Volcanic SO_2 Height SWIM Service

OPAS KTN Engage Catalyst funded project

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Abstract— **Volcanic ash and related gas cause a major risk for air traffic. To mitigate this risk and to improve situational awareness for ATM, information about the height of SO_2 plume is critical. This study presents a new SWIM Yellow Profile service, so called OPAS, with the aim of providing early warnings of volcanic SO_2 height from three satellite instruments (TROPOMI, IASI-A and IASI-B) with an accuracy of 1-2 km. This study describes our TROPOMI SO_2 height algorithm with a validation using synthetic data, a comparison with external observations, and highlights the potential impact of flying through an SO_2 cloud from the point of view of an engine constructor (Rolls-Royce) directly in relation with airlines and ATM. The SO_2 height alert from TROPOMI for the recent eruption of Nishinoshima volcano in June – July 2020, illustrates the interest of OPAS service in support of volcanic SO_2 plume avoidance by commercial airplanes.**

Keywords-component; Early Warning, Volcano Plume Height, Sulphur Dioxide- SO_2, SWIM Yellow Profile Service

I. INTRODUCTION AND MOTIVATION

Volcanic plumes, rich in ash and/or sulphur dioxide (SO_2), are major sources of hazards for aviation and Air Traffic Management (ATM). Potential safety and operability hazards include abrasion of windscreens and compressor blades, damage to avionic equipment and navigation systems, hot corrosion inside the engines, and most importantly, engine stalls due to melting ash in the combustion chamber [1][2]. The exposure to volcanic gases can also be dangerous for the health of the passengers. A volcanic eruption can cause partial or total closure of airspace over many countries which can led to social and economic upheaval (e.g. Eyjafjallajökull across Europe in April–May 2010) [3][4][5][6].

The potential impact of volcanic eruption on ATM is undeniable but to understand the full scope of this study, it is critical to highlight the point of view of aircraft manufacturer and the airlines, with respect to the potential impact for the engine for flying through a volcanic SO_2 cloud. A recent personal communication from Rolls-Royce indicated the level of impact SO_2 gas is believed to have on aviation; SO_2 gas has been implicated in a number of engine damage mechanisms. Figure 1 illustrates the flight routes of one operator potentially affected by sulphur damage, plus a selection of airports operations from which are associated with sulphidation damage.

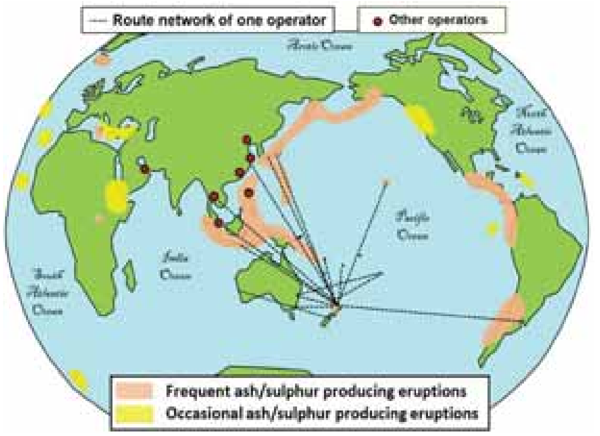

Figure 1: Illustration of areas with occasional and frequent volcanic emissions, and an example of a route network and operators seeing sulphur damage to engines.

The sulphidation mechanisms appear to be a function of:

1) the sequence of contamination exposure: Na/Ca, then SO_2/SO_4^{2-} and potentially Cl^-
2) Chronic versus acute SO_2 exposure

Figure 2 illustrates 4 types of hot corrosion within the gas turbine which has been associated with SO_2 exposure, i.e. sulphidation process with deposits on and inside the engines. The SO_2 contamination results in additional maintenance. The increase in the cost of the maintenance contract for the stakeholders and the turbine maintenance costs for the aircraft manufacturers, on top of the safety and health problems for the passengers during a long-line flight, are the main motivation for the development of the OPAS service (Operational alert Products for ATM via SWIM).

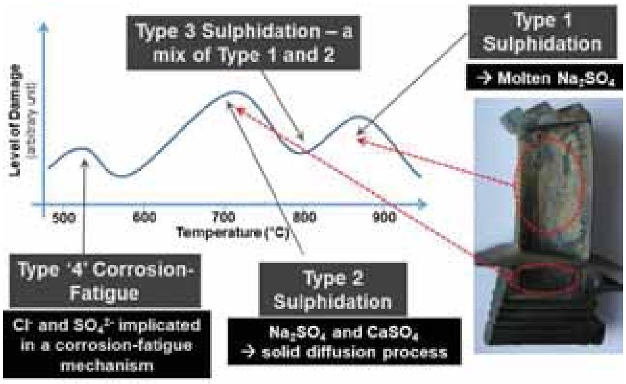

Figure 2: Illustration of the sulphidation mechanisms.

The work on the sulphidation mechanism at Rolls-Royce is a very convincing introduction to the scope addressed by OPAS service, i.e. the interest of the transfer to ATM stakeholders of information related to volcanic SO_2 (height and mass loading).

