User requirements for monitoring the evolution of stratospheric ozone at high vertical resolution

'Operoz': Operational ozone observations using limb geometry

Final Report

ESA 'Expro' Contract: 4000112948/14/NL/JK

Date: 1st of March 2015

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Executive Summary

I Introduction

The ESA study 'User requirements for monitoring the evolution of stratospheric ozone at high vertical resolution has been executed in the time period October 2014 to February 2015. The project has been referred to as the '*Operoz'* project where '*Operoz'* is an acronym for '*Operational ozone observations using limb geometry*'.

II Purpose and Scope of the Study

The purpose of the *Operoz* study has been threefold:

(i) To establish the user requirements for an operational mission targeting ozone profiles at high vertical resolution,
(ii) To identify the observational gaps with respect to these user requirements taking into account planned operational missions and observational ground networks, and
(iii) To perform a reality check on the observational requirements based on proven concepts and present-day knowledge of potentially available measurement techniques and to identify options for a small to medium size satellite mission.

Background information on operational ozone monitoring needs has been assembled and user requirements have been derived. The mission objectives call for operational, i.e. sustained long-term monitoring from space of ozone profiles (and possibly related observables) in the stratosphere in limb geometry at high vertical resolution. A small set of mission extensions has been defined and has been prioritized into desirable and other useful mission extensions. All mission extensions would significantly enhance the mission objectives of the minimum mission and would contribute fulfilling more than just mandatory user requirements.

Secondly, based on the mission objectives defined specific observational requirements have been defined in terms of satellite Level-2 products and auxiliary requirements. Observational requirements are provided for a minimum mission that would add significant value to the existing and planned suite of observations, as well as a set for the identified set of desirable mission extensions.

Thirdly, a detailed preliminary assessment has been made of available measurement techniques to fulfil the observational requirements for both the minimum mission and the desirable mission extensions. The capabilities of existing instrumentation have been assessed and for each of the different classes of space instrumentation relevant for an ozone monitoring mission, a reality check has been performed on the observational requirements. Finally, conclusions have been drawn and some general recommendations have been formulated.

During the study it has been appreciated that, next to stratospheric ozone (loosely referred to as the 'ozone layer'), also other important societal and science applications could be identified which potentially call for augmenting the operational monitoring of the atmosphere with high vertical resolution in the middle atmosphere using limb geometry. Identified applications specifically include numerical weather prediction, climate change, impact of large volcanic eruptions and (future) geo-engineering. Even though some of the observational requirements presented in this study are potentially relevant for these other applications, the definition of mission objectives and the prioritization for operational limb monitoring for other applications – i.e. other than targeting the 'Ozone Layer', has been considered out of the scope of the rather concise *Operoz* project.

III Background Information

The depletion of stratospheric ozone due to anthropogenic emissions of long-lived substances containing chlorine and other halogens was first identified as a matter of international concern in the mid-1970s through the paper by Molina and Rowland (1974) and has received increasing attention since the mid-1980s after the discovery of the ozone hole (Farman et al., 1985). Today, in spite of the Montreal Protocol and its amendments and adjustments, the atmospheric halogen loading is still enhanced substantially above natural levels and will remain so for decades. Substantial scientific progress has been made since the seventies and eighties. However, monitoring of stratospheric ozone remains extremely important, as the ozone layer has yet to recover from the atmospheric halogen loading caused by human action. Moreover, climate change is having an increasing influence on stratospheric ozone and the influence of changing ozone levels on climate has manifested itself.

Also, over the last decade operational services using stratospheric ozone observations have been developed in response to user requirements. The present-day ozone observations are essential for the services which assimilate and forecast ozone, in the troposphere and the stratosphere, and for numerical weather prediction. In Europe, the Copernicus Atmosphere Monitoring Service (CAMS) [1] provides stratospheric ozone analyses and forecasts (e.g. in relation to UV forecasting), forecast of global atmospheric composition (e.g. providing boundary conditions for regional air quality forecasts), as well as support to Numerical Weather Prediction (NWP). The future Copernicus Climate Change Service (C3S) [2] will stretch across application areas through the operational long-term provision of Essential Climate Variables (ECVs) from observations and analyses.

The World Meteorological Organisation has a mandate by the Parties of the Montreal Protocol to regularly report on the status of the ozone layer in support of the protocol and its amendments and adjustments. Recently the scope of the scientific needs of the Parties involved was defined as (WMO, 2014):

- Assessment of the state of the ozone layer and its future evolution, including with respect to atmospheric changes from, for example, sudden stratospheric warming or accelerated Brewer-Dobson circulation;
- Evaluation of the Antarctic ozone hole and Arctic winter/spring ozone depletion and the predicted changes in these phenomena, with a particular focus on temperatures in the polar stratosphere;
- Evaluation of trends in the concentration in the atmosphere of ozone-depleting substances and their consistency with reported production and consumption of those substances and the likely implications for the state of the ozone layer and the atmosphere;
- Assessment of the interaction between the ozone layer and the atmosphere; including: (i) The effect of polar ozone depletion on tropospheric climate and (ii) The effects of atmosphere-ocean coupling;
- Description and interpretation of observed ozone changes and ultraviolet radiation, along with future projections and scenarios for those variables, taking into account among other things the expected impacts to the atmosphere;
- Assessment of the effects of ozone-depleting substances and other ozone-relevant substances, if any, with stratospheric influences, and their degradation products, the identification of such substances, their ozone-depletion potential and other properties;
- Identification of any other threats to the ozone layer.

A series of nadir sounders is planned in order to continue the measurement of ozone and some other trace gases. ESA, in collaboration with the European Union, is planning to launch the Copernicus

[1] http://atmosphere.copernicus.eu/
[2] http://www.copernicus-climate.eu/

Sentinel-5 precursor (S5P; 2016), and to launch the Copernicus Sentinel-4 (S4) and Sentinel-5 (S5) instruments alongside IRS and IASI-NG, respectively, in Eumetsat's MTG-S and MetOp-SG series, commencing 2021 and 2022, respectively. In the United States, NOAA and NASA are collaborating on a series of operational satellites within the JPSS programme, which hosts the OMPS nadir ozone sounder (with planned launch dates 2017 and 2022). On JPSS-2 the addition of a limb capacity for OMPS similar to the current Suomi-NPP/OMPS is also foreseen.

The nadir view delivers information on total column ozone and on stratospheric ozone profiles at a coarse vertical resolution of about six kilometres at best. With this vertical resolution it is difficult to resolve vertical variations in ozone where there are sharp changes in vertical ozone gradients, such as close to the tropopause. Furthermore, UV nadir sounders (SBUV and GOME-type) are vulnerable to UV degradation of optical surfaces, which requires careful correction, and which is especially critical for long-term variability and trend detection. In this respect observations of upper stratospheric ozone are most vulnerable because the degradation is largest at the shortest UV wavelengths, which is problematic for trend analyses (Liu et al, 2007). Infrared nadir sounders like IASI retrieve ozone up to the mid-stratosphere, though provide very little information on upper stratospheric ozone (August et al., 2012; Hurtmans et al. 2012).

Stratospheric profile information from satellites has been shown to provide a valuable addition to total column ozone in data assimilation systems used by operational centres such as in the framework of MACC (Monitoring Atmospheric Composition and Climate), the current pre-operational service of CAMS. In contrast to limb observations, nadir profile observations strongly smooth out vertical structure; particularly in the lower stratosphere, where fine-scale vertical structure and short-term variability of ozone is large. For molecules other than ozone, nadir observations cannot provide stratospheric profiles with sufficient height resolution, which seriously limits their value for attribution of ozone changes to different processes at different altitudes.

It has long been recognised by the international community that there will be a lack of adequate limb measurements of ozone in future. For occultation measurements, a "gap" may open towards the end of this decade with the end of the lifetime of SAGE-III. Apart from the aging missions ODIN (with SMR and OSIRIS since 2001), AURA/MLS and SCISAT with ACE-FTS and Maestro (since 2004), and the more recent OMPS-limb on Suomi-NPP (launched in 2012 and with a nominal mission duration until 2016), the only subsequent planned limb-sounder is the OMPS follow-on in 2022 on JPSS-2.

IV Definition of Mission Objectives

Based on this information it has been concluded that operational observations of stratospheric ozone at high vertical resolution are essential

(1) In support of operational services, e.g., analyses and forecasts of atmospheric composition and support to numerical weather prediction, and

(2) For long-term (trend) monitoring

The long-term monitoring is required for the verification of the Montreal protocol and its amendments and adjustments, and, secondary, for the monitoring of the two-way interactions between stratospheric ozone and climate. For both objectives the required coverage of the entire globe can only be achieved from space.

<u>A minimum mission</u>

A minimum mission would have to add significant value to the existing and planned suite of nadir missions. A mission fulfilling this requirement is an ozone-only mission monitoring the evolution of the stratospheric ozone layer globally with dense spatial sampling (vertically and horizontally) at daily temporal resolution. Ozone distribution, variability, and trends shall be characterised in four areas: polar ozone, mid-latitude ozone, tropical ozone, and upper stratospheric ozone.

Improving the quality of operational products such as analyses, ozone forecasts and numerical weather prediction requires vertically resolved observations on a daily basis with good spatial coverage and extending into polar night. Such observations are critical for constraining the vertical distribution of ozone, both in the stratosphere and thus, indirectly, also in the troposphere.

Accurately monitoring the development of the ozone layer in a changing climate and with further decreasing ozone depleting substances for all relevant regions (polar, mid-latitudes, tropics) requires good vertical (1 to 2 km) and horizontal (100 to 200 km) resolution in the lower stratosphere. Good vertical and horizontal resolution is also required for the upper stratosphere, but the requirements are somewhat more relaxed than in the lower stratosphere (2 to 4 km vertically and 200 to 400 km horizontally). For deducing long-term ozone trends, considering zonally averaged data sets is typically sufficient. Long-term homogeneous ozone observations are needed that cover the upcoming time period of ozone recovery till the middle to end of the century. The long-term perspective calls for a series of small to medium size satellites with well (inter-) calibrated instrumentation.

<u>Mission extensions</u>
The minimum mission is an ozone-only mission and shall accurately monitor future changes in stratospheric ozone (mandatory, 'Priority A'). Three desirable ('Priority B') mission extensions have been identified: 'Brewer-Dobson Circulation', 'Stratospheric Chemistry', and 'Tropospheric Ozone'. These extensions would allow, in addition to the minimum mission, both near-real time and long-term monitoring of *why* ozone is changing (attribution), as well as a complete monitoring of both stratospheric and tropospheric ozone. The 'Brewer-Dobson Circulation' extension would focus on dynamical drivers of stratospheric ozone change and the 'Stratospheric Chemistry' extension would focus on the chemical drivers of stratospheric ozone change. Similarly, as for ozone, considering zonally averaged data of many of the desirable species may be sufficient for the long-term monitoring applications. The 'Tropospheric Ozone' extension specifically includes downward extension of ozone limb profiling into the upper troposphere and combination with (planned) operational nadir sounders.

Three other useful ('Priority C') mission extensions have been identified. These include 'Extension into the Mesosphere' , mainly expanding the vertical range of ozone observations up to about 85 km; secondly, 'Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols', extending the observations to include mainly stratospheric water vapour and aerosol extinction, which both have important interactions with stratospheric ozone, predominantly in the lower stratosphere; and thirdly, 'Climate Impact of Troposphere-Stratosphere-Transport and the Asian Monsoon', monitoring changes in climate that impact on stratospheric ozone and which are specifically driven through (changing) air pollution and transport patterns in the Asian monsoon circulation.

V Definition of Observational Requirements

Mandatory, desirable and other useful user requirements have been distinguished from which specific observational requirements have been derived. Mandatory observational requirements relate to the minimum mission and have been labelled 'Priority A' . Desirable requirements relate to the three desirable mission extensions and these have been labelled 'Priority B'. All other observational requirements have been labelled 'Priority C'. Even though it would be useful to also include 'Priority 'C' observations into an operational mission targeting stratospheric ozone these observations are not considered as potential mission drivers, e.g. in relation to instrumental design.

Table 1 provides a summary of the observational requirements with in black italics the observational requirements for the minimum mandatory mission targeting stratospheric ozone only and in green the requirements derived for the desirable mission extensions. For the long-term ozone monitoring auxiliary information is needed, most importantly on temperature and extinction coefficient in relation to the attribution of ozone changes. The information requirements for these products have been added at the bottom of the table. The required information on temperature might also be derived from other sources and the need for temperature observations - as part of the operational mission - would need to be evaluated carefully.

Table 1 combines the most stringent ozone requirements as derived from the mission objectives. Requirements on timeliness and update frequency specifically derive from the user requirements related to the operational services and data assimilation, while the requirements on stability and vertical coverage including the upper stratosphere (US; about 30 to 50 km altitude) derive from the user requirements for long-term monitoring.

Operoz **Summary of Observational Requirements Table**						
Operational services and Long-term monitoring ***Minimum Mission ('Priority A')*** + (a) Brewer-Dobson Circulation ('Priority B') + (b) Stratospheric Chemistry ('Priority B') + (c) Tropospheric Ozone ('Priority B')				***Timeliness: < 3h (LS, MS)*** ***Long-term stability (O_3 observations): 1% / 3% per decade*** Across-track sampling (O_3 observations): 100 / 200 km (UT, LS, MS) over a swath of ≥ 400 km (c)		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty[(1)]
O_3	***100 / 200***	***Global (incl. polar night)***	***1 / 2***	***LS***	***12h / 24h***	***8% / 16% or 50 / 100 ppbv***
O_3	***100 / 200***	***Global (incl. polar night)***	***1 / 2***	***MS***	***12h / 24h***	***4% / 8% or 50 / 100 ppbv***
O_3	***200 / 400***	***Global (incl. polar night)***	***2 / 4***	***US***	***Daily/weekly;*** 12h / 24h (b)	***4% / 8%***
O_3 (c)	100 / 200	Global	1 / 2	UT	12h / 24h	8% / 16% or 50 / 100 ppbv
H_2O (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	5% / 10%
HNO_3 (b)	100 / 200	Global	1 / 2	LS	12h / 24h	0.5 / 1 ppbv
HCl (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	0.2 / 0.4 ppbv
$ClONO_2$ (b)	100 / 200	50-90N; 50-90S	1 / 2	LS	12h / 24h	50 / 100 pptv
BrO (b)	100 / 200	Global	1 / 2	LS	12h / 24h	1.5 / 3 pptv
SF_6 (a)	100 / 200	Global	1 / 2	LS	12h / 24h	0.8 / 1.5 pptv
CFC-11[(2)] (b)	100 / 200	Global	1 / 2	LS	12h / 24h	15 / 30 pptv
CFC-12[(2)] (b)	100 / 200	Global	1 / 2	LS	12h / 24h	30 / 60 pptv
N_2O[(2)] (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	20 / 40 ppbv
CH_4[(2)] (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	0.1 / 0.2 ppmv
H_2O (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	5% / 10%
HNO_3(a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	0.5 / 1 ppbv
HCl (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	0.2 / 0.4 ppbv
$ClONO_2$ (b)	100 / 200	50-90N; 50-90S	1 / 2	MS	12h / 24h	50 / 100 pptv
BrO (b)	100 / 200	Global	1 / 2	MS	12h / 24h	1.5 / 3 pptv
SF_6 (a)	100 / 200	Global	1 / 2	MS	12h / 24h	0.8 / 1.5 pptv
CFC-11[(2)] (b)	100 / 200	Global	1 / 2	MS	12h / 24h	15 / 30 pptv
CFC-12[(2)] (b)	100 / 200	Global	1 / 2	MS	12h / 24h	30 / 60 pptv

$N_2O^{(2)}$ (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	20 / 40 ppbv
$CH_4^{(2)}$ (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	0.1 / 0.2 ppmv
H_2O (a,b)	200 / 400	Global	2 / 4	US	12h / 24h	8% / 16%
HNO_3 (b)	200 / 400	Global	2 / 4	US	12h / 24h	0.5 / 1 ppbv
HCl (a,b)	200 / 400	Global	2 / 4	US	12h / 24h	0.2 / 0.4 ppbv
SF_6 (a)	200 / 400	Global	2 / 4	US	Daily/weekly	0.8 / 1.5 pptv
$CH_4^{(2)}$ (a,b)	200 / 400	Global	2 / 4	US	12h / 24h	0.1 / 0.2 ppmv
Temperature (b)	100 / 200	Global	1 / 2	LS	12h / 24h	1 K / 2 K
Extinct. coef. (b)	100 / 200	Global	1 / 2	LS	12h / 24h	10^{-4} / 2.10^{-4} km^{-1}
Temperature (b)	100 / 200	Global	1 / 2	MS	12h / 24h	1 K / 2 K
Extinct. coef. (b)	100 / 200	Global	1 / 2	MS	12h / 24h	10^{-4} / 2.10^{-4} km^{-1}
Temperature (b)	200 / 400	Global	2 / 4	US	12h / 24h	2 K / 3 K

Table 1. *Observational Level-2 requirements for a (i) (in black italics) a minimum operational limb mission targeting stratospheric ozone and (ii) (in green) an extended mission including also 'Priority B' observational requirements. Notation B / T with B=Breakthrough; T = Threshold. Temperature and extinction coefficient are auxiliary data requirements, in support of ozone and the other Level-2 products. Per desirable ('Priority B') Level-2 products it is indicated in the first column (with either a,b and c) to which additional mission objective(s) the level-2 product is contributing. A (sub-)daily update frequency for ozone and possibly temperature (auxiliary information) in the US would be desirable for the operational services ('Priority B').*
(1) For the uncertainty requirement the least stringent of the relative and absolute requirements apply while the minimum ozone concentrations to be observed by 'Operoz' are mandatory (100 / 200 ppbv) in the LS and MS and desirable (50 / 100 ppbv) as well as extending in the UT.
(2) From the listed transport tracers (SF6, CFC-11, CFC-12, CH_4, and N_2O) the tracer SF_6 is considered the single best observable. An alternative could be a combination of tracers, e.g., CFC-11 or CFC-12(LS, MS) and N_2O (LS, MS) as well as CH_4 (MS, US).

The 'Brewer-Dobson Circulation' mission extension mainly targets the long-term monitoring mission objective while the 'Stratospheric Chemistry' and 'Tropospheric Ozone' extensions target both the operational services and the long-term monitoring mission objectives. Observations of SF_6 throughout the stratosphere or, alternatively, a combination of long-lived tracers including CFC-11 or CFC-12, N_2O and CH_4 are required for the 'Brewer-Dobson Circulation' mission extension. Apart from CH_4 also HCl might be an alternative tracer for SF_6 in the US. CFC-11, CFC-12, and N_2O have been considered less suitable in the US. Observations in the lower stratosphere (LS; up to about 20 km altitude) and mid-stratosphere (MS; between about 20 and 30 km altitude) of H_2O, HNO_3, HCl, CH_4, BrO, and $ClONO_2$ (in polar regions only) are required for the 'Stratospheric Chemistry' mission extension, while H_2O, HCl, HNO_3, and CH_4 are required in the US.

Dense horizontal sampling in the tropopause region is required for the operational services and across-track sampling has been suggested as 'Priority B' mission extension together with extension of the vertical coverage of the limb observations of ozone into the Upper Troposphere. In combination with the operational nadir sounders the extension into the upper troposphere would provide an optimized monitoring of both stratospheric and tropospheric ozone down to the surface.

For the operational services extension into the US as well as multiple observations per day (6-hourly update frequency) in at least the lower to mid-stratosphere would have been desirable for data assimilation. However a requirement 'better than 12h' for the update frequency would be hard to fulfil with a small to medium size limb mission on a single platform in Low-Earth orbit. The requirements on update frequency therefore should be read within the technological constraints.

Formation flying of the minimum mission with a planned nadir mission would potentially improve the three-dimensional ozone monitoring in the full atmosphere, i.e. including the lower and mid-troposphere, e.g. through the use of limb-nadir combination in retrieval techniques. The combination of the high spatial resolution offered by the nadir sounders with the vertical resolution in the stratosphere might well provide extra benefits for both types of observations. A similar benefit is expected in the combination of nadir and limb observations in the data assimilation framework. In that case the importance of co-location and thus formation flying is less direct and would need further investigations. An orbit in conjunction with planned operational nadir sounders, e.g. through formation flying, would however limit the selection of orbit altitude. Such orbit considerations have been considered out of scope in *Operoz*.

VI Reality Check on Minimum Mission Requirements

We have analysed the ability of different types of satellite instruments (shortwave, infrared, and (sub-)mm wave) to meet requirements for a minimum ozone-only observing mission, following the requirements summarised in Table 1. The basic requirements are high vertical resolution and daily global coverage of the whole stratosphere, including the ability to measure during polar night. Based on demonstrated performances, preliminary assessments have also been made of the different measurement techniques to address quantitative requirements specified for retrieval vertical resolution and uncertainty, horizontal sampling along-track, and long-term stability.

Measurement Type	***Along-track sampling (km)***	***Hori-zontal coverage***	***Night-time measure-ments***	***Vertical sampling (km)***	***Vertical coverage (km)***	***Update Frequency (hours)***	***Uncer-tainty***	***Stability***
Nadir UV	Green	Orange	Red	Red	Orange	Green	Orange	Red
Nadir IR	Green	Green	Green	Red	Orange	Green	Orange	Green
Occultation	Red	Red	Orange	Green	Green	Red	Green	Green
Infrared Limb Emission	Green	Green	Green	Green	Green	Green	Green	Green
(Sub-)mm Limb Emission	Green	Green	Green	Green	Green	Green	Green	Green
Shortwave Limb Scattering	Green	Green	Red	Green	Green	Green	Green	Green

Table 2. *Summary of the ability of the various instrument types to meet each of the minimum mission requirements. (Green = fully met, Orange = partly compliant, Red = cannot meet the requirement.*

Table 2 summarises the compliance of the different instrument types with the specified requirements. It is important to note that correlative non-space observations and solar occultation space observations may play an essential role in validation; not only during the commissioning phase but continuously, and that the stringent stability requirement could not be achieved without adequate provision of correlative observations as part of the overall observing system, to track and potentially correct in-flight changes to the instrument. For compliance with the daily global coverage and specifically the polar night, a mission that utilised emission sounding would be the most appropriate choice. This could encompass measurements in either the infrared or (sub-)mm wavelength ranges.

There are a range of ***infrared*** measurement types that could potentially meet the requirements. In the simplest case, a broad-band radiometer measuring in less than 10 channels would suffice, and this would be based on a long heritage of limb-sounding instruments, most recently HiRDLS. A Fourier Transform Spectrometer such as has been demonstrated by MIPAS on ENVISAT would also meet all the mission requirements, but with an increased complexity that is not needed for a minimum mission. In relation to the mission extensions, such an instrument would allow a greater number of species to be measured. The HiRDLS and MIPAS instruments were designed and built more than a decade ago. For the minimum mission, technology advances allow several alternative concepts for a compact infrared solution to be worthy of consideration.

Based on demonstrated performances of Aura/MLS and Odin/SMR, and retrieval simulations for the STEAM-R concept, it is evident that a limb-sounder operating in the ***(sub-)mm wave*** region could potentially meet the vertical resolution and uncertainty requirements for a stratospheric ozone minimum mission. The combination requirements on horizontal sampling, vertical resolution and uncertainty could more easily be met by an array receiver concept such as STEAM-R than by a purely limb-scanning concept. The MLS and SMR instruments were designed and built more than a decade ago. A concept derived for the minimum mission could benefit from technology developments such as those for STEAM-R. Vertical resolution is a driver for antenna size. Satellite height would be considered together with antenna and other instrument parameters to optimise a concept for the *Operoz* minimum mission.

Shortwave limb-scattering instruments, including OMPS-limb planned for JPSS-2, could fulfil requirements for the minimum mission, except for regions not illuminated by the sun, which specifically include polar night.

Occultation and nadir viewing instruments have been found to be not suitable for the minimum mission. In the case of occultation instruments, although providing high vertical resolution and highly accurate measurements, their sparse sampling patterns mean that global coverage can be accumulated only over an extended period (typically weeks to months) and not all seasons can be observed, which is a basic requirement. Such instruments are, however, a very valuable reference standards as they achieve the highest accuracy among all space measurements of vertical ozone profiles and, thus, are very well suited for validation of the entire altitude range of any limb sounders. Ozone sondes are limited to < ~30 km altitude, while ground lidar observations, depending on their configuration, can only cover limited altitude ranges. Nadir viewing instruments can provide data which meet horizontal sampling requirements, with daily, global coverage in the infrared and daytime-only in the shortwave, but they are unable to meet the fundamental requirement for high vertical resolution in the stratosphere. Nadir-viewing instruments with ozone capabilities will be available on the planned series of operational polar-orbiting platforms. Their horizontal sampling (across-track in particular) would complement that of a dedicated limb-sounder for stratospheric ozone monitoring. Furthermore, accurate characterisation of the stratospheric ozone distribution by the limb-sounder would benefit operational nadir viewing instruments' abilities to monitor tropospheric ozone.

The requirement placed on ***stability*** (1% /3% per decade; breakthrough/threshold) for long-term monitoring is exceedingly stringent. To achieve this level of stability over a timescale of decades, a series of satellites is needed, with overlaps of 2 years to ensure continuity. High-quality correlative observations from the global ozone sonde network and NDACC (Network for the Detection of Atmospheric Composition Change) will need to be maintained, preferably augmented by solar occultation missions such as the planned SAGE-III.

The ***timeliness*** of the data delivery will be primarily controlled by the satellite and ground-segment and is not therefore governed by the choice of instrument type. To monitor on a decadal timescale, a series of similar satellite instruments with sufficient overlap between them is needed.

VII Reality Check on the Requirements for Mission Extensions

For the mission extension '***Brewer-Dobson Circulation***' conventional infrared radiometry offers an established technique to observe a suite of tracers (CFC-12, N_2O, and CH_4) to cover the necessary height range, and high-resolution FTIR would enable the preferred age of air tracer (SF_6) to be observed. A sub-mm limb-sounder would enable HCl to be observed instead, along with the tracer N_2O. Temperature and H_2O would also be observed by infrared radiometry, FTIR or sub-mm techniques. The shortwave scattering technique provides H_2O and could potentially contribute temperature, N_2O and CH_4.

Abilities to meet each of the desirable ('Priority B') mission extensions

Mission Extension	Observable	Shortwave Scattering				Infrared Emission				(Sub-)mm Emission			
		UT	LS	MS	US	UT	LS	MS	US	UT	LS	MS	US
'Brewer-Dobson Circulation'	SF_6	Grey	Red	Red	Red	Grey	Yellow	Yellow	Yellow	Grey	Red	Red	Red
	CH_4	Grey	Yellow	Yellow	Yellow	Grey	Green	Green	Green	Grey	Red	Red	Red
	N_2O	Grey	Yellow	Yellow	Grey	Grey	Green	Green	Grey	Grey	Green	Green	Grey
	CFC-11	Grey	Red	Red	Grey	Grey	Green	Green	Grey	Grey	Red	Red	Grey
	CFC-12	Grey	Red	Red	Grey	Grey	Green	Green	Grey	Grey	Red	Red	Grey
	H_2O	Grey	Green	Green	Yellow	Grey	Green	Yellow	Yellow	Grey	Green	Green	Green
	HCl	Grey	Red	Red	Red	Grey	Red	Red	Red	Grey	Green	Green	Green
'Stratospheric Chemistry'	Temperature	Grey	Yellow	Yellow	Yellow	Grey	Green	Green	Green	Grey	Green	Green	Green
	HNO_3	Grey	Red	Red	Red	Grey	Green	Green	Green	Grey	Green	Green	Yellow
	HCl	Grey	Red	Red	Red	Grey	Red	Red	Red	Grey	Green	Green	Green
	H_2O	Grey	Green	Green	Yellow	Grey	Green	Yellow	Yellow	Grey	Green	Green	Green
	Ext. coef.	Grey	Green	Green	Grey	Grey	Green	Yellow	Grey	Grey	Red	Red	Grey
	CH_4	Grey	Yellow	Yellow	Yellow	Grey	Green	Green	Yellow	Grey	Red	Red	Red
	N_2O	Grey	Yellow	Yellow	Grey	Grey	Green	Green	Grey	Grey	Green	Green	Grey
	$ClONO_2$	Grey	Red	Red	Grey	Grey	Green	Green	Grey	Grey	Red	Red	Grey
	BrO	Grey	Green	Green	Grey	Grey	Red	Red	Grey	Grey	Yellow	Yellow	Grey
'Tropospheric Ozone'	O_3	Yellow	Grey	Grey	Grey	Green	Grey	Grey	Grey	Green	Grey	Grey	Grey

Table 3. *Summary of the ability of the various instrument types to meet requirements per desirable mission extension. Grey = N/A (no requirement for that altitude range); Green = Meets requirement; Yellow = Some info, but not completely meet requirements; Red = Species not available*

For the mission extension '***Stratospheric Chemistry***' conventional infrared radiometry offers an established technique to observe a suite of nitrogen oxides including $ClONO_2$ (chlorine reservoir gas) and extinction coefficient. High infrared spectral resolution would be needed specifically for 'Priority C' observables such as e.g. SO_2, PAN or CO. BrO cannot be observed in the infrared. A sub-mm limb-sounder would enable HCl and ClO to be observed instead of $ClONO_2$, along with

BrO, though not CH_4, PAN, and extinction coefficient. The shortwave scattering technique specifically covers BrO and extinction coefficient and could further contribute CH_4, CO, and NO_2. Temperature, H_2O and N_2O would be observed by all three techniques.

Either limb infrared (radiometry or spectrometry) or (sub-)mm wave could provide upper tropospheric ozone profiling for the '***Tropospheric Ozone***' mission extension. Less contribution would be possible using shortwave limb scattering to upper tropospheric ozone profiling.

Table 3 shows that no single measurement technique is capable of providing observations of all desired variables for either the 'Brewer-Dobson Circulation', 'Stratospheric Chemistry' or 'Tropospheric Ozone ' mission extensions. Limb infrared emission potentially could meet the requirements on the 'Priority C' mission extension 'Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols'.

VIII Summary and Conclusions

A set of mission objectives has emerged that are driven by the user requirements. The mission objectives specifically include support of operational services, e.g., analyses and forecasts of atmospheric composition and support to numerical weather prediction, and long-term (trend) monitoring in relation to the verification of the Montreal protocol. Two important additional mission objectives include the monitoring of geophysical variables that allow attribution of the observed ozone changes to forcings and objectives regarding the two-way interaction between stratospheric ozone and climate. The additional mission objectives have led to a prioritization of 'Brewer-Dobson Circulation', 'Stratospheric Chemistry' and 'Tropospheric Ozone' over other useful mission extensions. The three extensions would specifically allow observed ozone changes to be attributed to, respectively, changes in dynamics and chemistry, and provide optimal monitoring of both stratospheric and tropospheric ozone.

A minimum mandatory mission must add significant value to the existing and planned suite of operational nadir sounding missions. A mission fulfilling this requirement is an ozone-only mission monitoring the evolution of the stratospheric ozone layer globally with high vertical resolution and dense horizontal sampling at daily temporal resolution. The mandatory requirements include daily global coverage of the full stratosphere, as well as the ability to measure during polar night.

Nadir viewing instruments can provide data which meet horizontal sampling requirements, with daily, global coverage in the infrared and daytime-only in the shortwave, but they are unable to meet the requirements for high vertical resolution in the stratosphere. Nadir-viewing instruments with ozone capabilities will be available on the planned series of operational polar-orbiting (and geostationary) platforms, in Europe including IASI(-NG) and the Sentinels 4, 5, and 5p). Their horizontal sampling (across-track in particular) would complement that of a dedicated limb-sounder for stratospheric ozone monitoring. Furthermore, accurate characterisation of the ozone profile distribution by the limb-sounder would benefit the operational nadir viewing instruments' capabilities to monitor (lower) tropospheric ozone.

The OMPS-limb instrument planned for JPSS-2 (2022+), could fulfil requirements for the minimum mission, except for regions not illuminated by the sun, which specifically include polar night. For compliance with the daily global coverage and specifically the polar night, a mission that utilised emission sounding would be the most appropriate choice. Emission measurements in either the infrared or (sub-)mm wavelength ranges could further allow a breakthrough on sampling requirements (i.e. twice per day). Also, an observational gap is likely to appear between the present-day Suomi-NPP OMPS limb observations and the launch of JPSS-2.

Both the limb infrared and the limb (sub-)mm techniques offer considerable potential to contribute to the mission extensions. Shortwave scattering limb observations could contribute to the 'Brewer-Dobson Circulation' and 'Stratospheric Chemistry' mission extensions although with less extensive coverage of the desired (‘Priority B’) observables than infrared or (sub-)mm, and as yet undemonstrated capability for the extension on ‘Tropospheric ozone’. Across-track capabilities could be added as a mission extension to the limb emission or limb-scattering observational techniques.

IX Recommendations

Over more than a decade since the launches of Odin/OSIRIS, Odin/SMR, Envisat/SCIAMACHY, Aura/MLS, technology has advanced for both shortwave scattering and (sub-)mm, and new satellite instrument concepts have been developed, respectively, ‘CATS’ and ‘ALTIUS’ (both shortwave), and ‘STEAM-R’ (sub-mm). Together with new infrared concepts such as ‘Atmo-SAT’, these concepts are of direct relevance to *Operoz* requirements for the minimum mission and the extensions, along with diverse other instrument and technology developments initially for ground-based or airborne deployment, e.g. GLORIA (infrared) and MARCHALS (mm wave).

To identify an instrument concept dedicated to the *Operoz* minimum mission, or to accommodate the mission extensions, a substantial further study would be required. Other than NPP-Suomi/OMPS-limb, the current generation of satellite limb-sounders was designed more than a decade ago. Technology developments and evolution of proposed concepts over the last decade should therefore be taken into consideration, with a view to defining and optimising a compact, low cost concept for operational services and long-term monitoring and with maximum return for climate monitoring and stratospheric ozone assessments by the international science community.

1 Definition of Mission Objectives

1.1 Introduction

Global total ozone levels decreased through the 1980s and early 1990s, by about 2.5% in the global mean; the decrease was most pronounced in the Antarctic (related to the Antarctic ozone hole), noticeable but moderate in the mid-latitudes, with very little ozone change in the tropics (WMO, 2014). Total ozone is representative of ozone in the lower stratosphere. In the upper stratosphere ozone levels globally declined by about 10-15% from the late 1980s to the late 1990s (Steinbrecht et al., 2009, Jones et al. 2009).

During the 1980s and early 1990s, the abundance of ozone depleting substances (ODSs), in particular chlorofluorocarbons and halons, were increasing. Actions taken under the Montreal protocol and its amendments and adjustments reversed the increase of ODSs. Global ozone decline has stopped, with total ozone levels having approximately stabilized since stratospheric ODS abundances peaked between 1997 and 2000. Since 2000 the various upper stratospheric data records, however, show signs of an increase of up to 5% until 2013 (Kyröla et al. 2013; Bourassa et al., 2014; Gebhardt et al., 2014; Weber et al., 2014; WMO, 2014).

Atmospheric lifetimes of many ODSs used originally are long, ranging between years to many decades (SPARC, 2013) and emissions continue from currently existing banks containing a variety of ODSs. Furthermore, atmospheric concentrations of hydrochlorofluorocarbons (HCFCs) and halon-1301 are still increasing (WMO, 2014). Therefore, the removal of ODSs from the atmosphere and a recovery of the atmospheric halogen loading to natural levels will occur over a much longer timescale than the period (from about 1960 to 2000) during which their abundances increased. This slow decrease of ODSs in the atmosphere makes it difficult to unambiguously identify the influence of this decrease on the ozone layer.

In the future, with further declining ODS abundances, global ozone levels are expected to start increasing again at some point in time, but following a different pathway and proceeding at a different pace in different regions of the atmosphere. Furthermore, during the period of ozone recovery, ozone will also be affected by the expected anthropogenic increase in abundances of long-lived greenhouse gases, mainly carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O). Two of these gases (CH_4 and N_2O) affect ozone chemically. The impact of both these changes and the decline in ODSs will be different in different regions of the atmospheres (e.g. poles, mid-latitudes and tropics) and there is further an impact of natural influences and variability, like for example volcanic eruptions and solar activity.

1.1.1 Observed Changes in Stratospheric Ozone

Global

Total column ozone has remained relatively unchanged since 2000. There are indications of a small increase in global-mean total column ozone over 2000-2012. However, a total column ozone increase that can be unequivocally attributed to the observed ODS decreases in the atmosphere has not yet been observed (WMO, 2014).

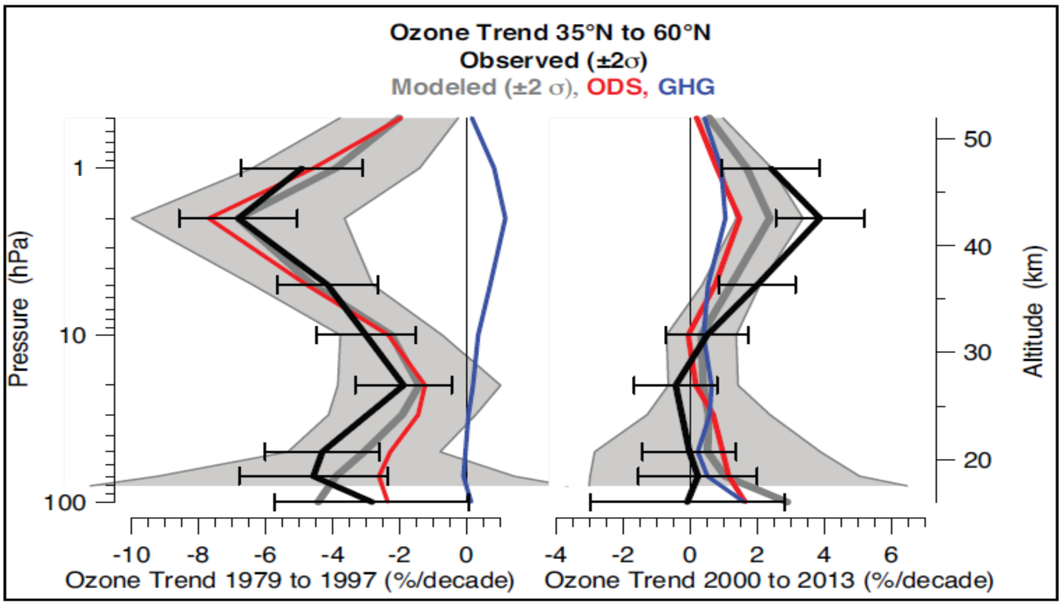

Figure 1.1 *Vertical profiles of observed annual mean ozone trends over 35°N–60°N (black) for the periods of stratospheric ODS increase (left) and ODS decline (right), with the corresponding trends based on model simulations (CCMVal-2) for ODS changes only (red), GHG changes only (blue), and both together (grey). The ±2 standard error uncertainty range for the trends is shown by the horizontal bars for the observations and by the grey shading for the all-changes modelled trend. (From WMO, 2014).*

In the upper stratosphere a clear ozone increase, by about 5% since 2000 (at about ~45 km altitude), is observed reversing the decline observed in the 1980s and 1990s (Figure 1.1). Based on model results, it is estimated that from 2000 to 2013, the decline in ODS abundances and the cooling due to increasing CO_2 have both made comparable contributions to the upper stratospheric ozone increase (Zubov et al., 2013).

In the extra-polar lower stratosphere (15 to 25 km altitude, 60°S−60°N), (total) ozone declined through the 1980s and early 1990s and has remained approximately stable since about 2000 at values about 2% lower than during 1964-1980. Northern and Southern Hemispheres mid-latitude (35°N–60°N and 35°S–60°S) ozone levels are currently 3.5% and 6% below the 1964-1984 average (WMO, 2014).

