

Interactive comment on “An empirical model of nitric oxide in the upper mesosphere and lower thermosphere based on 12 years of Odin-SMR measurements” by Joonas Kiviranta et al.

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We would like to thank the two anonymous referees and the editor for their attention to our paper “An empirical model of nitric oxide on 12 years of Odin-SMR measurements”. The comments were constructive and helped us to significantly improve the paper. Below, the reviewers’ comments are marked with (1), the author’s response with (2), and the change in the manuscript with (3).

Reviewer 1 comments:

(1) p2 l26: "Additionally, the amount of NO influences the thermal balance of the MLT,

especially at ultra-violet wavelengths (Richards et al., 1982)". The cited paper discusses the role of NO in modulating the thermospheric heating efficiency by infrared 5.3 μm cooling (not at ultra-violet wavelengths).

(2) The reviewer correctly points out a mistake in the content of the sentence.

(3) Changed sentence to refer to infrared cooling.

(1) p3 l25: "since night-time NO is expected to be higher than day-time NO". It should be mentioned that the day-night ratio of NO depends on latitude and altitude (see, e.g. Bermejo-Pantaleon et al., 2011)

(2) The original manuscript was inaccurate in its description of the day/night NO differences, although in reality the relationship is more nuanced.

(3) Manuscript modified to correctly represent the phenomenon.

(1) p3 l27: typo: based -> based on

(2) As pointed out, this was a typo.

(3) It has been corrected in the revised manuscript.

(1) p4 l25: "SANOMA will express NO in number density to accommodate chemical models" Why is number density over altitude better suited to accommodate chemical models than vmr over pressure level?

(2) The idea here was that certain models (e.g. WACCM) requires its constituents in number density. However, a more proximate reason was that the old model, NOEM, was in number density and hence comparison would be greatly facilitated if SANOMA was also in the same units.

(3) This point has been clarified.

(1) p8 l 6: the PC's mentioned here are not included in Eq. 1. It would be clearer to note that the PCs were replaced by polynomial fits to the geophysical parameters K_p ,

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delta, $\log(F10.7)$ in Marsh et al., 2004, represented in Eq 1 by f_1, f_2 , and f_3 .

(2) This connection was missing from the original manuscript.

(3) Added connection that Marsh et al. used polynomial fits to the geophysical parameters as substitutes for PC1-PC3.

(1) p10 l9: Have auto-correlations been considered in the regression? This would be important since explained variances might be overestimated otherwise (see, e.g. Hendrickx et al., GRL, 44, 2017)

(2) The reviewer raises a very good point here. Autocorrelation in the residual was tested using the Ljung-Box Q test. It was found to be present, although it is very low. The correlogram in Fig. 1 attached to this response is an example showing the autocorrelation in the residuals at 70°S and at an altitude of 102km, as a function of the time lag. The correlogram in Fig. 2 attached to this response corresponds to a random data set. We can see that auto-correlation in the residuals is only slightly higher than autocorrelation characteristic of a random time series. Moreover, P-values lower than 0.01 at high latitudes above 95km, as well as below 95km at all latitudes, indicate that there is no strong evidence to reject the null hypothesis that the residuals are not autocorrelated in these regions. (This can slightly vary according to the lag into consideration.) For these reasons, autocorrelation in the residuals can be considered as reasonable. It would of course be good to minimise it anyway, but we could not apply the Cochrane-Orcutt procedure to correct our NO data set, as it was done by Hendrickx et al. (2017). As we understand it, this procedure does not deal with long-term correlations. Koen et al. (2017) could use it in their study because they considered deseasonilised anomalies, hence short term variations only. The SMR data set is characterised by an uneven temporal sampling, with only four measurement days a month on an irregular basis. This makes the use of this procedure inappropriate in the context of our study. Moreover, considering autocorrelation is less crucial than in the study by Koen et al. (2017), where the conclusions were built upon R-squared values.

In our case, the coefficients of determination are not the actual result of the study, but rather a tool that indicates how well the model represent the data. Nevertheless, we agree that it is important to estimate these coefficients as accurately as possible. Finding the best way to do that requires further investigation and we keep that in mind for a next version of the model.

(1) p 11 l11: "R-squared" coefficient of determination

(3) This point has been clarified.

(1) p11 l8: Why aren't the mean differences between SANOMA and SMR zero in a given bin? This would be expected from a simple multilinear regression.

(2) The function of the figure is to indicate that the differences between SANOMA and SMR are extremely small in comparison to the measured values (10E7 vs. 10E-7). We assume this error to be negligible and due to numerical error in creating the model.

(3) A passage clarifying the significance of the figure has been added to the manuscript.

(1) p13 l10: "SANOMA includes no dynamics". Since SANOMA is an empirical model it does not include any physical process.

(2) Yes, as an empirical model, SANOMA does not intend to reproduce any physical processes. What we meant was that it does not include any parameter to account for dynamical processes, as it does with K_p , δ and $F_{10.7cm}$ to account for the geomagnetic activity, the seasonal variations and the solar activity, respectively.

(3) The manuscript has been modified to clarify what is meant by "no dynamics"

(1) p13 l11: "This could also be due to a lower signal-to-noise ratio in the measurements at lower altitudes." Isn't the measurement error already accounted for in Eq 5?

(2) Yes, Equation 5 accounts for measurement error, but since the measured NO number densities are comparatively small, a large relative error is unsurprising.

(3) We have changed the text in order to make that point clearer.

(1) p14 Table 1: Isn't ACE measuring at altitudes < 70 km as well?

(2) The reviewer is correct to point out this mistake in the table. However, we found that including the altitude range bears no significance for this particular study since the assumption is that all cover the upper mesosphere and lower thermosphere. The sole exception to this is the ACE-FTS instrument, whose maximum altitude is around 108 km but that is mentioned in the appropriate section.

(3) Removed altitude range column.

(1) p14 Table 1: Same for MIPAS. Also, the MIPAS latitude range should be 90S - 90N.

(3) MIPAS' latitude range has been corrected.

(1) p 15 Fig 12: I'm puzzled about the NOEM results, showing minimum polar summer NO concentrations in 2012-2014, i.e., well after the solar cycle minimum (2009-2010). How is this possible if NOEM uses F10.7 and Kp (both having lower values in solar min)?

(2) This is a very interesting and correct observation: the NOEM-simulated NO does indeed show a minimum between 2012-2014 instead of the expected 2009-2010. The reason for this seems to lie in the EOFs of NOEM. Figure 2 d) in the paper by Marsh et al. (2004) reveals that EOF 3 is positive between roughly -60 and +60 magnetic latitude, but negative close to the poles. The plotted time series in Figure 12 of our paper is taken at -70 degrees magnetic latitude and 102 km in altitude. At this location, the 3rd EOF has a value of roughly -2.5. Since this value is negative, a decrease in F10.7cm flux will result in an increase in modeled NO and vice versa. Concerning the negative values close to the poles, Marsh et al. (2004) wrote: "The third EOF shows an unexpected decrease at latitudes greater than 50° that also appears related to solar UV variability. A possible explanation is that this may again be related to an increase in the suppression of discrete auroral arcs as solar fluxes increase toward solar maximum.

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Alternatively, solar cycle induced variations in chemical composition or temperature of the lower thermosphere may be indirectly affecting NO production and loss and so the distribution of NO. " In short, the negative values were unexpected. We suspect that this negative value in EOF3 can lead to the minimum NO modeled by NOEM to occur at another time than 2009. For comparison, we can have a look at NOEM-modeled NO at the same dates as in Figure 12, but for the equatorial latitude band and the same height, see the attached Fig. 3. It shows that at the equator, where EOF 3 is positive, the time of lowest solar activity does coincide with the lowest NOEM NO. Therefore we believe that the NOEM minimum in Figure 12 is indeed caused by the negative value of EOF 3 in the study by Marsh et al. (2004) at that particular latitude.

(1) p18 l5 : The given reference is correct for MIPAS but for the NO data version mentioned here Bermejo-Pantaleon et al, 2011 would be more adequate. It is unfortunate that this study uses data version v5r 620 since it only covers the years 2010-2012. The newer version v5r 622 (available, for instance, at http://mesospheo.fmi.fi/data_service.html) covers the entire period 2005-2012.

(2) The new version of the data has been downloaded and used for all the analyses in the updated manuscript.

(3) The input data for the MIPAS section has been changed to v5r 622, meaning that the ensuing figures, values, and following conclusions have all been modified.

(1) p19 l2: "with a minimum of -60% at 115 km around 70 deg". It looks more like a minimum of -30 to -40% at 115 km in Fig. 22.

(2) This comment is no longer valid since we have revised this section due to the use of the newer v5r 622 MIPAS NO data.

(1) p21 Table 2: caption: "the mean of the mean percent difference". Do you mean the mean percent difference averaged over the respective latitude bands? Further: "between the various instruments and a) NOEM, b) SMRNOEM, and c) SANOMA".

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Shouldn't it be the other way round, i.e., model - instrument?

(2) We calculate the percent difference for each latitude band, and then calculate the average of these three. The difference is indeed model-instrument, not instrument-model as the caption might suggest.

(3) Changed caption to clarify the meaning of the values in the table.

(1) p21 l4: Since SMR measures both day and night time NO, a positive difference compared to the daytime measuring instrument SCIAMACHY was expected, but SANOMA shows a positive difference in comparison to SOFIE and ACE as well". SOFIE and ACE are solar occultation instruments. A diurnal sampling bias can therefore not be excluded when comparing to instruments that measure at both day and nighttime (like SMR or MIPAS).

(2) This is true.

(3) This point has been clarified in the revised manuscript.

(1) p21 l12-15: I wouldn't say that MIPAS measurements should be treated with care, particularly because MIPAS shows small absolute difference with respect to SANOMA (and hence SMR), as well as high R-squared values (Table 1). It is likely that the apparently different behavior of MIPAS compared to other datasets is related to the short time coverage of the MIPAS data version used here (2010-2012). It would be very interesting to check this by using the newer version v5r 622 (2005-2012).

(2) This comment is no longer valid since the v5r 622 MIPAS NO has been used and the ensuing conclusions have changed.

(1) p22 l5-7: see above.

(2) See above.

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(1) How was is the regression model built? We have the equation:

$$\text{NO}(\text{lamda}, h, t) = \text{Kp}(t)*c1 + \text{dec}(t)*c2 + \log(\text{F10.7}(t))*c3 + \text{com1}(\text{Kp}(t),\text{dec}(t))*c4 + \text{com2}(\text{Kp}(t),\text{dec}(t))*c5 + C$$

Firstly it is not clear how the authors formed com1 and com2. The paper says that they were a result of iteration, but there is no physical explanation for them or clear explanation of the iteration process. They do, however, introduce autocorrelation with all except term #3. I am worried that there are two terms which both have a linear (lagged) Kp term as well as linear/sin terms depending on solar declination in addition to the linear terms in #1 and #2 - without any explanation.

(2) Please refer to the response to the next comment.

(1) The final number of terms in #4 and #5 also depend on solar declination in a way that is not explained clearly. Why for summer solstice conditions are there a maximum number of lagged days (11)? Would it not be natural to assume a lag is needed for winter conditions when the lifetime of NO is larger and thus there might be build-up? Why was the Kp lag not built into the first term of the regression (and same for solar declination)? What is the physical meaning of having these extra Kp & dec dependent terms?

