RC2 — Anonymous Referee #2
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Review of Keune et al (2021) A holistic framework to estimate the origins of atmospheric moisture and heat using a Lagrangian model.

This study addresses uncertainty in the estimation of precipitation and heat sources derived from Lagrangian parcel trajectory methods. A framework is proposed to assess uncertainty in the input quantities and the associated trajectories, based on FLEXPART and ERA-Interim reanalysis. The study presents an important contribution to the field and the authors have done well to develop a framework that assesses a complex collection of uncertainties. I support the publication of this study, after the issues outlined here are addressed.

We thank the reviewer for their appreciation and support of our study, as well as their useful comments and suggestions. Our reply to all comments is detailed below. Underlined replies highlight planned changes in the manuscript.

General comments

1. I suggest it will be easier for the reader to understand the methodology if the need for such a methodology was more clearly explained in the introduction. The motivation of the study, besides estimating the uncertainty in identified sources, could be clarified by outlining the specific uncertainties you wish to examine. My understanding from reading the manuscript is that you wish to (i) evaluate the sensitivity of identified source regions to the air parcels released and (ii) the loss/gain of moisture/heat from/to those parcels along their trajectories. Is this correct? As for (i), it's unclear why this is necessary – what exactly is the issue with FLEXPART that you are trying to rectify? Is the issue that FLEXPART normally tracks all air, and you want to constrain it to only track moisture for precipitation (or heat) specifically? Why aren't the reanalysis fields of precipitation and evaporation used in the selection and tracking of parcels? And is the impact of the number and height of the parcels released, and trajectory timestep, considered? As for (ii), I'm unclear why it is necessary – could you expand on this? For instance, L53 states: "… moisture losses between source and sink regions are not accounted for." I'm a bit confused here – I thought FLEXPART intrinsically accounted for losses and gains between source and sink through the use of the positive and negative change in specific humidity along the trajectory (as stated in lines 49-50)? Is the problem that precipitation and evaporation must be inferred from the specific humidity change, and that you would like to quantify the precipitation/evaporation explicitly? This is an important point for the reader to understand the rest of the paper, including the need for linear or 'random' attribution of moisture – could you clarify please?

We agree with the reviewer that the need for the framework could be better motivated. We will adjust our introduction and explicitly mention the lacks that motivate this study along with the objectives that are going to be tackled in the study. Further, we will try to improve the comprehensibility of the method through a revision of the overall text, as well as through the addition of figures and examples to the main text and the supplementary material.

Here, we also clarify a few outstanding issues:

In general, the reviewer is absolutely right when they question "*Is the problem that precipitation and evaporation must be inferred from the specific humidity change, and that you would like to quantify the precipitation/evaporation explicitly?*". This is exactly the problem for the estimation of source regions of precipitation/moisture (addressing issue (ii)). While the simulations are driven with reanalysis data, including the surface fluxes, data is only available at the grid cell level and needs to be interpolated to the projected parcel locations. At this spatio-temporal resolution, only the specific humidity is available. While the sign of the specific humidity change is indeed a hint at the dominant process taking place (i.e., a gain or a loss of moisture through evaporation or precipitation; see Eq. 1), this criterion only reflects large scale evaporation and precipitation if integrated over sufficient large areas and longer times scales — which is also why a selection of parcels based on reanalysis fields of E and P is not straightforward. Integrating these specific humidity changes over large spatio-temporal scales and along multi-day backward trajectories, however, yields only a qualitative description of the source regions. The resulting source region maps show large areas of both positive (E–P > 0) and negative (E–P < 0) regions, with the former indicating general source regions and the latter general sink regions (e.g., between a source and the receptor region). In this setup, it remains difficult to *quantify* how much a specific source region contributes to, e.g., a precipitation event in the receptor region. Or in other words: the general sink regions between a source region and the precipitation event are not accounted for (l. 53). Hence, if one wants to detect those processes at smaller spatio-temporal scales and in a quantitative manner, additional criteria are needed.

