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Interactive comment on “Influence of under-sampled a priori data on tropospheric NO₂ satellite retrievals” by A. Heckel et al.

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This paper addresses the important issue of spatial undersampling of a priori information needed by NO₂ retrievals from space. Using low resolution a priori information for high resolution retrievals means that sharp spatial gradients in a priori NO₂ profiles, surface albedos and terrain height are not properly taken into account, resulting in systematic errors in the retrievals. For clouds, this problem is less relevant as cloud information is usually retrieved from the same instrument at the appropriate resolution.

The authors deserve considerable credit for taking up this issue that has been identified before, but was never quantified. The set-up of the experiment –comparing retrievals with high resolution a priori information to retrievals with spatially smoothed a priori information– makes sense, and the outcome is in line with expectations based on re-

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trieval theory. The paper has been written well, and the authors put their results in the perspective of what we know from literature. I also like the fact that the authors have quantified the error reduction when improving to 90 x 90 km² a priori NO₂ profile data. That resolution comes close to the global chemistry transport model capability of 1 x 1, which is expected to be the next feasible resolution generating a priori profiles that will be used in standard retrievals in the foreseeable future.

All in all, this paper makes an important contribution in pointing the way forward for improving satellite retrievals of minor trace gases with the DOAS approach. I absolutely support the main conclusion that state-of-science retrievals should focus on using a priori information with the appropriate spatial resolution. In case of sensors such as OMI and GOME-2, this means that especially the spatial resolution of the a priori profiles needs to be improved.

The difficulty I have with this paper is that the final error estimates to my opinion exaggerate the problem at hand. The abstract states that the relative uncertainties can be more than a factor of 2, but the paper does not make sufficiently clear that this factor of 2 uncertainty does not hold for current standard retrievals. The error presented by the authors is representative for a theoretical retrieval approach for a non-existing instrument with 15 x 15 km² spatial resolution that has to rely solely on 3 x 3 a priori information for both NO₂ profiles, albedos, and aerosols. But standard retrievals all use a priori information at significantly better resolution than the 3 x 3 used here, especially for albedo and terrain height, but also for a priori NO₂ profiles. Thus, the authors should either make clear that their error estimates are valid for such a theoretical retrieval based on 3 x 3 information, or use current, more realistic spatial resolutions for pixel sizes, NO₂ profiles, albedo, and aerosols, and come up with a better (and likely smaller) error estimate that would hold for standard retrievals. To underline this:

* The authors use a single a priori NO₂ profile on 3 x 3 resolution as a reference. The implicit assumption in the paper is that the air mass factors calculated for this 3 x 3 profile represent common practice in standard retrievals. But it's not. Standard

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retrievals use a priori profiles with resolutions of 2×2.5 (Dalhousie, NASA), 2×3 (KNMI), so the 3×3 profile is not so 'typical' as the authors claim: it is a factor of 1.5-1.8 too coarse. Therefore, the conclusion that single AMF errors lead to errors of 50-100% is too strong (P1903), and only holds for retrievals that use a 3×3 degree a priori NO_2 profile, and to my knowledge such retrievals do not exist.

* The authors conclude that the 'spread of AMF values', not captured by the single AMF value, leads to errors up to 100% (P1903). But even if the 15-km profile happened to be identical everywhere within the 3×3 domain, one would still observe a distribution of AMFs. Such a distribution reflects the variability of other a priori parameters (e.g. albedo, terrain height). Most standard retrievals do take high-resolution variability in surface albedo, terrain height, etc. into account (e.g. NASA, KNMI, EMPA to name a few), and their AMFs therefore capture at least part of the spread shown in Fig. 3(b). The authors should make a distinction between spread in AMFs caused by hi-res a priori profile variability not captured by current retrievals and spread caused by hi-res surface albedo, terrain height variability that is accounted for by current retrievals, and not report just the combined number as this may mislead readers into believing that the 50-100% is in fact the profile-shape undersampling error.

* The WRF-Chem a priori profiles at $15 \times 15 \text{ km}^2$ are too high-resolution to represent the spatial variability needed for current sensors such as OMI ($24 \times 13 \text{ km}^2$ at best) or SCIAMACHY ($60 \times 30 \text{ km}^2$), and too coarse to be representative for future missions such as TROPOMI ($7 \times 7 \text{ km}^2$). So the spread in Fig. 3(b) is too strong to be representative for OMI/SCIAMACHY resolutions, and inappropriate as a basis for error estimates for these instruments. Using WRF-Chem profiles on $30 \times 15 \text{ km}^2$ would be much more representative for OMI (as 60×30 would be for SCIAMACHY), and also lead to smaller differences and smaller error estimates between the distribution and the domain-average, single AMF values. This is in line with the 15 vs. 90 km study reported on in 3.4.

* Section 3.2: to my knowledge, none of the standard retrievals is still using 'single

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AMF' values based on 3x3 albedo maps. Instead most account now for high-resolution spatial variability in the surface albedo. The authors might consider comparing the use of MODIS-based pixel-size albedo estimates to the 0.5 x 0.5 or 1x1 albedos now used (NASA, KNMI, EMPA, Dalhousie, Bremen), and update their error estimate to relevancy.

