Interactive comment on “Improved OSIRIS NO$_2$ retrieval algorithm: Description and validation” by Christopher E. Sioris et al.

Anonymous Referee #2

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The authors present an improved algorithm for NO$_2$ vertical profile retrieval for the limb satellite instrument OSIRIS. They implement two main features: (1) apply larger fit window and (2) account for the diurnal variation along the LOS and Sun direction by combining two- or three dimensional forward model with a photochemical model. In validation studies they investigate statistical agreement between OSIRIS NO$_2$ profiles and a data set of balloon measurements obtained by different groups and instruments in the northern hemisphere. I acknowledge the presented concept, but at the same time I see the following critics which should be solved before the final publication (please find the motivation background within the detailed comments later):

(1) Algorithm description: the algorithm is rather poorly described. Neither there is structure of the algorithm sufficiently presented with clear references for details nor are the implementation of the new improvements (in particular the implementation of the C1
accounting for the diurnal gradient) clearly and in detail described.

(2) Besides that (but closely related) there is practically missing scientific discussion on the importance of the new improvements to the scientific community. It is not clear if the newly introduced concepts are new also outside the author team, are there alternatives, are they applicable or have perhaps already been applied for other algorithms, models, instruments? (3) validation study: there are either conclusions made based on a single profile or on a very general statistical behaviour without discriminating between type of balloon instrument, its measurement/retrieval technique, location, season, time (SZA) etc. Also it happens often that too much positive conclusions are suggested although plots indicate that it is not always the case.

Detailed comments:

P1, L19 "LOS column densities": is the definition the same as for slant column densities (SCDs) used later? If yes, be consistent, otherwise provide definition.

Introduction, 1st paragraph: The statement needs references.

P2, L17: be more specific what gradients do you aim to consider (nadir instruments also sees strong gradients). Maybe you want to say that a limb instrument has in addition to deal with horizontal gradients.

P3, L18-19 “The accuracy is due to two main factors: very high signal-to-noise…”: Higher signal to noise ratio mostly improves precision (not the accuracy), doesn’t it?

Last sentence P3 “occulation/limb occultation”: skip occultation on P4, L1

Sect. 2. The basic algorithm description is limited to 1(!) sentence, not to say that the chapter ‘methods’ starts right away with subsection “Algorithm settings”. To what then these settings are applied? Please provide background, an algorithm diagram would be helpful.

P4, L6-8: Also this statement requires references. The previous work of "many groups"
must be cited. From one side the methods and previous work cannot be known for unfamiliar readers, from another side the authors should give proper credit to previous work done in the field. When filtering in particular with regard to NO2 and limb satellite and balloon measurements the reference list is not long anymore.

P4, L9 What spectral fitting technique is used, is the fit done in optical thickness domain (e.g. DOAS) or radiance domain, or...? Some paragraphs above there are provided a number of references of author’s previous work. Please cite here the paper where the particular part of the algorithm is described in detail. And again, it is clear that brief introduction to the algorithm would be helpful, otherwise the reader must search through at least the 4 author’s papers cited above to puzzle the basic algorithm build-up.

P4, L15 “Water vapour absorption is neglected despite maximal absorptions of >0.1%”: There is an ongoing discussion about water vapour absorption on short wavelengths (e.g. Lampel et al., AMT, 8, 4329, 2015). On what source, absorption database, cross-sections etc. the considerations of authors are based? Have you investigated effect of possibly different placement of absorption lines and their strengths?

P4, L21 at this stage one can puzzle out that an iterative algorithm is used. Again please make the basic algorithm setup clear. E.g. what is done by simulated and measured radiances, fit results, perhaps a diagram might help.

P4, L26 what is SCIAMACHY? The instrument must be introduced already earlier as an example of another limb sounding satellite instrument since the OSIRIS is not the one and only limb instrument. In fact there are not so many limb sounding satellite instruments that it could be worth to introduce some of them, at least those, the authors are citing.

P5, L10; P6, L1 “Odin” -> “OSIRIS”

P5, L23 Perhaps add “since at least” before the reference in the brackets
Same sentence as above: “to recover . . . along-track distribution . . .”: While the retrieval of vertical distribution is described in authors’ earlier publications, this aspect for their algorithm is very new. It is also not clear from the manuscript if at all and, if yes, how in detail the along-track distribution is recovered. The text below in this subsection just suggests that one is inquiring (1D) profiles with a 2D or 3D photochemistry correction. If it is like that then citing here a more general publication where 2D fields are inquired from correlated scans along orbit without any comment is misleading.

P5, L29 “Five orders of scattering are used” Perhaps you mean "up to five orders". Anyhow, please explain what you mean here otherwise it reads as a technical slang. Are five orders enough for scenes above (thick) clouds? What is the accuracy then? Or do you filter complete scans for measurements above the cloud scenes out?

Sect 2.2. This short section hides the main improvement of the manuscript. Therefore it is much too short. More details are needed to understand your method and also scientific discussion in the context of the current state of the art is completely missing:

- it is important to say e.g. that photochemical correction capability has been demonstrated already earlier (McLinden et al., JGR, 2006 as an example) even without the 2D or 3D RTM model and discuss what is then benefit (is there benefit at all?) of the 2D or 3D model with respect to the previous corrections? Can now the gradient be accounted better? Why? Are there some studies done in that respect? What are the results?

