

# Exploitation of the Mesosphere (MesosphEO)



## User Requirement Document (URD)

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### DOCUMENT CHANGE RECORD

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1	0	30/01/2015	First draft of the document
2	0	26/02/2015	Rewrite of the document
2	1	10/03/2015	Minor revision; added requirements for N <sub>2</sub> O and OH
2	2	26/03/2015	Added requirement for retrieval sensitivity quantifier

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# 1 Introduction

## *1.1 Purpose*

This User Requirement Document (URD) of the MesosphEO project is summarising the user requirements for mesospheric data products. Information is required regarding the vertical and horizontal (spatial) distribution and temporal evolution of data products, like temperature, ozone, water vapour, methane, nitrogen oxides, metallic species, and polar mesospheric clouds.

The user requirements are defined from the point of view of climate modellers based on science needs independent of constraints such as spatial resolution, accuracy and observation frequency established by existing observational data sets. In this sense, the URD reflects what is needed in terms of observational data to achieve certain science goals, e.g. validation of long-term trends in climate models by observation. The scientific rationale behind the selection of the requirements is given as appropriate throughout the document.

## *1.2 Scope*

The scope of the URD is defined in relation to other project documents, most notably the project proposal. The user requirements include per science case and product type the quantitative data requirements, including horizontal resolution, vertical resolution, altitude range, observation frequency, local solar time resolution, time period, and accuracy. It also includes a clarification (rationale) for the given requirements for traceability. References are given where required accuracies are constrained by the goal to resolve or validate certain features seen in model data or existing observations.

## 2 Rationale for creating mesospheric climatologies

In recent years the science argument for creating mesospheric climatologies has become considerably stronger. On the one hand, the availability of a new generation of ‘high-top’ climate models generated increasing demand for mesospheric observed data sets needed for the model validation. In response to this demand, efforts are undertaken in homogenization and quality assessment of existing data to facilitate access. On the other hand, coupling to other regions of the atmosphere is still poorly understood. More and in some cases better observed data are needed to identify and study processes which couple the mesosphere to the troposphere and stratosphere, as well as to the thermosphere. Key science questions are:

- What is the mean state of the atmosphere from 40 to 110 km?
- What are the trends and decadal (solar cycle) variations?
- What is the mesospheric response to variability in waves originating in the lower atmosphere?
- What is the mesospheric response to impulsive solar events and how does it propagate downward?

Answering these questions requires studying atmospheric parameters (e.g. temperature, concentrations of trace gases) at different spatial and temporal scales ranging from long-term trends (several decades) to mesospheric responses to e.g. solar flares which happen on the scale of few hours. Trends are known mostly qualitatively, not quantitatively. Specifying trends in various parameters and studying various finer details of trend behaviour are tasks of current and future research. Certainly this would require long-term mesospheric observations in the order of 30 years, i.e. three solar cycles. Due to lack of such long-term observations, a combined study with model results derived from multi-decadal simulations could help to close this gap a bit. A prerequisite for these combined studies is the model validation on the basis of global observations.

The agreement between observations and models is still only qualitative for many parameters. Reducing the quantitative discrepancy between observed and simulated trends is of major importance. It will result in better understanding of mechanisms responsible for trends, but also deliver insight into processes which couple the mesosphere to the lower atmosphere and vice versa. A major coupling mechanism is energy and impulse transport via atmospheric waves. The key problem here is to identify trends in atmospheric wave activity in particular and atmospheric dynamics in general. Studying the mesospheric response to variability in waves propagating up from below is a task of current research. It is expected that trends in wave activity are of a complex spatial pattern.

The mesospheric response to impulsive solar events (e.g. energetic particle precipitation) is another task of current and future research. It is expected that long-term global observations provide significant contributions to assessment of the role of these impulsive events in climate studies. Of major importance is the question how mesospheric disturbances created by impulsive events propagate downward and affect the lower atmosphere. Simulations could help to investigate downward transport and horizontal distribution of reactive trace gases.

A wide range of specific requirements on observed data can be derived from research topics listed above. Some of these requirements are mutual exclusive. For instance, gravity wave studies require individual temperature profiles but can tolerate relatively large uncertainties in

estimated temperature. Temperature trend studies, on the other hand, may work with monthly averages but require high accuracy and stability. In order to disentangle requirements and, most important, to make requirements compatible with each other, science topics are grouped into five separate science cases:

- Mesospheric mean state
- Trend, interannual variability, and solar cycle
- Diurnal variation, planetary waves, stratospheric warmings and process studies
- Gravity waves
- Impulsive event studies

A set of specific requirements on observed data is defined for each science case in section 3.

Requirements are defined based on science needs independent of constraints such as e.g. sensor resolution and observational frequency established by existing observed data sets. In some cases these requirements match the constraints of existing data, while most often constraints are exceeded. This discrepancy can be interpreted as demand for new observation capabilities and specifications for future satellite missions can be derived from requirements listed in section 3.

