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Near Infrared Nadir Sounding of Vertical Column Densities: Methodology and Application to SCIAMACHY

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We would like to thank all reviewers for the useful remarks and recommendations. We have worked on all requests and the implementations in the manuscript are indicated by colors and a margin remark.

Figure assignments: As the positioning of subplots is still subject to change, we have not corrected all “left/right” versus “top/bottom” pointers.

1 Review 1

1.1 Suggestive Changes to the Main Body

R1.1. Section 2.1, page 3688, lines 12-13:
References and a brief justification for neglect of scattering added in text.

R1.2. Section 2.3.1, page 3694, line 18:
Replaced Buchwitz et al. (2000) by Buchwitz et al. (2006).

R1.3. Section 2.3.1, eqs. (19) and (20):
"XGas" has been replaced with "xGas" throughout the paper

R1.4. Section 3.1, page 3697, line 1:
Interval definition changed.

R1.5. Section 3.4, page 3700, line 9:
References added. The ice layer leads to a reduction of the instrument transmission and to a broadening of the spectrum. Lichtenberg et al. (2006); Gloudemans et al. (2005) pointed out a "continuous change of the slit function" due to the growth of an ice layer and, since scattering produces broadening, the change is indeed to a wider slit function.

R1.6. Section 4.2.2, page 3709, line 4:
Clarification added in text.

R1.7. Section 5, 2nd paragraph: We did not want to give the impression that BIRRA is better than a carefully designed DOAS algorithm. To be more precise we slightly reformulated the paragraph. See also Frankenberg et al. (2005) for a detailed discussion.

R1.8. Section 5, page 3711, line 17:
The SMR acronym has been repeated to make the summary self-contained.

R1.9. Figures general Some annotations have been enlarged.

R1.10. Figure 2: The caption has been corrected.

R1.11. Figure 6: The large scatter of the SMR values was due to bad/dead pixels, instrumental noise, and solar spectral lines. The intention was to show the impact of the ice layer in channel 8, so no pixel masking has been employed. For the sake of clarity we redrew the figure without bad/dead pixels.

R1.12. Axis Time Figure 11, 12, 16 Better time annotations to help to the understanding of the time series figures will be provided.

2 Review 2

2.1 Major remarks

R2.1. averaging kernels:
A discussion on altitude sensitivity has been added to subsection 2.2.3.

R2.2. instrument-noise related errors:
A new subsection 4.2.1 has been added addressing the carbon monoxide retrieval errors. Spatial and seasonal distributions of the errors have been included, as well as the associated histograms and the number of observations falling into longitude/latitude grid pixels.

The instrument-noise related errors affect the precision of the fit, whereas forward model errors lead to systematic errors affecting thus its accuracy. It is possible to deal with instrument-noise and model errors simultaneously by substituting the data errors with so-called "equivalent white noise" which combines both sources of errors (see e.g. Doicu et al. (2010)). The net effect of this substitution is the elimination of the model bias by the cost of increasing the noise error variance. Since BIRRA solves the optimization problem using this approach, the error analysis presented in subsection 4.2.1 is based in the combined retrieval errors, and consequently are expected to be larger than the instrument-noise related errors.

Note that under complicated scenarios (as e.g. observations containing broken convective clouds), the contribution of the forward model error to the retrieval error might be larger than the instrument-noise related error. Hence, only analyzing the total retrieval error is it possible to entirely explain the error spatial distributions whose maxima are located at low latitudes over the ocean.

2.2 Other questions/remarks

R2.3. Which a priori?
As we do not apply regularization (except for an optional positivity constraint), there is no a priori in BIRRA in the sense of optimum estimation. Atmospheric profiles are taken from climatology as discussed in section 3.8, i.e. US standard for VMR's and CIRA for p and T (see also response R2.8). The initial guess values of the molecular density scaling factors α_m (cf. eq. (11)) is one (our tests indicate that the fits are independent of the initial guess; note that in case of the separable least squares no initial value is required for the linear parameters β in subsection 2.2.2).

