LOng-LIved greenhouse gas PrOducts Performances (LOLIPOP)

User Requirements Analysis and Inventory of Satellite Products (URD)

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Document Authors	F. Fabiano (CNR-ISAC) P. Raspollini (CNR-IFAC) M. Gai (CNR-IFAC) M. Premuda (CNR-ISAC) E. Castelli (CNR-ISAC)
Document Approvers	S. Pinnock (ESA, Technical Officer)

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1 Introduction

1.1 Rationale

With ‘Other long-lived greenhouse gases’ (OLLGHGs) are collectively known a series of gases, except CO_2 and CH_4, which have a significant greenhouse effect or a strong impact on the ozone layer. Among those gases there are nitrous oxide (N_2O), sulfur hexafluoride (SF_6), and chlorocarbons such as carbon tetrachloride (CCl4) as well as groups of fluorinated species categorized as chlorofluorocarbons (CFCs), hydrochlorofluorocarbons (HCFCs), hydrofluorocarbons (HFCs), and perfluorocarbons (PFCs).

As reported in the (IPCC 2023), since 1750 the GHGs concentration increase is linked to their emissions connected to human activities. The 2019 data (IPCC, 2023), report a concentration of 410 ppm for CO_2, 1866 ppb for CH4 but also 332 ppb for N_2O. In addition, O_3 and halogenated gases are among the contributors to the GHGs increase.

In particular, the N_2O increase (23%) is similar to “the natural multi-millennial changes between glacial and interglacial periods over at least the past 800,000 years (very high confidence)” (IPCC, 2023, see Figure 2.1 of IPCC for N_2O growth). Agriculture is responsible for about 60% of the N_2O present in the atmosphere. N_2O acts as a catalyzer in the production of tropospheric O_3 and can contribute to the ozone layer depletion in stratosphere. Its global warming potential (GWP) of 298 (298 times the CO_2 GWP potential) in connection to its long lifetimes makes it a powerful GHG, (Hassan et al., 2022).

Other GHGs such as CFCs, HCFCs, HFCs, SF_6, and PFCs in the troposphere are well-monitored by surface networks. Their seasonal cycle, global trends and latitudinal gradients at the surface are well known. On the other hand, the short term and regional variability of these GHGs, as well as N_2O, is mainly located in the stratosphere where their chemical breakdown occurs. (GCOS, 2011), highlights how their study and monitoring in the stratosphere (that require limb/occultation measurements) “is needed for the assessment of radiative and dynamical feedback in the stratosphere related to composition changes.”

Most of the current anthropogenic radiative forcing is due to the increased concentration of CO_2 in the atmosphere, which is the main driver of the observed climate change in the historical period. However, N_2O and the halogenated gases (CFCs, HCFCs, ...) also contribute significantly to the radiative forcing, accounting for about 0.4 W/m^2 altogether, almost 20% of the total Radiative Forcing (RF) due to CO_2 alone (Forster et al., 2021). In terms of historical climate change, it is estimated that, of the total 1.3 K change in the global-mean surface temperature in 2019 with respect to the pre-industrial climate, about 0.1 and 0.2 K can be attributed to N_2O and the halogenated gases, respectively (Forster et al., 2021). Although less attention has been devoted to study the effects of minor GHGs, recently new studies have focused on the re-assessment of their Effective Radiative Forcing (ERF), including fast tropospheric adjustments (Hodnebrog et al., 2020), and on their impact on historical climate change (Sigmond et al., 2023). Due to their large GWP, it is important to monitor the concentrations of N_2O and halogenated gases and their role in current climate change, avoiding the risk of offsetting the difficult route towards the stabilization of climate at a safe level (Harmsen et al., 2023; Rogelj et al., 2024).

Recently, some studies reported anomalous behavior in the concentration of N_2O, some CFCs and HFCs. These include a slower-than-expected decrease in CFC-11 concentrations from 2012 to 2017, indicating a surge in global emissions, with a significant contribution from eastern China (Montzka et al., 2018; Rigby et al., 2019). Montzka et al. (2021) later reported that the anomalous CFC-11 emissions ceased during the following years and the decline went back to the 2008-12 trend, highlighting the importance of continued monitoring. Recent increased emissions of other species have also been reported, including HCFC-141b (Western et al., 2022) and various CFCs (CFC-13, CFC-112a, CFC-113a, CFC-114a and CFC-115 in Western et al., 2023; CFC-12 and CFC-113 in Lickley et al., 2021). A mismatch between reported and inferred emissions has been found for many HFCs (Velders et al., 2022). Emissions of N_2O also need to be closely monitored, since the current rate of increase of the atmospheric N_2O concentration is above the one projected by the CMIP6 scenarios (Tian et al., 2020). Despite Carbon tetrachloride (CCl_4) atmospheric abundances continue to decrease, they do it at slower rates than expected based on previous trends (UNEP report, 2024). Global CCl_4 emission estimates based on atmospheric observations averaged 44 ± 15 Gg yr–1 in both 2016 and 2020. The production of CCl_4 has increased in recent years due mainly to growing demand for feedstock use for production of HFCs, HFOs/HCFOs and perchloroethylene. Increasing CCl_4 production is likely to continue because of the increasing demand for HFO/HCFOs. Most emissions arise from CCl_4 production, handling, supply chain and use. Additional CCl_4 emissions likely arise from non-chloromethane production, such as in the vinyl chain production process, which is identified as a new potential source of CCl_4 emissions.

Regarding future projections, in the Shared Socio-economic Pathways framework (SSPs, Meinshausen et al., 2020), ozone-depleting substances follow a unique scenario compliant with the Montreal Protocol, with an immediate phase-out of the anthropogenic emissions. Other fluorinated gases (HFCs, PFCs, SF6 and NF_3) instead follow different future projections depending on the scenario, varying greatly from one scenario to the other. Meinshausen et al. (2020) observe that a more specific evaluation of single species and their potential future impact would be needed, moreover in light of the delayed phase-out. For example, Velders et al. (2022) assess the impact of different HFCs emission scenarios on future climate change, with an estimated additional warming of 0.28-0.44 °C in 2100 in the case without enforcement of the Kigali amendment to the Montreal protocol.

The Essential Climate Variables (ECVs) are biological, chemical or physical variables that characterize the Earth’s climate. ECVs contribute to the understanding and prediction of climate evolution, to mitigation and adaptation measures and to assess risk.
The current ECVs list by GCOS is composed by 55 variables (https://gcos.wmo.int/en/essential-climate-variables/). In these lists, ECVs for Atmosphere, Land and Ocean can be found.
Into the “Atmosphere-Atmospheric composition” category, Carbon Dioxide, Methane and Other Greenhouse gases are included. For all the reasons discussed above, the list of the GCOS ECVs now includes the OLLGHGs N_2O, CFCs, HCFCs, HFCs, PFCs and SF_6. However, among all the OLLGHGs ECVs, GCOS formulated the requirements for N_2O only, especially in the light of upcoming missions, but no requirement is provided for the other OLLGHGs species.

The relevance and requirements for the dataset of each of the OLLGHGs is strictly connected to their use in different applications. Thus, depending on the application, different requirements about time coverage, spatial and temporal resolution, timeliness as well as accuracy and precision are needed.

