a golden age of satellite observations of the polar middle atmosphere (the stratosphere and mesosphere, approximately 10 km - 90 km altitude, approximately 100 hPa – 0.01 hPa) that has continued to this day. The LIMS instrument was an early example of a research satellite instrument, typically deployed for scientific study of the Earth System. The LIMS instrument measured vertical profiles of temperature and various constituents (ozone, H_2O, HNO_3 and NO_2) within the pressure range 100 hPa – 0.1 hPa (see Table 3 in Gille and Russell, 1984). Although it only made measurements for the period October 1978 – May 1979, it provided a wealth of information which formed the basis for initial insights into the distribution of stratospheric H_2O (Jones et al., 1986; Remsberg et al., 2009). By combining LIMS and SAMS (also launched in 1978) measurements, Jones et al. (1986) used the concept of total hydrogen (H_2+H_2O+2×CH_4), a quantity roughly conserved in the stratosphere, to estimate the H_2O mixing ratio as it enters the stratosphere in the tropics from below. LIMS ozone measurements have also provided insight into the stratospheric ozone budget, improved our understanding of transport processes during polar winter (see Leovy et al., 1985; Manney et al., 1994) and helped test our understanding of ozone photochemical processes (Natarajan et al., 2002).

The first TOMS platform was launched by NASA in October 1978, heralding the start of intensive monitoring of ozone from space. The TOMS instruments (McPeters et al., 1998) measured total column ozone. Of the five TOMS instruments built, four entered orbit successfully. The Nimbus-7 and Meteor-3 TOMS provided daily global measurements of total column ozone for the period November 1978 – December 1994. After an eighteen month period during which the TOMS program had no on-orbit capability, ADEOS TOMS was launched in August 1996 and provided data until the failure of the ADEOS satellite in June 1997. Earth Probe TOMS (EP TOMS) was launched in July 1996 to provide additional measurements, but was boosted to a higher orbit to replace the failed ADEOS TOMS. The transmitter from EP TOMS failed in December 2006. Since January 2006, total ozone column data from OMI onboard EOS Aura has replaced EP TOMS. The TOMS total column ozone measurements have documented the long-term decline of global ozone levels and the emergence and development of the Antarctic ozone hole (see, e.g., Solomon et al., 1986; see also http://www.theozonehole.com/ozoneholehistory.htm). TOMS measurements have helped scientists understand the factors contributing to the stratospheric ozone distribution (e.g. Solomon, 1999), and helped society monitor the stratospheric ozone distribution and test the effect of societal actions addressing stratospheric ozone loss, e.g., the Montreal Protocol (http://www.unep.org/ozone/montreal.shtml; Sarma and Bankobeeza, 2000).

Since the LIMS experiment and the first TOMS platform, the leading research space agencies, including NASA, ESA and JAXA, have launched many satellite missions (Lahoz, 2010). These missions have made multiple observations of temperature and chemical species in the polar middle atmosphere. These observations, often from different instruments on the same satellite platform (as from NASA's UARS and EOS Aura, and ESA's Envisat), have provided, first, the opportunity to evaluate the observations themselves, notably checking for consistency; second, the opportunity to use the properties of trace gases to understand spatio-temporal variability in the polar middle atmosphere, including description of events such as major warmings and the final warming; third, the opportunity (based on the properties of trace gases) to investigate how dynamical and chemical processes contribute to the distribution of key stratospheric species such as ozone; and fourth, the opportunity to test understanding of middle atmosphere dynamical and chemical processes by confronting (and thus testing) model simulations with observations.

Information provided by research satellites has also helped address key societal issues of the last 30 years. These include: (i) the "ozone-hole" identified with massive ozone loss in the Antarctic stratosphere (Farman et al., 1985), and ozone loss in the Arctic stratosphere, with measurements for northern winter 2010-2011 identifying massive Arctic loss comparable to that measured in the Antarctic (Manney et al., 2011, and references therein); and (ii) monitoring of the lower atmosphere (the troposphere and lower stratosphere), with special interest in the Arctic as its environment is modified by climate change (WMO, 2011).

Remote sensing satellites are typically divided into research satellites (focused on research of the Earth System) and operational satellites (focused on Numerical Weather Prediction, NWP, and stratospheric ozone monitoring). Research satellites generally provide data off-line (data latency is typically at least 1-2 days after data acquisition), and use both nadir- and limb-viewing geometries. Operational satellites provide data in near-real-time, data latency being typically 1 hour or less after acquisition. Currently, the vast majority of operational satellites have nadir-viewing geometries. Recently, research satellite data have begun to be of interest to the NWP community; a requisite is their availability in near-real-time. Both research and operational satellites have contributed to our understanding of the polar middle atmosphere; in this review we focus on research satellites.

A recent development in middle atmosphere studies has been the assimilation of stratospheric constituents measured by instruments onboard various satellite platforms, including UARS, Envisat and EOS Aura (e.g., Lahoz et al., 2007a, b; Lahoz and Errera, 2010). There has been substantial progress over the last 15 years, with the field evolving from initial efforts to test the methodology to later efforts focusing on products for monitoring ozone and other constituents. Data assimilation has been used to study the stratosphere qualitatively and quantitatively: assimilation of ozone and other trace gas observations has been used to quantify wintertime ozone loss (e.g., El Amraoui et al., 2008; Jackson and Orsolini, 2008; Rösevall et al., 2008); analyses based on assimilation of stratospheric water vapour have been used to study sudden stratospheric warmings and quantify descent in the wintertime stratospheric polar vortex (Lahoz et al., 2011a). Over the last 15 years the production of ozone forecasts by a number of NWP centres has also become routine, e.g., at the European Centre for Medium-Range Weather Forecasts, ECMWF (Dethof, 2003).

This review paper complements the work of two relatively recent publications by Shepherd (2007) and Schoeberl and Douglass (2010), which provide an overview of stratospheric transport. Shepherd provides a picture of current understanding of transport in the stratosphere, with a strong focus on theoretical aspects, including strengths and weaknesses of this understanding; the key role of satellite observations in advancing this understanding is highlighted. Schoeberl and Douglass provide an integrated picture of trace gas transport in the stratosphere, with a focus on diagnostic tools and techniques for analysing observations. This report differs from these works of Shepherd and of Schoeberl and Douglass, in that the focus is the research satellite record over the last 30 years and discussion of the insights they have provided toward understanding middle atmosphere spatio-temporal variability.

Other studies of the middle atmosphere provide overviews of tropical processes such as the quasi-biennial oscillation (QBO), tropical waves and the tape recorder, and of how research satellite observations have helped improved our understanding of these processes (see, e.g., Baldwin et al., 2001). Finally, information on gravity waves derived from measurements of dynamical quantities such as temperature, has provided insight into middle atmosphere dynamical processes, and helped the development and testing of tools to model gravity waves (see Alexander et al., 2010, and references therein).

Section 2 discusses satellite observations and sets them in the context of the Global Observing System (GOS). Section 3 discusses how research satellite observations have contributed to our understanding of spatio-temporal variability in the polar middle atmosphere, focusing on the spatial and temporal characteristics of the wintertime polar stratosphere and the summertime circulation (Sect. 3.1); and the roles of chemistry and transport in determining the stratospheric ozone distribution (Sect. 3.2). Section 4 provides an overview of the role of data assimilation in understanding the polar middle atmosphere. Section 5 provides a discussion of how research satellite measurements of the middle atmosphere can continue to address the needs of science and society. Section 6 provides conclusions.

2 Satellite observations

2.1 Satellite types

Satellite observations provide large-scale geographical coverage, ranging from the continental scale to the global scale. They typically have lower spatial and temporal resolution, and less precision, than in situ measurements (e.g. from ground-based or aircraft platforms). Both types of data, satellite and in situ, contribute to the GOS, complementing each other (e.g., Thépaut and Andersson, 2010).

Within the satellite data GOS element, satellite observations of the Earth/ atmosphere can be broadly divided by remote sensing method (active vs passive technologies) and by geometry (nadir vs limb viewing). Satellites can also be classified according to their orbits: (a) geostationary (GEO); and (b) low Earth orbit (LEO), of which polar orbiting satellites are a considerable subset. Research satellites studying the polar middle atmosphere generally have LEO orbits, and can have sun-synchronous or non sun-synchronous orbits. Satellites with GEO orbits have been much less used to study the polar middle atmosphere owing to the limitations of the GEO geometry, which means the satellite cannot make good measurements poleward of approximately 60^{o}N or 60^{o}S. As of 2011, no satellites with a GEO orbit have been deployed to measure trace species (Lahoz et al., 2012); they have mainly contributed information on temperature (Thépaut and Andersson, 2010).

Sun-synchronous satellites have a fixed Equator crossing time, whereas non-sunsynchronous satellites do not. Sun-synchronous satellites (e.g. ESA’s Envisat and NASA’s EOS Aura; see Table 1 below) have the advantage that instruments always face away from the sun, so no periodic satellite yaw manoeuvre to avoid sunlight damaging the instruments is necessary. However, they have the disadvantage that they cannot observe the diurnal cycle at a particular location. For example, species such as NO and NO_2, which play a role in determining the distribution of ozone, have strong diurnal cycles. Non-sun-synchronous satellites (e.g. NASA’s UARS; see Table 1 below) have the advantage of being able to observe the diurnal cycle at a particular location, but the disadvantage that a periodic satellite yaw manoeuvre is needed to avoid sunlight damaging the instruments. In the case of the UARS MLS, this had the effect of the instrument either having a North Looking configuration (34°S–80°N) or a South Looking configuration (80°S–34°N).

Satellite instruments do not measure directly temperature or atmospheric gases, i.e., chemical species. What they measure is photon counts (level 0 data). Algorithms then transform the level 0 data into radiances (level 1 data). Subsequently, using retrieval techniques (Rodgers, 2000), retrievals of profiles or total column amounts are derived (level 2 data). Higher level data generally comprise of gridded data (level 3 data) and analyses derived using data assimilation methods (level 4 data).

The information that eventually becomes level 2 atmospheric gas data arises due to a variety of naturally-occurring physical processes (information on temperature is generally derived from information on gases such as CO_2, whose concentration varies little in the region of interest). Radiation is emitted from atmospheric gases undergoing vibrational or rotational oscillations in the microwave and infrared regions. These types of radiation are generally observed via limb-viewing geometry in order to determine vertical profiles of the gases. Nadir-viewing of emitted radiation can also provide limited information on gases such as ozone, H_2O, and CO_2 (e.g. from AIRS and IASI), but generally at too low a vertical resolution for polar process studies. Certain gases, such as ozone, can also scatter and absorb ultraviolet (UV) radiation. UV-scattering is observable at relatively high vertical resolution from limb-viewing sensors (e.g. from OSIRIS) or at lower vertical resolution from nadir (e.g. from SBUV and OMI). Horizontally scanning instruments such as OMI also provide good horizontal resolution compared to fixed nadir instruments. Another method that has been used is solar occultation in which the extinction of solar radiation is measured during sunrise/sunset as viewed from the satellite. This provides relatively high vertical resolution (~1 km) profiles with high precision. However, these instruments only provide limited geographic coverage - only one latitude in each hemisphere is measured each day for a typical solar occultation instrument (e.g., HALOE, and the POAM and SAGE instruments). A stellar occultation sounder like GOMOS has improved geographic coverage compared to a solar occultation sounder.

