GLYoxal Retrievals from TROPOMI
GLYRETRO

A proposal in response to the ESA ITT AO/1-9481/18/I-NS

Sentinel-5p+ Innovation (S5p+I) – Theme 1 Glyoxal (CHOCHO)

Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Belgium

Institute of Environmental Physics, University of Bremen (IUP-UB), Germany

Christophe Lerot

christophe.lerot@aeronomie.be, BIRA-IASB

Trissevgeni Stavrakou, Jean-François Müller, Jeroen Van Gent,
Isabelle De Smedt, Michel Van Roozendael (BIRA-IASB)

Andreas Richter, Leonardo Alvarado (IUP-UB)

1) TECHNICAL PART

1.1 <u>TECHNICAL REQUIREMENTS AND OBJECTIVES:</u>

1.1.1 Understanding of the main technical objectives of the RFP/ITT

The instrument TROPOMI aboard the Copernicus Sentinel-5p platform, successfully launched on 13th October 2017, is a nadir-viewing hyperspectral imager recording earthshine radiances in wavelength ranges from the ultraviolet to the shortwave infrared regions. With a swath of about 2600 km, TROPOMI covers the entire atmosphere every day with a spatial resolution of 3.5 x 7 km² (UV-VIS bands). Those measurements allow to derive information on key atmospheric species for the understanding and the monitoring of the Earth-atmosphere system, and more particularly of the ozone layer protection, air quality and climate change aspects.

A number of key data products are already generated operationally in near real time: columns of ozone, NO_2, HCHO, SO_2, CH_4, CO, cloud parameters, aerosol absorbing index… TROPOMI measurements offer the potential to derive additional information relevant to the mission objectives and this ITT aims at supporting parallel activities to develop scientific algorithms to further exploit the capability of the TROPOMI observations. The retrieval of glyoxal (CHOCHO) tropospheric columns is one of the themes this ITT focuses on and the object of this proposal.

Glyoxal is the most abundant dicarbonyl present in our atmosphere and is directly emitted from biomass burning and also results from the oxidation of precursor non-methane volatile organic compounds (NMVOC). Several attempts to establish a glyoxal global budget using chemistry transport models (Fu et al., 2008; Myriokefalitakis et al., 2008; Stavrakou et al., 2009) have estimated the production from natural sources and fires to about 70% and from human activities to about 30%. Owing to its short lifetime (~3 hours), elevated glyoxal concentrations are observed near emission sources. Measurements of atmospheric glyoxal concentrations therefore provide quantitative information on VOC emission and can help to better assess the quality of current inventories (e.g. Stavrakou et al., 2016; Cao et al., 2018). In addition, glyoxal is also known to contribute significantly to the total budget of secondary organic aerosols (e.g. Washenfelder et al., 2011), which impact both air quality and climate forcing.

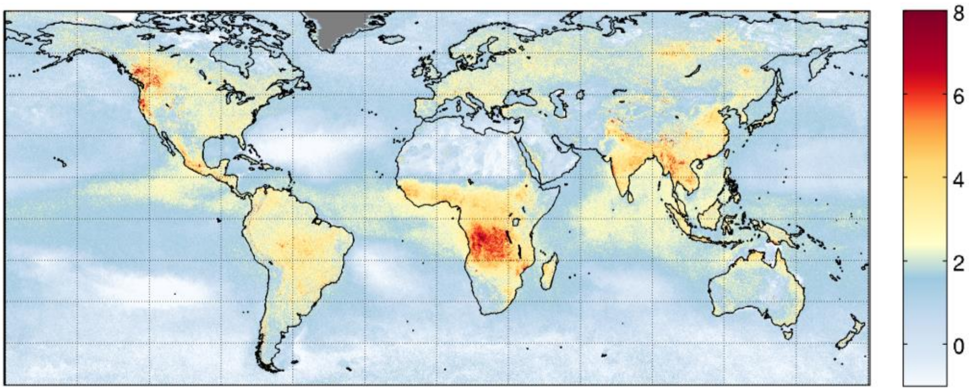

Figure 1: Preliminary evaluations of glyoxal vertical columns (10^{14} molec/cm²) retrieved from TROPOMI between November 2017 and October 2018

Glyoxal has three main structured absorption bands in the visible spectral range (420-460 nm), which offers the potential to use a DOAS (Differential Optical Absorption Spectroscopy) approach to retrieve tropospheric columns. However, typical glyoxal optical depths are very small (one order of magnitude smaller than optical depths of other absorbers in the same region) making the retrieval challenging and prone to noise and to systematic biases caused by spectral interferences. Nevertheless, the retrieval of glyoxal from space has already been demonstrated with several nadir sensors. First observations of glyoxal vertical columns from space have been realized by Wittrock et al. (2006) using nadir observations from the SCIAMACHY instrument aboard Envisat. Later, glyoxal VCDs have also been retrieved by different teams (Vrekoussis et al., 2009; Lerot et al. 2010) from the GOME-2/Metop-A/B instruments with a better signal-to-noise ratio owing to the better spatial coverage of the instrument. OMI, the precursor instrument of TROPOMI, has also been exploited to retrieve glyoxal (Alvarado et al., 2014; Chan Miller et al., 2014; Lerot et al., 2015) with a higher spatial resolution.

The main objectives of this activity are to develop a prototype glyoxal column retrieval algorithm for TROPOMI, to build a data pool of independent glyoxal data to be used to validate the TROPOMI glyoxal product generated with the prototype tools and to prepare a strategy to make this scientific algorithm operational. It is also required to highlight the added-value of the developed product for air quality studies and for the user community in regards of what is already available. For example, although the TROPOMI formaldehyde (HCHO) operational product can already provide information on the NMVOC emissions, the different production yields of glyoxal can bring complementary information. In that sense, the CHOCHO/HCHO ratio is often proposed as a metric to discriminate different types of emissions (Vrekoussis et al., 2010).