Polar region

The Antarctic ozone hole is the clearest example of how ODSs have impacted the stratospheric ozone layer; it continues to occur each austral spring and is expected to remain a recurring feature in the near future. Substantial polar ozone loss also occurs in the Arctic, albeit with much greater interannual variability. In winter/spring 2011, the Arctic stratosphere was particularly cold, which led to large ozone depletion (e.g. Manney et al., 2011; WMO, 2014). The current reduction in ODS abundances from their peak values is small (~10%), so that the observed variability in polar ozone in the last decade (Figure 1.2) is attributed to natural year-to-year changes in meteorology and not to recovery from the effect of the ODSs (WMO, 2014). The year-to-year variability in polar ozone loss is particularly pronounced in the Arctic, but has increased somewhat in the Antarctic in the recent decade (e.g. de Laat and van Weele, 2011; WMO, 2014).

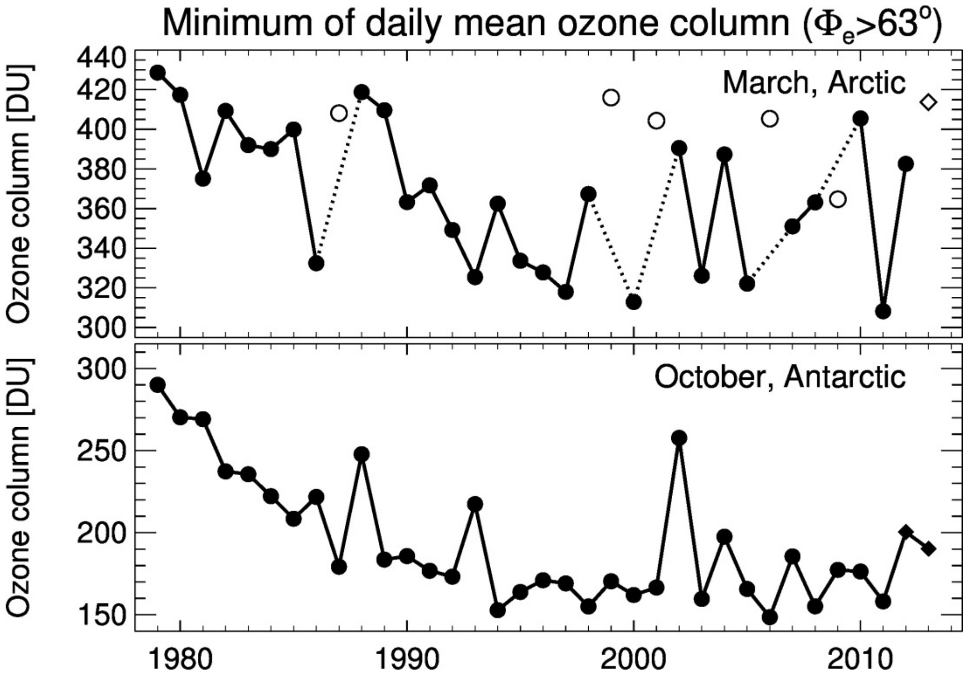

Figure 1.2 *Time series of the minimum of the daily average column ozone (Dobson units) within the 63° contour of equivalent latitude (Φ_e) in March in the Arctic and October in the Antarctic. Arctic winters in which the polar vortex broke up before March (1987, 1999, 2001, 2006, 2009, and 2013) are shown by open symbols; dotted lines connect surrounding years. Figure adapted and updated from Müller et al. (2008) and WMO (2014), using the Bodeker Scientific combined total column ozone database (version 2.8; circles) through the Arctic winter of 2012, and Aura OMI measurements thereafter (diamonds). (Figure courtesy of Jens-Uwe Grooß).*

Tropics

Over the past decades, changes in total ozone in the tropics were smaller than in any other region. While observations since the late 1970s show no apparent trend in total ozone (WMO, 2014), chemistry climate models (CCMs) seem to indicate that negative (before 2000) and positive trends (afterwards) are expected in the tropics. A very recent study indicates that recent lower stratospheric trends may have been compensated by tropospheric ozone trends possibly contributing to the absence of observed ozone column trends in the tropics (Shepherd et al., 2014).

The ozone trends as a function of altitude are quite variable in the tropics. Temperature and ozone in the lowermost tropical stratosphere declined continuously over the past three to five decades suggesting an increased upwelling of air in the tropical lower stratosphere (Randel and Thompson, 2011). These changes are dynamically driven and this observation is consistent with the results of model simulations, which simulate long-term increases in the tropical upwelling driven by the increase in greenhouse gases in the atmosphere and changes in the Brewer-Dobson circulation. But there are indications that tropical upwelling may undergo variabilities on time scales of up to a decade. Recent observations show that tropical lowermost stratospheric ozone has not continued the long-term decline since about 2002 (Aschmann et al., 2014). However, it has to be noted that ozone trends in this region are highly uncertain due to substantial uncertainties in the satellite data records below 20 km altitude (WMO, 2014).

In the tropical upper stratosphere ozone trends before and after the late 1990s are very similar to what is observed at middle latitudes (Figure 1.3); an increase since about the late 1990s following a long-term decline. In the middle stratosphere (30 to 35 km), however, a continuous and statistically significant decline in ozone up to 2012 has been observed and could be possibly related to N_2O and NO_X changes in connection with changes in the upwelling (Kyröla et al., 2013; Gebhardt et al., 2014; Nedohula et al., 2015).

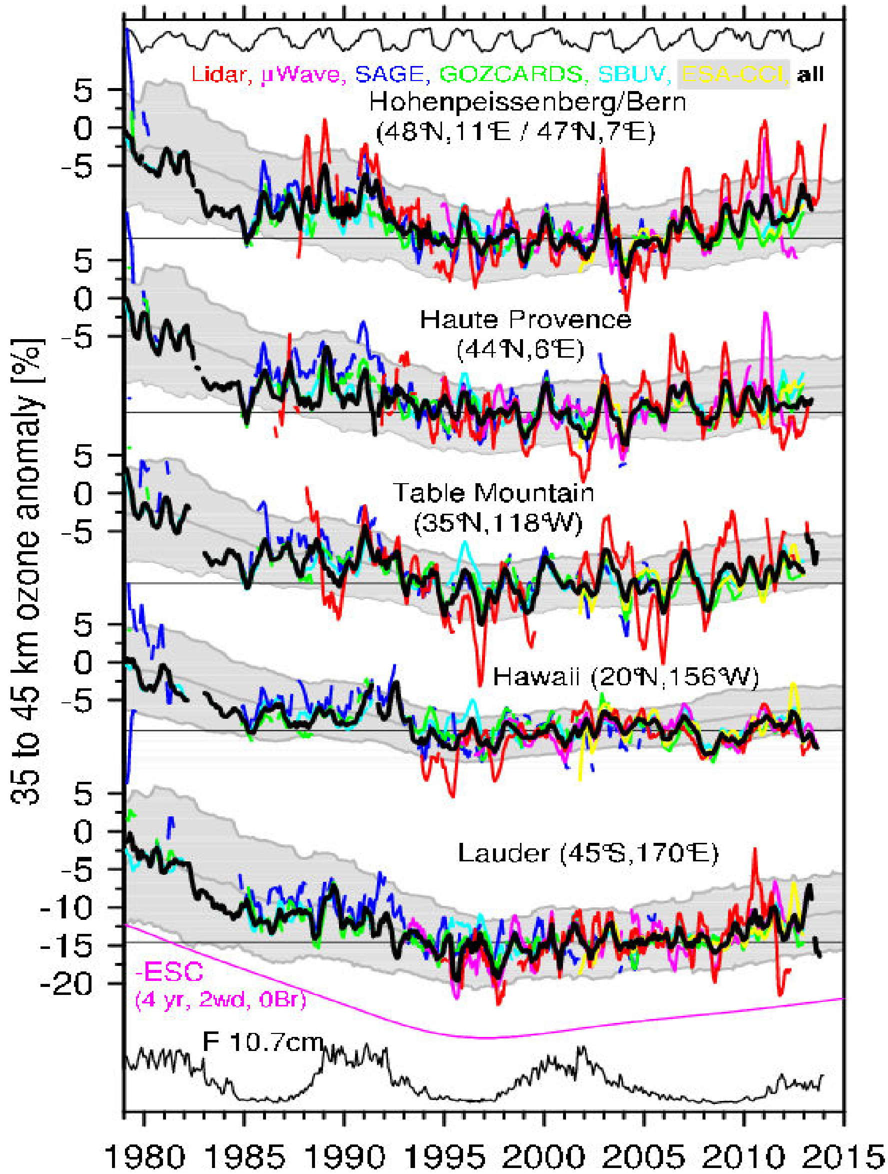

Figure 1.3 *Time series of ozone anomalies in the upper stratosphere as observed by ground-based lidars and microwave radiometers at five stations of the Network for the Detection of Atmospheric Composition Change (NDACC) and by satellite instruments. Anomalies are derived by subtracting the average annual cycle of each data record between 1998 and 2008, but the percent scale is set to zero at the beginning of data in 1979. Satellite data are 10° zonal means centred at the station latitudes. The GOZCARDS data record merges SAGE and HALOE data (up to 2005) with AURA-MLS data (since 2004) (Froidevaux et al., 2014). SBUV is the SBUV V8.6 merged dataset provided by NASA (McPeters et al., 2013). ESA-CCI is the average anomaly from the OSIRIS and SMR datasets (since late 2000), and the GOMOS, MIPAS, and SCIAMACHY satellite datasets (2002 to spring 2012) and was processed under the ESA Climate Change Initiative (Sofieva et al., 2013). The thick black line is the average anomaly from all available data sets. For clarity, data are smoothed by a 5 month running mean. The grey underlay is obtained from CCMVal-1 model simulations. It gives the running 24 month multi-model mean and ±2 standard deviations of individual model monthly means from this mean. The black lines at the top and bottom give proxies for QBO and solar flux. The pink line at the bottom gives an (inverted) proxy for stratospheric chlorine loading. Weber et al., 2014, updated from Steinbrecht et al. 2009.*

1.1.2 The Future of Stratospheric Ozone in a Changing Climate

As long as chlorine and bromine abundances in the stratosphere remain elevated, stratospheric ozone depletion will continue. In particular, the Antarctic ozone hole will continue to occur each austral spring. A large stratospheric sulphuric aerosol enhancement, either due to a strong volcanic eruption or due to an implementation of particular geoengineering measures (Crutzen, 2006, Rash et al., 2008) may result in substantial and additional chemical depletion of stratospheric ozone (Tilmes et al., 2008). However, under full compliance with the Montreal Protocol total column ozone will recover over most of the globe eventually. A recovery towards the 1980 benchmark levels is expected to occur before mid-century in mid-latitudes and in the Arctic, and somewhat later for the Antarctic ozone hole (WMO, 2014).

As ODSs decline in the atmosphere and the stratospheric halogen loading recovers towards natural levels, changes in CO_2, N_2O, and CH_4 will have an increasing influence on stratospheric ozone, both through chemical and climate effects. N_2O increases will lead to enhanced stratospheric ozone loss via the NO_X cycle, while increasing CH_4 and CO_2 will tend to increase ozone.

In particular, the expected future evolution of tropical total column and lower stratospheric ozone is strongly dependent on projected future abundances of CO_2, N_2O, and CH_4, which are highly uncertain. Tropical total column ozone is not only sensitive to changes in tropical upwelling, but is affected by changes in tropospheric ozone as well (Shepherd et al., 2014). Except for scenarios assuming large increases in methane, significant decreases in tropical total column and lower stratospheric ozone are projected during the 21st century (WMO, 2014).

The clearest impact of stratospheric ozone change on surface climate is caused by the Antarctic ozone hole. The Antarctic ozone hole has caused lower stratospheric cooling, which is very likely the dominant cause of observed changes in Southern Hemisphere tropospheric summertime circulation over recent decades that have an impact on surface temperature, precipitation, and the oceans (WMO, 2014). However, in the Northern Hemisphere, no robust link between stratospheric ozone changes and tropospheric climate has been established (WMO, 2014).

Ozone depletion has also an important impact on changes in the stratosphere; in the lower stratosphere, it has been the dominant cause of the observed globally averaged long-term cooling since about 1980. Ozone depletion has also caused cooling in the upper stratosphere, however, in this region there is about an equal contribution to the observed cooling by increasing greenhouse gases, particularly CO_2 (WMO, 2014).

The future development of stratospheric ozone will also depend very strongly on changes in the Brewer-Dobson circulation (Gerber et al., 2012). This impact is direct in the lower stratosphere and in the polar regions, where ozone is longer-lived and thus can be directly influenced by transport. It is indirect in the upper stratosphere and in the tropics, where the lifetime of ozone is shorter and the control of chemistry is more direct. However, ozone chemistry is driven by radicals that are influenced by long-lived precursor gases (e.g., N_2O, CH_4, H_2O, and CFCs), which in turn are also impacted by a changing Brewer-Dobson circulation.

Recently, Mahieu et al. (2014) presented ground-based and satellite data that show a recent and significant increase, in hydrogen chloride (HCl) starting around 2007 in the lower stratosphere of the Northern Hemisphere, which they attributed to a slowdown in the Northern Hemisphere atmospheric circulation occurring over several consecutive years. The pattern of variation in the stratospheric age of air distribution reported by Mahieu et al. (2014) is consistent with the analysis by Ploeger et al. (2015), which also showed that the simulated age of air distribution is in agreement with age of air deduced from stratospheric measurements of SF_6 by ESA's MIPAS instrument (Figure 1.4). The pattern of a change in the sign of the trend in age of air in the middle and upper stratosphere to positive values was also deduced based on four decades of *in situ* balloon-based measurements by Ray et al. (2014).

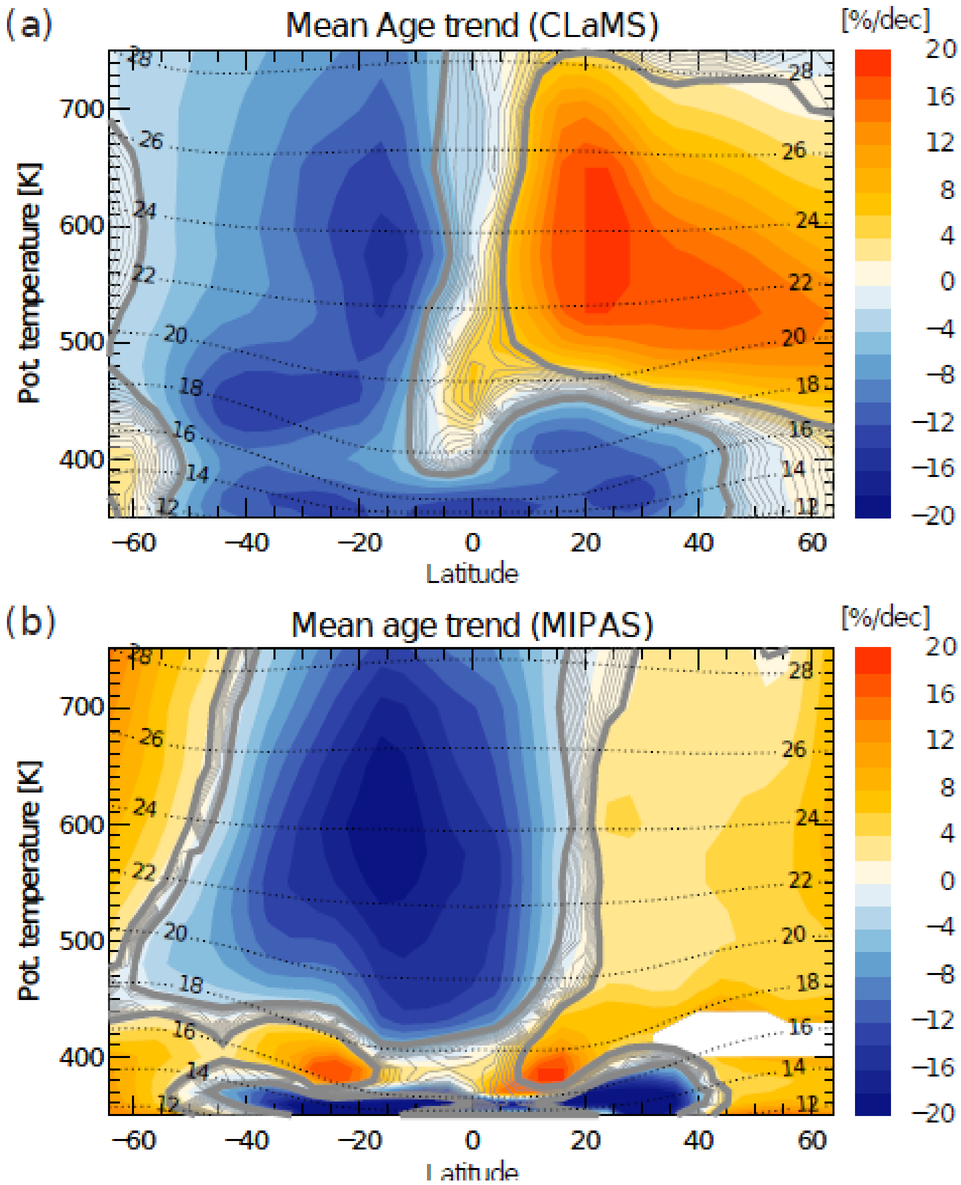

Figure 1.4 *Relative linear trend (in percent) of zonal mean age of air for the period 2002-2010 from (a) CLaMS and (b) MIPAS. The significance of the trend, measured in multiples of the standard deviation (σ), is shown as grey contours (2σ contour as thick lines, then decreasing with 0.2 steps as thin lines). Dashed lines show altitude levels in km. (From Ploeger et al., 2015).*

Most chemistry climate models indicate that the Brewer-Dobson circulation will accelerate (and age of air will decrease) in the future due to increases in greenhouse gases (Gerber et al., 2012; WMO, 2014). So far, observational evidence for such long-term trends in age of air is uncertain due to the sparsity of ground-based and *in situ* balloon measurements (Engel et al. 2009; Ray et al., 2014). In addition, age-of-air deduced from recent satellite measurements (e.g. by MIPAS, Stiller et al. 2008; 2012) also reveal short-term variability as well as distinct patterns dependent on regions observed (see Figure 1.4). Long-term measurements of global height-resolved and stratospherically stable tracers beyond a decade are missing.

1.2 Importance of Stratospheric Ozone Observations for Operational Services

The requirements for stratospheric ozone observations in operational services are driven by an extensive user community. The relevant users can roughly be split into three groups:

- Users of stratospheric ozone analyses and forecasts, both in near real-time and reanalysis mode. Examples are the World Meteorological Organization (WMO), which has a mandate to write annual scientific assessments of the status of the ozone layer, (meteorological) observation stations that launch ozone sondes and are interested in optimal timing of the release of these sondes, and in general the science community that studies the behaviour of the ozone layer.
- Users of global atmospheric composition and regional air quality forecasts. Air quality forecasting is a rapidly developing area which within Europe has had a considerable boost through the Copernicus programme. Users come from a wide range of application areas, such as policy makers, local/regional air quality and health authorities, and the general public.
- Users of numerical weather prediction (NWP) forecasts. As will be described below, having better stratospheric ozone measurements would improve the feedback on atmospheric temperatures and winds and therefore improve the weather forecast. This benefits users across the whole weather forecasting domain.

The first two areas are covered to a large extent within Europe by the Copernicus Atmosphere Monitoring Service (CAMS), although national operational centres could have their own systems as well. A similar set-up exists for numerical weather prediction (NWP), where ECMWF is a major user of satellite observations, but where national meteorological institutes also run their own data assimilation and forecasting systems. Finally, the future Copernicus Climate Change Service (C3S) stretches across the application areas through its operational provision of essential climate variables (ECVs) from observations and reanalyses.

Data assimilation is a tool to provide analyses that can be used for many purposes; one important application being monitoring of chemical species including ozone. The long-term monitoring objectives are discussed in Section 1.3.

Within the frame of this study an assessment of the potential impact of limb *temperature* observations on temperature assimilation was not possible so that this point in not further discussed in this report.

CAMS

The Copernicus Atmosphere Monitoring Service (CAMS) produces forecasts and analyses of global atmospheric composition. To provide accurate analyses and forecasts of stratospheric composition, profile information on key atmospheric constituents is essential. For example, Figure 1.5 shows a strong degradation of GEMS reanalysis ozone in the lower stratosphere relative to ozone sondes for the period July 2003 - September 2006, during which no limb ozone profile data were assimilated. This clearly shows the importance of high resolution vertical ozone profiles in the assimilation. These high resolution vertical ozone profiles are required globally and extending into polar night (such as observations from MIPAS and MLS). While ozone is central to these requirements, observations of other species could play a significant role as well.

The requirement for global height-resolved monitoring of atmospheric composition from space has been consistently identified by a number of international bodies (IGACO, 2004; Kelder et al., 2006; Reburn et al., 2008; GACS, 2009). These requirements are also reflected in the specification of limb-sounders in the post-EPS Mission Requirements Document (Schlüssel et al., 2010). Most recently, there have been clear recommendations from GCOS. To monitor atmospheric composition and critical links to climate, the GCOS Implementation Plan (GCOS, 2010) calls specifically for the development of a strategy for systematic global acquisition of height-resolved data on the three trace gases ozone, water vapour and methane (see Section 1.3 for long-term monitoring aspects).

To accurately monitor and forecast (up to 10 days) stratospheric ozone concentrations in a data assimilation system, high vertical resolution ozone profile observations are essential. With only total column ozone observations, analyses would depend too much on the model background and the background error covariances. The minimum requirement for an operational stratospheric ozone mission is therefore daily global ozone profiles at high vertical resolution.

In addition, other species can be assimilated to further constrain the ***ozone chemistry***, which is especially important for the short- to medium-range forecasts. Currently, based on MACC-III project results, experience exists with the assimilation of nitric acid (HNO_3), water vapour (H_2O), hydrochloric acid (HCl), as well as hypochlorous acid (HOCl), and nitrous oxide (N_2O) and so far this is planned to be continued for CAMS.

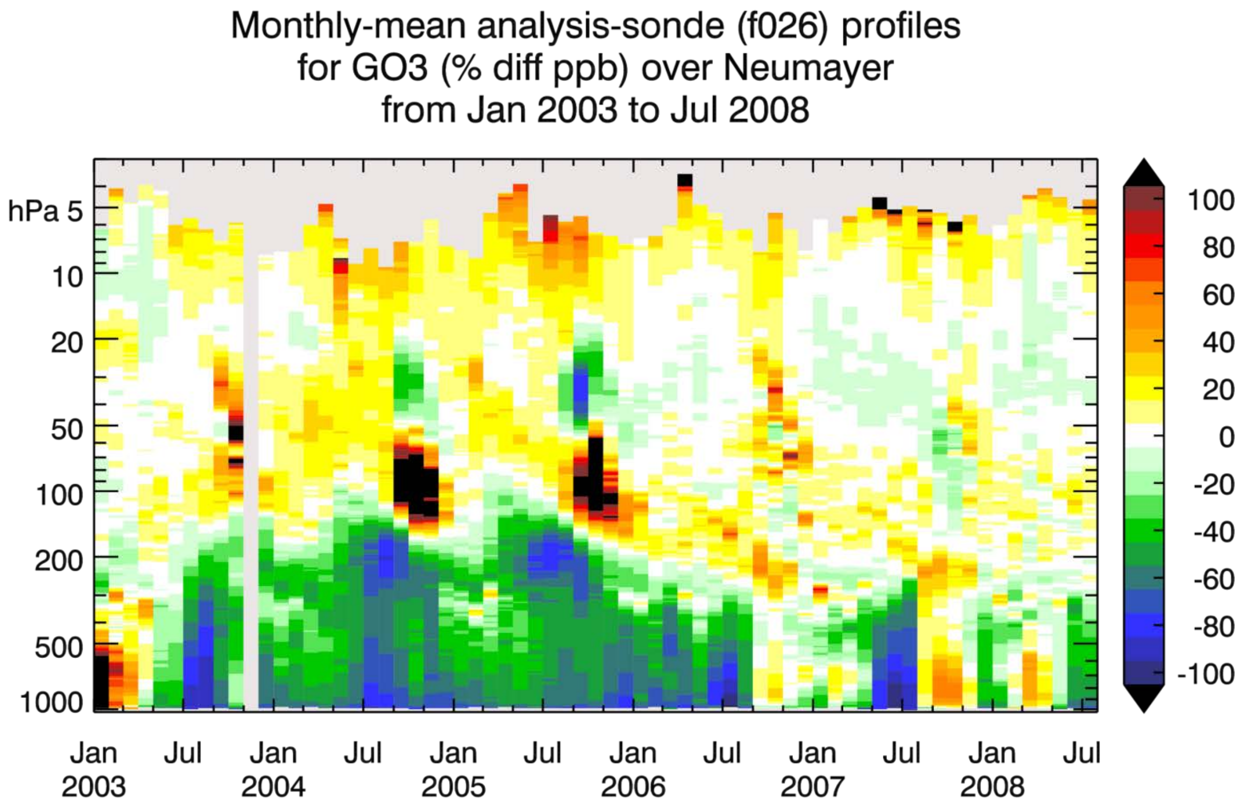

Figure 1.5 *Relative difference [%] between GEMS reanalysis ozone profiles and ozone sondes at Neumayer station. MIPAS data were assimilated between 10 January and 31 December 2003; MLS data were assimilated from 1 January 2006 onwards; and OMI total column data were assimilated from 30 July 2007 onwards. Strong degradation in the lower stratosphere and the troposphere is seen for the period July 2003 - September 2006, during which no limb profile data from either MLS or MIPAS were assimilated. This clearly shows the importance of high resolution vertical ozone profiles in the assimilation for both the stratospheric and the tropospheric ozone product.*

In general, to constrain the stratospheric chemistry, it will be important to constrain the nitrogen reservoir component through HNO_3 and the chlorine reservoir through measurements of HCl and in the polar lower and mid-stratosphere also $ClONO_2$. Information on water vapour is important as it constitutes the major source of HO_X radicals and N_2O as the source of the nitrogen reservoir species. Stratospheric bromine is responsible for a significant fraction of polar ozone destruction; BrO measurement help constraining the stratospheric bromine budget and are therefore important for polar ozone loss. The order of priority for observations constraining stratospheric chemistry is HNO_3, HCl, H_2O, N_2O, $ClONO_2$, and BrO, though with little difference in the importance of the three first compounds.

Additional parameters pertinent to ***monitoring stratospheric composition*** also have been considered in MACC-III, such as Polar Stratospheric Clouds (PSCs), volcanic sulphur dioxide (SO_2) and aerosol, and this will be continued in CAMS. For aerosol in particular it is currently very difficult to distinguish the various aerosol species and altitude ranges from available observations. Because of the very significant impact of stratospheric aerosol on radiation, it is important to account properly for the amount of stratospheric aerosol, which relies entirely on models with the current observing system.

Another cornerstone activity for CAMS is the ***monitoring and forecasting of air quality*** in Europe, up to several days ahead. Tropospheric ozone is a particular focus and long-range transport and local/regional contributions combine to build up high levels downwind of precursor emissions. This activity relies on a combination of modelling and assimilation of remote-sensing and in situ (at the surface and at altitude) instruments composing the Global Observing System.

As already noted above, assimilating only total column ozone observations puts large dependence on the model background and background errors, and this problem is even more pronounced for tropospheric ozone. Having detailed information about the stratospheric profile is essential here as was already clearly illustrated in, for instance, the GEMS reanalysis (Figure 1.5). In this 10-year reanalysis ozone profile measurements from Aura/MLS were not assimilated for certain periods resulting in an immediate degradation of the quality of the tropospheric ozone product.

There is currently insufficient experience with the (operational) assimilation of ozone profiles retrieved from the MetOp nadir sounders, either in the UV-VIS (GOME-2) or infrared (IASI). Previous studies using infrared nadir sounding (e.g. Parrington et al., 2008; Foret et al., 2009) show that while such observations are capable of constraining ozone in the free troposphere they have insufficient vertical resolution to have significant impact in the critical UT/LS altitude range. Also using UV-VIS nadir sounding have insufficient vertical resolution and again most critically in the UT/LS altitude range (e.g. Ziemke et al., 2014; see further the discussion in Section 3.2.1). Future limb sounding missions would therefore bring a very distinct contribution by constraining ozone around the tropopause, so stratospheric intrusions of ozone can be represented more realistically. This again defines the minimum mission requirements, as well as the potential extension to observe enhanced ozone levels in the upper troposphere.

Furthermore, operational stratospheric profile observations of species other than ozone would help to improve ***tropospheric services***. Assimilated NO_2 tropospheric columns currently depend very much on model information and would improve through measurements of stratospheric NO_2 profiles. CH_4 has a steep gradient in the stratosphere and is therefore difficult to constrain properly with only total column observations. The resulting uncertainty has an impact on the quality of methane forecasts, analyses and surface emission inversions. Vertically resolved information on stratospheric aerosol is important to allow the stratospheric contribution to total aerosol optical depth (AOD) observations (which is available from nadir sounders) to be determined.

NWP

The UT/LS and stratosphere are of specific interest for NWP as well, especially for medium- to long-range forecasting, through the impact of ozone and humidity on the radiation. Not resolving this well results in biases of stratospheric temperatures, which affect both the forecast scores and the quality of the assimilation of other satellite instruments.

The usefulness of a stratospheric mission is therefore two-fold as it fulfils:

- the need for vertically-resolved ozone and humidity data in the upper troposphere and lower stratosphere for assimilation into models to improve forecasts through their direct radiative effects.
- the need to account accurately for UT/LS distributions and variability of key species absorbing in the infrared in the assimilation of radiances from nadir-sounders.

For the reasons listed above, ozone has been a variable in leading NWP models for more than a decade. There is today a significant literature on the use of UT/LS and stratospheric ozone for NWP operations. The link between ozone and potential vorticity (Danielsen, 1968) makes UT/LS ozone information useful for forecasters to assess the validity of initial steps in the forecast trajectories in the case of fast-developing and high-impact weather systems. Recent developments have also shown the direct potential of ozone limb data to improve stratospheric winds analyses and forecasts (Semane et al., 2008).

Key observable ('Priority A') [3]*:* Stratospheric ozone

Key observables other than ozone ('Priority B'): HNO_3, HCl, H_2O

Further important observables ('Priority C'): N_2O, $ClONO_2$, BrO, PSCs, SO_2, NO_2, CH_4, stratospheric aerosols

Special requirements: Global measurements extending into polar night with high horizontal (100 km) and high vertical resolution (1-2 km in the LS and MS; 2-4 km in the US)[4]. Extension into the UT to observe enhanced ozone levels would be desirable.

Temporal density of the sampling: Global observations with dense and preferably sub-daily temporal resolution including (polar) night conditions.

[3] Three levels of priority are distinguished within *Operoz*: 'Priority A ' is referred to as mandatory, 'Priority B' is referred to as desirable, and 'Priority C' is referred to as useful, see also the discussion in Section 2.1

[4] Definitions of the altitude domains for Upper Troposphere (UT), Lower Stratosphere (LS), Mid Stratosphere (MS), and Upper Stratosphere (US) are provided in Section 2, Table 2.1

1.3 Long-term Monitoring of Stratospheric Ozone

Ozone is changing differently in different regions of the atmosphere and there are distinctive processes driving the changes. We will therefore discuss the long-term monitoring of ozone in the different regions in some detail in Section 1.3.1. This will set the stage for the definition of a “minimum mission” (‘Priority A’, i.e. using similar definitions as used in Section 1.2 above).

The two most important mission extensions related to the attribution of observed long-term ozone changes to forcings are “Brewer-Dobson Circulation” and “Stratospheric Chemistry”. These are discussed in Sections 1.3.2 and 1.3.3, respectively, as well as potential extensions of the minimum mission into the upper troposphere (Section 1.3.4). Observations under these thematic areas are considered ‘Priority B’. Additional mission extensions provide useful details on specific processes that also impact long-term stratospheric changes and they are considered ‘Priority C’ in *Operoz*: “Extension into the Mesophere” (Section 1.3.5), “Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols” (Section 1.3.6), and “Climate Impact of Troposphere-Stratosphere-Transport and the Asian Monsoon” (Section 1.3.7).

Obviously, temperature is clearly a central geophysical variable that determines the ozone levels throughout the stratosphere. At the same time, ozone, through its radiative interactions, is also a central parameter in setting the stratified thermal structure of the middle atmosphere. Temperature determines the speed of the ozone destruction reactions in the upper stratosphere. In the polar lower stratosphere low temperatures are a key trigger of heterogeneous chemistry, which is the ultimate cause of the occurrence of the ozone hole (see Section1.1.1). Accurate information on temperature is also needed in the retrieval of stratospheric ozone observations from Level-1 observations.

Important information on temperature will be available through the data assimilation systems utilised by meteorological services. Measurements of lower stratospheric temperatures by GPS type instruments will likely provide good constraints for the lower stratosphere. The situation in the upper stratosphere is less clear and the availability of temperature observations together with ozone profiling could become important. However, as also has been mentioned in Section 1.2, within the frame of this study an assessment of the potential impact of limb *temperature* observations on temperature assimilation was not possible so that this point is not further discussed in this report. However, temperature observations are considered to provide important auxiliary information for long-term monitoring.

1.3.1 Minimum Mission Objectives for an Ozone-only Mission

Ozone measurements are used for monitoring purposes in a variety of ways, e.g. through times series from particular instruments or by merging data sets into single homogenised data sets from different sources (e.g., WMO, 2010; WMO, 2014). Further, data assimilation aims at finding the best possible and comprehensive estimate of the state of the atmosphere taking into account interactions of as many parts of the system as feasible as initial conditions for providing forecasts of stratospheric ozone, tropospheric chemistry and NWP (see Section 1.2). This information may also be used to monitor the atmosphere over time. This can be achieved in a near real-time framework as well as in a reanalysis framework. The advantage of the latter is that it uses a frozen system, which allows more accurate interpretation of the results in terms of trends. Examples of the use of reanalysis can be found in Dee at al. (2014), Inness et al. (2013), and van der A et al. (2010). For monitoring purposes the long-term stability of the observations is extremely important.

Polar stratosphere

So far signatures of a trend reversal in Antarctic ozone have not been unequivocally established (Figure 1.2; WMO, 2014). Further, the question where in the Antarctic (edge of the vortex vs. core, which altitude range) the recovery should be first detectable is a matter of current scientific debate (Strahan et al., 2014). This question implies the requirement of good (100-200 km) horizontal resolution. Model projections suggest that the recovery of ozone will take longer in the Antarctic than in any other region. Measurements aimed at detecting a recovery of Antarctic ozone need to provide height resolved information in the lower stratosphere to allow an attribution of changing ozone to underlying processes.

In the Arctic, chemical ozone loss is generally less severe than in the Antarctic, in the sense that column ozone in spring is higher (Figure 1.2). However, in cold Arctic winters chemical ozone depletion is severe; the strongest chemical ozone loss observed so far occurred in winter 2011 (Manney et al., 2011). The analysis in the Arctic is further complicated by the large dynamical variability of the polar vortex causing both a strong inter-annual variability of Arctic ozone and a large spatial variability of the Arctic vortex in a particular year. However, the processes acting on ozone are similar in the Arctic and Antarctic, so that the requirements for ozone observations in terms of coverage and horizontal and vertical resolution are comparable for both polar regions. Part of the polar regions are covered in winter by polar night. Conditions in polar night are important for subsequent chemical ozone destruction in sunlight (e.g. the ozone level before the onset of ozone destruction), so that measurements throughout the polar night are important.

Mid-latitude lower stratosphere

Ozone loss due to the increase in ODSs has been observed in the mid-latitude lower stratosphere, but the reduction is much smaller than at polar latitudes. This calls for ozone measurements with good long-term stability. Furthermore, for monitoring long-term trends of mid-latitude lower stratospheric ozone, considering zonal averages is sufficient, which allows the random error of ozone measurements to be reduced. The information on ozone needs to be vertically resolved to allow a focus on the lower stratosphere, where ozone is long-lived. Similar to the polar region, lower stratospheric ozone undergoes large inter-annual and longer-term variability due to dynamical forcings. It is necessary to cover both hemispheres well (where different trends are observed and where different recovery pathways are expected).

Tropical ozone

Tropical ozone constitutes a major part of the global stratospheric ozone layer and is the only region where projections suggest decreasing ozone in the lower stratosphere and in total ozone (WMO, 2014). Lower stratospheric (and thus also column ozone in the tropics) is mostly sensitive to changes in the tropical upwelling and thus to changes in the Brewer-Dobson circulation (see Section 1.3.2). To detect changes in tropical ozone, a good coverage of the tropics is required (to separate tropical from mid-latitude issues), as well as a good vertical and horizontal resolution in the lower stratosphere (to allow changes due to circulation changes to be identified). For trend monitoring, considering zonal averages in the tropics will be sufficient.

Upper stratosphere

The upper stratosphere is the altitude region where fingerprints of ozone recovery are most easily detectable as transport processes play a minor role and changes are dominated by photochemistry (WMO, 2014). Indeed, first evidence of recovery was noted by Newchurch et al. (2003) and many other studies since then have confirmed that upper stratospheric ozone is recovering. Model studies indicate that both GHG and ODS have similar contributions to the observed upper stratospheric trends (WMO, 2014; Fleming et al., 2011; Gillett et al, 2011).

In the past, monitoring of these changes has largely relied on satellite measurements like SAGE and SBUV (WMO, 2011; WMO, 2014). Monitoring of upper stratospheric ozone requires observations that are sufficiently accurate and stable to quantify future trends. It also requires sufficient height resolution to capture the vertical structure of the trends. Model studies indicate that the vertical variability of chemically induced ozone changes in the upper stratosphere in the future will vary on vertical scales of a few kilometres (Figure 1.6; Zubov et al., 2013). Furthermore, temperature change is an important driver of increase in upper stratospheric ozone (WMO, 2014), such that a sufficiently accurate knowledge of upper stratospheric temperature trends is required see the discussion above on the use of either temperatures from (re-)analyses and/or observations by limb sounders in the Upper Stratosphere). Smaller scale processes on horizontal scales on the order of 100 km or below, which are important for the lower and middle stratosphere are less relevant for upper stratospheric ozone, such that horizontal resolution requirements are less stringent. Moreover, as when analysing ozone trends in mid-latitudes, considering zonal averages is sufficient.