The OPAS service can also be beneficial to the operational environment to enhance situational awareness and provide resilience in case of volcanic emissions affecting ATM. The International Civil Aviation Organization (ICAO) has designated nine Volcanic Ash Advisory Centres (VAACs) to provide their expertise to civil aviation in case of significant volcanic eruptions. Each VAAC is a meteorological centre (Civil Aviation Authority) designated by regional air navigation agreement to provide advisory information to Meteorological Watch Offices (MWO), area control centres, flight information centres, world area forecast centres and international OPErational METeorological information (OPMET) databanks regarding the lateral and vertical extent and forecast movement of volcanic ash in the atmosphere following volcanic eruptions.

The role of the VAACs is to provide:

- Volcanic Ash Advisory (VAA), an advisory information regarding the lateral and vertical extent and forecast movement of volcanic ash in the atmosphere following volcanic eruptions.
- Volcanic Ash Graphic (VAG), associated to the VAA, showing ash observations and forecasts.
- ASHTAM, provided in the VAA, are special series NOTAM (Notice to Airmen) notifying by means of a specific format change in activity of a volcano, a volcanic eruption and/or volcanic ash cloud that is of significance to aircraft operations.
- Volcanic Ash SIGMET, provided with the VAA, reports the presence of volcanic ash conditions.

A SIGMET (SIGnificant METeorological conditions), provided by a MWO, provides details concerning en-route weather phenomena which may affect the safety of aircraft operations.

The contamination of air by a volcanic SO_2 plume is considered as an atmospheric phenomena in the IWXXM (ICAO Meteorological Information Exchange Model). ICAO Annex 3 updates in 2023, 2026, and 2029 are scheduled to include modifications to the International Airways Volcano Watch (IAVW) that results in more quantitative VAAs, including the provision of ash concentration charts and a quantitative SO_2 information product (ICAO, 2019; CGMS-48, 2020). During the conjoint session of the 7th WMO VAAC Workshop and the 9th WMO VASAG Meeting (Volcanic Ash Scientific Advisory Group; on 21-22 Nov. 2019, Washington DC), London VAAC accepted to be in charge of the development/conception of the future SO_2 advisory.

The OPAS service aims to support the VAACs and the other stakeholders, with respect to SO_2 contamination during long-haul flights. Access to near real-time (NRT) data, with a time delivery of only few hours, is essential for the VAACs, to complete their task and deliver the volcanic advisory. A volcanic plume is composed, among others, by sulphur dioxide gas (SO_2). The layer height of an SO_2 plume (SO2LH), in addition to the selective detection of the vertical amounts of SO_2, can be retrieved using ultra-violet (UV) and infrared (IR) hyperspectral sensors. OPAS provides NRT information on the height of a volcanic plume (i.e. SO_2 height) and the associated SO_2 mass loading, which is relevant to the VAACs as it can substantially improve the forecast and the advisory created during a crisis. Information on the SO_2 height is also critical for the stakeholders (airlines, pilots, and aircraft manufacturers) to avoid health problem for passengers, unpleasant flights and especially to avoid SO_2 contamination of the engines, which represents consequent maintenance costs.

Section II presents the algorithmic development and the operational implementation of TROPOMI SO2LH. Section III describes OPAS Early Warning System (EWS) and its alert products. Section IV gives an overview of OPAS SWIM service and section V the conclusions and perspectives.

II. A NEW TROPOMI SO_2 LAYER HEIGHT PRODUCTS

A. *Overview of the algorithmic development*

From satellite SO_2 measurements, mostly from UV and IR sensors on board low Earth, polar orbiting satellites, information on SO_2 height can be inferred essentially using two methods: the model approach, which uses inverse modelling, or the measurement approach, which needs algorithm development. In the OPAS project, we consider the second approach.

The algorithmic developments to retrieve SO_2 plume height from space nadir hyperspectral measurements directly have been undertaken over the last 10 years. Based on the dependence of the spectral response to different altitude of the SO_2, the retrieved value is an SO2LH, i.e. an effective quantity over the averaged photon path in the SO_2 vertical layer. In the UV spectral range, the first studies were presented in 2010 and 2011, based on OMI and GOME-2 instruments [7][8]. SO2LH retrievals in the thermal IR have been reported in 2012 and 2014, both for the IASI – Infrared Atmospheric Sounding Interferometer – sensor [9][10]. In 2019 and 2020, the Full-Physics Inverse Learning Machine has been applied to TROPOMI (TROPOspheric Monitoring Instrument in the UV range), and a probabilistic algorithm to CrIS (Cross-track Infrared Sounder instrument) [11][12].

As a matter of fact, and in spite of its importance, there is currently no official operational algorithm available to retrieve SO2LH from any of the space nadir sensors on orbit. To our knowledge, there is only 2 scientific algorithms running in NRT and providing SO2LH images (from IASI and CrIS with spatial resolutions of 12 km² and 14 km² diameter, respectively; CrIS alerts available on-line; https://volcano.ssec.wisc.edu) [10][12]. The IASI product, operated by the Free University of Brussels (ULB) and recently implemented in SACS/EUNADICS EWS, is part of the SO2LH alerts considered by OPAS; see https://sacs.aeronomie.be [13][14].