1.1.2 Proposed approach to reach the main technical objectives of the RFP/ITT

The proposed work will be realized by BIRA-IASB and IUP-UB organizations, both with a strong expertise in DOAS retrievals from space and ground. More specifically, both partners have demonstrated experience with glyoxal retrievals and have already collaborated on this topic in other frameworks (e.g. as part of the prototyping of the Sentinel-5 L2 processor). The team is complemented by BIRA-IASB experts in modelling of the tropospheric composition. This work will be coordinated by BIRA-IASB.

The objectives of the ITT will be met with an approach that will follow three main activities: the actual development of the glyoxal algorithm, the validation of the prototype glyoxal product and the impact assessment of the activity. Note that these activities are not necessarily to be performed only in a sequential order, but can impact one another. For example, the validation of a beta TROPOMI glyoxal data set can influence the algorithmic developments.

1.1.1.1 Development of the glyoxal retrieval algorithm [BIRA-IASB]

As discussed before, tropospheric columns of glyoxal have already been retrieved from space with heritage missions following a DOAS approach. The concept of DOAS is relatively simple: the slant column (i.e. concentration integrated along the atmospheric effective light path) of the species of interest is first derived by means of a least-squares fit of the measured reflectance spectrum by laboratory cross-sections and then converted into a vertical column with an air mass factor (AMF), the latter requiring suitable radiative transfer calculations. For weak absorbers such as glyoxal, there is often an additional step which consists in normalizing the retrieved columns based on observations in a remote reference sector containing no or small amounts of the gas to be retrieved. This overall approach will remain unchanged and the focus will be on finding the optimal retrieval settings, which may have large impact in the case of glyoxal. Also, the unprecedented high spatial resolution of TROPOMI ideally requires the use of adapted data bases for the a priori information used in the AMF computation.

The glyoxal retrieval algorithm that we propose has been developed at BIRA-IASB and applied in the past to the GOME-2A/B and OMI instruments. Recently, the algorithm has been adapted to ingest the TROPOMI L1b data without significant change to retrieval settings, apart from the adaptation of the wavelength-dependent auxiliary data to the TROPOMI spectral resolution. The current version of the algorithm is described as part of the S5 glyoxal ATBD [Lerot et al., 2018]. Although those first results are promising and the glyoxal fields observed by TROPOMI are found to be well consistent with those of OMI, a number of further adaptations are needed to account for the TROPOMI specificities, in particular its high spatial resolution. Also some additional algorithmic developments will be investigated.

DOAS fit

As mentioned before, typical glyoxal optical depths are small compared to other species absorbing in the visible spectral range. This makes its retrieval very sensitive to spectral interferences and cross-section uncertainties included in the spectral fit, resulting in possible systematic errors. Those biases are reduced by the application of the reference sector normalization procedure. It is also common for weak absorbers to use as reference spectrum in the DOAS fit a mean radiance spectrum extracted from a remote area rather than using an irradiance spectrum (Alvarado, 2016). This may also help to reduce mean systematic biases. This procedure, which is the baseline for the HCHO and SO2 operational products, has not yet been applied to the TROPOMI glyoxal retrievals, an irradiance having been used as the reference so far. The added value of using a mean radiance as reference approach will be investigated.

Water vapour has absorption bands collocated with the glyoxal bands, which may lead to spectral interferences when the atmospheric water vapour content is large, as for example in Tropical Regions. The choice of the appropriate water vapour cross-sections is therefore important to limit as much as possible systematic errors. Also, recent analysis has shown that the reference temperature of the water vapour cross-section significantly influences the correlation with glyoxal. It will be investigated whether the temperature dependence of the water vapour absorption can be considered in the fit itself or if an optimal choice of the effective temperature can be made to reduce as much as possible biases in the glyoxal SCDs in large water vapour conditions. This is important in the Tropics, especially to better address the question of the glyoxal column enhancements observed over equatorial oceans.

AMF computation

The AMF computation step heavily relies on external auxiliary data. In particular, the albedo of the surface and a priori information on the vertical distribution of glyoxal need to be prescribed by external databases. For the surface albedo, the OMI LER climatology [Kleipool et al., 2008] with a spatial resolution of 0.5°x0.5° is currently used. A priori glyoxal profile information is prescribed over land by a climatology built on simulations carried out with the BIRA-IASB CTM IMAGES [Bauwens et al., 2016; Stavrakou et al., 2018] for the period 2005-2016. This climatology provides profiles with a spatial resolution of 2°x2.5° as a function of the day of the year. It is clear that the resolution of those two data bases is much too coarse with respect to the TROPOMI spatial resolution, which may introduce significant errors as shown by Heckel et. al [2011] for NO_2 retrievals.

It can be anticipated that new LER (possibly directionally dependent) climatologies based on TROPOMI observations themselves will be built in the coming years. Such data bases should logically be tested, their impact assessed, and finally used for the glyoxal retrievals. A link can also be made with the theme 5 (Aerosol Optical Depth and Bidirectional Reflectance Distribution Function). One of the activities of this theme is to develop a BRDF product. It has been shown [Lorente et al., 2018] that neglecting anisotropy in surface reflection may lead to significant errors in the visible spectral range, especially for large viewing angles. In case of successful release of a BRDF product, the best approach to optimally use it will be investigated.

Only a few models can provide a priori glyoxal information. TM5, which is currently used in the TROPOMI operational processing, has not that capability. We propose to replace the current source of a priori glyoxal profiles by new simulations realized with an updated chemical mechanism in the recent CTM MAGRITTE [Stavrakou et al., in preparation], successor of IMAGES. Those simulations will be run on a daily basis for the period 2018-2020 with a spatial resolution of 1°x1°. Errors related to the spatial resolution, but also due to neglecting the inter-annual variability of the emissions will be thus reduced.