(2) This was a very constructive comment, which warranted a closer inspection of the compound indices. We found an error in how they were built which has been corrected. The basic idea now is that com1 and com2 vary linearly with solar declination, see the updated equations in the manuscript. Com1 is zero during northern hemispheric summer and reaches a maximum during Arctic winter. Meanwhile com2 is zero during southern hemispheric summer, reaching its maximum during Antarctic winter. This means that com1 accounts for NO produced by energetic particle precipitation during previous days during northern winter, the time when the polar air mass receives least sunlight and dissociation of NO by sunlight is at a minimum. In essence, the closer to winter solstice we get, the longer back in time com1 goes in integrating over NO from

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previous days. We know that in the absence of sunlight, NO can persist for longer periods of time and therefore we can have a build-up of NO in the dark polar air mass. The same rationale applies for com2, but for the southern hemisphere. The newly added figure in the manuscript show the coefficients of the multivariate linear fits corresponding to com1 and com2. It confirms that com1 and com2 influence the measured NO only in the northern, and southern hemispheres, respectively. They act as a “memory” of the NO build-up from previous days during polar winter. Figure 11 b) and c) demonstrate that these added indices do in fact substantially improve SANOMA in the polar regions.

(3) A detailed description of the corrected indices, including comments on their physical meaning, has been added to the revised version of the manuscript.

(1) The actual regression coefficients “c1, c2, . . . c5” are not given (First 3 were plotted in Figure 8, I didn’t notice remarks on c4 and c5) and thus the equation can not be used. Please note that many readers will not have access to Matlab statistics toolbox used for the analysis.

(2) As mentioned at a later point in the paper, all the coefficients are available at odin.rss.chalmers.se.

(3) We have added a sentence at the point of introduction of the coefficients to clarify that these are available online. Moreover, a figure representing the coefficients c4 and c5 (Fig.9), was added to the manuscript, together with the corresponding detailed description.

(1) Other comments: Figure 2: This is plot of the F10.7 time series, clearly taken directly. Although the reference to the website is given, please plot the data yourself. This is a very simple figure with the actual monthly means and a running mean. The future prediction (red line) is not necessary for this paper.

(3) We have replaced the figure with a new one in which we plotted the relevant

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F10.7cm time series data ourselves.

(1) The indices you use here are not “space weather” indices, but rather geomagnetic and solar indices. The term space weather has a very specific meaning relating to impacts on technology (and these indices can be used for those), but as we are looking at impacts on the Earth’s atmosphere we should talk about geomagnetic and solar indices.

(2) Yes, we were using the term “space weather” rather inaccurately.

(3) This has been changed to “geomagnetic and solar indices”.

(1) The AE index (Auroral Electrojet) is mentioned in the same section, but this is not used anywhere after that, only Kp is mentioned.

(2) If we don’t mention the AE index in the paper, some readers could think that we should have considered the AE index instead of the Kp index. The function of mentioning the AE index is to indicate that we have tested it but found that the Kp index explains a larger portion of the variance of the Odin SMR NO measurements.

(3) Added clarification that AE is not used for the final model, but we did consider it.

Please also note the supplement to this comment:

<https://www.atmos-chem-phys-discuss.net/acp-2018-39/acp-2018-39-AC1-supplement.pdf>

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2018-39>, 2018.

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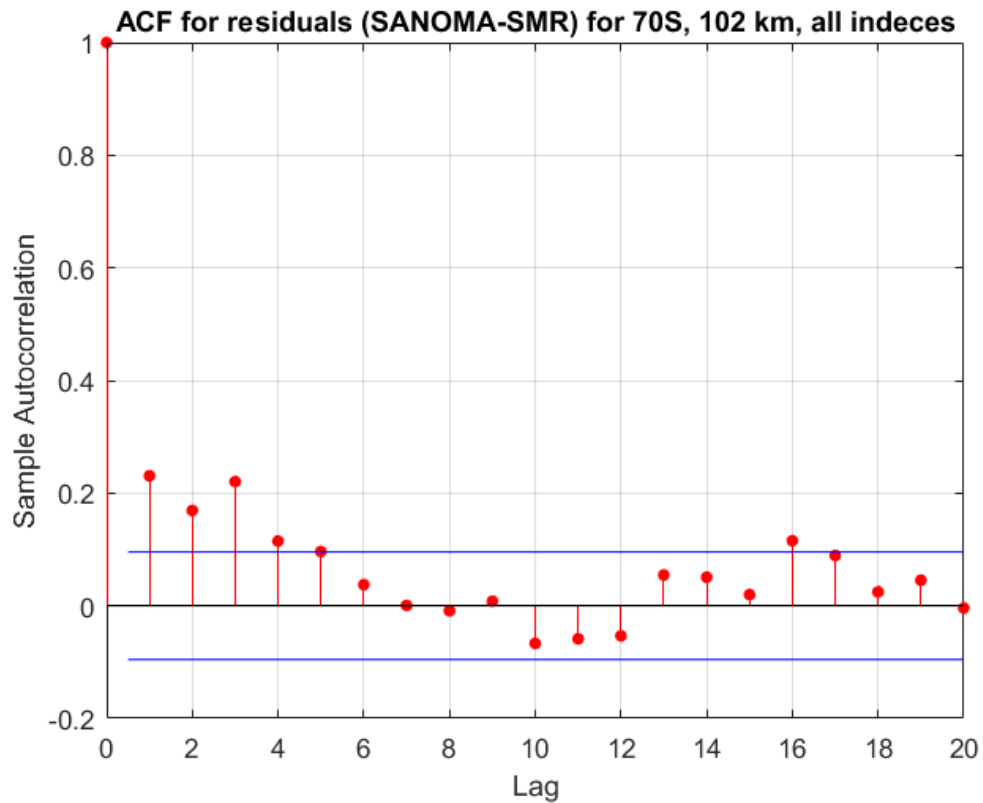


Fig. 1.

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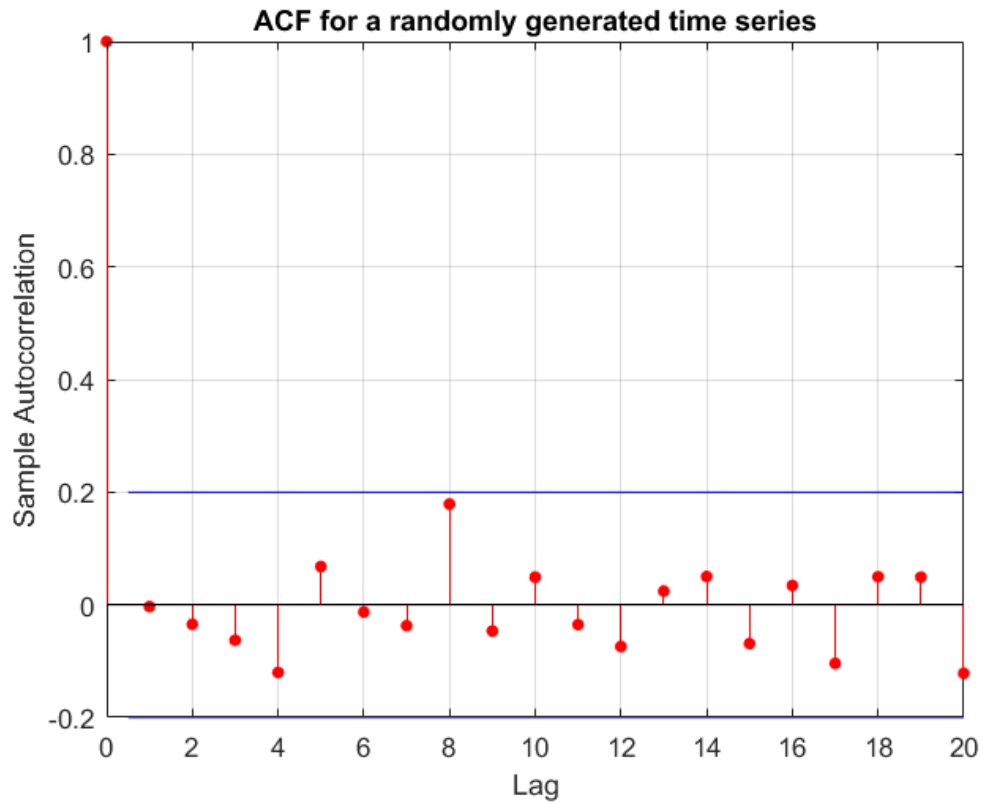


Fig. 2.

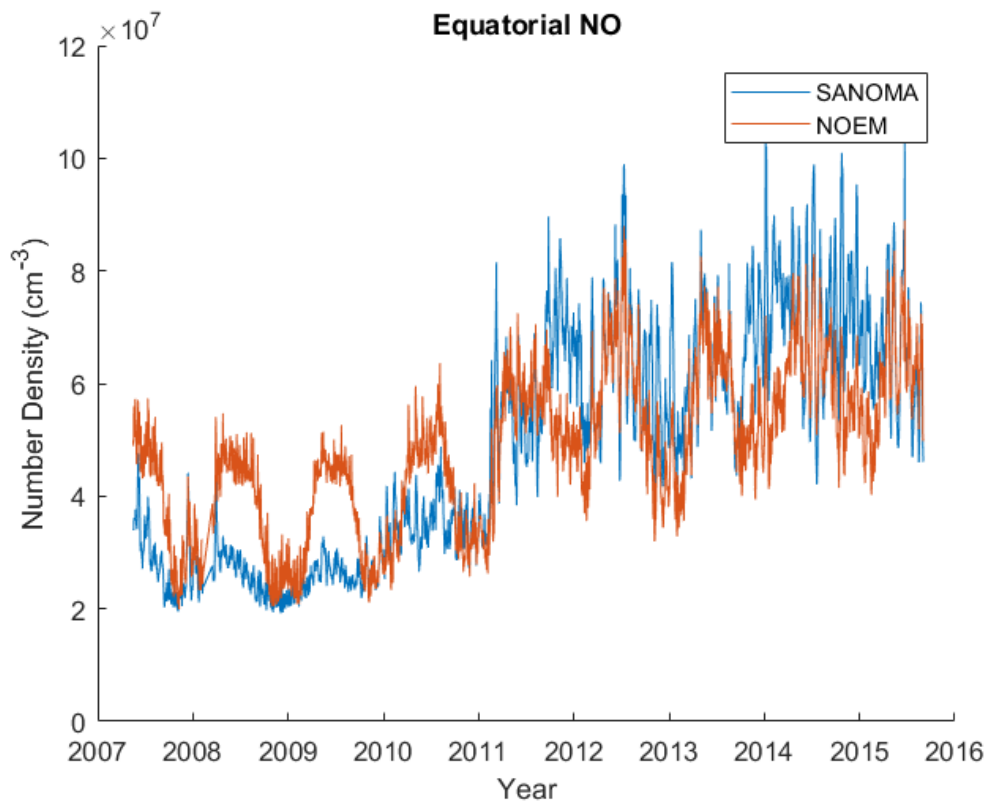


Fig. 3.