The LOng-LIved greenhouse gas PrOducts Performances (LOLIPOP) CCI+ project is one of the projects of the ESA's Climate Change Initiative (CCI). LOLIPOP is led by the Institute for Atmospheric Science and Climate (ISAC), of the National Research Council (CNR), Italy. The Science Leader is B.M. Dinelli supported by Project Manager M. Cardaci.

The LOLIPOP CCI+ project aims, among other objectives, at bridging the gap on the OLLGHGs requirements with user requirements resulting from applications in atmospheric and climate models and services.

1.2 Scope of the document

This document states users' requirements for the products of ESA's CCI LOLIPOP project.

The user requirements reported in this document, are, thus, based on peer-reviewed publications, other documents where user requirements have been formulated, and user consultation specifically performed in the frame of the project.

In addition, the document includes an inventory of available satellite data on OLLGHGs.

1.3 Structure of the document

The document is structured as follows: in Section 2, we report the outcome of the requirements already available from GCOS and the literature review of emissions, chemistry and climate models community. In Section 3 are reported the requirements obtained in the frame of the survey specifically produced in the frame of the LOLIPOP project. In Section 4 we report a summary of the inventory of satellite products [RD-2].

1.4 Reference Document

[RD-1] Inventory of OLLGHGs satellite products – Annex 2 of [D1.1 - URD]

1.5 Acronyms and Abbreviations

Abbreviation	Meaning
AerChemMIP	Aerosol Chemistry Model Intercomparison Project
AGAGE	Advanced Global Atmospheric Gases Experiment
AOGCM	atmosphere-ocean general circulation model
CCI	Climate Change Initiative
CCMI	Chemistry Climate Model Initiative
CESM	Community Earth System Model
CIMP6	Coupled Model Intercomparison Project Phase 6
CNR	National research Council
ECV	Essential Climate Variable
ERF	Effective Radiative Forcing
ESA	European Space Agency
ESRL	Earth System Research Laboratories
GCOS	Global Climate Observing System
GWP	Global Warming Potential
IFS	Integrated Forecasting System
IGAC	International Global Atmospheric Chemisry
IPCC	Intergovernmental Panel on Climate Change
ISAC	Institute of Atmospheric Sciences and Climate
LOLIPOP	Long Lived greenhouse gas PrOducts Performances
NOAA	National Oceanic and Atmospheric Administration
Obs4MIP	Observations for Model Intercomparison Projects
RFMIP	Radiative Forcing Model Intercomparison Project
SPARC	Stratosphere-troposphere Processes And their Role in Climate
SSPs	Shared Socio-economic Pathways
WACCM	Whole Atmosphere Community Climate Model
WCRP	World Climate Research Programme

2 Available Requirements

Specific user requirements can be found among the potential applications of OLLGHG datasets. Among the use for atmospheric studies we can find the assessment of satellite-based global/regional trends in GHG concentration, including an assessment of the statistical significance of the results and the monitoring of stratospheric chlorine levels and their impacts on the ozone recovery study. In modelling applications, satellite-based measurements of OLLGHGs can be used for atmospheric chemistry-climate model evaluation and data assimilation, but also to improve the knowledge in the forcings used for climate model simulations, e .g. via investigations of the uncertainty in the radiative forcing due to the uncertainties in observed 3D long-lived greenhouse gas distributions. Another recent and promising application is the emission inversion through chemistry-transport models, in order to track unreported emissions and complement emission inventories.GCOS ECV Requirements

As said in the introduction, the ECVs for the other greenhouse gases include N_2O, CFCs, HCFCs, HFCs, PFCs and SF_6 but only for the N_2O knowledge (3D distribution in ppb) the GCOS formulated the requirements. In general, the ECV requirements are expressed in terms of five criteria:

1. Spatial Resolution-horizontal and Vertical (if needed)
2. Temporal resolution (e.g. hourly, daily or annual)
3. Measurement Uncertainty (expressed in units of 2 standard deviations)
4. Stability – The change in bias over time
5. Timeliness - The time expectation for accessibility and availability of data.

For each of these requirements, a goal (**G**, above which further improvements are not necessary), breakthrough (**B**, intermediate between goal and threshold) and threshold (**T**, minimum requirement to be useful) value is presented.

The N_2O requirements, (as extracted from GCOS 245, (GCOS 2022)) from (https://library.wmo.int/viewer/58111?medianame=GCOS-245_2022_GCOS_ECVs_Requirements_#page=88&viewer=picture&o=bookmark&n=0&q= can be summarized as follows:

- Horizontal resolution 100km (**G**), 500 km (**B**), 2000km (**T**),
- Vertical resolution: 0.1 km (**G**), 1km (**B**), 3km (**T**)
- Timeliness: 1d (**G**), 30d (**B**), 180d (**T**)
- Temporal resolution: 1h (**G**), 30h (**B**), 168h (**T**)
- Uncertainty: 0.05 ppb (**G**), 0.1 ppb (**B**), 0.3 ppb (**T**)
- Stability: 0.05 ppb/decade (**G**), 0.05 ppb/decade (**B**), 0.2 ppb/decade (**T**)

These requirements on atmospheric compositions, however, are thought for future missions and may not be applicable at existing datasets from past and present missions.

In addition, GCOS provides requirements for N_2O anthropogenic emissions such as the direct one from fossil fuel use, industry, agriculture, waste, product use and the indirect ones from leaching and run-off or NOx emissions. In these cases the requirements in the units of Mg N_2O per year are:

- Horizontal resolution By country and sector (**G**), (**T**),

- Timeliness: within 1.25 years (**G**),(**T**)
- Temporal resolution: 1y (**G**), (**T**)
- Uncertainty: 40% (**G**), 80% (**T**)

Regarding anthropogenic emissions, the GCOS also formulated requirements for fluorinated gases (HFC, PFC, SF_6) originating from chemical industrial processes and product use. They are given in terms of Mg CO_2 per year and can be summarized in:

- Horizontal resolution By country and sector (**G**), (**T**),
- Timeliness: within 1.25 years (**G**),(**T**)
- Temporal resolution: 1y (**G**), (**T**)
- Uncertainty: 10% (**G**), 50% (**T**)

The N_2O GCOS requirements clearly differ for the different applications. For atmospheric applications the requirements on spatial and temporal resolutions as well as timeliness are much more stringent than the ones required for the monitoring of emissions: they go from km to country values in the spatial domain and from days to years in the temporal ones.

2.1 Usage of OLLGHGs data for climate modeling

We review here the recent literature regarding the usage of OLLGHGs data for climate modelling. In this context, the gases are considered for their global warming potential, thus entering the modelling activity as inputs to the computation of radiative fluxes in the atmosphere. Since OLLGHGs currently contribute to 20% of the total ERF due to CO_2 alone, their role is secondary but absolutely not negligible for determining the energetic balance of the system.

Currently the largest effort of the climate modelling community is represented by the activities of CMIP, the Coupled Model Intercomparison Project, now at its Phase 6 (Eyring et al., 2016). CMIP6 is organized in the contest of the activities linked with the periodic reports of the Intergovernmental Panel on Climate Change (IPCC) and is a major contributor to the policy briefs contained in the report. The last report (AR6) was published in 2021; CMIP6 saw the contribution of tenths of modelling groups around the world.