### **Selection of trace gases and metallic species**

Water vapor is the most efficient greenhouse gas. It plays an important role in ozone chemistry and its presence in the upper mesosphere is a prerequisite for the formation of polar mesospheric clouds. Water vapor is transported by the circulation and is thus a suitable tracer for dynamic processes. At higher altitudes, it is destroyed by photolysis from solar Ly- $\alpha$  radiation. The stratospheric source of water vapor, apart from vertical transport, is the oxidation of methane. Methane, a long-lived and well-mixed trace gas is biologically produced. Production rates increased due to anthropogenic activities. Another trace species of anthropogenic origin is carbon monoxide. Due to its long lifetime, it is often used as a tracer for polluted air masses. In the mesosphere, carbon monoxide is produced by photolysis of carbon dioxide. Carbon dioxide is an efficient greenhouse gas with strong impact on the energy budget of the atmosphere due to emission of infrared radiation. Also important for the energy budget is atomic oxygen. It is produced in the thermosphere by photo-dissociation of molecular oxygen and has a long lifetime in the upper mesosphere. Photo-dissociation of molecular oxygen is, by a large margin, the most significant heating process in the thermosphere.

The most important species regarding the atmospheric structure is ozone, which is the major source of heat in the middle atmosphere due to absorption of UV radiation. Ozone is destroyed in the stratosphere by catalytic processes driven by nitrogen oxides NO and NO<sub>2</sub>, while the most important catalyst in the mesosphere is HO<sub>x</sub>. Nitrogen oxides are produced in the thermosphere by auroral electrons and also in the mesosphere and upper stratosphere by processes related to energetic particle precipitation, e.g. during solar proton events and magnetic storms. In polar winter, the long lifetimes of nitrogen oxides coupled with downward transport inside the polar vortex facilitates destruction of stratospheric ozone. Thus NO<sub>x</sub> can connect the mesosphere-lower thermosphere region to the lower stratosphere.

Concerning metallic species, sodium is the so far best characterized species. Observations and modeling of metallic species can be used to derive the influx of meteoric dust particles.

## **Atmosphere dynamics**

The most important variables for studying atmosphere dynamics are temperature and wind. Temperature data products will be produced within the MesosphEO project and requirements are specified in Section 3. Wind is not included in the MesosphEO target list for the sole reason that so far there are very few satellite-based observations of wind in the mesosphere, and none of these observations cover the entire mesosphere. The lack of data notwithstanding, for the model validation wind information is equally important. The climate community wants to highlight the need for observed wind data.

## 3 Data requirements for the model validation

### 3.1 Introduction

This section briefly discusses five science cases and resultant requirements on observed data sets from the perspective of climate modellers. Requirements are defined independently of constraints established by existing data sets or performance data of existing or future satellite instruments. In ignoring these constraints, the resulting requirements are purely driven by science needs and can thus be regarded as baseline requirements for achieving certain science goals. By nature, this theoretical point of origin includes the “want everything” attitude which leads to requirements that usually can’t be met in reality. In order to converge toward performance characteristics of typical (future) satellite instruments, defined requirements are relaxed as much as possible without compromising science goals.

Requirements common to all science cases are defined in Section 3.2, while specific requirements are stated individually for each science case in Sections 3.3 – 3.8. Justifications for specific requirements are given whenever these requirements are not obvious results of a particular science problem. This mainly concerns the accuracy of observations which are often defined in the context of estimated trends and variability in certain atmospheric parameters. In this case, e.g. the estimated trend (taken from models or observations, in some cases both) is used as baseline and the accuracy of a given climate variable is chosen such that the trend is significant. This concept breaks down if the estimated trend is zero or if there is zero estimated variability. Accuracies are then defined as fraction of the peak value instead.

### 3.2 Common requirements

Observed data sets produced within the MesosphEO project provide vertically resolved products (limb sound profiles) with a global coverage. Each data value is required to have an error bar. For instance, in the case of temperature (expressed in K, T) the error will be given as a delta temperature value in K ( $\delta T$ ), such that  $T \pm \delta T$  represents a 68% confidence interval. A similar error bar will be given for the mixing ratio or concentration in case of trace gases and metal species. Data values will be organized along a vertical coordinate which is specified in both geometric altitude and pressure levels. The spacing of vertical levels reflects the vertical extent of typical features in the atmosphere. Major changes in the vertical domain happen typically in one scale height (approximately 7 km). Resolving features on this scale requires 2-3 independent observations per scale height, i.e. a vertical spacing of 3 km and 2-3 grid points per scale height, respectively. Some science goals e.g. gravity wave studies require a finer vertical spacing and more stringent requirements are defined for those studies.

#### **Time period**

Requirements for the time period covered in observed data sets are generally driven by the need to analyse a certain minimum amount of data in order to find a significant trend or averaging enough data in epoch analyses in order to determine a statistically significant signal. The longest relevant period is the 11-year solar cycle. There is a broad consensus within the climate community that reliable trend analyses should cover continuously at least three solar cycles. Based on this, the goal for observed data sets produced within the

MesosphEO project is 30 years. The requirement is deliberately formulated as goal because the typical lifetime of satellite missions is much shorter, and for some analyses it is sufficient if data are available for a minimum of 5 years in a given phase of the solar cycle.