- Also the possibility of simultaneous retrieval of different limb scans along orbit by a tomographic concept must be discussed being a really clear benefit of a 2D RTM model as e.g. already demonstrated for a rather similar retrieval of NO2 by Pukite et al., ACP, 2008 for SCIAMACHY. In such a case even photochemical modelling can be redundant to a large extent. Nothing is said if such a concept can be an alternative for the OSIRIS retrieval or it is even already considered at some retrieval step. If yes, please describe how the benefit by correlating the scans is considered in the described 2D
and 3D algorithm and how it matches with the photochemical modelling. Anyhow can you provide more details what you are doing in the new 2D and 3D algorithm, what exactly are implications to the parts of retrieval: forward modelling, spatial reconstruction, iteration process? Is there at least some correlative processing of the profiles obtained for different OSIRIS vertical scans in some of these steps to fully use 2D, 3D model capability or they are processed separately?

- The latitudinal resolution of 5 deg looks rather course (following this horizontal distance from TP means that LOS crosses altitude region of \( \sim 25 \) km, so almost the whole NO2 retrieval altitude range is within this horizontal region). Can the model assume at least liner variation between the grid points? Otherwise this could be a reason for the rather poor improvement of the 2D corrected retrieval with respect to its 1D alternative? Do sensitivity studies exist regarding this? How the horizontal model grid is matched with measurement and retrieval grid?

P7, L2: “the OSIRIS 2D and 3D profiles are retrieved…” if the profiles/OSIRIS scans along orbit are not correlated in any of the retrieval steps (which is not really clear from the few information provided, see one of the previous comments) then they are individual 1D profiles. One then cannot speak about 2D or 3D profiles like it would be if really a simultaneous (e.g. tomographic) retrieval for different scans would be performed. Please avoid misunderstanding and say e.g. “profiles with 2D or 3D photochemical correction”.

P8, L28 “1D inversion approach”: do you mean retrieval without modelling diurnal gradients?

P9, 1st paragraph: The difference in the figure is very small. I doubt that from so few measurements (just 33 scans and so small difference) it is possible to make a clear conclusion that the new fit window is better. Please indicate the sample standard deviation on the figure to clarify this. In order to increase the confidence could the improvement be proved on a much larger dataset? You do not need to stick to profiles
matching the balloon measurements here, do you? Another aspect: one should be certain that there are no covariance between the measurements and retrieved profiles for such a conclusion to be valid, e.g. if there is some kind of a-priori effect or correlated instrument feature at certain wavelengths (for what reason ever) one also could get lower variability.

P9, L5 add “left plot” or “left panel” after “Figure 2”

P9, L9 the improvement is very small, add “slightly” before “improved”

P9, L10 “and the upper altitude limit of the retrieval moves slightly higher...”: It is not said what do the colorshaded regions in Fig.2 mean? Supposing they represent error (one standard deviation), then this statement on L10 contradicts the figure: error for the extended window is larger at the uppermost altitudes. What is the reason for this strange result since one should expect better performance?

P9, L11 add “right plot” or “right panel” after “Fig. 2”

P9, L14 “The significant upper tropospheric NO2 enhancement...” The enhancement is not significant if comparing with the error: the relative enhancement for the new fit window might be large at these altitudes but both profiles still lay within the errorbars of each other. Therefore it would be good to skip "significant" here. Can you provide more proof that this is generally the case also for other profiles? At least it seems contradictory to other retrieval methods in Fig. 6 and 7 where the retrieval shows negative bias with respect to the validation dataset. Can you include 1D retrieved for the fitting window from v3.0 algorithm in Figs. 6 and 7 as well?

Paragraph discussing Fig. 3 on P8, L16-26: At 20 km altitude 2D&3D versions have larger values than 1D, is there an explanation? All versions disagree with balloon above 21 km or so, can you also explain this? I suppose you selected the best plot for the illustration here. How is about other individual profiles? I would recommend providing the comparisons of the individual profiles for the whole validation dataset as
a supplement.

P10, L1, Fig.4: Why sample size of 2D is not shown in the figure. Please mention if the sample agrees with that of 1D.

P10, L23-25: Can you comment what factors (RTM, forward modelling, chemical modelling, inversion) are impacting how the processing time for the different dimension versions, i.e. is the increased calculation burden in 2D and 3D just due to the chemical modelling?

P11, L10 & Conclusions P13, L28: the biases clearly exceed 10% (I see by eye up to 13% bias, i.e. by one third more than 10%). It is also evident that 2D product has larger bias than 1D, in particular at altitudes below 20 km. please discuss.

P11, L13-L15: “In contrast to ‘fast’ and v3.0 products, there are no altitudes in the lower stratosphere (below 24 km) with statistically significant average and median biases for the 1D and 2D products”: this statement is incorrect: in Fig. 7 the bias clearly exceeds error at 15.5 – 20.5 km for 2D...

P12, L11-16, Fig.9: There is no significant differences in the correlation for most of the altitudes between the different products, as a consequence clear conclusion on a better performance of a certain algorithm cannot be derived. Can you comment on the relatively high correlation of the fast product in the lowermost stratosphere? Is it due to the better forward model?

P14, L11-L14: Although the presented concept of photochemical correction seems promising, from the results shown (in particular on Figs. 6&7 but also on other plots as commented above) it is hard to speak about a clear improvement for the new algorithm. Especially at the lowest altitudes the bias (see Fig. 7) is the largest. I recommend to extend the study by investigating the behaviour of the agreement for different conditions (e.g. season, location, SZA, different instruments, techniques ...) A study comparing the real gradient (from OSIRIS), gradient simulated by the chem. model and the
correction on profile would be interesting. Do the gradients simulated by the chem.
model follow real gradients in all cases? Certainly also the effect of horizontal model
resolution should be investigated which seems to be much too coarse (see above).