With the advent of UV sounders with high spatial resolution like TROPOMI (3×5.5 km²), new possibilities are offered to retrieve SO2LH with clear scientific and societal added-values. The motivation for developing an SO_2 layer height retrieval algorithm for TROPOMI is driven by scientific and operational needs. The potential scientific users are from different communities (volcanologists, atmospheric researchers and climate modellers), while operational users are linked to the aviation sector (VAACs and other ATM stakeholders – airlines, pilots, aircraft manufacturers) or atmospheric modelling community (potentially the Copernicus Atmosphere Monitoring Service – CAMS).

Pioneering studies on SO_2 plume height retrievals from space UV measurements were based on retrieval schemes making use of demanding online radiative transfer modelling [7][8]. Thus, such algorithms are difficult to apply for TROPOMI NRT processing especially in the scenario of an extreme eruption, such as Pinatubo, or an SO_2-rich eruption, such as Raikoke, that could possibly solicit all the available hardware in a massive

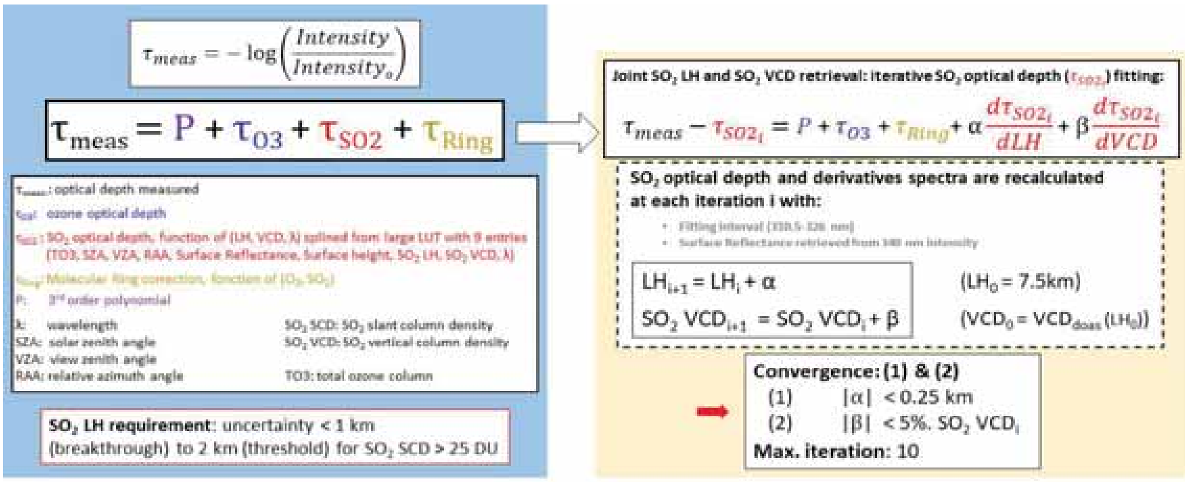

Figure 3: Algorithm concept of TROPOMI SO2LH retrievals.

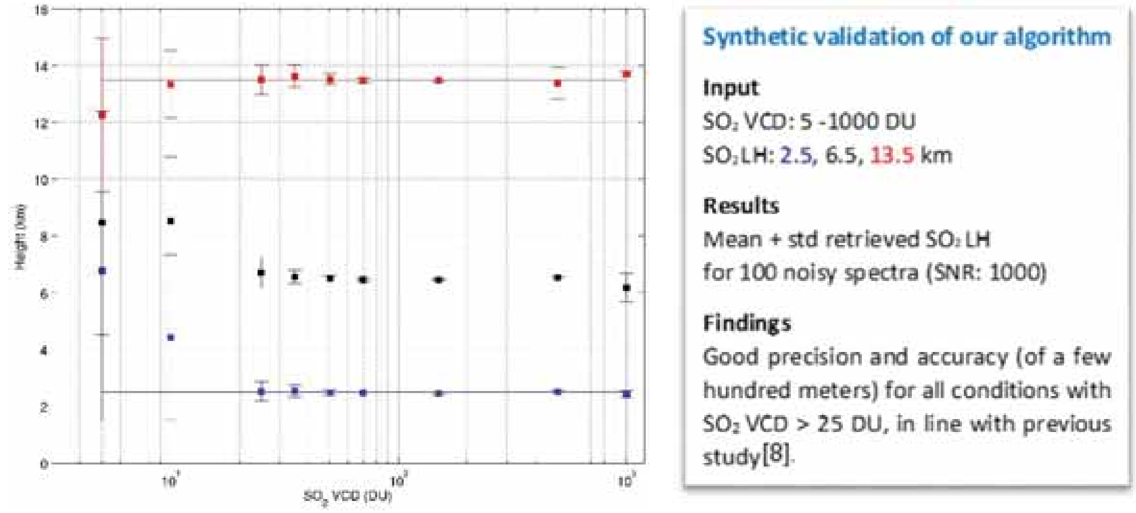

Figure 4: Illustration of synthetic validation of TROPOMI SO2LH retrievals (considering an O_3 VCD of 385 DU, a solar zenith angle of 30°, and an albedo of 5%).

