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Improving algorithms and uncertainty estimates for satellite NO_2 retrievals: results from the quality assurance for the essential climate variables (QA4ECV) project

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Supplement to:

Improving algorithms and uncertainty estimates for satellite tropospheric NO_2 retrievals from the Quality Assurance for Essential Climate Variables (QA4ECV) project

1. User needs and expert recommendations

The NO_2 users, mostly from academia and policy support, responded that NO_2 data products available at the time generally provide quality flags, but that the information is limited. They recommended that the data products should include more detailed quality flags describing the condition of low quality measurements, along with a master flag ('use' or 'do not use') for quick inspection. Figure 1 indicates that NO_2 data users ask for information on whether scenes are affected by cloud and aerosol contamination, sun glint, sensor status (e.g. row anomaly), and whether measurements were done over land or over sea, or over snow/ice.

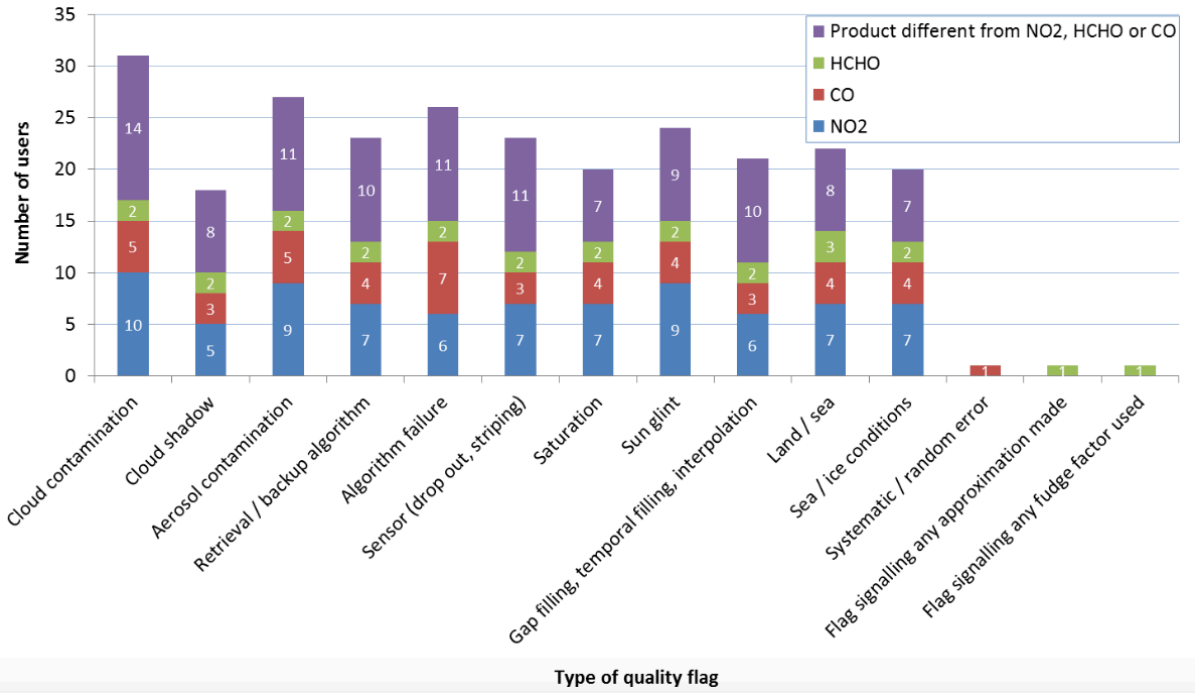

Figure S1. Response to the user survey question 'What additional information would you like to see provided as a quality flag?' in a NO_2 satellite data product (blue bars).

Current NO_2 data products often contain information on algorithm uncertainty on a per-pixel basis, but users indicated that they need specific information on the systematic and random error parts contributing to the stated uncertainties, on long-term stability of the data record, and on the dependence of the uncertainties on the ancillary parameters cloud fraction, cloud

pressure, surface albedo, aerosols, and temperature. Users said they needed this information in inverse modeling and data assimilation experiments in order to apply realistic weights to the observations and the modeled fields, and for weighting and filtering in trend analyses and mapping.