R2.4. Which methane columns?
CO retrievals utilize channel 8 data only (4282–$4303\,\mathrm{cm}^{-1}$), and the methane scaling factor or column is retrieved concurrently with the CO scaling factor.

R2.5. Section 2.3.2. Cloud data are taken from the SCIAMACHY Level 2 product, i.e. the cloud fraction has been calculated with OCRA (Optical Cloud Recognition Algorithm), and the cloud top height with SACURA (SemiAnalytical CloUd Retrieval Algorithm). Since the cloud information is available at the higher spatial resolution, cloud products have been averaged to the actual integration time of the fitting windows — in channels 6 (for CH4/CO2) and 8 (for CO). (A remark has been added at the beginning of section 3)

R2.6. Section 2.3.2. CO retrievals over ocean
Section 2.3.2 has been extended including a detailed discussion on retrievals over the ocean.

A glance to the retrieval error spatial distributions presented in section 4.2 illustrates that error maxima are located over the oceans — more precisely at the intertropical region where convective clouds are present —, indicating that they are subject to improvement. This is not a specific problem of BIRRA but a challenge for all atmospheric trace gas retrievals. Averaging over long time periods (increasing the number of observations) or over large areas (e.g. smoothing with a median or a mean filter) helps to reduce the errors of XCO over the ocean.

R2.7. Section 3 summary:
A brief summary has been given in the final section 5, paragraph 4 (mid of page 3711) (now paragraph 5).

R2.8. Atmospheric data
We are aware of the limitations of the CIRA climatology, and switching to better data (NCEP or ECMWF) is one of the more important items of our to-do list. Sensitivity studies using several AFGL atmospheres showed that the impact of the reference atmosphere is low.

R2.9. Channel 8 ice layer:
As already discussed by (Lichtenberg et al., 2006; Gloudemans et al., 2005), the ice layer leads to a broadening of the spectrum. To account for this effect, BIRRA treats the slit function width as an additional fit parameter in the channel 8 CO retrievals. The possibility to fit the slit function width has already been mentioned at the end of subsection 2.2. A note has been added in subsection 3.4 discussing the ice layer. See also response R1.5.

R2.10. Section 4.2 introduction to CO
Certainly the first paragraph is a very condensed "introduction to atmospheric CO" that nevertheless might be useful for an "understanding" of the results presented here. As it occupies only a very small fraction of the total paper the removal would not significantly reduces the size of the manuscript. The second paragraph should be useful for readers looking for similar results retrieved from other spaceborne sensors. Accordingly we would like to keep this introduction in its present form.

R2.11. Spatio-temporal patterns
As emphasized in the introduction, the objective of the manuscript is to present the algorithmic methodology, and section 4 is intended to provide only a brief snapshot of BIRRA's capabilities. We added some more references to SCIAMACHY, AIRS, and MOPITT papers discussing spatial/temporal patterns.

R2.12. Comparison with ground-based measurements
It is already mentioned in the section 4.3.2 (previously 4.2.2) that the comparison of "column" mixing ratios with "volume" mixing ratios present is delicate. However, in view of the good qualitative agreement (time evolution), the authors would like to keep the figure in the manuscript.

R2.13. Figures 3 or 5 vs. Figures 13 – 15
Since individual retrievals have large errors, specially over the ocean, the scatter of the data is evident. Further, figures 3 and 5 (now 4 and 6) represent results of sensitivity studies and, in some cases, under non-ideal configuration, what hampers the quality of the retrievals. On

the other hand, figures 3 and 5 (now 4 and 6) show monthly averages, whereas the figures in section 4 show seasonal or annual averages, what reduces the noise. The different grid pixel size also contributes to the appearance.

