

Review of “A light-weight NO₂ to NO_x conversion model for quantifying NO_x emissions of point sources from NO₂ satellite observations”

Sandro Meier, Erik F. M. Koene, Maarten Krol, Dominik Brunner, Alexander Damm, and Gerrit Kuhlmann

General Comments

This study investigates the method used to convert NO₂ emissions derived from TROPOMI to NO_x emissions. The current method tends to underestimate NO_x emissions by overestimating the NO_x decay time throughout the course of plume lifetime. The new model improves this representation by calculating a time-dependent NO_x:NO₂ ratio. The model is based on model simulations that consider detailed chemistry and meteorology over 4 NO_x emission sites. This paper logically explains the authors’ methods, reasoning, and results. This paper also does a good job of tracking error and explaining NO-NO₂-O₃ chemistry to explain the results. My concerns lie mostly in a lack of description of some background information, and the applicability of these results to greater time periods, regions, and weather conditions. I recommend publishing this paper after revisions by the authors, detailed below.

Specific Comments

1. More description of MicroHH and CSF would be very helpful in the Introduction. Information that I would find useful include inputs to each model, outputs from each model, general physical principles underlying each model, spatial and temporal resolutions, and the reason why each model was chosen for your project (i.e., the benefits of those models compared to similar model options). Some of these aspects are discussed in the Methods section, but it would be helpful to have more context for them when they’re first introduced, especially for people who are familiar with TROPOMI and NO_x chemistry, but not with this style of modeling.
2. I’m curious how important the NO:NO₂ split was when modeling the NO_x emissions in MicroHH (line 123). Were any sensitivity simulations performed by varying the split?
3. Line 134 states that only 2 days were selected to derive the fit parameters. I would suspect that the fit parameters are quite specific to those days (which is commented on in later sections). While it is shown that the new method improves NO_x emission estimates compared to the existing method with a constant NO_x:NO₂ ratio, I wonder whether this conclusion holds when different days are used. What were some of the meteorological qualities of the chosen days, e.g., were wind speed, wind direction, humidity, etc. typical? How would the simulation respond to days with abnormal weather or emissions phenomena?
4. When introducing Equation 5, it could be helpful to explain why a negative exponential function was used, e.g., to match observations or to fit a first order reaction rate.
5. The first paragraph of Section 3.2 comments on the limited availability of cloud-free, plume-detected images. I’m concerned about $N = 17$ for Janschwalde in Figure A3. Can these numbers of images provide statistically-significant results? This topic is further discussed in Section 4.2, which is helpful, and I think additional commentary about why these sites were chosen – despite their lack of data and the overlapping plumes – would provide helpful context.

6. In Figure 7, please state what the relative mean bias error is relative to. I assume it's relative to the bottom-up emission estimate since Lipetsk has no data, but the legend does not make that clear. I originally thought that the large, filled bars were for the bottom-up NO_x estimates because they do not have a black outline.
7. In the final paragraph of Section 3.2 (starting line 296), you comment on the fit parameters needing to be specific to each location. You comment on the error expected when applying this framework to other seasons or regions in Sections 4.1 and 4.2, which is helpful. Can you please comment on whether this framework is only intended to be used for local studies, and whether more research is being done to investigate its usage on global TROPOMI data?

Technical Corrections

1. For clarity when first introducing the topic of NO₂-to-NO_x conversion, please change the sentence beginning on line 51 to "To retrieve NO_x emissions, it is therefore necessary to convert NO₂ emissions to NO_x emissions". As-written, someone new to the field may think that the conversion is chemical, and not analytical, especially following the sentence about the chemistry of the NO_x family.
2. Figure A1 could benefit from a top axis showing distance as is done in Figure 4.