As mentioned before, non-negligible amounts of glyoxal are observed from space and ground over oceans, a feature currently not reproduced by models. For this reason, over oceans, instead of using a priori profiles coming from a model, we use a fixed parameterized profile reproducing profiles measured with an air-borne MAX-DOAS during the TORERO campaign in the tropical Pacific Ocean (January/February 2012) [Volkamer et al., 2015]. This option might be revisited in case of progress in modelling the oceanic glyoxal during the project.

Cloud correction

Cloud correction relying on the Independent Pixel Approximation is often applied for the retrieval of tropospheric species. It allows to relax the cloud coverage threshold from which satellite observations are advised to be rejected and also to implicitly account for aerosols, to some extent. However, applying such a correction turns out to be unstable due to a problematic increase of the glyoxal slant columns over bright surfaces (like clouds), which makes the retrieved slant column inconsistent with the typical glyoxal vertical profiles. For that reason, no cloud correction is currently applied in the glyoxal retrieval and only a very stringent filtering for cloud contamination is used. The reason for this behaviour is not well understood but is likely to originate again from spectral interferences (e.g. with the O_4 or Ring spectral signatures, which have strong cloud dependencies). At present, this appears to be a fundamental limitation but might be reconsidered if better insight into this issue is gained during the project.

The TROPOMI cloud parameters are retrieved operationally with the OCRA and ROCINN algorithms. OCRA provides the cloud cover fraction derived from broadband reflectance measurements in the UV-VIS-NIR bands, while ROCINN derives cloud optical thickness and cloud-top height using the O2-A band region. An alternative approach is to assume that the cloud is optically thick (cloud top albedo set to a high value, e.g. 0.8) and to derive a corresponding effective cloud fraction, similarly to what is done in the operational NO_2 product. We propose to test this approach and to derive the cloud fraction using the same spectral channels as those used for the glyoxal retrieval. This would ensure full independency with respect to the operational cloud product and would guarantee full co-registration between the determined cloud fraction and the glyoxal slant column.

Towards a TROPOMI glyoxal operational product

BIRA-IASB has been involved for many years into the support of the development and the implementation of operational products (Total Ozone, HCHO, SO2, BrO) for heritage nadir sensors (GOME, SCIAMACHY, GOME-2/Metop). As part of the TROPOMI Quality Working Group, the team has also defined the baseline algorithms for the tropospheric formaldehyde and SO2 operational products as well as for the offline total O3 product. It is also involved in the preparation of the future Copernicus Sentinel-4 and -5 instruments, including the definition of the glyoxal operational product. Therefore, the proposed team has all the expertise to prepare a strategy for the operationalisation of the TROPOMI glyoxal product. In addition, enhanced consistency between the retrieval approaches for formaldehyde and glyoxal is beneficial when combining products together to derive higher level quantities like, for example, the glyoxal-to-formaldehyde ratio.

1.1.1.2 Validation [IUP-UB]

Validation of the TROPOMI prototype glyoxal product will be an important activity of this work. One limitation of this activity is the scarcity of independent glyoxal data. It is therefore difficult to anticipate which data set will be available during the project. Glyoxal retrievals from the ground also suffer from similar limitations as from space, i.e. high sensitivity to spectral interferences and sensitivity to noise. As a result, validation activities are challenging on their own.
At BIRA-IASB, we have several time series of MAX-DOAS observations in different locations (Uccle, Xianghe, and Cabauw) which can be exploited for this work. At University of Bremen, glyoxal measurements from Bremen, Vienna and Athens are available for use in the validation.
It has to be noted that Rainer Volkamer, Associate Professor & CIRES Fellow at the University of Colorado, US, has shown interest in this proposal and proposed to act as a privileged user. He has long-standing expertise in glyoxal photochemistry and detection and will make independent validation datasets available to us. In particular, he participated in different campaigns over land and ocean during which glyoxal has been measured from ship- and air-borne MAX-DOAS.
The validation exercise will be realised by taking into account the respective instrumental sensitivity when external profile information is available and also considering the specificities of the validation sites. Because of the limited amount of independent glyoxal data, we propose to use also glyoxal columns simulated with the BIRA-IASB CTM MAGRITTE to evaluate the soundness of the TROPOMI glyoxal fields in terms of seasonal and inter-annual variability. In addition, the model can be used as a transfer function to compare with TROPOMI independent data which are either not collocated in time or which cannot be compared directly (e.g. in situ concentration measurements).

Anticipated available independent data sets:

- MAX-DOAS data in Xianghe, 2008-present
- MAX-DOAS data in Uccle, 2017-present
- MAX-DOAS data in La Reunion , 2018-present
- BBFlux campaign, US, August-September 2018
- MAX-DOAS data from Bremen during 2018 – end of project
- MAX-DOAS data from Athens during 2018 – end of project
- MAX-DOAS data from Vienna during 2018 – end of project
- CINDI campaigns, Cabauw, June-July 2009, September 2016
- TROPOMI validation campaign, to be defined
- COPMAR campaign, Atlantic Ocean, October 2016
- TORERO campaign, Equatorial Pacific Region, January-February 2012
- SENEX campaign, US, 2013
- SOAS campaign, US, 2013