R2.14. Figures 3, 5, 7, 9, 13, 14, 15, 17
Info on sampling area and smoothing have been added to figure captions. Data have been resampled on a regular grid with weighted averaging (with inverse variance) of single observations falling inside a grid pixel.

3 Review 3

3.1 Major points of criticism

R3.1. It is common practice to present first/preliminary results on conferences and workshops (ideally documented in proceedings that, however, are "probably not readily available" (quote from detailed points of criticism b)), and, once the material is more mature, to submit a manuscript to a well established journal (ideally recognized by ISI Journal Citation Report). Actually we were asked from several sides (e.g., ESA) to publish our methodology and results in a recognized scientific journal (conference proceedings are frequently considered as "irrelevant" or even "non–existent"). As BIRRA is the algorithmic basis of the operational SCIAMACHY carbon monoxide and methane nadir retrievals, this paper should be as complete and self-contained as possible. Moreover, we are convinced that our approach is sufficiently distinct from others to justify some "repetitions". In particular we do not have any concerns in "verbatim" reusing two or three of our own sentences published in "not readily available" proceedings.

Finally, the 6 pages proceedings paper (Schreier et al. 2007, co-authored with the Bremen group) describes BIRRA as of 2006 (actually BIRRA is described on about a half page, and the "application" is restricted to a single orbit), and clearly cannot reflect the code/algorithm upgrades and new applications of the past five years, e.g., modularization of the code (f77 $\rightarrow$ f2003), multiple spectral windows, methane retrievals in channel 6, ... Furthermore considerable effort has been put on development of pre– and post–processing tools mandatory for processing of large amounts of data beyond a single orbit. (See also last paragraph of this subsection, page 8.)

R3.2. Non-quantitative effects of various error sources:
Quantitative estimates of the effects of the error sources discussed in section 3 would clearly be useful for data applications. Since retrieval errors of individual observations estimated by BIRRA comprise instrumental noise of the spectra and systematic errors due to forward model deficiencies and imperfect auxiliary data, a quantitative estimation of every single contribution is unnecessary. The qualitative analysis presented in section 3 is helpful to improve the retrieval approach and complements the studies of Frankenberg et al. (e.g., 2005); Gloudemans et al. (e.g., 2008). Note the new subsection 4.2.2 giving a detailed discussion of the retrieval error spatial and temporal distributions.

R3.3. As stated in the manuscript, BIRRA serves a dual role as prototype / scientific retrieval code and as operational processor as part of ESA's D-PAC at DLR. We have tried to identify all input data (esp. external data) used by BIRRA as complete as possible. In particular, unless otherwise noted, we have used the dynamic pixel mask (Lichtenberg et al., 2006). University of Bremen providing the pixel mask used in Fig. 9 is given thanks in the Acknowledgments.

R3.4. In addition to University of Bremen and SRON, SCIAMACHY nadir NIR products (nb. CO and CH_4) have also been derived by the group at University of Heidelberg / Max Planck Institute for Chemistry, see, e.g., Frankenberg et al. (2005, 2008a), or, more recently, Liu et al. (2011). For comparisons with independent SCIAMACHY retrievals we have not included plots etc. in our manuscript, as these (data and/or plots) are readily available from, e.g., the Bremen and SRON web sites mentioned in the acknowledgments. We never stated that the "qualitative intercomparison" between BIRRA and WFM-DOAS presented in Schreier et al. (2007) is a validation. Moreover, we do not consider the present manuscript as a validation paper.

R3.5. To our knowledge public availability of data and/or algorithm is not mandatory for submission to AMT(D). Actually, the retrieval product derived with BIRRA as part of the operational SCIAMACHY L1-2 processor is available at D-PAC. However, because of the constraints of the operational processing environment we consider these products as sub-optimal (some effects will have to be corrected during the postprocessing of the data, e.g., impact of the ice layer), especially for years after 2005, where the loss of important spectral pixels dramatically influence the quality the operational product. Furthermore, as detailed in the product DISCLAIMER, individual data entries for a single ground pixel corresponding to a single nadir observation spectrum are not meaningful, and further filtering and averaging (e.g. monthly means) is required (Details of our filtering/averaging approach have been provided in the manuscript, the approach used by other groups is likely to be different).