2.2 Research satellite missions

We now describe selected key research satellite missions which have been used for Earth Observation of the polar middle atmosphere. A summary is provided in Table 1 and includes information on the space agency, the instrument, lifetime, observations, and height range and reference papers (associated with validation of the satellite dataset and/or description of the satellite mission). The exposition below sorts the missions by space agency and is based on Lahoz (2010).

NASA. The SAGE I mission was launched in 1979 and lasted for almost three years. It provided global measurements of aerosol extinction (at 0.45 and 1.0 µm), ozone, and NO_2. Its successor, the SAGE II mission, provided the scientific community with information on the global distribution of aerosol, ozone, H_2O and NO_2 over a period of 21 years (1984-2005). The successor to SAGE II was SAGE III, launched in collaboration between NASA and the Russian Space Agency in 2001. The data from SAGE III have been evaluated in a special issue in Atmos. Chem. Phys., "SAGE III Ozone loss and validation experiment II and the validation of international satellites and study of ozone loss (SOLVE-II/VINTERSOL)" (Ed. Carslaw), http://www.atmos-chem-phys.org/special_issue12.html (papers appeared over the period 2004-2007).

UARS was launched in September 1991, and ceased operations in December 2005. A number of UARS limb and occultation sounder instruments (CLAES, HALOE, ISAMS, MLS) have made middle atmosphere measurements of temperature, ozone, H_2O, ClO and other chemical species. The UARS data have been extensively evaluated (see UARS special issue in J. Geophys. Res., 1996, Vol. 101, 9539–10473), and have contributed to our understanding of many aspects of the atmospheric circulation and chemistry (see, e.g., the UARS special issue in J. Atmos. Sci., 1994, Vol. 51, 2781–3105).

EOS Aura (http://aura.gsfc.nasa.gov) was launched in July 2004. It carries on board four instruments: MLS, HIRDLS, OMI and TES. EOS Aura provides middle atmosphere information on: (i) chemistry of the middle and upper stratosphere (Aura MLS); (ii) temperature and constituents in the stratosphere and mesosphere (HIRDLS); and (iii) maps of total column ozone, which continue the TOMS record, and NO_2 (OMI). Aura MLS and HIRDLS are limb sounders; OMI is a nadir sounder. The EOS Aura data have been described in the literature (EOS Aura special issue in IEEE, 2006, Vol. 44), and in a special issue on EOS Aura validation in J. Geophys. Res., 2008, Vol. 113 (see also Schoeberl et al., 2008).

NRL. The Naval Research Laboratory (NRL) Polar Ozone and Aerosol Monitor III (POAM III) instrument was launched in March 1998, as a successor to the POAM II experiment (launched in September 1993), which provided data on ozone depletion in the polar stratosphere. POAM III provided profiles of ozone, NO_2, H_2O, and aerosol extinction. POAM III data have been used to validate research satellite datasets (e.g. Envisat MIPAS and SCIAMACHY) and for various polar process studies (e.g. Allen et al., 2003)

ESA. GOME is a scanning nadir sounder that has been making measurements of total column ozone and NO_2 since 1995. Since June 2003 the ERS-2 satellite which carries GOME has experienced problems. GOME-2, a successor to GOME, flies on the operational polar orbiting satellite METOP.

Envisat was launched in March 2002 with ten instruments on board; it ceased operations in April 2012. Envisat provided middle atmosphere information on temperature, ozone, H_2O and other atmospheric constituents using limb, nadir and occultation geometries (MIPAS, SCIAMACHY, GOMOS). The broad spectrum of information from Envisat reflects the paradigm that the Earth System should be treated as a whole, and that information from its various components should be integrated. However, the complexity and cost of Envisat mean it is unlikely that ESA (or other space agencies) will launch future missions of a size similar to Envisat.

Envisat data have been evaluated at a series of ESA workshops. Examples include the Envisat Validation Workshop held at ESRIN on December 2002 (http://envisat.esa.int/pub/ESA_DOC/envisat_val_1202/proceedings; ESA Special Publication SP-531); the Second Workshop on the Atmospheric Chemistry Validation of Envisat, ACVE-2, held at ESRIN on May 2004 (http://envisat.esa.int/workshops/acve2; ESA Special Publication SP-562); and the Third Workshop on the Atmospheric Chemistry Validation of Envisat, ACVE-3, held at ESRIN on December 2006 (ESA Special Publication SP-642). The data from MIPAS and SCIAMACHY have also been evaluated in special issues in Atmos. Chem. Phys.: (i) “Geophysical Validation of SCIAMACHY 2002–2004” (Eds. Kelder, Platt and Simon), http://www.atmos-chemphys.net/special_issue19.html (2005); and (ii) “MIPAS (Michelson Interferometer for Passive Atmospheric Sounding): Potential of the experiment, data processing and validation of results” (Eds. Espy and Hartogh), http://www.atmos-chemphys.net/special_issue70.html (2006). Data from the atmospheric chemistry instruments in Envisat have been used to study the unprecedented Antarctic ozone hole split of September 2002 (see the special issue in J. Atmos. Sci., 2005, Vol. 62).

JAXA. There have been two ADEOS missions: ADEOS (launched 1996) and ADEOS-II (launched 2002). Both missions lasted less than one year. The ADEOS mission carried several instruments on board, including ADEOS TOMS (which measured total column ozone) and ILAS (a limb instrument which measured temperature, ozone, H_2O and other atmospheric constituents). The ADEOS-II mission carried on board five instruments. ADEOS-II provided middle atmosphere information on temperature, ozone and other atmospheric constituents from ILAS-II. The ILAS-II products have been evaluated in several papers appearing in a special section of J. Geophys. Res., Vol. 111, 2006.

CSA. The SCISAT-1 platform was launched in 2003. It operates primarily in solar occultation mode, and carries the ACE-FTS and MAESTRO instruments (as well as visible and infrared imagers). The ACE-FTS instrument has several baseline species (and species retrieved as "research" products, e.g., HNO_4) providing middle atmosphere information: ozone, H_2O, CH_4, N_2O, NO_2 and others. It also retrieves several isotopes of H_2O, ozone and other species. The MAESTRO instrument measures ozone, NO_2 profiles, and wavelength-dependent optical depth. An evaluation of SCISAT-1 data was carried out in a special issue published in Geophys. Res. Lett., Vol. 32, 2005. ACE-FTS products are evaluated in a special issue of Atmos. Chem. Phys. (http://www.atmos-chem-phys.net/special_issue114.html, eds. Richter, Wagner). An evaluation of MAESTRO data was carried out by McElroy et al. (2007).

Other space agencies. ODIN, involving a number of space agencies, including the CSA (the Canadian Space Agency), CNES (the French Space Agency) and SNSB (the Swedish Space Agency), was launched in February 2001. It carries on board two instruments: OSIRIS and SMR. OSIRIS provides middle atmosphere information on ozone (Llewellyn et al., 2004). SMR provides middle atmosphere information on ozone, N_2O, ClO and HNO_3 (Murtagh et al., 2002).

Table 1: Measurements of temperature and/or chemical species in the middle atmosphere from selected research satellite missions (see also Lahoz, 2010). The latitudinal range of the measurements covers the polar regions (generally poleward of 60^{o}N and 60^{o}S). The height range reflects the region in the atmosphere where the measurements have information, typically as represented by averaging kernels.

Space Agency	Instrument	Lifetime	Observations	Height range (pressure, hPa, or height, km)	Reference papers	Notes
NASA	LIMS	Oct 1978 – May 1979	Temperature (T), ozone, H_2O, HNO_3, NO_2 profiles	70 hPa – 2 hPa (all observations)	Gille and Russell (1984)	Some measurements extend above 2 hPa and below 70 hPa
NASA	SAMS	Oct 1978 – June 1983	T, CO_2, CO, CH_4, NO_2, and H_2O profiles	20 km – 100 km	Drummond et al. (1980)	
NASA (Russian and Japanese space agencies also involved)	TOMS	Oct 1978 – Dec 2006	Ozone	Total column	McPeters et al. (1998)	Various instruments. Since Jan 2006 data from OMI has replaced EP TOMS
NOAA	SBUV and SBUV/2	Nov 1978 - present	Ozone layers	Nominally 25 km - 45 km	Miller et al. (2002)	SBUV (Nov 1978 – 1984); SBUV/2 on NOAA series (1984 – present)
NASA	SAGE I/SAGE II/SAGE III	SAGE I: Feb 1979 – Nov 1981; SAGE II: Oct 1984 – Aug 2005; SAGE III: Mar 2002 – Mar 2006	Ozone, H_2O, NO_2, aerosol	Stratosphere	McCormick et al. (1989) (SAGE I and SAGE II); Trepte et al. (2001) (SAGE III)	SAGE I, II and III use solar occultation. SAGE III was a joint mission between NASA and the Russian Space Agency
NASA	ATMOS	April 1985; Mar 1992; April 1993; Nov 1994	Ozone, NO, NO_2, N_2O_5, HNO_3, HO_2NO_2, HCN, $ClONO_2$, HCl, H_2O, CO, CO_2, CH_4, N_2O profiles	Stratosphere	Gunson et al. (1996); Irion et al. (2002)	Four space shuttle missions
NASA	UARS CLAES	Oct 1991- May 1993	T, ozone, H_2O, CH_4, N_2O, NO, NO_2, N_2O_5, HNO_3, $ClONO_2$, $CFCl_3$, CF_2Cl_2, aerosol extinction profiles	Nominally 10 km - 60 km	Roche et al. (1993); various papers in UARS special issue for J. Geophys. Res. (1996)	
NASA	UARS HALOE	Sep 1991- Nov 2005	T, ozone, N_2O, CH_4, H_2O, HCl, HF, NO, NO_2, aerosol extinction, aerosol composition profiles	Stratosphere; some species measured in the mesosphere; NO measured up to the thermosphere	Russell et al. (1993); various papers in UARS special issue for J. Geophys. Res. (1996)	Sun occultation geometry: HALOE data need to be averaged over long periods of time (order weeks) for global coverage
NASA	UARS ISAMS	Sep 1991- Jul 1992	T, ozone, CO, H_2O, CH_4, HNO_3, N_2O_5, NO_2, N_2O, aerosol	15 km – 80 km	Taylor et al. (1993); various papers in UARS special issue for J. Geophys. Res. (1996)	
NASA	UARS MLS	Sep 1991- Aug 2001	T, ozone, H_2O, ClO, HNO_3, volcanic SO_2, CH_3CN profiles	Stratosphere (upper troposphere also for H_2O)	Various papers in UARS special issue for J. Geophys. Res. (1996); Waters (1998)	Stratospheric H_2O measurements stopped April 1993; after Mar 1994 UARS MLS measurements became increasingly sparse

Table 1, cont.