As for (i): no, we do not evaluate the sensitivity of the source regions to the air parcels released. Our simulation is a global simulation that is initialized with a globally homogeneous distribution of 2 million air parcels. These move with the winds in space and time and can be used to establish multi-day backward trajectories, that in turn can be used to estimate source regions. However, the latter sounds rather simple, but it is not: first, criteria for a (reliable and accurate) detection of surface fluxes have to be determined; and subsequently, the quantitative source region contributions have to be estimated. Both steps are subject to uncertainty: in Fig. 2 (and 3), we show that it remains difficult to estimate the fluxes with the presented criteria — in most cases, considerable biases remain. However, these biases can be corrected; e.g., (re-)using the reanalysis data set that was used to force the simulations in the first place. And this is exactly what we do.

This framework for assessing uncertainty really only relates to FLEXPART-type studies. This is fine, but it needs to be discussed somewhere. For example, could you comment on how the framework might be applied to other types of models? This would make the proposed framework more widely applicable.

We thank the reviewer for this broad perspective. This framework could be applied to all models that trace air parcels — and FLEXPART is just one of them. LAGRANTO is another example, to which the framework could be directly applied. Further, parts of the framework (e.g., the different attribution methodologies) could also be applied to other models that trace 'water parcels'. We will add a sentence to the introduction and discuss the general applicability in the discussion and/or outlook parts of the manuscript.

2. The need for and steps involved in the random attribution of moisture needs further clarification. I find the explanation hard to follow, and I'm a bit lost in matching the notation in the 3 steps to the rest of the text. Could you clarify the general idea of

the approach, and each of the steps involved? This relates to the first comment above, that the need for such attribution needs further explanation.

We understand and agree with the reviewer, and all other reviewers, that the random attribution needs to be better explained. The general idea behind the random attribution is as follows: we determine a physical limit for the maximum contribution of a source location to the precipitation event under consideration. Consider, for example, a parcel that gains 5 g kg^{-1} of moisture through surface evaporation, but the parcel's total specific humidity content reduces to 2 g kg^{-1} through phase changes and/or precipitation *en route* afterwards—then the maximum contribution of this particular source location to the precipitation event is 2 g kg^{-1}. These limits are set for all identified source locations; and an iterative procedure then distributes the precipitation loss to all identified source locations. The distribution happens in two steps, which are randomly determined: First, a 'random' location among the identified ones is drawn. Second, a 'random' contribution between 0 g kg^{-1} and the maximum one for that source location is drawn. The procedure is repeated until the entire precipitation amount is attributed to all source locations.

We will add a figure to the main manuscript, revise the notation and the corresponding text, and further add examples to the supplementary material to describe the methodology.

3. The results figures are clear and well thought-out, but the meaning and implications of the numerical results could be further drawn out. For Figures 3 and onwards, what are the implications of these statistical results, both physically and for future studies? Furthermore, there is a clear difference in results that are based on the two attribution methodologies - but how can the reader assess if either are realistic or even necessary?

We thank the reviewer for this excellent question. We wish we had a straightforward answer. Unless there are observations available that facilitate a validation of the source–sink relationship, we do not know the ground truth and we cannot assess if the presented source regions are realistic.

This lack of observations, however, motivates the need for this uncertainty assessment. Thus, while we cannot assess the realism of the presented approaches, we can show that their assumptions do have an impact on the results. By presenting this uncertainty, we want to make the community aware of it, and we wish to encourage future studies to communicate these uncertainties.

We will add a sentence/paragraph to the discussion and/or the conclusion to better explain the meaning and the implications of our results.

Minor comments

5. L18: I'm not sure what is meant by 'synergistic impacts'. Do you simply mean that the bias corrections reduce the identified uncertainties?

Yes, this is exactly what we mean. We will revise this sentence/the wording.

6. L107 and 111 and other places in the document: I'm not sure what is meant by a 'diagnosis' of surface fluxes. Are you referring to an evaluation between simulated and observed fluxes, or something else?