Lack of a truly new retrieval approach combined with the missing justification of why a third set of CO and CH4 retrievals should be produced
We admit that we have not ”invented” a revolutionary new retrieval approach — we share the same physical basis and retrieval methodology (optimization). However, we are convinced that there are indeed significant conceptual and algorithmic differences between our approach and the three (!) “established” approaches:

- Separable least squares;
- Bound constrained least squares;
- “Online” line-by-line computation of molecular cross sections;
- Exact analytical Jacobians (automatic differentiation);
- “Direct fitting” of radiance (similar to SRON, but distinct from Bremen);
- “In-house” dynamic pixel mask;
- Methane retrieval: Parallel/concurrent fitting of two windows in channel 6;
- Carbon monoxide retrieval: Fitting of slit function width;
- Wavelength shift estimate.

Furthermore, although sensitivity studies have been presented by other groups as well (e.g., Frankenberg et al., 2005; Gloudemans et al., 2008), we believe our investigations (section 3) discusses novel aspects (e.g., subsection 3.3) and can be seen as complementary to the papers mentioned before.

3.2 Detailed points of criticism

R3a. BIRRA acronym: When starting this project some years ago we wanted to improve some early prototype having been developed at DLR, hence the term “better” in the original acronym. Later we recognized that this might be interpreted in a way we did not anticipate — we never wanted to indicate that our approach is better than other approaches developed elsewhere. As our forward model is essentially based on Beer’s law, we simply removed the “tt” in the first word, which results in the code acronym “Beer InfraRed Retrieval Algorithm”

R3b. Forward model acronym: BIRRA and its forward model are implemented in Fortran 2003, GARLIC is the modern Fortran re-implementation of the MIRART Fortran 77 code described in the IRS2000 proceedings (Schreier and Schimpf, 2001).

R3c. Line mixing is not yet considered in our BIRRA retrievals. To the best of our knowledge this is also the case for the U-Bremen and SRON retrievals.
Line mixing has been reported for a large number of molecules, including water, methane, carbon monoxide and dioxide. In the $\nu = 2 \leftarrow 0$ band of CO around $2.4\mu\mathrm{m}$, Brault et al. (2003) observed line shapes exhibit deviations on the order of 1% from the conventional Voigt profile, primarily due to speed-dependent broadening and secondarily to line mixing. Boone et al. (2011) notes that accounting for line mixing “in the analysis of remote sensing measurements of Earth’s atmosphere by the Atmospheric Chemistry Experiment (ACE) yields reduced residuals, which leads to improved performance in the volume mixing ratio retrievals for some molecules.” Frankenberg et al. (2008b) critically examined the spectroscopy of the $2\nu_3$ band of methane and its implications on atmospheric retrievals (for high resolution ground based FTIR and low resolution nadir measurements of SCIAMACHY), noting that despite improved line broadening parameters “some small systematic inconsistencies between modeled and measured methane spectra still exist, probably owing to line-mixing and Dicke-narrowing effects.” Tran et al. (2010) discusses consequences of line mixing in the $2\nu_3$ band of methane for molecular spectroscopy and atmospheric retrievals, concluding that “in the meantime, and from the point of view of atmospheric retrievals, neglecting LM (*line mixing*) with suitable effective line parameters is convenient and accurate (within current retrieval uncertainties).” This is in accordance with the recent GOSAT-2009 methane line list containing only Voigt profile parameters, i.e., “no attempt has been made to study line mixing effects” (Nikitin et al., 2010). (Note that we do not expect any significant computational problems when modeling line mixing, as this can be done

quite efficiently exploiting the imaginary part of the complex error function (Boone et al., 2011; Schreier, 2011).)