The CMIP6 protocol is constituted by various experiments:

- idealized experiments at constant forcing (pre-industrial control, abrupt 4xCO2), 150 years each;
- atmosphere-only experiment with observed concentrations of GHGs and aerosols and observed sea surface temperatures and sea-ice concentrations, from 1979 to 2014;
- coupled atmosphere-ocean historical experiment with observed concentrations of GHGs and aerosols, from 1850 to 2014;
- future scenarios, assuming different GHG concentration pathways that correspond to a set of Shared Socio-economic Pathways (SSPs), from 2015 to 2100 (extended to 2300);

The historical observed concentrations have been elaborated and distributed in a set of standardized inputs publicly available through the Input4MIP platform (https://esgf-data.dkrz.de/projects/input4mips-dkrz/).

The dataset is presented in Meinshausen et al. (2017). A total of 43 GHGs are considered in the study: "CO_2, CH_4, N_2O, a group of 17 ozone-depleting substances (ODSs) made up of 5 CFCs (CFC-12, CFC-11, CFC-113, CFC-114, CFC115), 3 HCFCs (HCFC-22, HCFC-141b, HCFC-142b), 3 halons (Halon-1211, Halon-1301, Halon-2402), methyl chloroform (CH_3CCl_3), carbon tetrachloride (CCl_4), methyl chloride (CH_3Cl), methylene chloride (CH2Cl2), chloroform (CHCl3), and methyl bromide (CH_3Br), and 23 other fluorinated compounds made up of 11 HFCs (HFC134a, HFC-23, HFC-32, HFC-125, HFC-143a, HFC-152a, HFC-227ea, HFC-236fa, HFC-245fa, HFC-365mfc, HFC43-10mee), 9 PFCs (CF_4, C_2F_6, C_3F_8, C_4F_{10}, C_5F_{12}, C_6F_{14}, C_7F_{16}, C_8F_{18}, and c-C_4F_8), NF_3, SF_6, and SO_2F_2".

The methodology used to prepare the datasets consists of three main steps:

- aggregation of existing observational data, from two main sources: the NOAA Earth System Research Laboratories (ESRL) network and the AGAGE network;
- the estimation of three quantities for the recent observational period: the global mean (as a function of time), the latitudinal gradient and the seasonality;
- the global mean is then extended backwards using ice core and firn data (before available observational data, to cover the whole historical period back to 1850).

For N_2O, AGAGE monthly station means (including pollution events) are used (Prinn et al., 1990), combined with NOAA/ESRL Monitoring Division data: this covers the 1990-2014 period. Before 1968, updated Law Dome data (MacFarling Meure et al., 2006) are used. In the period between 1968 and 1990, Law Dome data are merged with sparse observational data. For all gases, a detailed overview, comprising data sources and existing literature is provided in the supplement: https://dx.doi.org/10.5194/gmd-10-2057-2017-supplement.

As an example, we show in Figure 1 the global mean concentrations of CFC-11 as obtained by Meinshausen et al. (2017) for the historical period until 2014. Data sources are indicated in Fig. 1.

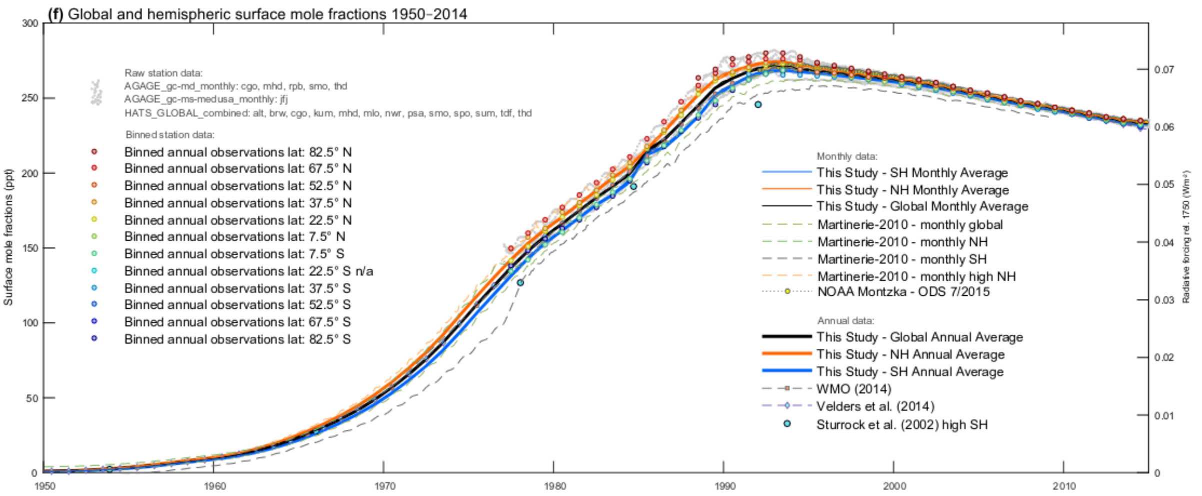


Figure 1: Global mean and latitudinal bin concentrations of CFC-11, as obtained by Meinshausen et al. (2017).

A particular point of interest is that the reconstruction made in Meinshausen et al. (2017) make use only of surface concentrations, while models need a vertical distribution too. A simplified method to provide a 3-D distribution is suggested in the paper, which is implemented in the CESM model and can be used by models that are not equipped with a chemistry module (most CMIP6 models). The approximation assumes a simplified vertically well-mixed troposphere and define a latitudinally varying tropopause height: the resulting latitude-height distributions for N_2O and CFC-12 are shown in Fig. 2.

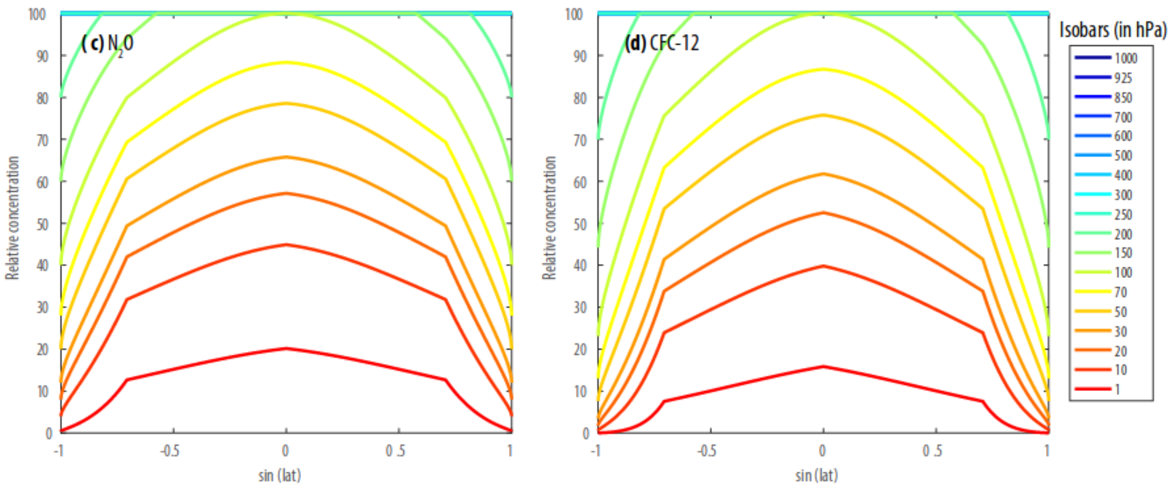


Figure 2: Assumed latitude-height distribution of N_2O (left) and CFC-12 (right) in Meinshausen et al. (2017). The gases are assumed to be well mixed below about 250 hPa.