### Averaging kernels

A major role in the model validation is attributed to averaging kernels used in retrievals. Because these kernels define the weighting of information content of retrieval parameters, knowledge of the kernels is essential when comparing model simulations to observational data. For this reason data sets produced within the MesosphEO project are required to contain a representation of the retrieval averaging kernels.

### A priori information

A priori information used in retrievals is crucial for the model validation in case the observed data is dominated by this information rather than actual observations. Knowledge of the a priori data is of particular importance if the data originates from models, as this may explain why the model comparison shows good agreement with one particular model while there may be large discrepancies with other models. For traceability the a priori information shall be either included in the observed data sets or made available as separate data sets which are then referenced within the observed data sets.

### Retrieval sensitivity

A numerical quantifier characterizing the retrieval sensitivity is necessary in order to assess the information content of observational data. Data products created within the MesosphEO project are required to have a numerical quantifier for each data value. A threshold value which defines a lower limit is to be included in the data sets.

### Quality flags

Quality flags are essential ingredients for automatic data selection and quality control in the model validations. Observed data sets produced within the MesosphEO project are required to include quality attributes assigned to each data value. Quality attributes will contain the following quality flags:

Flag	Exclusive	Meaning
High quality	Yes	High quality data; can be used without limitations
Bias	No	Fully characterized bias but otherwise high quality data
Contaminated	No	Contaminated data, e.g. problems with the instrument, unspecified biases
Experimental	No	Experimental (not validated) retrieval
Missing	Yes	Missing data

The middle column in the above table indicates whether flags are exclusive or can be combined with other flags.

### 3.3 Requirements for mesospheric mean state

The science case “Mesospheric mean state” calls for data products which allow the characterization of the mean state of the atmosphere, i.e. the state of the atmosphere in absence of trends, inter-annual variations, and diurnal variations. Separating the background from these disturbances requires sampling of observational data with high enough spatial and temporal resolution. Required accuracies for temperature, trace gases and metallic species are derived from expected latitudinal gradients (north-south difference, abbreviated N-S difference) where possible. In case there is no distinct latitudinal variation, one percent of the maximum concentration value between 60 and 90 km altitude is defined as required accuracy instead. Resultant requirements are listed in the following tables.

#### Requirements for temperature: *mesospheric mean state*

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Separating background from tides; (Regional) Mesospheric temperature trends	Latitude: 3 deg Longitude: 6 deg
Vertical resolution	(Regional) Mesospheric temperature trends	3 km 2-3 grid points per scale height
Altitude range	(Regional) Mesospheric temperature trends; seasonal cycle/ variability	40-110 km
Observation frequency	Seasonal cycle/ variability; short-term variability	3 days
Local solar time resolution	Separating background from diurnal variations	3 hours
Time period	Separating background from solar cycle effects and trends	As much as possible; goal 30 years; minimum 5 years in given phase of the solar cycle
Accuracy	Resolve latitudinal gradients and seasonal variations	3 K (Marsh et al., 2013a; 10% of mean N-S-difference)

**Requirements for H<sub>2</sub>O, CH<sub>4</sub>, CO, CO<sub>2</sub>, O, O<sub>3</sub>, NO, NO<sub>2</sub>, N<sub>2</sub>O, OH: *mesospheric mean state***

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Separating background from tides; latitudinal gradients	Latitude: 5 deg Longitude: 15 deg
Vertical resolution	(Regional) Mesospheric trends; resolve layers, e.g. night O <sub>3</sub> layer	3 km 2-3 grid points per scale heights
Altitude range	(Regional) Mesospheric trends; seasonal cycle/ variability	40-110 km
Observation frequency	Seasonal cycle/ variability	Monthly means
Local solar time resolution	Separating background from diurnal variation	1 hour
Time period	Separating background from solar cycle effects and trends	As much as possible; goal 30 years; minimum 5 years in given phase of the solar cycle
Accuracy	Resolve latitudinal gradients and seasonal variations	H <sub>2</sub> O: 200 ppbv (Seele and Hartogh, 1999; 50% inter-annual monthly variance) CH <sub>4</sub> : 20 ppbv (Schmidt et al., 2006; 10% of N-S-difference) CO: 200 ppb (Smith et al., 2011; 1% of maximum value, weak latitudinal gradient) CO <sub>2</sub> : 1 ppm (Smith et al., 2011; 10% of N-S-difference) O: 10 <sup>-4</sup> vmr (Smith et al., 2011; 1% of maximum value) O <sub>3</sub> : 50 ppbv (Schmidt et al., 2006; 1% of maximum value, 10% N-S-difference) NO: 10 <sup>-7</sup> vmr (Smith et al., 2011; 1% of maximum value) NO <sub>2</sub> : 0.1 ppbv (de Grandpré, 1997; 1% of maximum value)

		<p>N<sub>2</sub>O: 10 ppbv (Jin et al., 2009; 10% of N-S-difference)</p> <p>OH: 0.1 ppbv (Shapiro et al., 2012; 1% of maximum value)</p>
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**Requirements for Na, Mg, Mg<sup>+</sup>, Fe: mesospheric mean state**