R3d. Unphysical results, e.g., non-negativity:
We agree that statistical estimates can be regarded as “unphysical” only if they adopt forbidden values with “statistically significance”, i.e., within the confidence interval. We would not be seriously concerned about “unphysical results”, in particular negative molecular density scaling factors, if they are positive within the error bars. However, the negativity of the instrument slit function width would lead to a convolution of the high resolution spectrum with a non-defined instrumental function. Moreover, the simultaneous appearance of several “unphysical” fit parameters during the early steps of the iteration process is an indication that something is going wrong, and we hesitate to call the forward model with such inputs. To avoid these problems, BIRRA offers the option of (nonlinear or separable) least squares with bound constraints, i.e. regularization.

R3e. Last sentence in section 2.3.1 rewritten

R3f. Sun glint have not been considered.

R3g. Dead/bad pixel mask after 2009:
Data processing of SCIAMACHY is ongoing continuously at DLR–IMF, and accordingly the DBPM is updated, too. Admittedly, analysis of SCIAMACHY is becoming more challenging. However, we do not show any data for years beyond 2009 in the manuscript, and consequently the DBPM plot in Fig. 2 is considered adequate.

R3h. Adjective in first sentence in subsection 3.3 deleted (might be misleading). Yes, it is.

R3i. Sun mean reference:
Subsection 3.5 introduction slightly extended (see also response R4.8)

R3j. Solar spectrum: Clearly the Kitt Peak data utilized by Kurucz are observations. However, in order to “convert” these high mountain spectra to top-of-atmosphere irradiance some calculations are required. Indeed, this is indicated by the title of the Kurucz (1995) report cited in our manuscript and also in the MODTRAN documentation, e.g., “a new high resolution solar irradiance (based on a full calculated irradiance, after Kurucz 1995)” (Kneizys et al., 1996). New solar irradiance spectra for the most recent version of MODTRAN are discussed in Anderson

et al. (2007).
The “improved high-resolution solar reference spectrum” described in Chance and Kurucz (2010) has not been utilized in BIRRA because it does not cover the spectral range of interest.

R3k. Header of section 3.6 renamed ”Spectral Calibration”

R3l. Spectral calibration for SMR:
The SMR have been considered for the spectral calibration.

R3m. Least squares settings: References to the PORT web address and to the “Usage Summary” have been added.

R3n. Heading of section 4: ”Survey”
As indicated at the end of the introduction, section 4 does not aim to provide a (more or less) complete presentation of all retrieval results obtained so far (from mission start till today). Instead, we wanted to give the reader an idea of BIRRA’s capabilities (in addition to the “more technical” discussion of section 3), i.e. an overview or “survey”.

R3o. Section 4.1
All retrieved least squares fit parameters have been monitored.

R3p. Dynamic dead and bad pixel mask:
The description in subsection 3.6 has been slightly expanded. (Level 0-1 issues including the derivation of the dynamic dead & bad pixel mask are the subject of a forth-coming paper; see also Lichtenberg et al. (2009, 2010)). “M. Buchwitz private communication” added to the caption of the figure where U. Bremen pixel mask has been used.

R3q. Satellites vs. ground-based observations
The ground footprint of spaceborne-based atmospheric sensors covers typically an area of tens to hundreds of kilometers, whereas the quantities measured by means of ground-based spectrometers are bounded to the locations of the station. NIR infrared spaceborne-based spectrometers (SCIAMACHY among others) have also high sensitivity to the lower troposphere, so the authors still believe that the statement “Satellites [. . .] see in general a higher portion of the atmosphere” is true.

R3r. Sources of level 1 data and auxiliary data such as topography and clouds have been added to the introduction of section 3.