The authors comment that "While this study provides the main step from global-mean and annual-mean concentration histories towards zonally and monthly resolved ones, future research will be needed to provide more robust 4-D fields of concentrations". In this sense, improved vertically resolved measurements would be valuable.

CMIP6 models essentially rely on the input4mips datasets for all their needs regarding historical GHG concentrations. Regarding the implementation of the GHGs concentrations in climate models, three options are provided in Meinshausen et al. (2017):

- Option 1: All individual gases;
- Option 2: CO_2, CH_4, N_2O and CFC-12, all other 39 gases are summarized in an equivalent concentration of CFC-11 (scaled with the radiative forcing);
- Option 3: CO_2, CH_4, N_2O. All ODSs summarized as CFC-12-eq, other fluorinated gases as HFC-134a-eq (scaled with the RF);

As an example, the EC-Earth3 climate model (Doescher et al., 2022), which includes the IFS atmospheric component, and the WACCM model (Gettelman et al., 2019) both follow option 2. Notably, the WACCM model includes many more individual species in gas chemistry, but only accounts for their radiative effects in an aggregated way.
Typical CMIP6 model horizontal resolutions range from about 250 km down to 25 km for the highest resolution models. Models used for weather forecasts usually have finer grids, nowadays reaching 10 km and less at the global scale.
On the vertical, climate models tipically include between 30 and 100 vertical levels, covering at least troposphere and stratosphere and in some cases extending upwards to include the mesosphere. As an example on the upper end, the OpenIFS atmospheric model (cy47r3) developed by ECMWF, can run with a maximum of 137 levels, with a model top at 0.01 hPa (~80 km). Level width varies with the atmospheric density, from 20 m close to the surface, to about 200 m at the tropopause, to 1 km in the upper stratosphere.
Some more detail on individual models can be found at: https://wcrp-cmip.org/cmip-model-and-experiment-documentation/. A general tendency for the next CMIP phase is to go towards higher model resolutions, but still on the order of 10 to 100 km.

Summarizing, the main application of GHG data for climate modeling (without chemistry) is as input for radiative transfer calculations; current datasets are built from surface station measurements and extended backwards using proxies.
Another application consists in the calculation of the radiative forcing of minor species, in order to correctly weight their radiative effect when aggregating all minor species as equivalent species.
These two applications are well represented by two of the case studies proposed in this project, namely the sensitivity of the simulated climate to the 3D distribution of OLLGHGs (lat/height dependence) and the assessment of their radiative forcing. For these applications, an observed latitude-height climatology of the GHGs is sufficient (with a resolution of a few degree horizontally and few km vertically).

2.2 Usage of OLLGHGs data for chemistry-climate modeling and emission inversion

- **Chemistry-climate modeling**

Chemistry-climate models (CCMs) integrate the simulation of the climate system, through an atmosphere-ocean general circulation model (AOGCM), with a model of the atmospheric chemistry, including a comprehensive representation of chemical processes, such as the formation and destruction of ozone, aerosols, greenhouse gases, and other trace gases. CCMs are able to simulate chemical reactions, transport, and mixing of different chemical species in various atmospheric layers, usually encompassing the whole middle atmosphere.

The Chemistry Climate Model Initiative (CCMI) aims at advancing our understanding of chemistry-climate interactions within the Earth system (Morgenstern et al., 2017), focusing on coordinating inter-comparison of chemistry-climate models and evaluation with observations. Supported by Future Earth's IGAC and the WCRP's SPARC projects, CCMI addresses the need for improved understanding and modeling of the stratosphere and troposphere as a single entity. The scientific objectives encompass the simulation of the stratospheric ozone layer, tropospheric composition, air quality, and their complex interplay. The initiative seeks to explicitly address stratospheric gas-phase chemistry, which is well-understood and including all relevant reactions with published rate coefficients. Furthermore, it aims to improve understanding of heterogeneous chemistry, particularly in phenomena like ozone depletion and the tropospheric nitrogen cycle. Additionally, there's a notable emphasis on tropospheric climate-composition linkages within the initiative, prompting most models to include an explicit treatment of tropospheric aerosols due to their profound impact on climate and air quality.

About 20 models participated in the CCMI-1 initiative, most of which extending up to include the whole mesosphere (~80km, a few Pa) and some reaching even higher levels. One example is the WACCM model (Gettelman et al., 2019), which reaches up to the lower thermosphere. Horizontal resolutions of chemistry-climate models are usually comparable to the CMIP6 range. In fact, many such models are just climate models that add an atmospheric chemistry component, such as TM5 (Huijnen et al., 2010) or MOZART (Kinnison et al., 2007).

Connected to the CCMI is the Aerosol Chemistry Model Intercomparison Project (AerChemMIP; Collins et al., 2017), which is specifically focused on diagnosing climate forcings and feedback related to near-term climate forcers (NTCFs: methane, tropospheric ozone and aerosols, and their precursors) and chemically reactive well-mixed greenhouse gases (nitrous oxide and ozone depleting halocarbons). The project aims to document and understand past and future changes in atmospheric composition, estimating the global-to-regional climate response resulting from these changes. Some of the AerChemMIP models also participated in the Radiative Forcing Model Intercomparison Project (RFMIP, Pincus et al., 2016), aimed at assessing the ERF contribution of individual species.

Since CCMs simulate abundances of individual species throughout the lower and middle atmosphere, comprehensive datasets of N_2O and halocarbons in these altitude regions are potentially useful for model evaluation. Collins et al. (2017) highlight the importance of observational datasets such as the observations for Model Intercomparison Projects (obs4MIP) (Teixeira et al., 2014; Ferraro et al., 2015), the SPARC Data Initiative (Hegglin et al., 2017) for the stratosphere and the ESA CCI (Hollmann et al., 2013) for the troposphere.

Some works in literature report a systematic comparison of observations and model results regarding the concentration of individual species, including N_2O (Bruhl et al., 2007) and ozone (Kinnison et al., 2007; Lahoz et al., 2007), which gives an indirect information about ozone-depleting substances like CFCs.

More recently, an extensive study regarding the atmospheric lifetimes of N_2O, CFCs and other halogens has been performed in the context of the SPARC framework (SPARC, 2013). Atmospheric lifetimes inferred from existing observations were compared to those obtained by modelling results from a set of CCMs simulations. As reported in Chipperfield et al. (2014), the models show relative differences in the estimated lifetimes of up to 10% depending on the individual species (20% for CCl_4), highlighting the importance of a comparison with the observations. New satellite measurements in these altitude regions might be of use for an updated assessment of CCM performances.

- **Emission inversion through chemistry-transport models**

A recent evolution in the chemistry-climate community regards the inversion of measurements to trace back emissions of individual gas species to specific regions. One example is the work by Rigby et al. (2019), which attributed a significant part of the recent global rise in CFC-11 emissions to eastern Asia regions. Specifically, they used "high-frequency atmospheric observations from Gosan, South Korea, and Hateruma, Japan, together with global monitoring data and atmospheric chemical transport model simulations". This study relies on surface station data, but a comprehensive satellite dataset would certainly improve the spatial coverage.
More specifically, the analysis in Rigby et al. (2019) was performed with two regional Lagrangian chemical transport models, NAME (Manning et al., 2007) and FLEXPART (Stohl et al., 2005). The first one was driven with meteorological fields from the UK Met Office Unified Model, with a spatial resolution reaching up to about 0.1°×0.1° (for the most recent period) and a temporal resolution of 3 hours. FLEXPART was driven by operational ECMWF analysis with 1°×1° resolution globally and 0.2°×0.2° resolution for northeastern China.