Quantity	Driving Research Topic	Requirement
Horizontal resolution	(Regional) trends; separating background from tides; latitudinal gradients	Latitude: 5 deg Longitude: 15 deg
Vertical resolution	(Regional) Mesospheric trends	5 km 1-2 grid points per scale height <i>At peak of layer:</i> 1 km 5-6 grid points per scale heights
Altitude Range	(Regional) Mesospheric trends; topside studies	70-150 km
Observation frequency	Seasonal cycle/ variability	Monthly means
Local solar time resolution	Separating background from diurnal variations	1 hour
Time period	Separating background from solar cycle effects and trends	As much as possible; goal 30 years; minimum 5 years in given phase of the solar cycle
Accuracy for mixing ratio	Resolve latitudinal gradients	Na: 100/cm <sup>3</sup> (Fussen et al., 2010; 10% of N-S-difference) Mg: 50/cm <sup>3</sup> (Langowski et al., 2015; 2% of maximum value, 10% of N-S-difference) Mg <sup>+</sup> : 400/cm <sup>3</sup> (Langowski et al., 2015; ~10% of maximum value, 10% of N-S difference) Fe: 1000/cm <sup>3</sup> (Feng et al., 2013; 10% of N-S-difference)

### 3.4 Requirements for trends, inter-annual variability, and solar cycle studies

Trend analyses, analyses of inter-annual variability, and solar cycle studies share the common characteristic that analyses are generally based on long time series. There is broad consensus in the climate community that time series should cover at least three solar cycles (30 years). Because the lifetime of typical satellite missions is much shorter, it is expected that data from different instruments have to be merged. The most critical requirement is therefore stability of observations rather than accuracy. Values specified in the tables below are derived from expected trends and solar cycle effects where possible.

Requirements for the horizontal resolution follow from the wish to resolve regional trends (based on geographic sectors) such as trends in gravity waves (e.g. orographic gravity waves). Moreover, polar vortex related effects and auroral forcings are confined to high latitudes, and sufficiently high latitudinal resolution is needed to resolve these features.

#### Requirements for temperature: trends, interannual variability, and solar cycle studies

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Polar vortex dynamics; auroral forcings; trend in gravity waves sources;	Latitude: 5 deg Longitude: 45 deg
Vertical resolution	Mesospheric temperature trends	3 km 2-3 grid points per scale height
Altitude range	Mesospheric temperature trends	40-110 km
Observation frequency	Seasonal variability; inter-annual variability	Monthly means
Local solar time resolution	Separating background from diurnal variation; trends in diurnal variability	3 hours
Time period	Trends; solar cycle effects; inter-annual variability	As much as possible; goal 30 years; minimum 5 years in given phase of the solar cycle
Stability	Trends	0.5 K/decade (Beig et al., 2006; 30% of expected trend)

**Requirements for H<sub>2</sub>O, CH<sub>4</sub>, CO, CO<sub>2</sub>, O, O<sub>3</sub>, NO, NO<sub>2</sub>, N<sub>2</sub>O, OH: trends, inter-annual variability, and solar cycle studies**

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Polar vortex dynamics; auroral forcings	Latitude: 5 deg Longitude: 45 deg
Vertical resolution	Mesospheric trends	3 km 2-3 grid points per scale heights
Altitude range	Mesospheric trends; interannual variability	40-110 km
Observation frequency	Seasonal variability; interannual variability	Monthly means
Local solar time resolution	Separating background from diurnal variations and photochemical effects; trends in diurnal variability	1 hour
Time period	Trends; solar cycle effects	As much as possible; goal 30 years; minimum 5 years in given phase of the solar cycle
Stability	Trends; solar cycle effects	25% of expected trend or variation due to solar cycle; values per decade H <sub>2</sub> O: 100 ppbv (von Zahn, 2004, Langematz et al., 2005) CH <sub>4</sub> : 3 ppbv (Schmidt et al., 2006) CO: 100 ppbv (Forkman et al., 2012; 10% of interannual variation) CO <sub>2</sub> : 3 ppm (Akmaev et al., 2000) O: 50 ppm (Schmidt et al., 2006) O <sub>3</sub> : 5 ppbv (Langematz et al., 2005) NO: 50 ppbv (Schmidt et al., 2006) OH: 1 ppbv (Grygalashvyly et al., 2009)
Accuracy	Trends; solar cycle effects	NO <sub>2</sub> , N <sub>2</sub> O: No trend or solar cycle studies found, therefore same requirement as <i>mean state</i> : NO <sub>2</sub> : 0.1 ppbv N <sub>2</sub> O: 10 ppbv