Brief description of the CTM MAGRITTE

The MAGRITTE model calculates the distribution of 175 chemical compounds, among which 136 species undergo transport, and can be run either globally at 2°×2.5° or 1°x1° resolution depending on the application, or regionally at 0.5°×0.5° resolution. The lateral boundary conditions of the regional model are provided by the global model. In the vertical, the modelled troposphere is divided in 40 levels between the Earth's surface and the lower stratosphere. The meteorological fields are provided by ECMWF ERA-Interim analyses. Most model parameterizations, including the transport scheme, inherit from the IMAGES model (Müller and Brasseur, 1995; Stavrakou et al., 2009, 2015; Bauwens et al., 2016). The chemical mechanism and deposition scheme have been recently updated as described in Müller et al. (2018a) and Müller et al. (2018b), respectively.
The model uses anthropogenic emissions from the HTAPv2 dataset (Janssens-Maenhout et al.,2015). Anthropogenic NMVOC emissions are provided by the EDGARv4.3.2 inventory (Huang et al., 2017) for the year 2012. Biomass burning emissions are obtained from the Global Fire Emission Database version 4 (van der Werf et al., 2017). The global sources of glyoxal as calculated by the MAGRITTE model are estimated at 45 Tg/yr (Müller et al., 2018a), with significant contributions from glycolaldehyde oxidation by OH (11 Tg/yr), oxidation of aromatics (9 Tg/yr) and monoterpenes (9 Tg/yr), whereas direct emissions are believed to be small.

1.1.1.3 Impact assessment [BIRA-IASB]

The glyoxal prototype product generated with the retrieval algorithm will be distributed to potential users via the project website. Their feedbacks will help to identify the added-value of this product with respect to other products. The unprecedented spatial resolution of TROPOMI, its high signal-to-noise ratio and large

number of observations will clearly give new insights for the monitoring of atmospheric VOCs from space. The BIRA-IASB model team included in this consortium will also act as a privileged user and will make the link with the inverse modelling world.
As aforementioned, BIRA-IASB has been responsible for the development of the TROPOMI formaldehyde operational product, which is known to be an indicator of VOC emissions in the atmosphere. The advantage to have glyoxal in addition to formaldehyde originates from its different production yields. Therefore, combining the two products offers the potential to better discriminate the type of VOC emissions. In that sense, the glyoxal/formaldehyde ratio R_{gf} is often presented as a potential metric of which the value might indicate a type of emission (biogenic, anthropogenic or biomass burning). In practice, there are often discrepancies between the ratio estimated from the ground or from space in a given region. Both formaldehyde and glyoxal products are prone-to-noise owing to their weak optical depths, which makes the estimate of R_{gf} also sensitive to retrieval noise. In the past, such ratios have already been estimated at BIRA-IASB using OMI measurements and it was found that the larger values generally correlate with biomass burning conditions (Figure 2). This will be revisited using TROPOMI data. It is a clear advantage to have approaches to retrieve glyoxal and formaldehyde as consistent as possible to limit the risk of systematic bias when estimating R_{gf}. We will compare the estimated ratio to modelled values in different regions presenting different types of emissions (Southeast US and Tropics for biogenic emissions, US, Africa, Amazon for large fire events, and China and Indo-Gangetic plain for anthropogenic emissions). When possible, comparison with ground-based/aircraft data will be considered.

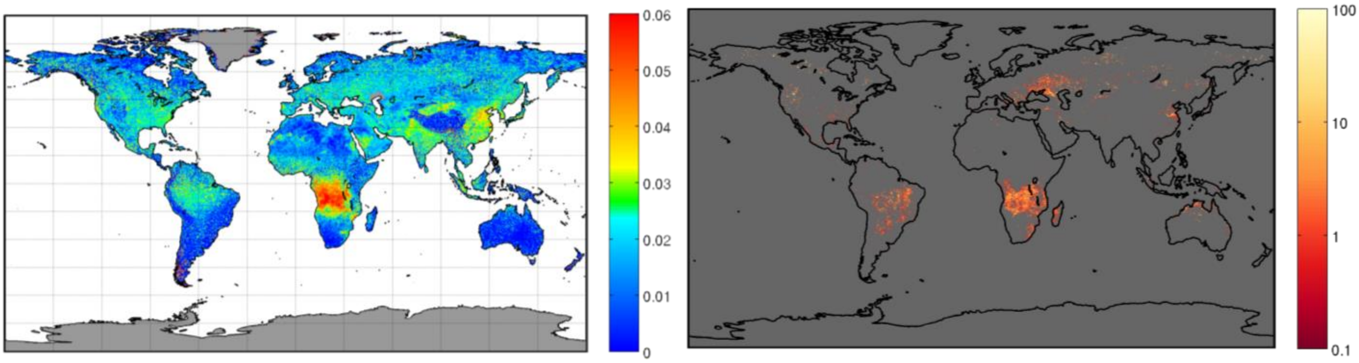

Figure 2: (left panel) Estimate of the glyoxal/formaldehyde ratio using OMI observations in June-July-August 2007; (right panel) MODIS fire counts (# fires/1000km^2/day) for the same period.

1.2 POTENTIAL PROBLEM AREAS:

1.2.1 Identification of the main problem(s) or problem area(s) likely to be encountered in performing the activity

1. Owing to weak CHOCHO optical depth, glyoxal products, from both satellite and ground-based instruments, are characterized by a large level of noise and are sensitive to spectral interferences, which may lead to systematic errors.

2. Another limitation is the scarcity of independent glyoxal observations in overlap with TROPOMI observations, which are needed for the validation activities.

1.2.2 Proposed solutions to the problems identified

1. This is a fundamental limitation. However, efficient background correction used for weak absorbers help to reduce systematic errors originating from spectral interferences but also from Lv1 calibration problems. Although the signal-to-noise ratio of TROPOMI is better than older instruments, a significant level of noise will remain, requiring spatial/temporal averaging to extract meaningful information. The large amount of TROPOMI observations help however to maintain higher time and spatial resolution than before.

2. We also propose to rely on glyoxal fields simulated with the CTM MAGRITTE to evaluate the TROPOMI glyoxal retrievals, the soundness of their spatial patterns and intra-annual variations. In addition, the CTM can play a role of transfer function between independent observations not collocated with TROPOMI and the latter.

