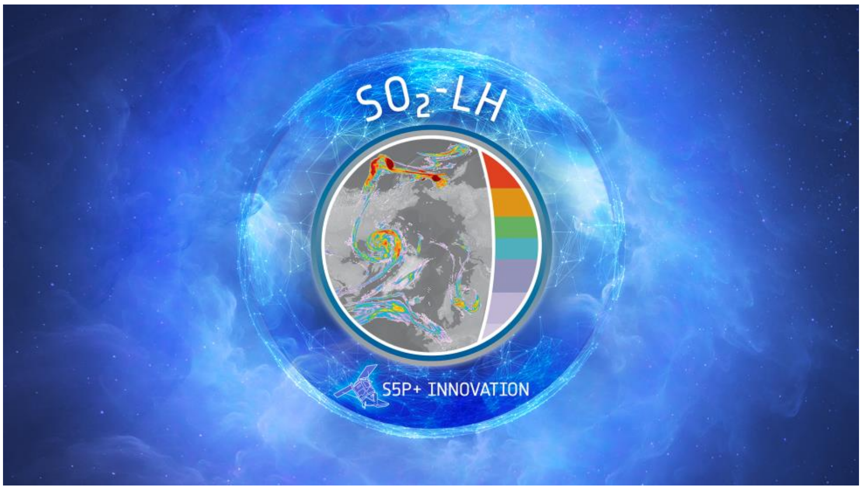

S5P+I: SO2LH project

Executive Summary [D17]

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0.9	2022-02-17	First initial version
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1. Introduction

1.1 Purpose

This document is the Executive Summary (Deliverable D16) as part of the Sentinel-5 precursor Innovation: SO2 LH project. This document summarizes relevant achievements of the project.

1.2 References

1.2.1 Applicable Documents

The following project documents contain provisions which, through reference in this text, become applicable to the extent specified in this document.

Table 1 Applicable Documents

Document Title		Document ID	Issue
[AD01]	Statement of Work, ESA Express Procurement Plus - [EXPRO+] Sentinel-5p Innovation (S5p+I)	EOP-SD-SOW-2018-049	2.0 (20.08.2018)

1.2.2 Reference Documents

The following standards or documents are referenced in this document. They have been used (in the sense of tailoring) to prepare the document on hand.

Table 2 Reference Documents

Title		Document ID	Issue
[RD01]	Sentinel-5P TROPOMI SO_2 LH ATBD	S5P+I-SO2LH-D4-ATBD-v4	4.0
[RD02]	Sentinel-5P TROPOMI SO_2 LH Validation Report	S5P+I-SO2LH-D5-VR-v2	2.0

1.3 Terms and Abbreviations

Abbreviations specific to the report are found in the following table:

Abbreviation	Meaning
DOAS	Differential Optical Absorption Spectroscopy
FP_ILM	Full-Physics Inverse Learning Machine
LH	Layer height
LUT	Look-up table
NN	Neural Network
PCA	Principal Component Analysis
RTM	Radiative Transfer Model
S5P	Sentinel-5 precursor
SCD	Slant column density
SO_2	Sulfur dioxide
TROPOMI	Tropospheric Ozone Measurement Instrument
VCD	Vertical column density

2. Overview about the S5p+I SO2LH project

The **ESA Sentinel-5p+ Innovation project (S5p+I)** has been initiated to develop novel scientific and operational applications, products and retrieval methods that exploit the potential of the Sentinel-5p mission's capabilities beyond its primary objective.

Accurate determination of the location, height and loading of SO_2 plumes emitted by volcanic eruptions is essential for aviation safety. The SO_2 layer height is furthermore one of the most critical parameters that determine the impact on the climate. The height of volcanic ash columns are often estimated by local observers with mostly unknown accuracy. The plume height can also be determined using aircraft, ground-based radar or LIDAR but such observations are often not available and many volcanic eruptions in remote areas remain not observed. In addition, volcanic plumes containing SO_2 but not ash cannot be seen directly. SO_2 in the atmosphere has important impacts on chemistry and climate at both local and global levels.

Although retrievals of SO_2 plume height have been carried out using satellite UV backscatter measurements from e.g. OMI (Ozone Monitoring Instrument) or GOME-2, until now such algorithms are up to now very time-consuming, since the spectral information content and its characterization require computationally demanding radiative transfer modelling. Due to the high spatial resolution of TROPOMI (Tropospheric Ozone Measurement Instrument) aboard S5p (Sentinel-5p) and consequent large amount of data, an SO_2 layer height algorithm has to be very fast.

The **SO_2 Layer Height (SO2LH)** theme is dedicated to the generation of an SO_2 layer height product for Sentinel-5p considering data production timeliness requirements. Within this project machine learning techniques have been applied to retrieve the SO_2 LH information from Sentinel-5p/TROPOMI data to overcome the issue of current state-of-the-art direct fitting approaches to directly retrieve the SO_2 LH, which use computationally expensive radiative transfer calculations.

The retrieval of the SO_2 LH based on Sentinel-5P/TROPOMI measurements is performed using the 'Full-Physics Inverse Learning Machine' algorithm (FP_ILM, Hedelt et al. 2019). combines a Principal Component analysis (PCA) and a Neural Network (NN) approach to retrieve the SO_2 LH based on Sentinel-5P/TROPOMI backscattered UV Earthshine measurements in the wavelength range between 311 and 335 nm.

