Review of gmd-2021-386
Anonymous Referee #2

Referee comment on "Effects of point source emission heights in WRF–STILT: a step towards exploiting nocturnal observations in models" by Fabian Maier et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-386-RC2, 2022

General

The manuscript "Effects of point source emission heights in WRF–STILT: a step towards exploiting nocturnal observations in models" by Fabian Maier and co-workers describes the use of vertical emission profiles for point sources in the time-reversed application of the Lagrangian particle dispersion model WRF-STILT. The authors convincingly show that ignoring vertical emission profiles and assuming surface emissions only, as done in many applications of LPDMs, may lead to serious biases for sites influenced by elevated point sources. The study is an important contribution for regional-scale inverse modelling of greenhouse gas emissions as it directly address shortcomings that can easily be remedied without major modifications on the transport description in LPDMs. The manuscript is well organized and written, methods and results are presented in an appropriate manner. Some minor concerns and considerations remain that I would like the authors to consider in a revised version of the manuscript.

Major comment

The way the introduction (L84-95) and section 4.2 states the problem of using nighttime observations tends to suggest that including vertical emission profiles (‘volume source approach’) alone may enable modelers to use such observations in inverse modelling
studies. However, an important prerequisite, and this is only mentioned rather weakly and hidden (e.g., citation of Geels et al., 2007), is the models ability to realistically reproduce nighttime stable boundary layers and the erosion of these stable layers in the morning hours. Analysis of simulated diurnal cycles and, where possible, vertical gradients against observations are inevitable before assimilating nighttime observations. This fact should be highlighted with more emphasize (introduction, section 4.2, and conclusion). The vertical emission profiles will not solve anything if, for example, the nighttime stable layers are only formed to weakly.

Minor comments

L55 & : This is specific for STILT. Other LPDMs (for example NAME, FLEXPART) use fixed sampling heights that do not vary with the boundary layer height.

L66f: There is another issue with point sources in time-reversed LPDM simulations. The source sensitivities (footprints) are usually stored on a horizontal grid with limited resolution. This adds to model uncertainties as well, since the limited resolution of the footprints may lead to false attribution of point source emissions in cases where a higher resolution footprint may actually have missed the point source. Since STILT is using an adaptive output grid that becomes coarser with distance to the receptor location, this problem may be more important for distant sources, but also for near sources and an inappropriate output resolution false attribution may happen. I think this issue deserves mentioning at this point.

L89-93: Another important point is that the average daytime footprint will differ significantly from the average nighttime footprint. Especially for tall towers the nighttime footprint is usually larger, sampling more distant sources, whereas the daytime (convective) footprint is often dominated by more local sources. Similar to point 2 this may lead to sampling of different source mixtures. The use of nighttime data would certainly extend the 'field of view' of tall tower sites in any inverse modelling study. One requisite is however that the diurnal cycle of boundary layer heights and mixing are captured correctly in the LPDM (point source representation or not; see main comment above).

L119-121: Could these point sources be highlighted in the map? Maybe panel b should be zoomed even further, in order to clearly see the location of these four sources relative to the site.

Figure 2: I find the depiction of model/emission domains a bit confusing. There seem to be two different resolutions and domains for WRF and TNO. However, the figure somehow
can be read as if there are 3 WRF domains. Maybe just indicate the higher resolution nests on the left (yellow and black rectangles, as is, but label them only with TNO 1km and WRF 2 km, respectively). Then produce a high resolution zoom that is smaller than the WRF high resolution domain in order to show the nearby point sources (see last comment).

L138: One hundred released air parcels per hour seems to be very small. How can one statistically resolve any vertical gradients with these? The VSI approach requires five different layers as applied here, the lowest two with a thickness of only 100 m. How can you be sure that one hundred air parcels can robustly represent any vertical gradient in such thin layers? The previous h_pbl/2 method may have allowed for such small air parcel numbers because no vertical gradient below h_pbl/2 had to be represented. The improved results with the VSI approach seem to justify the small number of air parcels, but they may merely result from improved separation between stable PBL and lower free troposphere at night. The lack of improvements during daytime (from SSI to VSI) may indicate that residence time gradients during the day are not well represented by the limited number of air parcels.