way (too long calculation; unacceptable for fast NRT retrievals). For this reason, we have developed in the frame of the Sentinel-5 L2 Prototype Processors ESA project (S5L2PP) and the OPAS project, a new SO2LH algorithm conceptually close to the Extended Iterative Spectral Fitting (EISF) algorithm [7]. It makes use of SO_2 slant optical depth (OD) look-up-tables (LUT) generated as a function of many parameters (geometry, Lambertian equivalent reflector, ozone optical depth τ_{O3}, SO_2 Vertical column density – VCD and height); see Fig. 3.

In brief, the slant column density (SCD) results from the spectral fitting of the DOAS technique (Differential Optical Absorption Spectroscopy) are first considered. For each of the measurements with a SO_2 SCD above a threshold of 25 Dobson Units (DU), SO_2 optical depth spectra are interpolated from the LUT. Starting from an a-priori pair of SO_2 VCD and height, an SO_2 optical depth spectrum is calculated and subtracted from the total measured optical depth. SO_2 OD height and VCD derivatives are also determined from the sub-LUT (by finite differences) and used in the forward model matrix. Then the results of the fit (updates on SO_2 height and VCD) are used to calculate new SO_2 spectra for the next calculation and few iterations are performed until convergence is reached ($\alpha < 0.25$ km, $\beta < 5\%$ SO_2 VCD; see the illustration of the algorithm concept in Fig. 3). At the final iteration, the retrieval delivers SO_2 VCD and height. From the computational point of view, the SO2LH retrieval takes less than 0.1 s/spectrum which is fast enough knowing that only a small part of the pixels need to be processed.

Application of the algorithm to synthetic spectra (closed-loop retrievals) demonstrated the capability of the scheme to retrieve SO2LH, with theoretical precision and accuracy of a few hundred meters for input SO_2 VCD typically larger than 25 DU, as show in Fig. 4, with mean bias and rms of 180 m and 600 m, respectively. The application of our algorithm to real spectra from TROPOMI, shows that the accuracy requirement of 1-2 km is fulfilled in most cases, except in the presence of high aerosol loadings (notably volcanic ash), conditions for which the algorithm dramatically underestimate the SO_2 height.
To fix this potential problem, a solution is to use of the cloud top height as a proxy for the SO_2 height. If an explicit aerosol treatment cannot be applied, the pixels affected are identified and the reduced quality of the data is reported through a flag, comprehensively documented. For these flagged pixels, there will be non-compliance of the accuracy requirement of 1-2 km on SO2LH. Note that for such scenes, a good estimate of the SO2LH could still be obtained for the surrounding pixels of a dense ash cloud, where lower Aerosol Optical Depth (AOD) will take place (so called umbrella cloud effect).

The description of the quality flag of our SO2LH product is the following (AAI is the Absorbing Aerosol Index):

- Quality flag associated to SO2LH retrieval (activation for SO_2 SCD > 25DU).
- VCD is the SO_2 vertical column established assuming SO_2 profile with a centre of mass altitude of 15 km.
- flag = 0: SO2LH module not activated.
- flag = 1: SO2LH module activated but no convergence (number of iterations: max allowed).
- flag = 2: SO2LH module activated, low level of confidence due to absorbing aerosols (AAI > 4 or AAI missing).
- flag = 3: SO2LH module activated, medium level of confidence due to low signal (SO_2 improved for VCD >= 10 DU and VCD < 25 DU).
- flag = 4: SO2 LH module activated, medium level of confidence due to absorbing aerosols (AAI>4) with the use of nearest cloud altitude.
- flag = 5: SO2 LH module activated, high level of confidence, convergence with good data quality.

B. Operational implementation

TROPOMI SO2LH products have been created since April 2020 in automatic mode. As these data are obtained in the frame of a research application, the current time delivery for the spectral radiances from TROPOMI (used in our SO2LH algorithm) is ~ 6 hours. This will probably decrease to less than 2 hours in the future by using the official TROPOMI SO2LH products from ESA, which should be delivered in 2021-2022. This will definitely be of interest for the activity developed by the OPAS service.

III. Early warning and OPAS notification

The SO2LH alert products developed by OPAS and the implementation of early warnings are built on an existing EWS, so called SACS (Support to Aviation control Service) [13]. This system is dedicated to aviation and ATM, and was upgraded in the EUNADICS-AV (European Natural Disaster Coordination and Information System for Aviation) H2020 project with a total of 13 alert products of airborne hazards, based on the detection of volcanic SO_2 and 3 aerosols (volcanic ash, desert dust and smoke from wildfire) [14][15][16].

SACS provides alert products in NRT (images, email notifications and homogenised alert data products, so called NCAP – NetCDF Alert Products; NetCDF is a data format, i.e. Network Common Data Form). The two alert products from SACS/EUNADICS directly linked to the OPAS project are the SO2LH from IASI–A and IASI–B sensors.