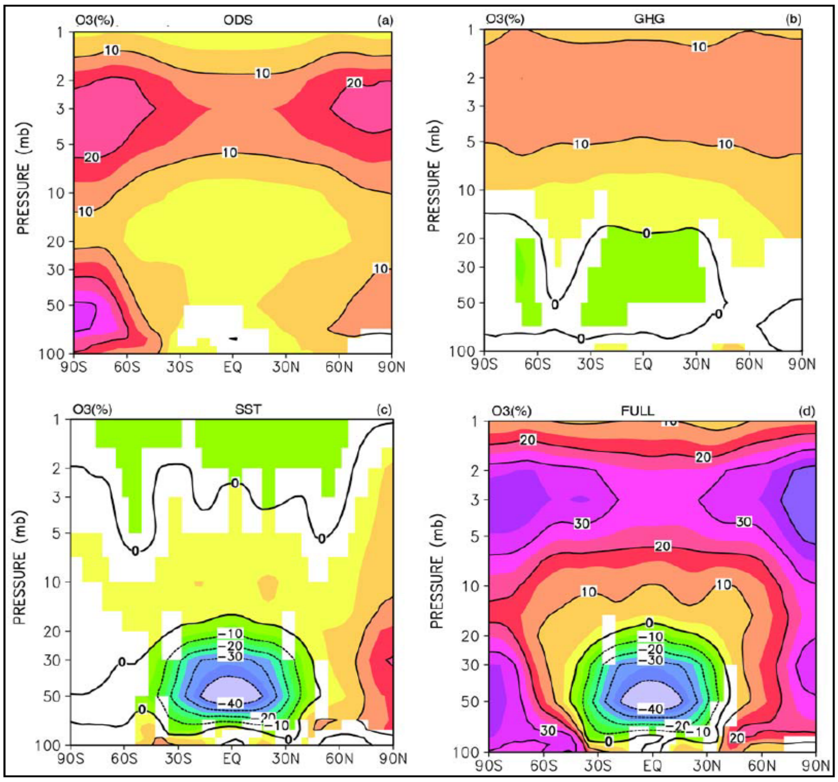

Figure 1.6 *Zonal, annual and ensemble mean percentage changes of the ozone mixing ratio between different timeslice integrations of the SOCOL CCM for 2100 and for 2000 conditions. (a) Ozone changes from 2000 to 2100 when only ODSs are changed. (b) Ozone changes from 2000 to 2100 due to GHG changes only. (c) Ozone changes due to changes in sea surface temperature and sea ice, driven by tropospheric warming. (d) Ozone changes when ODS, GHG, sea surface temperature, and sea ice are all changed together. White regions indicate non-significant changes at the 5% confidence level. Adapted from Zubov et al. (2013) and WMO (2014).*

Key observable ('Priority A'): Stratospheric ozone

Special requirements: Global measurements extending into polar night with high horizontal (100 km) and high vertical resolution (1-2 km in the LS and MS; 3-4 km in the US)[5]. For analysing ozone trends consideration of zonal averages will be sufficient in most cases, which might allow for more relaxed requirements on the random error component of individual ozone observations.

Temporal density of the sampling: Global observations with daily/weekly temporal resolution.

[5] Definitions of the altitude domains for Lower Stratosphere (LS), Mid Stratosphere (MS), and Upper Stratosphere (US) are provided in Section 2, Table 2.1

1.3.2 Brewer-Dobson Circulation

Changes in the Brewer-Dobson circulation are an important driver of stratospheric change as they impact stratospheric ozone both directly and indirectly (Gerber et al., 2012; see also Section 1). These changes affect both the speed of the mean meridional overturning and the mixing intensity across transport barriers in the stratosphere, e.g., across the 'tropical pipe' (Ploeger et al., 2015). Changes in the Brewer-Dobson circulation have indeed been observed in past years (e.g., Mahieu et al., 2014; Ray et al., 2014; Ploeger et al., 2015) and are projected to continue into the future in a changing climate (e.g., WMO, 2014). These changes affect ozone and also other stratospheric tracers and need to be accounted for when studying the evolution of the stratospheric ozone layer. For example, changes in the abundance of CFCs and thus of inorganic chlorine (at a given altitude) indirectly influence chemical ozone loss.

A widely used measure for the strength of the stratospheric circulation is 'age of air' (AoA), which is variable in time and latitude and throughout the stratosphere (e.g. Stiller et al., 2012; Mahieu et al., 2014; Moore et al., 2014; Ray et al., 2014; Ploeger et al., 2015). Observations of SF_6 have been shown to be very well suited for observing variability in stratospheric age of air, because SF_6 does not have stratospheric sources and sinks and a relatively constant tropospheric growth rate (Stiller et al. 2008; 2012). These studies using SF_6 for deducing stratospheric age of air or its trends have relied on strongly averaged data (in particular zonal averages and relatively coarse latitudinal resolutions). Averaging of SF_6 measurements over zonal bands would also be possible for operational applications, which allows the random error of the individual measurements to be reduced.

An alternative to SF_6 is CO_2 (e.g., Schmidt and Khedim, 1991; Ray et al., 2014), but the determination of mean age values below 2 years based on CO_2 is hampered by the seasonal cycle in the troposphere, which propagates into the stratosphere. CO_2 also has a stratospheric source through the production of CO in the oxidation of methane followed by the reaction $CO + OH \rightarrow CO_2 + H$, which can however be corrected for if methane would be measured simultaneously (Stiller et al., 2012). However, CO_2 is difficult to measure from space; there are no examples of measurements at high vertical resolution of CO_2 in the stratosphere. Limited studies on age of stratospheric air have also been conducted using CF_4 (Harnisch et al., 1999) and HF (Russell et al., 1996).

Other long-lived stratospheric tracers (e.g., CH_4, N_2O, CFCs, though also O_3 itself) are influenced by varying age of air and can thus provide some information on age of air. However, the analysis is complicated by the fact that these tracers have a stratospheric chemical sink. Nonetheless, multi-year, global-scale distributions of long-lived stratospheric tracers would be useful for diagnosing large-scale changes and variability of the net transport within the middle atmosphere (Pommrich et al., 2014; Remsberg, 2014). Furthermore, stable degradation products of the CFCs, namely HF and HCl may also provide useful observations to deduce changes in stratospheric transport patterns and age of air (Russell et al., 1996; Mahieu et al., 2014). Recently, Moore et al. (2014) have put forward a concept to monitor stratospheric age-of-air based on long-term measurements of long-lived stratospheric tracers and also discussed the benefits of SF_6 and CO_2 measurements.

Moreover, zonally averaged water vapour (H_2O) in the tropical lower stratosphere shows an anomaly pattern (the so called "tape recorder" pattern) and the speed of the upward propagation of this pattern is a measure of tropical upwelling. Tropical upwelling and stratospheric water vapour are thus closely related to changes in the Brewer-Dobson circulation (e.g. Randel et al., 2006; Dhomse et al., 2008). However, for directly monitoring changes in the Brewer-Dobson circulation on a global scale sustained observations of the stable tracers have a higher priority.

Key observables other than ozone ('Priority B'): SF_6, CO_2, CH_4, N_2O, CFCs, H_2O, HCl, HF, CF_4

Special requirements: In order to resolve patterns of AoA change (Figure 1.4), a vertical resolution of 2 to 4 km and a horizontal sampling of 100-200 km is required throughout the stratosphere (threshold). In the case of SF_6 the requirements are on zonal averages which might allow for more relaxed requirements on the random error component of individual observations.

Temporal density of the sampling: Changes in the Brewer-Dobson circulation are in the order of months per decade. Since seasonal effects are important, global observations with weekly/monthly temporal resolution are required.

1.3.3 Stratospheric Chemistry

Polar ozone

Chemical ozone destruction at the poles is initiated by heterogeneous chlorine activation on the surfaces of cold stratospheric aerosol and polar stratospheric clouds (PSCs). Activation occurs through the conversion of reservoir chlorine species (HCl and $ClONO_2$) to active chlorine (ClO). Chlorine activation rates are mainly controlled by temperature with a limited dependence of heterogeneous activation rates on the different particle types. Nonetheless, the formation of different types of particles is important as these particles may significantly alter gas-phase chemistry through the uptake or permanent removal (through particle sedimentation) of HNO_3 (Wegner et al., 2012; Wohltmann et al., 2013; Grooß et al., 2014). Monitoring HCl, $ClONO_2$, and ClO in the polar stratosphere puts additional constraints on the polar chemistry responsible for polar ozone depletion. Temperature information is essential, because low temperatures not only trigger activation but also allow rapid chemical ozone loss to proceed. In this part of the atmosphere, reliably temperature information is provided through the meteorological (re-)analyses.

In spring 2011, the extent of polar ozone loss in the Arctic was in the range of observations of weak Antarctic ozone holes (Manney et al., 2011); however, the abundance of ozone above the Arctic was still substantially larger than in Antarctic ozone holes, where still the strongest polar ozone losses are observed (WMO, 2014). Variability and recovery of Antarctic ozone will be different at the vortex edge and the vortex core, e.g., because of different temperatures different solar insolation and transport barriers in the polar vortex (Lee et al., 2001; Tilmes et al., 2006b). Moreover, a distinction between polar vortex and mid-latitude air is necessary. Therefore, a good horizontal coverage (extending into polar night) and resolution of measurements in the polar lower stratosphere (100 to 200 km) is required. Polar ozone loss occurs rapidly, requiring weekly to daily temporal resolution.

Water vapour affects the chemistry of polar ozone loss through its impact on polar stratospheric cloud formation and on heterogeneous reactivity (e.g., Vogel et al., 2011; Drdla and Müller, 2012). Water vapour is also important for the formation of ice clouds in the polar winter stratosphere (PSC Type II); however, ice clouds rarely form in the Arctic stratosphere (e.g., Pitts et al., 2013) and in the Antarctic they have only a minor impact on polar ozone depletion (Kirner et al., 2015).

Height resolved observations of ozone and long lived tracers (e.g., CH_4, N_2O) allow the chemical ozone loss in an Antarctic season to be diagnosed through the tracer correlation technique (e.g., Müller et al., 1996; Tilmes et al., 2006a), provided a good coverage of the Antarctic vortex region (including polar night) over the winter and spring is given. A good spatial coverage of vertically well resolved ozone measurements allows for an application of the "Match" technique (von der Gathen et al., 1995; Terao et al., 2002). In this way it is possible to distinguish chemical change from dynamically caused ozone change.

Mid-latitude ozone

Total ozone in mid-latitudes has also been affected by chemical ozone depletion from ODSs, albeit to a much lesser extent than polar ozone (WMO, 2014). Mid-latitude total ozone is dominated by ozone in the lower stratosphere, where a large variability complicates the identification of long-term ozone changes. Further, the dominant ozone loss cycle in the stratosphere is driven by NO_X radicals for which HNO_3 is the major reservoir species and N_2O is the main source gas.

Ozone in the lowermost stratosphere at mid-latitudes is also influenced strongly by loss through HO_X radicals for which water vapour is the source species. However, water vapour trends and variability in the lowermost stratosphere are highly uncertain (Kunz et al., 2013; Hegglin et al., 2014) and, furthermore, depend on season. This calls for water vapour monitoring in this region with monthly to weekly resolution.

Tropical ozone

Future abundances of gases like H_2O, N_2O, and CH_4 impact tropical ozone through chemical effects and via their influence on climate change. Changes in the Brewer-Dobson circulation, and thus in tropical upwelling also have an impact on tropical ozone in the lowermost stratosphere, with an increase in upwelling leading to a reduction in ozone. Based on SAGE II data, negative ozone trends in the tropical lower stratosphere (about 18-19 km) for 1985–2005 were reported in WMO (2011). Chemical climate models consistently simulate a long-term decline of ozone in the lowermost tropical stratosphere by up to 20% between 1960 and 2060 (WMO, 2014). However, recent analyses of shorter satellite data sets, between 2002 and 2012, do not show significant lower stratospheric ozone trends (Gebhardt et al., 2014; Eckert et al., 2014).

Further, a combined SAGE II-GOMOS data set for 1984-2011 (Kyrölä et al., 2013) shows a significant negative trend between 20-22 km for the period 1984-1997 but an insignificant trend for 1997-2011. Nedoluha et al. (2015) report a significant decrease in tropical ozone at 10 hPa over the time period 1991-2013, which they attribute to an increase in NO_y caused by a decreasing upwelling in the tropics. These recent studies indicate a substantial decadal variability of ozone in the tropical lowermost stratosphere (WMO, 2014). Therefore, high vertical resolution is required in the tropical lower stratosphere and a long term coverage with good stability. To determine the tropical ozone trends and variability and their seasonal dependencies, monthly/weekly time resolution would be sufficient.

Stratospheric sulphate layer

Stratospheric ozone is influenced by the stratospheric sulphate layer. The stratospheric sulphate layer is fed both from natural sources (mainly COS), volcanic eruptions, and from tropospheric pollution (Brühl, et al., 2012). The stratospheric “background” aerosol layer is strongly enhanced by major volcanic eruptions, like El Chichon in 1982 and Mount Pinatubo in 1991, with direct injections into the stratosphere. However, smaller volcanic eruptions have been shown to also have an impact on the lowermost stratosphere (Vernier et al., 2011a; Fairlie, et al., 2014; Fromm et al., 2014; Ridley, et al., 2014).

Enhanced aerosols distributed globally in the lower stratosphere in both hemispheres directly affect stratospheric temperatures and can also provide additional surfaces for heterogeneous chemical reactions on liquid particles in polar regions (e.g., Kawa et al., 1997; Tilmes et al., 2008; Drdla and Müller, 2012). Stratospheric aerosol particles are further of great relevance for the NO_X chemistry throughout the stratosphere because they catalyse the reaction $N_2O_5 + H_2O \rightarrow 2\ HNO_3$ (which is not dependent on temperature) and thereby lead to a reduction of NO_X levels.

Very Short-Lived Species

In addition to the long-lived ozone depleting substances (such as CFCs and halons) also very short-lived substances (VSLS) can contribute significantly to the stratospheric halogen loading (WMO 2010, WMO 2014). In particular short-lived bromine compounds have a significant impact on the ozone layer. Observations of bromine monoxide (BrO) from SCIAMACHY/Envisat provided for the first time a global picture of the stratospheric bromine loading. A number of different studies based upon stratospheric BrO observations from balloon and satellites indicate that VSLS contribute about 5 (2-8) pptv (the total stratospheric bromine is about 20 pptv) to the current stratospheric bromine loading (WMO, 2010; WMO, 2014).

Although important progress has been made in the recent past to better quantify the contribution of stratospheric bromine from VSLS and to investigate the processes that transport VSLS into the stratosphere via the tropical UT/LS, little is currently known how the impact of VSLS on the stratospheric ozone layer will evolve in the next decades under the influence of a changing climate.

Upper stratosphere

Change in upper stratospheric ozone driven by chemical change is dominated by changing upper stratospheric chlorine, which can be best monitored by HCl measurements. CH_4 constitutes an important sink for upper stratospheric chlorine radicals (through the reaction $CH_4 + Cl \rightarrow HCl + CH_3$). In addition upper stratospheric ozone is affected by small diurnal variations of a few percent, which is relevant for trend studies (Studer et al., 2014; Sakazaki et al., 2013; Parrish et al., 2014).

To minimise the diurnal effect, a sun-synchronous orbit with a fixed local equator crossing time could be chosen. For consecutive missions with varying local times at the equator some harmonisation in the long-term data record is required when combining data from the different missions. In case a more inclined orbit would be selected, to enhance revisiting times, local time variation will need to be accounted for in trend monitoring, In principle, diurnal corrections can then be derived by binning data according to different local times as was done in studies by Sakazaki et al., 2013 and Studer et al., 2014.

Summary

Observing the chemical species which are key to the processes driving ozone destruction in the various regions of the atmosphere will allow the monitored behaviour of ozone to be attributed to processes driving the changes in ozone. The importance of particular species varies with region, but the anthropogenic impact on stratospheric ozone is clearly dominated by chlorine species. The strongest ozone depletion occurs in the polar regions, driven by very low temperatures and heterogeneous reactions on stratospheric particles and clouds.

Key observables other than ozone (‘Priority B’): HCl, HNO_3, H_2O, $ClONO_2$, BrO, N_2O, CH_4

Further important observables (‘Priority C’): PSCs, aerosol (surface area density), ClO, NO, NO_2, N_2O_5, $BrONO_2$

Special requirements: Measurements in the polar regions (including polar night), high horizontal (100-200 km in the LS and MS, and 300-400 km in the US) and vertical resolution (1-2 km in the LS and MS; 3-4 km in the US)[6].

Temporal density of the sampling: Global observations with daily to weekly temporal resolution.

[6] Definitions of the altitude domains for Lower Stratosphere (LS), Mid Stratosphere (MS), and Upper Stratosphere (US) are provided in Section 2, Table 2.1

1.3.4 Tropospheric Ozone

Tropospheric ozone is an important greenhouse gas and an air pollutant (e.g. Jacobson, 2012). It is responsible for significant damage to crops and forests, and has adverse effects on the human respiratory system. On the other hand, it is a precursor of hydroxyl radicals (OH), which determine the oxidizing capacity of the lower atmosphere. Thus, tropospheric ozone is important for the removal of other pollutants from the troposphere. Ozone in the upper troposphere in the tropics also has a significant impact on radiative forcing (Riese et al., 2012; see also Figure 1.7).

A significant contribution to tropospheric ozone, particularly in the upper troposphere, comes from the stratosphere, the exact amounts are still uncertain, but are believed to be governed in part by stratospheric circulation changes (Wang et al., 2011; Neu et al., 2014). Lightning-induced NO_X (NO + NO_2) plays an important role in ozone chemistry in the tropical troposphere as well. In general upper tropospheric ozone levels are very low and may be in most cases below detection limits. However in case of enhanced ozone levels from stratospheric intrusions they become measurable from limb sounders.

Several approaches have been used to determine tropospheric ozone from space-based observations. Direct retrieval of tropospheric ozone profiles is possible by exploiting spectral information with peak sensitivity in the troposphere from infrared measurements: Tropospheric Emission Spectrometer (TES, e.g., Bowman et al., 2006) and the Infrared Atmospheric Sounding Instrument (IASI, e.g., Coheur et al., 2005); and UV-Vis measurements such as GOME-2 (e.g. Miles et al., 2015). Profiles retrieved from nadir viewing instruments typically have coarse vertical resolution (approximately 6 km) and much of the ozone information in the UT also comes from the LS (e.g. Parrington et al., 2008).

Another approach is to derive tropospheric ozone columns from the combination of limb and nadir sounders is the subtraction of the stratospheric column (limb) from the total column (nadir). This residual method was first successfully applied by Fishman et al. (1990) by combining data from the nadir viewing Total Ozone Mapping Spectrometer (TOMS) and limb viewing Stratospheric Aerosol and Gas Experiment (SAGE-I and II) instruments. Ebojie et al. (2014) was the first to combine nadir and limb observations derived from the same instrument, here SCIAMACHY. The OMPS/JPSS also provides the same possibility to combine their nadir and limb ozone observations. Accurate knowledge of stratospheric ozone is critical to retrieving and interpreting tropospheric ozone. High vertical resolution in the UT/LS (1-2 km) from a limb sounder is required to improve observational sensitivity over this altitude range and for separating the tropospheric and stratospheric regime.

Key observable ('Priority B'): Ozone profiles in the UT for enhanced tropospheric ozone levels.

Special requirements: Tropospheric ozone, either by targeting tropospheric columns in retrievals through limb-nadir matching or through combined assimilation of both nadir and limb-based ozone observations. Global observations with high horizontal (100 km) and vertical resolution (1-2 km in the UT/LS; 3-4 km in the US).

Temporal density of the sampling: Global observations with daily to weekly temporal resolution.

1.3.5 Extension into the Mesosphere

In the mesosphere ozone is strongly influenced by solar radiation and exhibits a distinct diurnal cycle. Over an 11-year solar cycle, depending on the level of UV solar activity assumed, ozone may change anti-cyclic with solar activity (e.g. Merkel et al., 2011, WMO 2014). In the upper stratosphere solar cycle changes are currently uncertain to within a factor of two. Solar UV activity is an important climate factor as it influences stratospheric temperatures and, consequently, atmospheric circulation (Grey et al., 2010).

Large ozone depletion may be observed following enhanced solar proton precipitation producing elevated NO_X level that can descend down into the stratosphere causing substantial ozone depletion lasting for several months (e.g. Seppälä et al., 2004; Lópes-Puertas et al., 2005; Rohen et al., 2005; Vogel et al., 2008). CO may furthermore be an additional species of interest as a tracer of intrusions of mesospheric air into lower stratosphere (Müller et al., 2007).

Important observables ('Priority C'): ozone, NO, NO_2, CO, temperature

Special requirements: In the mesosphere, the vertical resolution can be relaxed to 3 to 4 km.

Temporal density of the sampling: For assessing trends, global observations with weekly/monthly time resolution would be sufficient.

1.3.6 Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols

Water vapour is a very important greenhouse gas in the atmosphere. At higher altitudes in the troposphere it is responsible for the "water vapour feedback" (Dessler and Sherwood, 2009), which substantially enhances the radiative forcing induced through the increased concentrations of the greenhouse gases including CO_2, N_2O, CH_4, chlorofluorocarbons and ozone. Water vapour accounts for about half of the present day (natural) greenhouse effect and is the most important gaseous source of infrared opacity in the atmosphere (Schmidt et al., 2010).

A particular large climatic impact of H_2O and ozone changes is expected in the UT/LS, which is a region of rather low temperatures and plays an important role for atmospheric cooling to space and radiative forcing of the atmosphere. For example, Figure 1.7 (left, top) shows that the impact on surface temperature of an ozone unit mass change at 100 hPa at the equator is about a factor of 2 larger than the impact of the same change at 10 hPa (Riese et al., 2012). Methane changes are also important but the peak impact occurs at somewhat lower altitudes (Figure 1.7, right). A strong impact of changes in concentration at the tropopause levels is also found for water vapour (Figure 1.7, middle, see also Solomon et al., 2010). Stratospheric water vapour has also been suggested as an important driver of decadal global surface climate change (Solomon et al., 2010; Riese et al., 2012; Dessler et al., 2013).

Large volcanic eruptions cause elevated levels of stratospheric sulphate aerosols (Fairlie et al., 2014; Fromm et al., 2014) and episodic cooling of global average surface temperatures for a few years and thus have an impact on climate (Solomon et al., 2011). Long-term satellite measurements of stratospheric aerosols have been mainly provided by SAGE II until 2005 (Thomasson et al., 1997, ASAP, 2006). A higher global sampling has been achieved with the UV/VIS limb sounders OSIRIS (Rieger et al. 2014) and SCIAMACHY (Ernst et al., 2012) since 2001. The spaceborne CALIPSO lidar has also contributed important global aerosol measurements (Vernier, et al., 2012a; Fairlie et al., 2014).

Also, hyperspectral infrared limb instruments, such as MIPAS, have been found well suited for aerosol observations, both at day and night time. Especially the detection, classification and quantification of volcanic aerosol has been a focus in the past (Echle et al. 1998, Griessbach et al. 2012, Grainger et al. 2013, Griessbach et al. 2014). Nonetheless, there is evidence that currently available satellite instrumentation can not observe a substantial amount of the volcanic aerosol between the tropopause and 15 km at middle to high latitudes, leading to an underestimate of total radiative forcing resulting from the recent volcanic eruptions (Ridley, et al., 2014). Thus, vertically resolved measurements of stratospheric aerosol down to the tropopause would be of particular importance.

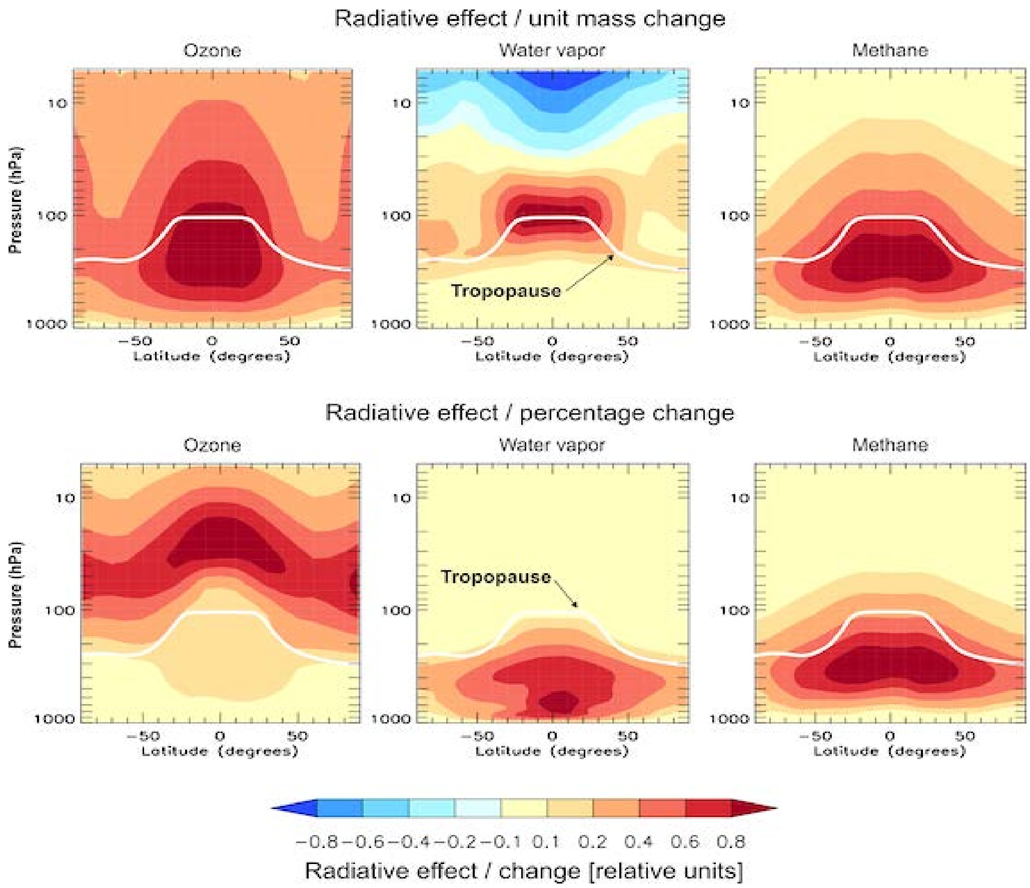

Figure 1.7 *Sensitivity of surface temperature to the altitude and latitude of (left) ozone, (middle) water vapour, and (right) methane changes. Shading shows relative impact on surface temperature, measured as radiative effect, from either (top) unit mass increases or (bottom) 1% increases applied at individual latitudes and altitudes (1 km thick layers). For each trace gas, the calculated radiative effects have been normalized to the respective maximum value. Red colours are indicative of warming, blue colours indicate cooling. (Figure taken from Riese et al. (2012)).*

Over the time period of available observations (since 1970) no significant trends in background aerosols were found (Deshler, 2008), however, minor volcanic eruptions (Ernst et al., 2012; Fromm et al., 2014; Ridley, et al., 2014; see also Figure 1.8), pyro-convection (Damoah et al., 2006) as well as the Asian monsoon lifting tropospheric sulphur pollutant (Notholt et al., 2005; Bourassa et al., 2012) may be responsible for significant variability in "background" stratospheric aerosol. For the period 2000 to 2010, Solomon et al. (2011), using data from several independent data sets (including lidar and satellite data), deduced that stratospheric aerosols increased by about 7% per year. Such an increase implies a change in radiative forcing of about –0.1 Watt per square meter over this period, which constitutes a significant effect (Solomon et al., 2011).

One suggestion of human "geo-engineering" to actively counteract global warming is the injection of sulphur aerosols into the stratosphere (Crutzen, 2006; Rash et al., 2008). A better understanding of the impact of a hypothetical geo-engineering with sulphate aerosols on the ozone layer is needed. Enhanced sulphate aerosols could substantially delay the recovery of Antarctic ozone and cause enhanced Arctic ozone losses (Tilmes et al., 2008).

Satellite limb observations would be very helpful to refine our knowledge on the aerosol effect on climate as well as on stratospheric ozone and also would provide reasonable constraints for assessing geo-engineering concepts. Addressing these questions requires observations of vertically resolved aerosol properties (e.g. extinction) and, possibly, also sulphate species.

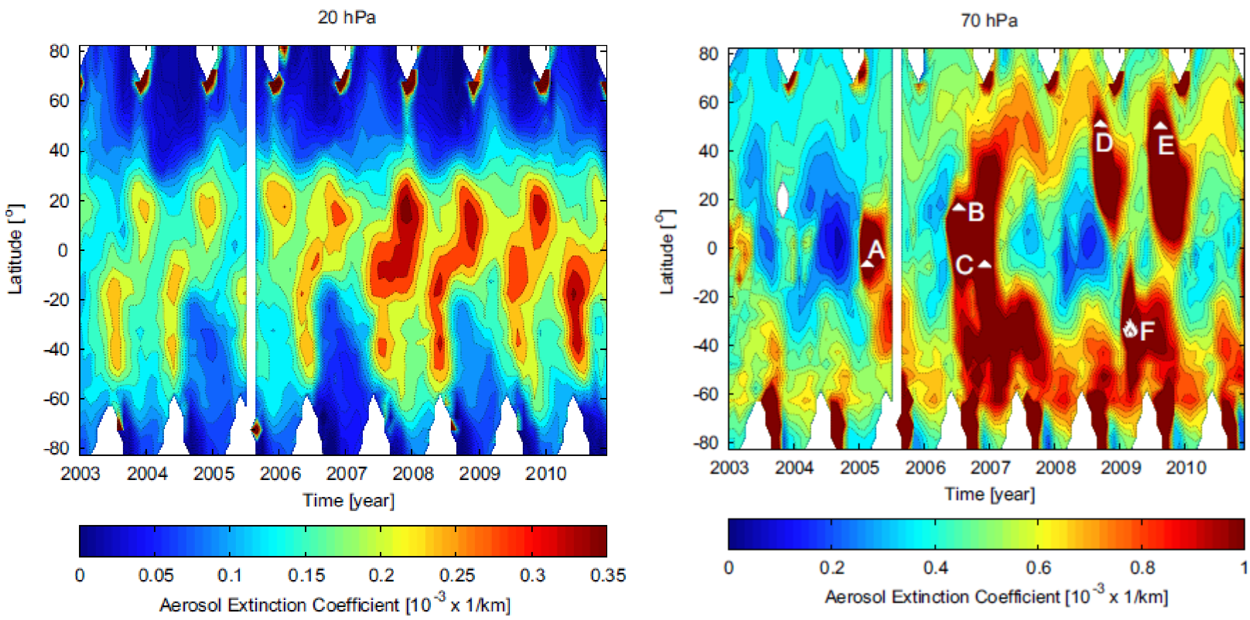

Figure 1.8 *Variation of stratospheric aerosol extinction at 20 hPa (left panel, approx. 27 km altitude) and 70 hPa (bottom panel, approx. 18 km altitude) retrieved from SCIAMACHY limb scatter observations. Volcanic eruptions indicated by strong stratospheric aerosol extinction signals at 70 hPa level: (A) Manam (January 2005, 4°S); (B) Soufriere Hills (May 2006, 16°N); (C) Tavurvur (October 2006, 4°S); (D) Kasatochi (August 2008, 52°N); (E) Sarychev Peak (June 2009, 48°N). (F) indicates the Australian bush fires in February 2009 at 38°S. (Figure from Ernst et al., 2012).*

Important observables other than ozone ('Priority C'): water vapour, stratospheric sulphate aerosols (number, surface and volume density), OCS, SO_2

Special requirements: high vertical/horizontal resolution in lower stratosphere and upper troposphere.

Temporal density of the sampling: Weekly to monthly time resolution is required to resolve seasonal cycle effects and to characterize the evolution of sulphate aerosol after small volcanic eruptions.

1.3.7 Climate Impact of Troposphere-Stratosphere-Transport and the Asian Monsoon

Most source gases enter the stratosphere via tropical convection and slow uplifting through the tropical UT/LS. The strongest uplift occurs in Northern Hemisphere winter. However, the Asian summer monsoon anticyclonic vortex is known to provide an additional pathway for vertical transport of tropospheric air to the stratosphere (e.g., Park et al., 2007, Vogel et al., 2014). For example, enhanced stratospheric hydrogen cyanide (HCN; Randel et al., 2010) and of peroxy acetyl nitrate (PAN; Fadnavis et al., 2014) were observed in the Asian monsoon region.

In general the Asian monsoon anticyclonic circulation at altitudes of 18-20 km is characterized by high concentrations of tropospheric source gases (e.g. CO, H_2O, SO_2) and low concentrations of stratospheric source gases (e.g. ozone). Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO) measurements have identified a coincident layer of enhanced aerosol concentrations near the tropopause (Vernier et al., 2011b). Substantial amounts of stratospheric aerosols from a more minor volcanic eruption have been identified being transported through the Asian monsoon (Bourassa et al., 2012).

The Asian monsoon region is also a favoured region for water vapour entry into the stratosphere (e.g., Ploeger et al., 2013). The nature of the transport pathways from boundary layer sources through the Asian monsoon into the lowermost stratosphere in Northern Europe is not well known; recently rapid uplift by typhoons and eastward eddy shedding from the main Asian monsoon anticyclone have been discussed as additional fast transport pathways (Vogel et al., 2014).

Important observables other than ozone ('Priority C'): H_2O, aerosols, HCN, CO, SO_2, PAN

Special requirements: high vertical (1-2 km) and horizontal resolution in the UT/LS

Temporal density of the sampling: Daily to weekly resolution allows the analysis of transport patterns; a monthly sampling the large-scale effects of the Asian monsoon on the global stratosphere.

1.4 Summary and Conclusions

From the discussion of the different applications of possible data products that may be obtained in the frame of a mission monitoring stratospheric ozone at high vertical resolution, a set of objectives emerges. These objectives are driven by the requirements of the different usages of the products of such a mission. The usage includes primarily operational services (e.g., analyses and forecasts of atmospheric composition and support to numerical weather prediction) and verification of the Montreal protocol and its amendments and adjustments, and, secondary, monitoring of the two-way interactions between stratospheric ozone and climate.

1.4.1 Minimum Mission

A “Minimum Mission” would have to add significant value to the existing and planned suite of nadir missions. A mission fulfilling this requirement is an ozone-only mission monitoring the evolution of the stratospheric ozone layer globally with dense spatial sampling (vertically and horizontally) at daily temporal resolution. The scientific background as well as a brief discussion of spatial/temporal requirements is given in Sections 1.2 and 1.3.1.

Ozone distribution, variability, and trends must be characterised in four areas: polar ozone, mid-latitude ozone, tropical ozone, and upper stratospheric ozone.

Improving the quality of operational products such as analyses, ozone forecasts and numerical weather prediction requires vertically resolved observations on a daily basis with good spatial coverage and extending into polar night. Such observations are critical for constraining the vertical distribution of ozone, both in the stratosphere and thus, indirectly, in the troposphere.

Accurately monitoring the development of the ozone layer in a changing climate and with further decreasing ozone depleting substances for all relevant regions (polar, mid-latitudes, tropics) requires good vertical (1-2 km) and horizontal (100-200 km) resolution in the lower stratosphere. Good vertical and horizontal resolution is also required for the upper stratosphere, but the requirements are somewhat more relaxed than in the lower stratosphere (3-4 km vertically and 300-400 km horizontally). For deducing long-term ozone trends, considering zonally averaged data is sufficient.

Long-term homogeneous observations are needed that cover the time period of ozone recovery (mid to end of this century). This calls for a series of small to medium size satellites with well (inter-) calibrated instrumentation.

1.4.2 Mission Extensions

The minimum mission is an ozone-only mission and shall accurately monitor future changes in stratospheric ozone (‘Priority A’). Highest priority components for a mission extension (‘Priority B’) are, “Brewer-Dobson Circulation” (Section 1.3.2) and “Stratospheric Chemistry” (Section 1.3.3) , together with extension of ozone observations into the troposphere (Section 1.3.4).

These extensions would allow, in addition to the minimum mission, both near-real time and long-term monitoring of why ozone is changing, as well as a complete monitoring of both stratospheric and tropospheric ozone. The “Brewer-Dobson Circulation” extension would focus on dynamical drivers of stratospheric ozone change and the “Stratospheric Chemistry” extension would focus on the chemical drivers of stratospheric ozone change. For both extensions a number of additional chemical species next to ozone would be required to be observed. The requirements on coverage and spatiotemporal resolution of these chemical species resemble those of ozone. Similarly, as for ozone, considering zonally averaged data of many of the desirable species may be sufficient for the long-term monitoring applications.

The “Extension into the Mesosphere” (Section 1.3.5) would expand the vertical range of ozone observations up to about 85 km.

The additional mission objective of the mission extension “Radiative impact of Stratospheric Water Vapour and Sulphate Aerosols” (1.3.6) would be monitoring changes in radiative forcing due to these two compounds, which both interact with stratospheric ozone. This extension requires predominantly a good characterization of water vapour and sulphate aerosols in the lower stratosphere.

Similarly, the additional mission objective of the mission extension “Climate Impact of Troposphere-Stratosphere-Transport and the Asian Monsoon” (1.3.7) would be to monitor changes in climate that impact on stratospheric ozone and which are driven through the changing transport patterns in the Asian monsoon circulation. This extension requires the measurement of a number of additional trace species (as has been specified in sub-section 1.3.7).

Throughout this report, the focus is on developing mission objectives and discussing user requirements for a limb mission measuring ozone at high vertical resolution. The priorities for measuring stratospheric constituents other than ozone presented above were set on this basis. Had we considered the priorities in a more general sense, namely the priorities for a high resolution limb mission for stratospheric composition, the issue of climate change (as well as volcanic eruptions) would have been more prominent than in the above discussion. In particular, this would have led to a much higher prioritization of measurements of stratospheric water vapour and sulphate aerosols, especially in the lower and middle stratosphere.

2 Definition of Observational Requirements

2.1 Introduction

Based on the mission objectives and associated user requirements presented in Section 1, technologically free – though not technologically ignorant, in this section geophysical observational requirements are identified. The priority settings for the observational requirements follow the definitions used in prioritizing the user requirements in Section 1. Mandatory observational data products are denoted as ‘Priority A’ requirements, desirable observational data requirements as ‘Priority B’ requirements and further useful data products are denoted as ‘Priority C’.

In Section 2.2 the observational requirements are identified for a minimum mandatory (‘Priority A’) *ozone-only* mission targeting the operational services (user area ‘U1’). Also desirable mission extensions (‘Priority B’) in response to the user requirements for the operational services are derived as well as a few other useful extensions (‘Priority C’).

In Section 2.3 the observational requirements are identified for a minimum *ozone-only* mission targeting long-term monitoring (user area ‘U2’). Further, desirable (‘Priority B’) and other useful (‘Priority C’) observational requirements are presented for the mission extensions suggested in Section 1.

In Section 2.4 the ‘Summary Observational Requirements (SOR)’ are presented in one overall summary table containing the mandatory and desirable quantitative mission and data requirements. The summary table contains both threshold and breakthrough requirements, where the breakthrough requirements refer to user area ‘U3’ which is mainly considered to represent the R&D user domain. The distinction between the user areas U1, U2, and U3, the role of science and R&D for application development, and the relation between the user areas and the use of threshold and breakthrough requirements is further detailed in Appendix A. The SOR-table (Table 2.7) is carried forward to Section 3 for the ‘reality check’.

2.1.1 Target, Breakthrough and Threshold Requirements

In the WMO/ESA response to GCOS (WMO/ESA, 2011) definitions are given for what should be understood with target, threshold and breakthrough requirements. *Target* (or *goal*) requirements refer to maximum requirements, i.e. an ideal value above which further improvement of the observation would not cause any significant improvement in performance for the application in question. Target requirements are not considered in *Operoz* because the focus in this project is on a minimum mission for operational applications.

Breakthrough requirements provide an intermediate requirement, in between threshold and goal which, if achieved, would result in a significant improvement for the targeted application. The *Threshold* requirements provide the minimum requirement which have to be met to ensure that data are useful. Below this minimum, the benefit derived does not compensate for the additional cost involved in using the observation.

Threshold requirements for any given observing system cannot be stated in an absolute sense. Always some assumptions have to be made concerning which other observing systems are likely to be available. As discussed in Section 1, in the case of *Operoz* concerning the need for stratospheric ozone observations from limb-view the defined thresholds are based on the assumed presence of planned operational nadir observations (MetOp-SG and the Sentinels 4/5/5P) as well as the continuation of present-day ground-based networks for ozone observations such as the ozone sonde and ozone lidar networks. Surface networks are crucial for the validation of the satellite observations of ozone.

2.1.2 Entries for the Level-2 Product Requirements

In the next sections we will discuss for ozone observations as well as other observables the required spatial coverage, horizontal sampling, vertical resolution, temporal resolution and update frequency, as well as measurement uncertainty, timeliness and long-term stability requirements. These requirements refer to the Level-2 data requirements for an individual observation even though different sampling strategies might be used to comply with the Level-2 data requirements.