R3s. Figures:

i. Fonts: see note R1.9 above

ii. Pixel mask figure:
We would like to keep both panels of the figure.

iii. Figure 5 (now 6):
A detailed figure of South-East Asia is included in section 4.2.2.

iv. Effect of H2O on retrieval coverage:
Since the inclusion of strong H2O absorption lines lead to errors (discussed in 3.3), and the quality criteria are based on these retrieval errors, the number of good retrievals using all H2O lines in the fit is lower than when excluding the three strongest lines within the CO fitting window in channel 8.

v. SMR spectra: see response R1.11

vi. Although scarce, there are some negative values distributed over land as well as over the ocean. Keeping the color bar symmetric, it is easier to identify positive and negative biases.

vii. "Kurucz" corrected

viii. IUP mask:
Figure caption accordingly extended.

ix. Wavenumber shift $\Delta\nu$ (in accordance with the unit)

x. Three of the four scatter plots have been removed. Linear regression and correlation coefficients for n2g vs. nsg are given.

4 Review 4

4.1 General comments

The relevant missing information has been added in several sections of the paper. The results presented in this work are either dry-air vertical column densities (CO), column mixing ratios (CH4) or volume mixing ratios (CO measured at Assekrem ground station). It has been clarify, that for comparisons with ground stations, the SCIAMACHY CO product has been presented as (dry-air) column mixing ratios instead of vertical column densities. The altitude sensitivity ("averaging kernels") of the retrievals has been added to the script, together with a-priori and cloud information. Global maps as well as histograms of retrieval errors are included in order to provide information about the precision of the results. Additionally, the spatial distribution of the number of observations that survived the quality criteria are also included.

4.2 Specific comments

R4.1. Replaced "Sounding" $\longrightarrow$ "Retrieval" in the title.

R4.2. Optical depth: superscript "prior" removed in eq. (8), note added at end of sentence.

R4.3. Separable least squares: due to the highly efficient forward modeling computing, time is not really critical (the relatively costly LBL evaluation of the cross sections is done only once per state) and we have not performed an elaborate benchmark comparison of separable vs. nonlinear least squares. The main advantage is the numerical robustness and reliability of the separable least squares: Using synthetic noisy "observed" spectra with constant reflectivity ($r_0 > 0,\ r_1 = r_2 = 0$) and fitting with a second order reflectivity polynomial, the separable least squares delivers the "true" state vector (molecular scaling factors and aux parameters) correctly in all cases, whereas the nonlinear least squares fails for about half of the spectra.

R4.4. Altitude sensitivity: See response R2.1 regarding "averaging kernels"

R4.5. What a priori is used for CO and CH4?
See response R2.3

R4.6. Random-noise retrieval errors:
14-day averaged retrieval errors are provided in Fig. 12
See also response R2.2

R4.7. Fraction of retrievals rejected, treatment of clouds
A new plot showing the number of observations accepted has been added to section 4.2.

Clouds are not treated as a scattering body nor as a Lambertian reflector. Clouds are neglected in the forward model, but the impact that they have on the photon path is taken into account by the use of a proxy. Subsection 2.3.2 has been substantially extended discussing retrievals over ocean, with special focus on the influence of clouds.

R4.8. The sun mean reference is derived as an average of a daily series of measurements. (This explanation is added in subsection 3.5)

R4.9. Artificial features: wording changed.

R4.10. Microwave Limb Sounder:
We did not attempt to give a complete listing of spaceborne CO sounders, the list given here includes the currently operating nadir sounders and MIPAS as SCIAMACHY's sister instrument on ENVISAT. Adding MLS would have opened another list, and we should then mention also ODIN, ACE/FTS, SMILES, . . .

R4.T. The technical corrections have been implemented.

5 Further Changes

C1. expanded abstract and/or summary listing novel aspects and operational vs prototype results from prototype.

C2. Added reference to Hedelt et al. (2011) Venus,
Feng and Zhao (2009) Hitran NIR (and some info to subsection 3.7)

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