Space Agency	Instrument	Lifetime	Observations	Height range (pressure, hPa, or height, km)	Reference papers	Notes
CNES/U.S. Navy	SPOT-3 POAM II, SPOT-4 POAM III	POAM II (Sep 1993 – Nov 1996); POAM III (Mar 1998 – Dec 2005)	Ozone, H_2O, NO_2, aerosol extinction profiles	Stratosphere, upper troposphere	Lucke et al. (1999)	
NASA	CRISTA	Nov 1994; Aug 1997	Ozone, CH_4, N_2O, CFC-11, HNO_3, $ClONO_2$, N_2O_5 profiles	Nominally 10 km - 55 km	Offermann et al. (1999)	Two space shuttle missions
ESA	ERS-2 GOME	April 1995 – Jul 2011	Total column ozone, NO_2; ozone profiles	Total column; Mid and lower stratosphere (sub-column profiles)	Burrows et al. (1999)	
EUMETSAT	MetOP GOME-2	Oct 1996 - present	Ozone, NO_2, H_2O, O_2, BrO, other gas profiles		Callies et al., 2000	Flies on operational satellite platform; continues GOME mission
SNSB	ODIN SMR and OSIRIS	2001 - present	Ozone (and isotopes), N_2O, HNO_3, H_2O (and isotopes), CO, ClO profiles	7 km - 110 km	Murtagh et al. (2002) – ODIN; Llewellyn et al. (2004) - OSIRIS	Built jointly with France, Finland and Canada. ODIN is a joint astronomy and aeronomy mission, and the observations are shared equally among these disciplines
NASA	TIMED SABER	2002 - present	T profiles	10 km – 105 km	Mertens et al. (2001)	Coverage is 54°S-82°N or 82°S-54°N depending on yaw cycle
ESA	Envisat GOMOS	March 2002 – April 2012	T, ozone, NO_2, NO_3 profiles	Troposphere to mesosphere (nominally up to 120 km)	Bertaux et al. (2000, 2010)	Stellar occultation sounder: better coverage than solar occultation sounder; height of validity range varies between species and/or stars used for occultation
ESA	Envisat MIPAS	March 2002 – April 2012	Ozone, H_2O, NO_2, HNO_3, N_2O, CH_4 profiles	Nominally 6 km - 68 km	Fischer et al. (2008)	Problems since 2004 affected performance
ESA	Envisat SCIAMACHY	March 2002 – April 2012	Total column ozone; ozone, H_2O (and HDO), NO_2, BrO, CH_4, SO_2, HCHO, OClO, CO, CO_2	15 km – 45 km (limb geometry)	Bovensmann et al. (1999)	SCIAMACHY has limb, nadir and occultation modes
NASA	EOS Aqua AIRS	May 2002 - present	T, ozone	Stratosphere (T), ozone total column	Chahine et al. (2006)	Planned as an operational mission, it has been used for research purposes. T data extends down to ~900 hPa.
JAXA	ADEOS-II ILAS-II	Dec 2002 – Oct 2003	T, ozone, NO_2, HNO_3, aerosols, H_2O, CFC-11, CFC-12, CH_4, N_2O, $ClONO_2$ profiles	Stratosphere	Nakajima et al. (2006)	A previous JAXA mission, ADEOS, was launched in 1996 and lasted ten months. ILAS-II is a solar occultation instrument
CSA	SCISAT-1 ACE-FTS and MAESTRO	2003 - present	Ozone, H_2O, CH_4, N_2O, NO_2 and others (ACE-FTS). Ozone, NO_2 profiles, and wavelength-dependent optical depth (MAESTRO)	Stratosphere	Bernath et al. (2005) – ACE-FTS; McElroy et al. (2007) - MAESTRO	ACE-FTS and MAESTRO are solar occultation instruments (ACE-FTS in the infrared; MAESTRO in the UV-Vis-near infrared)

Table 1, cont.

Space Agency	Instrument	Lifetime	Observations	Height range (pressure, hPa, or height, km)	Reference papers	Notes
NASA	EOS Aura HIRDLS	2004 - present	T, ozone, HNO_3, CFC-11, CFC-12 profiles	Range covering all species is 415 hPa – 0.1 hPa, but vertical range varies between species	Gille et al. (2008)	After launch, HIRDLS optical path was blocked. Measurements at high vertical resolution can be made at one scan angle
NASA	EOS Aura MLS	2004 - present	T, ozone, H_2O, ClO, CO, HCl, HCN, HNO_3, HO_2, SO_2, N_2O profiles	316 hPa – 0.002 hPa (all species)	Waters et al. (2006); various papers in Aura special issue in J. Geophys. Res. (2008)	Vertical range varies between species and often is a subset of overall range
NASA	EOS Aura OMI	2004 - present	Total column ozone, NO_2; ozone profiles	215 hPa – 0.22 hPa (ozone profiles)	Levelt et al. (2006); various papers in Aura special issue in J. Geophys. Res. (2008)	
EUMETSAT	METOP-A IASI	May 2007 - present	T, ozone	Lower stratosphere (top ~50 hPa) (T); ozone total column	Chalon et al. (2001)	Planned as an operational mission, it has been used for research purposes. T data extends down to ~900 hPa.
NASA	NPP/OMPS	Oct 2011 - present	Ozone	Total column; 15 km – 60 km profiles	-	Launched 28 Oct 2011 as part of the NPOESS mission

2.3 The Global Observing System

The GOS consists of the suite of observing platforms used for Earth Observation, and includes in situ observations from ground-based networks and aircraft, and observations from operational and research satellites (Thépaut and Andersson, 2010; Lahoz, 2010). Research satellites are valuable additions to the GOS and provide several benefits to the Earth Observation and atmospheric sciences communities. Because they often have both limb and nadir-viewing instruments, the combination provides better atmospheric analyses of the middle atmosphere (see, e.g., Struthers et al., 2002). Because they have instruments which often focus on middle atmosphere measurements of ozone and of photochemical species that affect the ozone distribution, they provide information for studying stratospheric ozone depletion, and information that helps develop coupled climate/chemistry models (SPARC CCMVal, 2010).

A number of research satellite missions are being planned and/or proposed in Europe to make measurements in the middle atmosphere. ESA’s Sentinel-5 LEO atmospheric mission will provide information on the middle atmosphere (e.g. ozone and NO_2). It will be embarked on post-EPS and operated by EUMETSAT. Launch is planned for after 2017. A Sentinel 5 precursor is planned for the period 2013–2019 to fill the data gap between the expected end of the Envisat and EOS Aura missions (before 2014) and the expected launch dates of MTG-S (2017) and post-EPS (2020). See ESA (2007) for more details on Sentinel-5.

NASA’s NPP mission satellite (see Table 1) carries five science instruments, including four new state-of-the-art sensors, which will provide critical data to help scientists understand the dynamics of long-term climate patterns and help meteorologists improve short-term weather forecasts. The mission will extend more than 30 key long-term datasets NASA has been tracking, including measurements of the ozone layer. NPP serves as a bridge mission between NASA's EOS satellites and the next-generation Joint Polar Satellite System (JPSS), a NOAA programme that will also collect weather and climate data. The Joint Polar Satellite System is planned for launch in the timeframe of 2015-2018.

Synergy between research and operational satellites, and the potential benefits to the operational agencies accruing from this synergy, can make it attractive to use research satellites in an operational capability. This can happen in a number of ways: (i) one-off use of research satellite data, e.g., measurement of a key photochemical species such as ozone, or of a novel geophysical parameter such as stratospheric winds (these were provided by the UARS HRDI instrument – the UARS WINDII instrument provided mesospheric winds); (ii) regular use of research satellite data, e.g., a satellite series that can extend the time record of key geophysical parameters such as ozone and H_2O; and (iii) use of the research satellite instrument design in future operational missions. Increased interest by the meteorological centres in ozone and chemical forecasting makes research satellites more attractive to them. An example are the operational services for monitoring and forecasting atmospheric composition developed within the EU-funded GEMS and MACC projects in the context of the GMES European programme (Hollingsworth et al., 2008).

It is worth insisting on the complementarity of the research and the operational approach to satellite data, in particular in the sense that often research instruments are precursors of operational instruments. Thus, operational centres exercise the science on research satellites to improve their readiness when operational satellites come by. The best illustration of this is provided by the AIRS and IASI instruments (see Table 1). The science community, in particular at the operational centres, was able to use AIRS to prepare for the assimilation of data from multi-spectral sounders, and this minimized the delay when IASI started to provide data to operational centres.

Satellite observations and in situ observations are complementary. In particular, satellite observations rely on ground-based observations for calibration and validation (USGEO, 2010). In operational meteorology, data assimilation is used to combine the high accuracy of in situ observations (including ground-based and aircraft platforms) with the high spatial coverage of satellite platforms (Andersson and Thépaut, 2010). The relative merit of planned and/or proposed ground-based observational networks and satellite platforms (impact on the GOS, observing system versus cost), as well as the combination of ground-based and satellite observations for various elements of the Earth system, is being studied using the notion of Observing System Simulation Experiments, OSSEs (Masutani et al., 2010a, b). Details of the GOS requirements regarding satellite measurements (mainly from an operational perspective) are provided in Thépaut and Andersson (2010). Similarly, details of the GOS requirements (including ground-based and satellite observations) for studying atmospheric chemistry processes are provided in IGACO (2004). In Sects. 4-5 we discuss the role of OSSEs in designing the future GOS with respect to observations of the middle atmosphere.

3 Understanding the spatio-temporal variability of the polar middle atmosphere

After the discovery of the Antarctic ozone hole (Farman et al., 1985), there was a strong focus on understanding the factors involved in ozone depletion in the wintertime stratosphere, both in the Arctic and the Antarctic. After launch in September 1991, the resources of the UARS mission were deployed to study ozone depletion in the wintertime stratosphere. This included considering both dynamical and chemical processes involved in determining the ozone distribution in the stratosphere. The UARS satellite was the first time a multi-instrument platform was available for such studies. As a result, it provided an unprecedented opportunity for the use of ozone and tracer data from multiple instruments (MLS, HALOE, CLAES and ISAMS; see Table 1) to study the spatio-temporal characteristics of the wintertime polar stratosphere. UARS provided measurements of both the same tracer species from different instruments (e.g. H_2O from MLS and HALOE) and of different but complementary tracer species (e.g. H_2O from MLS, N_2O from CLAES). The UARS measurements provided, first, the opportunity to validate the measurements by inter-instrument comparisons and, second, the observational evidence to strengthen inferences from consistency between the chemical species (including ozone) measurements and the tracer measurements.