Definition of the 3 types of alert products delivered by SACS:

NRT imaging on a dedicated web interface

Email notifications (with key information and link to dedicated tailored images)

Creation of homogenised alert data products (SO_2 height information, improved SO_2 mass loading, SO_2 contamination of the flight level, identification of source, and links to images)

Figure 5 illustrates the achievement of the OPAS project, presenting a snapshot of SACS/OPAS SO2LH alert products. The SO2LH products is only shown for IASI–A, IASI–B and TROPOMI. The SACS web-interface shows currently 5 UV instruments (TROPOMI and 4 others) and 3 IR instruments (IASI–A, IASI–B and another instrument).

In case a TROPOMI SO_2 slant column is over 25 DU, our algorithm is activated and SO2LH observations are retrieved. If the quality flag of at least one of the TROPOMI pixels reaches the value 5 (i.e. a high level of confidence; convergence with good data quality), an email notification is sent to subscribers.

SO_2 heights and improved SO_2 vertical columns (in DU) are simultaneously retrieved using our algorithm. A new SO_2 maximum can be obtained in the SO2LH notifications (Fig. 6),

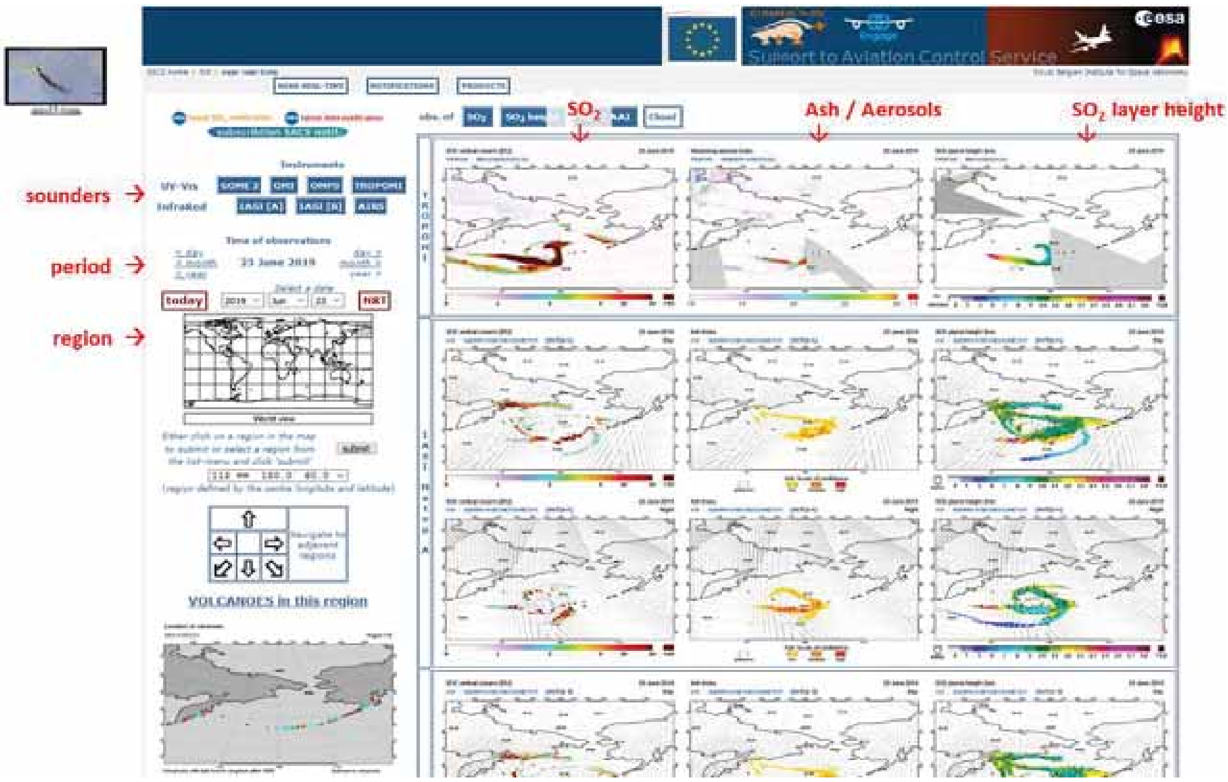

Figure 5: Snapshot of SACS website (http://sacs.aeronomie.be) showing an example of images (archive) for the Raikoke eruption on 22 June 2019.

especially if the SO_2 height is lower than 15 km, which is the assumed height considered in the SO_2 notification. An improved SO_2 mass loading is estimated using the new SO_2 vertical columns (with quality flags 3, 4 and 5). The notification level is based on the new SO_2 mass loading (if this mass is higher than 5 kt, the level is HIGH, otherwise it is LOW). The most likely name of the erupting volcano is mentioned.

The third OPAS SO2LH alert product is the delivery of a NetCDF data file. This file is an upgraded version of the existing SO_2 alert product developed in EUNADICS–AV project (Fig. 7). This existing NCAP data file is already created in NRT by SACS EWS in case of an exceptional SO_2 detection. Simultaneously with an SO2LH email notification, SACS EWS upgrades of the TROPOMI SO_2 NCAP file, incorporating the SO2LH data (see blue tags on data field in Fig. 7).