Similar works have been carried out by Manning et al. (2007) and Corazza et al. (2011) regarding the inversion of N_2O emissions.
Another example of a chemistry transport model that can be used at high resolution to invert measurements is the ICOsahedral Nonhydrostatic model with Aerosols and Reactive Trace gases (ICON-ART, Schröter et al., 2018). ICON-ART resolutions range from tens of km down to less than 1 km, depending on the domain, the application and the timescale considered.

Summarizing, there is a potential for more challenging applications of observational OLLGHG datasets that involves atmospheric chemistry models. The first application regards the evaluation/validation of chemistry-climate models through comparison of simulated and observed concentrations or trends, or inferred atmospheric lifetimes of individual species. For this application, various data format may be suitable, ranging from monthly latitude-height climatology to time-varying 3D distribution of the individual species, with a moderate horizontal/vertical resolution (few degrees/few km). Another application involves data assimilation of measured VMR profiles, for example to get a regularized distribution of chemical species (an example in this sense is represented by the third case study proposed in this project): in this case the data need to be at high temporal frequency (~daily).

Finally, there is a great interest in using observational datasets for inversion of GHG emissions through chemistry-transport models. In this case, the spatial and temporal resolution required are much higher: ideally a few hours frequency or less, and at a horizontal scale of tens of km (but dependent on the model resolution and on the dimension of the region analyzed).

3 Requirements from user consultation in the frame of the LOLIPOP ESA CCI project

A survey has been produced to gather information about the interest in improved observational datasets of OLLGHGs, including input from the modelling community, but not only. The questionnaire is available in Annex 1 - Questionnaire. The questionnaire was answered by 42 scientists. Among the participants, about 60% are modelers. Other participants indicated the

following as their main research field: atmospheric radiative transfer, remote sensing, atmospheric composition measurement and atmospheric chemistry/physics.
As a first indication, most of the users agreed on the need for improved observational datasets, with an average score of 4.5 over 5. Regarding the modeling community, the respondents are representative of two modeling activities:

- weather forecasts and climate modelling without chemistry (about one third of the users);
- atmospheric and climate models including chemistry (other: chemistry-climate, chemistry-transport modeling) -> more than half of the users);

Depending on the main activity, the users need gas concentrations for the following purposes, ordered starting from the most common choice, along with the preferred data format:

- model validation and diagnostics (chemistry): many data formats are suitable in this case, ranging from a monthly latitude-height climatology to high-frequency 3D distribution and individual VMR profiles;
- analysis of atmospheric transport and emission inversion: this application requires very high-frequency and high resolution data, either in the form of 3D distribution or individual VMR profiles;
- model input for radiative transfer computation: monthly latitude-height climatologies are sufficient for this use;
- data assimilation in chemistry-climate models: requires individual VMR profiles or high-frequency 3D distribution of the individual species;
- assessment of radiative forcing: monthly latitude-height climatologies are sufficient in this case.

Fig. 3 shows the distribution of the individual species judged more interesting by the users (only gases with more than one choice are listed).

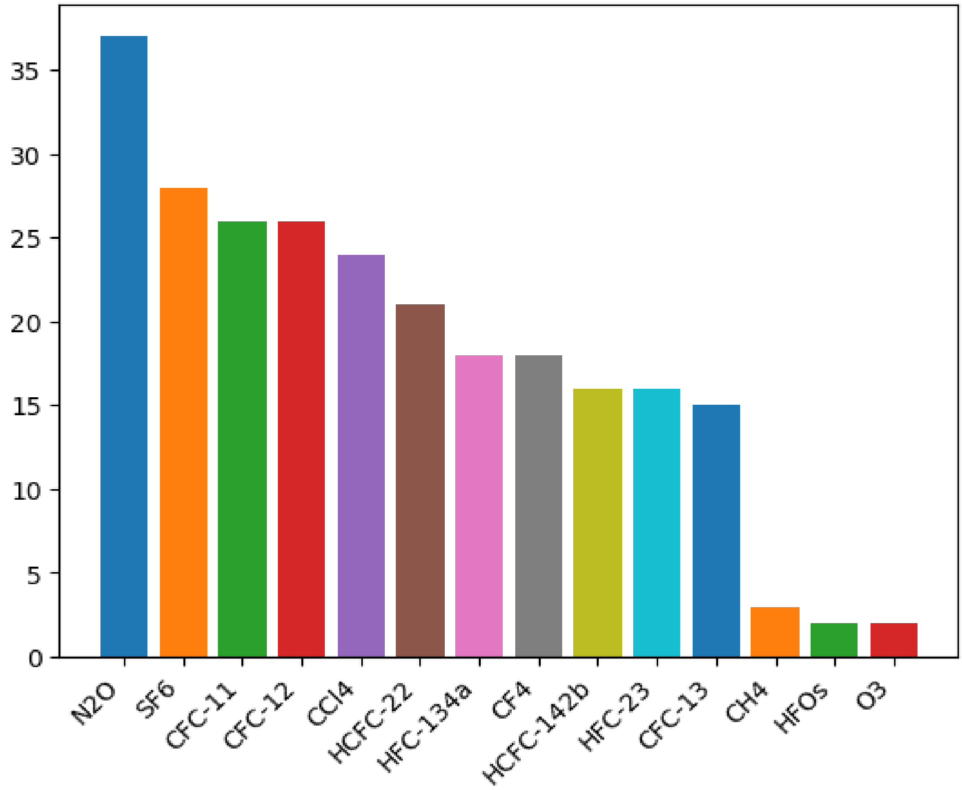
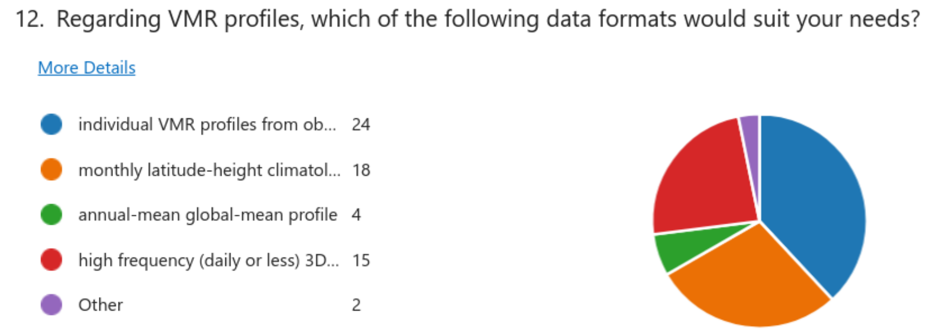


Figure 3: For which gases there is a specific interest?

Other gases, indicated by only one user, are: CFC-113, halon 1211, H1301, VSLS Org. Chlorine, HFC-125, HFC-143a, HFC-227ea, Hydrogen, NF_3, PFC-116 (C2F6), PFC-218, PFC-318, HF, CH_3CCl_3, CH_3Br, CH_3Cl, H1211.

