Interactive comment on “Using photochemical models for the validation of NO$_2$ satellite measurements at different solar zenith angles” by A. Bracher et al.

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Response to Anonymous Referee #1 Letter to ACPD 4, p2599-2601

General comment by Referee #1: The presented paper describes a first validation of ENVISAT/SCIAMACHY Limb NO2 observations by collocated observations of the SAGE II and HALOE satellite instruments. Temporal mismatches of the individual observations - important due to the diurnal cycle of stratospheric NO2 - are accounted for by photochemical model calculations. Spatial mismatches of the individual observations are accounted for by selecting those pairs of observations that were likely conducted in air masses of the same stratospheric circulation regimes. While the former
two approaches can be considered to be state of the art, the latter approach falls short with respect to similar studies conducted earlier (i.e., Bacmeister et al., JGR, 104, 16379, 1999; Lu S2599 et al., JGR, 105, 4563, 2000; Harder et al., 2000, GRL, 27, 3695, 2000; Randall et al., 2002, JGR, 107, doi:10.1029/2001JD001520; Vogel et al., JGR, 108, 8334, doi:10.1029/2002JD002564, 2003 and others).

Reply by author: We added more information on why we think that the method to separate collocations within the same air mass from others is adequate for our study and state of the art. In Chapter 2.5 the text was changed to the following: "Validation at the edge of different air masses is more difficult, because gradients in the horizontal distribution result from transport processes, e.g., at the polar vortex or at the upper troposphere lower stratosphere region (UTLS). Therefore, besides to identifying collocated measurements by limiting time difference and distance between two observation points, additional criteria were selected to ensure that collocations were made in the same air masses according to the method described in Bracher et al. (2004). The tropopause height and the position of the polar vortex were determined by analysis of the potential vorticity (PV) distribution. PV values measured at the same geolocation and day of each collocated measurement were taken from the United Kingdom Meteorological Office (UKMO) assimilated meteorological dataset available in a 3.75° X 2.5° (longitude-latitude) grid resolution (Swinbank and O’Neill, 1994) and spatially interpolated to the observation point. As a result of the relatively large ground scene of a SCIAMACHY profile, the corner coordinates of the ground scene for each SCIAMACHY profile were checked for their homogeneity of PV. For samples outside the tropics, the tropopause was assumed to be the 3.5 PVU level, which was shown by Hoerling et al. (1991) to be a good estimate for the dynamical tropopause height. Inside the tropics where the dynamical tropopause is not defined, the 380 K isentropic level was a proxy for the tropopause. To separate collocations, where the four corners of a SCIAMACHY ground pixel and the collocated HALOE or SAGE II tangent point were inside the polar vortex or outside the vortex, matches where the PV of both measurements at the isentropic level of 475 K were selected having either greater than 40 or less than -40
PVU (i. e. inside the vortex) or between -30 and 30 PVU (i. e. outside the vortex), respectively. For the tropopause height, deviations within 1 km for collocations were tolerated. This applied method is fast in screening a larger number of collocations for their coincidence in air mass. Bracher et al. (2004) showed that including these atmospheric dynamics criteria regarding tropopause height and polar vortex for the selection of collocated measurements improves significantly individual comparisons. Opposed to that, for comparisons of multi-platform measurements where only a small amount of matches have been found within a chosen spatial-temporal vicinity the methods developed by Bacmeister et al. (1999), Lu et al. (2000), and Danilin et al. (2002) to enlarge the number of matching by using a trajectory hunting technique is more appropriate. The results of these studies showed that in this case with the trajectory hunting technique comparisons were statistically more robust than just limiting the comparisons to the traditional correlative analysis." We also discuss approaches in other validation studies (Bacmeister et al. 1999, Lu et al. 2000, Danilin et al. 2002). Other citations given by the referee were cited elsewhere: Randall et al. 2002 did not separate for different air masses, but a reference to this study was necessary and now made in Chapter 2.2.1 ("Randall et al. (2002) compared HALOE v19 NO2 data to data from Atmospheric Trace Molecule Spectroscopy Experiment (ATMOS). Results show that between 25 and 42 km the measurements from the two instruments agree within 10%. ATMOS NO2 data have an estimated accuracy of about 6% in the 20 to 45 km range (Abrams et al., 1996.") and in Chapter 3.1.5 (see answer to point 4). Also references were made in the introduction to a number of previous studies that use photochemical models to investigate different aspects of measured trace gases, or to make trace gas measurements obtained during different times intercomparable (Harder et al., 2000; Sinnhuber et al., 2002; Stowasser et al., 2003; Vogel et al., 2003; Marchand et al., 2003). To our knowledge, no photochemistry models have been used so far to validate NO2 satellite measurements made at different solar zenith angles. However, there is a study by Marchand et al. (2004) that assimilates NO2 and ozone measured by GOMOS into a model to investigate the self-consistency of GOMOS night-time NO2,
ozone and NO3 measurements, and a reference to this has been added as well.