The horizontal sampling requirements relate to *along-track* sampling. Across-track sampling is considered as a potential mission extension and for that extension across-track sampling requirements are provided. Vertical resolution requirements are specified because these drive the user requirements, while different vertical sampling strategies could be used in limb geometry.

Temporal resolution is directly related to the coverage and required revisiting time at a certain location. While user requirements are typically specified in terms of spatio-temporal resolution, e.g. a global distribution at specified spatial resolution every 12 h, 1d, 1 week, etc., observational requirements should combine coverage requirements, e.g. global, with realistic revisit time requirements, e.g., a (sub-)daily, weekly, repeat of an observation at either a specific location, or (e.g.) within a specified longitude and latitude range. Different observation geometries (occultation vs. scattering, choice of orbit) intrinsically leads to different revisit times.

As indicated above the observational requirements in *Operoz* are to be defined technologically free, though not technologically ignorant. Basic assumption for *Operoz* is that a small to medium size limb mission will be flown on a low-Earth polar orbit revisiting all latitudes about 32 times daily (including night and day). The mission will not make use of multiple platforms. These assumptions intrinsically limit the update frequency at a specific geographical (latitude/longitude) location. The update frequencies provided in the next sections are to be read with acknowledgement of these practical limitations.

Where applicable, and in order to satisfy specific user requirements, the requirements on the total uncertainty (or ‘total error’) are further detailed, e.g. in relation to required knowledge of random and systematic contributions to the total uncertainty. Also, in response to user requirements on ozone trends requirements on stability are specified. Stability has been identified of prime importance for long-term monitoring and the construction of climate data records and thus stability requirements have been formulated. Similarly, timeliness has been identified of prime importance for operational services (Section 1) and therefore timeliness requirements are also defined.

2.1.3 Definition of Altitude Domains

Within *Operoz* six altitude domains have been defined. These altitude domains are needed to exactly define the vertical coverage for the ozone data requirements and to be able to differentiate these requirements as a function of altitude in the atmosphere.

The stratosphere is divided into an upper stratosphere (US) between 30 and 50 km altitude, a middle stratosphere (MS) between 20 and 30 km altitude and a lower stratospheric region between the tropopause and 20 km altitude. Outside the tropical belt the stratospheric region between the tropopause and 20 km is commonly referred to as the lowermost stratosphere (LMS). The tropopause varies as a function of latitude. Different definitions of the tropopause can be used, e.g. based on the temperature profile or dynamically through potential vorticity.

Because in *Operoz* the focus is on stratospheric ozone observations we loosely refer to the tropopause as the altitude below which the ozone concentrations are smaller than about 100 ppbv. Climatologically the tropopause varies from about 6 km at the poles to about 17 km at the equator. In the sub-tropics as well as the mid-latitudes multiple tropopauses may be encountered with alternating layers of tropospheric and stratospheric origin. Typically the altitude range between 6 and 20 km will be referred to as UT/LS. The stratopause (i.e. the top of the stratosphere) is also dependent on latitude and may vary from day-to-day as well. Here the upper altitude limit for the stratosphere is set to a global climatological value of about 50 km altitude. The definitions of the different altitude domains as used within *Operoz* for the definition of the observational requirements are summarized in Table 2.1.

Abbreviation	Full name of the atmospheric domain	Altitude range used in *Operoz*
T	Troposphere	SFC - TP
UT	Upper Troposphere	6 km - TP
LS	Lower stratosphere	TP - 20 km
MS	Middle stratosphere	20 - 30 km
US	Upper stratosphere	30 - 50 km
M	Mesosphere	50 - 85 km

Table 2.1 *Definition of the altitude regions in the atmosphere within Operoz. SFC = Earth's surface; TP is tropopause (typically at ~6 km at the poles and at ~17 km in the tropics). The UT has been defined to contain the tropospheric layers above 6 km and below the tropopause. The UT/LS refers to the 6 to 20 km altitude region. For the stratopause a constant altitude is used which is set at 50 km altitude.*

2.2 Operational Services

The CAMS and NWP services to which the operational ozone observations from limb geometry will provide additional observational constraints include forecasting and analysis as well as model validation through data assimilation. The exact scope of the (end-)user requirements has been defined in Section 1. Here we distinguish the observational requirements for a mandatory minimum ozone-only mission (section 2.2.1) and suggest desirable mission extensions (2.2.2) in response to the user requirements.

2.2.1 Role of Service Providers in Relation to Setting Observational Requirements

Recently, in the EU FP7 project GMES-Pure (see http://www.gmes-pure.eu) service providers such as CAMS and NWP centres have been identified to play an important role for the translation and traceability of (end-)user requirements (such as formulated in Section 1) into observational requirements as relevant for e.g. space agencies.

In GMES-Pure several illustrative decision trees have been constructed. (see http://gmes-pure.eu/wpcms/wp-content/uploads/2014/04/D3_4-GMES-PURE-ServiceDataRequirements-v1C.pdf). An excerpt of one of these decision trees is copied below (Figure 2.1). The figure shows that feedback and confirmation from service providers is in the centre of the decision tree because the knowledge of the service providers is needed to define the observational requirements. These observational requirements shall be fully traceable to the provider's service specifications and further to the (end-)user requirements for the information services to be provided.

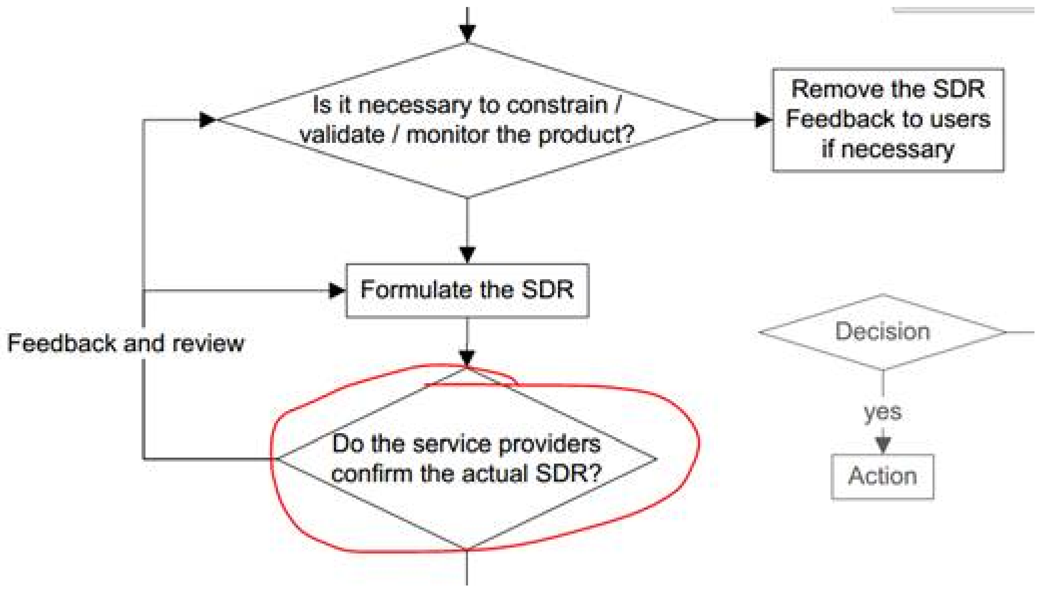

Figure 2.1 *Excerpt from the decision tree on service data requirements and the role of the service provider on the traceability of observational requirements to (end-)user needs (GMES-Pure EU project deliverable on Service Data Requirements (http://gmes-pure.eu/wpcms/wp-content/uploads/2014/04/D3_4-GMES-PURE-ServiceDataRequirements-v1C.pdf).*

Service data requirements such as for the CAMS and NWP services are drive by finding the balance between the contributions from the operational model on the one hand and constraints by ground-based, in-situ and spaceborne remote sensing observations on the other. The *Operoz* observational requirements for operational services have been derived together with the CAMS service provider and therefore are the expression of the added value estimated to meet user needs and to provide continuation (threshold) as well as significant improvement (evolution through the breakthrough) of the Copernicus and NWP services.

This basic understanding for a proper translation of user requirements into observational requirements has been applied in *Operoz*, i.e. the service providers (e.g. CAMS) define the exact observational needs to optimally serve their users.

2.2.2 Minimum Mission

The operational services (user area 'U1') targeted by the *Operoz* mission are being delivered through near-real time assimilation of the ozone observations into an operational system providing regularly updated forecasts and analyses. Consequently, stringent ***timeliness*** requirements (**< *3 hours***) apply. For model validation, timeliness requirements are much less stringent so this specific application is not driving the timeliness requirement.

In order to be useful for the operational services a ***global*** coverage is needed on a daily basis (24h) at a minimum. An update frequency of 12h has defined as breakthrough to include information on the diurnal cycle. For all requirements, breakthrough and threshold requirements will be denoted as B /T, so for the update frequency the requirements are written (12h / 24h).

For the use of observations in a data assimilation system there is no specific need to measure the exact same point every day or twice daily. More frequent observations than twice per day would still be desirable for data assimilation to increase spatial sampling but have been considered impossible to obtain with a small to medium size limb mission on a single platform in Low-Earth orbit. The requirements on update frequency therefore should be read within these basic technological constraints that have been imposed on the study.

High vertical resolution (1 km / 2 km) for user area U1 is required in the LS and MS. From a data assimilation point of view there are no strong requirements for operational ozone observations from limb geometry in the US between ~30 and 50 km altitude as part of the minimum mission requirements. The quality of the present-day services for the 30 to 50 km altitude range is currently not well-known due to limited availability of validation data above 30 km. Ozone sondes typically do not reach above 30 km altitude and there is still a general lack of experience with the operational use of the convoluted vertical ozone profiles from present-day operational nadir missions such as GOME-2. Consequently in *Operoz* no mandatory requirements have been formulated for ozone observations above 30 km targeting user area U1.

The vertical coverage requirement for the operational services is therefore to provide compliant stratospheric ozone profile observations from about 30 km down to the tropopause. As discussed in Section 2.2 different definitions could be used to define the tropopause, e.g. based on the temperature gradient, or dynamically through potential vorticity. For practical reasons the ozone requirements are to be met for ozone concentrations down to about a mixing ratio of (100/200 ppbv). Atmospheric layers with lower ozone concentrations are typically considered to be tropospheric in origin and are thus considered outside of the vertical domain to be covered by limb observations of stratospheric ozone. Translated into ozone number densities at e.g. the 150 hPa level and with a climatological tropopause temperature of ~210 K mixing ratios of 100 ppbv and 200 ppbv correspond with ozone number densities of approximately 5.18·10(17) molec.m^{-3} and 1.04·10(18) molec.m^{-3}, respectively.

Table 2.2 summarizes the minimum mission Level-2 requirements for ozone targeting the user requirements for user area U1. The horizontal sampling requirements (100/200 km) relate to the need to observe mesoscale ozone variability in the lower and mid-stratosphere. The vertical resolution requirements of (1/2 km) are traced to the spatial scales of observed ozone profile variability.

The threshold requirements provide the minimum observational needs for user area U1. By fulfilling the breakthrough requirements in Table 2.2 the minimum mission is considered also to be robust for the currently envisioned future evolution of the assimilation services (user area U3).

It has been explicitly stated in Section 1 that ozone observations during polar night are needed. This has been indicated in Table 2.2 under the horizontal coverage requirements. The polar observations need to cover the layers with chemical ozone depletion. The vertical resolution requirements as provided in Tables 2.2 suffice also in the polar region.

Good horizontal spatial coverage of the polar regions is required to distinguish polar vortex and mid-latitude air. Also in this respect the tabulated horizontal sampling requirements for the polar region are not different than defined globally. Because of the low Earth polar orbit which is mostly chosen for operational missions the sampling will be in practice a bit better at high latitudes than for the global average.

Operational Services (user area U1)				**Timeliness: <3h**		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty (*)
O_3	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	8% / 16% or 50 / 100 ppbv
O_3	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	4% / 8% or 50 / 100 ppbv

Table 2.2 *Observational 'Priority A' Level-2 requirements for a minimum mission targeting user area U1. Notation B / T with B=Breakthrough; T = Threshold.*
(*) For the uncertainty requirement the least stringent of the relative and absolute requirements apply while the minimum ozone concentrations to be observed by 'Operoz' are (100 / 200 ppbv) below which the layer is considered tropospheric and thus outside the required vertical domain to be covered.

The uncertainty requirements in the LS (8%/16%; 50/100 ppbv) are less stringent than those in the MS (4%/8%; 50/100 ppbv) mainly because the relative ozone variability is much larger in the LS than in the MS. The least stringent of the relative and absolute requirement applies, i.e. for small ozone concentrations, which mainly will apply to the lowest ozone concentrations in the LS and also in the MS within the polar ozone hole, the relative uncertainty is allowed to exceed 16% in the LS and 8% in the MS. Atmospheric layers with ozone concentrations below (100/200 ppbv) are considered tropospheric and the ozone observations do not need to comply. For the lowest required (threshold) minimum ozone concentration of 200 ppbv the required *relative* uncertainties for a single observation increase ultimately to (25%/50%). For the (breakthrough) minimum ozone concentration of 100 ppbv these numbers are 50% and 100%, respectively.

The uncertainties are to be understood as total errors and to include all random observational errors as well as (quasi-)systematic error components ('biases'). Furthermore, the total uncertainty includes both instrument-related Level-1 error components and retrieval errors. Retrieval biases may include for example latitudinal and height dependent observational biases as well as complex varying bias contributions that are a function of observation geometry, certain atmospheric conditions, etc. The random error component is likely to be mainly related to signal-to-noise ('precision') and is required to be sufficiently small such that in the total uncertainty the quasi-systematic error components are expected to dominate over pure random error components. Note that for use in data assimilation a detailed characterisation of both the random and (quasi-)systematic error components is more important than their exact weighing in the total uncertainty and therefore only the (total) Level-2 uncertainty is tabulated per observable.

Finally, the important assumption made is that the *Operoz* project is about defining an ozone limb mission for CAMS and NWP and not, also, about defining e.g. a (stratospheric) temperature mission to serve CAMS and NWP. Clearly, to define a high vertical resolution limb mission for temperature is outside the scope of the *Operoz* project. CAMS is being built on the NWP infrastructure, which means that benefit is obtained from the work that has been done over the last decades but also that *Operoz* would have to stay in-line with the developments in the NWP community. The *Operoz* project team therefore cannot specify user requirements on meteorological observations as this would need to be coordinated with the full NWP community.

Profile observations of temperature, as well as the extinction coefficient in relation to (e.g. volcanic) aerosols and clouds, would however provide important auxiliary data to a minimum ozone-only mission for the retrieval of ozone from level-1 observations and for the error analysis of the operational limb ozone observations.

2.2.3 Mission Extensions

Based on the discussion in Section 1.2 it would be desirable ('Priority B') for the mission objectives related to the operational services to extent the mandatory observations of ozone with (i) extension of the limb ozone observations into the upper troposphere, and (ii) improved horizontal sampling using across-track limb observations.

The required sub-daily sampling in the LS could be significantly improved using across-track sampling. The sampling requirements would be similar to the along-track, i.e. 100 /200 km. Using a swath width of ~300 to 400 km such three dimensional sampling would allow for the observation of important mesoscale ozone variability around the tropopause related to, for example, tropospheric and stratospheric intrusions (Pan et al., 2009).

The extension of the ozone observations into the UT would also require the capability to observe ozone to lower concentrations. Observations of enhanced ozone levels in the upper troposphere, i.e. ozone concentrations above ~50/100 ppbv (instead of 100/200 ppbv for the minimum along-track, LS only mission) are most important for CAMS and observations of tropospheric ozone will also lead to improved boundary conditions for regional air quality models. The required limb observation of *enhanced* levels of tropospheric ozone excludes requirements on the variations in background tropospheric ozone concentrations below ~50 ppbv, which would exceed present-day detection limits for ozone observations using limb geometry.

The other 'Priority B' mission extensions in support of operational services mission objectives include:

Extension of the ozone observations into the Upper Stratosphere

This extension would require the timeliness requirements (<3h) to include the ozone profile observations in the US (above 30 km altitude), with all other requirements similar as for the minimum mission targeting long-term monitoring including the US (Section 2.3.1)

Stratospheric Chemistry

This extension for the operational services would require observations of HNO_3, HCl, and H_2O ('Priority B'), as well as N_2O, $ClONO_2$, BrO, PSCs, SO_2, NO_2, CH_4 and stratospheric aerosols ('Priority C'). This mission extension is discussed together with the similar extension on 'Stratospheric Chemistry' in relation to Long-term Monitoring (Section 2.3.3) with for this application only differences with respect to the update frequency (12h/24h) and the timeliness requirements (<3h) for the Priority 'B' observations listed above. Also, the 'Priority B' list for stratospheric chemistry in support of the operational services is a sub-set of the 'Priority B' list for the 'Stratospheric Chemistry' mission extension in relation to long-term monitoring (see further Section 2.3.3).

Additional mission extensions in relation to the Operational Services have been assigned 'Priority C'. These extensions include observations of H_2O profiles at high vertical resolution in the UT/LS in support of NWP and observations of stratospheric NO_2, CH_4 and aerosol profiles in support of CAMS tropospheric services. The observational requirements on stratospheric profiles of H_2O, CH_4 and NO_2 are discussed in the 'Priority C' mission extensions in relation to long-term monitoring (Section 2.3 below). The update frequency and timeliness requirements for these 'Priority C' observables would need to be similar as for ozone in the minimum mission in support of operational services.

2.3 Long-term Monitoring

2.3.1 Minimum Mission

As discussed in Section 1 the continuation of ozone profile trend monitoring is required for verification of the Montreal Protocol and its amendments and adjustments. Long-term monitoring of ozone as Essential Climate Variable (ECV) has been recommended by GCOS(2011). Continuation of existing data records has been recommended as well as the need for follow-up limb and/or occultation missions in the coming decades with expected ozone layer recovery. Stringent stability requirements apply for decadal trend monitoring, extending the observational requirements on stability to sequentially planned operational missions. The exact scope of the (end-)user requirements has been defined in Section 1.

For long-term monitoring (user area U2) it has been derived in Section 1 that vertically resolved measurements are mandatory in the upper stratosphere with 'HALOE-like' vertical resolution of 2 to 4 km. The extension into the US is thus a mandatory element of a minimum mission for user area U2 on top of the minimum mission for user area U1

For long-term monitoring limb observations at high vertical resolution would be an essential enhancement to the planned operational nadir missions. One important argument is that upper stratospheric ozone is central in the ozone assessment and protocol monitoring questions. Furthermore, experience over the last decades has learned that calibration issues are difficult to handle for the nadir-based short UV observations. Rapid degradation so far has made the nadir UV profiles much less suitable for trends and monitoring than for near-real time use and data assimilation (user area U1).

Table 2.3 summarizes the minimum mission Level-2 requirements for ozone targeting the user requirements for user area U2. The horizontal resolutions are identical to user area U1 in the lower and mid stratosphere, though a factor 2 relaxed in the upper stratosphere. The vertical resolution requirements of (1/2 km) in the LS and MS are more relaxed in the US (2/4 km). The threshold requirements provide minimum observational needs for user area U2. By fulfilling breakthrough requirements the minimum mission is considered also robust for future assessments as well as more detailed attribution studies (R&D domain, user area U3 (see also Appendix A).

It has been made explicit in Section 1 that ozone observations during polar night are needed, and also for user area U2. This has been indicated in Table 2.3 under the horizontal coverage requirements. The vertical resolution requirements as provided in Tables 2.3 suffice also in the polar region. Good horizontal spatial coverage of the polar regions is required to distinguish polar vortex and mid-latitude air. Also in this respect the tabulated horizontal sampling requirements for the polar region are not different than defined globally. Because of the low Earth polar orbit which is mostly chosen for operational missions the sampling will be in practice a bit better at high latitudes than for the global average.

Uncertainty requirements on individual observations in the stratosphere follow the requirements for user area U1. This is not surprising because the uncertainty requirements are primarily driven by the relevant dynamical range and variability of ozone in the atmosphere at the spatial scales accessible with limb observations. Similarly as for user area U1, the uncertainty numbers as expressed in the table are to be understood as total errors and to include all random observational errors as well as (quasi-)systematic error components ('biases'). Furthermore, the total uncertainty includes both instrument-related Level-1 error components and retrieval errors. Retrieval biases may include e.g. latitudinal and height dependent observational biases as well as complex varying bias contributions that are a function of observation geometry, certain atmospheric conditions, etc. The random error component is likely mainly related to signal-to-noise ('precision') and is required to be sufficiently small such that in the total uncertainty the quasi-systematic error components are expected to dominate over pure random error components.

Long-term monitoring (user area U2)				Long-term stability (O_3 observations): 1% / 3% per decade		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty (*)
O_3	100 / 200	Global (incl. polar night)	1 / 2	LS	Daily/weekly	8% / 16% or 50 / 100 ppbv
O_3	100 / 200	Global (incl. polar night)	1 / 2	MS	Daily/weekly	4% / 8% or 50 / 100 ppbv
O_3	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	4% / 8%

Table 2.3 *Observational 'Priority A' Level-2 requirements for a minimum mission targeting user area U2. Notations similar to Table 2.2.*
(*) For the uncertainty requirement the least stringent of the relative and absolute requirements apply while the minimum ozone concentrations to be observed by 'Operoz' are (100/200 ppbv) below which the layer is considered tropospheric and thus outside the required vertical domain to be covered.

The stability requirement of 1% per decade (breakthrough) is similar to GCOS (2011). The threshold stability requirement of 3% per decade e.g. follows user requirements on stability as formulated in the e.g. User Requirements Documents for the ESA Ozone_cci project (van der A et al., 2011) and the user requirements defined in CMUG (2012). The stability requirement in the context of the CCI programme has been formulated in relation to the existing decadal records using on (combinations of) past satellite missions measuring ozone vertical profiles. This implies that the 3% per decade threshold stability requirement should be read as a multi-mission requirement for operational monitoring of ozone in case a decade (and longer) would have to be covered with more than one operational mission.

2.3.2 Mission Extensions

Brewer-Dobson Circulation

The Level-2 requirements for the mission extension 'Brewer-Dobson Circulation' are listed in Table 2.4 ('Priority B'). Observations of SF_6 throughout the stratosphere are required, or, alternatively, a combination of long-lived tracers including CFC-11 or CFC-12, N_2O and CH_4. Both HCl and CH_4 might be alternative tracer for SF_6 in the US region. CFC-11, and to a lesser extent CFC-12 and N_2O, are less suitable for age-of-air studies in the US because of their chemical losses and thus these species are not required above 30 km altitude for this mission extension. Uncertainty requirements derive from the need to resolve the observed spatiotemporal atmospheric variability of the observables. An equivalent sampling of both hemisphere is required.

The full list of candidate atmospheric constituents to diagnose the Brewer-Dobson (B-D) circulation and referred to in Section 1 include SF_6, CO_2, CH_4, N_2O, CFCs, H_2O, HCl, HF, CF_4 and CO. However, CO serves mainly as a tracer for occasional mesospheric intrusions, rather than monitoring the B-D circulation *per se*. CO_2 also has several disadvantages (seasonal cycle, stratospheric source through CO+OH. Both CO and CO_2 will therefore not be considered further. Because spaceborne observations of HF and CF_4 have not yet been demonstrated these gases have not considered further in the setting the observational requirements for an operational mission.

Long-term monitoring (user area U2) **+ Brewer-Dobson mission extension ('Priority B')**				***Long-term stability (O_3 observations): 1% / 3% per decade***		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty (*)
O_3	*100 / 200*	*Global (incl. polar night)*	*1 / 2*	*LS*	*Daily/ weekly*	*8% / 16% or 50 / 100 ppbv*
O_3	*100 / 200*	*Global (incl. polar night)*	*1 / 2*	*MS*	*Daily/ weekly*	*4% / 8% or 50 / 100 ppbv*
O_3	*200 / 400*	*Global (incl. polar night)*	*2 / 4*	*US*	*Daily/ weekly*	*4% / 8%*
SF_6	100 / 200	Global	1 / 2	LS	Daily/ weekly	0.8 / 1.5 pptv
CFC-11	100 / 200	Global	1 / 2	LS	Daily/ weekly	15 / 30 pptv
CFC-12	100 / 200	Global	1 / 2	LS	Daily/ weekly	30 / 60 pptv
N_2O	100 / 200	Global	1 / 2	LS	Daily/ weekly	20 / 40 ppbv
CH_4	100 / 200	Global	1 / 2	LS	Daily/ weekly	0.1 / 0.2 ppmv
HCl	100 / 200	Global	1 / 2	LS	Daily/ weekly	0.2 / 0.4 ppbv
H_2O	100 / 200	Global	1 / 2	LS	Daily/ weekly	5% / 10%
SF_6	100 / 200	Global	1 / 2	MS	Daily/ weekly	0.8 / 1.5 pptv
CFC-11	100 / 200	Global	1 / 2	MS	Daily/ weekly	15 / 30 pptv
CFC-12	100 / 200	Global	1 / 2	MS	Daily/ weekly	30 / 60 pptv
N_2O	100 / 200	Global	1 / 2	MS	Daily/ weekly	20 / 40 ppbv
CH_4	100 / 200	Global	1 / 2	MS	Daily/ weekly	0.1 / 0.2 ppmv
HCl	100 / 200	Global	1 / 2	MS	Daily/ weekly	0.2 / 0.4 ppbv
H_2O	100 / 200	Global	1 / 2	MS	Daily/ weekly	5% / 10%
SF_6	200 / 400	Global	2 / 4	US	Daily/ weekly	0.8 / 1.5 pptv
CH_4	200 / 400	Global	2 / 4	US	Daily/ Weekly	0.1 / 0.2 ppmv
HCl	200 / 400	Global	2 / 4	US	Daily/ weekly	0.2 / 0.4 ppbv
H_2O	200 / 400	Global	2 / 4	US	Daily/ weekly	8% / 16%

Table 2.4 *As Table 2.3 for the minimum mission ('Priority A', in black italic) with in addition (in green) the observational requirements related to the mission extension 'Brewer-Dobson Circulation' ('Priority B') .*

Stratospheric Chemistry

The Level-2 requirements for the mission extension 'Stratospheric Chemistry' are listed in Table 2.5 ('Priority B'). Apart from the O_3 observations extending into the US, the desirable observables for stratospheric chemistry are HCl, H_2O and CH_4 throughout the stratosphere and N_2O, HNO_3, BrO, and $ClONO_2$ (required only poleward of 50 degrees latitude) are required only in the LS and MS. Uncertainty requirements derive from the need to resolve observed spatiotemporal atmospheric variability of the observable. The update frequency for ozone in the US follows the requirements on the update frequency in the LS and MS for the minimum mission with this mission extension, the other ozone requirements are the same as for the minimum mission. Auxiliary data requirements in relation to the attribution of (chemical) ozone changes include information on temperature (in LS, MS and US), and information on extinction in LS and MS.

Operational Services (user area U1) and Long-term monitoring (user area U2) **+ Stratospheric Chemistry ('Priority B')**				***Timeliness: < 3h*** ***Long-term stability (O_3 observations): 1% / 3% per decade***		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty (*)
O_3	*100 / 200*	*Global (incl. polar night)*	*1 / 2*	*LS*	*12h / 24h*	*8% / 16% or 50 / 100 ppbv*
O_3	*100 / 200*	*Global (incl. polar night)*	*1 / 2*	*MS*	*12h / 24h*	*4% / 8% or 50 / 100 ppbv*
O_3	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	4% / 8%
HNO_3	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	0.5 / 1 ppbv
H_2O	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	5% / 10%
HCl	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	0.2 / 0.4 ppbv
$ClONO_2$	100 / 200	50-90N; 50-90S	1 / 2	LS	12h / 24h	50 / 100 pptv
BrO	100 / 200	Global	1 / 2	LS	12h / 24h	1.5 / 3 pptv
N_2O	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	20 / 40 ppbv
CH_4	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	0.1 / 0.2 ppmv
HNO_3	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	0.5 / 1 ppbv
H_2O	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	5% / 10%
HCl	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	0.2 / 0.4 ppbv
$ClONO_2$	100 / 200	50-90N; 50-90S	1 / 2	MS	12h / 24h	50 / 100 pptv
BrO	100 / 200	Global	1 / 2	MS	12h / 24h	1.5 / 3 pptv
N_2O	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	20 / 40 ppbv
CH_4	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	0.1 / 0.2 ppmv
H_2O	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	8% / 16%
HCl	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	0.2 / 0.4 ppbv
CH_4	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	0.1 / 0.2 ppmv

Temperature	100 / 200	Global	1 / 2	LS	12h / 24h	1 K / 2 K
Extinct. coef.	100 / 200	Global	1 / 2	LS	12h / 24h	10^{-4} / 2.10^{-4} km^{-1}
Temperature	100 / 200	Global	1 / 2	MS	12h / 24h	1 K / 2 K
Extinct. coef.	100 / 200	Global	1 / 2	MS	12h / 24h	10^{-4} / 2.10^{-4} km^{-1}
Temperature	200 / 400	Global	2 / 4	US	Daily/weekly	2 K / 3 K

Table 2.5 *As Table 2.3 for the minimum mission ('Priority A', in black italic) with in addition (in green) the observational requirements related to the mission extension 'Stratospheric Chemistry' ('Priority B') .*

Tropospheric Ozone

The Level-2 requirements for the mission extension 'Tropospheric Ozone' are listed in Table 2.6 ('Priority B'). Across-track sampling requirements would improve horizontal sampling in the UT/LS. There are no 'Priority C' requirements for this mission extension.

Operational Services (user area U1) and Long-term monitoring (user area U2) **+ Tropospheric Ozone ('Priority B')**				***Timeliness: < 3h*** ***Long-term stability (O_3 observations): 1% / 3% per decade*** Across-track sampling: 100 / 200 km (in UT, LS and MS) over a swath of ≥ 400 km		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty (*)
O_3	*100 / 200*	*Global (incl. polar night)*	*1 / 2*	*LS*	*12h / 24h*	*8% / 16% or 50 / 100 ppbv*
O_3	*100 / 200*	*Global (incl. polar night)*	*1 / 2*	*MS*	*12h / 24h*	*4% / 8% or 50 / 100 ppbv*
O_3	*200 / 400*	*Global (incl. polar night)*	*2 / 4*	*US*	*Daily/weekly*	*4% / 8%*
O_3	100 / 200	Global (incl. polar night)	1 / 2	UT	12h / 24h	8% / 16% or 50 / 100 ppbv

Table 2.6 *As Table 2.3 for the minimum mission ('Priority A', in black italic) with in addition (in green) the observational requirements related to the mission extension 'Tropospheric Ozone' ('Priority B').*

For the other three mission extension there are no 'Priority B' requirements:

Extension into the Mesosphere

'Priority C' observables in the mesosphere (M) include temperature, NO, NO_2 and CO. Along-track sampling, vertical resolution and update frequency requirements are similar to in the US.

Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols

'Priority C' observables include temperature throughout the stratosphere and in the LS and MS in addition sulphate aerosols, OCS and SO_2. For sulphate aerosols information on particle size and surface area density need to be retrieved from observations of the ***spectral dependency*** of the extinction coefficient. While the extinction coefficient is already basically required as auxiliary data product for a minimum ozone-only mission, only through observation of the spectral dependency of the extinction coefficient higher order products such as particle size and surface area density can be retrieved.

Along-track sampling, vertical resolution and update frequency are similar as for ozone. Across-track sampling as for the tropospheric ozone mission extension would be improve on the sampling most importantly in the LS.

Climate Impact of Troposphere-Stratosphere Transport and the Asian Monsoon

'Priority C' observables in the UT/LS include H_2O, aerosols, CO, HCN, PAN, and SO_2. For aerosols characterisation information on size and surface area density need to be retrieved from observations of the spectral dependency of the extinction coefficient. Across-track sampling as for the tropospheric ozone mission extension would improve on the sampling in the UT/LS.

2.4 Summary of Observational Requirements

The mandatory ('Priority A') and desirable ('Priority B') observational requirements that have been presented in Section 2.2 and 2.3 are summarized. The requirements differentiate between the observational requirements to observe stratospheric ozone only, i.e. the minimum mission, as well as the observational requirements including the most important mission extensions suggested in Section 1 and further in Sections 2.2 and 2.3 ('Priority B'). Other requirements that have been labelled 'Priority C' will not be considered quantitatively in Section 3 because even though these observations would be useful to have, these won't be potential mission drivers. The longer products listed in the tables of Section 2.3 still provide a useful reference gross list of potentially desirable and useful additional observations. The mandatory and desirable summary of observational requirements (SOR) includes the need for profiling of some auxiliary information, most importantly temperature and extinction coefficient.

Table 2.7 provides the SOR-table with in black italics the observational requirements for the minimum mandatory mission targeting stratospheric ozone only and in green the requirements derived for the desirable mission extensions. The table combines the most stringent ozone requirements from Tables 2.2 and 2.3. The required timeliness and required update frequency in the LS and MS are determined by the operational services, while the requirements on stability and the extension of the vertical coverage into the US are derived from the long-term monitoring requirements.

The mission extensions that have been prioritized in Section 1 are 'Brewer-Dobson Circulation', 'Stratospheric Chemistry' and 'Tropospheric Ozone'. The 'Brewer-Dobson Circulation' mission extension mainly targets the long-term monitoring mission objective while the 'Stratospheric Chemistry' and 'Tropospheric Ozone' extensions target both the operational services and the long-term monitoring mission objectives.

Observations of SF_6 throughout the stratosphere or, alternatively a combination of long-lived tracers including CFC-11 or CFC-12, N_2O and CH_4 are derived from Table 2.4 for the 'Brewer-Dobson Circulation' mission extension. Note that - apart from CH_4 – also HCl can be seen as an alternative tracer for SF_6 for 'Brewer-Dobson Circulation' in the US region. CFC-11, CFC-12, and N_2O have been considered less suitable in the US (above 30 km altitude) and thus are not required in the US. Observations in the LS and MS of H_2O, HNO_3, HCl, CH_4, BrO, and $ClONO_2$ (in polar regions only) are derived from Table 2.5 for the 'Stratospheric Chemistry' mission extension, while H_2O, HCl, HNO_3, and CH_4 are required in the US.

Further, dense horizontal sampling in the tropopause region is required for the operational services for which across-track sampling has been suggested as 'Priority B' mission extension in Section 2.2.2 together with extension of the vertical coverage of the limb observations into the Upper Troposphere (Table 2.6). In combination with the operational nadir sounders the extension into the upper troposphere would provide an optimized monitoring of both stratospheric and tropospheric ozone down to the surface.

For the operational services extension into the US as well as multiple observations per day (6-hourly update frequency) in at least the lower to mid-stratosphere would have been desirable for data assimilation. The upward extension into the US for operational services extends only the timeliness requirement to the US because the US is already part of the minimum mission for the mission objectives on long-term monitoring. The requirement on better than 12h for the update frequency has been found hard to obtain with a small to medium size limb mission on a single platform in Low-Earth orbit. The requirements on update frequency therefore should be read within this basic technological constraint on mission orbit. Across-track sampling would however provide significantly more dense sampling and therefore has been suggested as ‘Priority B’ mission extension together with coverage of upper tropospheric ozone in support of the dense sampling required in the UT/LS for the operational services.

Operoz Summary of Observational Requirements Table

Operational services and Long-term monitoring ***Minimum Mission (‘Priority A’)*** + (a) Brewer-Dobson Circulation (‘Priority B’) + (b) Stratospheric Chemistry (‘Priority B’) + (c) Tropospheric Ozone (‘Priority B’)				***Timeliness: < 3h (LS, MS)*** ***Long-term stability (O_3 observations): 1% / 3% per decade*** Across-track sampling (O_3 observations): 100 / 200 km (UT,LS, MS) over a swath of ≥ 400 km (c)		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty[1]
O_3	***100 / 200***	***Global (incl. polar night)***	***1 / 2***	***LS***	***12h / 24h***	***8% / 16% or 50 / 100 ppbv***
O_3	***100 / 200***	***Global (incl. polar night)***	***1 / 2***	***MS***	***12h / 24h***	***4% / 8% or 50 / 100 ppbv***
O_3	***200 / 400***	***Global (incl. polar night)***	***2 / 4***	***US***	***Daily/weekly;*** 12h / 24h (b)	***4% / 8%***
O_3 (c)	100 / 200	Global	1 / 2	UT	12h / 24h	8% / 16% or 50 / 100 ppbv
H_2O (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	5% / 10%
HNO_3 (b)	100 / 200	Global	1 / 2	LS	12h / 24h	0.5 / 1 ppbv
HCl (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	0.2 / 0.4 ppbv
$ClONO_2$ (b)	100 / 200	50-90N; 50-90S	1 / 2	LS	12h / 24h	50 / 100 pptv
BrO (b)	100 / 200	Global	1 / 2	LS	12h / 24h	1.5 / 3 pptv
SF_6 (a)	100 / 200	Global	1 / 2	LS	12h / 24h	0.8 / 1.5 pptv
CFC-11[2] (b)	100 / 200	Global	1 / 2	LS	12h / 24h	15 / 30 pptv
CFC-12[2] (b)	100 / 200	Global	1 / 2	LS	12h / 24h	30 / 60 pptv
N_2O[2] (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	20 / 40 ppbv
CH_4[2] (a,b)	100 / 200	Global	1 / 2	LS	12h / 24h	0.1 / 0.2 ppmv
H_2O (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	5% / 10%
HNO_3(a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	0.5 / 1 ppbv
HCl (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	0.2 / 0.4 ppbv
$ClONO_2$ (b)	100 / 200	50-90N; 50-90S	1 / 2	MS	12h / 24h	50 / 100 pptv
BrO (b)	100 / 200	Global	1 / 2	MS	12h / 24h	1.5 / 3 pptv
SF_6 (a)	100 / 200	Global	1 / 2	MS	12h / 24h	0.8 / 1.5 pptv
CFC-11[2] (b)	100 / 200	Global	1 / 2	MS	12h / 24h	15 / 30 pptv

CFC-12[(2)] (b)	100 / 200	Global	1 / 2	MS	12h / 24h	30 / 60 pptv
N_2O[(2)] (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	20 / 40 ppbv
CH_4[(2)] (a,b)	100 / 200	Global	1 / 2	MS	12h / 24h	0.1 / 0.2 ppmv
H_2O (a,b)	200 / 400	Global	2 / 4	US	12h / 24h	8% / 16%
HNO_3 (b)	200 / 400	Global	2 / 4	US	12h / 24h	0.5 / 1 ppbv
HCl (a,b)	200 / 400	Global	2 / 4	US	12h / 24h	0.2 / 0.4 ppbv
SF_6 (a)	200 / 400	Global	2 / 4	US	Daily/weekly	0.8 / 1.5 pptv
CH_4[(2)] (a,b)	200 / 400	Global	2 / 4	US	12h / 24h	0.1 / 0.2 ppmv
Temperature (b)	100 / 200	Global	1 / 2	LS	12h / 24h	1 K / 2 K
Extinct. coef. (b)	100 / 200	Global	1 / 2	LS	12h / 24h	10^{-4} / 2.10^{-4} km^{-1}
Temperature (b)	100 / 200	Global	1 / 2	MS	12h / 24h	1 K / 2 K
Extinct. coef. (b)	100 / 200	Global	1 / 2	MS	12h / 24h	10^{-4} / 2.10^{-4} km^{-1}
Temperature (b)	200 / 400	Global	2 / 4	US	12h / 24h	2 K / 3 K

Table 2.7 *Observational Level-2 requirements for a (i) (in black italics) a minimum operational limb mission targeting stratospheric ozone and (ii) (in green) an extended mission including also 'Priority B' observational requirements. Notation B / T with B=Breakthrough; T = Threshold. Temperature and extinction coefficient are auxiliary data product requirements, in support of ozone and the other Level-2 products. Per desirable ('Priority B') Level-2 products it is indicated in the first column (with either a,b and c) to which additional mission objective(s) the level-2 product is contributing. A (sub-)daily update frequency for e.g. ozone and temperature (auxiliary product) in the US would be desirable for the operational services ('Priority B').*
(1) For the uncertainty requirement the least stringent of the relative and absolute requirements apply while the minimum ozone concentrations to be observed by 'Operoz' are mandatory (100 / 200 ppbv) in the LS and MS and desirable (50 / 100 ppbv) as well as extending in the UT.
(2) From the listed transport tracers (SF6, CFC-11, CFC-12, CH_4, and N_2O) the tracer SF_6 is considered the single best observable. An alternative could be a combination of tracers, e.g., CFC-11 or CFC-12(LS, MS) and N_2O (LS, MS) as well as CH_4 (MS, US).