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An empirical model of nitric oxide in the upper mesosphere and lower thermosphere based on 12 years of Odin-SMR measurements

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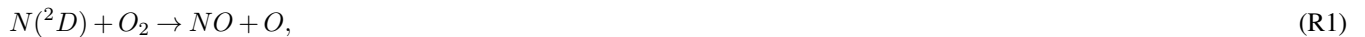
Abstract. Nitric Oxide (NO) is produced by solar photolysis and auroral activity in the upper mesosphere and lower thermosphere region and can, via transport processes, eventually impact the ozone layer in the stratosphere. This work uses measurements of NO taken between 2004 and 2016 by the Odin Sub Millimetre Radiometer (SMR) to build an empirical model which links the prevailing solar and auroral conditions with the measured number density of NO. The measurement data are averaged daily and sorted into altitude and magnetic latitude bins. For each bin, a multivariate linear fit with five inputs, the planetary K-index, solar declination, and the F10.7cm flux, and two newly devised indices which take the planetary K-index and the solar declination as inputs in order to take NO created on previous days into account, constitutes the link between environmental conditions and measured NO. This results in a new empirical model, SANOMA, which only requires the three indices to estimate NO between 85 km-115 km and 80° S-80° N in magnetic latitude. Furthermore, this work compares the NO calculated with SANOMA and an older model, NOEM, with measurements of the original SMR-dataset, as well as measurements from four other instruments: ACE, MIPAS, SCIAMACHY, and SOFIE. The results suggest that SANOMA can capture roughly 31-70% of the variance of the measured datasets near the magnetic poles, and between 16-73% near the magnetic equator. The corresponding values for NOEM are 12-38% and 7-40%, indicating that SANOMA captures more of the variance of the measured datasets than NOEM. The simulated NO for these regions was on average 20% larger for SANOMA, and 78% larger for NOEM, than the measured NO. Two main reasons for SANOMA outperforming NOEM are identified. Firstly, the input data (Odin SMR NO) for SANOMA spans over 12 years, while the input data for NOEM from the Student Nitric Oxide Experiment (SNOE) only covers 1998-2000. Additionally, some of the improvement can be accredited to the introduction of the two new indices, since they include information of auroral activity on prior days which can significantly enhance the number density of NO in the MLT during winter in the absence of sunlight. As a next step, SANOMA could be used as input in chemical models, as a priori information for the retrieval of NO from measurements, or as a tool to compare Odin SMR NO with other instruments. SANOMA and accompanying scripts are available on odin.rss.chalmers.se

1 Introduction

Nitric oxide (NO) is a reactive free radical, and together with Nitrogen dioxide (NO₂), constitutes the NO_x compounds. Whereas tropospheric NO_x may originate from both natural sources, such as forest fires, and anthropogenic sources, such as combustion engines (Wallace and Hobbs, 2006), NO in the mesosphere and lower thermosphere (MLT, ~50-150 km) has a

purely natural origin. Knowledge about NO in this region is of great importance, because it can affect the atmospheric layers below. To understand how, we need basic knowledge on the chemical reactions which create and destroy NO. In the MLT, NO can be produced by two mechanisms: either direct radiation from the sun in the form of solar-soft x-rays ($8 \leq \lambda \leq 12 \text{ \AA}$) or energetic particle precipitation (EPP) (Barth et al., 1999; Sinnhuber et al., 2012). These particles can include electrons, protons, or heavier ions. These may originate directly from the sun, from aurorae and the radiation belts during geomagnetic storms, or from outside of the solar system.

Previous studies have established that EPP from auroral activity dominates the variation of NO near the magnetic poles, while solar-soft x-rays contribute more near the magnetic equator (Gérard and Barth, 1977; Barth et al., 1999; Sinnhuber et al., 2012). NO in the MLT is created through the reaction between molecular oxygen and an excited nitrogen according to the equation



in which $N(^2D)$ denotes an excited nitrogen atom. Excited nitrogen is created by the two reactions



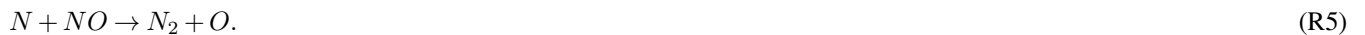
and



in which e^* indicates an energetic electron, originating from either EPP or solar soft x-rays (Marsh et al., 2004). This implies, that auroral or solar activity is necessary to form NO in the presence of an oxygen molecule. On the other hand, solar light destroys NO in the cannibalistic reaction



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Therefore the amount of NO is affected by seasonal variation of sunlight. Under sunlight conditions in the MLT region, NO has a chemical lifetime of less than one day, whereas during the polar night in winter, it may persist for several weeks (Minschwaner and Siskind, 1993). This increased lifetime, together with a stable polar vortex, can eventually result in the descent of NO into the stratosphere where it can partake in catalytic cycles to destroy ozone (Siskind et al., 2000; Pérot et al., 2014). Additionally, the amount of NO influences the thermal balance of the MLT, especially at ultra-violet wavelengths via infrared cooling (Richards et al., 1982). These effects highlight the importance of understanding the mechanisms by which solar and auroral activity create and destroy NO.

This study focuses on the effect of solar and auroral activity on the amount of NO in the MLT. Over the past several decades, at least six satellites have measured NO in the MLT region. These include the past instruments, SNOE (Student Nitric Oxide Experiment), SCIAMACHY (Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY), MIPAS (Michelson Interferometer for Passive Atmospheric Sounding), as well as the currently active Odin SMR (Sub Millimetre Radiometer), SOFIE (Solar Occultation for Ice Experiment), and ACE (Atmospheric Chemistry Experiment) instruments. The limitation of satellite measurements is that they only cover certain locations and periods of time. Yet, many applications, such as chemical models of the upper atmosphere, require information on the amount of NO at any given time or location. To help bridge this gap, a model which connects known environmental conditions, such as auroral activity, with measured NO can help to provide an estimate of NO at any time and place. Such a model can also help validate and constrain poorly resolved or underdetermined parameters of first principle models.

Marsh et al. (2004) derived an empirical model, NOEM (Nitric Oxide Empirical Model), which calculates the zonally averaged number density of NO on a grid of magnetic latitude and altitude using the Kp-index, solar declination, and the 10.7 cm solar flux as inputs. Section 2.3 describes the Kp-index and 10.7 cm solar flux while Section 4 specifies the parameters of NOEM in more detail. Empirical Orthogonal Function (EOF) analysis of NO measured with SNOE, which operated between 1998-2000 and measured UV-fluorescence scattering of incident solar radiation (Barth et al., 2003), forms the basis for the derivation of NOEM. Bender et al. (2015) and Bermejo-Pantaleon et al. (2011) use the NO calculated with NOEM as a priori in the NO retrievals of the SCIAMACHY and MIPAS instruments respectively. Moreover, NOEM constitutes the upper boundary for the NCAR (National Center for Atmospheric Research) WACCM (Whole Atmosphere Community Climate Model) at 140 km and helps to evaluate the response of WACCM to variability around 100 km in altitude.

However, no study has validated NOEM nor proposed a contending model since its release. This study aims to fill these two gaps by building a new empirical model based on NO measurements in the MLT by Odin SMR for the period 2004-2016. We hypothesize that an empirical model derived from Odin SMR should be more accurate than NOEM because the Odin SMR measurements include a larger range of solar conditions over a period of over 12 years. Furthermore, SNOE measured only daytime NO whereas SMR provides NO measurements during both day and night. This might introduce some discrepancy between NOEM and the resulting empirical model, since ~~night-time NO is expected to be higher than day-time NO due to its dissociation by sunlight~~the concentration of NO is characterized by a strong diurnal variation, depending of latitude and altitude (Bermejo-Pantaleon et al., 2011).

This study primarily aims to derive a new empirical model based on the 12 years of Odin SMR measurements to calculate NO in the MLT. This new model will be named the SMR Acquired Nitric Oxide Model Atmosphere (SANOMA). Additionally, this study aims to evaluate the performance of both SANOMA and NOEM by comparing simulated NO with measurements from the independent NO-measuring instruments SOFIE, SCIAMACHY, ACE, and MIPAS.

Section 2 describes the SMR NO data set ~~and space weather as well as geomagnetic and solar~~indices, while section 3 thoroughly describes the method used to derive SANOMA from the Odin SMR observations. Finally, Section 4 assesses the performance of both NOEM and SANOMA by comparing their simulated NO with measured NO from aforementioned satellites, followed by a discussion in Section 5.

2 Data Description

This section outlines the Odin SMR data set which forms the basis for SANOMA. Section 2.1 describes the contents of the original data set of Odin SMR measurements while Section 2.2 presents the steps taken from this data set to the NO data used for the analysis. Finally, Section 2.3 offers an overview of the indices used in this study to describe auroral and solar activity.

5 2.1 Odin SMR

The Odin SMR instrument scans the limb of the atmosphere and has been observing NO thermal emission lines in a band centered around 551.7 GHz since October 2003 (Sheese et al., 2013). Frisk et al. (2003) provide a description of the Odin SMR instrument. Odin orbits the Earth in a sun-synchronous orbit with ascending and descending nodes around 06:00 and 18:00 local time, respectively (Murtagh et al., 2002), and provides near-global coverage between approximately 82° S and 82° N, although some measurements can be located at higher latitudes, as the satellite is turned to point towards the poles when conditions allow for this. From 2003 to 2007, the Odin SMR instrument split its measurement time between aeronomy and astronomy modes. Consequently, during this period the NO mode of the SMR instrument operated a 24 hour period approximately once per month whereas subsequent to 2007, it has measured approximately four 24-hour periods each month. Since the SMR instrument measures microwave emission, the data set also contains both day- and night-time measurements.

15 Using the measured emission spectra, an inversion algorithm derives the Volume Mixing Ratio (VMR) of NO as a function of altitude for the location of the measurement with an altitude resolution of ~ 4 km. This inversion technique uses the measured brightness temperatures of the NO emission from the various tangent altitudes of a single limb scan as well as a priori NO climatology to ascertain an estimate for the VMR of NO as a function of altitude. Version 3.0 Level 2 NO VMR constitute the Odin SMR data used in this study.

20 Only measurements in which the measurement response, a measure of the relative contributions of the measurement and the a priori, exceeds 0.75 are considered for our analysis. Although no study has validated the version 3.0 Level 2 data, Bender et al. (2015) found that version 2.1 SMR NO measurements were consistent with NO measurements from the ACE, MIPAS, and SCIAMACHY instruments.

2.2 Daily Zonal Averages

25 SANOMA will express NO in number density to ~~accommodate chemical models. The~~ facilitate its comparison to NOEM. The Odin-SMR measured VMR at each altitude is converted to number density, molecules/cm³, with the ideal gas law in which the pressure and temperature originate from an apriori background atmosphere. For the analysis, an algorithm calculates the daily averages of NO number density as a function of altitude and altitude-corrected magnetic latitude. Since the original data set contains measurements on geographical coordinates, a Matlab routine based on the IGRF-12 (International Geomagnetic Reference Field) internal field model, converts the geographical latitude to altitude-corrected magnetic latitude (Thebault et al., 30 2015), denoted with Λ .

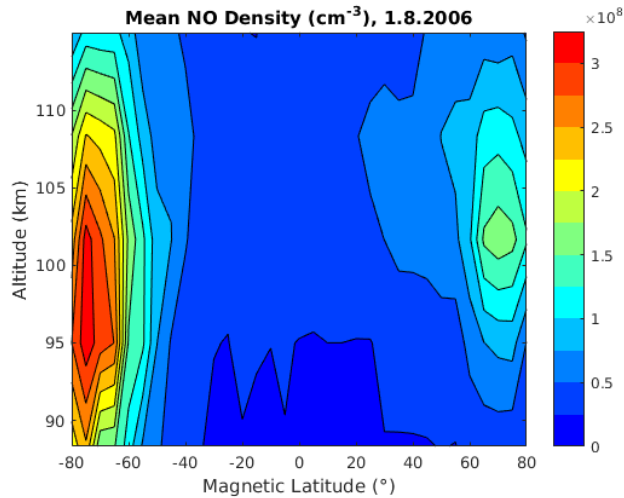


Figure 1. Mean NO density in molecules/cm³ for 1.8.2006 calculated from V3.0 Level 2 Odin SMR data.

For each measurement day, the NO number density is sorted into bins according to altitude and magnetic latitude. Prior to sorting, each individual measurement is interpolated in altitude with grid points at the centers of the altitude bins. The bins for altitude run from 85 km to ~118.33 km with a bin width of ~6.67 km. This altitude range reflects the area in which the measurement response of the SMR-measured NO typically exceeds 0.75, while the resolution reflects that of the measurement.

5 The bins for magnetic latitude run from -82.5°Λ to 82.5°Λ with a bin width of 5°Λ. Once the algorithm has sorted the individual measurements for the measurement day, it calculates the mean NO number density in each bin. Although the Odin orbit should ensure near-global coverage, on some days the data covers only a limited range of altitudes and latitudes due to gaps in the measurements. Figure 1 illustrates an example of the average NO number density for the 1st of August 2006. Maximum NO concentrations can be seen around -70°Λ and 70°Λ and reflect the locations of maximum auroral activity. With all measurement

10 days, the resulting NO number density data comprises 442 individual days from January 2004 to April 2016, each containing 33 latitude and 5 altitude bins. Therefore, a 3D-matrix with the dimensions 442×5×33 contains all the necessary information on NO. Although Odin has continued measuring subsequent to 2016, the used period already contains one solar cycle and is thus deemed sufficient for the analysis in this work.