**Requirements for Na, Mg, Mg<sup>+</sup>, Fe: trends, interannual variability, and solar cycle studies**

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Polar vortex dynamics (e.g. response to stratospheric warmings); latitudinal variations in altitude of layer peak	Latitude: 5 deg Longitude: 45 deg
Vertical resolution	(Regional) Mesospheric trends; variability in altitude of layer peak	5 km 1-2 grid points per scale height <i>At peak of layer:</i> 1 km 5-6 grid points per scale heights
Altitude range	(Regional) Mesospheric trends; topside studies	70-150 km
Observation Frequency	Seasonal variability; interannual variability	Monthly means
Local solar time resolution	Separating background from diurnal variations and photochemical effects	1 hour
Time period	Trends; solar cycle effects	As much as possible; goal 30 years; minimum 5 years in given phase of the solar cycle
Accuracy	Trends; solar cycle effects	No trend or solar cycle studies found, therefore same requirements as <i>mean state</i> : Na: 100/cm <sup>3</sup> (Fussen et al., 2010; 10% of N-S-difference) Mg: 50/cm <sup>3</sup> (Langowski et al., 2015; 2% of maximum value, 10% of N-S-difference) Mg <sup>+</sup> : 400/cm <sup>3</sup> (Langowski et al., 2015; ~10% of maximum value, 10% of N-S difference) Fe: 1000/cm <sup>3</sup> (Feng et al., 2013; 10% of N-S-difference)

**Requirements for polar mesospheric clouds: *trends, interannual variability, and solar cycle studies***

Quantity	Driving Research Topic	Requirement
Horizontal resolution	(Latitudinal) Trends and interannual variability	Latitude: 10 deg Zonal average
Vertical resolution	Albedo and occurrence frequency studies	Column integral
Observation frequency	Trends, interannual variability; solar cycle effects	Seasonal
Local solar time resolution	Separating background from diurnal variations	1 hour
Time period	Trends; solar cycle effects	As much as possible; goal 30 years; minimum 5 years in given phase of the solar cycle
Accuracy	Trends	10% of expected trend Occurrence frequency: 0.01 % (Fiedler et al., 2011; Shettle et al., 2009) Albedo: $5 \times 10^{-9}$ (DeLand et al., 2007)

### ***3.5 Requirements for diurnal variation, planetary waves, stratospheric warmings, and process studies***

The common theme of diurnal variation studies, planetary wave studies, and stratospheric warming studies is variability on the time scale of few days. The observation frequency is here defined by planetary waves and diurnal variations. Both show significant day-to-day variability in phase and amplitude. Three days is the maximum time period, as longer averaging times result in significantly reduced perturbation amplitudes.

The horizontal resolution is driven by the wish to resolve regional variations (per sector) in planetary wave amplitudes and diurnal variations. Also, stratospheric warmings are confined to high latitudes. Resolving effects associated with stratospheric warmings thus requires a sufficiently high resolution in latitude. In the northern hemisphere, major stratospheric warmings occur about once every second year. A minimum of 10 years is required in order to capture a sufficiently large number of events.

Polar mesospheric cloud process studies take on a special position. In order to gain insight into microphysical processes, high resolution observations are required. Suitable data sets are generally available only for selected campaigns. The required observation frequency is one day with one hour local solar time binning.

Requirements for the accuracy of observations are derived from estimated diurnal variations and mean planetary wave amplitudes where possible. These values represent the smallest perturbation amplitudes, as perturbations resulting from the mesospheric response to stratospheric warmings are generally larger.

**Requirements for temperature: *diurnal variation, planetary waves, stratospheric warmings, and process studies***

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Polar vortex dynamics; auroral forcings; trend in gravity waves sources, e.g. orographic waves	Latitude: 5 deg Longitude: 45 deg
Vertical resolution	Tides; planetary waves	3 km 2-3 grid points per scale height
Altitude range	Mesospheric response to planetary waves and tides; mesospheric coolings associated with stratospheric warmings	40-110 km
Observation frequency	Short-term variability; variability of tides; variability of planetary waves; development of the mesospheric cooling in response to stratospheric warmings	3 days
Local solar time resolution	Diurnal variation	3 hours
Time period	Stratospheric warmings	As much as possible; goal 30 years; minimum 10 years
Accuracy	Vertical propagation of planetary waves; diurnal variation	50% of mean planetary wave amplitude (Limpasuvan and Wu, 2003) Lower mesosphere: 1 K Upper mesosphere: 3 K

**Requirements for CO, CO<sub>2</sub>, O, O<sub>3</sub>, NO<sub>x</sub>: diurnal variation, planetary waves, stratospheric warmings, and process studies**

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Polar vortex dynamics; auroral forcings	Latitude: 5 deg Longitude: 15 deg
Vertical resolution	Tracer studies	3 km 2-3 grid points per scale heights
Altitude range	Tracer studies	40-110 km
Observation frequency	Short-term variability	3 days
Local solar time resolution	Diurnal variation; photochemical effects	1 hour
Time period	Stratospheric warmings	As much as possible; goal 30 years; minimum 10 years
Accuracy	Resolve diurnal variation	O: 10 <sup>-4</sup> vmr (Smith et al., 2011; 10% of temporal variation) O <sub>3</sub> : 80 ppbv (Marsh et al., 2003, Schmidt et al., 2006; 10% of temporal variation) NO: 20 ppbv (Marsh and Roble, 2002; 10% of diurnal variation at 89 km) NO <sub>2</sub> : 50 ppbv (Hauchecorne et al., 2007; 10% of Jan 2004 event) No diurnal variation studies found for CO and CO <sub>2</sub> ; therefore same requirements as <i>mean state</i> : CO: 200 ppb (Smith et al., 2011; 1% of maximum value) CO <sub>2</sub> : 1 ppm (Smith et al., 2011; 10% of N-S-difference)