1.2.3 Proposed trade-off analyses and identification of possible limitations or non-compliances

Apart from the product limitations presented before, we do not expect non-compliances with respect to tasks defined in the SoW. Errors associated to glyoxal products from space and from ground are generally large and will be better assessed as part of the study.

1.3 TECHNICAL IMPLEMENTATION / PROGRAMME OF WORK

1.3.1 Proposed Work Logic

Figure 3 illustrates the work logic proposed to achieve the objectives associated to the glyoxal theme of the Sentinel-5p+ Innovation project. The activities will start with an initial review of the current and past activities in relation with the theme as well as of the currently defined scientific requirements. In parallel, independent glyoxal data, which are needed to meet the study objectives, will be collected from different sources (e.g. MAX-DOAS, airborne, in situ, model). Those initial activities will serve as input to the main task of the project, consisting in the development of the glyoxal retrieval scientific algorithm from TROPOMI/S-5p observations and in its validation. This task can be seen as an iterative process in which validation feedback can be ingested within the algorithm development activities. Owing to the sparsity of independent glyoxal data, we also include in this process comparison with glyoxal fields simulated with the BIRA-IASB Chemical Transport Model MAGRITTE. A task subsequent to the algorithm development is the preparation of a potential transfer of the tools to an operational environment. During the algorithmic development, typical constraints related to such an operational environment will be considered and potential mitigation means proposed. Based on the final scientific prototype, TROPOMI/S-5p data will be processed to generate a glyoxal tropospheric column product, which will be used for investigating its impact on relevant fields of research (e.g. emission inventories assessment). In this context, the developed glyoxal product will also be used in combination with the S-5p operational formaldehyde product to compute glyoxal/formaldehyde ratios and investigate whether this metric can help to discriminate type of emissions and how consistent these ratios estimated from TROPOMI measurements are with estimates from ground-based or models. The outcome of the project and its different tasks will be promoted in different ways: website, communications at conferences, publications.

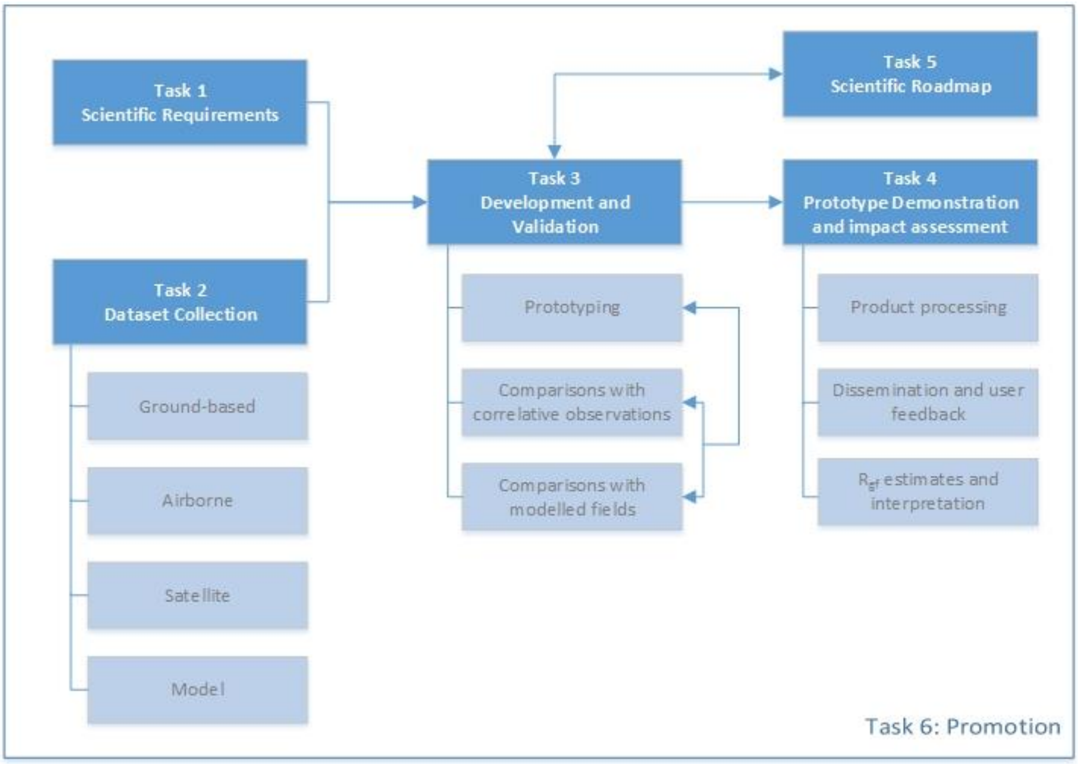

Figure 3: Proposed work logic for the theme glyoxal of S5p+I

1.3.2 Contents of the proposed work

1.3.2.1 Work Breakdown Structure (WBS)

The WBS follows closely the six tasks as defined in the Statement of Work:

- Task 1: Scientific Requirement Consolidation
- Task 2: Dataset Collection

- Task 3: Development and Validation
- Task 4: Prototype Demonstration and Impact Assessment
- Task 5: Scientific Roadmap
- Task 6: Promotion

We have added Task 0 grouping together all management activities.

Figure 4 illustrates the WBS as we have defined it. One work package (WP) has been assigned to every task, except Tasks 3 and 4 that have been split in two WPs:

- WP 00: Project management, led by BIRA-IASB (DOAS team)
- WP 10: Requirement Baseline, led by BIRA-IASB (DOAS team)
- WP 20: Dataset Collection, led by BIRA-IASB (DOAS team)
- WP 31: CHOCHO Product Development, led by BIRA-IASB (DOAS team)
- WP 32: Validation, led by IUP-UB
- WP 41: Prototype Demonstration, led by BIRA-IASB (DOAS team)
- WP 42: Impact Assessment, led by BIRA-IASB (TMOD team)
- WP 50: Scientific Roadmap, led by BIRA-IASB (DOAS team)
- WP 60: Promotion, led by BIRA-IASB (DOAS team)

Please refer to section 1.3.1 for the interactions between the different WPs.