2.3 **Space Weather** Geomagnetic and Solar Indices

15 Since auroral and solar activity create NO in the MLT, proxies which describe these two phenomena constitute key parts of SANOMA. In the search for appropriate proxies, this chapter introduces some of the most common ones **used**.

Measurements of the irregular variations of the horizontal component of the Earth's magnetic field constitute an auroral activity index, the Kp-index (Menvielle and Berthelier, 1991). It ranges from 0-9 on a quasi-logarithmic scale with higher values corresponding to higher activity. It is derived every 3 hours from a network of measurements stations located between

20 ~40° N-60° N as well as at ~40° S geographical latitude. A similar index, the Ap-index is exponentially proportional to the

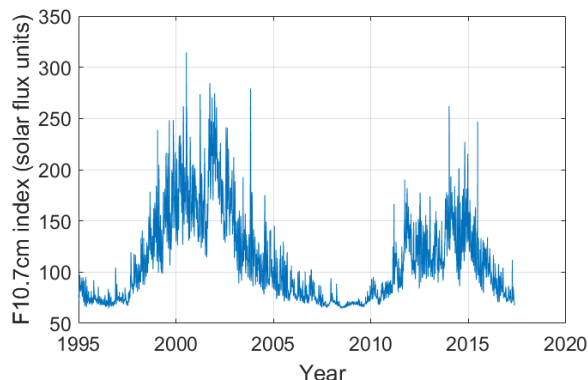


Figure 2. Daily mean F10.7cm flux over time. (NOAA, 2017)

Kp-index. Finally, the Ae-index is another measure for auroral activity and has been suggested to correlate more directly with NO in the MLT region than the Kp- or Ap-index (Hendrickx et al., 2015). The Ae-index derives from measurement stations closer to the magnetic poles than the Kp-index (Menvielle et al., 2011). ~~The Kp- and Ap-indices for this study are~~ However, this study uses only the Kp-index because the empirical model created with the Kp-index explains a larger percentage of
 5 the variance of the original Odin-SMR NO measurements, than an empirical model using the Ae-index. The Kp-index is obtained from the National Oceanic and Atmospheric Administration (NOAA) ~~whereas the Ae-index originates from~~ <http://wdc.kugi.kyoto-u.ac.jp/aedir/>.

To describe solar activity, the 10.7 cm solar radio flux is among the most widely used indices. It constitutes a proxy for the incoming solar soft x-rays and is based on the solar radio emission in a 100 MHz-wide band centered around 2800 MHz (Tapping and Detracey, 1990). This study uses the observed daily mean 10.7 cm from the NOAA. The total radiation flux centered around the Lyman- α line defines an alternative proxy for solar activity and originates from <http://lasp.colorado.edu/lisird/data.html>.
 10 Figure 2 shows the F10.7cm flux over time. Over the measurement period of Odin SMR, solar activity decreased from 2003 to 2009, subsequent to which it rose to reach a maximum in 2014, followed by another decline. In the context of this work, the solar cycle is integral to understanding radiation-related variations of NO.

15 3 SANOMA

This section describes the method used to derive SANOMA from the original Odin SMR measurements. Section 3.1 presents the evidence on how various environmental conditions are linked to the amount of measured NO and presents the underlying equations of SANOMA. Section 3.2 compares SANOMA as well as an empirical model derived from Odin SMR NO but using the principle of NOEM, with NO measured with Odin SMR.

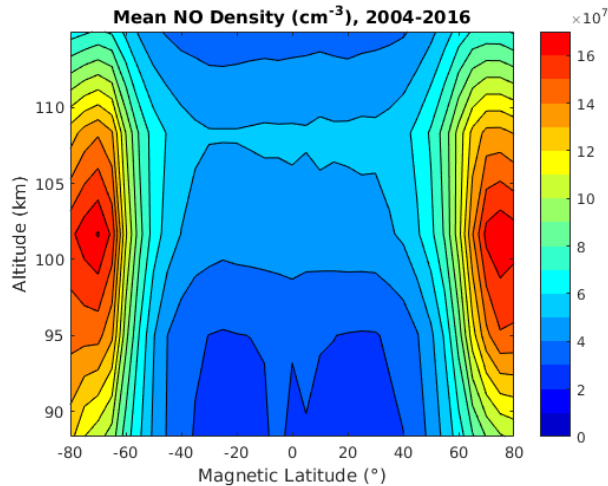


Figure 3. Mean NO density of NO measured by Odin SMR from 2004-2016.

3.1 Linking Environmental Conditions and Measurements to Form SANOMA

Figure 3 displays the mean NO from the Odin SMR dataset. Distinct maxima of up to $16 \times 10^7 \text{ cm}^{-3}$ around $\pm 70^\circ \Lambda$ can be observed at an altitude of roughly 102 km. Figure 4 shows the time series of the daily means of NO derived from the V3.0 Odin SMR data at the altitude-latitude bin centered around a) 102 km and $-70^\circ \Lambda$ and b) 102 km and $0^\circ \Lambda$. Figure 4a) displays strong seasonal variability, while the time series in Figure 4b) exhibits long-scale variability which can be associated with the solar cycle (Baker et al., 2001). The highest peaks in Figure 4a) are most likely produced by high levels of auroral activity. These enhancements are also linked to the seasonal variation, with highest levels during winter, during which NO created in the lower thermosphere is transported downwards in the polar vortex (Pérot et al., 2014).

To investigate the link between auroral activity and the NO number density, Figure 5 zooms in on the year 2015 from the same time series as in Figure 4 along with the daily mean of the a) K_p and b) 10.7 cm fluxes from one day prior to the measurements. Figure 5a) suggests that the K_p index correlates with the amount of NO at the chosen location. Further, Figure 5b) illustrates the link between tropic NO and the $F10.7 \text{ cm}$ flux.

(Marsh et al., 2004) used the K_p -index and $F10.7 \text{ cm}$ flux as a proxies for auroral and solar activity, respectively. (Marsh et al., 2004) used these two indices as well as solar declination as inputs for a model, NOEM, to calculate the variations of NO in the MLT. Understanding the theory behind NOEM is necessary to have a foundation upon which we build SANOMA. NOEM is based on principle component analysis of two years of measurements from the Student Nitric Oxide Experiment (SNOE) between 1998 and 2000, in which the variation of daily mean NO in time is described using Empirical Orthogonal Functions (EOF's) in space, and their Principal Components (PC's) in time, ~~with the~~ In the study by Marsh et al. (2004), these

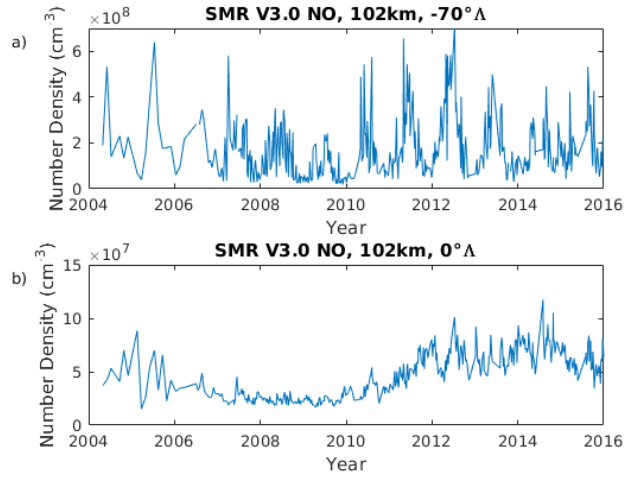


Figure 4. a) Daily mean NO density of Odin SMR NO at a) 102 km and $-70^\circ \Lambda$ and b) 102 km and $0^\circ \Lambda$, from 2004 to 2016.

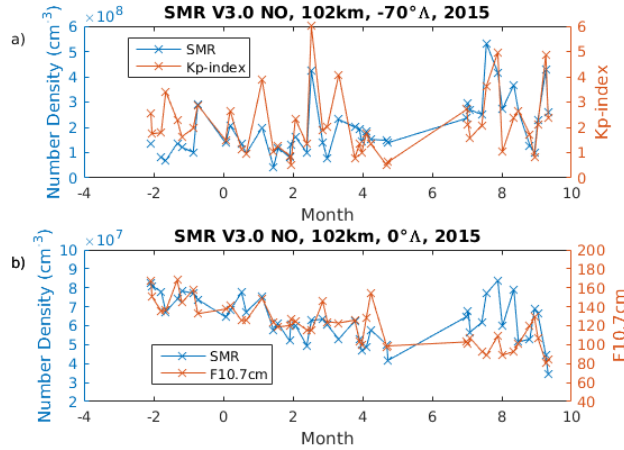


Figure 5. a) Daily mean NO derived from Odin SMR at 102km and -70° magnetic latitude with the Kp-index b) 102 km and $0^\circ \Lambda$ with the F10.7cm flux.

PC's were replaced by polynomial fits to the planetary K-index, the solar declination, and the F10.7cm flux. This led to the following equation

$$NO(\Lambda, h, t) = \overline{NO}(\Lambda, h) + EOF_1(\Lambda, h) \cdot f_1(Kp) + EOF_2(\Lambda, h) \cdot f_2(\delta) + EOF_3(\Lambda, h) \cdot f_3(\log(F10.7)), \quad (1)$$

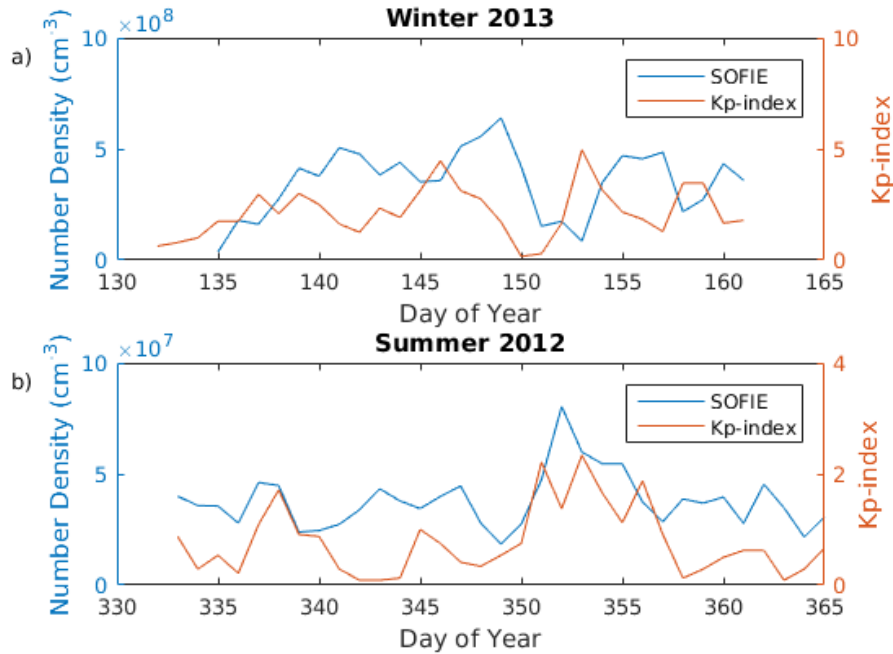


Figure 6. NO number density measured with SOFIE and Kp-index over time for a) 101 km altitude, 75° S magnetic latitude, winter 2013, and b) 101 km altitude, 75° S magnetic latitude, summer 2012.

in which f , h , t , Kp , δ , and $F10.7$ denote a polynomial fit, the altitude, time, planetary K-index, solar declination, and F10.7cm flux, respectively. However, Kp , δ , and $F10.7$ may be insufficient to describe the processes responsible for the creation and depletion of NO in the MLT region.