**Requirements for Na, Mg, Mg<sup>+</sup>, Fe: diurnal variation, planetary waves, stratospheric warmings, and process studies**

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Mesospheric response to stratospheric warmings; tides	Latitude: 5 deg Longitude: 15 deg
Vertical resolution	Planetary waves, tides	5 km 1-2 grid points per scale height <i>At peak of layer:</i> 2 km 3 grid points per scale
Altitude range	Response of metal layers to planetary waves and tides; topside studies	70-150 km
Observation frequency	Short-term variability; variability of tides and planetary waves; response to stratospheric warmings	3 days
Local solar time resolution	Diurnal variation; photochemical effects	1 hour
Time period	Stratospheric warmings	As much as possible; goal 30 years; minimum 10 years
Accuracy	Resolve diurnal variation; short-term variability	Fe: 500/cm <sup>3</sup> (Yu et al., 2012; 10% of diurnal variation) Mg: 50/cm <sup>3</sup> (Langowski et al., 2015; 10% of seasonal variation) Mg <sup>+</sup> : 300/cm <sup>3</sup> (Langowski et al., 2015; 10% of seasonal variation) Na: 200/cm <sup>3</sup> (Dunker et al., 2014; variability within a few days)

**Requirements for polar mesospheric clouds: *diurnal variation and process studies (microphysics)***

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Process studies (microphysics)	2 km
Vertical resolution	Process studies (microphysics)	1 km
Observation frequency	Process studies (microphysics)	1 day; non-continuous (campaigns)
Local solar time resolution	Diurnal variation	1 hour
Time period	Process studies (microphysics)	Campaigns
Accuracy	Diurnal variation	Ice water content: $9 \times 10^{-16} \text{ cm}^3/\text{cm}^3$ (Fiedler et al., 2011, 10% of diurnal variation) Particle size distribution: Best effort Total area: Best effort

### 3.6 Requirements for gravity waves studies

Gravity wave amplitudes can be extracted from high-resolution temperature profiles. In this connection the resolvable vertical wave spectrum is limited by the vertical resolution of the temperature profile. There is broad consensus in the climate community that a lower limit of 1 km vertical wavelength is sufficient. The required vertical resolution is thus 0.5 km.

The horizontal resolution is driven by the wish to identify individual gravity wave hot spots associated with orographic features such as islands or (small) mountain ranges. In order to capture diurnal variations in gravity wave activity (e.g. convectively generated gravity waves), the same geographic region must be observed at different local times. The accuracy is derived from expected mean gravity waves amplitudes. Because gravity wave amplitudes grow with height, accuracy requirements are defined separately for the lower and upper mesosphere.

#### Requirements for temperature: *gravity waves*

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Identification of gravity wave hot spots	50 km
Vertical resolution	Resolve gravity waves with vertical wavelength of 1 km	0.5 km 14 grid points per scale height
Altitude range	Vertical propagation of gravity waves in the mesosphere	40-110 km
Observation frequency	Gravity wave amplitudes; diurnal variability of gravity wave activity	By profile; no averaging; one profile every 4 hours
Time period	Gravity wave trends; interannual cycle/ variability	As much as possible; goal 30 years; minimum 5 years
Accuracy	Gravity wave amplitudes; energy dissipation	50% of mean gravity wave amplitude (Rauhe et al., 2008) Lower mesosphere: 0.8 K Upper mesosphere: 2.5 K

### 3.7 Requirements for impulsive events studies

Impulsive event studies stand out due to the special requirements on observed data. Because events occur on the time scale of several hours to few days, a three-hour observation cycle is required in order to map the temporal evolution of the initial event and subsequent mesospheric response. The three-hour observation cycle is achieved with a local time resolution of three hours in combination with a daily observation frequency.

The driver for the horizontal resolution is the wish to independently characterize the mesospheric response to impulsive events for different geographic sectors. The minimum time period of 10 years ensures that a sufficiently large number of events suitable for statistical analyses are captured.

#### Requirements for temperature: *impulsive events studies*

Quantity	Driving Research Topic	Requirement
Horizontal resolution	Particle precipitation; auroral forcings	Latitude: 5 deg Longitude: 45 deg
Vertical resolution	(Regional) Mesospheric effects	3 km 2-3 grid points per scale height
Altitude range	Mesospheric response to impulsive events; downward propagation or response	40-110 km
Observation frequency	Evolution of the initial event and subsequent mesospheric response	Daily
Local solar time resolution	Evolution of the initial event and subsequent mesospheric response	3 hours
Time period	Variability of impulsive events; solar cycle effects	As much as possible; goal 30 years; minimum 10 years
Accuracy	Identify response to particle precipitation events	1.5 K (von Savigny et al., 2007; 50% of variation caused by particle precipitation event)

#### Requirements for CO, CO<sub>2</sub>, O<sub>3</sub>, NO<sub>x</sub>, N<sub>2</sub>O, HNO<sub>3</sub>, OH: *impulsive events studies*

Requirements for trace gases are limited to making available well characterized Level-2 data. Observations which cover polar regions are required only.