In fact, chemistry-climate models (CCMs) consider all those individual species or a good fraction of those, at least for the representation of the chemical reactions. Climate models without chemistry only need information regarding the major radiatively active GHGs, therefore only N_2O and CFC-12, and (most of them) aggregating all other gases as a CFC-11 equivalent (as in option 2 in Meinshausen et al., 2017).

The questions regarding the most useful data format and the representation of gases in the model also highlight two different modelling communities (Fig. 4). On one side, weather and climate models (without chemistry) represent gases either through a latitude-height distribution, some including seasonality, or only through a global mean concentration in the troposphere. This community prefers to have new data as a monthly latitude-height climatology. On the other side, chemistry-climate models represent gases through a 3D time-varying distribution, so prefer either high-frequency 3D distributions or the individual VMR profiles from single observations.



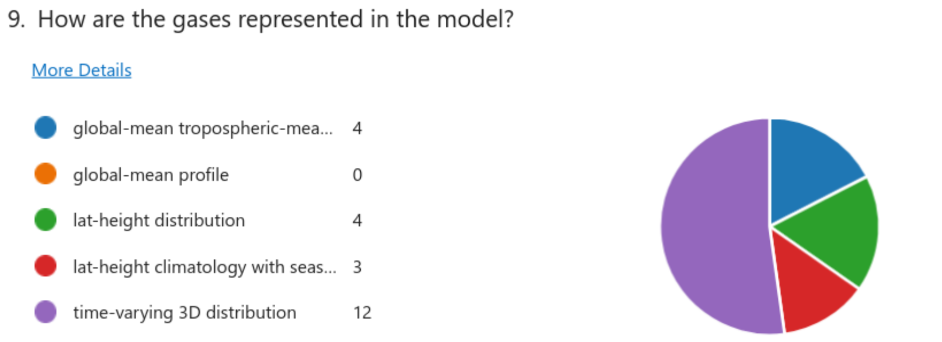


Figure 4: Gas representation in the models (top) and preferred data format (bottom).

Additional requirements can be extracted from the questions regarding the horizontal and vertical resolution, and the data accuracy. For climate applications and general chemistry-climate model evaluation, a horizontal resolution of a few degrees is sufficient. For emission inversion and transport studies, a much higher horizontal resolution is needed, down to 50 km or even 10 km (about 0.1 deg).
For the vertical resolution, the general indication is at least 3 km (the higher, the better) and a coverage of at least troposphere and stratosphere, with a particular focus on the UTLS region, and some interest also in the mesosphere.
The relative accuracy is indicated by most to be reasonable around 10% (but better at 2-5%), although some stricter requirement is present for N_2O (~0.1ppb). Beside the accuracy, there is a strong indication for avoiding drifts in the dataset and evaluating the systematic error.

Additional requirements regard the time coverage, with all users requiring a long and stable dataset. Most users also are in favour of an easy and public access to the datasets, which are preferred to be in netcdf format.

4 Summary of user's requirements for OLLGHGs from the survey and the literature review

The literature review provides a background to interpret the results from the user survey, which is turn has proven to be extremely useful in indicating quantitative requirements for the different applications.

We summarized the results reported in Section 2 and 3 regarding user requirements in the following tables, separating N2O, CFC-11 and CFC-12, which are of interest for both weather/climate models and chemistry-climate models, and other species, mostly of interest for chemistry-climate and chemistry-transport applications. However, most requirements are common for the different species, the main difference being in the weather and climate models only directly using the major species (N2O, CFC-11, CFC-12).

Different applications have significantly different requirements on the data format and resolution, from the simpler (low resolution monthly latitude-height climatology) to the more challenging (high-frequency high resolution 3D distribution). Some of the requirements may prove hard to satisfy with existing measurements, but in general users rely on the best that the observational community can deliver.

Species of Interest	**N2O, CFC-11 and CFC-12**			
Application	Evaluation (Chemistry-climate models)	Assimilation (Chemistry-climate models)	Emission inversion (chemistry-transport models)	input for radiative transfer (weather and climate models)
Data format	monthly latitude-height climatology/time-varying 3D distribution	individual VMR profiles/high-frequency 3D distrib.(~daily)	high-frequency 3D distrib. (~3 hourly)/individual VMR profiles	monthly latitude-height climatology
Horizontal resolution	Few degrees		Around 10 km	Few degrees
Vertical resolution	1-3 km (less in upper atm)		high resolution close to surface	1-3 km
Vertical extension	troposphere to mesosphere		surface/lower troposphere	Troposphere and stratosphere
Accuracy	10% (but better at 2-5%), N_2O about 0,1 ppbv			
Additional requirements	Stability over time (no value) and assessment of systematic errors			

Species of Interest	**SF6, CCl4, HCFC-22, HCFC-134a, CF_4, HCFC-142b, HFC-23, CFC-13**			
Application	Evaluation (Chemistry-climate models)	Assimilation (Chemistry-climate models)	Emission inversion (chemistry-transport models)	Assessment of radiative forcing
Data format	monthly latitude-height climatology/time-varying 3D distribution	individual VMR profiles/high-frequency 3D distrib. (~ daily)	high-frequency 3D distrib. (~3 hourly)/individual VMR profiles	monthly latitude-height climatology
Horizontal resolution	Few degrees		Around 10 km	Few degrees
Vertical resolution	1-3 km (less in upper atm)		high resolution close to surface	1-3 km
Vertical extension	troposphere to mesosphere		surface/lower troposphere	troposphere and stratosphere
Accuracy	10% (but better at 2-5%)			
Additional requirements	Stability over time (no value) and assessment of systematic errors			

Table 1: Summary of the requirements from the user's survey and the literature review.

5 Inventory of satellite products for OLLGHG

The user survey, reported in the previous section, highlighted how most of the users agreed on the need for improved observational datasets. One of the objectives of the LOLIPOP project is to produce an inventory of existing satellite data on OLLGHGs.

Here we summarize the main information on the available datasets for each molecule. We found satellites datasets for N_2O, SF_6, CFC-11, CFC-12, CCl_4, HCFC-22, HCFC-134a, CF_4, HCFC-142b, HFC-23, CFC-13. Each table, from 2 to 12, reports the information about the mission, the type of product, the observation geometry, the spatial coverage, the resolutions, the useful vertical range and the temporal coverage of each product. Due to the large amount of information found for the different datasets and molecules, we prefer to move the complete description of each dataset for each molecule in [RD-1].

The inventory is composed of datasets from both nadir and limb missions and particular attention was given in finding data for the main OLLGHGs, as indicated by the user survey, N_2O, SF6 and CFCs 11 and 12.