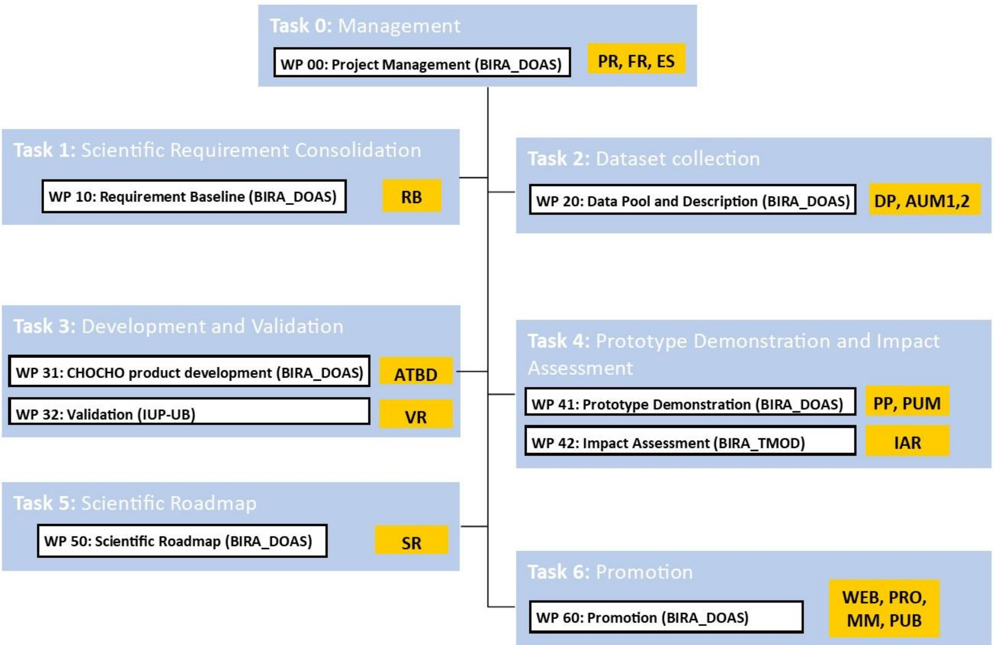

Figure 4: Work breakdown structure of the proposed study.

1.3.2.2 Work Package Description (WPD)

The following tables provide detailed Work Package (WP) descriptions with WP Title, Name of responsible company/institute, Name of the WP Manager, Input required to start the work under the WP, Output expected and a description of the tasks included in the WP.

Table I: WP00 description

PROJECT: GLYRETRO	PHASE: 1	WP: WP00
WP Title: Project Management Company: BIRA-IASB WP Manager: Christophe Lerot, BIRA-IASB		Sheet of 1/1 Issue Ref 1

Start Event: Kick-off (KO) End Event: KO+24M	Planned Date: 01/07/2019 (tbc) Planned Date: 01/07/2021 (tbc)	Issue Date 24/01/2019
Inputs: – SOW, proposal, signed (sub)contracts – WP description – Deliverables D1-14 Tasks: – Management of all project activities and administrative matters. – Coordination of different WPs, monitoring of time schedule, budget and realization of activities. – Identification of potential issues. – Liaison between ESA and partners – Writing of monthly progress reports, final report and executive summary. Outputs: – Monthly Progress Reports (PR, D15) – Final Report (FR, D16) – Executive Summary (ES, D17)		

Table II: WP10 description

PROJECT: GLYRETRO	PHASE: 1	WP: WP10
WP Title: Requirements Baseline Company: BIRA-IASB, IUP-UB WP Manager: Christophe Lerot, BIRA-IASB		Sheet of 1/1 Issue Ref 1
Start Event: Kick-off (KO) End Event: KO+2M	Planned Date: 01/07/2019 (tbc) Planned Date: 01/09/2019 (tbc)	Issue Date 24/01/2019
Inputs: – Literature – Copernicus Sentinels 4 and 5 Mission Requirements Traceability Document [XX]. Tasks: – Review and assessment of currently existing glyoxal products from satellite and ground-based measurements as well as from models. – Identification of datasets useful for the proposed study. – Overview of current initiatives in relation with the proposed work. – Overview of current scientific and operational requirements for space glyoxal retrievals. Outputs: – Requirements Baseline document (RB, D1)		

Table III: WP20 description

PROJECT: GLYRETRO	PHASE: 1	WP: WP20
WP Title: Dataset collection Company: BIRA-IASB, IUP-UB WP Manager: Jeroen Van Gent, BIRA-IASB		Sheet of 1/1 Issue Ref 1
Start Event: Kick-off (KO) End Event: KO+12M	Planned Date: 01/07/2019 (tbc) Planned Date: 01/07/2020 (tbc)	Issue Date 24/01/2019

Inputs: – RB Tasks: – Make available a data pool of independent glyoxal data (ground-based, airborne, satellite, models) and ancillary information useful for validation on the project website and publish the relevant description. – Coordination with other themes. Outputs: – Data Pool (DP, D2) – Auxiliary Dataset User Manual v1, v2 (AUM1/2, D3/ D8).	