## 4 Data format requirements

All data will be made available in netCDF format and CF (Climate and Forecast) conventions for metadata will be adopted. The metadata provide a definitive description of what the data in each variable represents as well as the temporal and spatial properties of the data. The netCDF CF metadata conventions are available at: <http://cfconventions.org/>

Data values will be organized along a vertical coordinate which is specified in both geometric altitude and pressure levels.

## 5 References

- Akmaev, R. A., and V. I. Fomichev. A model estimate of cooling in the mesosphere and lower thermosphere due to the CO<sub>2</sub> increase over the last 3–4 decades. *Geophysical research letters* 27.14 (2000): 2113-2116.
- Beig, G., Trends in the mesopause region temperature and our present understanding - An update, *Phys. Chem. Earth*, 31, 3-9, doi:10.1016/j.pce.2005.03.007, 2006.
- DeLand, M.T., E.P. Shettle, G.E. Thomas, and J.J. Olivero, Latitude-dependent long-term variations in polar mesospheric clouds from SBUV version 3 PMC data, *J. Geophys. Res.*, 112, D10315, doi:10.1029/2006JD007857, 2007.
- Dunker, T., Hoppe, U. P., Feng, W., Plane, J. M., and Marsh, D. R., Mesospheric temperatures and sodium properties measured with the ALOMAR Na lidar compared with WACCM. *Journal of Atmospheric and Solar-Terrestrial Physics*, 2015.
- Feng, W., D. R. Marsh, M. P. Chipperfield, D. Janches, J. Höffner, F. Yi, and J. M.C. Plane, A global atmospheric model of meteoric iron, *J. Geophys. Res. Atmos.*, 118, 9456–9474, doi:10.1002/jgrd.50708, 2013.
- Fiedler, J., Baumgarten, G., Berger, U., Hoffmann, P., Kaifler, N., and Lübken, F.-J., NLC and the background atmosphere above ALOMAR, *Atmos. Chem. Phys.*, 11, 5701-5717, doi:10.5194/acp-11-5701-2011, 2011.
- Forkman, P., Christensen, O. M., Eriksson, P., Urban, J., & Funke, B.. Six years of mesospheric CO estimated from ground-based frequency-switched microwave radiometry at 57° N compared with satellite instruments. *Atmospheric Measurement Techniques*, (5), 2827-2841, 2012.
- Fussen, D., Vanhellemont, F., Tétard, C., Mateshvili, N., Dekemper, E., Loodts, N., Bingen, C., Kyrölä, E., Tamminen, J., Sofieva, V., Hauchecorne, A., Dalaudier, F., Bertaux, J.-L., Barrot, G., Blanot, L., Fanton d'Andon, O., Fehr, T., Saavedra, L., Yuan, T., and She, C.-Y., A global climatology of the mesospheric sodium layer from GOMOS data during the 2002–2008 period, *Atmos. Chem. Phys.*, 10, 9225-9236, doi:10.5194/acp-10-9225-2010, 2010.
- de Grandpré, J.W. Sandilands, J.C. McConnell, S.R. Beagley, P.C. Croteau, M.Y. Danilin, Canadian middle atmosphere model: Preliminary results from the chemical transport module. *Atmosphere-Ocean*, Vol. 35, Iss. 4, 1997.
- Grygalashvily, M., Sonnemann, G. R., and Hartogh, P.: Long-term behavior of the concentration of the minor constituents in the mesosphere – a model study, *Atmos. Chem. Phys.*, 9, 2779-2792, doi:10.5194/acp-9-2779-2009, 2009.
- Hauchecorne, A., J.-L. Bertaux, F. Dalaudier, J. M. Russell III, M. G. Mlynczak, E. Kyrölä, and D. Fussen, Large increase of NO<sub>2</sub> in the north polar mesosphere in January–February 2004: Evidence of a dynamical origin from GOMOS/ENVISAT and SABER/TIMED data, *Geophys. Res. Lett.*, 34, L03810, doi:10.1029/2006GL027628, 2007.