Response to open issues in the detailed evaluation: 1.-3., 5., 6., 9., 12., 15. no changes requested

4. Are the scientific methods and assumptions valid and clearly outlined? Comment by Referee #1: Yes, at most places except some obscurities in chapter 3.1.5. Here a major problem comes with the author’s confusion with the technique of solar occultation measurements and the correctly stated notation of ‘solar zenith variations along the line-sight’. I largely recommend therefore to rethink and correct the sentence. ‘This means that the variation of the solar zenith angle... Reply by author: The referee is right and the text was rewritten as follows in chapter 3.1.5: "Newchurch et al. (1996) state that the variation of the solar zenith angle along the line-of-sight of an occultation instrument does influence the retrieved density of NO2 especially below 20 km, where errors can grow as large as 20%. The $1^\circ$ change we assumed probably is a fairly conservative estimate that overpredicts the uncertainty due to this effect because the variations at least partly cancel out. Still, this seems to be a fairly large source of model uncertainty, though maybe not the largest, as originally stated. It is possible to correct for this variation during the NO2 retrieval as it is done for the HALOE retrieval (see Gordley et al., 1996), but this carries its own sources of additional errors, and is not done for all occultation measurements (Randall et al., 2002)."

7. Do the authors give proper credit to related work and clearly indicate their own new/original contribution? Comment by Referee #1: In part, for the reminder part see the refs. provided above. Reply by author: The references were added in the manuscript as pointed out in the reply to the general comment, and point 14.

8. Does the title clearly reflect the contents of the paper? Comment by Referee #1: No! My impression is that the authors used only a single photochemical model (which is no fault), therefore the used notation ‘models’ is incorrect. Please skip the ‘s’ in the word models. Reply by author: The referee is right and the title was changed accordingly:
"Using a photochemical model for the validation of NO2 satellite measurements at different solar zenith angles"

10. Is the overall presentation well structured and clear? Comment by Referee #1: While in the first two thirds of the manuscript the English has considerably be improved from the first version, the English of the remaining last 1/3 part is still poor. Please English correct the latter part as well! Reply by author: The manuscript, especially the last third, was read by a native English speaker and corrected to improve significantly its structure and language.

11. Is the language fluent and precise? Comment by Referee #1: See point 10. Reply by author: See comments to point 10.

13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated? Comment by Referee #1: See point 10! Reply by author: See comments to point 10.

14. Are the number and quality of references appropriate? Comment by Referee #1: See the points above! Also according to what has been said already in the previous iterations of the review process, the manuscript would benefit to correctly cite earlier studies at the appropriate places, i.e. von der Gathen, Nature, 375, 131, 1995; McKenna et al., JGR, 107, doi:10.1029/2000JG00114, 2002; Roscoe, H. K., J. R. Drummond, and R. F. Jarnot, Infrared Measurements of Stratospheric Composition III. The Daytime Changes of NO and NO2 , Proc. Roy. Soc. (Lond.), A375, 507, 1981) and others.

Reply by author: Most of the reference concerning the use of trajectory calculations were added in the chapter 2.5, describing the method on selecting collocations from the same air masses, except for the paper by von der Gathen et al. (1995) because although the match technique is using trajectories we think only references regarding validation work considering air masses are appropriate to cite in the context of this paper. Concerning the use of photochemical models, of course a very large number
of studies exist, and it is certainly not possible to cite them all. However, we now referenced a number of more recent model in the introduction, as stated already in our reply to the general comment.