Formation flying of the minimum mission with a planned nadir mission would potentially improve the three-dimensional ozone monitoring in the full atmosphere, i.e. including the lower and mid-troposphere, through the use of limb-nadir combination in retrieval techniques. The combination of the high spatial resolution offered by the nadir sounders with the vertical resolution in the stratosphere might well provide extra benefits for both types of observations. Studies performed in the context of the Premier mission clearly indicated important added-value of combining nadir and limb observations. Extension of the limb observations of ozone to below the tropopause into the upper troposphere would significantly improve the 3-D characterisation of ozone in the UT/LS region and therefore has been suggested as 'Priority B' mission extension.

A similar benefit is expected in the combination of nadir and limb observations in the data assimilation framework. In that case the importance of co-location and thus formation flying is less direct and would need further investigations. We conclude that the objective to monitor tropospheric and stratospheric ozone 3-D distribution together would potentially provide an additional observational requirement with respect to an orbit in conjunction with planned operational nadir sounders, e.g. through formation flying. This would however limit the selection of orbit altitude. Such orbit considerations have been considered out of scope in *Operoz*.

3 Reality Check

3.1 Introduction

This section follows on from Sections 1 and 2 and aims to check the reality of their requirements for an operational ozone monitoring mission, and to assess the suitability of different types of instruments to meet these requirements.

In the first part of this report, the types of potential space instruments are discussed, alongside the strengths and weaknesses of each instrument type, illustrated by the instruments that have been flown or are planned. This study in particular focuses on limb sounding instruments, as these have been identified to be an important missing operational space component in providing high vertical resolution stratospheric measurements of ozone in particular as well as many other relevant atmospheric constituents. It is emphasised in Section 1 that the vertical resolution required could only be met globally by a limb sounding mission.

In addition, the requirement for ‘global coverage including polar night’ has implications for the different types of instruments, and these will be discussed below. In particular, occultation cannot meet the requirement for global measurements on the order of a few days, due to its sampling pattern. In the case of solar occultation, only two latitudes are sampled per day, at sunset and sunrise. Nevertheless, solar occultation measurements are very attractive for validation of any ozone profile measurements from ground and space as they provide the highest accuracy among all limb sounders and high vertical resolution.

In the later parts of this report, the potential of each of the instrument types to meet quantitative requirements for the minimum mission are assessed, and summarised. Types of instrument that could potentially achieve these aims within the additional constraint of an ‘Existing technology or modest advancements and a small to medium size space mission’ are identified. The potential of the planned operational missions to meet the *Operoz* requirements is also discussed.

3.2 Capabilities of Existing Space Instrumentation Relevant for an Ozone Monitoring Mission

There is a long heritage of satellite instruments measuring ozone throughout the atmosphere and data from a variety of these instruments have been used operationally by NWP and other data assimilation services, or in monitoring trends in global and polar ozone. In this section we discuss the heritage and capabilities of these past and present missions.

3.2.1 Operational Nadir Sounding Missions

There is a long history of measurements of ozone and other species by nadir instruments, and this capability will be continued operationally with future instruments on Sentinel 5P, MTG-S/Sentinel-4[7], MetOp-SG/Sentinel-5 and OMPS nadir sounders. Therefore, as operational instruments of these types will be available in the future, they provide a baseline from which to judge what is additionally required by a limb-sounding instrument to meet the missions specified here. Vertical ozone profile information can be retrieved from nadir sounders operating in the UV/visible, e.g. SBUVs, GOME, and OMI (Barthia et al., 1996, 2013; Meijer et al., 2006; Kroon et al., 2011; Miles et al., 2015) and thermal IR, e.g. IASI (Clerbaux et al., 2009).

Instrument	Satellite	Instrument type	Time period	Max Vertical Resolution	Horizontal
SBUV / SBUV/2	NOAA (various satellites)	UV/VIS	1978-present	6 at 3hPa To >15km in LS	170x340km (340=along track
GOME	ERS-1 (ESA)	UV/VIS	1995-2003	~7-15km	40x320km
GOME-2	METOP (EUMETSAT)	UV/VIS	2006->	~7-15km	40x80km
OMI	AURA (NASA)	UV/VIS	2004->	6-10km	13×24 km(308-500nm) 13x48 km (<308nm)
IASI	METOP (EUMETSAT)	IR	2007->	>8km	12x12km at nadir
OMPS	Suomi-NPP / JPSS NOAA/NASA/DoD	UV/VIS	2012 ->	~8km (30-50 km), > below	250x250 / 50x50 (mapper – not profiles)

Table 3.1 *Characteristics of key instruments measuring nadir ozone profiles. Their global record will be carried on with the planned next generation of instruments on operational polar platforms such as Sentinel 5P and MetOp-SG/Sentinel-5.*

Table 3.1 identifies several key nadir missions capable of profiling stratospheric ozone. The nadir viewing geometry allows high horizontal sampling and resolution, but with a much coarser vertical resolution (typically 6 to 8 km at best) than limb sounders (1 to 3 km). This means that nadir instruments do not meet the basic requirement for high vertical resolution in the stratosphere specified for the minimum and extended missions in Section 1 and 2. This conclusion, that there is a need for a limb-sounding instrument above the currently planned operational nadir missions, is discussed further below.

Vertical Ozone Profiles from nadir sounders

For the subsequent discussion it is useful to consider diagnostic properties of nadir retrieved ozone profiles. Figure 3.1 shows simulated vertical averaging kernels for ozone profiles measured by both thermal infrared (IASI-Next Generation) and UV (Sentinel-5) instruments, to be co-located on MetOp-SG, along with the combination of the two. These calculations were conducted in a science

[7] MTG-S/Sentinel-4 is in geostationary orbit so will provide regional rather than global coverage.

support study for PREMIER (Kerridge et al, 2012) and show results from an idealised case with a very loose a priori constraint. This loose constraint (100% a priori error and 3 km correlation length) does not reflect what would be done in practice but illustrates the maximum attainable vertical resolution. This shows that the maximum vertical resolution achieved by either instrument is 6 km, with the UV having somewhat greater sensitivity in the mid to upper stratosphere, and the thermal infrared in the lower stratosphere.

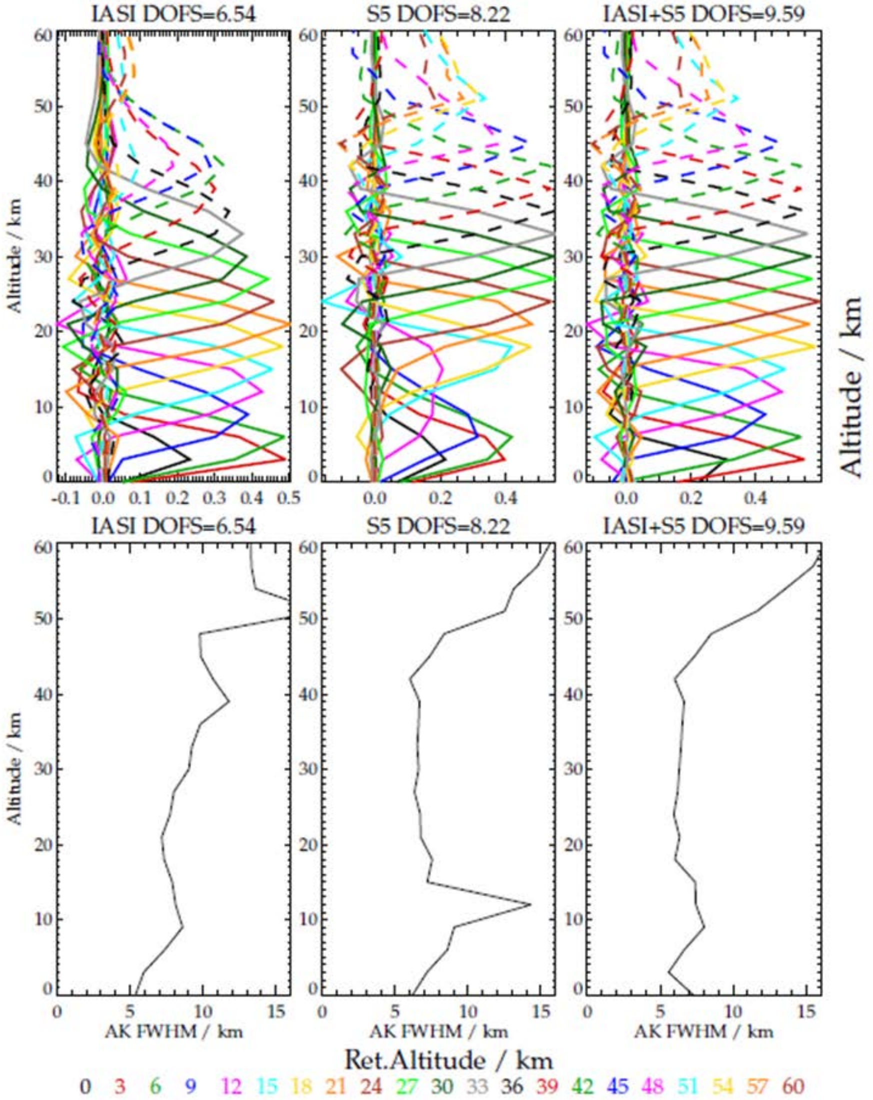

Figure 3.1 *Theoretical averaging kernels for left: the next generation IASI instrument on METOP-SG (thermal infrared), Sentinel 5 (UV/visible) and the combination of the two. Simulations have been performed assuming 100% a priori error and a correlation length of 3km only; this is a looser constraint than would be applied in reality but allows the theoretical information that could be provided by the instrument to be assessed. The bottom row of plots shows the achievable vertical resolution, represented by the full width half maximum of the averaging kernels.*

Figure 3.2 shows contribution functions and averaging kernels for typical nadir retrievals for the SBUV instruments. The contribution function provides information on how certain wavelengths contribute to ozone at various altitudes. The averaging kernels provide information on the vertical resolution. Typical widths of averaging kernels are about 7 km. Below the ozone number density maximum (~23 km), the widths of averaging kernels become larger and their shapes become more asymmetric, which means that the smoothing errors are getting larger as well. The shorter wavelengths (below ~300 nm) are used by SBUV to provide profile information, while the longer wavelengths are used to provide total ozone information[8]. The widths and asymmetry in the averaging kernels have to be carefully accounted for in any comparisons with correlative observations or model data, or else one has to limit comparison to extended vertical layers or partial columns (Liu et al., 2010; Kramarova et al., 2013a; Miles et al., 2015).

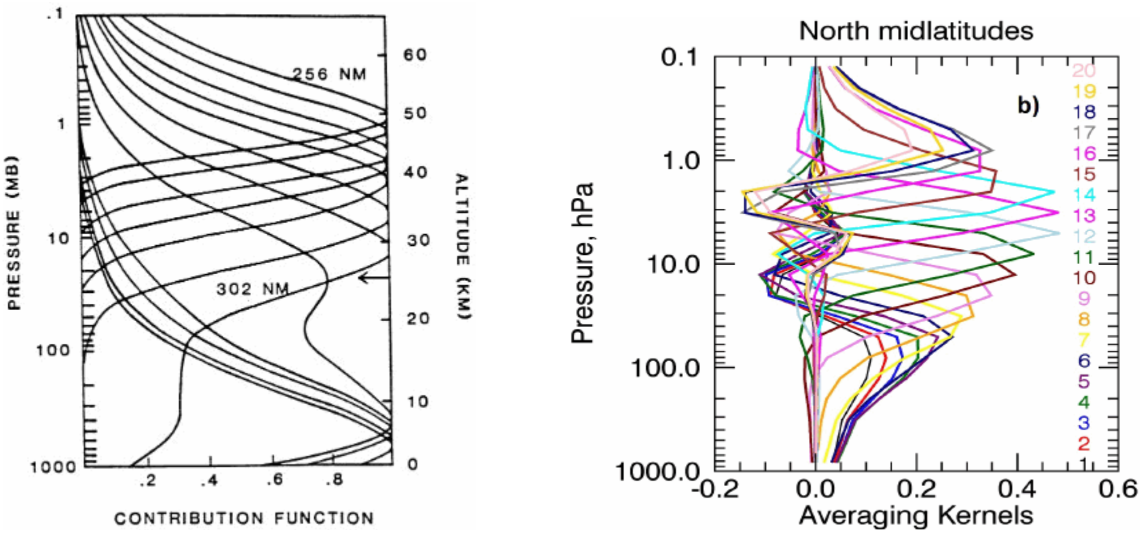

Figure 3.2 *Contribution functions (left, Fleig et al., 1990) and averaging kernels (right, Kramarova et al., 2013) typical for SBUV nadir ozone profile retrievals. Twelve discrete wavelengths between about 255 nm and 340 nm are used in the SBUV-type retrieval (Barthia et al., 2013). The wavelengths below about 300 nm contain profile information (upper curves in left panel), while the longer wavelengths (lower curves) provide total ozone information. The averaging kernels (right panel) for altitudes below the ozone number density peak (~ 22 km, ~40 hPa) are getting broader (lower vertical resolution) and more asymmetric (larger smoothing errors).*

Do we need limb ozone?

The question therefore arises as to whether ozone profiles of this vertical resolution could be suited to application areas or usage, as outlined in the previous Sections. This question is particularly important when discussing the value of an ozone only limb mission. For an extended mission that includes requirements to stratospheric profiling of other trace gases and other geophysical parameters (e.g. aerosols), which is generally not feasible from nadir sounders, the extended capabilities of limb observations over nadir are obvious.

Figure 3.3 shows typical smoothing errors for UV/visible nadir sounders, showing the error that is introduced into the measurement by not resolving the vertical profile. In the upper stratosphere above 30 km (10 hPa) this error is quite low, so that this region is generally suitable for monitoring upper stratospheric ozone recovery, although for attribution studies the vertical resolution is not sufficient. In the lower stratosphere where ozone shows quite some variability and larger smoothing errors, the short-term variations, like the QBO (quasi-biennial-oscillation) signal, can become distorted (change in phase and amplitude of QBO signal) compared to high vertical resolution limb data (Kramarova et al., 2013b, see Figure 3.4). In this case the limb data indeed provide much better details on the variability. A distorted QBO signal in ozone can severely affect data assimilation by providing incorrect constraints on assimilated ozone.

[8] For the GOME-2 class of instrument temperature dependent spectral information in the Huggins bands (315-345nm) is used to extend profile information down into the troposphere, as for the Sentinel-5 simulation in Figure 3.1.

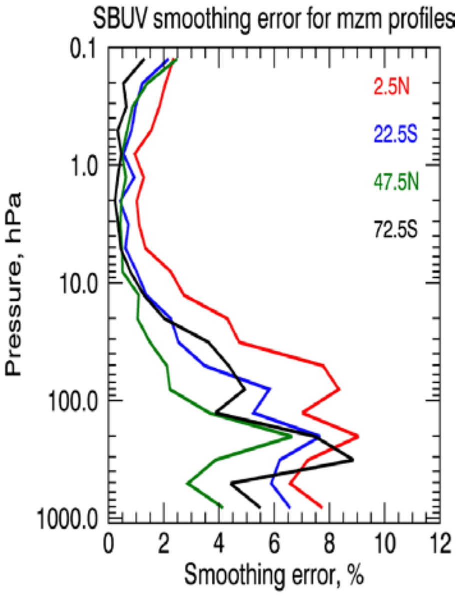

Figure 3.3 *Smoothing errors of monthly mean zonal mean (mzm) ozone. From Kramarova et al. (2013a).*

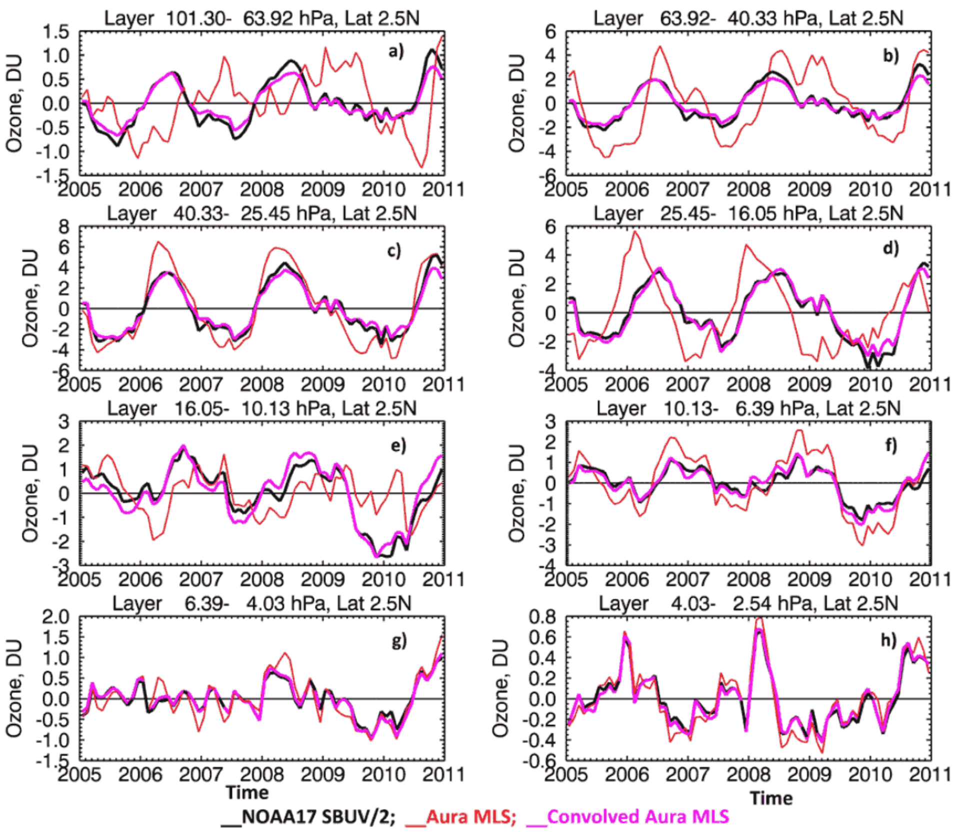

Figure 3.4 *Monthly mean zonal mean de-seasonalised ozone (anomaly) timeseries from SBUV2 and MLS/Aura (limb) for different altitudes in the inner tropics. Note the change in the phase and amplitude of the SBUV2 QBO signal due to the averaging kernels in the lower stratosphere. From Kramarova et al. (2013b).*

Another advantage of the limb data is that it can provide more detailed vertical structure in the trend as shown in Figure 3.5. Because of the better vertical resolution in the limb data, the dynamical and chemical effects on ozone changes on short- and long-term timescales, in particular in the lowermost stratosphere, are easier to detect and are distinguishable. In addition, in the upper stratosphere it is important to distinguish between layers controlled by chlorine (Cl) and the layers above and below in which HO_X and NO_X cycles control the chemistry, along with changes in thermal and dynamical structure. To distinguish such layers the higher vertical resolution provided by limb sounders is key.

Another important issue is the high sensitivity of the UV/visible nadir profile retrieval to the radiometric calibration. While limb sensors are more or less self-calibrating (e.g. taking reference spectra at tangent-height above significant ozone absorption), the optical degradation seen in the UV/visible nadir sun-normalized radiances due to hard radiation and contamination/polymerization of optical surfaces have to be corrected for (e.g. Krijger et al. 2014).[9,10]

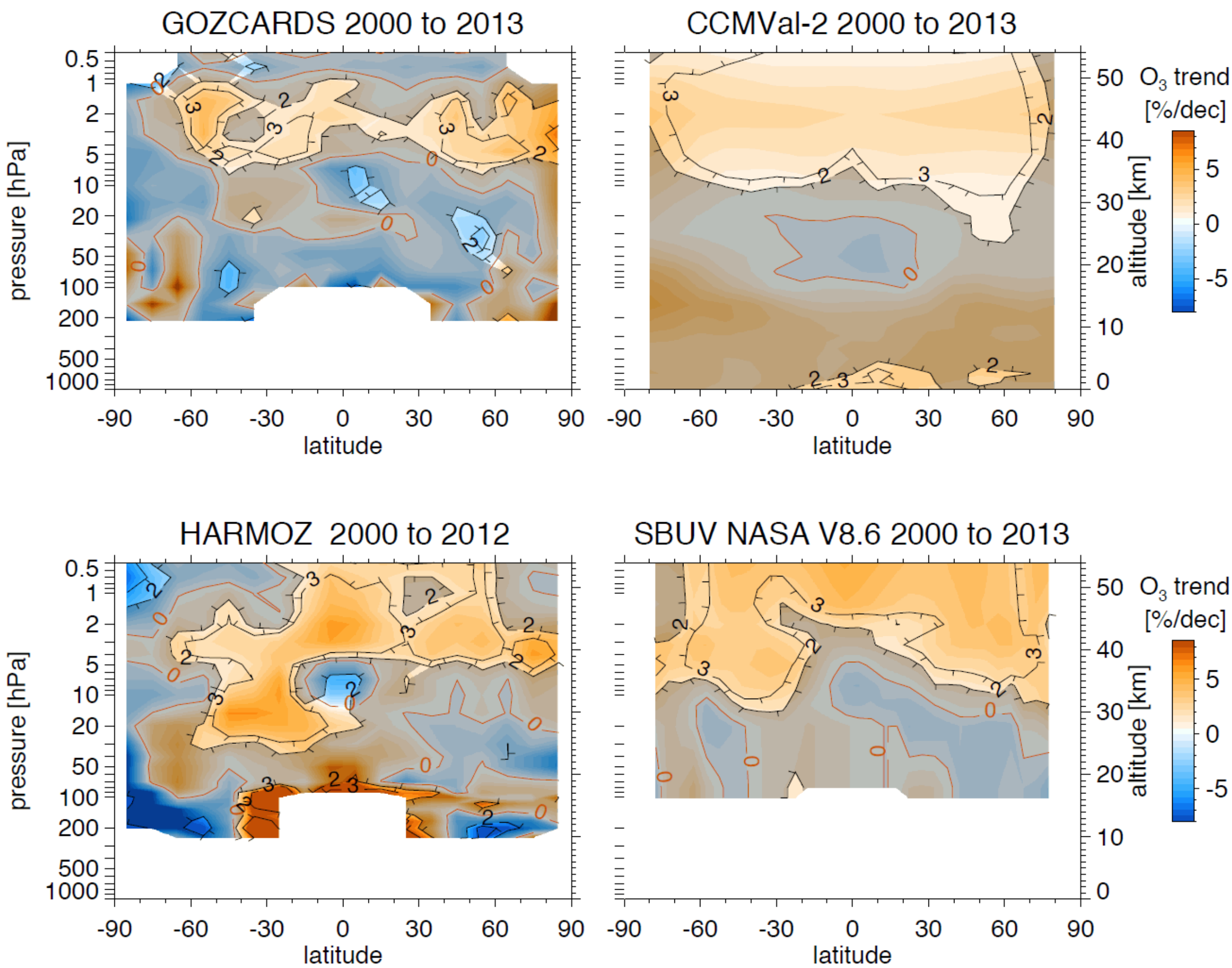

Figure 3.5 *Ozone profile trends in %/decade after 2000 from different profile datasets. Left top: GOZCARDS limb data (merged SAGE II and MLS/Aura data), top right: CCMVal-2 dataset combining several chemistry climate models (CCM), bottom left: HARMOZ (merged ENVISAT and ODIN limb data), bottom right: SBUV V8 nadir profile data. Magnitudes of trends are given by the colour scale. The black contour lines give the ratio of trend to uncertainty, i.e., the statistical significance of the trends. The line labelled 3 corresponds to 3σ, 2 corresponds to 2σ. Gray shading indicates regions where the trends are not significant at the 2σ level. (WMO, 2014).*

[9] The wavelength dependence for the UV degradation is correlated to the ozone Hartley band absorption, which makes it hard to distinguish these. If the degradation is similar for solar and nadir observations, the degradation cancels out in taking the ratio of earthshine and sun spectra. However, the degradation in case of the GOME type instruments is scan angle dependent (solar and earth measurements are done using different mirror scan angles) (Krijger et al.,2014).
[10] Degradation corrections are optimised with long time series (e.g. de Land et al,, 2012), so those to be applied in NRT would not be so accurate.

For the shortest UV wavelengths used in the nadir retrieval the degradation with time means a reduction in the SNR, thus affecting strongly the retrieval in the upper stratosphere, in particular between 40 and 50 km, which is the region most suitable for Montreal Protocol monitoring. Infrared instruments such as IASI are not affected by UV degradation, but have lower sensitivity in this region of the upper stratosphere (Figure 3.1) and current retrievals only extend up to 40 km (Hurtmans 2012). If stratospheric ozone columns are needed, for instance to constrain (indirectly) tropospheric ozone in data assimilation or to derive tropospheric ozone from limb-nadir matching, accurate measurements in the upper stratosphere (see Appendix B) are required, as well as a good vertical resolution in the lower stratosphere.

The main conclusion is that only limb sounders provide complete coverage of the stratosphere with adequate vertical resolution as required per the Summary of Observational Requirements Table (Table 2.7). Nadir UV sounders are unable to provide sufficient high vertical resolution to meet the mission requirements, and fall short especially in the upper stratosphere. Infrared sounders such as IASI contain little information above ~40 km. thus providing no additional information on the upper stratosphere (e.g. Hurtmans et al., 2012). While insensitive to UV degradation issues, the extent to which infrared nadir sensors can extend on the heritage from UV nadir sounders since the late 1970s is still to be established.

3.2.2 Limb Sounding Missions

Measurements looking through the limb of the atmosphere have the advantage of having a much higher inherent vertical resolution than those looking downwards. Resolution is limited by the field of view of the instrument which then scans through the atmosphere to create the profile. This can then lead to a vertical resolution of a few kilometres (which is of the order required to meet the observational requirements specified in Table 2.7).

Conversely, this viewing geometry gives limb sounders coarser along-track resolution (typically of the order of a few 100 km), and, while measurements across-track can have a small horizontal footprint, satellite swaths are separated by several thousands of kilometres. Use of either an across-track scan or a horizontal array would be possible to achieve across-track coverage. However, this would likely increase complexity and therefore costs of such an instrument. In general, the observational requirements include daily global coverage with moderate spatial resolution in the zonal direction (i.e. across-track) and rather high spatial resolution (up to 100 / 200 km) in the meridional direction (i.e. along-track). It would be possible to meet these threshold horizontal sampling requirements with a limb mission which only viewed in the along-track direction.

As mentioned above limb sounding can be undertaken using different spectral regions ranging from solar shortwave (UV/VIS/NIR/SWIR) to (sub-)millimetre wave and in between the thermal infrared (IR). Limb sounding techniques basically encompasses (i) measuring atmospheric emission in the infrared or the (sub-)millimetre wave, (ii) measuring scattered solar radiation in the shortwave (UV/VIS/NIR/SWIR); and, (iii) occultation techniques using direct infrared or shortwave light from the sun, moon or stars which has been transmitted through the upper atmospheric layers. These different techniques will be discussed further in the sections below.

Shortwave (UV/VIS/NIR/SWIR) Limb Instruments

Ultraviolet(UV), visible (VIS), and near-infrared (NIR) remote sensing has a strong heritage as the first measurements were available by the end of the 1970s. Among the first of these limb sounders were solar occultation instruments from the series of SAGE type instruments (SAGE I: 1979-1981, SAGE II: 1984-2005, and SAGE III: 2001-2006).

The first shortwave limb-scattering instrument was the Solar Mesosphere Explorer (1981-1989), which observed ozone and NO_2 in the stratosphere and mesosphere from their absorption in discrete bands in Rayleigh-scattered sunlight (Barth et al, 1983). Demonstration experiments using limb scatter covering broad spectral bands contiguously were done aboard the space shuttle with the SOLSE/LORE instruments in the late 1990s (McPeters et al., 2000). The first regular limb scatter measurements were provided by the OSIRIS instrument launched in 2001 aboard ODIN (Murtagh et al., 2002) and this instrument is still operating. Other limb scatter missions are SCIAMACHY aboard ENVISAT (2002-2012, Bovensmann et al., 1999), and OMPS aboard Suomi-NPP (2012-present, Flynn et al., 2006, Rault and Loughman, 2013). An overview of all past and current UV/VIS limb sounders is given in Table 3.2.

The biggest advantage of limb scatter missions, typically in a near polar orbit, is the large sampling of the sunlit part of the earth thus providing over the full latitude-longitude range revisiting times of a few days – compared to 1-2 months for solar occultation observations. Depending on the width of across-track scans daily coverage is potentially feasible. A limb scattering instrument operating in the UV/VIS could therefore fulfil the requirement for daily coverage under sunlit conditions.

Experiment	**Period**	**Primary Observation Type**	**Stratospheric Observations**	**Comments**
SAGE I/ AEM-2	1979-1981	solar occultation	ozone, aerosol, NO_2	some ozone bias w.r.t. to SAGE II
SAGE II/ ERBS	1984-2005	solar occultation	ozone, aerosol, NO_2, H_2O	– „gold standard“ for ozone – includes SWIR (H_2O)
OSIRIS/ ODIN	2001-today	limb scatter	ozone, aerosol, NO_2, H_2O, BrO	terminator orbit (due to astronomy mode of SMR/ODIN)
SAGE III/ Meteor	2001- 2006	solar occultation	ozone, aerosol, NO_2, H_2O, NO_3	lunar occultation & limb scatter
SCIAMACHY/ ENVISAT	2002-2012	limb scatter	ozone, aerosol, NO_2, H_2O, BrO, OClO	– lunar/solar occultation SWIR (H_2O) – Limb/nadir matching
GOMOS/ ENVISAT	2002-2012	stellar occultation	ozone, aerosol, NO_2, H_2O, BrO, NO_3, T, OClO	„bright limb“ in preparation (daytime measurements), complementing night-time measurements
MAESTRO/ SCISAT	2004-today	solar occultation	O_3, NO_2, aerosol	– incl. near nadir mode – back scatter mode
OMPS/ SNPP	2012-today	limb scatter	O_3, aerosol	– limb-nadir matching possible

Table 3.2 *Current and past UV/VIS/NIR/SWIR limb sounders with extended time coverage.*

Trace gases other than ozone that can be retrieved from UV/VIS limb scatter sounders include NO_2 and BrO (the latter up to 30 km). Ozone retrievals using the combination of Hartley (UV), Huggins (near-UV), and Chappuis bands (VIS) cover the altitude range up to the mesosphere (~65 km). The vertical resolution varies from 2 km (OSIRIS, OMPS) to 4 km (SCIAMACHY). In addition to trace gases, aerosol extinction and cloud properties (cirrus, polar stratospheric clouds, noctilucent clouds) can be derived. BrO profiles in the LS and aerosol extinction profiles are unique to UV/VIS limb sounders. BrO in the MS/US can also be detected from sub-mm observations, e.g. SMILES.

From Short Wave InfraRed (SWIR) wavelengths water vapour profiles up to about 24 km altitude can be retrieved (Rozanov et al., 2011). Extensive validation of SCIAMACHY water vapour profiles retrieved near 1.4µm show an accuracy of about 10% between 14 and 20 km and 20% above 20 km (Weigel et al., 2015). In principle, CO_2, CH_4, and N_2O can be observed in the SWIR as well (Bovensmann et al., 1999) but this requires sufficient SNR. Further improvements in the SWIR setup as was available from SCIAMACHY will be needed to show the true potential to retrieve these data.

Several further occultation missions were flown as well, They are SAGE III aboard Meteor (2001-2006, solar), GOMOS aboard ENVISAT (2002-2012, stellar), and MAESTRO (2004-present, solar) (Wang et al.,2006, Bertaux et al.,2010, McElroy et al., 2007). Stellar occultation observations from GOMOS provide night time measurements and a better global sampling in comparison to solar occultation. By accounting for limb scatter effects (“bright limb”) daytime measurements are also possible. In the following we focus on limb scatter observations as these observations provide the best spatial coverage for an operational mission.

Table 3.3 summarises the UV/VIS data products from OSIRIS and SCIAMACHY. The largest uncertainties from limb scatter measurements come from stray light (limb radiances vary over four orders of magnitudes from the LS to the mesosphere) and altitude registration. There are several techniques that reduce the uncertainty in the altitude registration to about 200 meters or less in the tangent point altitude.

Instrument	Ozone	NO_2	BrO	Aerosol
Vertical resolution	~2km 3-4 km	~2 km 3-4 km	3-5 km 3-4 km	2 km 3-4 km
Accuracy/ precision	5% 5-10%	6-16% 10-20%	30% 30-50%	10% 10%
altitude range	CTH-60km CTH(8)-65km	CTH-45km CTH(12)-45km	16-36km 15-32km	CTH-35km CTH(12)-35km

Table 3.3 *UV/VIS retrieval products from OSIRIS/SCIAMACHY. Top numbers (blue) refers to OSIRIS and bottom number (green) to SCIAMACHY. In cases of clouds the lowest altitude is the cloud top height (CTH).*

From OMPS, the first ozone limb data (accuracy ~10%, 10-60 km) and aerosol extinction profiles are available (Rault et al., 2013). The along-track horizontal resolution for limb scatter observations is about 250 km and due to multiple scattering into the line-of-sight it is hard to improve further. Using tomographic retrievals it is feasible to improve the along-track horizontal resolution down to 100 km (e.g. Petrenko et al., 2003, Degenstein et al., 2009). Across-track horizontal resolution depends on the design geometry (slit width and orientation, across-track scan pattern) and can be as low as 100 km (OMPS). The OMPS-limb sounder therefore fulfils the broad requirements for a minimum mission, except that for fully global coverage to include polar night as well as uncertain long-term data continuity.

Experiment	Launch	Primary Observation Type	Stratospheric Observations	Comments
Programmatically approved missions				
SAGE III/ISS	2016	solar occultation	ozone, aerosol, NO_2, H_2O, NO_3	launch preparation
OMPS/JPSS-2	~2022	limb scatter	ozone, aerosol	approved
OMPS/JPSS-3	~2027	limb scatter	ozone, aerosol	approved
Potential future mission concepts				
ALTIUS		limb scatter	ozone, aerosol, NO_2, BrO	- 2D observations in across track plane using AOTF - tested in field campaigns
CATS		limb scatter	ozone, aerosol, NO_2, BrO	- OSIRIS heritage - industry studies - multiple slits optimised for tomographic retrievals
SCIAMACHY/ ISS		limb scatter	ozone, aerosol, NO_2, H_2O, BrO	- SCIAMACHY heritage - combined with IR spectrometer - multiple slits
SAGE III		solar occultation	ozone, aerosol, NO_2, H_2O, NO_3	- second spare available

Table 3.4 *Future shortwave (UV/VIS/NIR/SWIR) limb satellite missions.*

Approved future UV/VIS sensors are currently SAGE III aboard ISS (2016), and the OMPS limb follow-on to be launched in 2022 aboard JPSS-2 (Table 3.4). Mission concepts for new type of limb scatter instruments uses multiple slits (for different altitude ranges) to further reduce straylight sensitivity and at the same time better support tomographic retrievals. This is proposed for CATS (Canadian Atmospheric Tomography System) (Degenstein, 2013), which is a follow-up on to OSIRIS. Another new concept is the ALTIUS design (Dekemper et al., 2014) which uses acousto-optical tunable filters and array detectors to provide 2D spatial imaging with high spatial resolution in the forward viewing direction. It will allow the application of several methods (incl. horizon viewing and stellar occultations) to improve altitude registration. A UV and thermal infrared spectrometer in combination are proposed for the Japanese module on ISS (SCIAMACHY/ISS) (ICACGP/DLR,2013).

Infrared Limb Instruments

The requirements for the "Minimum Mission" are specified in black italics in Table 2.7. They can be fulfilled by infrared limb-emission measurements. In particular, global horizontal coverage with an update frequency of 12h (24h) throughout the stratosphere (LS, MS, US) requires limb-emission sounding (including measurements in polar night). Limb-emission sounding has also the potential to provide numerous additional chemical species, which are required in the context of mission extensions.

Global observations of atmospheric infrared limb-emissions represents a reliable technique to obtain vertically resolved profile data of ozone, temperature, a variety of additional trace substances simultaneously, at daytime and night-time (e.g. Drummond et al., 1980; Gille and Russell III, 1984; Roche et al., 1993; Taylor et al., 1993; Bingham et al., 1997; Offermann et al., 1999; Russell et al., 1999; Fischer et al., 2008; Gille et al., 2008). The technique can provide high vertical (up to 1 km) resolution and good horizontal sampling along the flight track (about 100 km), and thus can fulfil the temporal/spatial sampling requirements specified in Table 2.7.

Two classes of ozone measuring infrared limb-emission instruments have been utilised in the past: "broadband radiometers" and spectrally higher resolving spectrometers such as Fourier Transform Spectrometers (FTS). The "radiometric" limb-sounding technique was pioneered by the LRIR (Limb Radiance Inversion Radiometer) and LIMS (Limb Infrared Monitor of the Stratosphere) experiments on Nimbus 6 and 7. LRIR employed four filters for radiometric channels to measure p/T via CO_2 at 15 µm (649-672 cm^{-1}, 592-700 cm^{-1}), ozone at 9.6 µm (984-1169 cm^{-1}), and water vapour at 25 µm (412-445 cm^{-1}). Limb measurements were made in the 15 to 55 km altitude range with a vertical resolution of about 3 km. To extend the number of measurable trace species, LIMS used six-channels measuring pressure/temperature via CO_2 at 15 µm (645-673 cm^{-1}; 595-739cm^{-1}), ozone at 9.6 µm (947-1103 cm^{-1}), H_2O at 6.3 µm (1396-1527 cm^{-1}), NO_2 at 5.3 µm (1580-1613 cm^{-1}), and HNO_3 at 11.3 µm (859-900 cm^{-1}). Vertical resolution was also in the range of 3 km.

The most advanced radiometric observations with increased vertical resolution (1-2 km) were made by the High Resolution Dynamics Limb Sounder (HIRDLS). HIRDLS is an infrared limb-scanning radiometer designed to sound the upper troposphere, stratosphere, and mesosphere to determine pressure/temperature O_3, H_2O, CH_4, N_2O, HNO_3, N_2O_5, CFC-11, CFC-12, $ClONO_2$, and aerosols with a horizontal along track sampling of about 100 km. Limb scans are made in the vertical measuring infrared emissions utilising a detector subsystem with 21 channels ranging from 6.12 to 17.76µm (see Table 3.5). The 21 HgCdTe detector elements were cooled by a mechanical Stirling cycle cooler.

The second class of ozone measuring instruments in the infrared region are spectrometers, providing continuous spectral coverage in a broad spectral range at a wide range of spectral resolutions. The CRyogenic Infrared Spectrometers and Telescopes for the Atmosphere (CRISTA) experiment utilized 4 Ebert-Fastie spectrometers to cover the spectral range from 4 to 15 µm at moderate (2 cm^{-1}) spectral resolution. The list of detectable species is comparable to HIRDLS, with some extensions (e.g. PAN, CCl_4).