Figure 6 demonstrates a situation in which the Kp-index may not suffice to model the NO number density near the magnetic pole. We use SOFIE measurements in this context since contrary to Odin SMR, SOFIE measures on consecutive days. Figures 6a) and 6b) compare SOFIE NO with the Kp-index at 102 km and -75°A during the Antarctic winter in 2013 and Antarctic summer in 2012 respectively.

Figures 6a) and 6b) display two key differences. Firstly, during summertime the NO number density is one order of magnitude lower than during winter. Additionally, Figure 6b) suggests that SOFIE NO varies with little or no lag with respect to fluctuations in the Kp-index. However, NO in Figure 6a) seems to have a lag of several days in comparison to the Kp-index. For instance, the Kp-index increases between days 142 and 146, while SOFIE NO follows an increase between days 146 and 149. Other examples can be seen between the increase in the Kp-index on days 151 and 157, as well as the corresponding increases in NO on days 153 and 158. Such a lag could be due to the longer lifetime of NO in dark conditions. Although Figure 6 offers no conclusive evidence of a major difference in the behavior of measured NO with respect to the Kp-index, it does warrant a need for further investigation. Perhaps the fact that NOEM disregards any effect of the Kp-indices of previous has an effect on

Table 1. Constant n in Equations 2 and 3 as a function of solar declination (δ).

<u>n</u>	<u>com₁</u>	<u>com₂</u>
<u>3</u>	<u>$\delta > 0$</u>	<u>$\delta < 0$</u>
<u>4</u>	<u>$-5 < \delta < 0$</u>	<u>$5 > \delta > 0$</u>
<u>6</u>	<u>$-10 < \delta < -5$</u>	<u>10 days. The values in $> \delta > 5$</u>
<u>8</u>	<u>$-15 < \delta < -10$</u>	<u>$15 > \delta > 10$</u>
<u>12</u>	<u>$-20 < \delta < -15$</u>	<u>$20 > \delta > 15$</u>
<u>22</u>	<u>$\delta < -20$</u>	<u>$\delta \geq 20$</u>

the accuracy of the final model. This is why we propose two additional indices which take into account the Kp-index on prior days as well. These are defined as:

$$com_1 = \frac{Kp_{d=1} + \sum_{d=2}^n Kp_d \cdot e^{-d/4 - (d-2)/5} \cdot \frac{\delta + 23.4 - \delta + 23.4}{46.8}}{46.8}, \quad (2)$$

$$com_2 = \frac{Kp_{d=1} + \sum_{d=2}^n Kp_d \cdot e^{-d/4 - (d-2)/5} \cdot \frac{\sin(\frac{\delta * \pi}{46.8}) \cdot \delta + 23.4}{46.8}}{46.8}, \quad (3)$$

- 5 in which Kp_d is the Kp-index on day where d , which is indicates the number of days prior to the simulated day, e is Euler's number, and n is a constant which depends on the solar declination. If the magnitude of the solar declination is less than 10° , 15° , 20° , or more than 20° , n is assigned the value 2, 4, 6, or 11 respectively. A solar declination of $23.523.4^\circ$ corresponds to summer solstice in the northern hemisphere. The two new indices aim to account for NO which has been created on previous days, since During this time com_1 is equal to zero, and the solar declination term in com_2 is equal to one, while the opposite holds true for the winter solstice of the northern hemisphere when the solar declination is -23.4° . Therefore, com_1 pertains to an NO build-up from previous days in dark conditions, NO in the MLT can persist for up to in the northern hemisphere, while com_2 has the same function for the southern hemisphere. Equations 2 and 3 assume that the influence of NO from previous days reduces exponentially with an increasing number of days prior to measurement. The constant n for com_1 and com_2 depends on the solar declination, as listed in Table 1.
- 15 The constant n regulates the number of days from which the Kp-index is taken into account by com_1 and com_2 . We expect that with decreasing sunlight, the longer back in time the Kp-index affects the measured NO, therefore warranting a larger n . These exact values for n are the results of an iteration scheme on Equations 2 and 3 were chosen through iteration such that SANOMA would explain the largest percentage of variance of the Odin SMR dataset. This iteration scheme contained two variables: the constant n as a function of the solar declination bins in Table 1, and the factor in the denominator of the exponential, $e^{-d/5}$, which describes how quickly the influence of the Kp-index from previous days diminishes. The criterion for finding these values was to maximize the adjusted R-squared averaged over the entire spatial domain of the resulting
- 20

empirical model compared to the original measurements, described later on in Section 3.2 and depicted in Figure 11 c). With an initial guess of n for the various solar declination bins of 3,4,5,7,10, and 12, the denominator which maximizes the adjusted R-squared value in Figure 11 is 5. Similarly, with the now determined denominator, each solar declination bin was optimized individually, such that the adjusted R-squared averaged over the entire spatial domain in Figure 11 would reach a maximum.

5 This iteration resulted in the values presented in Table 1. Section 3.2 demonstrates that these two compound indices lead to a significant improvement in the model.

SANOMA uses the three indices from NOEM and the two indices defined in Equations 2 and 3, to build a multivariate linear fit.

The simulated NO for each altitude-latitude bin as a function of time becomes

$$10 \quad NO(\Lambda, h, t) = K_p(t) \cdot c_1 + dec(t) \cdot c_2 + \log(F10.7cm(t)) \cdot c_3 + com_1(K_p, dec) \cdot c_4 + com_2(K_p, dec) \cdot c_5 + C \quad (4)$$

in which the Kp-index and the logarithm of the F10.7cm flux both have a lag of 1 day for the best fit. This lag is in accord with previous similar studies (Hendrickx et al., 2015; Marsh et al., 2004; Solomon et al., 1999). Solomon et al. (1999) attribute this lag to the one-day lifetime of NO. Taking the logarithm of the F10.7cm flux instead of the flux itself results in a better fit between SANOMA and Odin SMR. This observation agrees with the findings of Marsh et al. (2004) and Fuller-Rowell (1993).

15 The indices c are obtained as an output of a multivariate linear fit function called 'regress' in MatLab 2015b, in which a matrix containing all of the input indices as a function of time, and a corresponding matrix containing the measured NO time series in a given altitude and latitude bin, constitute the two inputs. Figure 7 shows the measured and simulated time series of NO for 102 km and $-70^\circ \Lambda$. Although SANOMA generally follows the SMR measurements, it misses some of the highest peaks of NO. Either these peaks are results of random variation of the measurements, or SANOMA fails to simulate some physical or

20 chemical process which would result in such peaks of NO. One such effect could be the dynamics of the MLT region, which would transport NO.

The complete SANOMA model comprises of a total of 165 individual multivariate linear fits, one for each altitude-latitude bin. The coefficients of these fits indicate which of the input indices influence NO at the various locations. Figures 8a)-c) present the coefficients of the multivariate linear fits for the Kp-index, solar declination, and $\log(F10.7cm)$ flux, respectively.

25 These figures offer an insight to where each of the physical drivers influence the NO number density the most. The effect of geomagnetic activity seems to be strongest around $\pm 70^\circ \Lambda$, while the solar radiation affects NO over the latitude range between $\pm 70^\circ \Lambda$ in the altitudes from 100 to 110 km. Figures 8a)-c) are also reminiscent of the EOF's obtained by Marsh et al. (2004). Furthermore, Figure 8b) shows the anti-symmetric effect of season on either contributing to an increase, or decrease of NO, as the coefficient changes sign from negative in the southern hemisphere, to positive in the northern hemisphere. Finally, Figure

30 9 a) and b) depicts the coefficients corresponding to the new indices, com_1 and com_2 , respectively. The two exhibit maxima at roughly 95 km in altitude close to the northern and southern magnetic poles. Figure 9 indicates, that the indices function as planned as com_1 significantly deviates from zero only in the northern hemisphere, while the same is true for com_2 in the southern hemisphere. The entire set of coefficients can be downloaded from odin.rss.chalmers.se.

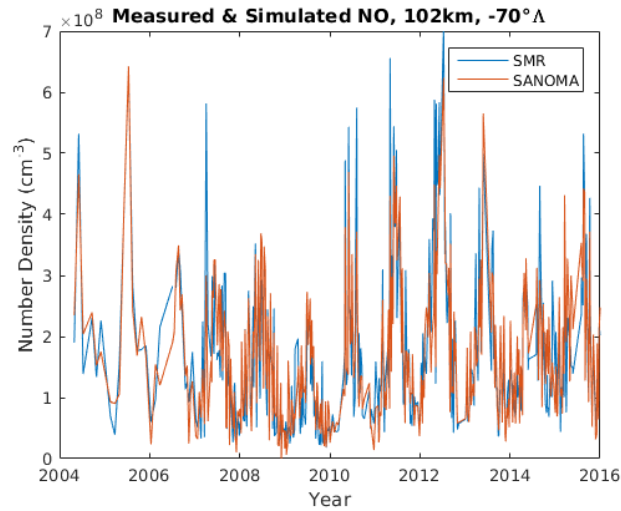


Figure 7. SMR-measured and SANOMA-simulated time series of NO at 102 km and $-70^\circ\Lambda$

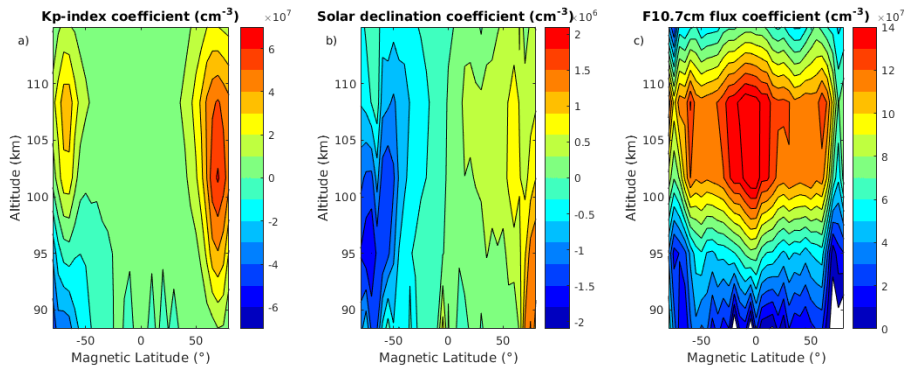


Figure 8. The coefficients of the a) Kp-index b) Solar declination c) F10.7cm flux, in Equation 4.

3.2 Comparing SANOMA to Odin SMR-measured NO

This section compares NO simulated with SANOMA with the original SMR-measured NO to confirm that the model has been successfully built. SANOMA has a resolution of 6.66 km in altitude and $5^\circ\Lambda$ in latitude. Figure 10 illustrates the mean of the difference of the time series of SMR and SANOMA NO at each location in cm^{-3} . The largest mean difference is $-2.8 \times 10^{-7-8}$ cm^{-3} , which means that on average, SANOMA can simulate the Odin SMR NO measurements with relatively low systematic error. Considering that the actual measured number density of NO is within the order of magnitude 10^7 cm^{-3} , this difference can be considered negligible and the result of numerical error in the creation of the model.