In a series of papers using UARS tracer data; tracer data from other satellites (e.g. Envisat, EOS Aura, ACE-FTS, SAGE series, POAM series); and in situ tracer data (e.g. from ATMOS onboard the space shuttle), a picture was built of the wintertime evolution of the polar stratosphere, and the key features determining the large-scale wintertime flow. This was done for both the Arctic and the Antarctic and provided the opportunity to compare and contrast the flow regimes of the Polar regions. Comparison of tracer data with analysed meteorological fields (e.g. geopotential height; potential vorticity, PV) from NWP centres such as the Met Office and ECMWF helped support the evidence provided by the satellite data.

To highlight the role of research satellites such as UARS in understanding the spatio-temporal variabililty of the polar middle atmosphere, we discuss two key aspects where research satellite tracer and ozone data have provided insights: (i) the spatio-temporal characteristics of the wintertime polar stratosphere and the summertime circulation (Sect. 3.1); and (ii) the role of chemistry and transport in determining the stratospheric ozone distribution (Sect. 3.2).

3.1 Spatio-temporal characteristics of the wintertime polar stratosphere

Meteorology. The early winter stratosphere is characterized by the build-up of a cyclonic polar vortex at high latitudes, identified by relatively low temperatures, relatively high PV magnitudes and westerly winds. It is circumscribed by a belt of strong westerly winds accompanied by high latitudinal gradients in PV. These high PV gradients often denote the edge of the polar vortex, differentiating air masses poleward and equatorward of this belt of strong westerlies. Depending on the sources and sinks of stratospheric tracers, these air masses may have different values for the tracer field, and thus be identifiable from global tracer data.

In both the Arctic and Antarctic, the large-scale wintertime flow is organized by the interaction between a strong cyclonic polar vortex and anticyclonic circulations. The polar vortex in the Arctic is generally weaker than that in the Antarctic; this is associated with temperatures in the former being generally higher than in the latter. In the Arctic during early winter there develops a quasi-stationary anticyclone typically located over the Aleutian Islands. This anticyclone, the Aleutian High, tends to displace the Arctic polar vortex off the Pole. In the Arctic there can also develop eastward travelling anticyclones that merge with the Aleutian High and contribute to displace and distort the polar vortex (see, e.g., O'Neill et al., 1994). Different from the Arctic, two distinct flow regimes are identified in the winter-spring period in the Antarctic: in mid and late winter, a flow organized by the interaction between a relatively strong polar vortex and eastward travelling anticyclones; in spring, a flow regime organized by the interaction between the relatively weaker polar vortex and a quasi-stationary anticyclone located south of Australia, the "Australian High" (Lahoz et al., 1996). Lahoz et al. (1996) also documented the phenomenon of merger of anticyclones in the Antarctic (already documented for the Arctic by, e.g., O'Neill et al., 1994), and provided a detailed study of tracer transport during merger by computing the isentropic advection of thousands of particles using the technique of domain-filling trajectory calculations (see Sutton et al., 1994).

During late winter, the polar vortex weakens as the final warming approaches. The final warming is associated with the transition between the wintertime and summertime circulations, during which the polar vortex breaks up and the circulation changes from westerly winds to easterly winds. In the Arctic, the polar vortex break-up is typically much earlier and more abrupt than that in the Antarctic (e.g., Waugh and Randel, 1999), often being triggered by stratospheric sudden warming events. During the final warming in the Antarctic stratosphere, the break-up of the polar vortex, accompanied by a strengthening of the quasi-stationary anticyclone, generally is top-down, taking place first in the upper stratosphere and progressing to the mid and lower stratosphere over a period of approximately two months. For the Arctic stratosphere, the way the vortex break-up occurs varies from year to year.

A climatology of stratospheric polar vortices and anticyclones for the Arctic and Antarctic was compiled by Harvey et al. (2002). The frequency distributions illustrate the climatological location and persistence of polar vortices and anticyclones. Harvey et al. (2002) showed that preferred locations of anticyclogenesis are related to cross-equatorial flow and weak inertial stability, and discussed regimes of eastward travelling and quasi-stationary anticyclones. In a follow up paper, Harvey et al. (2004) focused on the differences in the ozone distribution in the anticyclones and the ambient air outside the anticyclones, and found that differences resulted from both anomalous transport and photochemistry in the neighbourhood of the stratospheric anticyclones.

Transport inferred from satellite data. A number of ways to treat satellite tracer data (e.g. the along-orbit track, equivalent latitude-theta, and zonal mean pictures – described below) have been used to identify a number of elements of the three-dimensional transport taking place during the wintertime stratosphere. The main elements that have been identified are: descent of air in the polar vortex associated with the Brewer-Dobson circulation; the presence of mixing barriers associated with the edge of the polar vortex; the presence of a surf zone, with strong mixing processes, found between the transport barriers associated with the edge of the polar vortex and the subtropical jets; and the presence of filamentary structures.

The along-orbit track picture considers satellite data along the 1-D orbit track (see Lahoz et al., 2009, and references therein). The geometry of this 1-D picture provides a physically meaningful (coordinate independent) pole-centred picture of the atmosphere. An advantage of the pole-centred picture is that it retains the information content in the data without the blurring effect of gridding by interpolation between viewing tracks and averaging along latitude circles. The equivalent latitude-theta picture, where theta is potential temperature, provides a 2-D picture of the atmosphere (see Manney et al., 2009, and references therein). The 2-D equivalent latitude-theta picture involves some interpolation and averaging, but since the averaging is done along PV contours, preserves much of the pole-centred viewpoint; this picture provides information on the roles of quasi-horizontal transport and vertical transport in determining tracer distributions. The merits of the along-track orbit approach and the equivalent latitude-theta approach are discussed in, e.g., Lahoz et al. (2011a). The zonal mean picture takes averages along latitude circles to provide a 2-D picture (latitude-height) of the atmosphere. Its main advantages are the simplicity of application and the way it summarizes often complex atmospheric information. Ruth et al. (1994) discusses pitfalls associated with the zonal mean picture, for example, that it can miss longitudinal variations during dynamically active periods when the stratospheric flow can become strongly asymmetric.

A first use of satellite data to study the evolution of the wintertime middle stratosphere was done by Leovy et al. (1985) using gridded maps of ozone data from LIMS (the data were mapped globally in the form of Fourier coefficients at fixed latitudes using a Kalman filter algorithm). They showed that the ozone distribution, in particular the total column of ozone, was affected by both the zonal mean diabatic circulation (i.e., the Brewer-Dobson circulation) and other dynamical events, notably: (i) planetary wave breaking; (ii) and major and minor warming events (a major warming took place in February 1979 – see later for a discussion of this dynamical feature of the stratosphere).

Using the along-orbit track picture, Lahoz et al. (1994) showed by comparison of MLS H_2O tracer data and CLAES N_2O tracer data with the diabatic heating field (plotted along isentropic surfaces), that these tracer data exhibited strong diabatic descent through isentropic surfaces at polar latitudes (in the polar vortex) and quasi-horizontal transport at mid latitudes (in the Aleutian High). The along-orbit track cuts further showed strong latitudinal gradients between the tracer data at high latitudes and at lower latitudes, and relatively weak latitudinal gradients at mid latitudes. Comparison with analysed meteorological fields from the Met Office (Swinbank and O'Neill, 1994), including PV, and diabatic heating rates calculated using UARS MLS data as input, identified the distribution of the tracer fields with the distribution of geopotential height, with tracer values at polar latitudes associated with the cyclonic stratospheric polar vortex, and tracer values at mid latitudes associated with the anticyclonic Aleutian High. Similar results were obtained for ISAMS N_2O tracer fields for early winter using both the zonal mean picture and the along-orbit track picture (Ruth et al., 1994).

The distribution of the MLS H_2O and CLAES and ISAMS N_2O tracer fields in the stratospheric polar vortex (relatively high H_2O values; relatively low N_2O values) and the surf zone (relatively low H_2O values; relatively high N_2O values) was shown to be consistent with the known stratospheric sources and sinks of H_2O and N_2O, and the Brewer-Dobson circulation. These tracer distributions also provided evidence of stratospheric transport barriers, for example between the high latitude air confined in the polar vortex, and the mid latitude air in the surf zone, where mixing between low latitude and mid latitude air masses takes place. Evidence for these stratospheric transport barriers was provided by Manney et al. (1994) using trajectory calculations based on meteorological analyses.

In the Antarctic winter stratosphere, as for the Arctic wintertime stratosphere, comparison with the diabatic heating field (plotted along isentropic surfaces) shows tracer values exhibiting strong diabatic descent through isentropic surfaces at polar latitudes (in the polar vortex) and quasi-horizontal transport at mid latitudes (in the anticyclonic circulations). In particular, as documented by Lahoz et al. (1996) using the along-orbit track picture, the distribution of the H_2O tracer fields in the Antarctic winter stratosphere is consistent with the known stratospheric sources and sinks of H_2O, and the Brewer-Dobson circulation. The strength of the descent rates in the Antarctic and Arctic polar vortex are found to be associated with the extent to which the temperature field differs from radiative equilibrium, with descent being stronger where temperatures are higher than expected from this equilibrium. As a result, descent rates in the Antarctic polar vortex are found to be generally weaker than in the Arctic polar vortex. Descent of air in the wintertime polar upper stratosphere (for both the Arctic and the Antarctic) has been also documented by other authors (e.g. Lahoz et al., 1993; Manney et al., 1994; Schoeberl et al., 1995).

Manney et al. (1999) applied the 2-D equivalent latitude-theta picture to tracer data (CH_4 and total nitrogen, NO_y) from the ATMOS mission to study the Arctic and Antarctic stratospheric polar vortex in late winter and spring. They showed evidence for strong descent in the polar vortex in the upper stratosphere, weaker descent at lower altitudes, and evidence of greater descent at the edge of the polar vortex than at the centre of the polar vortex. These results confirm the general picture provided by the 1-D along-orbit track picture discussed above.

In an extension of the work in Lahoz et al. (1996), Lahoz et al. (2006) applied the along-track orbit picture to Envisat MIPAS H_2O, CH_4 and N_2O tracer data throughout the stratosphere to study the evolution of the Antarctic winter stratosphere; this included comparison of these data against meteorological data from the Met Office and PV analyses from ECMWF. The CH_4 field in the stratosphere has a vertical and latitudinal distribution similar to that of N_2O (but opposite to that of H_2O), as their stratospheric sources and sinks are similar in nature. Lahoz et al. (2006) documented and analysed a number of salient dynamical and transport features: (i) merger of anticyclones in the Antarctic stratosphere; (ii) development of an intense, quasi-stationary anticyclone in spring; (iii) top-down breakdown of the polar vortex; (iv) systematic descent of air into the polar vortex; and (v) formation of a three-dimensional structure of a tracer filament on a planetary scale. This work confirmed and extended the paradigms of the Antarctic polar vortex temporal evolution and spatial characteristics identified previously in Lahoz et al. (1996) and references therein.