In order to acquire the most complete set of stratospheric composition data, covering pole to pole over almost a full solar cycle, the Fourier transform spectrometer (FTS) MIPAS on ESA's Envisat was focusing on high spectral rather than high spatial resolution. It was operating from 2002 until 2012. By observing the 4 to 15 µm range at very high-spectral sampling, up to 40 atmospheric trace gases could be measured in the nominal altitude range from 6 to 68 km at 2 to 4 km vertical spacing and 300 to 500 km along-track sampling (Fischer et al., 2008).

To fulfil more stringent spatial sampling requirement (and to include across-track sampling) the infrared limb-imaging technique was proposed (Riese et al., 2005; Friedl-Vallon et al., 2006), which combines the FTS technique with two-dimensional detector arrays for about 1000 simultaneous limb views in the mid-infrared spectral region. The capabilities of this technique were further studied for the PREMIER Infrared Limb Sounder (IRLS) in the framework of the ESA's Earth Explorer (EE-7) program (ESA, 2012). This technique is also the basis for new FTS concepts. For example, the German ATMO-SAT concept provides the same spectral resolution as the PREMIER IRLS, but at somewhat coarser vertical resolution (1-2 km). Since the PREMIER IRLS chemistry mode offers a large list of additional chemical species, it will be considered further in the discussion of potential mission extensions (see Section 3.4).

The characteristics of previous "conventional radiometers" and new concepts for "Fourier Transform Spectrometers" are summarized in Table 3.6 in terms of detectable species, vertical sampling, along-track sampling and altitude range.

In addition to these two well-demonstrated "existing technologies", the conventional radiometer and Fourier Transform Spectrometers, several new concepts may be worthy of consideration as "modest advancements for a small to medium sized mission":

- 2D detector array observing simultaneously a set of tangent-heights (vertical) through a set of interference filters (horizontal). Detectable species include p, T, O_3, H_2O, CH_4, N_2O, HNO_3, N_2O_5, CFC-11, CFC-12, $ClONO_2$, and aerosols.
- 2D detector array observing simultaneously a set of tangent-heights (vertical), acquiring samples of an interferogram at each tangent height through a static interferometer (micro-FTS).
    - Potentially offers a compact solution with coarse spectral resolution over broad bandwidth
- Limb-scanning laser heterodyne radiometer (LHR)
    - Potentially offers compact solution with very high spectral resolution over comparatively narrow bandwidth

Channel	Purpose	Spectral Band Pass (Half-Maximum Points, cm^{-1})
1	N_2O, aerosol	566.9–584.3
2	temperature	599.8–615.1
3	temperature	612.1–636.5
4	temperature	629.4–652.7
5	temperature	657.1–680.8
6	aerosol	819.9–834.9
7	$CFCl_3$	834.6–850.7
8	HNO_3	862.0–900.9
9	CF_2Cl_2	915.6–932.0
10	O_3	991.8–1008.5
11	O_3	1013.7–1044.0
12	O_3	1120.5–1139.7
13	aerosol	1202.6–1221.4
14	N_2O_5	1230.5–1257.7
15	N_2O	1255.9–1278.5
16	$ClONO_2$	1279.2–1299.5
17	CH_4	1327.0–1366.0
18	H_2O	1387.0–1432.2
19	aerosol	1401.4–1415.5
21	NO_2	1585.2–1632.9

Table 3.5 *HIRDLS spectral channels (Gille et al., 2008).*

Instrument	Detectable Species	Vertical Sampling	Along-track Sampling (approx.)	Altitude Range
LRIR	p/T, ozone, H_2O	2-3 km	500 km	Mesosphere, Stratosphere
LIMS	p/T, ozone, H_2O, HNO_3, NO_2	2-3 km	200 km	Mesosphere, Stratosphere
HIRDLS	p/T, ozone, H_2O, HNO_3 CH_4, N_2O, CFC-11, CFC-12, N_2O_5, $ClONO_2$	1 km	100 km	Stratosphere, Upper Troposphere
MIPAS	p/T, ozone, H_2O, HNO_3, CH_4, N_2O, CFC-11, CFC-12, N_2O_5, $ClONO_2$, PAN, HCN, COS, SO_2, SF_6, C_2H_6, $BrONO_2$, ClO. Aerosol and cloud extinction (a.o)	1.5-3.0 km	~ 400 km	Lower Thermosphere Mesosphere, Stratosphere, Upper Troposphere
Potential Future Mission Concepts				
PREMIER-type or ATMOSAT-type	p/T, ozone, H_2O, HNO_3, CH_4, N_2O, CFC-11, CFC-12, N_2O_5, $ClONO_2$, PAN, HCN, COS, SO_2, SF_6, C_2H_6, $BrONO_2$, ClO. Aerosol and cloud extinction	1-2 km	50 / 100 km	Mesosphere, Stratosphere, Upper Troposphere

Table 3.6 *Observational parameters of relevance, vertical sampling, and along track sampling of previous thermal infrared missions. HIRDLS did not measure CO and NO. However, these trace gases could be included in an advanced radiometer. While LRIR, LIMS, HIRDLS and MIPAS were successfully flown in space, PREMIER and ATMO-SAT represent concept studies. The restricted spectral range of the PREMIER IRLS concept also excluded CO and NO. For SO_2 and COS, single profiles can only be retrieved after volcanic eruptions. Under undisturbed conditions, monthly zonal averages are available. SF_6 data are also restricted to monthly zonal means. However, this is sufficient for Age-of-Air (AoA) analyses. $BrONO_2$ can be retrieved in terms of weekly zonal means.*

(Sub-)mm Limb Instruments

Another wavelength range which can be used for limb-emission sounding is the millimetre (mm) wave and sub-millimetre (sub-mm) wavelength region. This uses measurement techniques which employ the coherent detection of electromagnetic waves rather than incoherent detection of photons as is used at infrared wavelengths. Measurement at these wavelengths is much less sensitive to the presence of cirrus clouds than in the IR, so in a cloudy atmosphere (sub-)mm wave instruments can penetrate further down into the atmosphere. However, penetration into the troposphere is limited by absorption of water vapour and oxygen, and hence (sub-)mm wave instruments cannot penetrate as far into the troposphere as infrared instruments in the absence of clouds. There is also a trade off in instrument design between the vertical and horizontal resolution, the achievable lowest altitude measurable and the instrument noise which will be discussed further in the minimum mission requirements section.

Table 3.17.1: Summary for MLS ozone

Pressure / hPa	Resolution Vert. × Horiz.	Precision[a] ppmv	Precision[a] %	Accuracy[b] ppmv	Accuracy[b] %	Comments
≤ 0.01	—	—	—	—	—	Unsuitable for scientific use
0.02	5.5 × 200	1.4	300	0.1	35	
0.05	5.5 × 200	0.9	150	0.2	30	
0.1	4 × 400	0.5	60	0.2	20	
0.2	3 × 450	0.5	40	0.1	7	
0.5	3.5 × 550	0.3	20	0.1	5	
1	3 × 450	0.2	7	0.2	7	
2	3.5 × 450	0.15	3	0.2	5	
5	3 × 450	0.15	2	0.3	5	
10	3 × 500	0.1	2	0.3	5	
22	2.5 × 400	0.1	2	0.2	5	
46	2.5 × 350	0.06	3	0.2	8	
68	2.5 × 350	0.04	3–10	0.05	3–10	
100	2.5 × 300	0.04	20–30	[0.05 + 5%]		
150	2.5 × 400	0.03	5–100	[0.02 + 5%]		
215	3 × 400	0.02	5–100	[0.02 + 20%]		
261	3 × 450	0.03	5–100	—	—	Requires further evaluation
316	2.5 × 500	0.05	—	—	—	Not recommended (until further evaluation)
1000 – 464	—	—	—	—	—	Not retrieved

[a]Precision on individual profiles
[b]As estimated from systematic uncertainty characterization tests. Stratospheric values are expressed in ppmv with a typical *equivalent* percentage value quoted. 215 – 100 hPa errors are the sum of the ppmv *and percentage* scaling uncertainties quoted. Accuracy values, especially for pressures from 100 to 316 hPa will be re-evaluated, but the estimates for v2.2 data are currently used in this Table.

Table 3.7 *Resolution and uncertainty estimates for v3.3/v3.4 Ozone data taken from the MLS/AURA data quality document (Livesey et al., 2013).*

Limb emission sounding of this type began with the Microwave Limb Sounder (MLS) on the UARS satellite in 1991 (Barath et al 1993) and the Millimetre-wave Atmospheric Sounder (MAS) on the ATLAS Space Shuttle Missions (Croskey et al 1992). UARS/MLS measured in frequency bands below 220GHz, using narrow bandwidth (~500MHz) channels to profile the stratosphere with around 3 to 4.5 km vertical resolution. MAS consisted of three radiometers operating at frequencies 61 to 64 GHz, 183 GHz and 204 GHz targeting O_2 (for temperature and pointing), H_2O and O_3, and chlorine monoxide (ClO), respectively. MAS provided simultaneous information on the temperature and ozone distribution in the 20 to 90 km region and information on H_2O and ClO with a vertical resolution of up to 4 km.

A second MLS instrument was launched on the AURA satellite in 2004 (Waters et al 2006), and this is currently still functioning and providing important inputs into operational data assimilation systems. For AURA/MLS sub-millimetre and THz bands were added to allow additional species to be measured, and also had increased penetration into the upper troposphere by selection of bands in mm-wave windows. Species measurable include O_3, T, H_2O, BrO, CH_3Cl, CH_3CN, ClO, CO, HCl, HCN, HNO_3, HO_2, HOCl, N_2O, OH, SO_2, and ice water content (IWC) and path (IWP), and relative humidity w.r.t. ice (RHi).

In respect to ozone, the latest AURA/MLS retrieval algorithms are able to achieve a vertical resolution of approximately 2.5 to 3.5 km in the stratosphere, with an along-track horizontal resolution of 300 to 500 km, and an accuracy and precision ranging from 5 to 10%, and 2 to 10%, respectively, in the altitude range between 68 and 1hPa (see Table 3.7; Livesey et al., 2013).

Table 1. Theoretical and Typically Achieved Capabilities of Odin/SMR for the Observation of Stratospheric ClO, N_2O, O_3, and HNO_3[a]

Species	Frequency, GHz	Precision (1-σ)	Altitude Resolution	Altitude Range	Number of Iterations
		Theoretical Capabilities[b]			
O_3	501.5	0.5–2 ppmv (25–30%)	~2 km	~19–50 km	2–3
ClO	501.3	0.15–0.2 ppbv	1.5–2 km	~16–67 km	2–3
N_2O	502.3	15–35 ppbv (10–20% <30 km)	~1.5 km	~15–70 km	2–3
O_3	544.9	0.2–0.4 ppmv (10–20%)	~1.5 km	~18–70 km	3–4
HNO_3	544.4	≤1 ppbv (15–25% <30 km)	1.5–2 km	~21–67 km	3–4
		Achieved Capabilities CTSO-v222[c,d]			
O_3	501.5	0.25–1.5 ppmv (20–25%)	~2.5 km	~17–45 km	2–3
ClO	501.3	0.15–0.25 ppbv	2–2.5 km	15–55 km	2–3
N_2O	502.3	10–45 ppbv (5–15% <30 km)	~2 km	13–55 km	2–3
O_3	544.9	0.2–0.5 ppmv (10–25%)	~2 km	14–70 km	3–4
HNO_3	544.4	≤1 ppbv	2–3 km	20–50 km	3–4
		Achieved Capabilities CTSO-v223[c,e]			
O_3	501.5	0.25–1.5 ppmv (20–25%)	3–3.5 km	~18–45 km	2–3
ClO	501.3	0.15–0.25 ppbv	2–2.5 km	15–55 km	2–3
N_2O	502.3	15–45 ppbv (15–20% <30 km)	~1.5 km	14–55 km	2–3
O_3	544.9	0.2–0.8 ppmv (10–40%)	~1.5 km	14–70 km	3–4
HNO_3	544.4	≤1.5 ppbv	1.5–2 km	18–35 km	3–4
		Achieved Capabilities Chalmers-v1.2[c,e,f]			
O_3	501.5	0.25–0.75 ppmv	3.5–4 km	21–45 km	4–5
ClO	501.3	0.05–0.15 ppbv	2–4 km	15–45 km	4–5
N_2O	502.3	10–30 ppbv (5–15% <30 km)	2–4 km	15–35 km	4–5
O_3	544.9	0.2–0.4 ppmv (10–20%)	2–3 km	17–60 km	5–6
HNO_3	544.4	≤1 ppbv	2–2.5 km	18–35 km	5–6

[a]Indicated are target line frequencies, single-scan precisions and altitude resolutions (FWHM) in the lower stratosphere, approximate altitude ranges for a polar scenario, and the typical number of iterations required for reaching convergence.
[b]Retrieval grid given by nominal tangent-altitudes of stratospheric mode scan: $\Delta z = 1.5$ km ($z \leq 50$ km), $\Delta z = 3$ km ($z > 50$ km).
[c]Based on single-scan retrieval (latitude ~78.4°S, 20/9/2002, orbit 217F).
[d]Retrieval grid $\Delta z = 2$ km ($z \leq 50$ km), $\Delta z = 6$ km ($z > 50$ km).
[e]Retrieval grid given by tangent-altitudes of scan: $\Delta z \sim 1.5$ km ($z \leq 50$ km), $\Delta z \sim 6$ km ($z > 50$ km).
[f]Smoothed in altitude (using non-diagonal a priori covariance matrix).

Table 3.8 *Theoretical and achieved capabilities of ODIN/SMR (Urban, 2005).*

The first sub-millimetre radiometer in space was the Swedish instrument, ODIN/SMR, which was launched in 2001 and is still functioning. This radiometer employs frequencies of up to 580 GHz for both atmospheric and interstellar sounding. These higher frequencies have the advantage of allowing a higher vertical resolution for a given antenna size and orbit height, but have the disadvantage of reducing the penetration into the troposphere as water vapour absorption is stronger. Odin/SMR is capable of measuring stratospheric ozone with a vertical resolution of around 1.5 to 2 km using the spectral line at 544.9 GHz, but with a precision of 10 to 20% (Table 3.8; Urban, 2005). Species that can be measured by Odin/SMR include O_3, ClO, N_2O, HNO_3, H_2O, CO, and isotopes of H_2O and O_3. Due to the viewing geometry of the instrument it however has a very coarse along-track resolution (Table 3.8).

The Sub-Millimetre Wave Limb Emission Sounder (SMILES) (Inatani et al, 2000, Shtotani et al 2002) was flown on the International Space Station from September 2009 to April 2010, and measured O_3 with a vertical resolution of 2 to 4 km and a horizontal resolution of 100 km. It had a much greater sensitivity due to the use of (< 4K) superconducting receivers, although measurements were restricted to the stratosphere due to the frequency bands used (625 GHz and 650 GHz). Due to the need for cryogenic cooling, such an instrument is unlikely to be appropriate for the type of satellite mission considered here.

More recently, instrument studies have put forward designs for new mm-wave or sub-mm-wave instruments. These included the STEAM-R instrument, which would have formed a component of the PREMIER mission (Kerridge et al., 2012). This instrument type has a direct heritage from ODIN/SMR, and use of the STEAM-R frequency bands is being demonstrated by an airborne precursor instrument (MARSCHALS). The STEAM-R concept exploits the 310-350 GHz band, and in the PREMIER configuration used a receiver array to sound up to 30 km with high vertical and along-track resolution (sampling every 50 km along track).

In the subsequent evolution for a potential national or bilateral mission (ALiSS) vertical coverage has been extended through the upper stratosphere. It is therefore envisaged that such an instrument could be compliant with the requirements formulated in Section 1 and 2. The characteristics for the (sub-)mm wave region are summarised in Table 3.9.

Instrument	**Lifetime**	**Detectable Species**	**Vertical Resolution (O_3)**	**Along-track Sampling (O_3)**
MLS (UARS)	1991 - 2001	O_3, ClO, H_2O, T, cloud ice water content, HNO_3, volcanic SO_2, CH_3CN	3.5 - 4km	
MLS (AURA)	2004 - present	O_3, T, H_2O, BrO,CH_3Cl, CH_3CN, ClO, CO, HCl, HCN, HNO_3, HO_2, HOCl, N_2O, OH, SO_2, IWC, IWP, RHi	2.5 - 3.5km	300 - 500km
MAS (ATLAS)	1992	O_3, H_2O, ClO, T	3km	
SMR (ODIN)	2001 - present	O_3, ClO, N_2O, HNO_3, H_2O, CO, isotopes of H_2O and O_3	1.5 - 3 km	900 - 1140 km
SMILES	2009 - 2010	O_3, O_3 isotopes (3 types), BrO, CH_3CN, ClO, HCl, HNO_3, HOCl, and HO_2	2 - 4 km	100 km
Potential Future Mission Concepts				
STEAM-R		O_3, H_2O, CO, HNO_3, N_2O, HCN, CH_3CN, SO_2	2km[11]	50 km

Table 3.9 *Information on programmatically approved (past) millimetre-wave and sub-millimetre wave instruments and proposed potential future mission concepts (STEAM-R).*

[11] In the STEAM-R design for PREMIER, vertical coverage was up to 30km. In subsequent evolution for a potential national or bilateral mission (ALiSS) vertical coverage extended through the upper stratosphere.

3.3 Assessment of Potential Contributions of Different Classes of Space Instrumentation to Meet Minimum Mission Observational Requirements

The minimum mission has been defined in Section 1 to be a mission focussing on the measurement of ozone only, at good vertical resolution throughout the stratosphere, and at daily or weekly global sampling depending on the height range. An important requirement is the necessity to measure globally at all seasons, including during polar night. More details of the geophysical data requirements, broken down into user areas are given in Section 2 and are summarised in Table 2.7 (minimum mission in black). These include requirements on the timeliness of the data and the instrument stability.

In this section we assess the potential contributions of all these different classes of space instrumentation to meet these specific requirements. A specific analysis of occultation missions has not been included here as the sparse sampling pattern of such instruments precludes their ability to meet the requirement for global sampling on a daily basis. Solar occultation only samples two latitudes per day (sunset and sunrise) and does not provide along-track resolution.

3.3.1 Operational Nadir Sounding missions

A fundamental requirement of the minimum mission is that measurements are made *throughout the stratosphere with a high vertical resolution*. This cannot be met by any of the future operational nadir missions, and is a fundamental difficulty for any nadir mission measuring either scattered shortwave sunlight, or infrared emission. It is therefore concluded that a nadir mission is not suitable for the minimum mission required. For UV nadir-sounders the need for sunlight also means that the requirement for measurement in the polar night cannot be met. Furthermore, UV degradation requires correlative external measurements, such as O_3 sondes, or other measures (e.g. soft calibration) to correct for the long-term record. Although neither restriction is shared by infrared instruments such as IASI, these are, however, much less sensitive than UV instruments to especially the upper stratosphere.

Minimum mission observational requirements				**Timeliness: <3h Stability: 1% / 3% per decade**		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty (*)
O_3	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	8% / 16% or 50 / 100 ppbv
O_3	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	4% / 8% or 50 / 100 ppbv
O_3	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	4% / 8%

Table 3.10 *Summary of the ability of nadir sounders to meet the minimum mission requirements. Green = compliant, Red = non-compliant, yellow = some compliance. In the case of nadir sounders, they are unable to meet the vertical resolution requirements. Although they have the potential to measure throughout the stratosphere and can therefore comply broadly with the vertical range the coarse resolution means that locating information purely in a given range (e.g. from the tropopause upwards) is not feasible. Additionally, uncertainty requirements can only be met for retrieval of layers much broader than the required 2 km (typically 6 to 8km).*

The nadir instruments do provide good horizontal resolution and global coverage, however, so there will be important benefits from such instruments in conjunction with a limb sounder; both through increased information on horizontal structure and extending ozone information through the troposphere. This aspect will be further elaborated with respect to possible mission extensions. The ability of nadir sounders to meet the minimum mission requirements is summarised in Table 3.10.

3.3.2 Limb Sounding Missions

Shortwave (UV/VIS/NIR/SWIR) Limb Instruments

From the experience of past and current limb shortwave scatter instruments as well as design considerations for future missions (see Section 3.2.2), the following minimum ozone only mission (if operating in the UV/VIS spectral range) can be proposed as shown in Table 3.11. For a simple spectrometer the SWIR spectral range need not be covered. Using a multiple slit design in combination with CCD detectors is most suitable to meet the needs for tomographic retrievals with high accuracy and sufficiently high horizontal resolution in the along-track direction. Wavelengths covered are in the range between 260 and 800 nm. For lower data amounts and speedier retrievals selected wavelength bands in the UV/VIS may suffice. Several other species like NO_2, BrO and aerosols are automatically covered in this spectral range. Aerosol extinction retrieval is important to properly constrain the ozone retrieval. The ability of shortwave limb instruments to meet the minimum mission requirements is summarised in Table 3.12.

Parameter	**Requirements**	**Comments**
instrument type	Limb scatter	high global sampling
Orbit	sun-synchronous/near polar	best latitude coverage
local time	10am - 14am (fixed equator crossing time)	for trend monitoring fixed equator crossing time is important, e.g. minimizing diurnal effects
Revisit time	24h / 72h	Revisit times can be tuned by horizontal scanning specific design (side viewing)
Accuracy	5% (20% in the UT/LS and cloud free)	
Precision	5% (10% in the UT/LS)	
Stability	1%/decade	
altitude range (operation)	0-60 km	must be larger than the valid range for ozone
vertical sampling	0.5 km	oversampling in the vertical is important
altitude range (ozone)	TP/CTH-50 km	Retrievals are feasible up to about 65km
along-track resolution	100km	Multiple slit design, 2D imaging, and / or tomographic retrievals will be required
Across-track resolution	50 km	
Vertical resolution	2 km	Needs to be checked if tomographic retrievals in combination with slit design can improve this
Wavelength range	260-800 nm	longer wavelengths may be needed to constrain aerosols in ozone retrievals, for ozone-only retrievals an upper limit of 680 nm may suffice.

Table 3.11 *Potential minimum ozone-only mission operating in the UV/VIS.*

Minimum mission observational requirements				Timeliness: <3h Stability: 1% / 3% per decade		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty
O_3	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	8% / 16% or 50 / 100 ppbv
O_3	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	4% / 8% or 50 / 100 ppbv
O_3	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	4% / 8%

Table 3.12 *Ability of shortwave (UV/VIS/NIR/SWIR)limb scattering instrument to meet the requirements of the minimum mission. This type of mission is limited by being unable to measure in the (polar) night.*

Infrared Limb Instruments

For the "Minimum Mission", a relatively simple *radiometer* measuring p/T and ozone, and aerosol/cloud extinction (11.3 µm) in less than 10 spectral channels would be sufficient. Radiometric infrared limb-sounding from a low earth orbit (LEO) with high inclination provides global ozone maps with twice-daily synoptic sampling (Salby et al., 1982) of a zonal resolution of eight wavenumbers (update frequency 12 hours). The resolution in the meridional direction depends on the along-track sampling, which is better than 100 km for a HIRDLS-type radiometer.

Ozone vertical profile observations from HIRDLS on NASAs Aura platform (Gille et al., 2008) provided vertical resolution of ~1 km, combined with 65 km profile spacing along track. The instrument measured ozone in three of its 21 infrared channels (see Table 3.5) centred around wave-numbers of about 1000 cm^{-1} (channel 10), 1030 cm^{-1} (channel 11) and 1130 cm^{-1} (channel 12), respectively. The corresponding full widths are 20 cm^{-1}, 20 cm^{-1}, and 37 cm^{-1}, respectively. The design sounding ranges are: 8 to 75 km for channel 10, 30 to 85 km for channel 11 and 8 to 55 for channel 12.

A major issue in the reduction of data to geophysical parameters has been an unanticipated large visual obstruction in the HIRDLS field of view. This is a serious challenge for the data analysis methods and their implementation. Comparisons with independent observations indicate, however, that HIRDLS stratospheric ozone is well recovered.

Precision and accuracy estimates in these altitude regions for HIRDLS are based on in-orbit measurements and comparisons to independent observations (Nardi et al., 2008). Accuracy of better than 10% is indicated between 25 and 50 km by the majority of the comparisons with coincident measurements, and 5% between 30 and 45 km based on comparisons with lidar soundings. Between 15 and 20 km, at middle and high latitudes, the accuracy is 10–20%. These accuracies, which are obtained from validation measurements, are quite remarkable, when considering the enormous unforeseen technical difficulties encountered by HIRDLS.

The precision estimates are based on observed ozone variability in different bins (equivalent latitude, potential temperature, for details see Nardi et al. 2008). The results obtained from regions (and seasons) with low atmospheric variability indicate that ozone precision is approximately 5 to 10% between about 400/500 and 2000 K potential temperature vertically (15/20 to 50 km). Below 400/500 K, the atmospheric variability becomes larger and precision estimates based on observed variability become less meaningful. However, Pan et al. [2009] show that HIRDLS resolves laminae with tropospheric origin with a vertical extension of about ~2 km in the mid-latitude lowermost stratosphere. This relatively good performance in term of accuracy and precision is remarkable, considering the technical difficulties of HIRDLS.

HIRDLS along-track sampling is higher than the required horizontal along-track sampling of the "Minimum Mission". Its vertical resolution (1 km) corresponds to the breakthrough value for the altitude range from TP to 30 km and is better than the breakthrough values for the altitude range from 30 to 50 km. A HIRDLS-type instrument covering its subset of p/T, ozone, and aerosol channels would therefore be compliant with the "Minimum Mission", with some room for trade-offs between spatial sampling and accuracy.

An FTS-type instrument employing a 2D detector array can fulfil all uncertainty requirements given in Table 2.7. This was demonstrated in the PREMIER CORSA study (Kerridge et al., 2012) based on single profile retrieval studies and is also valid, if MTG detectors are used as they are. An FTS-type instrument would also fulfil all "breakthrough" values in terms of vertical sampling (even with some spatial averaging). However, such an instrument appears to be too complex for an ozone-only "Minimum Mission".

A simpler approach would be the utilization of 2D detector arrays to observe simultaneously a set of tangent-heights (vertical) through a set of interference filters (horizontal) that cover similar spectral ranges (micro-windows) as used in the PREMIER consolidation of requirements study for the Infrared Limb Sounder (IRLS) . A filter covering the same pixel area as the IRLS in the dynamics or chemistry mode would provide at least a factor of two better signal-to-noise ratio (Friedl-Vallon, private communication). In first order, the uncertainty ranges derived for the PREMIER IRLS can therefore serve as estimates of the uncertainty ranges achievable by such a radiometer. We will use this approach also to assess the performance for additional trace gases, considered for mission extensions in Section 3.4.

The ability of infrared limb instruments to meet the minimum mission requirements is summarised in Table 3.13.

Minimum mission observational requirements				**Timeliness: <3h** **Stability: 1% / 3% per decade**		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty
O_3	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	8% / 16% or 50 / 100 ppbv
O_3	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	4% / 8% or 50 / 100 ppbv
O_3	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	4% / 8%

Table 3.13 *An infrared limb emission instrument seems able to meet the requirements of the minimum mission.*

(Sub-)mm Limb Instruments

For the minimum mission, a frequency band in the mm-wave or sub-mm region should be sufficient to observe ozone rotational line(s), for which the measurement technique has been well-established (UARS/MLS, Aura/MLS, Odin/SMR, and JEM/SMILES). Stratospheric ozone observations would be unaffected by aerosol or PSCs. As for the IR, mm-wave limb-sounding is continuous through day and night. Vertical resolution is determined primarily by the half-power beam-width and is a function of frequency, antenna size and orbit height, and also by the vertical spacing of tangent-heights.

To define and optimise a mm-wave concept specifically to meet *Operoz* requirements for a "minimum mission" would involve trade-offs between different frequency bands, considering vertical resolution, and radiometric sensitivity.

Aura MLS or derivative

For its primary ozone frequency band at 240GHz, the retrieval precision (Table 3.7) meets the *Operoz* requirement of 8%, although vertical resolution is significantly coarser (~2.5 to 3km) than that specified for *Operoz* (1 to 2 km), due to the beam-width at that frequency. Beam-width varies inversely with measurement frequency, so is >2.5 times narrower in the MLS 650GHz band, which targets ClO and HCl primarily, but which also observes ozone.

Aura/MLS might achieve the *Operoz* 2 km threshold vertical resolution in its 240 GHz band by spacing tangent-heights more finely than in the standard limb-scan pattern. This starts ~8 km below the TP and ends ~ 30 km above the stratopause, thereby covering a vertical range approximately double that needed for *Operoz*. So the MLS limb-scan range and tangent-height spacing could both potentially be halved while retaining a comparable scan time and hence along-track spacing of limb-scans.

Horizontal resolution in the limb-viewing direction is controlled by radiative transfer. MLS has implemented a 2D (tomographic) retrieval from which a horizontal resolution of ~400 km is achieved for ozone. With appropriate along-track spacing and measurement sensitivity, a horizontal resolution of ~100 km has been shown to be theoretically possible for water vapour, facilitated by its very strong and spectrally varying limb-opacity. This seems likely not achievable for ozone. To improve upon 400 km horizontal resolution would require a much closer spacing of limb-scans, which could not be achieved simultaneously with a factor two reduction in tangent-height spacing, while retaining measurement integration time and hence sensitivity.

Aura/MLS ozone from the 240 GHz band is compliant in retrieval precision over (most of) the required height range, and could potentially be configured to achieve better compliance with either the vertical or horizontal resolution requirements of *Operoz*; though not both. Moving to a higher frequency, such as the 325-360 GHz band specified for STEAM-R and by improving the antenna beam-width the *Operoz* vertical resolution requirement could be met. Moving to a vertical array of receivers could improve sensitivity (through increased integration time, to compensate for the increase in system noise from operating at frequency) while also potentially allowing horizontal sampling to be increased.

Odin SMR or derivative

The *Operoz* 2 km vertical resolution requirement is met by Odin/SMR ozone retrievals from lines at 501.5 and 544.9 GHz region, due in part to the 2 times higher frequency (and observing from a lower satellite altitude of 600 km, cf. 705 km for AURA/MLS) providing a narrower beam-width than MLS using 240GHz. Single-scan retrieval precision does not, however, comply with the *Operoz* requirement of 8%, although is generally within a factor of 1.5 to 2.5 (Table 3.8). The SMR altitude range from tropopause to 70 km exceeds the *Operoz* requirement, offering scope for reductions to increase overall measurement time in the required vertical range in *Operoz*, either by reducing tangent-height spacing or increasing integration time. This should improve retrieval precision, to come close(r) to the requirement.

The Odin/SMR horizontal resolution along-track is solely determined by scan-time, because the instrument views perpendicular to the flight track. It is not straightforward to gauge what would be achievable by viewing instead along-track. Moving to a lower frequency, such as the 325-360GHz as specified for STEAM-R, may be anticipated to increase sensitivity (lower system noise achievable at lower frequency) while reducing vertical resolution. To ensure that the *Operoz* 2 km vertical resolution is met, an increase in antenna size and/or reduction in satellite height might be necessary. Moving to a vertical array of receivers could improve retrieval precision (through increased integration time) and would also optimise horizontal sampling and resolution along-track.

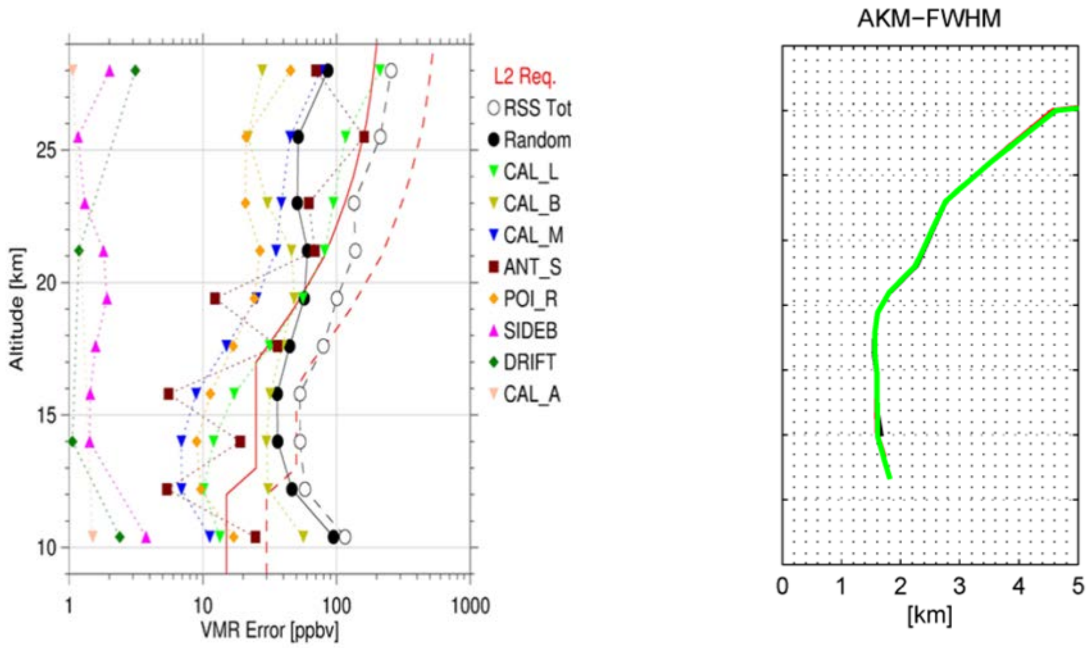

Figure 3.6 *STEAM-R simulations of uncertainties and vertical resolution for an instrument measuring at tangent altitudes from 6 to 28 km (in the context of the study for the PREMIER mission). In subsequent studies the limb-viewing range has been extended to include the whole stratosphere leading to compliance with the minimum mission 'Operoz' requirements over the full required altitude range.*

STEAM-R or derivative

On the basis of sophisticated retrieval simulations performed by Jo Urban for the STEAM-R concept in the PREMIER mission context (Kerridge et al, 2012), *Operoz* requirements on ozone uncertainty and vertical resolution would be met in the height-range below 30km (Figure 3.6). In the context of the subsequent study for ALiSS, the STEAM-R concept subsequently evolved to extend the tangent-height range to the upper stratosphere, and to move from a fixed, staring receiver array to introduce limb-scanning of the array, to acquire the full set of tangent-heights.

Summary

Aura MLS (240 GHz): complies with the *Operoz* (8%) uncertainty requirement. With a reduction in limb-scan range to that required by *Operoz* and a corresponding reduction in tangent-height spacing, the vertical resolution requirements (2 km) could be closely met. However, AURA/MLS is at least a factor of two coarser in horizontal resolution than the *Operoz* (200km) requirement.

Odin SMR (500 GHz): complies with the *Operoz* vertical resolution requirement. With a reduction in limb-scan range to that required by *Operoz* and corresponding increase in measurement time within that range, its precision could meet or be close to meeting the *Operoz* (8%) requirement.

STEAM-R (325-360 GHz)[12]: complies in simulations with *Operoz* requirements on vertical resolution and uncertainty in the height-range below 30 km. Performance has yet to be quantified in depth for the ALiSS concept, in which tangent-height range is extended to the upper stratosphere. Such a concept is, however, anticipated to remain compatible with *Operoz* requirements. Updated

[12] Retrieval performance was assessed extensively in simulations for the proposed PREMIER mission, during Phase 0 and Phase A. The satellite altitude was specified to be 817km for PREMIER, in order to co-fly with the operational MetOp-SG satellite.

retrieval simulations[13] for the scanning 7-beam array of STEAM-R in ALiSS have shown that the vertical resolution of such an instrument is not degraded from the original 14-beam fixed array of STEAM-R PREMIER, and could indeed be slightly improved. (This is in part due to specifying an orbit height substantially lower than the 817 km selected for PREMIER).

Minimum mission observational requirements				**Timeliness: <3h** **Stability: 1% / 3% per decade**		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty
O_3	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	8% / 16% or 50 / 100 ppbv
O_3	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	4% / 8% or 50 / 100 ppbv
O_3	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	4% / 8%

Table 3.14 *A millimetre-wave / sub-millimetre wave limb-sounding instrument is potentially able to meet the requirements of the minimum mission.*

The horizontal sampling threshold requirement of 200 km could more likely be met by an array receiver concept than by a purely limb-scanning concept, due to the challenge of also meeting stringent vertical resolution and precision requirements. To optimise a mm/sub-mm concept to meet the *Operoz* requirements, an initial trade-off study would need to consider: frequency coverage and resolution, use of receiver array and/or limb-scanning. The ability of (sub-)mm limb instruments to meet the minimum mission requirements is summarised in Table 3.14.

3.3.3 Minimum Mission Summary

In Section 3.3 we have analysed the ability of different types of satellite instruments (shortwave, infrared, and (sub-)mm wave) to meet requirements for a minimum ozone-only observing mission, following the requirements set out in Section 1 and 2, and these are summarised again in Table 3.15 below.

The basic requirements are high vertical resolution and daily global coverage of the whole stratosphere, including the ability to measure during polar night. Based on demonstrated performances, preliminary assessments have also been made of the different measurement techniques to address quantitative requirements specified in Section 2 (Table 2.7) for retrieval vertical resolution and uncertainty, horizontal sampling along-track, and long-term stability.

Table 3.15 below summarises the compliance of the different instrument types with the specified requirements. It is important to note that correlative non-space observations and solar occultation space observations may play an essential role in validation; not only during the commissioning phase but continuously, and that the stringent stability requirement could not be achieved without adequate provision of correlative observations as part of the overall observing system, to track and potentially correct in-flight changes to the instrument. For compliance with the daily global coverage and specifically the polar night, a mission that utilised emission sounding would be the most appropriate choice. This could in encompass measurements in either the infrared or (sub-)mm wavelength ranges.

[13] Private communications, courtesy of Prof. D. Murtagh, Chalmers UT, Gothenburg, Sweden

Infrared Limb Instruments

There are a range of infrared measurement types that could potentially meet the requirements. In the simplest case, a broad-band radiometer measuring in less than 10 channels would suffice, and this would be based on a long heritage of limb-sounding instruments, most recently HiRDLS. A Fourier Transform Spectrometer such as has been demonstrated by MIPAS on ENVISAT would also meet all the mission requirements, but with an increased complexity that is not needed for the minimum-mission concept detailed here[14].

However, looking forward to the mission extensions, such an instrument would allow a greater number of species to be measured and extended goals to be met. The HiRDLS and MIPAS instruments were designed and built more than a decade ago. For the minimum mission, technology advances allow several alternative concepts for a compact infrared solution to also be worthy of consideration.

(Sub-)mm Limb Instruments

Based on demonstrated performances of Aura MLS and Odin SMR, and retrieval simulations for the STEAM-R concept, it is evident that a limb-sounder operating in the (sub-)mm wave region could potentially meet the vertical resolution and uncertainty requirements for a stratospheric ozone minimum mission. The combination requirements on horizontal sampling, vertical resolution and uncertainty could more easily be met by an array receiver concept such as STEAM-R than by a purely limb-scanning concept. The MLS and SMR instruments were designed and built more than a decade ago. A concept derived for the minimum mission could benefit from technology developments such as those for STEAM-R. Vertical resolution is a driver for antenna size. Satellite height would be considered together with antenna and other instrument parameters to optimise a concept for the *Operoz* minimum mission.

Measurement Type	***Along-track sampling (km)***	***Hori-zontal coverage***	***Night-time measure-ments***	***Vertical sampling (km)***	***Vertical coverage (km)***	***Update Frequency (hours)***	***Uncer-tainty***	***Stability***
Nadir UV	Green	Orange	Red	Red	Orange	Green	Orange	Red
Nadir IR	Green	Green	Green	Red	Orange	Green	Orange	Green
Occultation	Red	Red	Orange	Green	Green	Red	Green	Green
Infrared Limb Emission	Green	Green	Green	Green	Green	Green	Green	Green
(Sub-)mm Limb Emission	Green	Green	Green	Green	Green	Green	Green	Green
Shortwave Limb Scattering	Green	Green	Red	Green	Green	Green	Green	Green

Table 3.15 *Summary of the ability of the various instrument types to meet each of the minimum mission requirements. (Green = fully met, Orange = partly compliant, Red = cannot meet the requirement.*

[14] However, looking forward to the mission extensions, such an instrument would allow a greater number of species to be measured and is relevant to addressing an extended set of mission objectives (Section 3.4).

