The manuscript “Estimation of OH in urban plume using TROPOMI inferred NO2/CO” presents an analysis of OH derived from urban plume information using TROPOMI satellite observations combined with WRF model simulations. Analysis focuses on the city of Riyadh, and assumptions regarding plume decay away from the city center, background conditions, and emissions are used to optimize the model to best match the TROPOMI products. Optimization of both the NO2/CO ratio and individual components (i.e., NO2 and CO separately) produce similar results for the OH derived for the two seasons examined.

General comments

This paper describes an interesting analysis and a potentially useful technique, enabling inference of NO2 lifetime (and OH) from a single TROPOMI overpass. This more instantaneous view could have benefit over previously used Exponentially Modified Gaussian function fit methods, which require substantial temporal averaging. However, the analysis relies on many assumptions, the implications of which are in some cases discussed, in other cases not. Some larger context is missing, regarding how the work might be applied on a wider scale, or else used for case studies of interest. Many metrics and side analyses are presented, and the main analysis has many “moving parts,” (i.e., TROPOMI, WRF, CAMS, the main least squares optimization vs. the EMG optimization, etc.), making it difficult to interpret the results and muddling the main messages. As a result, there is opportunity to streamline the writing and improve the presentation quality. Since the analysis appears to be robust, given the convergence on OH from the two optimization methods (ratio vs. component wise), I would consider this work suitable for publication in ACP and of interest to its audience once the following comments are addressed.
For presentation quality, I usually try to stay away from commenting on writing style, but I do think some re-organization would be beneficial to the reader. Instances that could help clarify confusion are noted under “Specific comments,” but I might also suggest reframing the results in an “easier to digest” way. Currently, Section 3 follows the steps of the analysis quite closely, which gets quite overwhelming when discussing model vs. TROPOMI differences, then ratio optimization vs component wise differences and those differences vs. CAMS or EDGAR, then those differences vs. EMG, etc., each with an emissions, a background, and an OH component. Perhaps an easier to follow organization would first discuss emissions only, in terms of the evolution of the emissions over the course of the optimization, then OH, then background? This is only a suggestion, but I think it would improve the readability of the paper.

In terms of providing more context/motivation for this work, I would interested in seeing discussion on topics such as: how difficult would it be to apply this method to other cities? What are the limitations that might make this hard to do for some locations? How do these findings influence our understanding of urban pollution, or what role could they play in better quantifying emissions? Etc.

Specific comments

L19: From the one-sentence description of the method in the abstract (that OH concentration, NOx and CO emissions are iteratively optimized), the referencing to “NO2/CO ratio optimization” and “XNO2 optimization” is unclear without having read the full paper. I would suggest clarifying further the concept of ratio and component-wise optimization. Also, aren’t background conditions also optimized? This could be included in the method description.

L20: Again, on first reading of the abstract, the mention of CAMS comes as a surprise; I thought WRF was being used. Further elaboration on the method could help clarify.

L30: Air pollution from cities doesn’t just threaten the health of those living in the cities, but also populations downwind; this statement seems overly general.

L82: Please provide the months used in Fig. S1 (i.e., is summer the average of June-July-Aug?)

L100: I believe the newer v.2.2.0 of the retrieval should help with the bias in NO₂ seen in the analysis, according to the statement here: http://www.tropomi.eu/data-
Is it feasible to try this analysis with the newer products? It is understandable that results cannot always be published immediately after they are produced, but if an update to the analysis cannot be undertaken, at least a discussion of how the analysis might be affected by newer data products or a suggestion for future directions should be included.

L102: I’d be curious if the WRF-chem model does a better job of simulating urban NO2, in general, compared against TM5? So, is it fixing the bias issue for the right reasons?

L111: The authors assessed NO2 data quality vs ground-based measurements from prior studies; is there a similar analysis that can be done for CO? Or is there reason to believe that the reference CO profile from TM5 is more reliable than it was for NO2?