To explore the added value of the two new indices and the SANOMA equation, Figure 11 illustrates the adjusted coefficient of determination, denoted R-squared values, of three empirical models based on Odin SMR NO measurements. These models

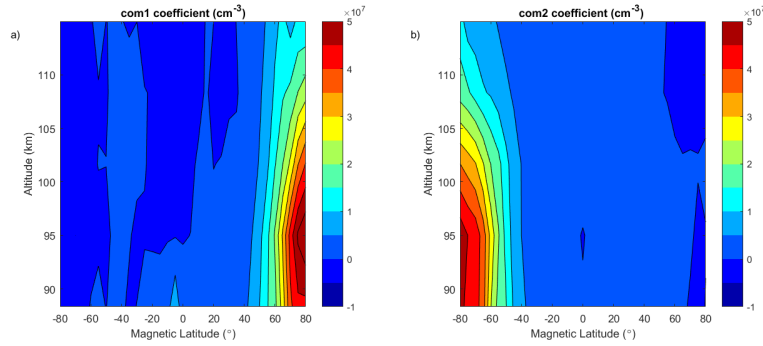


Figure 9. The coefficients corresponding to the a) com1 b) com2 indices.

are a) a model built up according to Equation 1, called SMRNOEM, as a function of magnetic latitude and altitude, b) a model built with Equation 4 but without the compound indices, and c) with Equation 4. The R-squared value represents the percentage of the variance in the original SMR dataset which each model can explain. From left to right, we can observe an increasing trend in which the mean explained variances in each subplot is 0.509, 0.552, and 0.639, 0.506, 0.541, and 0.643. Figure 11b) demonstrates that using a multi-variate linear method instead of EOF analysis increases the R-squared somewhat in comparison to 11a), but the more obvious improvement is provided by the inclusion of Kp-index information from earlier days, as illustrated by Figure 11c). The most striking difference between Figures 11b) and c) is the great increase in the explained variance close to the magnetic poles and lower down in altitude, brought by the compound indices com_1 and com_2 . This improvement can be explained with by fact that these two indices take the lifetime of upper-atmospheric NO into account, hence yielding more accurate results in the polar regions in which the accumulation of NO in the absence of sunlight plays an important role. Using Equation 4 to build an empirical model therefore increases the overall explained variance by 13%, and by up to 40% near the poles. The figures imply, that Equation 4 would describe the variation of NO best around the magnetic poles, in which geomagnetic activity dominates its variation. Although the adjusted R-squared attains 0.8-0.9 close to the magnetic poles and exceeds 0.5 in most areas, values down to 0.1 indicate that SANOMA fails to accurately simulate the variability of NO at magnetic latitudes closer to the equator than $\pm 40^\circ$ and below altitudes of roughly 95 km.

So far we have presented how well SANOMA explains SMR measurements. However, the SMR measurements themselves include measurement error and hence a model will be unable to perfectly reproduce the measurements. We can attempt to separate the discrepancy between SANOMA and SMR into two parts: the measurement error from Odin SMR and the modeling error from SANOMA. Having an understanding of the error of SANOMA can help to assess the reliability of its simulations. Assuming that all errors are normally distributed, we estimate the variance of the modeling error with

$$\sigma_{SANOMA}^2 = \sigma_{total}^2 - \sigma_{OdinSMR}^2, \quad (5)$$

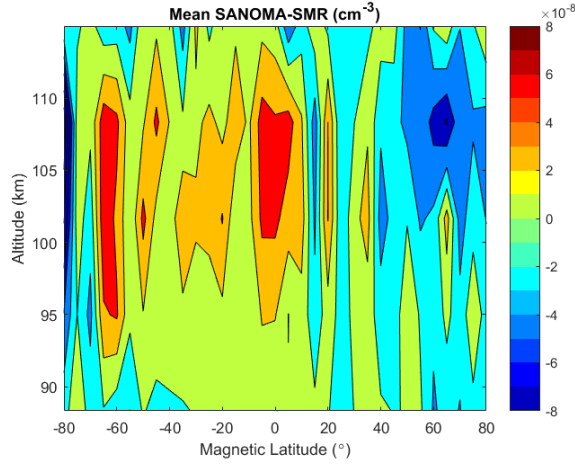


Figure 10. Mean of the differences between the time series of SANOMA-simulated and SMR-measured NO in cm^{-3} .

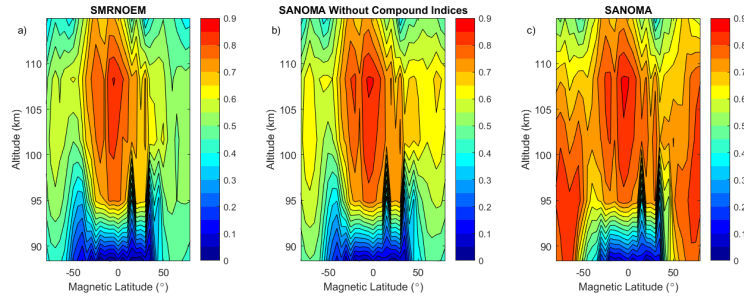


Figure 11. Adjusted R-squared between SMR and an empirical model from Odin SMR NO using a) Equation 1 b) Equation 4 without *com1* or *com2* c) Equation 4.

in which σ_{SANOMA}^2 , σ_{total}^2 , and $\sigma_{OdinSMR}^2$ are the estimated variances of the model error, total error, and measurement error, respectively. For each location, we estimate σ_{total}^2 is estimated as the variance of the time series of SANOMA-SMR. The mean of the daily means of the known measurement error constitutes $\sigma_{OdinSMR}^2$. In some cases, σ_{SANOMA}^2 is close to zero, or slightly negative. If this occurs, σ_{SANOMA}^2 is set to zero, so we can calculate the square root of the variance to yield the standard deviation of the modeling error. Figure 12 illustrates the standard deviation of the modeling error in absolute and relative values. Figure 12b) suggests that the highest relative modeling error is located at the lowest altitudes. One explanation could be that dynamics start to play a larger role lower down, and since This is not surprising as it corresponds to the altitude range where we find lower values of NO number densities. Moreover, the transport of NO starts to play a non-negligible role in this region, affecting the number density of NO. SANOMA includes no dynamics, it fails to model the variations of NO accurately. This could also be due to a lower signal-to-noise ratio in the measurements at lower altitudes parameter to account for this effect, possibly explaining the higher relative standard deviation of the modeling error.

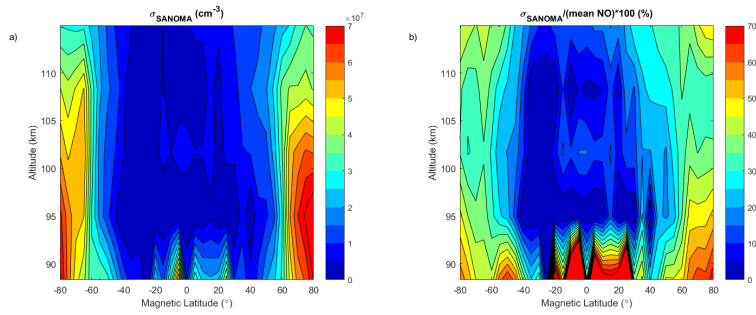


Figure 12. a) Standard deviation of the modeling error b) Standard deviation of the modeling error relative to the mean NO.

Table 2. Overview of all the compared NO datasets

Instrument	Period	Latitudes	Altitudes (km) -Technique	Wavelength
SMR	2003-	82° S - 82° N	85-115 -Microwave Emission	544 μm
SNOE	1998-2000	82° S - 82° N	100-150 -UV Scattering	215 nm, 237 nm
SOFIE	2007-	80° S - 60° S, 60° N - 80° N	40-140 -Solar Occultation	5.316 μm
SCIAMACHY	2008-2012	88.75° S - 88.75°	60-160 -UV Scattering	230-314 nm
ACE	2004-	8285° S - 8285° N	70-110 -Solar Occultation	5.18-5.43 μm
MIPAS	2005-2012	8290° S - 8290° N	70-120 Infrared emission	5.3 μm

4 Assessment of SANOMA and NOEM

So far, we have presented SANOMA, its underlying principle, and a comparison of its simulations with NO measured by Odin SMR. This section evaluates the performance of SANOMA and NOEM by comparing simulated NO number density with measured NO from the four independent instruments, SOFIE, SCIAMACHY, ACE-FTS, and MIPAS. SANOMA can be seen as a tool to compare the SMR dataset with the other data, and therefore these comparisons can provide valuable information regarding the accuracy of SMR-NO measurements. For an overview, Table 2 lists the underlying techniques behind the instruments as well as the time and regions of operation.

SANOMA has a resolution of 6.66 km in altitude and $5^\circ\Lambda$ in latitude while NOEM has corresponding resolutions of 3.33 km and $5^\circ\Lambda$. For direct comparison, we average two adjacent NOEM altitude bins to result in an altitude resolution of 6.66 km. To prepare each data set comparison with these models, an algorithm sorts the NO measurements from each instrument into the same bins as in SANOMA and calculates daily average NO number density. The following four subsections present the comparisons of SANOMA and NOEM to the four independent instruments, while Section 4.5 summarizes these results.

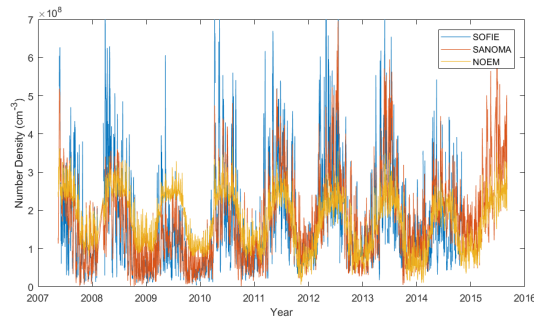


Figure 13. Time series of NO number density measured with SOFIE over the entire measurement period as well as simulated NO with SANOMA and NOEM, 102 km altitude, $-70^\circ \Lambda$.

4.1 SOFIE

This section compares the SANOMA and NOEM simulated NO number density with Level 2 V1.3 SOFIE measurements (Gordley et al., 2009) (available at sofie.gats-inc.com) between 102 km to 115 km. These altitudes reflect the range in which NOEM, SANOMA, and SOFIE all overlap. According to Figure 13, especially prior to 2011, NOEM-simulated NO exceeds that of both SOFIE-measured and SANOMA-simulated NO. A possible cause for this effect is discussed in Section 4.5. Additionally, the SOFIE measurements show high peaks of NO, which are partially absent in SANOMA, and completely absent in NOEM. The SANOMA time series seems to generally agree better with the SOFIE measurements than NOEM.

To examine the accuracy of SANOMA and NOEM as a function of magnetic latitude and altitude, Figure 14 depicts the median of the difference between the simulated NO and SOFIE as a percentage of the mean SOFIE number density. Although SOFIE predominantly measures at geographic latitudes between 60° and 80° in both hemispheres, some measurements from the southern hemisphere originate from as low as $40^\circ \Lambda$ due to a changing orbit and greater offset between the geomagnetic and geographic poles in the southern hemisphere. Generally, the difference between SANOMA and SOFIE lies between $\pm 40\%$ in the region from $60^\circ \Lambda$ to $80^\circ \Lambda$ in both hemispheres while the NOEM-modeled NO exceeds SOFIE with up to 160%.

To assess the amount of variation that each model captures of the original SOFIE data, Figure 15 presents the R-squared values of linear fits between SANOMA and SOFIE as well as NOEM and SOFIE, respectively. Whereas SANOMA exhibits up to 0.65 R-squared at $-70^\circ \Lambda$ and 102 km, NOEM falls significantly shorter with a maximum R-squared value of 0.35 at $-55^\circ \Lambda$ and 102 km. Furthermore, Figure 15 emphasizes that SANOMA outperforms NOEM at all altitudes in the auroral zone of $60^\circ \Lambda$ to $80^\circ \Lambda$ in both hemispheres and that SANOMA captures more variability of the SOFIE measurements in the southern than in the northern hemisphere.