N2O							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	temporal coverage
HIRDLS	VMR prof.	limb	80 / -64	1-1.2km	300x10k m	100-0.46hPa	Jan. 2005- March 2008
MLS	VMR prof.	limb	82 / -82	5/8km	200-300 km	100-5.1hPa	2004-today
MIPAS-KIT	VMR prof.	limb	global	3/4km strato – 4/6 km above	300-500 km below 45 km, 500-700 km above	5-70km	2002-2012
MIPAS-ESA	VMR prof.	limb	global	4/30km	400-500km NOM	6-60km	2002-2012
SMR/ODIN	VMR prof.	limb	82.5/-82.5	5km		15-50km	2002-today
ACE-FTS	VMR prof.	limb	82 / -82	3 km		5-95km	Febr. 2004-today
ILAS II/ ADEOS II	VMR prof.	limb	56-70 ºN and 63-88 ºS	1.5/3km	25 degreees		Jan-Oct 2003
TES	column+prof	nadir(manly)	global				Aug. 2004- Jan. 2018
AIRS-CLIMCAPS	partial column	nadir	global	100plev	13.5km	1000-100hPa	Aug. 2002- Sept.2016
CrIS-CLIMCAPS	partial column	nadir	50x50km				2015-2021
IASI (EUMETSAT)	total column	nadir	global	Total column	IASI FOV	Total column	2009-today
TANSO-FTS	total column	nadir	global	total column	10km	total column	2019-2021
IASI(NOPIR)	Profile	nadir	global	variable 2 DOF	12km	800-80hPa	2011-2020
IASI(SOFRID)	Total column, VMR, mean VMR in 700-350 hPa	nadir	global				2014
IASI(TN2OR)	scientific/profile	nadir		14 p. lev.			2011
IASI-MUSICA	VMR prof.	nadir	global				2014-2019
BEFORE 2002							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	1984
ATMOS	VMR prof.	limb	-180.0,-73.0,180.0,75.0	1km	2x2 km	5-96km	1985-1994 few days
ISAMS/UARS	VMR prof.	limb	-180.0,-80.0,180.0,80.0	2.5km	495km	15-80km	Sept. 1991- July1992
CLAES/UARS	VMR prof.	limb	34S and 80N and 80S and 34N	2.5km	300km	10-60km	Oct. 1991- May 1993
ILAS/ADEOS	VMR prof.	limb	57-73 ºN and 63-88 ºS	1.9-3km		10-70km	Sept. 1996- June1997
CRISTA	VMR prof.	limb		2-3km	500 km x 650 km	15-150km	November 3 to 12, 1994, August 8 to 16, 1997

Table 2: Inventory of datasets for N_2O.

SF6							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	temporal cov.
MIPAS-KIT	VMR prof.	limb	global	3-4 km at 10km, 5 km at 20 km, 7 km at 30 km, 11 km at 40 km	300-500 km	5-40km	2002-2012
ACE-FTS	VMR prof.	limb	82 / -82	3 km		8-32km / 12-32km	Feb. 2004-today
IASI	total column	nadir	23.27◦N—66.32◦N	total column	average over region	0-40km	2008-2023
BEFORE 2002							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	temporal cov.
ATMOS	VMR prof.	limb	-180.0,-73.0,180.0,75.0	1km	2x2 km	5-96km	1985-1994 few days

Table 3: Inventory of datasets for SF_6.

CFC-11							
Mission	pr. Type	Geom	coverage	Vert. Res	H res	useful range	temporal cov.
HIRDLS	VMR prof.	limb	80 / -64	1-1.2km	100km	316-17.8hPa	Jan. 2005-March 2008
MIPAS-KIT	VMR prof.	limb	global	2 km tropo., 6km strato.	300-500 km	5-60km	2002-2012
MIPAS-ESA	VMR prof.	limb	global	4/30km	400-500km for NOM	full range	2002-2012
ACE-FTS	VMR prof.	limb	82 / -82	3 km		5-30km	Feb. 2004-today
ILAS II/ADEOS II	VMR prof.	limb	56-70 ºN and 63-88 ºS	1 km	25 degreees	5-60km	Jan-Oct2003
IASI	total column	nadir	23.27◦N—66.32◦N	total column	average over region	0-40km	2008-2023
BEFORE 2002							
Mission	pr. Type	Geom	coverage	Vert. Res	H res	useful range	temporal cov.
ATMOS	VMR prof.	limb	-180.0,-73.0,180.0,75.0	1km	2x2km	5-96km	1985-1994 few days
CLAES/UARS	VMR prof.	limb	34S and 80N and 80S and 34N	2.5km	300km	10-60km	Oct. 1991-May 1993
CRISTA	VMR prof.	limb		2-3km	500 km x 650 km	15-150km	November 3 to 12, 1994, August 8 to 16, 1997

Table 4: Inventory of datasets for CFC-11.

CFC-12							
Mission	pr. Type	geom	Coverage	Vert. Res	H res	useful range	temporal cov.
HIRDLS/AURA	VMR prof.	limb	80 / -64	1-1.2km	100km	316-8.3hPa	Jan. 2005-March 2008
MIPAS-KIT	VMR prof.	limb	Global	2 km tropo., 6km strato.	300-500km	5-50km	2002-2012
MIPAS-ESA	VMR prof.	limb	Global	5/7.5km	400-500km for NOM	full range	2002-2012
ACE-FTS	VMR prof.	limb	82 / -82	3 km		5-30km	Feb. 2004-2012
ILAS II/ADEOS II	VMR prof.	limb	56-70 ºN and 63-88 ºS	1 km	25 degreees		Jan-Oct2003
IASI	total column	nadir	23.27◦N—66.32◦N	total column	average over region	0-40km	2008-2023
BEFORE 2002							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	temporal cov.
ATMOS	VMR prof.	limb	-180.0,-73.0,180.0,75.0	1km	2x2 km	5-96km	1985-1994
CLAES/UARS	VMR prof.	limb	34S and 80N and 80S and 34N	2.5km	300km	10-60km	Oct. 1991-May 1993
ILAS/ADEOS	VMR prof.	limb	57-73 ºN and 63-88 ºS	1.9-3km		10-70km	Sept. 1996-June1997
CRISTA	VMR prof.	limb		2-3km	500 km x 650 km	15-150km	November 3 to 12, 1994, August 8 to 16, 1997

Table 5: Inventory of datasets for CFC-12.

CCl4							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	2002
MIPAS-KIT	VMR prof.	limb	global	3 km at tropopause increasing to 6 km at 30 km	300-500km	5-30km	2002-2012
MIPAS-ESA	VMR prof.	limb	global	10 km at 6 km and 5-7.5 km between 10 and 30 km	400-500km for NOM	full range	2002-2012
ACE-FTS	VMR prof.	limb	82 / -82	3 km		6-25/8-30km	Feb.2004-today
IASI	total column	nadir	23.27◦N—66.32◦N	total c.	average over region	0-40km	2008-2023
BEFORE 2002							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	1984
ATMOS	VMR prof.	limb	-180.0,-73.0,180.0,75.0	1km	2x2km	5-96km	1985-1994 few days
CRISTA	VMR prof.	limb		2-3km	500 km x 650 km	15-150km	November 3 to 12, 1994, August 8 to 16, 1997

Table 6: Inventory of datasets for CCl_4.

HCFC-22							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	temporal cov
MIPAS-KIT	VMR prof.	limb	global	2 km at tropopause increasing to 6 km at 30 km	300-500km	5-50km	2002-2012
MIPAS-ESA	VMR prof.	limb	global		400-500km	6-36km	2002-2012
ACE-FTS	VMR prof.	limb	82 / -82	3 km		5-25km	Feb. 2004-today
IASI	total column	nadir	23.27◦N—66.32◦N	total column	Average over region	0-40km	2008-2023
BEFORE 2002							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	temporal cov
ATMOS	VMR prof.	limb	-180.0,-73.0,180.0,75.0	1km	2x2km	5-96km	1985-1994 few days

Table 7: Inventory of datasets for HCFC-22.