- Hervig, M., M. McHugh, and M.E. Summers, Water vapor enhancement in the polar summer mesosphere and its relationship to polar mesospheric clouds, *Geophys. Res. Lett.*, 30(20), 2041, doi:10.1029/2003GL018089, 2003.
- Jin, J. J., Semeniuk, K., Beagley, S. R., Fomichev, V. I., Jonsson, A. I., McConnell, J. C., Urban, J., Murtagh, D., Manney, G. L., Boone, C. D., Bernath, P. F., Walker, K. A., Barret, B., Ricaud, P., and Dupuy, E.: Comparison of CMAM simulations of carbon monoxide (CO), nitrous oxide (N<sub>2</sub>O), and methane (CH<sub>4</sub>) with observations from Odin/SMR, ACE-FTS, and Aura/MLS, *Atmos. Chem. Phys.*, 9, 3233-3252, doi:10.5194/acp-9-3233-2009, 2009.
- Langematz, U., J. L. Grenfell, K. Matthes, P. Mieth, M. Kunze, B. Steil, and C. Brühl, Chemical effects in 11-year solar cycle simulations with the Freie Universität Berlin Climate Middle Atmosphere Model with online chemistry (FUB-CMAM-CHEM), *Geophys. Res. Lett.*, 32, L13803, doi:10.1029/2005GL022686, 2005.
- Langowski, M. P., von Savigny, C., Burrows, J. P., Feng, W., Plane, J. M. C., Marsh, D. R., Janches, D., Sinnhuber, M., Aikin, A. C., and Liebing, P.: Global investigation of the Mg atom and ion layers using SCIAMACHY/Envisat observations between 70 and 150 km altitude and WACCM-Mg model results, *Atmos. Chem. Phys.*, 15, 273-295, doi:10.5194/acp-15-273-2015, 2015.
- Limpasuvan, V., and D. L. Wu, Two-day wave observations of UARS Microwave Limb Sounder mesospheric water vapor and temperature, *J. Geophys. Res.*, 108, 4307, doi:10.1029/2002JD002903, D10, 2003.
- Marsh, D. and R. Roble, TIME-GCM simulations of lower-thermospheric nitric oxide seen by the halogen occultation experiment, *Journal of Atmospheric and Solar-Terrestrial Physics*, 64, 8–11, doi:10.1016/S1364-6826(02)00044-5, 2002.
- Marsh, D., A. Smith, and E. Noble, Mesospheric ozone response to changes in water vapor, *J. Geophys. Res.*, 108, 4109, doi:10.1029/2002JD002705, D3, 2003.
- Marsh, D., Michael J. Mills, Douglas E. Kinnison, Jean-Francois Lamarque, Natalia Calvo, and Lorenzo M. Polvani, Climate Change from 1850 to 2005 Simulated in CESM1(WACCM). *J. Climate*, 26, 7372–7391, doi:10.1175/JCLI-D-12-00558.1, 2013a.
- Marsh, D. R., D. Janches, W. Feng, and J. M. C. Plane, A global model of meteoric sodium, *J. Geophys. Res. Atmos.*, 118, 11,442–11,452, doi: 10.1002/jgrd.50870, 2013b.
- Rauthe, M., Gerding, M., and Lübken, F.-J., Seasonal changes in gravity wave activity measured by lidars at mid-latitudes, *Atmos. Chem. Phys.*, 8, 6775-6787, doi:10.5194/acp-8-6775-2008, 2008.
- von Savigny, C., M. Sinnhuber, H. Bovensmann, J. P. Burrows, M.-B. Kallenrode, and M. Schwartz, On the disappearance of noctilucent clouds during the January 2005 solar proton events, *Geophys. Res. Lett.*, 34, L02805, doi:10.1029/2006GL028106, 2007.
- Schmidt, H., G.P. Brasseur, M. Charron, E. Manzini, M.A. Giorgetta, T. Diehl, V.I. Fomichev, D. Kinnison, D. Marsh, and S. Walters, The HAMMONIA chemistry climate model: Sensitivity of the mesopause region to the 11-year solar cycle and CO<sub>2</sub> doubling, *J. Climate*, 16(19), 3903-3931, 2006.

- Seele, C., and P. Hartogh, Water vapor of the polar middle atmosphere: Annual variation and summer mesosphere conditions as observed by ground-based microwave spectroscopy, *Geophys. Res. Lett.*, 26, 1517-1520, doi: 10.1029/1999GL900315, 1999.
- Shapiro, A. V., Rozanov, E., Shapiro, A. I., Wang, S., Egorova, T., Schmutz, W., and Peter, Th.: Signature of the 27-day solar rotation cycle in mesospheric OH and H<sub>2</sub>O observed by the Aura Microwave Limb Sounder, *Atmos. Chem. Phys.*, 12, 3181-3188, doi:10.5194/acp-12-3181-2012, 2012.
- Shettle, E. P., M. T. DeLand, G. E. Thomas, and J. J. Oliver, Long term variations in the frequency of polar mesospheric clouds in the Northern Hemisphere from SBUV, *Geophys. Res. Lett.*, 36, L02803, doi:10.1029/2008GL036048, 2009.
- Smith, A. K., R. R. Garcia, D. R. Marsh, and J. H. Richter, WACCM simulations of the mean circulation and trace species transport in the winter mesosphere, *J. Geophys. Res.*, 116, D20115, doi:10.1029/2011JD016083, 2011.
- von Zahn, U., Baumgarten, G., Berger, U., Fiedler, J., and Hartogh, P., Noctilucent clouds and the mesospheric water vapour: the past decade, *Atmos. Chem. Phys.*, 4, 2449-2464, doi:10.5194/acp-4-2449-2004, 2004.
- Yu, Z., X. Chu, W. Huang, W. Fong, and B. R. Roberts, Diurnal variations of the Fe layer in the mesosphere and lower thermosphere: Four season variability and solar effects on the layer bottomside at McMurdo (77.8°S, 166.7°E), Antarctica, *J. Geophys. Res.*, 117, D22303, doi:10.1029/2012JD018079, 2012.