The application to other seasons (section 4.2) is interesting, but it is not clear to me whether also seasonal changes in NO₂ profile shape have been accounted for. From the description on P1911, it seems that only the solar zenith angle has changed to reflect lower sun in wintertime, and all other variables have been kept constant. Keeping the surface albedo constant is perhaps justifiable, but we know that the vertical and spatial distribution of the NO₂ profiles differs significantly between seasons (as the authors also acknowledge on lines 9-12). So to properly evaluate seasonal differences in the errors, I would encourage the authors to use an appropriate WRF-Chem simulation for a wintertime day and evaluate the combined effects of low sun and wintertime NO₂ profile on the retrievals.

Some aspects of the influence of a priori profiles on retrievals, irrespective of their spatial resolution, have not been addressed at all. Previous work (e.g. Hild et al., 2002; Martin et al. 2006, Beirle-papers) has clearly shown that NO₂ in the upper troposphere for instance from lightning leads to increased values for the air mass factors. Because the authors do not state whether lightning NO_x production is included in WRF-Chem in the first place, and neither whether free and upper tropospheric NO₂ contributed significantly to the NO₂ burden on 29 August 2005, we can only guess whether the results presented here are truly representative. Suppose that WRF-Chem does not include the lightning NO_x source, then the conclusions presented here are too strong. On the other hand, if we suppose that WRF-Chem simulated to much NO₂ aloft, then the conclusions might even be at the cautious side. The authors should inform us to what extent NO₂ in the free troposphere is taken into account in WRF-Chem, and also to what extent the simulation of 29 August 2005 can be regarded as typical.

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On page 1897, the authors state that the ‘uncertainty in the a priori information used’ (in the calculation of the air mass factor – KFB) is a factor that is ‘systematic’, and contrast it to measurement noise, which they characterize as of ‘random nature’. I presume the authors actually refer to the error contributions from both noise and a priori here (instead of the ‘factors’), and imply that a priori information leads to systematic errors in the retrieval. But a priori information error contributions are not strictly systematic in the sense that they represent a fixed and unchangeable bias. To illustrate this: the assumed surface albedo might be too low for one particular pixel on a particular day (due to e.g. vegetation growth), and too high for the same location one day later (e.g. soil darkening due to precipitation). So I do not think that a strict distinction between fitting errors as random errors on the one hand, and air mass factors as systematic errors on the other hand does justice to the complexity of the issue. Certainly, air mass factors have significant systematic components, but sometimes can be regarded –at least partially- as consisting of random contributions as well.

Minor issues

P1895, L20: the papers cited are concerned with changes in emissions or NO₂ columns over periods of more than a decade, so I would suggest not to call this ‘short trends’.

P1895, L29: ‘quantitative analysis with high accuracy’. Any analysis obviously needs to be of the highest possible accuracy, but I think the authors are actually referring here to the need for accurate absolute retrieved quantities. I suggest they rephrase.

P1896, below equation (2), delta z should also be defined for completeness.

P1896, L18-22: I suggest to point out here that bAMF_z depends on the assumed albedo, aerosols, clouds, and terrain pressure to make clear where ‘This step’ actually relies on the appropriate a priori data.

P1896, L24: I suggest the authors specify what ‘on average’ here means.

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P1897, L9: I dispute that ‘the resolution of the a priori dataset . . . has often not been improved from that used for GOME-1’. Improvements in the terrain height resolution were the topic of papers by Schaub et al. [2007], and Zhou et al. [2009]. OMI NO₂ products switched to higher-resolution albedo datasets as of 2009.

P1898, L21: does ‘atmospheric profile’ here refer to one a priori NO₂ profile?

P1899, L16-17: I think the statement that ‘this kind of spatial variability’ (in the NO₂ distribution - KFB) is not represented in standard retrievals is too strong. I think it would be more appropriate to state that the spatial variability is not sufficiently represented in the a priori information used for standard retrievals (and perhaps also state which retrievals you refer to as standard retrievals: are these are the Dalhousie, Bremen, NASA, and KNMI retrievals?). The KNMI algorithm for instance calculates a more representative a priori profile based on the closest 4 (2 x 3 native resolution) grid cells to the centre of the pixel. Such a smoothing step will not completely resolve the gradients discussed in this study, but it results in a better representation of the NO₂ spatial distribution compared to the single large model grid cell case studied here as reference case.

P1901, L19-20: it was not clear to me why all data from August 2005 were averaged. Previously the authors stated that the authors intend to evaluate the effect of under-sampling a priori data for a single day, so why now use a monthly mean here? Is MODIS AOT for 29 August 2005 not covering the whole domain?

P1902, L223: typo ‘obtaine’.

P1905, L26-27: I think the authors should clearly state here that aerosols enhance the photon path length in the boundary layer over shielding, provided that the aerosol and NO₂ vertical profiles are identical, as they assumed in this calculation.

P1906, end of 3.3: it would be interesting to still put a number on the aerosol effect. This can then be directly compared to the error estimates for the hi-res profile and

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surface albedo effects.

P1915, L13: the uncertainties range here from -5×10^{15} to $+5 \times 10^{14}$ molec. cm^{-2} . Is it really 10^{14} ? Later on I see that this can be read off from Figure 10, which has not been presented before. Perhaps it is good to remind us that the -5×10^{15} effect mainly illustrates the AMF decreases because of improved sampling over polluted landscapes, whereas the $+5 \times 10^{14}$ molec. cm^{-2} illustrates the increases in AMF because of better spatial sampling over oceans.

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