A study of the Antarctic final warming was performed by Orsolini et al. (2005). They used Envisat MIPAS observations of H_2O and ozone to study the period (October – November) after the major warming that took place in the Antarctic in September 2002; these were combined with meteorological analyses from ECMWF and the Met Office. The 2002 Antarctic final warming occurred early, following an unusually active winter and the first recorded major warming in the Antarctic (Roscoe et al., 2005). Mapped H_2O and ozone data from MIPAS and analysed PV, displayed on potential temperature surfaces, showed the break-up of the polar vortex. A large tongue of vortex air was pulled out westward and coiled up in an anticyclone, while the vortex core remnant shrank and drifted eastward and equatorward over the South Atlantic. By roughly mid-November, the vortex remnant at 10 hPa had shrunk below scales resolved by the satellite observations, while a vortex core remained in the lower stratosphere. Comparison with other satellite data (HALOE, POAM III, and SAGE II and SAGE III), and with fine-scale fields derived from reverse-trajectories based on MIPAS or climatological data, confirmed these features seen in the MIPAS data. This confirmed the value of, first, comparison between various satellite datasets (the same species; different but complementary species) and, second, comparison between satellite datasets and other complementary data, in this case from reverse-trajectories. A comparison between trajectory calculations and observed tracer fields from UARS MLS (H_2O) and UARS CLAES (N_2O, CH_4) performed by Manney et al. (1995b) showed that large-scale features agreed well, supporting the utility of trajectory calculations for diagnosing tracer transport in the wintertime polar vortex (for both the Arctic and the Antarctic).

Other tracers besides H_2O, N_2O and CH_4 have been used to study transport in the middle atmosphere. For example, the long-lived nature of CO allows it to be a very useful diagnostic of transport, particularly in the upper stratosphere and mesosphere, since the mixing ratio of CO increases with altitude due to CO_2 photolysis. Allen et al. (1999) used ISAMS CO observations to study the evolution of the polar stratosphere during the January 1992 major warming (stratospheric warmings are discussed immediately below) and Allen et al. (2000) examined the Antarctic polar region. Clear evidence of planetary wave-induced transport of CO was observed in both hemispheres, and descent rates calculated from ISAMS CO for the Antarctic from April to July 1992 were consistent with diabatic trajectory analyses.

An UARS climatology for the tracers H_2O and CH_4 compiled from HALOE, CLAES and UARS MLS for the period 1991-1997 (Randel et al., 1998) revealed well-known seasonal variations with unprecedented detail, and which have been described above. In particular, the data showed during winter and spring: (i) the presence of enhanced latitudinal gradients (mixing barriers) in the sub-tropics and across the polar vortices; and (ii) strong descent inside the polar vortices.

Stratospheric warmings. A dynamical phenomenon generally associated with the Arctic polar stratosphere is that of the major stratospheric warming (Charlton and Polvani, 2007), which tends to occur with regularity in midwinter or late winter. The major stratospheric warming is a significant dynamical event that dramatically disrupts the typical wintertime circulation of the stratosphere, and affects the location of the polar vortex and its temporal evolution during winter. After a major warming the polar vortex may recover; if the major warming occurs late in winter, the polar vortex may not fully recover and decay as the final warming takes place.

Major warmings can be classified as vortex displacement (also wavenumber-1) or vortex split (also wavenumber-2) events. During these events the polar vortex is strongly disrupted, and in the mid stratosphere (e.g. 10 hPa) polar temperatures increase dramatically over a few days and zonal mean zonal winds reverse sign from westerly to easterly at latitudes poleward of 60^{o}N; wintertime warmings that do not satisfy this criterion are termed minor warmings. Minor warmings can occur in the Arctic and the Antarctic winter stratosphere. The major stratospheric warming phenomenon was discovered using ground-based temperature observations made at Berlin (Scherhag, 1952). In contrast to the situation in the Arctic, since records began, only once (in September 2002) has a major warming been documented in the Antarctic winter stratosphere (see, e.g., Roscoe et al., 2005). Because the major warming that took place in the Antarctic in September 2002 was associated with the split of the Antarctic ozone hole, studies of this phenomenon using satellite data focused on the information provided on the stratospheric ozone distribution: from the ozone data itself, and from photochemical data and tracer data. These studies confirmed the usefulness of satellite data for studying a major warming event. They were published in a special issue of the Journal of Atmospheric Sciences (Vol. 62, March 2005).

Although the major warming of February 1979 was described using LIMS data (see, e.g., Leovy et al., 1985), only in the past few years have sufficient satellite data and meteorological data been available to thoroughly study the dynamics and transport during a major stratospheric warming throughout the upper troposphere to the mesosphere. These recent studies have investigated major stratospheric warmings using satellite observations of tracers; meteorological analyses of geopotential height, temperature and horizontal winds; and fields of PV derived from meteorological analyses. An example of the application of these data to the study of major warmings is provided by Manney et al. (2009), who studied the major stratospheric sudden warming that took place in the Arctic winter in January 2009.

The major stratospheric sudden warming in January 2009 was the strongest and most prolonged on record. Manney et al. (2009) used Aura MLS observations of CO, H_2O and N_2O in the stratosphere and mesosphere (in potential temperature, levels between 400 K and 2500 K) to provide an overview of dynamics and transport during the major warming. Manney et al. (2009) used the 2-D equivalent latitude-theta approach for their analysis. This work built on a study of the major warming in January 2006 by Manney et al. (2008), which used temperature (and wind and geopotential height) observations from the Aura MLS and SABER instruments, and analysed meteorological and PV fields from ECMWF and the Goddard Earth Observing System, GEOS-5.

In the study of Manney et al. (2009), the 2006 and 2009 major warmings were compared and contrasted. This included quantifying the amount of mixing of trace gases from high latitude and mid latitude air masses during the major warming; documenting the decay of polar vortex fragments and the persistence of vortex (cyclone and anticyclone) fragments; and documenting the impact of the major warmings on the stratospheric temperature distribution and descent rates in the polar vortex. The work in Manney et al. (2009) was extended by Lahoz et al. (2011a) using Envisat MIPAS measurements of H_2O and H_2O analyses produced by assimilation of MIPAS H_2O data into the BASCOE chemical data assimilation system (Errera et al., 2008). The results from Lahoz et al. (2011a) were consistent with those of Manney et al. (2009), and demonstrated the advantages of using data assimilation for studying the stratosphere – more details of the application of the data assimilation method to studying the middle atmosphere are provided in Sect. 4.

Summertime circulation. To understand the summertime circulation in the stratosphere it is helpful to understand the transition between the wintertime and summertime circulations. This is associated with the break-up of the wintertime polar vortex, the final warming. In the Arctic, the polar vortex break-up is typically much earlier and more abrupt than that in the Antarctic (e.g., Waugh and Randel, 1999), often triggered by stratospheric sudden warming events. Of particular interest in studies of the final warming is how high and mid latitude air masses (typically, containing relatively low and relatively low ozone amounts, respectively) mix after the break-up of the polar vortex. One motivation for these studies is concern that low ozone values in summertime (e.g. from low ozone events, LOEs) can impact human health and ecosystems, e.g., through erythemal UV dose enhancement at high Arctic latitudes (Jackson et al., 2003) and at high Antarctic latitudes (Orsolini et al., 2011).

The spatio-temporal characteristics of the summer middle atmosphere have been relatively little studied compared to those of the winter middle atmosphere; this is reflected in that relatively few studies have been made of the summertime circulation (dominated by the summertime high, an axi-symmetric anticyclone centred over the Pole) using research satellite data. Although research satellite data have been available, or are available, to study the summertime circulation, the interest on ozone depletion (WMO, 1999) has tended to focus research using these data on the wintertime stratosphere. However, over the last ten years the value of measurements of long-lived tracers for studying the summer stratosphere has been recognized (Orsolini, 2001), and a number of studies of the summertime circulation, including the transition between the wintertime and summertime circulations, have been performed. For example, the dynamics and chemistry of the summer stratosphere have been discussed, respectively, by Wagner and Bowman (2000) and Fahey and Ravishankara (1999); the dynamics and chemistry of springtime vortex remnants in the Arctic have been studied by Konopka et al. (2003).

FrIACs. In a study of the final warming of the Arctic winter of 2005, Aura MLS tracer observations of H_2O and N_2O were used to discover a hitherto unreported phenomenon, that of the "frozen-in anticyclone", FrIAC (Manney et al., 2006). Manney et al. (2006) analysed the tracer data by constructing 2-D isentropic maps from the Aura MLS along-track orbit data. The FrIAC contained relatively high N_2O values and relatively low H_2O values. It was a remnant of the high latitude anticyclone present during the Arctic winter (the Aleutian High). The main features of the FrIAC were its vertical coherence (initially it extended from 25 km to 45 km in the stratosphere) and its persistence well into the Northern summer (late August), although by early summer it had become weaker at higher levels in the stratosphere. A feature similar to the FrIAC is that of a low ozone pocket, seen in the wintertime stratosphere (e.g. Harvey et al., 2004), where high ozone amounts from low latitudes are confined in an anticyclone at high latitudes. Because of the photochemical properties of ozone in the stratosphere (in contrast to those of the tracers H_2O and N_2O), ozone amounts in the low ozone pocket quickly relax to values consistent with local sunlight conditions.

Allen et al. (2011) extended the work of Manney et al. (2006) by comparing Aura MLS N_2O data for the period after the break-up of the 2005 Arctic winter vortex with simulations from various transport models. Allen et al. (2011) identified three phases during the evolution of the 2005 FrIAC: (i) the "spin-up phase" in late winter/early spring; (ii) the "anticyclonic phase" in spring; and (iii) the "shearing phase" in summer. Comparison between Aura MLS N_2O data and model simulations provided an important test of the understanding of the chemistry and transport responsible for the development and maintenance of the FrIAC. Confronting models with observations is a key feature of data assimilation (Lahoz et al., 2010) and will be discussed in Sect. 4.

Work on FrIACs was further extended by Thiéblemont et al. (2011), who used Aura MLS N_2O, H_2O and ozone data for the northern spring and summer of 2007. Their focus was the role of structures such as FrIACS in the balance between chemical and dynamical processes associated with the ozone budget (in Sect. 3.2 we discuss the roles of dynamics and chemistry in determining the ozone distribution in the middle atmosphere). To better understand the dynamical conditions required for FrIACs and associated processes, Thiéblemont et al. (2011) constructed a climatology of tropical air mass intrusions using a PV contour advection model. This climatology revealed a preferred path for exchanges between the polar and tropical stratospheres. Using ERA-interim wind and temperature reanalyses from ECMWF, Thiéblemont et al. (2011) were able to establish links between FrIAC occurrences and Rossby wave activity. Furthermore, they found evidence that FrIACs could exist if no major sudden stratospheric warmings occurred during the polar vortex phase, and their development appeared favourable if the tropical QBO was in the easterly phase. In a further paper, Allen et al. (2012) identified an unusually large FrIAC in 2011, studied links between the FrIAC and the final warming, and compared and contrasted the FrIAC with those from other years.