4.2 SCIAMACHY

This section compares the SANOMA- and NOEM-simulated NO number density with v1.8.1 SCIAMACHY (Bender et al., 2013) measurements of NO in the altitudes from 102 km to 115 km. Figure 16 draws the time series of SCIAMACHY-measured,

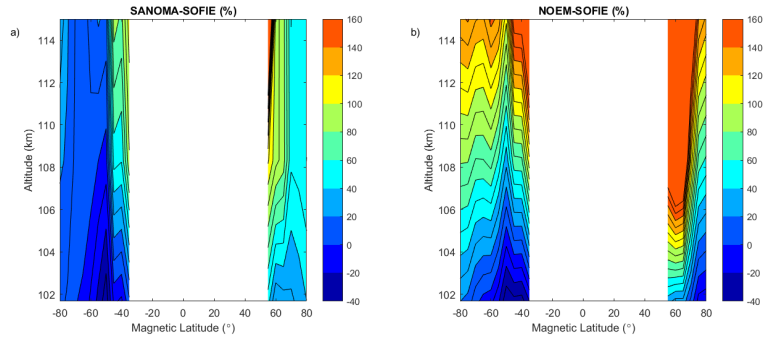


Figure 14. a) Median difference between SANOMA and SOFIE as a percentage of mean SOFIE NO number density. b) Median difference between NOEM and SOFIE as a percentage of mean SOFIE NO number density.

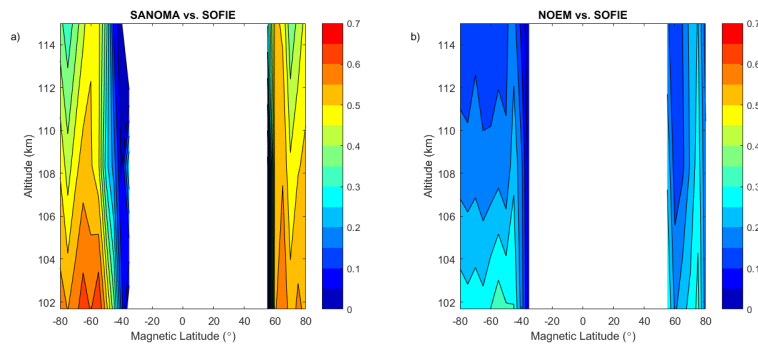


Figure 15. a) Adjusted R-squared of linear fits between SANOMA and SOFIE NO number density. b) Adjusted R-squared of linear fits between NOEM and SOFIE NO number density.

as well as SANOMA- and NOEM-simulated NO for 102 km and $-70^\circ\Lambda$. As in Figure 13, NOEM NO exceeds that of both SANOMA and SCIAMACHY whereas SANOMA follows SCIAMACHY measured NO more accurately over the entire measurement period. Another clear feature is that SANOMA NO increases significantly more than SCIAMACHY NO during Antarctic winter. One possible explanation is that SCIAMACHY only measures day-time NO, whereas the Odin SMR data which resulted in SANOMA also included measurements from the polar night, during which the NO number density is enhanced.

Figures 17a) and b) display the mean difference between SANOMA and SCIAMACHY as well as NOEM and SCIAMACHY as a percentage of the mean SCIAMACHY number density. NOEM NO exceeds SCIAMACHY with over 200% while SANOMA reaches maximum differences up to 150% at $-70^\circ\Lambda$ and 102 km.

As can be seen in Figures 18a) and b), SANOMA reaches maximum R-squared values of roughly 0.5 in the areas of high auroral activity while NOEM attains only 0.25 at 102 km and $-60^\circ\Lambda$. The results suggest that SANOMA captures significantly more variability of the SCIAMACHY dataset than NOEM.

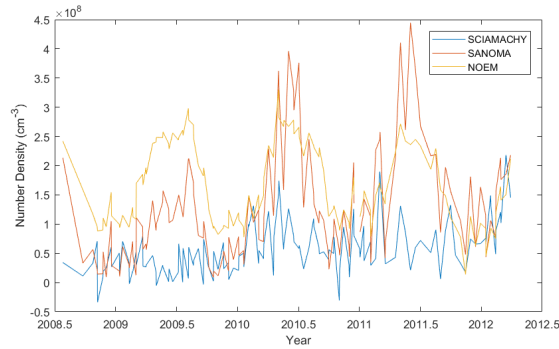


Figure 16. Time series of NO number density measured with SCIAMACHY and simulated with SANOMA as well as NOEM, 102 km altitude, $-70^\circ \Lambda$.

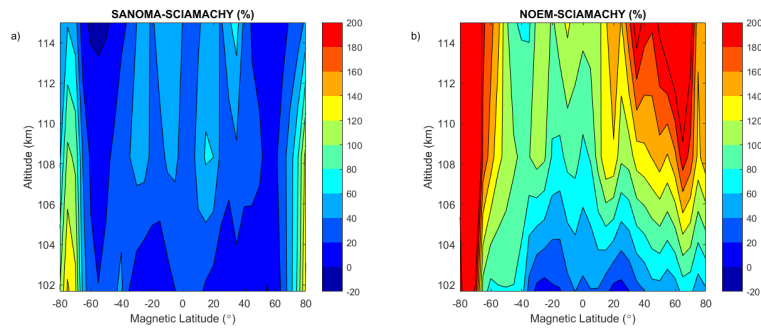


Figure 17. a) Median difference between SANOMA and SCIAMACHY as a percentage of mean SCIAMACHY NO number density. b) Median difference between NOEM and SCIAMACHY as a percentage of mean SCIAMACHY NO number density.

4.3 ACE

This section compares the SANOMA and NOEM simulated NO number densities with V3.5 ACE measurements (Bernath et al., 2005) between 102 and 108 km. Quality filtering of the ACE NO measurements constitutes the reason for the upper limit of the altitude in these comparisons. Figure 19 provides an overview of almost nearly one entire solar cycle of ACE, SANOMA, and NOEM NO. It can be seen that both models miss the highest spikes of NO in the ACE measurements, although SANOMA manages to capture several between 2005 and 2012. Figure 20a) suggests that the difference between SANOMA and ACE is generally zero or positive above 105 km with a maximum difference of 60% within $30^\circ \Lambda$ of the magnetic equator at 108 km. Negative differences can be observed below 105 km, with a minimum of -50% near the magnetic equator at 102 km. On the contrary, Figure 20b) shows that the difference between NOEM and ACE is positive at nearly all locations, with a maximum of 160% at 20°N magnetic latitude at 108 km. The patterns in Figure 20 could be due to the different height at which each model places the maximum NO. The maximum of NO number density in ACE is located close to 100 km, while the corresponding SANOMA and NOEM NO maxima are located between 102-108 km.

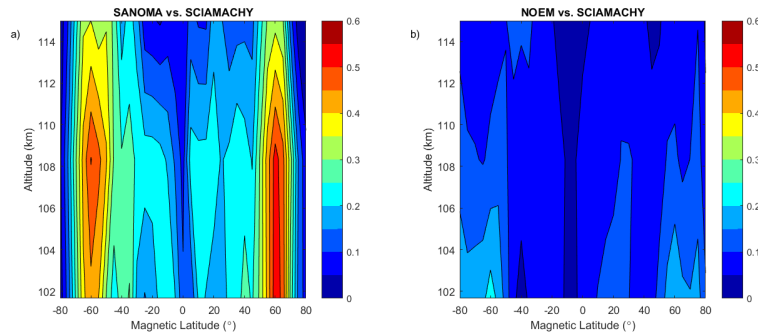


Figure 18. a) Adjusted R-squared of a linear fit between SANOMA and SCIAMACHY NO number density. b) Adjusted R-squared of a linear fit between NOEM and SCIAMACHY NO number density.

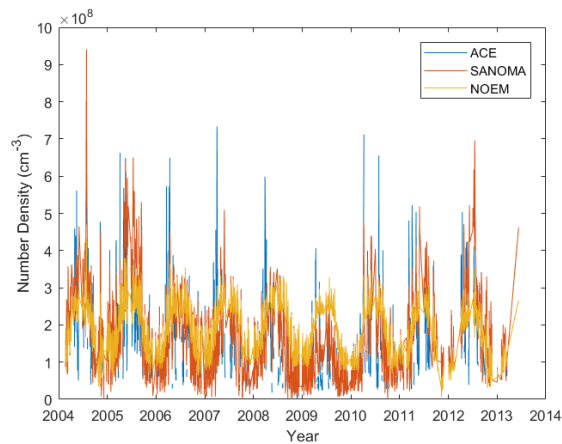


Figure 19. Time series of NO number density measured with ACE and simulated with SANOMA as well as NOEM, 102 km altitude, $-70^\circ \Lambda$.

The SANOMA R-squared values in Figure 21a) reach a maximum of 0.65 at $70^\circ \Lambda$ magnetic latitude while Figure 21b) indicates that NOEM only attains 0.35 at $35^\circ \Lambda$ at 102 km. Figure 21a) also shows a band of lower R-squared from $-45^\circ \Lambda$ to $-25^\circ \Lambda$, the cause of which remains unknown.

4.4 MIPAS

- 5 Finally, this section compares the simulated NO number densities with v5r [MIPAS-620 \(Fischer et al., 2008\)](#) [622 MIPAS \(Bermejo-Pantaleon et al., 2011; Fischer et al., 2008\)](#) measured NO in the altitudes from 102 km to 115 km. In Figure 22, although both NOEM and SANOMA seem to follow the variations of MIPAS-measured NO, SANOMA more accurately reproduces the number density of MIPAS. [Especially during the period of low solar activity around 2009-2010 as indicated in Figure 2, NOEM overestimates MIPAS NO, whereas SANOMA follows it more closely. Both models miss some highest spikes of NO, for instance during 2011.](#) Figures 23a) and 23b) display the median differences between SANOMA and MIPAS as well

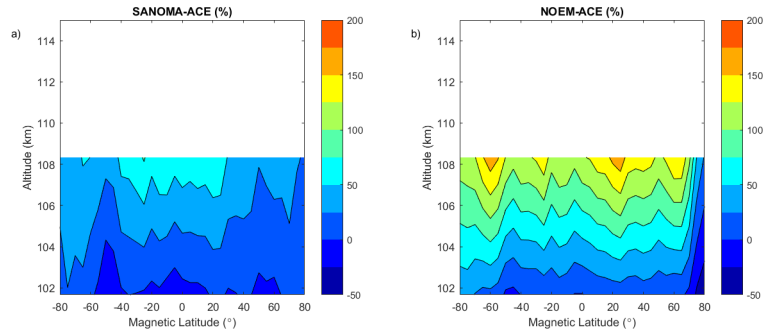


Figure 20. a) Median difference between SANOMA and ACE as a percentage of mean ACE NO number density. b) Median difference between NOEM and ACE as a percentage of mean ACE NO number density.

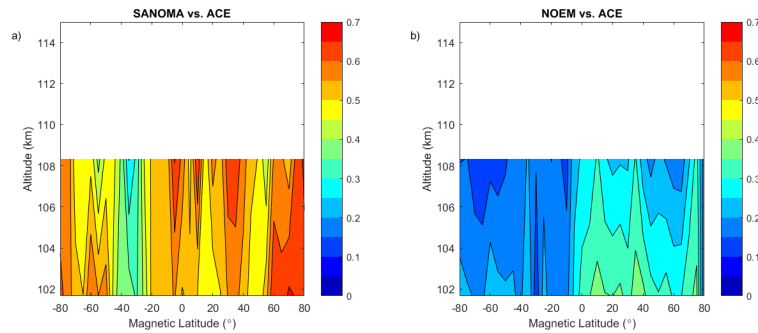


Figure 21. a) Adjusted R-squared of a linear fit between SANOMA and ACE NO number density. b) Adjusted R-squared of a linear fit between NOEM and ACE NO number density.

as NOEM and MIPAS as a percentage of the MIPAS-measured NO. SANOMA ~~underestimates MIPAS NO at all locations, with a minimum of -60~~ ranges between -40% at 115 km around 70° Λ . ~~Meanwhile, the difference between NOEM and MIPAS changes from positive in the higher altitudes to less positive or negative in the lower altitudes, and +100% at 102 km at 30° Λ in comparison to MIPAS. The corresponding values for NOEM are -20% at 80° Λ and +160% at 115 km and 50° Λ .~~ Finally,

5 Figures 24a) and 24b) suggest that in both models, the R-squared varies ~~strongly~~ with latitude. SANOMA explains up to 80% of the variance of MIPAS NO at the lower altitudes around ~~70°N-80° Λ~~ , while NOEM only reaches ~~50~~40% at 20°N° Λ .