Respondents also stated that it was important to provide traceability information and processing information along with the NO_2 data product. Full schematic details of a processing chain for the NO_2 satellite data product should be provided. When asked why they needed such information, the most common answers were: "to understand the data", "to identify sources of uncertainty" (in the retrieval algorithm), to apply appropriate "data filtering", and "to account for uncertainty in further processing" of the NO_2 data for their own purposes. Traceability information would have to be made available at a point of central access, along with other documentation on the data processing, such as an Algorithm Theoretical Baseline Document (ATBD) and a Product Specification Document (PSD) with guidance on how to use or not use the data.

Last but not least, the users found a systematic validation of the NO_2 data product with coherent independent reference data to be desirable, especially if the independent reference data itself is properly quality-assured. Information on the validation status of the product would preferably be gathered in a central access point, along with the traceability information. Within the QA4ECV project, these recommendations have led to the development of a so-called Quality Assurance (QA) System. Within this system (available at: http://www.qa4ecv.eu/qa-system), data producers have the possibility to provide all these pieces of information, and users can obtain a quick overview of the maturity and completeness of the data product.

2. Producer requirements

We did a survey of data producer requirements for quality assurance in satellite data records. We interviewed producers of satellite data other than those involved in QA4ECV. The response told us that satellite data producers recognize that traceable input (ancillary data) files, read-in software, sensitivity analysis documentation, and publications are not always provided along with the data, but preferably should be. Data producers stated that direct communication with their data users is important, mostly on issues including read-in software, product format, flagging and filtering procedures, and the uncertainty budget. In general, data

producers thought that the necessary traceability and quality information is in principle available, but cannot always be easily found. These recommendations helped shape the QA4ECV QA System [Nightingale et al., 2018]. Within this system, data producers have the possibility to provide all these pieces of information, and users can obtain a quick overview of the maturity and completeness of the data product. Data producers were generally positive about benchmarking their satellite data product against other scientific standards, such as from cross-calibrated global validation networks. They noticed that quality information for independent reference data is often not available. For more detailed outcomes of the ECV data producer survey, please see QA4ECV Deliverable 1.1 [Nightingale et al., 2015].

3. GCOS guidelines for generation of NO_2 ECV datasets

The guidelines established in GCOS report 138 [GCOS, 2010] are paraphrased below in Table S1, together with the response by the QA4ECV NO_2 consortium.

Table S1. Summary documenting point-by-point the extent to which GCOS guidelines for the generation of an ECV dataset [GCOS, 2010] has been followed, here for NO_2.

	GCOS guideline	**Addressed how?**
1.	Full description of all steps taken in the generation of the QA4ECV NO_2 product, including algorithms used, and characteristics and outcomes of validation activities.	This paper, QA4ECV D4.2 (Muller et al. [2016]), QA4ECV D4.5 (Muller et al. [2018]), QA4ECV D6.1 (Compernolle et al. [2018]).
2.	Application of appropriate calibration/validation activities.	This paper, QA4ECV D4.2 (Muller et al. [2016]), QA4ECV D5.6 (Compernolle et al. [2017])
3.	Statement of expected accuracy, stability and resolution (time, space) of the product, including, where possible, a comparison with the GCOS requirements.	This paper (section 6, Section 2.3) QA4ECV D5.5 (Boersma et al. [2017])
4.	Assessment of long-term	QA4ECV D6.3 (Boersma et al. [2018]), Zara et al.

	stability and homogeneity of the product.	[2018]
5.	Information on the scientific review process related to FCDR/product construction (including algorithm selection), FCDR/product quality and applications	This paper (section 4), QA4ECV D4.2 (Muller et al. [2016]), Lorente et al. [2017], Zara et al. [2018]
6.	Global coverage of products where possible	Global coverage is achieved in 1 or more days, depending on the sensor. See daily QA4ECV NO_2 maps on www.qa4ecv.eu/ecv/no2-pre/data.
7.	Version management of products, particularly in connection with improved algorithms and reprocessing.	Thusfar a QA4ECV NO_2 ECV algorithm v1.0 and v1.1 have been developed. The former contained a bug in the stratospheric correction, and was superseded with v1.1, which constituted the final product. v1.1 is publicly available from www.qa4ecv.eu/ecv/no2-pre/data, and via digital object identifiers.
8.	Arrangements for access to the products and all documentation.	QA4ECV NO_2 ECV data are freely available via the project website (www.qa4ecv.eu/ecv/no2-pre/data), and relevant documentation including a Product Specification Document and the DOI's is provided along with the data.
9.	Timeliness of data release to the user community to enable monitoring activities.	Data for July 1995 – November 2017 has been released.
10.	Facility for user feedback	The QA4ECV website contains a so-called 'NO_2 ECV Forum' (http://www.qa4ecv.eu/forum/267), where users can ask questions and provide feedback.
11.	Application of a quantitative maturity index if possible	A maturity matrix analysis has been carried out twice for the QA4ECV OMI NO_2 products, once via self-assessment in the QA4ECV Quality Assurance Report (http://ec2-52-56-155-184.eu-west-2.compute.amazonaws.com/#/summary-reports?id=04335219574c), and once by EUMETSAT in