Yes, by diagnosis we mean the (unconditional) detection and quantification of surface fluxes and precipitation from the Lagrangian model. To detect and diagnose these fluxes, the difference between two consecutive timesteps are considered for all air parcels — and evaluated using one of the criteria detailed in the methods section. The integration of all parcel differences then represents the 'diagnosed' flux on a global grid — and can be validated with observations and/or reference data sets, such as ERA-Interim. We will add a clear definition to the main manuscript.

7. L131: 'all air parcels … are evaluated independently…' – what is the aim here?

The aim is to detect how well the criteria detect the fluxes; i.e. to estimate the (biased) fluxes from the model and to determine bias correction factors. The 'independently' refers to the fact that we do not condition this on any receptor region but apply it globally using two consecutive timesteps. We will make sure that this becomes clear in the revised version of the manuscript.

8. L113: Which 'other existing methods' are you referring to? Could you cite some examples please?

We will add references to this sentence.

9. L140: '…source contributions can be further constrained by means of a receptor quantity…'. Do you mean source contributions can be scaled to match the precipitation in the sink?

Yes, and no… This is exactly what can be done and is done in many cases (and a bias correction with precipitation yields the same result). With this sentence, we wanted to generalize this meaning a bit as also other receptor quantities could be used; e.g., the integrated water vapor over a region could be used as a target variable instead of precipitation. On the contrary, for heat advection as defined here, no receptor quantity can be applied and the source region contributions are not constrained by a receptor quantity. This is, however, not explicitly stated. We will revise our wording in this sentence to something more explicit and add a few more sentences at the appropriate places in the method description.

10. L232: Could you expand a little on the importance of only using parcels that are within the ABL? L235 states the impact is considerably small for 6h time steps. Does this mean that back-trajectory methods don't need to consider the height of the ABL, or that it has a minor impact?

In l. 235, we were referring to the difference of the results if one considers only one or both occurrences to be within the (maximum) ABL. For our case studies and the 6-hourly timesteps, the resulting source locations did not differ much. Our speculation – i.e., that this is impacted by the 6-hourly time steps – was, however, misplaced (as also mentioned by another reviewer). We will revise this sentence and remove this speculation.

As for the importance of considering ABL changes only: the answer to this question appears to be almost philosophical. While we wish to determine only the *direct* surface source locations, Fremme and Sodemann (2019) argue that changes above the ABL should be considered as they are indirectly influenced by the surface. In turn, other studies (e.g., Stohl and James, 2004; Stohl and James, 2005; Nieto et al., 2006; Drumond et al., 2008; and others), are more interested in the general sources of moisture and examine large-scale convergence and divergence zones of atmospheric moisture transport; and hence do not limit themselves to surface sources only. With our interest to identify only the direct surface source locations, the ABL criterion helps to increase the likelihood that changes in state variables reflect surface fluxes.

11. L393: '…the timesteps for the calculation of trajectories are adapted to Lagrangian timescales…'. What is the trajectory timestep? How was is determined?

In FLEXPART, parcel trajectories are determined using the grid scale wind, as well as turbulent and mesoscale wind fluctuations. FLEXPART was run in with 900 seconds synchronization and sampling timesteps; which correspond to the default setting of FLEXPART (see Stohl et al., 2005). Turbulence is not well described at this timescale (Stohl et al., 2005) — and hence the timestep can be adjusted through a modification of the Langevin equation, which parameterizes turbulence in FLEXPART.

We do not wish to dive further into this aspect, thus reference to the technical description of FLEXPART in Stohl et al. (2005) for details. However, we will adjust the corresponding sentence in the main manuscript to better reflect the simulation settings.

12. L36: Suggest rephrase grammar to "Tracking air parcels enables the state of the atmosphere and its changes in space and time to be inferred, …"

We thank the reviewer for the suggestion, and we will revise the sentence accordingly.

13. L156: The first sentence of section 2.2. makes it sound as though it follows from what is said above. Perhaps rephrase to something like: 'To characterize the physical processes influencing the air parcels, the changes in air parcel properties…'.

We thank the reviewer for the suggestion. We will revise this sentence to something along the lines of the reviewer's suggestion.

14. L497: Change 'he3at' to 'heat'.

We will fix this typo.

References

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