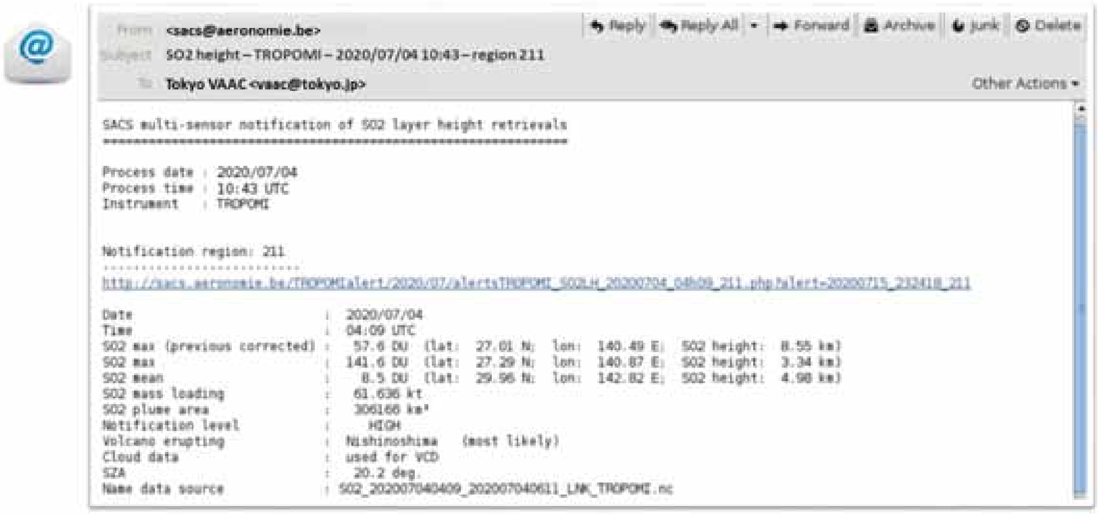

Figure 7: Illustration of the key information received by subscribers in the SO2LH email notification (with a link to dedicated web page).

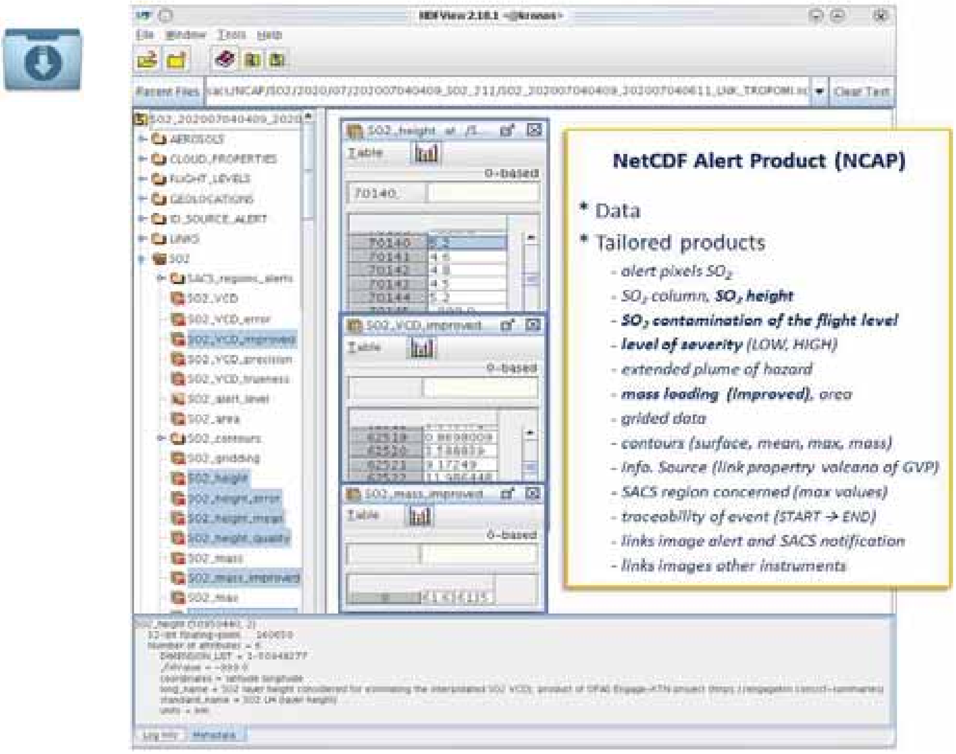

Figure 6: Illustration of the SO2LH NCAP data provided by OPAS.

Figure 7 illustrates NCAP data using the visualisation tool *HDFview*. This provides an overview of the field and variable accessible in the upgraded SO_2 NCAP file. The right yellow panel displays all the available information. The NCAP data provide detailed information, notably the SO_2 contamination of the flight level (FL).