Lahoz et al. (2007b) used CH_4 tracer and ozone data from Envisat MIPAS, supplemented by meteorological data from the Met Office and PV analysed fields from ECMWF, to study the evolution of the Arctic stratosphere during spring and summer, focusing on the evolution of the summertime high. Lahoz et al. (2007b) used both the along-track orbit and equivalent latitude-theta pictures. This paper found evidence in the CH_4 data for the FrIAC feature described by Manney et al. (2006) (identified by relatively high values of CH_4), and of the slowness of isentropic mixing processes in the mid and upper stratosphere during summertime. The results for the CH_4 and PV data were consistent (e.g. relatively high CH_4 values and relatively low PV values were seen in the FrIAC), and provided robustness to inferences regarding the FrIAC made from the satellite tracer data (similar consistency is found between satellite tracer data and the PV data for the wintertime stratosphere). The ozone data showed that as the summertime high became dominant during June–August, net photochemical ozone loss produced a low ozone pool in the lower and mid stratosphere. (A similar feature was documented by Orsolini et al. (2003) from ozone analyses derived from the assimilation of GOME total column ozone data.) As the summertime high decayed and the wintertime polar vortex built up from September onward, the low ozone pool extended vertically throughout the stratosphere, and the tracer isopleths at high latitudes started to dip, showing the effects of wintertime diabatic descent as the stratospheric circulation changes from summer to winter conditions

Filamentary structures in the stratosphere. One potential problem with satellite tracer data regarding their ability to study stratospheric transport phenomena is their relatively low spatial resolution, which can mean that fine structures (e.g. filaments) can be missed. One way to address this shortcoming is to use the technique of back trajectories to construct high-resolution tracer fields from low-resolution satellite observations. Sutton et al. (1994) applied this technique to N_2O observations from ISAMS. The resulting high-resolution tracer fields revealed fine-scale transport features such as mixing equatorward of the polar vortex, in the surf zone, and a complex pattern of transport in the Aleutian High, where low latitude and mid latitude air mix and persistent filamentary structures are seen.

Fully Lagrangian particle advection methods have shed some light on the nature of the stratospheric transport barriers (WMO, 1994). However, due to ambiguity in the choice of initial and end states and due to the lack of a useful flux gradient relationship, it is difficult to build a coherent picture of how the tracer transport is occurring. A conceptual leap in quantifying and understanding these transport processes has been facilitated by the modified Lagrangian mean (MLM) diagnostics introduced by Nakamura (1996).

The key diagnostic quantity that results from this approach is the equivalent length, which is a measure of the geometric structure of the tracer field, being large for complex structure and small for simple structure. It is also, in effect, a measure of the actual length of the tracer contour. Therefore, increasing equivalent length enhances mixing by making a larger interface available for microscale diffusion. Equivalent length in the stratosphere is enhanced mainly through chaotic advection (stirring), such as that due to large-scale planetary waves. In the MLM framework, the equivalent length multiplied by the microscale diffusion coefficient can be thought of as a Lagrangian effective diffusivity, analogous to the Eulerian eddy diffusivity K_{yy}. The advantage of this approach is that barriers to horizontal mixing are easily identified by minima in equivalent length, and the strength of a barrier is determined by the depth of the minima. Conversely, regions with large equivalent length are identified as regions of significant isentropic mixing.

Early applications of the equivalent length concept to the real atmosphere were done using long-lived tracers N_2O and CO both from satellite observations and 3-D models (Nakamura and Ma, 1997; Allen et al., 1999). In order to provide a more coherent global picture with continuous temporal coverage, later studies used passive tracer simulations as the test field for calculating the MLM diagnostics (Haynes and Shuckburgh, 2000a, b; Allen and Nakamura, 2001).

The conceptual and computational advantages afforded by the MLM diagnostics have significantly increased understanding of mixing processes in the stratosphere. It is expected that these tools will continue to provide useful information for future modelling and observational work. A further step has been made by Nakamura (2001) in formulating a diagnostic called "mixing efficiency", analogous to equivalent length, that can be defined for particular geographical regions, rather than for equivalent latitude surfaces. Application of equivalent length along with this new diagnostic will continue to provide further insight into the transport processes that affect the stratospheric ozone distribution.

Mesosphere-stratosphere coupling. Coupling between the mesosphere and stratosphere is an area of increasing interest, chiefly because the former is a source region of key stratospheric species such as NO_x (= NO + NO_2), which is the major driver for catalytic ozone loss in the mid stratosphere (Brasseur and Solomon, 2005). Research satellite data from Envisat MIPAS and ADEOS-II ILAS-II have been used to document transport between the mesosphere and the stratosphere (see, e.g., Funke et al., 2005; Ejiri et al., 2006; Juckes, 2007). However, Lahoz et al. (2009) argue that these studies have not looked in sufficient detail at this transport, and have not identified the elements of this transport; for example, detailed explanation is not forthcoming for anomalous features in the CH_4 distribution for southern autumn where the vertical gradient is reversed. Such identification and explanation is crucial for a proper understanding of mesosphere–stratosphere coupling.

Lahoz et al. (2009) use Envisat MIPAS CH_4 data, supplemented by meteorological analyses from the Met Office and ECMWF, to study the middle atmosphere during southern autumn (March – June 2003). They use the along-track orbit picture. Based on these data they hypothesize that the CH_4 distribution can be explained as a combination of two transport processes: (i) isentropic transport in the lower mesosphere and upper stratosphere of CH_4-rich air from low/mid latitudes to high latitudes during early autumn, and (ii) diabatic descent at high latitudes of CH_4-poor air from the lower mesosphere during autumn. Calculations of stratospheric effective diffusivity (Allen and Nakamura, 2001) provide broad support for this hypothesis. The CH_4 along-track orbit data are shown to provide more information than studies using spatial and temporal averages of the same MIPAS CH_4 data, and to explain anomalous features in the CH_4 distribution, where the vertical gradient is reversed. These results show the value of comparing observed quantities (e.g. CH_4 MIPAS data) and simulated quantities (e.g. effective diffusivity) for strengthening inferences made on atmospheric processes.

3.2 The role of chemistry and transport in determining the stratospheric ozone distribution

Introduction. The distribution of ozone in the stratosphere is determined by transport and chemistry (photochemistry and heterogeneous chemistry) processes (WMO, 1999). Since the discovery of the Antarctic ozone hole (Farman et al., 1985) it has been of interest to quantify the contributions of transport and chemistry to ozone depletion in both the Antarctic and the Arctic. Quantification of these contributions has been made possible by various observational platforms of the middle atmosphere, including UARS, Envisat and EOS Aura (see Table 1). This observational information has been complemented by, first, meteorological data, and second, information from model simulations of the middle atmosphere (either from a chemistry transport model, CTM, a general circulation model, GCM, or from trajectory calculations). Combination of observational, meteorological and model information has helped to further our understanding of the processes contributing to ozone depletion, and quantify this ozone depletion.

Stratospheric processes. Measurements of ozone and various tracers from UARS MLS provided one of the first examples of the value of research satellite for studying Antarctic and Arctic ozone loss. Early results from UARS MLS included the first global maps of stratospheric ClO (Waters et al., 1993), the predominant form of chemically-reactive chlorine in the destruction of stratospheric ozone. These results showed the lower stratosphere polar vortex was filled with ClO in the regions where ozone was depleted, confirming earlier conclusions from ground-based and aircraft measurements that chlorine chemistry is the cause of the Antarctic ozone hole. Waters et al. (1993) showed that ClO in the Antarctic polar vortex can become enhanced by June (early Antarctic winter), and that ozone destruction by ClO is masked in early Antarctic winter by diabatic descent in the polar vortex of relatively ozone-rich air – an indication of the need to disentangle transport and chemistry processes when attributing ozone depletion and quantifying it (methods used to do this are discussed below). Waters et al. (1993) also used UARS MLS ClO data to quantify ozone depletion during Arctic winter - more recently, Manney et al. (2011) used Aura MLS ozone, HNO_3, HCl and ClO, together with PV analysed fields, to document substantial ozone loss (comparable to that of the Antarctic ozone hole) in the Arctic winter of 2010-2011. In a demonstration of the value of combining observational and model information for understanding ozone depletion, results from 3-D CTMs (Douglass et al., 1993; Geller et al., 1993; Lefèvre et al., 1994) produced shortly after the UARS MLS data were obtained, showed the observed distribution of enhanced Arctic ClO was consistent with CTM predictions. Furthermore, the value of trajectory studies for understanding ozone depletion was demonstrated in the work of Schoeberl et al. (1993), who found a clear relationship between predicted polar stratospheric cloud (PSC) formation and enhanced Arctic ClO observed by UARS MLS.

Definitive evidence of loss of Arctic ozone due to chemistry associated with enhanced ClO was provided by analyses of combined UARS MLS and CLAES data by Manney et al. (1994). Additional confirmation of the paradigm of chemical processing by PSCs leading to activation of stratospheric chlorine was shown in the analyses of Arctic UARS CLAES, MLS and HALOE data by Geller et al. (1995), and in Antarctic UARS MLS and CLAES data by Ricaud et al. (1995). Differences between the Arctic and Antarctic winter polar vortex ozone conditions as deduced from UARS MLS observations were described by Santee et al. (1995), and as deduced from combined UARS MLS, CLAES and HALOE data were described by Douglass et al. (1995).

The ozone stratospheric distribution is determined by both transport and chemistry (photochemistry, and chemistry on the surface of PSCs), with the stratospheric regions were these are dominant dependent on transport and chemical timescales (WMO, 1999).Transport timescales dominate in the lower stratosphere, except in ozone hole conditions; chemical timescales dominate in the upper stratosphere; and transport and chemical timescales are comparable in the mid stratosphere.

Randall et al. (1995) used POAM III ozone data to elucidate the different roles of photochemistry and dynamics in determining the stratospheric ozone distribution. Two results from this work were a transition between summertime photochemical control and dynamical control around 25 km, and that ozone mixing ratios inside the Arctic wintertime polar vortex were indicative of enhanced descent within the vortex, as well as other dynamical processes and possibly chemical loss. The temporal evolution of MIPAS ozone data in the Antarctic wintertime stratosphere (e.g. Lahoz et al., 2006) reflects the roles transport and chemistry play in determining the ozone stratospheric distribution, including the role of the polar vortex break-up and mixing of high latitude ozone-poor air (associated with ozone loss in the polar vortex coupled to the wintertime isolation of the polar vortex) and mid latitude ozone-rich air (associated with ozone production due to the Chapman photochemistry cycle).

Pockets of low ozone have been observed in many occasions in anticyclones at mid to high latitudes in the middle stratosphere (Leovy et al., 1985; Rood et al., 1993; Manney et al., 1995a; Harvey et al., 2008). Trajectory calculations performed by Morris et al. (1998) show that much of the air within the pockets originates in the tropics or sub-tropics at higher levels several weeks earlier. Their results show that the development of the low ozone pockets can be explained by current understanding of chemistry and dynamics. The primary mechanism responsible for the development of these low ozone regions is the isolation of air at high latitudes for periods of time long enough that significant ozone loss toward local photochemical equilibrium can occur. Such behaviour is different from that of the surrounding air masses that move from mid to high latitudes and back again over the course of a few days. The dynamical behaviour associated with these latter air masses results in ozone concentrations more consistent with lower latitude photochemical equilibrium values. Nair et al. (1998) showed that a Lagrangian photochemical model was able to reproduce the observed formation of low ozone pockets at mid stratosphere levels. They deduced that the rapid ozone loss localized in these pockets was due to a decrease in the odd oxygen production rate and not to an increase in the loss rate by reaction with halogen species, as in the standard ozone hole scenario.