Shortwave (UV/VIS/NIR/SWIR) Limb Instruments

Shortwave limb-scattering instruments, including OMPS-limb planned for JPSS-2, could fulfil requirements for the minimum mission, except for regions not illuminated by the sun, which specifically include polar night[15].

Occultation and Nadir Viewing Instruments

The remaining classes of instruments, occultation and nadir viewing instruments, assessed here have been found to be not suitable for the minimum mission.

In the case of occultation instruments, although providing high vertical resolution and highly accurate measurements, their sparse sampling patterns mean that global coverage can be accumulated only over an extended period (typically weeks-months) and not all seasons can be observed, which is a basic requirement as discussed in Sections 1 and 2. Such instruments are, however, a very valuable reference standards as they achieve the highest accuracy among all space measurements of vertical ozone profiles and, thus, are very well suited for validation of the entire altitude range of any limb sounders (ozone sondes are limited to MS and below, while ground lidar observations, depending on their configuration, can only cover limited altitude ranges. Nadir viewing instruments can provide data which meet horizontal sampling requirements, with daily, global coverage in the infrared and daytime-only in the shortwave, but they are unable to meet the fundamental requirement for high vertical resolution in the stratosphere.

Nadir-viewing instruments with ozone capabilities will be available on the planned series of operational polar-orbiting platforms. Their horizontal sampling (across-track in particular) would complement that of a dedicated limb-sounder for stratospheric ozone monitoring. Furthermore, accurate characterisation of the stratospheric ozone distribution by the limb-sounder would benefit operational nadir viewing instruments' abilities to monitor tropospheric ozone (Appendix B).

Sections 1 and 2 also specify requirements for timeliness of data delivery and long term time series of data. The timeliness of the data delivery will be primarily controlled by the satellite and ground-segment and is not therefore governed by the choice of instrument type. To monitor on a decadal timescale, a series of similar satellite instruments with sufficient overlap between them is needed.

[15] The use of the UV/VIS/NIR/SWIR frequency range is relevant to addressing an extended set of mission objectives (Section 3.4).

3.4 Mission Extensions

3.4.1 Assessment of the Summary of Observational Requirements (SOR) Table

The requirements for the suggested mission extensions have been detailed in Section 1 and 2, and a consolidated Summary of Observational Requirements (SOR) Table has been provided (Table 2.7).

There are also lower priority requirements discussed in Section 2, which are not included in the SOR-Table. The ability of the various types of instruments to also measure these species are discussed in the following tables. A detailed assessment of the quantitative requirements for these species has not been performed because these observables would not drive mission concepts.

Nadir Sounders

In general, nadir sounders cannot meet the vertical resolution requirements specified for the extended missions in the stratosphere and mesosphere, with measurements of species generally being either column measurements or of species primarily located in the troposphere. The two exceptions to this case are temperature and humidity, where radiances from millimetre wave and infrared nadir instruments are routinely assimilated in NWP and provide profile information throughout the troposphere and stratosphere, though at a much lower vertical resolution than is required for the mission detailed here. The role of nadir sounders is however very important for the add-on mission looking at tropospheric ozone, which can be measured by both infrared and shortwave instruments as has already been described in Section 2 above.

Infrared instruments such as IASI can measure various trace gases, but in most cases the vertical resolution would be extremely poor, and it is only in the case where species are predominantly located in the stratosphere that infrared nadir sounders could contribute. As noted above, instruments such as IASI are able to measure temperature and water vapour in both the troposphere and lower stratosphere at high vertical resolution, but they are not able to cover the full altitude range required here with sufficient vertical resolution to meet the requirements.

At a very coarse resolution, it is possible to obtain information on HNO_3, SO_2 (assuming absence of significant tropospheric pollution), and also some information on CO and CH_4 profiles which extend into the lower stratosphere, although the coarse resolution means that it is not possible to completely separate the lower stratospheric information from that from the upper troposphere.

Other trace gases which have been shown to be detectable by IASI such as N_2O, CFC-11 and CFC-12 are dominated by the tropospheric signal and have little vertical information obtainable, so will not be suitable for meeting the extended mission requirements.

In general in the shortwave, species other than ozone are only detectable as column amounts, and for many species these are dominated by tropospheric concentrations (e.g. H_2CO, CHOCHO, CH_4), so are not suitable for meeting the extended mission requirements. Column values of BrO, NO_2, SO_2 and AOD (which could provide information on stratospheric sulphate at certain locations and times, for instance after a volcanic eruption) can provide information on the stratospheric column in certain situations where the tropospheric column can be assumed to be very small. However, none can meet the vertical resolution requirements.

Shortwave Limb Scattering Instruments

In the UV/VIS/NIR/SWIR limb observations from the tropopause region up to the thermosphere are feasible on a global scale. Stratospheric observations in limb scatter geometry are limited to the sunlit portion of the earth but air glow emissions in the SWIR allow measurements under night-time conditions mainly in the mesosphere. Stellar occultation observations as successfully demonstrated by GOMOS provide mainly night-time measurements (Bertaux et al., 2010) with some limited measurements under daylight conditions using the brightest stars as a light source.

In the UV/visible spectral range (up to about 800 nm) dominated by ozone absorption in the Hartley (UV), Huggins (near UV), and Chappuis (visible) bands several other trace gases (NO_2, BrO, OClO) aerosols and clouds (e.g. sub-visible cirrus and polar stratospheric clouds (von Savigny et al., 2005, Wiensz et al., 2013) can be observed in the stratosphere.

Table 3.3 (Section 3.2) summarises the uncertainty, altitude range, and vertical resolution for ozone, BrO, NO2, and aerosols for typical limb scatter observations. For NO_2 from limb scatter uncertainties are 10-20% (10-45 km), BrO 30% (10-35 km) and aerosols 10% (10-35 km). OClO is a photoactive species which can be only observed at twilight conditions (near 90° solar zenith angle) (Krecl et al.,20006, Kühl et al., 2008) mainly in the polar vortex when chlorine gets activated, e. g. under ozone hole conditions. In the UV/visible ozone can be retrieved up to ~65 km (lower mesosphere) using limb scatter geometry and up to 100 km altitude using stellar occultations. Using air glow emission from oxygen bands upper mesospheric ozone can be inferred (e. g. Thomas et al., 1983).

In the SWIR it is in principle possible to retrieve N_2O (up to 40 km), CO (up to 35km), CO_2 (up to 55 km), and CH_4 (up to 40 km) as was originally planned for SCIAMACHY (Bovensmamnn et al., 1999). Due to the low signal-to-noise and many bad detector pixel of the InGeAs detectors retrievals of these trace gases was not possible. In addition sufficient high spectral resolution in the SWIR is needed. Using the visible oxygen bands in combination with CO_2 from the SWIR, temperature and pressure retrievals are possible. Temperature retrievals up to about 35 km altitude from observations in the oxygen A-band have been successfully demonstrated using stellar occultations (Bertaux et al., 2010). LS water vapour has been successfully retrieved from SWIR observations near 1.4μm (Rozanov et al., 2011).

The minimum mission scenario (ozone only) using a UV/visible spectrometer (excluding SWIR) as described in Table 3.12 using a continuous spectral range would automatically cover NO_2, BrO , OClO, and aerosols, which are relevant for the extended mission themes: stratospheric chemistry, stratospheric water vapour and stratospheric aerosols, and troposphere-stratosphere-transport and the Asian monsoon. An extension into the SWIR is required in order to observe stable tracers like N_2O, CO_2, CH_4, and CO as relevant for the mission theme BD circulation. Mesospheric observations from airglow measurements in the SWIR extend the measurement capabilities up to the upper mesosphere and lower thermosphere, e.g. NO, temperature from OH* and oxygen A-bands, metals and metal oxides, oxygen, water vapour, noctilucent clouds, and ozone (Bovensmann et al., 2011, Evans et al., 2010, Stevens et al.,2008, Petelina et al., 2006).

Table 3.16 on the next page summarises the summary of observational requirements met by current UV/VIS/SWIR techniques.

An across-track sampling capability could potentially be implemented for this class of sensor through azimuth scanning, with associated trade-off with along-track sampling and integration time (hence noise). For the ALTIUS design, using acousto-optical tunable filters, it could alternatively be attained by a 2-D limb-imaging array.

Capabilities to Meet *Operoz* Summary of Observational Requirements

Shortwave (UV/VIS/NIR/SWIR) Limb Scattering

Operational services and Long-term monitoring	
MM Minimum Mission ('Priority A')	***- Timeliness: < 3h (LS, MS)*** ***- Long-term stability (O_3 observations): 1% / 3% per decade*** ***- Vert. resolution: 1/2km (LS, MS); 2/4km (US)*** ***- Along-track sampling: 100/200km (LS, MS); 200/400km (US)***
BD Brewer-Dobson Circulation ('Priority B') **SC Stratospheric Chemistry ('Priority B')** **TO Tropospheric Ozone ('Priority B')**	**- Across-track sampling (O_3 observations): 100 / 200 km (UT, LS, MS)**

Observable	Mission	Horizontal coverage	Uncertainty		
			LS	MS	US
O_3	***MM***	***Global (incl. polar night)***	***4% / 8% or 50 / 100 ppbv***	***4% / 8% or 50 / 100 ppbv***	***4% / 8%***
UT O_3	**TO**	**Global (enhanced only)**	**8% / 16% or 50 / 100 ppbv (UT)**		
H_2O	**BD, SC**	**Global**	**5% / 10%**	**5%/10%**	**8%/16%**
HNO_3	**SC**	**Global**	**0.5 / 1 ppbv**	**0.5 / 1 ppbv**	**0.5 / 1 ppbv**
HCl	**BD, SC**	**Global**	**0.2 / 0.4 ppbv**	**0.2 / 0.4 ppbv**	**0.2 / 0.4 ppbv**
$ClONO_2$	**SC**	**50-90N; 50-90S**	**50 / 100 pptv**	**50 / 100 pptv**	
BrO	**SC**	**Global**	**1.5 / 3 pptv**	**1.5 / 3 pptv**	
SF_6	**BD**	**Global**	**0.8 / 1.5 pptv**	**0.8 / 1.5 pptv**	**0.8 / 1.5 pptv**
CFC-11	**BD**	**Global**	**15 / 30 pptv**	**15 / 30 pptv**	
CFC-12	**BD**	**Global**	**30 / 60 pptv**	**30 / 60 pptv**	
N_2O*	**BD, SC**	**Global**	**20 / 40 ppbv**	**20 / 40 ppbv**	
CH_4*	**BD, SC**	**Global**	**0.1 / 0.2 ppmv**	**0.1 / 0.2 ppmv**	**0.1 / 0.2 ppmv**
Temperature*	**SC**	**Global**	**1 K / 2 K**	**1K / 2K**	**2K / 3K**
Extinct. coef.	**SC**	**Global**	**10^{-4} / 2.10^{-4} km^{-1}**	**10^{-4} / 2.10^{-4} km-1**	

Table 3.16 *Summary of current abilities using limb scattering to meet 'Priority A' (in italics) and 'Priority B' observational requirements. (Green = fully met, Orange = partly compliant, Red = cannot meet the requirement.*
**these quantities can be in principle measured, but uncertainties have to be confirmed by further studies.*

Infrared Limb Emission Sounders

Limb-emission sounding offers global horizontal coverage with an update frequency of 12h (24h) throughout the stratosphere (LS, MS, US) during daytime and nighttime (e. g. under polar night conditions). In addition to ozone, it can provide pressure / temperature as well as numerous additional chemical species, which are required in the context of mission extensions. The number of additional species primarily depends on spectral coverage and spectral resolution. Previous broadband radiometers measured single profiles of p/T, ozone, H_2O, HNO_3, CH_4, N_2O, CFC-11, CFC-12, NO_2, N_2O_5, $ClONO_2$, as well as aerosol and cloud extinction (see Table 3.6).

CO and NO have widely spaced emission bands in the 4.7 and 5.3 µm wavelength regions which have been detected, for example, by ISAMS onboard UARS using gas-correlation radiometry and by the MIPAS FTS onboard Envisat.

The number of detectable species increases with increasing spectral resolution. For example, a PREMIER-type InfraRed Limb Sounder (IRLS) provides, in addition, single profiles of PAN, HCN, C_2H_6 and ClO for pollution events or active chlorine conditions. For SO_2 and OCS single profiles are available after volcanic eruptions as well as monthly zonal averaged for undisturbed conditions. The most important age-of-air-tracer, SF_6, is available as monthly zonal average, a quantity which is commonly used for age-of-air and circulation analyses. $BrONO_2$ can be obtained as weekly zonal average. The list of detectable species potentially also includes CF_4, however, there is the need for improved spectroscopic data (M. Höpfner, private communication).

A possible mission extension compared to a classical radiometer or FTS is an across-track capability. This would mainly enhance operational applications in the LS. For data assimilation, a scanning mechanism providing similar along-track and across-track coverage/resolution would be most useful. It could be implemented by an additional horizontal scanning mirror. Monitoring STE and transport by the Asian monsoon would also benefit from across-track sampling provided by a two dimensional detector array. In addition to better across-track coverage/resolution, such an array could also be used to enhance the precision of the observations (across-track averaging), if necessary.

Compliance with the ‘Priority B’ extensions

The desirable requirements with ‘Priority B’ are summarized in Table 2.4 in green. They address “Brewer-Dobson Circulation”, “Stratospheric Chemistry” and “Tropospheric Ozone” as mission extensions with highest priority. A large number of the desirable species can be obtained from infrared limb-sounding (see Section 4.2). SF_6 can be retrieved in terms of monthly zonal averaged, which is generally sufficient for age-of-air analyses. Note that the Level-2 data requirements are based on a daily to weekly update frequency from which zonal monthly means could be derived.

Table 3.17 (see next two pages) gives a summary of the capability of infrared limb sounding to meet the ‘Priority A’ and ‘Priority B’ observational requirements. For an FTS-type instrument employing a 2D detector, a detailed uncertainty analysis for ozone, temperature, CH_4, HNO_3, and CFC-11 was performed in the framework of the PREMIER CORSA study (Kerridge et al., 2012), based on single profile retrieval studies. For HNO_3, CFC-11, and CH_4 the retrieval simulations approximately covered the altitude range of the UT, LS, and MS. For HNO_3, the derived uncertainties remain well below the breakthrough value specified in Table 2.7 (0.5 ppbv) in the whole altitude range. This also applies to MTG detectors, if they are used as they are.

For CFC-11, the derived uncertainties remain well below the breakthrough value of 15 pptv in the UT and LS and below the threshold value of 30 pptv in the MS, even for MTG detectors. The results for CH_4 also suggest a high degree of compliancy as well. For water vapor, the estimated uncertainties are somewhat dependent on the type of detector. For an MTG detector, the uncertainties are of the order of 20 to 30 % in the altitude range of the LS and MS, somewhat larger in the US, and below 10% in the UT. These values exceed the threshold of 10%. The errors are, however, dominated by detector noise and can be mitigated below 10% by averaging over a view profiles (e. g. by utilizing the across-track dimension of the detector array.).

A future radiometer could utilize 2D detector arrays to observe simultaneously a set of tangent-heights (vertical) through a set of interference filters (horizontal) that cover similar spectral ranges (micro-windows) as used in the PREMIER study. For such an instrument a similar range of uncertainties can be expected. A filter covering the same pixel area as the IRLS in the dynamics or chemistry mode would provide at least a factor of two better signal-to-noise ratio (F. Friedl-Vallon, private communication.)

Uncertainty ranges obtained by HIRDLS can only be considered as an upper limit due to the technical difficulties described in Section 3.2. For HNO_3 the accuracy is between 20 and 30% between 20 and 50km. The corresponding in-orbit precision is 0.2 to 0.3 ppbv. LIMS achieved an accuracy of stratospheric water vapor of about 20% (35 years ago).

Capabilities to Meet *Operoz* Summary of Observational Requirements **Infrared Limb Emission Sounding**					
Operational services and Long-term monitoring ***MM Minimum Mission ('Priority A')*** **BD Brewer-Dobson Circulation ('Priority B')** **SC Stratospheric Chemistry ('Priority B')** **TO Tropospheric Ozone ('Priority B')**				***- Timeliness: < 3h (LS, MS)*** ***- Long-term stability (O_3 observations): 1% / 3% per decade*** ***- Vert. resolution: 1/2km (LS, MS); 2/4km (US)*** ***- Along-track sampling: 100/200km (LS, MS); 200/400km (US)*** **- Across-track sampling (O_3 observations): 100 / 200 km (LS, MS)**	
Observable	Mission	Horizontal coverage	Uncertainty LS	Uncertainty MS	Uncertainty US
O_3	***MM***	***Global (incl. polar night)***	***4% / 8% or 50 / 100 ppbv***	***4% / 8% or 50 / 100 ppbv***	***4% / 8%***
UT O_3	**TO**	**Global (enhanced only)**	**8% / 16% or 50 / 100 ppbv (UT)**		
H_2O	**BD,SC**	**Global**	**5% / 10%**	**5%/10%**	**8%/16%**
HNO_3	**SC**	**Global**	**0.5 / 1 ppbv**	**0.5 / 1 ppbv**	**0.5 / 1 ppbv**
HCl	**SC**	**Global**	**0.2 / 0.4 ppbv**	**0.2 / 0.4 ppbv**	**0.2 / 0.4 ppbv**
$ClONO_2$	**SC**	**50-90N; 50-90S**	**50 / 100 pptv**	**50 / 100 pptv**	
BrO	**SC**	**Global**	**1.5 / 3 pptv**	**1.5 / 3 pptv**	
SF_6	**BD**	**Global**	**0.8 / 1.5 pptv**	**0.8 / 1.5 pptv**	**0.8 / 1.5 pptv**
CFC-11	**BD**	**Global**	**15 / 30 pptv**	**15 / 30 pptv**	
CFC-12	**BD**	**Global**	**30 / 60 pptv**	**30 / 60 pptv**	
N_2O	**BD,SC**	**Global**	**20 / 40 ppbv**	**20 / 40 ppbv**	
CH_4	**BD, SC**	**Global**	**0.1 / 0.2 ppmv**	**0.1 / 0.2 ppmv**	**0.1 / 0.2 ppmv**
Temperature	**SC**	**Global**	**1 K / 2 K**	**1K / 2K**	**2K / 3K**
Extinct. coef.	**SC**	**Global**	**10^{-4} / 2.10^{-4} km^{-1}**	**10-4 / 2.10-4 km-1**	

Table 3.17 *Summary of current abilities using limb emission sounding in the infrared to meet 'Priority A' (in italics) and 'Priority B' observational requirements. (Green = fully met, Orange = partly compliant, Red = cannot meet the requirement.*

An across-track sampling capability could potentially be implemented for this class of sensor through azimuth scanning, as HIRDLS had been designed to have, with associated trade-off with along-track sampling and integration time (hence noise). For FTIR concept of the PREMIER IRLS design, it could alternatively be attained over a restricted swath by 2-D limb-imaging array.

(Sub-)mm Limb Emission Sounders

Instruments using the (sub-)mm wavelength region are capable of profiling several of the 'Priority B' (and 'Priority C') species identified in Section 2, and thereby contribute useful information both to the Brewer-Dobson and Stratospheric Chemistry mission extensions, and also to the other mission extensions.

General information on measuring at this frequency range and details of the current instruments, including a summary of all the species measured have been described previously in Section 2. A plot of simulations for STEAM-R done in support of the PREMIER mission is also included below, showing the expected performance of a number of species in the lower to mid-stratosphere. A more detailed assessment as to for which species observations using the (sub-)mm wavelength region can meet the requirements is summarised in Table 3.18.

Based on established performances of Aura MLS and Odin SMR, and also simulations for STEAM-R[16], compliant or close to compliant measurements of H_2O, HNO_3 and N_2O and temperature would be expected in the millimetre or sub-mm wave length regions (see Figure 3.7 for some key examples of performance estimates), and of HCl in the 625 GHz (sub-millimetre) band specifically, unique to MLS. In the case of HNO_3, it may not be possible to meet the uncertainty requirement, except in cases of high HNO_3 concentrations.

Measurements of BrO have been demonstrated by Aura MLS, although they required averaging to provide a useful product, so would not meet the daily sampling requirements. It is likely that BrO measurements in this frequency range would therefore not be fully compliant with the requirements from this study, but would still provide useful information.

Information on upper tropospheric ozone can be obtained in mm-wave windows down to a depth limited by humidity, dependent on the frequency of the ozone line chosen. Atmospheric windows in the mm-wave (<360GHz) allow penetration down into the troposphere (as demonstrated by Aura MLS 240GHz and also by an airborne limb-sounder (MARSCHALS) in the 300-350GHz range designated for the STEAM-R concept. Those in the sub-mm range (above 360GHz) allow coverage of the full stratosphere (e.g. Odin/SMR around 500 GHz), although not much lower than the tropopause. The advantage of (sub-)millimetre over infrared wavelengths is a greatly decreased sensitivity to cirrus, allowing measurements in the tropical upper troposphere, where cirrus is ubiquitous, as well as mid- and high latitudes. However, being more affected by water vapour attenuation, mm-wave observations cannot penetrate as far down as infrared measurements in the absence of clouds.

The other 'Priority B' species would not be measurable by a mm- or sub-mm wave instrument. However, a number of the 'Priority C' species would be available. For instance, for the 'Stratospheric Chemistry' extension, information is available on ClO, SO_2, NO_2 and NO. ClO in particular is measured by both MLS and ODIN-SMR, and it should be possible to meet the mission requirements for this species. The other species (SO_2, NO_2 and NO) would not be completely compliant, being limited both in altitude range and accuracy.

HCN, CO and SO_2 are also detectable in this frequency range, and are of relevance for the 'Troposphere-Stratosphere Transport and the Asian Monsoon' extended mission. Such species have

[16] In the context of PREMIER, simulations were performed for a STEAM-R concept designed to cover the altitude range below 30km only. As mentioned in the previous section of this report concerning the "minimum mission", this concept has subsequently been extended to the upper stratosphere in the context of a Swedish national or bilateral mission.

all been detected by MLS albeit with a high uncertainty, meaning that either averaging, or use of profiles only in elevated concentrations is required. Such species would also be detectable by an instrument such as STEAM-R, but would not be fully compliant with the detailed requirements.

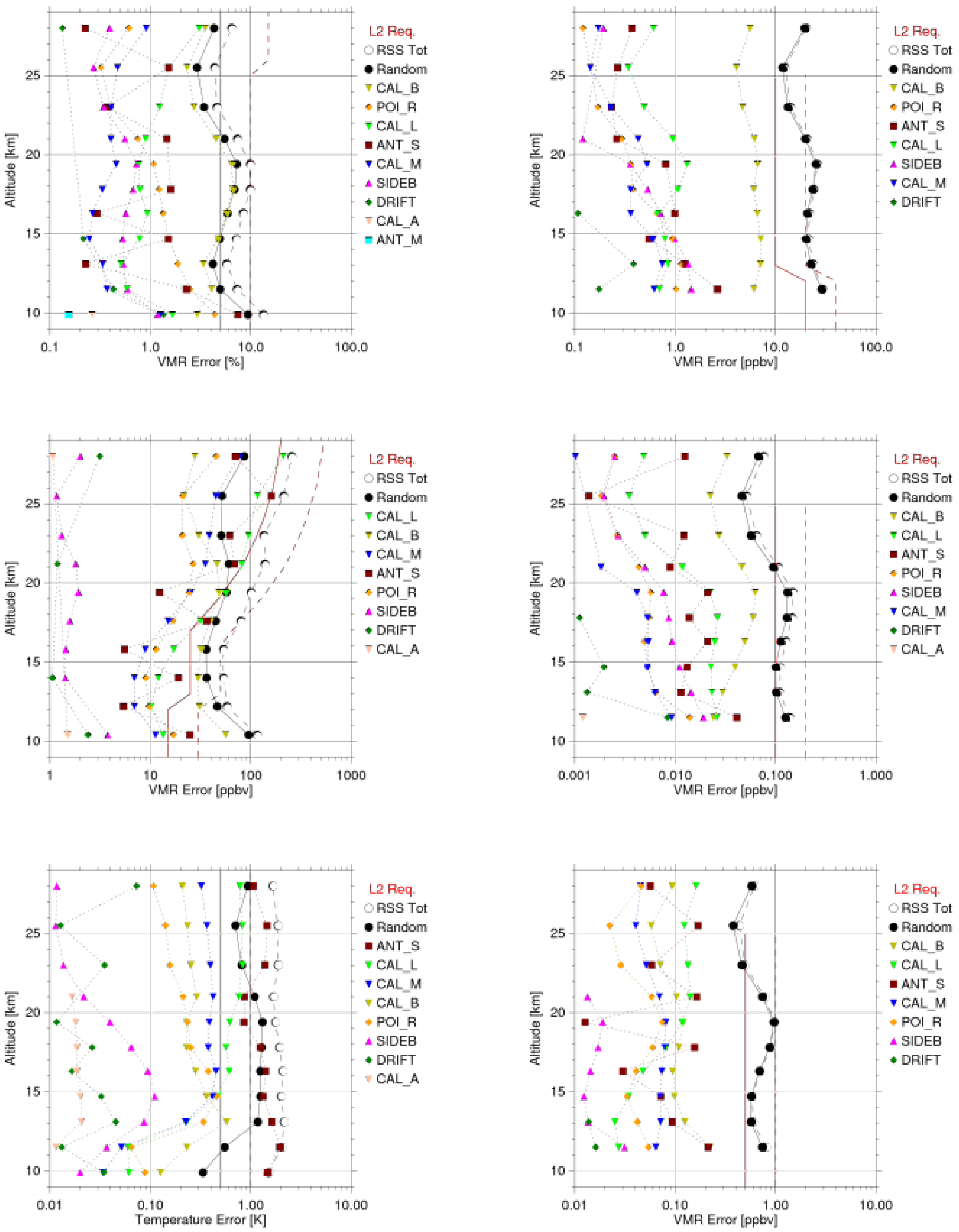

Figure 3.7 *From the PREMIER study (CORSA study final report) – Summary plots for H_2O (top left), CO (top right), O_3 (centre left), HCN (centre right),T (bottom left), HNO_3 (bottom right) based on STEAM-R Level 1 performance estimates for the industrial phase-A study. Error budgets calculated by J.Urban are according to Level-1 instrument performance estimates reported in the report for mission selection and a standard retrieval set-up for linear simulations. Only instrumental errors are considered, spectroscopic errors are not included.*

Capabilities to Meet *Operoz* Summary of Observational Requirements

(Sub-)mm Limb Emission Sounding

Operational services and Long-term monitoring	
MM* *Minimum Mission ('Priority A') **BD Brewer-Dobson Circulation ('Priority B')** **SC Stratospheric Chemistry ('Priority B')** **TO Tropospheric Ozone ('Priority B')**	***- Timeliness: < 3h (LS, MS)*** ***- Long-term stability (O_3 observations):*** ***1% / 3% per decade*** ***- Vert. resolution:*** ***1/2km (LS, MS); 2/4km (US)*** ***- Along-track sampling:*** ***100/200km (LS, MS); 200/400km (US)*** **- Across-track sampling (O_3 observations):** **100 / 200 km (LS, MS)**

Observable	Mission	Horizontal coverage	Uncertainty LS	Uncertainty MS	Uncertainty US
O_3	***MM***	***Global (incl. polar night)***	***4% / 8% or 50 / 100 ppbv***	***4% / 8% or 50 / 100 ppbv***	***4% / 8%***
UT O_3	**TO**	**Global (enhanced only)**	**8% / 16% or 50 / 100 ppbv (UT)**		
H_2O	**BD,SC**	**Global**	**5% / 10%**	**5%/10%**	**8%/16%**
HNO_3	**SC**	**Global**	**0.5 / 1 ppbv**	**0.5 / 1 ppbv**	**0.5 / 1 ppbv**
HCl	**SC**	**Global**	**0.2 / 0.4 ppbv**	**0.2 / 0.4 ppbv**	**0.2 / 0.4 ppbv**
$ClONO_2$	**SC**	**50-90N; 50-90S**	**50 / 100 pptv**	**50 / 100 pptv**	
BrO	**SC**	**Global**	**1.5 / 3 pptv**	**1.5 / 3 pptv**	
SF_6	**BD**	**Global**	**0.8 / 1.5 pptv**	**0.8 / 1.5 pptv**	**0.8 / 1.5 pptv**
CFC-11	**BD**	**Global**	**15 / 30 pptv**	**15 / 30 pptv**	
CFC-12	**BD**	**Global**	**30 / 60 pptv**	**30 / 60 pptv**	
N_2O	**BD,SC**	**Global**	**20 / 40 ppbv**	**20 / 40 ppbv**	
CH_4	**BD, SC**	**Global**	**0.1 / 0.2 ppmv**	**0.1 / 0.2 ppmv**	**0.1 / 0.2 ppmv**
Temperature	**SC**	**Global**	**1 K / 2 K**	**1K / 2K**	**2K / 3K**
Extinct. coef.	**SC**	**Global**	**10^{-4} / 2.10^{-4} km^{-1}**	**10-4 / 2.10-4 km-1**	

Table 3.18 *Summary of current abilities using limb emission sounding in the (sub-)mm range to meet 'Priority A' (in italics) and 'Priority B' observational requirements. (Green = fully met, Orange = partly compliant, Red = cannot meet the requirement.*

As described in the section of this report on ozone for the "minimum mission", Aura MLS and Odin SMR observing attributes are such as to comply more closely with requirements on, respectively, vertical coverage and vertical resolution. To optimise the selection of frequency band(s) and other instrument specifications for stratospheric trace gases to be targeted by *Operoz*, trade-off studies would need inter alia to consider carefully the frequency dependences of line strength, antenna beamwidth and system noise. Penetration below the tropopause would also be relevant, to ensure ozone requirements could be met over the required altitude range. An across-track sampling capability could potentially be implemented for this class of sensor through azimuth scanning, with associated trade-off with along-track sampling and integration time (hence noise).

Table 3.18 gives a summary of the capability of (sub-)mm limb emission sounding to meet the 'Priority A' and 'Priority B' observational requirements.

3.4.2 Discussion of Individual Mission Extensions

Brewer-Dobson Circulation ('Priority B')

The key observables required to address this mission extension are included in Table 2.4.

Shortwave Limb Scattering

Lower stratospheric water vapor retrieval has been successfully demonstrated in the SWIR by SCIAMACHY (Rozanov et al., 2011, Hegglin et al., 2014). It is in principle possible to also retrieve CH_4 and N_2O (up to 40 km) in SWIR bands, as was originally planned for SCIAMACHY (Bovensmamnn et al., 1999). Considering other observables identified to be useful for this mission extension and assigned 'Priority C' in *Operoz*: CO should be possible (up to 35km) and CO_2 (up to 55 km. Using the visible oxygen bands in combination with CO_2, temperature (and pressure) retrievals are possible.

Infrared Limb Emission Sounding

All the 'Priority B' species, except HCl, can be obtained from the type of infrared instrumentation discussed in 3.2.2. Radiometers can provide CH_4, N_2O, CFC-11, CFC-12, and H_2O. A high-resolution FTS (MIPAS or PREMIER IRLS type) would provide SF_6 in addition. SF_6 is best suited for age-of-air and corresponding circulation analyses. The SF_6 measurements are only available in terms of monthly zonal averages. However, these would be sufficient to analyze the relatively slow changes of the Brewer-Dobson circulation and their spatial and seasonal dependencies. In conclusion, infrared radiometers already provide a wealth of information on tracers affected by changes in the Brewer-Dobson circulation. Temperature would be covered by either a radiometer or spectrometer. The most prominent age-of-air measure, SF_6, can however only be provided by a high-resolution Fourier Transform Spectrometer.

(Sub-)mm Limb Emission Sounding

On the basis of Aura/MLS, Odin/SMR and simulations performed for STEAM-R, limb emission in the mm/sub-mm range would be expected to provide observations on the stratospheric constituents N_2O, H_2O and HCl for diagnosing and monitoring the Brewer-Dobson circulation. Temperature would be covered, as would CO ('Priority C'). The age of air tracer SF_6 does not have rotational lines detectable in the mm/sub-mm, however, and nor do CH_4, CFC-11 or CFC-12.

Stratospheric Chemistry ('Priority B')

The key observables required to address this mission extension are included in Table 2.5.

Shortwave Limb Scattering

The required reactive species BrO can be measured in the UV (Sinnhuber et al, 2005; McLinden et al., 2010; Bourassa et al., 2011; Bauer et al., 2012). In the Lower Stratosphere, BrO measurements are only demonstrated in this spectral range. As in the case of the B-D circulation, lower stratospheric water vapor, CH_4 and N_2O (up to 40 km) are accessible in the SWIR domain In addition the (spectral) extinction coefficient can be measured and temperature can be derived. Considering the 'Priority C' observables NO_2 can be measured as well as OClO as an indicator for chlorine activation in the polar vortex.

Infrared Limb Emission Sounding

All ‘Priority B’ species, except HCl and BrO, can be obtained from the types of infrared instrumentation discussed on 3.2.2. Radiometers can provide HNO_3, H_2O, CH_4, N_2O, and $ClONO_2$ (see Table 3.6). In addition, temperature and spectral extinction coefficient (for aerosol surface area density) can be obtained from filter radiometers next to a number of ‘Priority C’ species (NO_2, N_2O_5, NO[17]. From an Fourier Transform Spectrometer the same list as for the filter radiometers can be obtained with in addition NO, SO_2 and $BrONO_2$. In conclusion, most of the species can be provided by radiometric limb-sounding. Valuable additional information on ClO could be obtained from a high resolution FTS. The lack of HCl and BrO would affect, in particular, monitoring and studies of polar chemistry.

(Sub-)mm Limb Emission Sounding

On the basis of Aura/MLS, Odin/SMR, and also simulations performed for STEAM-R, (sub-)mm observations would be expected to provide data uniquely on the ‘Priority B’ species HCl and on the other ‘Priority B’ species N_2O, HNO_3, and H_2O for diagnosing and monitoring stratospheric chemistry. The ‘Priority C’ observables ClO, BrO, NO and NO_2 would also be covered, with some averaging required. Neither CH_4 nor the heavy molecule $ClONO_2$ (and N_2O_5) are detectable in the (sub-)mm, however, nor the extinction coefficient in relation to aerosols.

Tropospheric Ozone (‘Priority B’)

The key observables required to address this mission extension are included in Table 2.6.

The required O_3 observations in the UT can be provided directly by a limb sounding instrument, down to either cloud top or, in the case of (sub-)mm, to an altitude determined by atmospheric humidity. Across-track sampling capability, to achieve denser horizontal coverage, could potentially be introduced either by azimuth scanning or by the horizontal dimension of a 2-D detector array, both in the case of shortwave and limb emission.

While nadir sounders in the UV/visible or Infrared do not meet the required vertical resolution in the troposphere, their combination with a limb sounding instrument would allow the greatest information to be obtained over the entire vertical profile, extending into the lower troposphere. The limb information would, by constraining the stratosphere, localise the nadir sounder information in the troposphere. An assimilation scheme, such as those used in MACC/CAMS, would not require the instruments to be observing the same location at the same time. However, for combined retrievals, it would be beneficial for the limb- and nadir- sounding observations to be collocated as closely as possible.

Shortwave Limb Scattering

Assuming no clouds and good constraints on aerosols (joint retrievals) it may be possible to obtain UT ozone. This, however, needs to be demonstrated.

Infrared Limb Emission Sounding

Infrared limb-sounding can provide ozone in the upper troposphere. Among other factors (nb . cloudiness), the penetration depth into the troposphere depends on the selected wavelength and spectral resolution.

(Sub-)mm Limb Emission Sounding

As discussed in earlier sections, (sub-)mm observations extend down into the troposphere in

[17] NO is measurable in the stratosphere by gas correlation radiometry.

atmospheric windows <360 GHz[18], and Aura/MLS has demonstrated retrieval of ozone profiles in the UT. By virtue of being much less sensitive to cirrus, ozone observations can be made in the UT under most conditions.

Extension into the Mesosphere ('Priority C')

Key observables needed to address this mission extension are identified in Section 2.3.2.

Shortwave Limb Scattering

Mesospheric observations of airglow in the shortwave provide capabilities in the upper mesosphere and lower thermosphere. These include temperature from OH* and oxygen A-bands and the 'Priority C' observable NO. Other relevant observations in this height range could be metals and metal oxides from meteoric and cometary impact, oxygen, noctilucent clouds, and ozone (Bovensmann et al., 2011, Evans et al., 2010, Petelina et al., 2006). From OH emission in the UV mesospheric water vapour can be derived (Stevens et al., 2008).

Infrared Limb Emission Sounding

An extension of the altitude range of infrared limb-sounding into the mesosphere is feasible (see Table 3.6). Temperature and all 'Priority C' observables could be provided, i.e., NO, NO_2, CO, together with O_3. While CO_2 (for T) and NO_2 have quite closely spaced lines and have therefore been measured in the mesosphere by conventional filter radiometry (e.g. HIRDLS, LIMS), NO and CO have narrow, widely spaced lines, and mesospheric observations have instead been made either by gas-correlation radiometry (ISAMS) or by spectrometry (MIPAS). In addition, new concepts such as laser heterodyne radiometry, with capability of very high spectral resolution over selected bands, might be relevant for NO and CO as well as other species required in the mesosphere. In conclusion, infrared limb-sounding provides all species required to monitor and investigate mesospheric processes impacting on the stratosphere such as the downward transport of NO_X.

(Sub-)mm Limb Emission Sounding

Aura/MLS and Odin/SMR have observed – next to O_3, temperature, NO and CO in the mesosphere. The strongest rotational lines of NO and CO are ~1THz. A limb-sounder dedicated to the mesosphere and lower thermosphere (e.g. LOCUS concept) would employ THz bands to target atomic O, O_2 and OH as well as NO, CO and possibly NO_2 and HO_2.

Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols ('Priority C')

Key observables needed to address this mission extension are identified in Section 2.3.2.

Shortwave Limb Scattering

Using selected wavelengths distributed across the visible and near-infrared (NIR) spectral range, aerosol extinction profiles can be retrieved assuming a given particle size distribution (e.g. Thomasson et al., 2007, Ernst et al.,20112, Rieger et al. 2014). H_2O is retrievable in the SWIR (Rozanov et al., 2011). Subvisible cirrus clouds are detectable (Wiensz et al. 2013). Although SO_2 can be observed in the UV in nadir view, saturation in the UV ozone bands (LS, MS) in limb view prevents any reasonable retrieval of this species, and nor is OCS detectable

Infrared Limb Emission Sounding

[18] Atmospheric windows >360 GHz (i.e. sub-mm) do not extend below the tropopause, however, so Odin SMR ozone retrievals are limited to the stratosphere.

Temperature, H_2O and (spectral) extinction coefficient can be obtained from radiometric observations (see Table 3.6). SO_2 or OCS observations require a high-resolution FTS.

(Sub-)mm Limb Emission Sounding

On basis of established performances of Aura/MLS and Odin/SMR, and also simulations for STEAM-R, the (sub-)mm wavelength range would provide H_2O and (volcanically enhanced) SO_2, along with temperature, OCS (and ozone) in support of this mission extension. Sulphate aerosol and other stratospheric particulates are, however, generally too small for their extinction to be detected in this wavelength range.