4.5 Summary of the Results

~~The~~This section aims to summarize and elaborate on the results of the previous sections. To achieve an overview of the results, Table 3 presents R-squared values between the measurement instruments and three different models: a) NOEM b) SMRNOEM, a model built using the NOEM equations, but Odin SMR data, and c) SANOMA. Comparing NOEM and SMRNOEM informs

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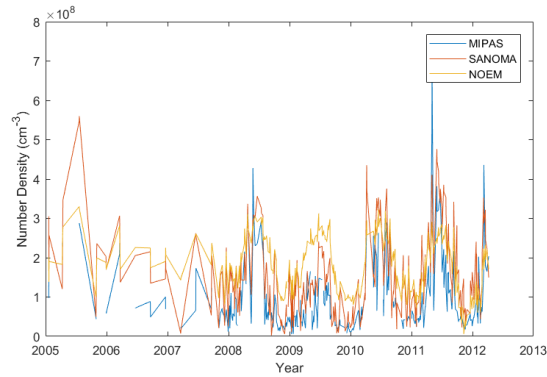


Figure 22. Time series of NO number density measured with MIPAS and simulated with SANOMA as well as NOEM, 102 km altitude, $-70^{\circ}\Lambda$.

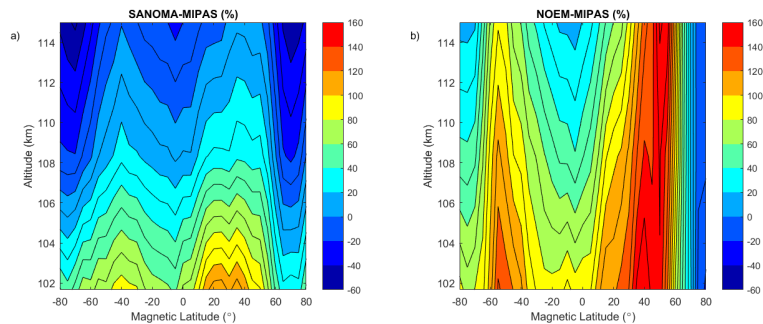


Figure 23. a) Median difference between SANOMA and MIPAS as a percentage of mean MIPAS NO number density. b) Median difference between NOEM and MIPAS as a percentage of mean MIPAS NO number density.

us on any improvement provided by using the Odin SMR NO dataset instead of the SNOE dataset, while differences between SMRNOEM and SANOMA are results of the different approach to developing the two models.

Table 3 reveals that SANOMA consistently explains a similar amount, or more variance than SMRNOEM in all regions and for all instruments, which in turn explains more variance than the SNOE-based NOEM. With SOFIE, ACE, and SCIAMACHY, the median difference between SANOMA and these instruments is closer to zero than for NOEM, ~~while the opposite holds true for MIPAS.~~

Generally, the models capture more variance in the northern, than in the southern hemisphere. Perhaps the larger offset between the geomagnetic and geographic pole, or the more stable polar vortex in the souther hemisphere affect the amount of NO in ways which are beyond the reach of these simple models.

10 The SMRNOEM values in Table 3 highlight how much the Odin SMR dataset itself improves the resulting empirical model and the consistently higher R-squared values in SANOMA compared to SMRNOEM justify the use of the compound indices. Using the SANOMA- instead of the NOEM-equation with SMR-measured NO increased the percentage of explained variance

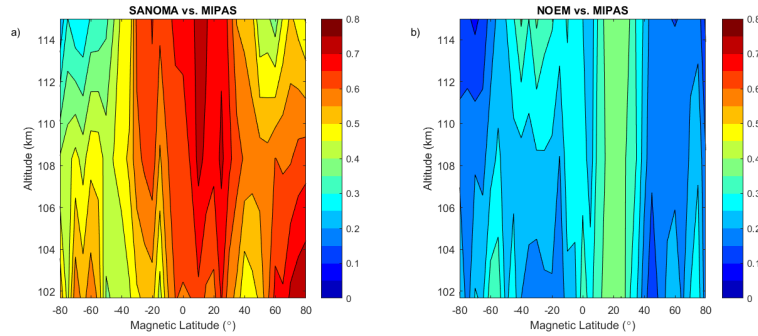


Figure 24. a) Adjusted R-squared of a linear fit between SANOMA and MIPAS NO number density. b) Adjusted R-squared of a linear fit between NOEM and MIPAS NO number density.

Table 3. Mean Adjusted R-squared between 102 and 115 km averaged over the entire altitude range (102-115 km) over three latitude bands: southern high latitudes, tropics, and northern high latitudes, as well as the mean average of the mean percent difference differences over these three domains between the various instruments and a) NOEM, b) SMRNOEM, and c) SANOMA, and the various instruments.

Instrument	R-sq ($-75^{\circ}\Lambda$ to $-55^{\circ}\Lambda$)			R-sq ($-30^{\circ}\Lambda$ to $30^{\circ}\Lambda$)			R-sq ($55^{\circ}\Lambda$ to $75^{\circ}\Lambda$)		
	a	b	c	a	b	c	a	b	c
SMR	0.287	0.509	0.645 0.646	0.544	0.704	0.730 0.732	0.356	0.487	0.696
SOFIE	0.193	0.307	0.495 0.500	N/A	N/A	N/A	0.212	0.207	0.424
SCIAMACHY	0.124	0.292	0.309 0.317	0.069	0.148	0.159 0.161	0.118	0.095	0.316
ACE	0.169	0.423	0.507 0.514	0.246	0.469	0.509 0.510	0.272	0.381	0.572
MIPAS	0.325 0.206	0.483 0.350	0.470 0.426	0.350 0.291	0.456 0.581	0.459 0.621	0.378 0.197	0.378 0.342	0.632

by up to 100% near the magnetic poles. Moreover, these comparisons stem from 102 km and upwards, but as indicated by Figure 11, SANOMA outperforms SMRNOEM by even more in the altitudes below 102 km.

Since SMR measures both day and night time NO, a positive difference compared to the daytime measuring instrument SCIAMACHY was expected, ~~but SANOMA shows a positive difference.~~ SANOMA is also characterized by a slight positive bias in comparison to ~~SOFIE and ACE as well~~ the solar occultation instruments 'SOFIE and ACE-FTS, which could be due to differences in the diurnal sampling. The magnitude of the relative differences between SANOMA and each satellite is similar, although slightly higher than the differences between the SMR dataset and the other instruments described by (Bender et al., 2015). As the time series in Figures 13, 16, 19, and 22 showed, NOEM overestimates the measured NO prior to 2011. The fact that NOEM was derived from SNOE data between 1998-2000, a time of high solar activity, as indicated by Figure 2, might explain why it fails to accurately reproduce the lower NO number densities observed at times of lower solar activity. SANOMA profits from the wider variety of solar conditions experienced over the Odin SMR measurement period from 2004 to 2016 to provide more accurate NO number density over the entire solar cycle.

~~On average, NOEM NO seems to be more accurate than SANOMA only in comparison to MIPAS. However, the MIPAS measurements should be treated with care, since Bender et al. (2015) found that MIPAS NO is 80-120% higher at altitudes between 100 and 120 km. Because the two empirical models can be regarded as extensions of the original measurement instruments, a high MIPAS NO relative to SANOMA was expected.~~

5 5 Conclusion and Discussion

This study presented a new empirical model called SANOMA to simulate NO in the MLT. This model is based on V3.0 Odin SMR NO, to which we fit multivariate linear functions using the Kp-index, solar declination, the logarithm of the F10.7cm flux, as well as two compound indices based on the Kp-index and solar declination. These two compound indices attempt to account for the lifetime of NO in the absence of sunlight. SANOMA can capture an average of 63.9% of the variance of the Odin SMR NO between 88 and 116 km and $-80^\circ \Lambda$ to $80^\circ \Lambda$. The comparisons of SANOMA, the model developed in this study, and NOEM, a similar model by Marsh et al. (2004), with measurements from the SOFIE, SCIAMACHY, ACE, and MIPAS instruments suggest that SANOMA explains significantly more variance of the NO measured by each instrument than NOEM. The percentage of explained variance by SANOMA spans from a minimum of 16% in the magnetic tropics ($-30^\circ \Lambda$ to $30^\circ \Lambda$) with SCIAMACHY, to 73.2% in the magnetic tropics with SMR. Similarly, NOEM captures a minimum of 6.9% of the variance with SCIAMACHY NO in the magnetic tropics, and a maximum of 54.5% of the variance with SMR NO in the same region. Furthermore, the results ~~suggest that over the entire measurement period in this study, NOEM~~ show that SANOMA slightly overestimates the amount of NO ~~for all of the satellites, while SANOMA either over- or underestimates it. The difference between SANOMA and measured NO is closer to zero than NOEM for SOFIE, SCIAMACHY, and ACE, while the opposite holds true for MIPAS. This difference to MIPAS NO is consistent with the findings of Bender et al. (2015), who found that MIPAS NO is roughly 100% higher in the altitudes 100-120 km than in ACE, SMR, or SCIAMACHY. However, this overestimation is significantly lower than for NOEM, when compared with the measurements of the five instruments considered in this study.~~

An alternative to the multivariate linear fit in this study would have been EOF analysis such as in (Marsh et al., 2004). We attempted this approach and compared the resulting model to SANOMA, with roughly equivalent success. The multivariate linear fit approach was then chosen for its simplicity.

Our original hypothesis that a model similar to NOEM, but derived using Odin SMR data, would result in a more accurate model was proven to be true. Comparing the results of NOEM and SANOMA with measured NO showed that especially during times of low solar activity, NOEM overestimates NO by roughly 100%. This could be attributed to the fact that NOEM was built on only two years of SNOE NO data from 1998-2000, a period of high solar activity. Hence, when the model is applied to low-activity periods, such as 2009-2010, the extrapolation from high-activity to low-activity conditions is inaccurate, resulting in large errors of NOEM NO compared to the measurements.

In terms of explaining the variation of NO, unlike NOEM, SANOMA manages to recreate more of the highest concentrations of NO. SANOMA still fails to explain some of the highest spikes of NO and suffers from a relatively coarse (6.5 km) altitude

resolution as well as a narrow altitude range (85 km-115 km). The results from Figures 12 suggested that SANOMA fails to model some physical processes which govern the amount of NO. Perhaps dynamical processes cause fluctuations in the concentration of NO at 85 km, causing the model to miss some of the variation of NO. However, the error associated with SANOMA has been estimated and is available to any potential user of the model.

- 5 Creating SANOMA with all SMR-measurements will have likely introduced a positive bias compared to day-measuring instruments, such as SCIAMACHY, since night-time NO is expected to be higher than day-time NO. An alternative to the current model would be to provide two versions of SANOMA: one for day, and one for night.

Although no rigorous validation of Odin SMR NO in the MLT regions exists, Bender et al. (2015) proposed that the Odin SMR is consistent with measurements from other satellites. However, it is conceivable that all of these measurements could deviate from the true concentration of NO. Even so, SANOMA offers an estimate which reflects the physical processes behind the creation of NO. As long as no in-situ measurements are available, remote sensing is the only way to provide some estimate of the true state. SANOMA could be used in the future as an input for chemical models of the atmosphere, as apriori information for satellite retrievals of NO, or as a transfer function to compare NO observational data sets with each other, to name a few possible applications. SANOMA and accompanying scripts are available on odin.rss.chalmers.se

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- 15 *Author contributions.* Joonas Kiviranta: main body of text, work behind SANOMA, analyzed satellite and indices data, all plots Kristell Pérot: initiated the study, scientific consulting, editing of text, input on correctness of facts, etc. Donal Murtagh, scientific consulting, editing of text, Patrick Eriksson, scientific consulting, editing of text.

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