In general, the FP_ILM algorithm creates a mapping between the spectral radiance and the atmospheric parameter (here the SO_2 LH) using machine learning methods. The main advantage of the FP_ILM algorithm over classical direct fitting approaches is that the time-consuming training phase involving complex radiative transfer (RT) modelling and NN training is performed offline; the final trained inversion operator itself is robust and computationally simple and therefore extremely fast and can be applied in near-real-time (NRT) processing environments. The algorithm is described in detail in the SO_2 LH Algorithm Theoretical Baseline Document (ATBD, [RD01])

The algorithm has been extensively validated against other datasets, which is described in detail in the SO_2 LH Validation Report (VR,) as well as Koukouli et al. (2021).

3. Executive summary of the project

The ESA S5P+I: SO2LH project led by DLR with the collaboration of AUTH Greece, University of Oxford UK and ECWMF/CAMS UK has been successfully kicked-off on 3rd July 2019 and successfully finished on 31st of March 2022.

DLR has led the project and performed the algorithm development task, whereas AUTH performed the validation exercise together with University of Oxford, which provided a reference SO_2 LH product based on Metop/IASI measurements. ECMWF/CAMS have assimilated the prototype data and analyzed the product generated throughout the algorithm development. They also provided input to the validation exercise led by AUTH.

The algorithm development was based on an SO_2 LH algorithm initially developed for S5P/TROPOMI by Hedelt et al. (2019). In the framework of this S5P+I: SO2LH project, the algorithm has been improved and optimized for operational application and implementation. During the project several algorithm and product versions have been released, reflecting minor and major algorithm and L2 format updates.

During the SO_2 LH product validation direct validation against IASI SO_2 LH results from the University of Oxford and against IASI SO_2 LH results from ULB/LATMOS, which is an official EUMETSAT AC-SAF product has been performed. Indirect validation has been performed against CALIOP/CALIPSO aerosol layer height data as well as SO_2 LH forecasts from ECWMW based on assimilated Metop/GOME-2 and S5P/TROPOMI SO_2 total column data and assimilated S5P/SO_2 LH prototype products generated in the framework of this project.

In August 2019, DLR has set-up a project website (https://atmos.eoc.dlr.de/so2-lh/) where the project and partners are described. On this website, project-related documents were made available to the public. This website was maintained and updated throughout the entire project. This website also hosted the datapool (Deliverable D2) in which the input and auxiliary data for the SO_2 LH algorithm was provided internally. A dedicated Twitter account has been generated (https://twitter.com/DlrSo2), in which users are informed about recent and ongoing volcanic eruptions.

In March/April 2020, DLR has provided the first version of the Algorithm Theoretical Basis Document (ATBD). First prototype SO_2 LH L2 products based on this ATBD version were used for the validation exercise, including results for several volcanic eruptions that occurred during the project lifetime.

After initial tests with ECWMF/CAMS, an automated algorithm chain generating SO_2 LH results at DLR for ongoing volcanic eruptions and their assimilation by CAMS has been set-up: DLR is reading the incoming S5P/TROPOMI NRT data and automatically applying the SO_2 LH retrieval algorithm once per hour. The results are automatically pushed to a dedicated CAMS FTP server, where they are picked up and assimilated in a dedicated CAMS forecast experiment. The results are also used in automated Twitter tweets on https://twitter.com/DlrSo2 to inform the users about the SO_2 LH and additional information about ongoing volcanic eruptions.

In September 2020, the second version of the ATBD was released as well as the first version of validation report, already showing the very good agreement against direct and indirect independent SO_2 LH datasets.

In March 2021, the third version of the ATBD was released including a major revision of the algorithm baseline. However, only shortly after this revision it was found that the results for several volcanic eruptions were worse than in the former version. Due to this and concerns from ESA it was decided to roll back to a previous algorithm version.

In July 2021, the final version of the algorithm (Version 4.0), the L2 prototype products covering the entire S5P/TROPOMI timeframe along with the final ATBD (Version 4.0, [RD01]) and validation report (Version 2.0, [RD02]) have been released. The validation results have been summarized in a paper, which is currently under review, see Koukouli et al. 2021. The ECMWF/CAMS assimilation results and SO_2 forecasts have been published in Inness et al. 2022.

The entire S5P+I: SO2LH project has been successfully finalized. An SO_2 LH retrieval algorithm has been developed that is fast and accurate and has been extensively validated against several independent datasets. The SO_2 LH L2 product enables for the first time the precise determination of the total vertical SO_2 column and thus the SO_2 mass and flux after a volcanic eruption as well as the accurate forecast of the volcanic SO_2 plume movement. It is able to meet the requirements imposed by entities related to aviation, forecast, disaster mitigation and society.

The L2 prototype products already fulfill the scientific requirements of near-future satellite missions. Moreover, the algorithm and L2 prototype products also fulfill the processing requirements on timeliness of current operational processing facilities and are therefore capable for implementation in an operational retrieval framework. Most notably, the algorithm has already been implemented in a semi-operational quasi-NRT retrieval environment in the framework of the DLR INPULS project and the products are actively assimilated by ECMWF/CAMS for SO_2 forecasts.

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