Climate Impact of Troposphere-Stratosphere Transport and the Asian Monsoon ('Priority C')

Key observables needed to address this mission extension are identified in Section 2.3.2.

Shortwave Limb Scattering

Aerosol extinction is available in the visible and near-infrared. The 'Priority C' NO_2 is available in the UV/visible and CO, and H_2O in the SWIR.

Infrared Limb Emission Sounding

The specified 'Priority C' observables can be obtained from infrared limb-sounding. CO and PAN are both very suitable transport tracers to diagnose troposphere-to-stratosphere transport. While H_2O, and extinction coefficient can be measured with a radiometer, the other species (HCN, PAN and SO_2) require a FTS. This means that biomass-burning and sulphur related science questions can only be addressed by observations with an FTS.

(Sub-)mm Limb Emission Sounding

On basis of established performances of Aura/MLS and Odin/SMR, and also simulations for STEAM-R, specifically for a monsoon uplift event, the sub-mm wavelength range would provide CO, HCN (and CH_3CN), H_2O and (elevated) SO_2, along with temperature (and ozone) in support of this mission extension. However, the heavy molecule PAN does not have rotational lines detectable in the (sub-)mm and, apart from the large size component (>100 micron) of cirrus, particulates in the UT/LS and stratosphere are generally too small for their extinction to be detected in this wavelength range.

3.4.3 Mission Extensions Summary

For the desirable ('Priority B') mission extension 'Brewer-Dobson Circulation' conventional infrared radiometry offers an established technique to observe a suite of tracers (CFC-12, N_2O, and CH_4) to cover the necessary height range, and high-resolution FTIR would enable the preferred age of air tracer (SF_6) to be observed A sub-mm limb-sounder would enable HCl to be observed instead, along with the tracer N_2O. Temperature and H_2O would also be observed by infrared radiometry, FTIR or sub-mm techniques. The shortwave scattering technique provides H_2O and could potentially contribute temperature, N_2O and CH_4.

For the desirable ('Priority B') mission extension 'Stratospheric Chemistry' conventional infrared radiometry offers an established technique to observe a suite of nitrogen oxides including $ClONO_2$ (chlorine reservoir gas) and extinction coefficient. However, BrO cannot be observed in the infrared. A sub-mm limb-sounder would enable HCl and ClO to be observed instead of $ClONO_2$, along with BrO. The shortwave scattering technique specifically covers BrO and extinction coefficient. Temperature, H_2O and N_2O would be observed by all three techniques.

Abilities to meet each of the 'Priority B' mission extensions													
Mission Extension	Observable	Shortwave Scattering				Infrared Emission				(Sub-)mm Emission			
		UT	LS	MS	US	UT	LS	MS	US	UT	LS	MS	US
'Brewer-Dobson Circulation'	SF_6	Grey	Red	Red	Red	Grey	Yellow	Yellow	Yellow	Grey	Red	Red	Red
	CH_4	Grey	Yellow	Yellow	Yellow	Grey	Green	Green	Green	Grey	Red	Red	Red
	N_2O	Grey	Yellow	Yellow	Grey	Grey	Green	Green	Grey	Grey	Green	Green	Grey
	CFC-11	Grey	Red	Red	Grey	Grey	Green	Green	Grey	Grey	Red	Red	Grey
	CFC-12	Grey	Red	Red	Grey	Grey	Green	Green	Grey	Grey	Red	Red	Grey
	H_2O	Grey	Green	Green	Yellow	Grey	Green	Yellow	Yellow	Grey	Green	Green	Green
	HCl	Grey	Red	Red	Red	Grey	Red	Red	Red	Grey	Green	Green	Green
'Stratospheric Chemistry'	Temperature	Grey	Yellow	Yellow	Yellow	Grey	Green	Green	Green	Grey	Green	Green	Green
	HNO_3	Grey	Red	Red	Red	Grey	Green	Green	Green	Grey	Green	Green	Yellow
	HCl	Grey	Red	Red	Red	Grey	Red	Red	Red	Grey	Green	Green	Green
	H_2O	Grey	Green	Green	Yellow	Grey	Green	Yellow	Yellow	Grey	Green	Green	Green
	Ext. coef.	Grey	Green	Green	Grey	Grey	Green	Yellow	Grey	Grey	Red	Red	Grey
	CH_4	Grey	Yellow	Yellow	Yellow	Grey	Green	Green	Yellow	Grey	Red	Red	Red
	N_2O	Grey	Yellow	Yellow	Grey	Grey	Green	Green	Grey	Grey	Green	Green	Grey
	$ClONO_2$	Grey	Red	Red	Grey	Grey	Green	Green	Grey	Grey	Red	Red	Grey
	BrO	Grey	Green	Green	Grey	Grey	Red	Red	Grey	Grey	Yellow	Yellow	Grey
'Tropospheric Ozone'	O_3	Yellow	Grey	Grey	Grey	Green	Grey	Grey	Grey	Green	Grey	Grey	Grey

Table 3.19 *Summary of the ability of the various instrument types to meet requirements per mission extension for the 'Priority B' mission extensions. Grey = N/A (no requirement for that altitude range); Green = Meets requirement; Yellow = Some info, but not completely meet requirements; Red = Species not available; White = Better spectroscopic data are needed.*

Abilities to meet the 'Priority C' mission extension 'Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols'													
Mission Extension	Observable	Shortwave Scattering				Infrared Emission				(Sub-)mm Emission			
		UT	LS	MS	US	UT	LS	MS	US	UT	LS	MS	US
'Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols'	Temperature	Grey	Yellow	Yellow	Yellow	Grey	Green	Green	Green	Grey	Green	Green	Green
	H_2O	Grey	Green	Green	Yellow	Grey	Green	Yellow	Yellow	Grey	Green	Green	Green
	Ext. coef	Grey	Green	Green	Grey	Grey	Green	Yellow	Grey	Grey	Red	Red	Grey
	OCS	Grey	Red	Red	Grey	Grey	Green	Green	Grey	Grey	Green	Green	Grey
	SO_2	Grey	Red	Red	Grey	Grey	Yellow	Yellow	Grey	Grey	Yellow	Yellow	Grey

Table 3.20 *Summary of the ability of the various instrument types to meet requirements for the 'Priority C' mission extension on 'Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols'. For infrared, performance of high-resolution FTS is adopted here. Grey = N/A (no requirement for that altitude range); Green = Meets requirement; Yellow = Some info, but not completely meet requirements; Red = Species not available;*

For ‘Priority C’ observational requirements, conventional infrared radiometry offers an established technique to observe, next to ozone and temperature, several major constituents. Higher infrared spectral resolution would be needed specifically for SO_2, PAN, NO or CO[19]. A sub-mm limb-sounder could cover several major constituents, though with the exception of CH_4, PAN, and extinction coefficient. The shortwave scattering technique could further contribute CH_4, CO, NO_2, and extinction coefficient and, but is less capable than emission techniques in O_3 profiling in the upper troposphere and does not cover NO_2 and CO in the mesosphere.

In summary: no single measurement technique is capable of providing observations of all desired variables for either the ‘Brewer-Dobson Circulation’, ‘Stratospheric Chemistry’ or ‘Tropospheric Ozone ‘ mission extensions (Table 3.19), nor for the ‘Priority C’ extensions with the exception of limb infrared emission potentially meeting the requirements on ‘Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols‘ (Table 3.20).

Either limb infrared (radiometry or spectrometry) or (sub-)mm wave could provide upper tropospheric ozone profiling. The infrared and mm/sub-mm techniques therefore offer considerable potential to contribute to three most desirable (‘Priority B’) mission extensions as well as to the minimum mission. Infrared (high-res spectrometry) or (sub-)mm could also provide required mesospheric observations (‘Priority C’). Shortwave limb scattering could contribute to ‘Brewer-Dobson Circulation’, ‘Stratospheric Chemistry’, although with less extensive coverage of required species than limb infrared or limb (sub-)mm. Less contribution would be possible using shortwave limb scattering to upper tropospheric ozone profiling for the ‘Tropospheric Ozone’ mission extension. Shortwave limb scattering could contribute to the ‘Priority C’ mission extensions with several required species as well as with the (spectral) extinction coefficient.

In addition to conventional infrared radiometry and high-resolution FTIR techniques, novel infrared radiometry, microFTS or LHR concepts would also be potentially applicable to temperature and additional constituents required for the mission extensions.

Over more than a decade since the launches of Odin OSIRIS, Envisat SCIAMACHY, Aura MLS and Odin SMR, technology has also advanced for both shortwave scattering and (sub-)mm, and three new satellite instrument concepts have been developed, respectively, CATS, ALTIUS and STEAM-R. Together with infrared Atmo-SAT, these concepts are of direct relevance to *Operoz* requirements for the minimum mission and extensions, along with diverse other instrument and technology developments initially for ground-based or airborne deployment, e.g. GLORIA (infrared) and MARCHALS (mm wave).

[19] NO or CO would be measurable also by gas correlation radiometry.

4 Summary and Conclusions

From the discussion of the different applications of possible data products that may be obtained in the frame of a mission monitoring stratospheric ozone at high vertical resolution, a set of objectives emerges. These objectives are driven by the requirements of the different usages of the products of such a mission. The usage includes operational services and long-term monitoring for the verification of the Montreal protocol and its amendments and adjustments, as well as the interaction between stratospheric ozone and climate.

4.1 The Minimum Mission

The minimum mission must add significant value to the existing and planned suite of operational nadir sounding missions. A mission fulfilling this requirement is an ozone-only mission monitoring the evolution of the stratospheric ozone layer globally with high vertical resolution and dense horizontal sampling at daily temporal resolution. The general mission objectives of the minimum mission are (i) to provide support to operational ozone services (CAMS, NWP) and (ii) to accurately monitor the future evolution of the ozone layer in a changing climate with anticipated further reductions in the major ozone depleting substances during the next decades (long-term monitoring). The vertical resolution needed for the minimum mission in the lower stratosphere (LS) and middle stratosphere (MS) is 1 to 2 km with a horizontal resolution of about 100 to 200 km for all relevant regions (polar, mid-latitudes, tropics). For long-term monitoring good vertical and horizontal resolution is also required for the upper stratosphere (US), but the requirements are somewhat more relaxed than in the lower and middle stratosphere (2 to 4 km vertically and 200 to 400 km horizontally). Also, the strict timeliness requirements (<3h) in the LS and MS do not apply in the US because the observations in the US are needed for long-term monitoring though not considered mandatory for the operational services. Long-term observations are needed that cover the time period of ozone recovery (through to the mid / end of this century). This calls for a series of overlapping missions.

Observational requirements for the minimum mission have been tabulated in the 'Summary of Observational Requirements' (SOR) Table (Table 2.7). The requirements tabulated in black italics in the SOR-Table refer to the *mandatory* requirements ('Priority A') and these have been copied in a shortened 'Priority A' table here (Table 4.1). Table 4.1 provides the summary of observational requirements derived for a minimum operational mission targeting stratospheric ozone at high vertical resolution. Table 4.1 combines the most stringent requirements in response to the combined mission objectives for operational services and long-term monitoring. Timeliness and update frequency in the LS and MS are determined by the requirements for the operational services, while stability and vertical coverage (i.e. including the US) are determined by the requirements related to long-term monitoring. The mandatory requirements include daily global coverage of the full stratosphere (LS, MS and US), as well as the ability to measure during polar night.

Based on demonstrated performances, preliminary assessments have been made of the different measurement techniques to address the observational requirements. Shortwave limb-scattering instruments, including OMPS-limb planned for JPSS-2 (2022+), could fulfil requirements for the minimum mission, except for regions not illuminated by the sun, which specifically include polar night. For compliance with the daily global coverage and specifically the polar night, a mission that utilised emission sounding would be the most appropriate choice. Emission measurements in either the infrared or (sub-)mm wavelength ranges could further allow a breakthrough on sampling requirements (i.e. twice per day). Note also that an observational gap is likely to appear between the present-day Suomi-NPP OMPS limb observations and the launch of JPSS-2.

Summary of Observational Requirements for a Minimum Mission Targeting Stratospheric Ozone				Timeliness: <3h Stability: 1% / 3% per decade		
Observable	Along-track sampling (km)	Horizontal coverage	Vertical resolution (km)	Vertical coverage (km)	Update frequency	Uncertainty (*)
O_3	100 / 200	Global (incl. polar night)	1 / 2	LS	12h / 24h	8% / 16% or 50 / 100 ppbv
O_3	100 / 200	Global (incl. polar night)	1 / 2	MS	12h / 24h	4% / 8% or 50 / 100 ppbv
O_3	200 / 400	Global (incl. polar night)	2 / 4	US	Daily/weekly	4% / 8%

Table 4.1 *Observational Level-2 requirements for a minimum operational mission targeting stratospheric ozone. Notation B / T with B=Breakthrough; T = Threshold. The horizontal sampling refers to the along-track sampling. Only the mandatory requirements ('Priority A') are presented.*
(*) For the uncertainty requirement the least stringent of the relative and absolute requirements apply while the minimum ozone concentrations to be observed by 'Operoz' are (100/200 ppbv) below which the layer is considered tropospheric and thus outside the required vertical domain to be covered.

There are a range of limb infrared measurement types that could potentially meet the requirements. In the simplest case, a broad-band filter radiometer measuring in less than 10 channels would suffice, and this would be based on a long heritage of limb-sounding instruments, most recently HiRDLS. Technology advances over the last decade would however allow several alternative concepts for a compact infrared solution to also be worthy of consideration for the minimum mission.

Based on demonstrated performances of Aura/MLS and Odin/SMR, and retrieval simulations for the STEAM-R concept, it is evident that a limb-sounder operating in the (sub-)mm wavelength range could potentially meet the vertical resolution and uncertainty requirements for a stratospheric ozone minimum mission. A concept derived for the minimum mission could benefit from technology developments such as those for STEAM-R. Vertical resolution is a driver for antenna size. Satellite height and frequency band would therefore be considered together with antenna and other instrument parameters to optimise a concept for the *Operoz* minimum mission.

Occultation and nadir viewing instruments have been found to be significantly less suitable for the minimum mission. In the case of solar occultation instruments, although providing high vertical resolution and highly accurate measurements, their very sparse sampling patterns mean that global coverage can be accumulated only over an extended period (typically weeks to months) and not all seasons can be observed; which is a basic requirement for the minimum mission. Occultation instruments are, however, a valuable reference standard as they achieve the highest accuracy among all space measurements of vertical ozone profiles and, thus, are well suited for validation of the entire altitude range of any limb sounder. SAGE-III instrument is planned for launch on ISS which could provide important observations for validation over its mission lifetime of about 2 years.

Although geographical sampling would be much denser in the case of stellar occultation, e.g. based on the GOMOS concept, especially if stellar ozone retrievals during daytime could be made with a similar quality as during night-time (yet to be demonstrated) , the coverage would still be less complete than for a limb scattering or limb emission instrument. Furthermore, data quality and vertical coverage would vary with the magnitude (intensity) of each star.

Nadir viewing instruments can provide data which meet horizontal sampling requirements, with daily, global coverage in the infrared and daytime-only in the shortwave, *but they are unable to meet the requirements for high vertical resolution in the stratosphere*. Nadir-viewing instruments with ozone capabilities will be available on the planned series of operational polar-orbiting (and geostationary) platforms, in Europe including IASI(-NG) and the Sentinels 4, 5, and 5p). Their horizontal sampling (across-track in particular) would complement that of a dedicated limb-sounder for stratospheric ozone monitoring. Furthermore, accurate characterisation of the ozone profile distribution by the limb-sounder would benefit the operational nadir viewing instruments' capabilities to monitor (lower) tropospheric ozone.

The requirement placed on *stability* (1% /3% per decade; breakthrough/threshold) for long-term monitoring is exceedingly stringent. To achieve this level of stability over a timescale of decades, a series of satellites is needed, with overlaps of 2 years to ensure continuity. High-quality correlative observations from the global ozone sonde network and NDACC (Network for the Detection of Atmospheric Composition Change) will need to be maintained, preferably augmented by solar occultation missions such as the planned SAGE-III.

Finally, the timeliness of the data delivery will be controlled by the satellite downlink and ground-segment, and is therefore not governed primarily by the choice of instrument type, although the degree of flexibility in orbit selection is somewhat greater for emission sounding than for solar scattering. To monitor on a decadal timescale, a series of similar satellite instruments with sufficient overlap between them is needed.

4.2 Mission Extensions

Desirable mission extensions building on the minimum mission have been identified. For these elements we distinguish between mission extensions (in terms of observational requirements) and additional mission objectives. The 'Priority B' mission extension 'Tropospheric Ozone' includes vertical coverage of the limb ozone observations into the UT and preferably an azimuth viewing capacity to provide across-track sampling. Together with the operational nadir sounders, these extensions respond to the two minimum mission objectives (operational services and long-term monitoring) but now include the monitoring of both stratospheric and tropospheric ozone, whereas the minimum mission targets stratospheric ozone only.

Two important additional mission objectives have been formulated in Section 1: 'Monitoring of geophysical variables that allow attribution of the observed ozone changes to forcings', and 'Objectives regarding the two-way interaction between stratospheric ozone and climate'. These additional mission objectives have led to a prioritization of 'Brewer-Dobson Circulation' and 'Stratospheric Chemistry' over other mission extensions. These extensions would specifically allow observed ozone changes to be attributed to, respectively, changes in dynamics and chemistry.

Three other useful mission extensions are assigned 'Priority C': 'Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols', 'Climate Impact of Troposphere-Stratosphere Transport and the Asian Monsoon' and 'Extension into the Mesosphere'. The 'Priority C' observational requirements are presented in Section 2 although they do not appear in the final 'Summary of Observational Requirements' (SOR) Table (Table 2.7). The SOR-Table presented in Section 2.4 includes both the 'Priority A' observational requirements (in black italics) and the 'Priority B' observational requirements (in green).

In Section 3 a preliminary assessment ('reality check') of the SOR-Table has been performed. No single measurement technique has been found capable of providing observations of every required observable for either the 'Brewer-Dobson Circulation' or 'Stratospheric Chemistry' extension. Limb infrared emission (radiometry or spectrometry) or limb (sub-)mm emission could provide upper tropospheric ozone. Both the limb infrared and the limb (sub-)mm techniques thus offer considerable potential to contribute to the mission extensions. Shortwave scattering limb observations could contribute to the 'Brewer-Dobson Circulation' and 'Stratospheric Chemistry' mission extensions although with less extensive coverage of the desired ('Priority B') observables than infrared or (sub-)mm, and as yet undemonstrated capability for the extension on 'Tropospheric ozone'. In addition to conventional infrared radiometry and high-resolution FTS techniques, novel infrared radiometry, microFTS or LHR concepts would be potentially applicable to temperature and additional constituents required for the mission extensions as well as the minimum mission.

As we have discussed in Section 1.4.2 the priorities could also have been set in a more general sense, namely the priorities for a high resolution limb mission for stratospheric composition (instead of mission targeting stratospheric ozone at high vertical resolution). In this more general setting the issue of climate change as well as the impact of volcanic eruptions and potentially geo-engineering would have become more prominent.

In particular, this would have led to a much higher prioritization of measurements of stratospheric water vapour and sulphate aerosols, especially in the lower and middle stratosphere. In Section 3.4 we found that both limb scattering and limb infrared emission (radiometry or spectrometry) might be capable of providing most of the required observations for the mission extension on 'Radiative Impact of Stratospheric Water Vapour and Sulphate Aerosols', while in the (sub-)mm wavelength range the small sulphate aerosols are not detected – which in turn would be an advantage of (sub-) mm wavelength range for the continuity of the operational ozone monitoring during potential conditions with high volcanic aerosol loading in the stratosphere.

4.3 Conclusion and Recommendation

The analysis and preliminary assessment in this report indicates that requirements for the Operoz ozone-only mission could potentially be met by limb-emission at infrared or (sub-)mm wavelengths or by limb-scattering in daytime only, therefore excluding observations during (polar) night.

Requirements to also profile upper tropospheric ozone and to observe additional geophysical variables of relevance to the identified mission extensions could be met to a greater extent by limb-emission in either wavelength range than by limb-scattering. Across-track capabilities could be added as a mission extension to the limb emission or limb-scattering observational techniques.

To identify an instrument concept dedicated to the *Operoz* minimum mission, or to accommodate the mission extensions, a substantial further study would be required. Other than NPP-Suomi/ OMPS-limb, the current generation of satellite limb-sounders was designed more than a decade ago. Technology developments and evolution of proposed concepts[20] over the last decade should therefore be taken into consideration, with a view to defining and optimising a compact, low cost concept for operational services and long-term monitoring and with maximum return for climate monitoring and stratospheric ozone assessments by the international science community.

[20] Relevant concepts include e.g. STEAM-R (in (sub-)mm), AtmoSAT (in infrared), CATS and ALTIUS (both in shortwave).

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Appendix A. *Definition of User Areas within Operoz*

Three user areas are distinguished in *Operoz* (see Table A.1), including (U1) the users served by the providers of the Copernicus core services, mainly the Copernicus atmosphere monitoring service (CAMS), (U2) users served by providers of non-operational long-term ozone and climate data records, and (U3) users involved in the domain of Research and Development (R&D). Users in U3 are, e.g., involved in the evolution of the services provided in U1 and U2. The R&D domain typically provide the response to advances in scientific knowledge, technology and societal demands, and/or involved in assessments, attribution and process understanding to support policy makers.

User requirements expressed in the three user areas need to be considered together for the definition of space mission objectives targeting the next decade(s). However, requirements for user area U3, including service evolution and improved assessments and scientific research are considered more demanding. The *breakthrough* requirements in *Operoz* have been defined such to target all three user areas, i.e. while the threshold requirements basically respond to the user areas U1 and U2, the breakthrough requirements include user area U3 and relate to a significant step in improving the operational services based on R&D..

User area	Priority	User area	Services and/or key products
U1	A; Threshold	Operational forecasting and reanalysis through data-assimilation	Copernicus Atmosphere Monitoring Service (CAMS) NWP
U3	A; Breakthrough	Service evolution	Present-day anticipated needs for the future evolution of the Copernicus Atmosphere Monitoring Service (CAMS) and NWP
U2	A; Threshold	Long-term monitoring	Ozone and other Climate Data Records (CDRs); continuation of present-day ozone and other climate data records
U3	A; Breakthrough	Improved policy support through assessments and attribution	Improvement on the present-day ozone and other climate data records; better support for future Scientific assessments and process understanding

Table A.1 *Three user areas (U1, U2 and U3) are distinguished in Operoz for the definition of future operational limb observations of ozone and related observables.*

User area U1: Copernicus Atmosphere Monitoring Service (CAMS) and NWP centres

Operational is here defined in the strict sense of the meteorological services of 24/7 availability and updating of quality assured data sets and forecasts. The observations for operational services are characterized by rather strict requirements on timeliness w.r.t. forecasting. The present-day MACC integrated forecasting system including data assimilation is taken as the principal backbone for the CAMS operational atmosphere services in the foreseeable future. C3S is not as well defined, but components could consist of reanalyses and Essential Climate variable time series. Long-term reanalyses however are considered part of user area U2.

User area U2: Long-term monitoring and climate data records

User needs on ozone and climate data records are non-operational in the strict meteorological sense. A Climate Data Record (CDR) is here defined as (NRC, 2004): 'A series of observations over time that measures variables believed to be associated with climate variation and change. These changes may be small and occur over long time periods (seasonal, interannual, and decadal to centennial) compared to the short-term changes that are monitored for weather forecasting. Thus a CDR is a time series of a climate variable that tries to account for systematic errors and noise in the measurements.'

Fundamental CDRs (e.g. radiances) and thematic CDRs (e.g. ozone vertical profile) have been endorsed by e.g. GCOS and WMO. No further distinction has been made based on the current status of a CDR, e.g. operational vs. developmental CDRs. There might be partial overlap with the reanalysis products in the U1 user area, also depending on the evolution of the C3S. Climate data records typically require to cover 30 years continuously.

User area U3: Service evolution, improved scientific assessment and scientific research

Present-day user requirement include foreseeable service evolutions on the medium term (here, tentatively <2020). However, on the longer term (here, tentatively, >2020) significant further evolution of the present-day monitoring services might be expected. New services might emerge as well as additional monitoring needs in society might come up. The longer term evolution of the monitoring services is intrinsically difficult to predict. Future monitoring needs will follow yet unknown advances in science and technology, as well as new developments in societal and policy demands. At the same time this longer time horizon is very relevant for the development of an operational space component because of the long time involved in the development and implementation of new space missions. Scientific research is considered to provide important components for service evolution and future assessments.

Service providers in relation to the user community for operational limb ozone observations

Important end users include international (scientific) bodies such as WMO, IPCC, WCRP, CMUG, EEA, as well as regional and national operational centers and institutions. Individual users in the research domain typically will make use of the services, although some researchers might prefer to use the raw satellite observations (radiances) for their analyses. Although individual researchers do not provide user requirements directly, their indirect advice, e.g. through international scientific bodies, is important to enhance scientific process understanding, to help define the required observational needs for future scientific assessments and to help define the desired long-term evolution of the monitoring services.

The U1 and U2 service provider's observational needs for present-day core and downstream monitoring services are driven by the needs of the end users of the services. Because service providers add value to the observations these providers principally have the required knowledge to define the observational service needs. End users are less well equipped and typically care most about the (overall) quality of the service and less about the service machinery.

Within *Operoz* user requirements such as presented in Section 1 therefore refer to high-level requirements that reflect both user and end-user needs and are driven by specific space mission objectives. Even though user requirements could include specific quantitative requirements on pre-selected data products, user requirements should typically refrain from specific geophysical observational requirements. Observational requirements such as presented in Section 2 are specific in terms of geophysical products and derive directly from the user requirements though are to be defined by service providers. Observational requirements are assumed to obey the laws of physics and should not be technologically ignorant, though should refrain from considerations on specific technological implementation options and performance of potentially available observational techniques.

Figure A.1 provides a complete overview of the user and data community finally serving end-user needs, with on the bottom of the pyramid the general public.

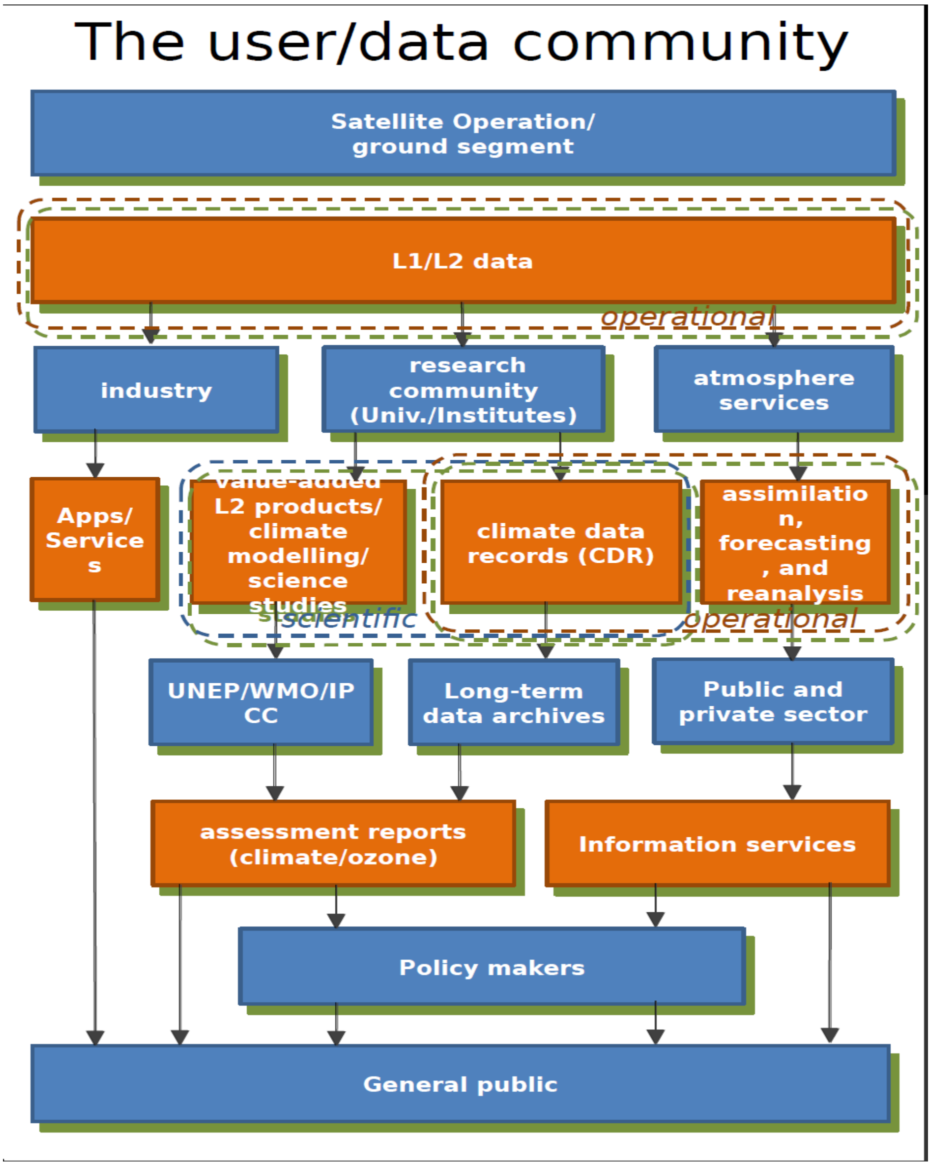

Figure A.1 *The user/data community for an operational mission targeting stratospheric ozone with high vertical resolution.*

Appendix B. *Impact of Upper Stratospheric Ozone on the Derived Tropospheric Ozone Column*

The tropospheric ozone column can be retrieved by subtracting the stratospheric ozone column from a limb sounder from the total ozone column retrieved by a collocated nadir sounder. If a limb sounder measures ozone only up to 30 km, the question arises how the missing stratospheric ozone above 30 km may introduce an error in the tropospheric ozone column when using limb-nadir matching.

This has been investigated using an available ozone profile climatology, here the climatology from Lamsal et al. (2004) as available from http://www.iup.uni-bremen.de/gome/o3climatology. This profile climatology classifies ozone profiles according to zonal bands (tropics, middle and high latitudes in each hemisphere), seasons (winter/spring and summer/fall in extra-tropics), and total ozone. This profile climatology has been constructed by combining ozone sondes and satellite occultation data (SAGE II and POAM III) to cover altitudes from the ground to 60 km. Figure AB.1 shows the various ozone profiles from this climatology

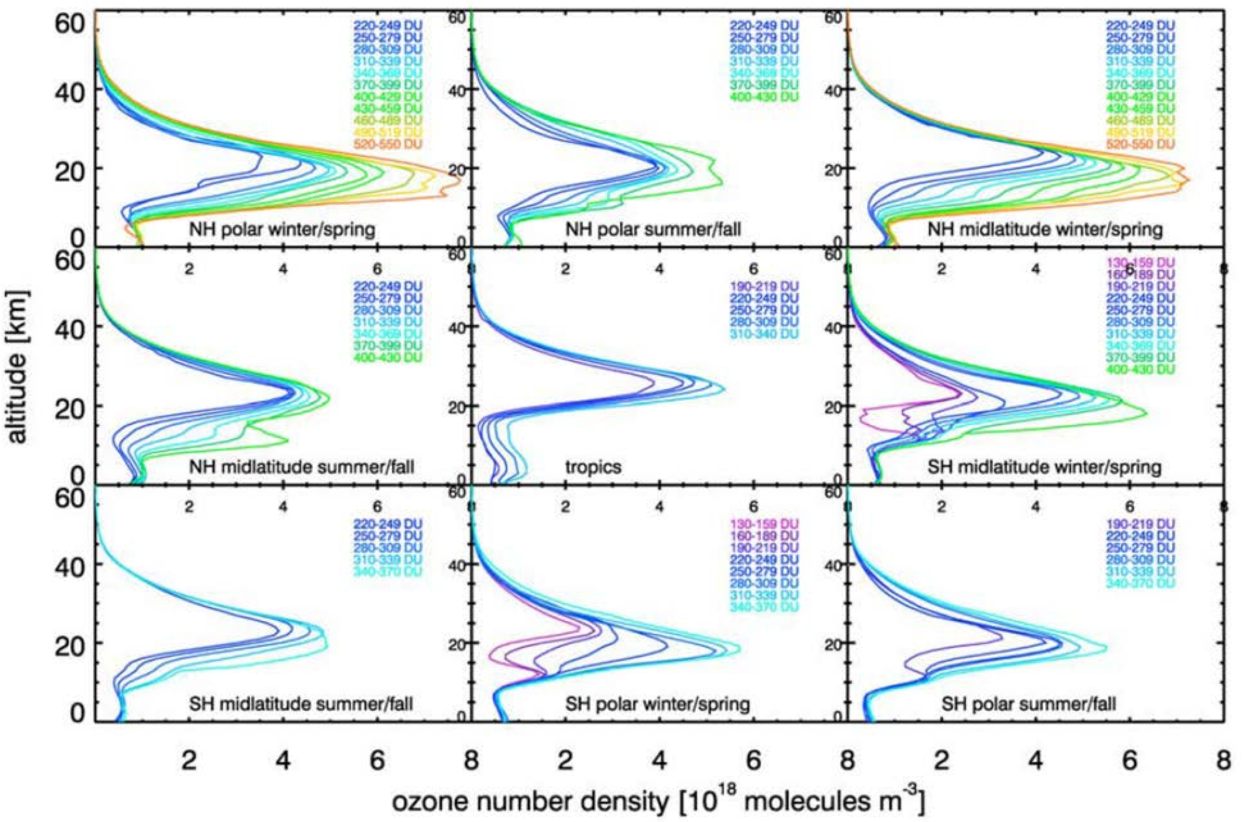

Figure AB.1 *Climatological ozone profiles from Lamsal et al. (2004).*

From these climatological profiles, the stratospheric ozone column (SOC) above 30 km and tropospheric ozone (TOC) were determined. In order to determine the tropopause the temperature climatology derived from the temperature data that were either measured by the ozone sondes or used in the satellite ozone retrievals was used (Lamsal et al., 2004). The tropopause height was determined using the WMO definition based upon lapse rates and the ozone profiles integrated up to the thermal tropopause for deriving TOC. The results for SOC above 30 km and TOC are shown in Figure AB.2 as a function of total ozone. It is feasible to estimate SOC above 30 km by assuming a constant ozone volume mixing ratio and using a standard atmosphere (air density from the US standard atmosphere). The difference of the estimated SOC to the climatological SOC (ΔSOC) is shown as well.

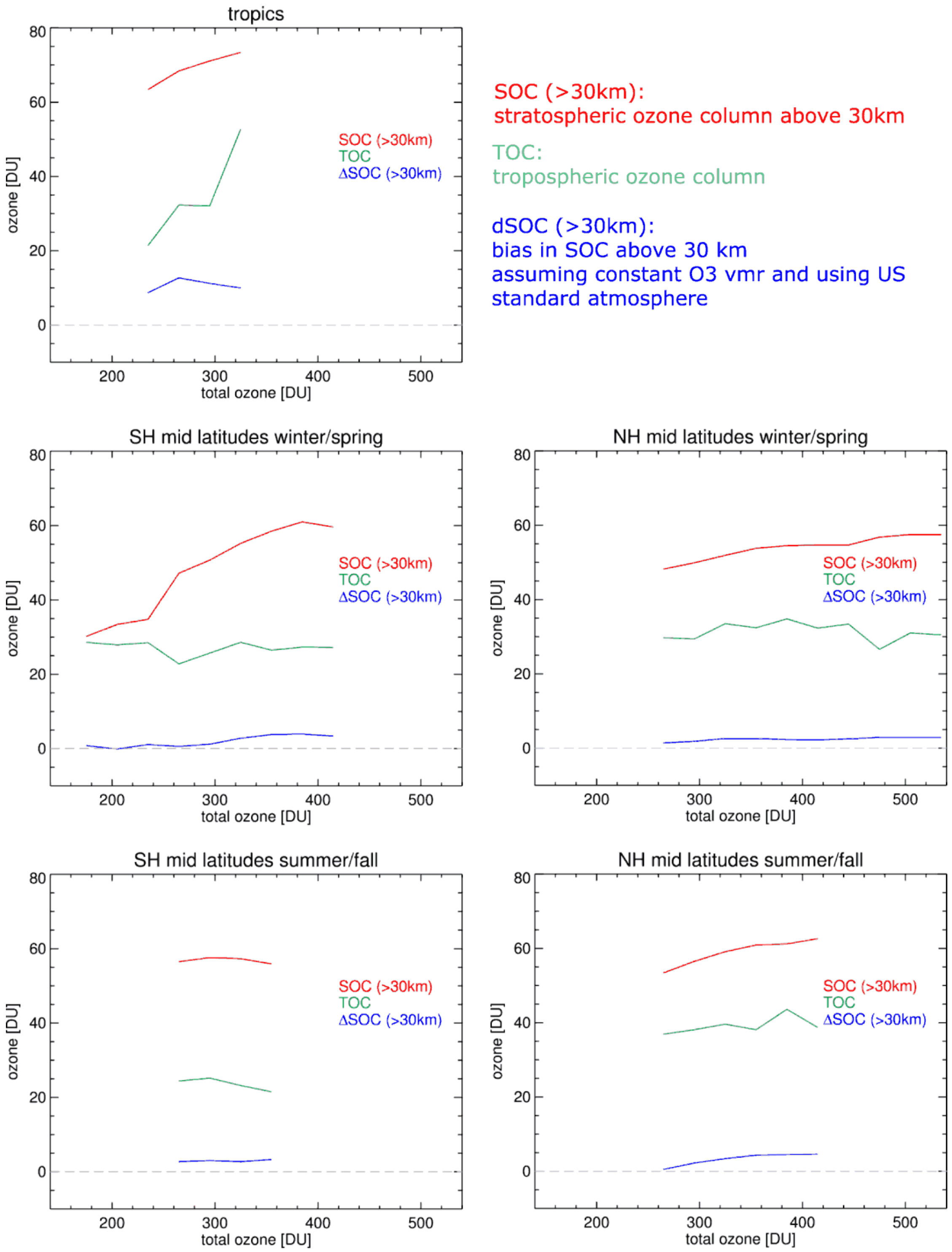

Figure AB.2 *Stratospheric ozone columns (SOC) and tropospheric ozone columns (TOC) as derived from the Lamsal et al. (2004) ozone profile climatology (Fig. BOX1). Top panel: tropics; middle panel: middle latitudes in the SH (left) and NH (right) in winter/spring; bottom panels: same as the middle panels but for summer/fall.*

In most cases the SOC above 30 km is about 60 DU, roughly 20% of the total ozone column. Tropospheric ozone (here mainly background ozone) is on the order of 30 DU, which is about 10% of the total ozone column, except for the NH summer/fall where values are closer to 40 DU. In all cases SOC above 30 km is larger than TOC, which means that the upper stratosphere is important when determining the ozone column above the tropopause. It is, however, conceivable to estimate the missing SOC above 30 km by extending the ozone profile to upper altitudes assuming a constant ozone volume mixing ratio and air density from standard atmospheres. The bias between the estimated upper stratospheric ozone column to the observed one (as derived from the ozone profile climatology) is shown as ΔSOC in Figure AB.2 and can be considered as an error in the total SOC if no measurements are available above 30 km. In the extra-tropics this bias is about 5 DU (about 15% of TOC), however, in the tropics this value can reach 10 DU (30-50% of the TOC).

Upper stratospheric ozone from limb sounders is, thus, important for achieving the highest possible accuracy in tropospheric ozone when using the limb-nadir matching technique or to constrain tropospheric ozone in data assimilation. The error in total SOC as calculated here provides rather a lower limit as the ozone profiles used for the calculation are averages over large samples. It is very likely that the uncertainties in TOC will be even larger for individual measurements and much smaller sample averages.

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