L139: Considering the outer WRF domain, this backward integration time seems to be rather short. What is the reason for the selected 3 days? How frequently do particles remain within the domain after 72 hours?

L139: There is no information here about the output resolution of STILT. Was this identical to the input resolution of WRF (2 km) or to that of the TNO emissions (1 km). As far as I know STILT output resolution varies with distance from the release location. What was the typical output resolution at distances covered by the synthetic source experiment?

L157: As mentioned before: other LPDMs use a fixed sampling heights in the order of 50 m to 100 m. A smaller sampling height actually assures that the assumption of instant vertical mixing is met. However, it also may require the use of larger particle ensembles in order to sufficiently represent particle distributions in more shallow layers.

L173: This may need further explanation. Wouldn't h' depend on may factors like wind speed, stability, etc. Is this 'effective mixing depth' used in any LPDM? Maybe this should be discussed in the previous section when STILT's sampling height is introduced. It seems to be unrelated to the 'volume source' approach.

Section 2.2.2: This being GMD, I have a technical question: How are the height profiles implemented in STILT? Are these fixed levels according to the TNO suggestions or is the user able to specify them.

L214f: This baseline assumption is most likely not very accurate for the eastern domain border and easterly advection. A note of caution should be added here.
L244 (“The standard deviation ...”): What does this aim at? Put observed variability and unexplained variability into perspective? Should't this be done by simply giving the coefficient of determination of linear regression or by an analysis of variance?

L243ff: The use of RMSD may be a bit misleading as it contains the bias as well. A bias-corrected (centered) RMSD (CRMSD) would allow analysing if the representation of variability beyond the bias was improved or not (CRMSD = sqrt(RMSD^2 – BIAS^2)). A quick check of the values in Fig4 suggests that the VSI approach mostly improves the bias but not the representation of variability.

Figure 4, caption: 'standard error of the mean': Not clear which mean this refers to. That of the observations? Why give the standard error? The standard deviation could be more easily compared to RMSD.

Figure 6: Are these surface footprints or obtained from the VSI approach for a specific height?

L315: Which times does this refer to? Hours of release at the receptor or hours of the backward calculation? One particle back-trajectory seems to be a rather poor sample size for a LPDM. How can this be justified.

L318: Are these the PBLH regimes at the time of arrival at the receptor? They may not be representative for the whole transport duration and the considered domain. Travelling times from the furthest power plant were probably larger than 8 hours. So arriving at nighttime in Heidelberg could mean that the power plant plume was still well-mixed over a large boundary layer during the previous day. Could be one reason why differences between the two PBL regimes seem to become smaller again for the largest power plant distance.

Figure 7: Wouldn't it make sense to show the differences as relative differences (e.g. 2(A-B)/(A+B))? The different logarithmic axis (compared to the individual SSI and VSI plots) make it difficult to judge if the differences are important. It would also allow for a more detailed discussion in the text.

L334 and elsewhere: Since sub-panels of Figure 7 are labeled, please refer to them as a,b,c in the text as well.

L363f ('The SSI approach ...'): I don't see this. In Fig 7f (SSI-VSI) most differences are
positive, exceptions being power plants at 15 and 20 km, but those are not the closest. Discussion in relative terms would be helpful. See comment on Figure 7.

L386 (‘quite low’): Please quantify and explain why these would be smaller. Uncertainty type 3 seems clear since the location is known. But especially uncertainty type 4 could be an important factor when it comes to the current study.

L394: Connected to the previous comment. Is this true? What is the diurnal profile that is applied to large point sources in the present simulations? This may well be different for different point sources. Can you be sure that the nearby point sources mentioned in section 2.1 can be represented well by the applied diurnal profile? A day/night difference of 50 % seems likely for a combined heat and power plant that can react relatively quickly to energy demands.

L461ff: I am not sure if this is the right location for this paragraph. Could also go to the introduction. It certainly does not fit the section title. Maybe also in the context of the Brunner et al 2019 publication L87, which also highlights the importance of representing point sources correctly in Eulerian models.

Code availability: It is not clear to me if the modifications of the ‘volume source approach’ have been made available in the latest STILT version and how they can be activated. A few more technical details on how to use the approach and from which version these are available would be appreciated.