		QA4ECV D6.1 (Compernolle et al. [2018]).
12.	Publication of a summary (a webpage or a peer-reviewed article) documenting point-by-point the extent to which this guideline has been followed.	This table.

4. Mapping QA4ECV OMI NO_2 columns to the MAX-DOAS location of Tai'an

In our validation of OMI QA4ECV NO_2 columns with independent MAX-DOAS data, we account for the location of the pixel relative to Tai'an. Figure S2 below shows the average (June 2006) OMI NO_2 columns as a function of distance to Tai'an. It shows that, on average, OMI pixels within 20 km of Tai'an are within the 5-7×10^{15} molec. cm^{-2} range, i.e. within 1×10^{15} molec. cm^{-2} of the June 2006 average value at Tai'an. This shows that the correction factor in Eq. (6), the ratio of the climatological column at Tai'an to the climatological column at the location of the individual OMI pixel, is always in the range 0.85-1.15.

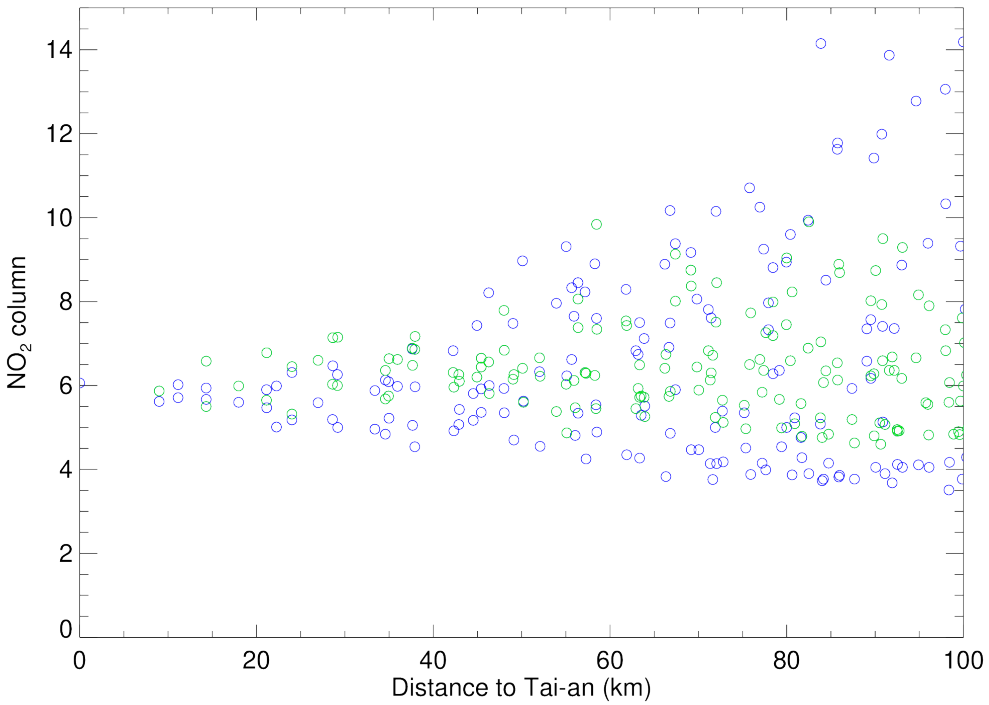

Figure S2. Campaign-mean QA4ECV OMI tropospheric NO_2 columns (May-June 2006, in 10^{15} molec.cm^{-2}) as a function of distance to Tai'an. Blue circles indicate values of cells east of Tai'an (Figure 13), green circles west of Tai'an. The value for a distance of 0 km, is the campaign-mean tropospheric NO_2 column over Tai'an itself (6.06×10^{15} molec.cm^{-2}).

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