Quantifying ozone loss. To determine the variation of ozone due solely to chemical processes, dynamical and chemical variations must be separated in the observed ozone fields (here we focus on satellite data). Four methods have primarily been used to isolate photochemical loss (see, e.g., Harris et al., 2002; Rex et al., 2002; Newman and Pyle, 2003). These methods are described below.

The Lagrangian "Match" technique uses multiple sampling of an air mass by measurements to infer ozone loss along the assumed trajectory (Rex et al., 2003, and references therein). "Matches" occur when trajectories indicate that the same air parcel is observed multiple times by one or more instruments, within some prescribed tolerance limits. If the polar vortex is sampled homogeneously, the ozone loss result reflects vortex average conditions (Harris et al., 2002).

The "Tracer Correlation" technique removes the effect of transport by comparing the pre-winter and post-winter relationships between ozone volume mixing ratio and a tracer, such as N_2O or CH_4, inside the polar vortex (Proffitt et al., 1990; Müller et al., 1997, 2001). This method assumes that in the absence of ozone production or loss, the ozone/tracer relationship remains constant; thus, any post-winter deviations from the pre-winter relationship are interpreted as chemically induced.

The "Vortex Average" technique quantifies dynamical variation of an average ozone profile inside the polar vortex by calculating vortex average descent rates from a radiative transfer model. This technique assumes that the dynamical contribution to ozone change inside the vortex is dominated by diabatic descent (Sect. 3.1 discusses the observational evidence for diabatic descent in the polar vortex), and that mixing between vortex and extra-vortex air is minimal; therefore, only vertical transport is considered (Hoppel et al., 2002). This method requires that the vortex edge be defined (the vortex edge is often assumed to be at the location of the maximum of the westerly winds circumscribing the polar vortex, but other definitions exist – see Nash et al. (1996)). A modification of this approach involves estimating horizontal mixing across the vortex edge; however, such calculations can incur significant errors (see, e.g., Jackson and Orsolini, 2008).

The "Passive Subtraction" technique requires ozone to be simulated as a passive tracer. This method compares observed ozone with a reference field which represents the evolution of ozone in the absence of chemical depletion (see, e.g., Manney et al., 1995b, 2003; Goutail et al., 1997; Deniel et al., 1998; Hoppel et al., 2002; Singleton et al., 2005). Note that Manney et al. (2011) used several versions of this method to quantify the unprecedented ozone loss that took place in the northern winter of 2010-2011. Typically, an ozone reference field for the stratosphere is initialized from climatology or observations, and passively transported through the winter using an off-line model forced by meteorological analyses. To separate the effects of ozone transport, the reference ozone is then subtracted from the ozone observations. The reference ozone can also be pseudo-passive, with heterogeneous chemical reactions on PSCs switched off, but gas phase catalytic cycles still active. The approach of assuming the ozone to be pseudo-passive is suitable at longer timescales (greater than around a month) and also in the mid and upper stratosphere, where the impact of NO_x chemistry is greater.

To address some of the shortcomings of the vortex-averaged method mentioned above, namely, the definition of the vortex edge, and estimates of mixing across the vortex edge, Jackson and Orsolini (2008) have assimilated ozone data from Aura MLS and SBUV/2 into the Met Office assimilation system to estimate ozone loss in the Arctic winter stratosphere (a similar study was also carried out by Rösevall et al., 2008). Their results show that the data assimilation method is very promising and can lead to potentially more accurate ozone-loss estimates than the established methods mentioned above. A follow-on study (Sovde et al., 2011) showed the benefit of using the 4-D variational method (4D-Var) instead of 3D-Var in assessing ozone loss using data assimilation notions. El Amraoui et al. (2008) also used data assimilation notions to estimate ozone loss in the polar vortex – they assimilated ozone and N_2O fields from Aura MLS into the MOCAGE-PALM assimilation system, and used the information on N_2O (a passive tracer) to remove the contribution from diabatic descent to the ozone distribution. Section 4 provides more details of the application of data assimilation notions to studying the middle atmosphere.

4 The role of data assimilation in understanding the middle atmosphere

We have two broad sources of information for the middle atmosphere: (i) measurements (“observations”); and (ii) understanding of the temporal and spatial evolution of the atmosphere (“models”). Observations (or measurements) sample the middle atmosphere in space and time, with spatial and temporal scales dependent on the technique used to make the measurements (e.g. satellites, ground-based). These measurements provide information on the middle atmosphere and contribute to building an understanding of how it evolves in space and time.

To make use of the information embodied in observations and models it is necessary to understand the characteristics of this information. One characteristic is that both observations and models have errors, namely, systematic, random and of representativeness. These are discussed in some detail in Lahoz et al. (2010). Another key feature of observations is that they are discrete in space and time, with the result that the information provided by observations has gaps. It is desirable to fill the gaps in the information provided by observations: first, to make this information more complete, and hence more useful; second, to provide information at a regular scale to quantify the characteristics of this information. Information at an irregular scale can be quantified, but this procedure is more tractable when done with a regular scale. An objective method to fill in the observational gaps is data assimilation (see, e.g., Kalnay, 2003; Lahoz et al., 2010). Data assimilation combines the information from the observations and the prior knowledge of the state of the atmosphere (and their associated errors), the latter typically embodied in a numerical model.

Data assimilation of research satellite data is increasingly being used to study the middle atmosphere, notably to provide analyses of, e.g., ozone and tracers such as H_2O, that help study middle atmosphere phenomena such as the evolution of the polar vortex, major warmings, or the final warming (see Sect. 3.1); estimate descent rates in the polar vortex (see Sect. 3.2); quantify ozone loss (see Sect. 3.2); and perform budget studies of species such as ozone (see Sect. 3.2). The review by Lahoz and Errera (2010) includes a comprehensive list of references in this area. As shown in Lahoz et al. (2011a), data assimilation produces analyses that add value to both observations and models: to observations by filling in observational gaps; to models by constraining them with observations; to observations and models by producing datasets that are closer to independent data than the observational and model information input into the data assimilation system.

We illustrate the role data assimilation plays in middle atmosphere studies by posing two questions that data assimilation helps address. These questions are: (i) What is the “best” estimate of the atmospheric state? and (ii) What is the incremental value of observations from a proposed instrument?

What is the “best” estimate of the atmospheric state? To answer this question we must address the following issues: the nature of the atmospheric system under study, in this example concerning ozone and/or other variables (chemical species, meteorological quantities) in the middle atmosphere; that obtaining the best estimate, i.e., the analysis, requires combination of observational and model information, including their errors; and that there is a need to define what is the best way of combining the observational and model information. Many publications provide evidence of how the analyses obtained in data assimilation of ozone and tracer species add value (i.e., provide benefit) to the observational and model information used as input in the method (see, e.g., Lahoz and Errera, 2010; Lahoz et al., 2011a). Note, however, that analyses generally obtained using data assimilation are sub-optimal due to the models and observations being biased and/or having non-Gaussian errors. However, arguably, using data assimilation is the best we can do.

Besides finding the analysis, it is important to assess the quality of the analysis. To address this we need to consider the following issues: that a model has several components, e.g., transport and chemistry; and that (as stated above) analyses are a combination of observational and model information, including their errors. When addressing the quality of the analysis we thus have to consider the quality of the elements that comprise it, i.e., the observational and model information that goes into providing the analysis. To do this we need to consider the following: (i) the consistency of observational data, e.g., whether observations of different stratospheric tracers such as H_2O, CH_4 and N_2O are consistent among themselves (see, e.g., discussion in Chipperfield et al., 2002); (ii) looking at the self-consistency of data (observational or model) using data assimilation diagnostics - this tests, for example, whether prior assumptions on observational and/or model errors are correct (e.g. Struthers et al., 2002; Jackson, 2007); (iii) comparison of the analyses against independent data (i.e., data not used in the assimilation procedure) – this provides an estimate of biases in the observations and/or the model (e.g. Geer et al., 2006); and (iv) observational data monitoring - this looks at whether observational data characteristics change in time (e.g. Štajner et al., 2004). The evaluation of data assimilation analyses (points (ii) and (iii) above) is discussed in detail in Talagrand (2010).

By assimilating different sets of ozone observations, Jackson (2007) was able to infer information both about the impact of the assimilated observations and on the quality of the assimilation system. He showed that assimilating SBUV data alone degraded ozone analysis in certain locations (such as the polar vortex edge and near the tropopause) compared to a reference assimilation experiment where no ozone data were assimilated and the analysed ozone was simply advected by assimilated winds. Only with the addition of Aura MLS observations was the quality of the ozone analyses considerably improved. This study showed that: (i) at the level of current understanding high quality, high vertical resolution observations such as Aura MLS are key to producing accurate ozone analyses; and (ii) the difficulty in accurately representing background error covariances combined with the low vertical resolution of observations such as those from SBUV will lead to poor ozone analyses.

Another solution is to perform an intercomparison of analyses (see Geer et al., 2006, 2007). An advantage of an intercomparison of analysis systems is that it can reveal shortcomings more quickly than an investigation focusing on just one analysis system. Geer et al. (2006, 2007) discuss two intercomparisons of ozone analyses in which most of the data assimilation systems involved assimilated Envisat MIPAS ozone profiles (one system assimilated Envisat SCIAMACHY total column ozone). These intercomparisons revealed a number of features of interest when developing an ozone data assimilation system: (i) only analyses that correctly modelled heterogeneous ozone depletion were able to reproduce the ozone destruction over the South Pole – this was independent of whether the model included a relatively simple Cariolle scheme (Cariolle and Déqué, 1986) or a comprehensive chemical scheme; (ii) where some models performed better than others, in general, the improved performance could be explained by better modelling of transport and chemistry; and (iii) it is important to account for observational and model resolution when comparing analyses against independent data, e.g., taking account of the different vertical resolutions of the MIPAS ozone data assimilated and the independent ozonesonde data used for evaluation.

The general conclusions drawn from the intercomparison described in Geer et al. (2006) were that for ozone data assimilation systems developed in the timeframe of 2005 and later, and in regions of good data quality and coverage, similarly good ozone analyses are obtained regardless of the data assimilation method, or the model used. In the intercomparison described in Geer et al. (2006) this reflected the generally good quality of the MIPAS ozone observations.