Table III: WP31 description

PROJECT: GLYRETRO PHASE: 1	WP: WP31
WP Title: CHOCHO Product Development Company: BIRA-IASB WP Manager: Christophe Lerot, BIRA-IASB Start Event: Kick-off (KO) Planned Date: 01/07/2019 (tbc) End Event: KO+18M Planned Date: 01/01/2021 (tbc)	Sheet of 1/1 Issue Ref 1 Issue Date 24/01/2019
Inputs: – RB – DP – TROPOMI L1 data – Ancillary information (a priori profiles, cloud parameters,…) – WP32 Tasks: – Study of current algorithms to retrieve glyoxal tropospheric columns from nadir UV-VIS observations. – Development of the algorithm; o Selection of optimal ancillary information. o Testing and optimization of retrievals settings. o Investigation of different approaches to handle cloud contamination – Iterative algorithmic development based on activities carried out within WP32. – Error analysis and definition of validity domain based on defined requirements. Outputs: – ATBDv1, v2, v3 (D4)	

Table IV: WP32 description

PROJECT: GLYRETRO PHASE: 1	WP: WP32
WP Title: Validation Company: IUP-UB, BIRA-IASB WP Manager: Andreas Richter, IUP-UB Start Event: KO+4M Planned Date: 01/11/2019 (tbc) End Event: KO+18M Planned Date: 01/01/2021 (tbc)	Sheet of 1/1 Issue Ref 1 Issue Date 24/01/2019

Inputs: – RB – DP – AUMv1,v2 – Beta and final glyoxal data sets produced within WP31 Tasks: – Support to algorithmic developments by comparisons of produced TROPOMI glyoxal columns with independent observed and modelled glyoxal data. – Support to selection of ancillary information (e.g. a priori profiles) – Assessment of the final product quality (VCDs and error estimates. – Check of compliance with defined requirements. Outputs: – VRv1, v2 (D5)	

Table V: WP41 description

PROJECT: GLYRETRO	PHASE: 1	WP: WP41
WP Title: Prototype Demonstration Company: BIRA-IASB WP Manager: Christophe Lerot, BIRA-IASB Start Event: KO+12M End Event: KO+18M	 Planned Date: 01/07/2020 (tbc) Planned Date: 01/01/2021 (tbc)	Sheet of 1/1 Issue Ref 1 Issue Date 24/01/2019
Inputs: – WP31 – WEB – TROPOMI L1 data – Ancillary information (a priori profiles, cloud parameters,…) Tasks: – Production of a glyoxal tropospheric column product using the developed algorithm for the entire TROPOMI time series. – Development of a L2 format consistent with the Observation File Format Standard for the S5p Ground Segment. Outputs: – Prototype Products (PP, D6) – Products User Manual (PUM, D7) – Auxiliary User Manual v2 (AUM2, D8); See WP 20.		

Table VI: WP42 description

PROJECT: GLYRETRO	PHASE: 1	WP: WP42
WP Title: Impact Assessment Company: BIRA-IASB WP Manager: Trissevgeni Stavrakou, BIRA-IASB Start Event: KO+14M End Event: KO+21M	 Planned Date: 01/09/2020 (tbc) Planned Date: 01/04/2021 (tbc)	Sheet of 1/1 Issue Ref 1 Issue Date 24/01/2019
Inputs: – L2 glyoxal product generated as part of WP41 – DP – RB		

– VRv1,v2 – User community Tasks: – Perform comparison of the generated L2 glyoxal product with state-of-the art models and evaluate the meaningfulness of provided error estimate – Investigate the added-value of the developed product for air quality studies and for the associated user community. – Investigate the synergistic use of the developed product with other retrievals (e.g. glyoxal/formaldehyde ratio) and the corresponding added information for the characterization of the atmospheric processes – Evaluate the maturity of the product, its possible limitations and its readiness to be included in the operational product line of TROPOMI Outputs: – Impact Assessment Report (IAR, D9)	

Table VII: WP50 description

PROJECT: GLYRETRO	PHASE: 1	WP: WP50
WP Title: Scientific Roadmap Company: BIRA-IASB WP Manager: Christophe Lerot, BIRA-IASB Start Event: KO+18M End Event: KO+24M	Planned Date: 01/01/2021 (tbc) Planned Date: 01/07/2021 (tbc)	Sheet of 1/1 Issue Ref 1 Issue Date 24/01/2019
Inputs: – User community – IAR Tasks: – Critical analysis of the user community with respect to the prototype product. – Identification of a strategy to include the developed product within the S5p operational environment. Proposal of possible mitigation means considering operational constraints. – Definition of future strategies and potential activities to further improve satellite glyoxal retrievals, to enhance the product impact on air quality studies. – Reviewing the product requirements. Outputs: – Scientific Roadmap (SR, D10)		

Table VIII: WP60 description

PROJECT: GLYRETRO	PHASE: 1	WP: WP60
WP Title: Promotion Company: BIRA-IASB, IUP-UB WP Manager: Christophe Lerot, BIRA-IASB Start Event: K End Event: KO+24M	Planned Date: 01/07/2019 (tbc) Planned Date: 01/07/2021 (tbc)	Sheet of 1/1 Issue Ref 1 Issue Date 24/01/2019
Inputs:		

– Material from all WPs – PP – DP Tasks: – Development of a project website, in coordination with other themes promoting the project activities, but also serving of platform for data access (DP) and document storage for the consortium. – Present the project and associated activities to the community at conferences and forums. Multimedia material adapted to different target audiences will be created. – Publication as one of several peer-reviewed articles of the scientific outcome of the project. Outputs: – Project Website (WEB, D11) – Promotion Summary Report (PRO, D12) – Multimedia Summary Report (MM, D13) – Papers (PUB, D14)	

1.4 BACKGROUND:

1.4.1 Existing own concepts/products relevant to the activity and/or to be used

BIRA-IASB has developed in the past tools to retrieve glyoxal from heritage sensors and that has been recently adapted to TROPOMI in the framework of the S5L2PP project. These tools will be further developed within this study.
The DOAS fits make use of the QDOAS software, which has been continuously developed for more than two decades and used for analysing spectra recorded by many satellite, ground-based or mobile instruments. Also a series of look-up tables are generated using the radiative transfer model VLIDORT. The latter won't be part of the retrieval software but is nevertheless needed in the development phase. We will also make use of extraction, gridding, mapping and intercomparison tools that are being continuously used for all projects.