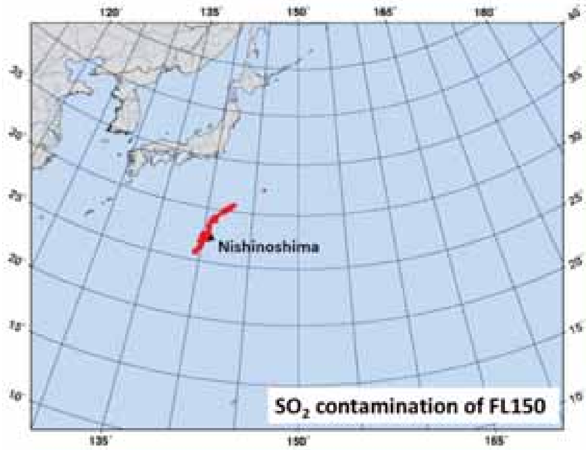

Figure 8: Illustration of the SO_2 contamination for FL150, as retrieved by TROPOMI on 4 July 2020 at 04:00 UTC.

For the example of the SO_2 height notification related to the eruption of Nishinoshima volcano, on 4 July 2020, the NCAP tailored products indicate that the most contaminated FL are FL090 to FL170 (between a range of altitude of about 2750 to 5200 m). Figure 8 illustrates the SO_2 contamination which could be of great interest for the VAACs if they take the responsibility of producing advisory report related to volcanic SO_2 plume.

IV. OPAS SWIM YELLOW PROFILE SERVICE

The registry of OPAS as a System-Wide Information Management (SWIM) Yellow Profile notification service requires a definition aligned with the ATM Information Reference Model (AIRM). This means the creation of information model, design of the service and a service description in SWIM terms. We have implemented the *OPAS SO2LH Dataset Service Definition* to complete the SWIM Yellow Profile service specifications.

The first transfer of information to SWIM Technical Infrastructure proposed by OPAS is the volcanic SO2LH alert product. This kind of transfer of information related to atmospheric volcanic emission, is considered, in the AIRM semantic, as a '*Meteorological Information Exchange*'.

The specification of the requirements and the Technical Infrastructure (TI) of a SWIM Yellow Profile is completed [17].

The steps in transitioning to SWIM Yellow Profile are the following:

1. Ensure information exchanges are properly defined and understandable for the stakeholders.
2. Create information model ("information definition" in SWIM terms).
3. Design the service ensuring it uses options from the SWIM TI Yellow Profile.
4. Implement and deploy the service (creation of a "service description").
5. Register the service in the SWIM Registry.

The OPAS project has achieved steps 1 – 4. A definition of OPAS notification service has been written in JSON (JavaScript Object Notation) format. In addition, OPAS information definition (xlsx file) has been written to provide Concept Definition and conformance to AIRM. The service description of OPAS Yellow Profile captures the fact that

- subscription is by email. Notifications of SO_2 alerts with SO2LH are sent to subscribers.
- an Internet Protocol (IP) address has to be provided, giving access right to BIRA *https* server.

The registry of OPAS as a SWIM service, is nearly completed (i.e. step 5) and a first draft of what it will look like has been created (see Fig. 9).

V. CONCLUSIONS AND PERSPECTIVES

The OPAS project offered an opportunity to create a bridge between SACS/EUNADICS EWS and SESAR (Single European Sky ATM Research) SWIM. The following achievements were reached:

- the algorithm development and the operational run of TROPOMI SO2LH retrieval,
- the implementation of TROPOMI SO2LH alert product and the upgrade of IASI–A & –B SO2LH alert products, with FL SO_2 contamination information,
- the definition of the OPAS dataset notification service, with the creation of an information model, the design of the service and its description in SWIM terms.

Such an achievement is promising for the next goal, i.e. the creation/registry of a SWIM Yellow Profile service dedicated to the notification of early warnings of natural airborne hazard. The SESAR ALARM (multi-hAzard monitoring and earLy wARning system) project, recently awarded, will take OPAS on board and upgrade SACS EWS.

The OPAS Engage-KTN project was also a great opportunity to consider some recent communications from the industry (Rolls-Royce), and to convincingly highlight the consequent risk of the SO_2 contamination in term of maintenance costs (contract for the stakeholders and turbine maintenance for the aircraft manufacturers), in addition to safety and health problems for the passengers during a long-line flight exposure.