What is the incremental value of observations from a proposed instrument? To answer this question we need to consider the following: what new observations are of interest; what is the likely nature of the future GOS (this includes building on information provided by the current GOS) and what are the errors of the observing platforms; and that although, in principle, adding new information should be beneficial, this may not always be the case (see, e.g., Rood, 2010). Thus, as well as testing the incremental value of new observations, we are also testing the current data assimilation system. A solution is to set up an observing system simulation experiment, OSSE (Masutani et al., 2010a, b) to test if adding a new observation has a significant impact. OSSEs are related to observing system experiments (OSEs), where one assesses the incremental value of existing observations (Masutani et al., 2010b). OSEs are extensively used by the meteorological agencies to assess the relative contribution to the skill of the NWP forecast of each element of the GOS (see Talagrand, 2010).

OSSEs are well-established in the work of the meteorological agencies, and over the last ten years have become increasingly established in the work of the research space agencies (e.g. at ESA and NASA). In both cases, OSSEs are used to assess the value of potential additions to the GOS, for example from satellites (operational and/or research). However, the object of the OSSEs is different: for the meteorological agencies it is to assess whether there is significant improvement in the skill of the NWP forecast; for the space agencies it is to assess whether there is significant improvement in the information provided on the Earth System (e.g. from fields of stratospheric ozone or stratospheric winds; from air quality information, e.g., ozone fields, in the lowermost atmosphere). Examples of the use of OSSEs by the space agencies include assessment of the value of lower stratospheric horizontal wind speed information from ESA's ADM-Aeolus (Stoffelen et al., 2006); and assessment of the value of stratospheric ozone and horizontal wind information from the formerly proposed (but now shelved) CSA's SWIFT instrument onboard the CHINOOK platform (Lahoz et al., 2005). Regarding the middle atmosphere, OSSEs are also being planned for the proposed EE-7 PREMIER satellite, in this case on gravity wave information provided by temperature measurements of the stratosphere (Lahoz et al., 2011b).

OSEs and OSSEs benefit from conceptual simplicity, but can often be expensive to run. Accordingly, alternative methods for assessing the impact of observations have been developed. For example, Cardinali et al. (2004) developed influence matrices which were used to show the impact of subsets of observations within a data assimilation system. Furthermore, in OSSEs the estimated absolute observation impact is obtained through comparison with a simulated reference atmosphere (called the Nature Run). Such comparison has associated short-comings, including the realism of the Nature Run, and likely overoptimistic results if the same model is used to create the Nature Run and perform the OSSE (see discussion in Masutani et al., 2010a). These shortcomings can be overcome by instead assessing the impact of new observations using ensembles (e.g. Tan and Andersson, 2005), which does not require a reference atmosphere. Although not yet directly applied to the stratosphere, the abovementioned methods may potentially be used as an alternative to OSSEs in the future.

Summary of the role of data assimilation in research satellite missions. It is recognized that space agencies involved with research satellite missions (current and future) should position data assimilation at the centre of their activities. In particular, data assimilation should be used for:

(i) Adding value to satellite data by combining observational and model information;
(ii) Providing the "best" estimate of the state of the middle atmosphere;

(iii) The objective evaluation of the incremental value of current satellite data (using OSEs); and
(iv) The objective evaluation of the incremental value of future satellites (using OSSEs or similar methods).

5 Discussion and forward look

The examples discussed in Sect. 3 show how research satellite data over the last 30 years has provided insight into our understanding of the spatio-temporal characteristics of the middle atmosphere, notably on the evolution of the wintertime stratosphere and the summertime circulation (Sect. 3.1); and the role of transport and chemistry processes in determining the stratospheric ozone distribution (Sect. 3.2). These insights have come from the observational capabilities provided by a wealth of satellite platforms (see Table 1 in Sect. 2.2) and, in particular, from the extensive use of observations of tracer and chemical species together with meteorological information (temperature, winds, geopotential height) and PV analyses derived from meteorological information. The use of model information, e.g., from CTMs or GCMs, and its comparison against observational information, has also contributed toward this understanding, in particular by providing a means to test hypotheses.

In Sect. 4 we discuss the role data assimilation plays toward our understanding of the middle atmosphere. In Sect. 4 we illustrate how, by combining observational and model information (and their errors), data assimilation adds value to either of these pieces of information. The synergistic use of satellite observational information and model information with meteorological information, as well as the objective way in which data assimilation brings together this information, is crucial to our understanding of the middle atmosphere.

Notwithstanding the insights on the middle atmosphere gained from wealth of research satellite data in the last 30 years, maintaining a capability to observe the middle atmosphere from satellite platforms is essential to continue to benefit from these insights. This means continuing the line of research satellite platforms that runs from LIMS and TOMS to the Envisat and EOS Aura missions, via the UARS mission. Beyond Envisat and EOS Aura there are plans for the Sentinel-4 and -5 platforms, as well as for the Sentinel-5 precursor to fill in the gap between Envisat and EOS Aura and the geostationary (GEO) MTG and the low Earth (LEO) orbit post-EPS satellite platforms. It is essential that temporal gaps in the satellite record of the middle atmosphere are filled in or, at least, reduced.

As well as filling in or reducing the temporal gaps in the satellite record, it is important to make the best use of the research satellite, including the use of multiple satellite platforms (an example of this concept is the A-train; http://www.nasa.gov/mission_pages/a-train/a-train.html); the use of different satellite platforms to provide observational information of the same variable (e.g. ozone, tracer species); the evaluation of the satellite data; and confronting model information with observational information. Furthermore, it is also important to continue to combine meteorological data with research satellite data, as well as use data assimilation to add value to observational and model information.

Finally, it is important to assess additions to the future GOS for the middle atmosphere, in particular to quantify the additional benefit from satellite platforms (GEOs/LEOs), relative to other satellite platforms, and relative to in situ data (e.g. ground-based observations). OSSEs (or similar methods) will play a key role in these activities. This will require continuing to develop models and data assimilation systems in parallel with developments in the GOS. OSSEs are recognized as being an essential part of the development of the GOS for monitoring various key aspects of the Earth system for humankind in the 21st Century (e.g. air quality; see Lahoz et al., 2012). Studying the middle atmosphere to understand important scientific and societal issues such as the stratospheric ozone distribution and climate change remains an important activity, and the very recent discovery of severe Arctic loss (Manney et al., 2011) shows that the middle atmosphere can still surprise us. A robust GOS of the middle atmosphere provides information on how it changes over time, and provides constraints on models that bring model improvement and increased understanding of processes affecting the spatio-temporal characteristics of the middle atmosphere. This will help us deal with the expected and the unexpected concerning the spatio-temporal evolution of the middle atmosphere.

6 Conclusions

Over the last 30 years there has been a wealth of research satellite observations of the middle atmosphere from various research space agencies (NASA, ESA, JAXA, CSA and others). These observations have augmented our knowledge of the polar middle atmosphere: (i) the spatial and temporal characteristics of the wintertime polar stratosphere and the summertime circulation; and (ii) the role of chemistry and transport in determining the stratospheric ozone distribution. This augmentation of knowledge has been accomplished by the synergistic use of these research satellite observations together with information from meteorological analyses; information from model simulations; and, increasingly, information from analyses of chemical species and tracers derived using data assimilation.

The knowledge gained on the middle atmosphere has helped establish international agreements such as the Montreal Protocol negotiated in 1987 (Sarma and Bankobeza, 2000) and five subsequent amendments, that largely stopped the production of ozone depleting substances. Numerical simulations of this “world avoided” (Newman et al., 2009) provide evidence of the value of the Montreal Protocol in preventing massive ozone collapse in the stratosphere during the second half of the 21st Century, which would have had adverse effects on human health through an increase in the UV radiation reaching the ground. Furthermore, it is recognized that changes in the ozone distribution in the middle atmosphere will affect the climate of the 21st Century, for example by modifying the stratospheric circulation (WMO, 2011). The middle atmosphere thus plays a crucial role in a number of societal challenges humankind faces in the 21st Century. It is thus important that observations of this critical region of the Earth System continue for the foreseeable future – the recent demise of ESA’s Envisat satellite (http://www.esa.int/esaCP/SEM1SXSWT1H_index_0.html) has made this need even more urgent.

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Appendix A

List of acronyms

ADEOS: Advanced Earth Observing Satellite
ATOVS: Advanced TOVS (TIROS Operational Vertical Sounder)
CLAES: Cryogenic Limb Array Etalon Spectrometer
CNES: Centre National d'Études Spatiales
CSA: Canadian Space Agency
EOS: Earth Observing System
EPS: EUMETSAT Polar System
ESA: European Space Agency
EUMETSAT: European organization for the exploitation of METeorological SATellites
GEMS: Global Earth system Monitoring using Space and in-situ data
GMES: Global Monitoring for Environment and Security
GOME: Global Ozone Monitoring Experiment
HALOE: HALogen Occultation Experiment
HRDI: High Resolution Doppler Imager
IASI: Infrared Atmospheric Sounding Interferometer
ILAS: Improved Limb Atmospheric Spectrometer
ISAMS: Improved Stratospheric And Mesospheric Sounder
JAXA: Japan Aerospace space eXploration Agency
LIMS: Limb Infrared Monitor of the Stratosphere
MACC: Monitoring Atmospheric Composition and Climate
MAESTRO: Measurements of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation
MLS: Microwave Limb Sounder
MTG: Meteosat Third Generation
NASA: National Aeronautics and Space Administration
NOAA: National Oceanic and Atmospheric Administration
NPOESS: National Polar-orbiting OPerational Environmental Satellite System
NPP: Suomi National Polar-orbiting Partnership
NRL: Naval Research Laboratory
OMI: Ozone Monitoring Instrument
OMPS: Ozone Mapping and Profiler Suite
POAM: Polar Ozone and Aerosol Measurement
SABER: Sounding of the Atmosphere using Broadband Emission Radiometry
SAGE: Stratospheric Aerosol and Gas Experiment
SAMS: Stratospheric and Mesospheric Sounder
SBUV/SBUV2: Solar Backscatter UltraViolet/2
SPOT: Système Pour l'Observation de la Terre (System for observing the Earth)
SWIFT: Stratospheric Wind Interferometer For Transport studies
TIMED: Thermosphere Ionosphere Mesosphere Energetics Dynamics
TOVS: TIROS (Television and InfraRed Observations Satellite) Operational Vertical Sounder
UARS: Upper Atmosphere Research Satellite
WINDII: WIND Imaging Interferometer

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ABSTRACT
We discuss the insights that research satellite observations from the last 30 years have provided on the spatio-temporal variability of the polar middle atmosphere. Starting from the time of the NASA LIMS (Limb Infrared Monitor of the Stratosphere) and TOMS (Total Ozone Mapping Spectrometer) instruments, both launched in 1978, we show how these observations have augmented our knowledge of the polar middle atmosphere, in particular how information on ozone and tracers has augmented our knowledge of: (i) the spatial and temporal characteristics of the wintertime polar stratosphere and the summertime circulation; and (ii) the roles of chemistry and transport in determining the stratospheric ozone distribution. We address the increasing joint use of observations and models, in particular in data assimilation, in contributing to this understanding. Finally, we outline requirements to allow continuation of the wealth of information on the polar middle atmosphere provided by research satellites over the last 30 years.

KEYWORDS		
Middle atmosphere	Satellite observations	Spatio-temporal variability

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