In Table 1, the term “XNO2(emis,OH)” is used in its own definition; I expected it was intended to say “As XNO2(emis)...” – please check.

L181: I’m not sure I agree with this justification for not allowing XNOx,Bg to be lost by OH; NOx will continue to be oxidized, even if the plume it resides in was previously exposed to OH. Is there any sort of sensitivity test that can be done to see how large an effect this would have on the results?

L194: Please explain why the lifetime of NOx is the more relevant quantity to this analysis than the lifetime of NO2.

Figure 1 caption: Please indicate “(right)” to describe the right panel, presumably after “wind direction” or “boundary layer.”

L248: Is it possible that the NOx/NO2 conversion factor may not hold for emissions, since all NOx emissions from combustion processes occur in the form of NO, strictly speaking? While NO converts relatively rapidly to NO2, this still might be something to consider. Please discuss any anticipated implications of this assumption.

Fig. 4c: It seems very counterintuitive that the optimization for XCO increases emis by so much, barely decreases Bg, yet you still achieve a decline in the XCO quantities such that TROPOMI values are well matched. Am I interpreting this correctly?
Fig. 4 caption: How exactly are the f values shown here derived? It looks as though they are not simply the sum of f_1 and f_2 values shown in Fig. S17. Please either explain or point to the location in the text where this is explained.

L345: I’m concerned that this test is more likely to work since you are dealing with an internally consistent system. Using the model, it is easier to be sure that it can replicate a hypothetical scenario posed in the model with enough adjustments. The real world and what TROPOMI are detecting could be very different systems, though, so if the model is missing underlying processes, there is less confidence that this optimization process is robust.

I suppose the pseudo data experiment is still worth doing, and I’m not sure what test I would suggest in its place, but perhaps some qualification should be added that the promising results of the experiment may stem from this being an ideal/consistent system.

L352: I was initially confused that the f values in Figs. S17 and S18 changed so much between the first iteration and the second. I later realized that the second iteration values represented adjustments made to the first iteration values (i.e., f_emis doesn’t go from being +158.5 to –1.3 from iteration 1 to 2 in Fig. S17a; it goes from 158.6 to 157.2, or however you derive the 155.1 f_emis in Fig. 4a). It may be worth describing this more fully, so other readers aren’t confused.

Also, for Fig. S17c, please place the values of f_emis1 and f_Bg1 on the left side, 2nd iteration f’s on the right, to avoid confusion. And, why is there not a green line in this panel corresponding to XCO_WRF,1st iter?

L371: It would be helpful to state the value from Lama et al. (2020) here.

L417: Looking at Fig. S19, if this is done by linear extrapolation from data that is present for 2000-2015, why does year 2016 CO emissions drop followed by increases in 2017 and 2018?

L426: Please state why this model simulation is well suited to evaluate emissions changes – how does it calculate emissions, if not by relying on the EDGAR inventory?

L447: What is CAMS-TEMPO based on? Is there a reason why its temporal emission factors for Riyadh should be especially trustworthy?
L464: Why give a range for summer but a precise value for winter?


L475: It’s not just sources, but also some sinks are missing (for NO2), right?

L500: Is it possible to give a title to Appendix B, as was done for Appendix A?

L504-505: Why not write this in its simplified form, XCO_emis*0.10? The same goes for the next line.

Technical corrections

L30: “threating” should be “threatening”

L65: Beginning “OH estimates from...” is not a complete sentence

L107: This URL returns a “Not found” message

L175: “save” should be “safe”

L310: “emission” repeated twice

L313: either “estimates” should be singular or “an” should be removed

L355: f_B should be f_Bg
L392: “a” should be removed, or else “days” should not be plural

L397: “compare” should be “compared”

L407: “it the solution” should be “at the solution”

L419: “yield” should be “yields”

L422: “has” should be “have”

L481: “allows” should be “allow”

L509: Again, the link to the TROPOMI data appears to be invalid. The Zenodo link for the WRF simulations requires a login, so I could not access the data; I’m unsure if this is typical or not.