1.4.2 Third Party's concepts/products relevant to the activity and/or to be used

For verification and validation activities, third party data will be collected and used. They will certainly include the data listed in section 1.1.1.2., as well as other satellite glyoxal products (e.g. from OMI) generated either at BIRA-IASB or elsewhere. Availability of additional data will be investigated as part of WP20. While access to correlative data originating from IUP-UB and BIRA-IASB is guaranteed, the access to data from other parties will have to be confirmed. Their publication in the data pool will be made only if permission is given by the data provider.

1.4.3 Other technical achievements relevant to the activity and/or to be used

Background intellectual property rights (BIPR) exist for some tools intended to be used during this study. The following table lists tools and software that are owned by the institutes working in this project or by third parties.

Table 1: BIPRs associated to tools that will be used during the study.

Name of BIPR item	Owner	Description	WP impacted
LIDORT VLIDORT LIDORT-RRS	RT Solutions Inc.	LIDORT (LInearized Discrete Ordinate Ra-diative Transfer) is a family of discrete ordinate scattering code with a simultaneous facility for the generation of both radiances and analytic Jacobians.	WP31
QDOAS	BIRA-IASB	QDOAS is a generic multi-sensor DOAS retrieval tool developed at BIRA-IASB, being used for development and prototyping pur-poses. QDOAS is	WP31 WP41

		free software distributed under the terms of the GNU General Public License.	
BeTV	BIRA -IASB	Tool library to calculate tropospheric air mass factors, vertical columns, averaging kernels and error estimates (linked with input from QDOAS and LIDORT).	WP31 WP41
SCIATRAN	V. Rozanov, A. Rozanov, J.P. Burrows (IUP-UB)	Coupled radiative transfer model SCIATRAN	WP3.2
NLIN	A. Richter (IUP-UB)	DOAS analysis package	WP3.2

1.4.4 Background of the company(ies)

Royal Belgian Institute for Space Aeronomy (BIRA-IASB)

Since its creation in 1964, the main tasks of the Belgian Institute for Space Aeronomy (BIRA-IASB) are research and public service in the field of space aeronomy, which includes the study of the physics and chemistry of the atmospheres of the Earth and other planets, and of outer space. BIRA-IASB has a strong expertise in designing and operating instruments and experiments to monitor atmospheres and space environment. It has also developed a strong know-how in the exploitation of measurements from ground, air and space, as well as their geophysical interpretation using, among others, theoretical and numerical models.
The BIRA-IASB UV-visible Remote Sensing group has acquired considerable expertise in the retrieval of atmospheric trace gases and aerosols based on observations performed using the Differential Optical Absorption Spectroscopy (DOAS) from ground-based, aircraft and satellite instruments. The activities of the group are performed in the context of international ground-based networks and atmospheric chemistry satellite missions, such as GOME, SCIAMACHY, GOME-2, OMI, TROPOMI and forthcoming missions (Sentinels-4 and -5). The group is leading the algorithmic development of the Sentinel-5 Precursor TROPOMI operational Level-2 processor for SO_2, HCHO and total ozone, and is part of the TROPOMI ESA mission performance centre (MPC). For Sentinel-4 and Sentinel-5, the group is also leading the development of L2 algorithms for SO2, HCHO, ozone and glyoxal (only for Sentinel-5).

Institute of Environmental Physics at the University Bremen (IUP-UB)

Roughly 23,000 people are currently active as students, teachers, researchers, or employees of the University of Bremen. The department “Physics and Chemistry of the Atmosphere” (PCA), at the IUP-UB of the University of Bremen, Germany, is one of the leading European research institutions in the field of ground-based and space-borne remote sensing of the atmosphere. It is led by Prof. Dr. John P. Burrows, the SCIAMACHY PI and Lead Scientist of GOME. The PCA at IUP-UB comprises more than 60 employees (professors, technical staff, permanent scientists, postdocs and PhD students) and is supported by third-party funding by more than 3000 k€ annually. The satellite sensors GOME and SCIAMACHY were proposed and supported by the IUP-UB team since the early 1990’s when the institute was founded. The IUP-UB team was directly involved in the SCIAMACHY definition and building phases and has been involved for more than 20 years in the development of innovative radiative transfer models (e.g., SCIATRAN) and retrieval algorithms (e.g., DOAS, Weighting Function Modified (WFM)-DOAS, Bremen optimal EStimation DOAS (BESD)) for the analysis of GOME, SCIAMACHY, GOME-2, OMI, OMPS and TROPOMI data from the troposphere towards the mesosphere for gases such as O3, NO2, BrO, IO, SO2, H2O, HCHO, CHOCHO, CH4, CO2 and CO as well as clouds (including NLCs and PLCs) and aerosol parameters. IUP-UB also holds excellent experience and skills in ground-based and satellite retrievals and in the area of software design, software engineering, as well as build-up of databases available to the public. IUP-UB has successfully completed and is currently involved in a large number of national and international projects and studies related to algorithm development, improving the data quality of operational algorithms and validation of satellite data (e.g., ESA projects: GHG-CCI, ESA Aerosols-CCI, ESA Clouds-CCI, ESA Ozone CCI, PROMOTE, SQWG, ADVANSE, FRM4DOAS, S5L2PP, S4; EU-projects EU ACCENT, AMFIC, GEMS, GEOmon, IMECC, MACC, NORS, PANDA, QA4ECV, SHIVA).

1.5. TECHNICAL RESERVATIONS – TECHNICAL COMPLIANCE:

1.5.1 Reservations

This proposal includes no reservation with respect to the technical requirements of the ITT.

1.5.2 Technical Compliance Matrix (Statement of Work / Technical Requirements)

The proposed work with the clarifications made in this proposal is technically fully compliant with the SoW.

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