

## **Reply to Juan A. Añel (Feosc. Mod. Dev. Exec. Editor)**

Our paper uses SO<sub>2</sub> **data** or **products** and we often referred to them as ‘retrievals’ in the original version of the paper. No work with any retrieval code has been carried out for this paper, it is simply a data assimilation paper. It should be possible to reproduce the work described in this paper by just using the TROPOMI SO<sub>2</sub> data and the model output, and no access to the TROPOMI retrieval algorithm is required.

We realize that we used the term ‘retrieval’ a lot when referring to the data and have made some changes to the document and replaced a lot of those ‘retrievals’ with ‘data’ or ‘products’ in the text. This makes it clearer that the paper is utilizing data and not developing or refining a retrieval algorithm. We have also replaced the one location where we used ‘retrieval algorithm’, i.e. “Improvements to the FP\_ILM retrieval algorithm are on-going” with “Improvements to the TROPOMI SO<sub>2</sub> LH product are on-going”.

We have added a DOI for the TROPOMI LH data used in this study, a link to the ESA S5P website where the operational S5P SO<sub>2</sub> data can be downloaded and additional information about the ECMWF code and availability. Note, that we had already provided DOIs for the data assimilation experiments used in this paper.

We will upload a modified version of the paper.

### **Code and Data availability**

This study was based on the IFS model cycle 47R1. The ECMWF IFS code is only available subject to a licence agreement with ECMWF. ECMWF member-state weather services and their approved partners will get access granted. The IFS code without modules for assimilation can be obtained for educational and academic purposes as part of the openIFS release (<https://confluence.ecmwf.int/display/OIFS>, last access 26/10/2021). A software licensing agreement with ECMWF is required to access the OpenIFS source distribution: despite the name it is not provided under any form of open-source software license. License agreements are free, limited to non-commercial use, forbid any real-time forecasting, and must be signed by research or educational organizations. Personal licenses are not provided. OpenIFS can-not be used to produce or disseminate real-time forecast products. ECMWF has limited resources to provide support and thus may temporarily cease issuing new licenses if it is deemed too difficult to provide a satisfactory level of support. Provision of an OpenIFS software license does not include access to ECMWF computers or data archives other than public datasets. A detailed documentation of the IFS code is available from <https://www.ecmwf.int/en/publications/ifs-documentation> (last access 26/10/2021). The output from the assimilation experiments used in this study is available from <https://apps.ecmwf.int/research-experiments/expver/> (last access 26/10/2021) using the following DOIs for the 6 experiments:

- [hhu5: 10.21957/cygt-xf49](https://doi.org/10.21957/cygt-xf49)
- [hgze: 10.21957/qfam-7474](https://doi.org/10.21957/qfam-7474)
- [hhbu: 10.21957/zpdt-f079](https://doi.org/10.21957/zpdt-f079)
- [hhtm: 10.21957/jraa-s174](https://doi.org/10.21957/jraa-s174)
- [hhtn: 10.21957/ddxs-2v95](https://doi.org/10.21957/ddxs-2v95)
- [hgz7: 10.21957/81bh-7h58](https://doi.org/10.21957/81bh-7h58)

The TROPOMI V3.1 SO<sub>2</sub> LH data are available from <https://doi.org/10.5281/zenodo.5602935>, the operational TROPOMI SO<sub>2</sub> data from the Copernicus Open Access Hub (<https://scihub.copernicus.eu/>) and the IASI SO<sub>2</sub> plume height data from <https://en.aeris-data.fr/>.