HCFC-134a							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful Range	Temporal cov.
ACE-FTS	VMR prof.	limb	82 / -82	3 km		5-25km	Feb. 2004-today
IASI	total column	nadir	23.27◦N—66.32◦N	total column	average over region	0-40km	2008-2023

Table 8: Inventory of datasets for HCFC-134a.

CF_4							
Mission	pr. Type	geom	Coverage	Vert. Res	H res	useful range	temporal cov.
MIPAS-ESA	VMR prof.	limb	Global	3-5-7km	400-500km for NOM	full range	2002-2012
ACE-FTS	VMR prof.	limb	82 / -82	3 km		15-55km	FEb. 2004-today
IASI	total column	nadir	23.27◦N—66.32◦N	total column	average over region	0-40km	2008-2023
BEFORE 2002							
Mission	pr. Type	geom	Coverage	Vert. Res	H res	useful range	temporal cov.
ATMOS	VMR prof.	limb	-180.0,-73.0,180.0,75.0	1km	2x2km	5-96km	1985-1994 few days
CRISTA	VMR prof.	limb		2-3km	500 km x 650 km	15-150km	November 3 to 12, 1994, August 8 to 16, 1997

Table 9: Inventory of datasets for CF_4

HCFC-142b							
Mission	pr. Type	geom	Coverage	Vert. Res	H res	useful range	temporal cov.
ACE-FTS	VMR prof.	limb	82 / -82	3 km		6-12km	Feb. 2004-today
IASI	total column	nadir	23.27∘N—66.32∘N	total column	average over region	0-40km	2008-2023

Table 10: Inventory of datasets for HCFC-142b.

HFC-23							
Mission	pr. Type	Geom	coverage	Vert. Res	H res	useful range	temporal cov.
ACE-FTS	VMR prof.	limb	82 / -82	3 km		5-35km	Feb. 2004-today

Table 11: Inventory of datasets for HFC-23.

CFC-13							
Mission	pr. Type	geom	coverage	Vert. Res	H res	useful range	temporal cov.
ACE-FTS	VMR prof.	limb	82 / -82	3 km		5-25km	Feb. 2004-today

Table 12: Inventory of datasets for CFC-13.

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Annex 1 - Questionnaire

ESA-CCI - LOLIPOP - Climate applications and user needs

The ESA Climate Change Initiative (CCI) provides high-quality datasets of climate-sensitive variables measured by satellite instruments, covering atmospheric gases like ozone, water vapour and the most important greenhouse gases (GHG), carbon dioxide and methane. However, a complete understanding of the Earth's climate requires other atmospheric gases with significant greenhouse effects or a strong impact on the ozone layer. This is the case for nitrous oxide (N2O), sulfur hexafluoride (SF6), and chlorocarbons such as carbon tetrachloride (CCl4) as well as groups of fluorinated species categorized as chlorofluorocarbons (CFCs), hydrochlorofluorocarbons (HCFCs), hydrofluorocarbons (HFCs), and perfluorocarbons (PFCs). These gases are collectively known as 'Other long-lived greenhouse gases' (OLLGHGs) and are recognised as one of the GCOS Essential Climate Variables (ECVs). While GCOS has outlined requirements for N2O, no user requirements have been identified for the other OLLGHGs.

To bridge this gap, the LOng-LIved greenhouse gas PrOducts Performances (LOLIPOP) CCI+ project, aims to establish a baseline for the user requirements for these OLLGHGs and to compare it to the quality of satellite observations, assessing whether existing data is sufficient for selected applications in climate and atmospheric chemistry models and services.

We invite you to participate in this questionnaire to gather information on your specific needs as a potential user of the OLLGHGs datasets. Your valuable insight will shape future observational products, directly influencing the upcoming stages of the project and will be at the core of a user meeting planned for 2025.

Completing it will only take a few minutes of your time (14 + 3 questions)!

(We adhere to the General Data Protection Regulation (GDPR) guidelines, ensuring the confidentiality of personal information (name, e-mail). For data queries or modifications, contact Bianca M. Dinelli - CNR-ISAC.)

1. Name, affiliation *

2. E-mail (optional, for re-contact in the next stages of the project)

3. Main research field *

4. In your opinion, how critical is the need for improved/updated observational datasets of N2O and/or minor long-lived GHGs (CFCs, HCFCs, ..)? *

☆ ☆ ☆ ☆ ☆

5. Among the gases listed here, select those that are of specific interest to you. (You can choose as many as you like) *

- ☐ N2O
- ☐ CFC-11
- ☐ CFC-12
- ☐ CFC-13
- ☐ HCFC-22
- ☐ HFC-23
- ☐ HCFC-142b
- ☐ HFC-134a
- ☐ CCl4
- ☐ CF4
- ☐ SF6
- ☐ HCFC-141b
- ☐ HFC-143a
- ☐ HFC-125
- ☐ HFC-32
- ☐ HFC-227ea
- ☐ HFOs
- ☐ Other

6. Does your activity include climate/atmospheric modelling? *

- ○ Yes
- ○ No

7. If yes, which type of model(s) do you use?

- ☐ global climate model
- ☐ atmospheric chemistry
- ☐ weather forecast
- ☐ Other

8. Apart from CO_2 and CH_4, which GHGs are considered in your model?

- ○ only N_2O and CFC-12
- ○ N_2O, the others aggregated as CFC-12_eq and HFC-134a_eq
- ○ N_2O and CFC-12, the others aggregated as CFC-11_eq
- ○ All individual species (list in question 5)
- ○ Other

9. How are the gases represented in the model?

- ◯ global-mean tropospheric-mean value
- ◯ global-mean profile
- ◯ lat-height distribution
- ◯ lat-height climatology with seasonal cycle
- ◯ time-varying 3D distribution

10. Regarding N2O and minor GHGs, how are the gas concentrations useful for your activity? *

- ◯ model input (radiative transfer)
- ◯ model validation/diagnostics (chemistry)
- ◯ data assimilation
- ◯ assessment of radiative forcing
- ◯ Other

11. In what form is it preferable to have the gas concentrations? *

- ◯ VMR profiles
- ◯ total columns
- ◯ partial columns

12. Regarding VMR profiles, which of the following data formats would suit your needs? *

- [ ] individual VMR profiles from observations
- [ ] monthly latitude-height climatologies
- [ ] annual-mean global-mean profile
- [ ] high frequency (daily or less) 3D data
- [ ] Other

13. Which other dataset characteristics would be desirable? (you can choose as many as you like)

- [ ] long term coverage (> 10 yrs)
- [ ] regularization (no "holes" in the data)
- [ ] netcdf format
- [ ] easy, direct download with public access
- [ ] merged multi-instrument
- [ ] high frequency (daily)
- [ ] high spatial resolution
- [ ] upper atmosphere included
- [ ] troposphere included
- [ ] Other

14. Do you have specific requirements regarding the horizontal resolution of the data?
    (you can specify different needs for different gases/groups and applications)

15. Do you have specific requirements for the vertical resolution and vertical range?
    (you can also specify different needs for different gases/groups and applications)

16. Do you have any requirement for the data accuracy (max relative error)?
    (you can also specify different needs for different gases/groups and applications)

17. If you have any additional comment/suggestion, we'll be happy to hear it:

Annex 2 - Inventory of OLLGHGs satellite products

The “Inventory of OLLGHGs satellite products”, annex 2 of the [D1.1 – URD] “User Requirements Analysis and Inventory of Satellite Products”, is provided as a separate document.

***** End of Document *****