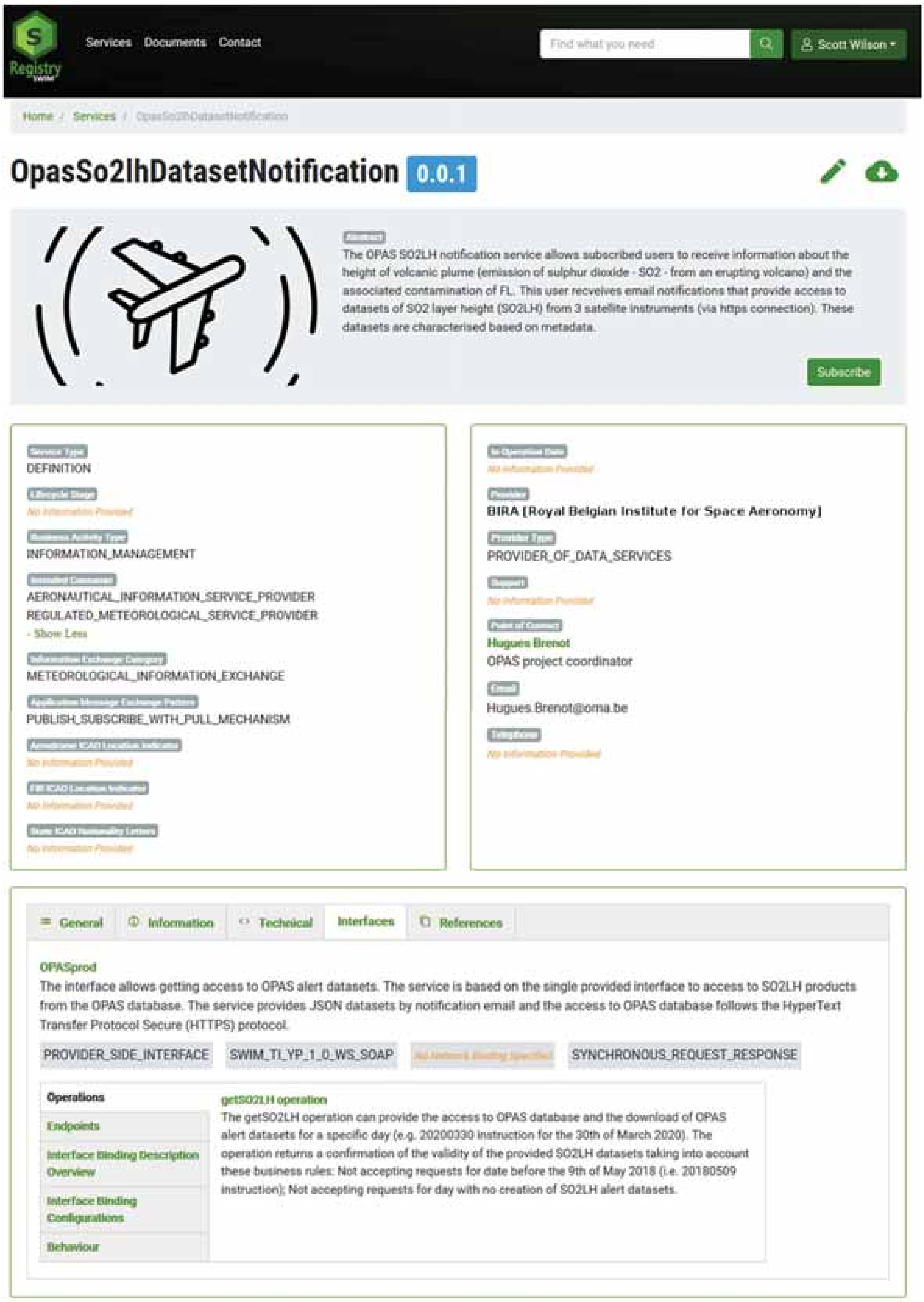

Figure 9: Draft of OpasSo2lhDatasetNotification SWIM Registry.

The transfer of homogenised NRT SO2LH observation via a SESAR SWIM Yellow Profile service, providing unambiguous (i.e. with selective SO_2 detection) and easy to interpret information, may benefit to all the operational ATM users for supporting aviation safety. The development of NRT information about the FL SO_2 contamination represents a real interest for the stakeholders, especially to the airlines and aircraft manufacturers.

The next step of the OPAS project, that will help increase the maturity towards such an activity, are the following:

- The finalisation of the SWIM registry of OPAS as a Yellow Profile service.
- The achievement of consolidated results of validation for the TROPOMI SO2LH using several external sensors.

To complete the first results of TROPOMI SO2LH validation, additional comparison with data from IASI, CrIS, SEVIRI (Spinning Enhanced Visible and Infrared Images), CALIOP Cloud-Aerosol LIdar with Orthogonal Polarization) instruments, GNSS (Global Navigation Satellite System) radio-occultations and ground-based data from FLAME (FLux Automatic Measurements) network at Etna, are being investigate [10][12][18][19][20]. Reports from pilots and trajectory of flights will also be considered in the validation process, showing the impact on air traffic of recent volcanic eruptions and highlighting the interest of OPAS new development (SO2LH) to mitigate the risk for ATM.

ACKNOWLEDGMENT

We thank the Engage-KTN (Knowledge Transfer Network) catalyst funding for the development achieved in the frame of OPAS project (Thematic Challenge 3; https://engagektn.com) of SESAR Joint Undertaking (https://www.sesarju.eu). This was a great opportunity to bring together research institution, aircraft manufacturer and company providing decision intelligence to aviation. This project has received funding from the SESAR Joint Undertaking under the European Union's Horizon 2020 research and innovation programme under grant agreement No 783287. The opinions expressed herein reflect the authors' view only. Under no circumstances shall the SESAR Joint Undertaking be responsible for any use that may be made of the information contained herein.

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