RC1 — Anonymous Referee #1
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Review of paper

A holistic framework to estimate the origins of atmospheric moisture and heat using a Lagrangian model

by J. Keune et al.

submitted to *Geosci. Model Dev.*

This is a much-needed study contributing to quantitatively assess the reliability of Lagrangian source diagnostics. As pointed out by the authors, these diagnostics potentially provide very valuable insight into the atmospheric moisture and heat budgets; however, it is intrinsically difficult to quantify errors and uncertainties associated with these methods. I therefore fully support the intention of this study, and to a large degree also the used methodologies; however, in its current version the paper is difficult to read. I find the notation confusing in several (important) places and I could not understand the idea and implementation of the "random attribution method". Therefore, major revisions are required to streamline the paper, clarify concepts and notation, and make the paper in the end more reader friendly. It will then be a valuable contribution to the field.

We thank the reviewer for their thoughtful evaluation and support of our study. We will reply to all comments in detail in the following, highlighting planned changes in the manuscript. In particular, we understand the confusion with the random attribution method and some notations. We aim to revise some of our notations, to provide figures that illustrate the concepts and notations, and to provide examples in the supplementary material that underlie our statements with numbers.

Major comments

A) Line 89: "the application of these models and tools to assess diabatic heating and heat transport lags behind". I am not sure that I agree with this statement. The study by Pfahl et al. (2015) is an important one but certainly not the first one in this direction. Early applications of trajectory computations with reanalysis data in the 1980ies and 1990ies looked at latent heating in cyclones and warm conveyor belts, and how this latent heating affects the potential vorticity structure of the systems (e.g., Whitaker et al., 1988; Reed et al., 1992; Wernli and Davies, 1997; Rossa et al., 2000). These were not yet full budget studies, but I would claim that Lagrangian methods first looked at latent heating and only about 1-2 decades later also at moisture sources and transport.

References:

Reed, R. J., Stoelinga, M. T., Kuo, Y.-H., 1992: A model-aided study of the origin and evolution of the anomalously high potential vorticity in the inner region of a rapidly deepening marine cyclone. Mon. Weather Rev., 120, 893–913.

Rossa, A. M., H. Wernli, and H. C. Davies, 2000. Growth and decay of an extratropical cyclone's PV-tower. Meteorol. Atmos. Phys., 73, 139-156.

Whitaker, J. S., Uccellini, L. W., Brill, K. F., 1988: A model-based diagnostic study of the rapid development phase of the President's Day cyclone. Mon. Weather Rev., 116, 2337–2365.

We thank the reviewer for noticing insight and the references. <u>We will change 'adiabatic heating' to 'sensible heating'</u> to better reflect what we meant: while many Lagrangian studies investigate the history of moisture in the air, very few studies have focused on the history of heat — or dry static energy; and even fewer studies have outlined regions where the air was warmed by sensible heating. To better highlight that the concept of tracking latent heating was already applied in earlier studies, <u>we will add an additional sentence on the latent heating of air during the development of cyclones.</u> However, we also wish to note that the cited statement referred to the number of models and studies published, rather than the temporal occurrence of studies and models to estimate the origins of moisture and heat. <u>We will make that clear in the revised version of the manuscript.</u>

B) Line94:I think this is a slightly misleading summary of the Quinting and Reeder (1997) study. They mainly emphasized the role of adiabatic descent, and their last sentence of the abstract says "Likewise, the role of the local surface sensible heat fluxes is deemphasized.".

We thank the reviewer for his comment and will <u>rephrase this sentence</u> to better reflect the study findings.

C) I am completely lost with understanding the "random attribution" method (section 2.3.2) for several reasons. First, I don't understand the notation "length nt": is this n times t? And then later, what is ix, nx, ... an later n_min ... ?? Most likely this requires a schematic where you explain also the notation. Then how can you use Delta q,random in step 1 if you calculate it only in step 3? Then I am completely lost with step 2, and I also don't understand the general motivation for doing this. Can you explain this method and the motivation for it in a much better way?

We agree with the reviewer that a bit more work is needed here. We aim to <u>polish this section, add a figure that visualizes the concepts (and notations) and provide examples for both attribution methods, the random attribution and the linear discounting/attribution, to the supplementary material.</u>

D) Fig.3b is a key figure of this study. Since,e.g.,the methods SOD08 and RH-20 vary in multiple ways (additional RH criterion, different Delta q threshold) it would be interesting to know which change had the largest effect. It would be very useful to have a more in-depth discussion of which criteria affect the results shown in Fig. 3b.

We wish to highlight that the RH-20 criterion does not explicitly consider a minimum Delta(q) threshold and that the SOD08 criterion does not consider a maximum Delta(RH) threshold (see Table 1). Hence, a direct comparison on the effects of temperature and specific humidity changes on these criteria is difficult. However, the criterion ALL-ABL was introduced to provide a criterion that lies in between SOD08 and RH-20: compared to SOD08, it does not consider a minimum Delta(q) threshold and hence indicates if filtering for a minimum threshold improves the detection of E. Compared to RH-20, the ALL-ABL does not consider a maximum Delta(RH) threshold and hence allows to infer the suitability of this temperature-dependent threshold. We will make sure that <u>the corresponding differences are clarified in the text.</u>

E) While I agree that this study addresses important technical aspects of moisture and heat source identification, the text is rather heavy to read, and the results are mainly presented in a statistical way, which is hiding a bit what is going on technically. To me, it would be useful to have a didactic example, starting with a single trajectory and then a set of trajectories, which helps me better understand the differences between the methods and the effects of the bias corrections etc.

We will <u>add a new diagram to the main text/the supplementary material</u> in order to highlight the differences between the criteria (Table 1) and the attribution methods.

F) The random attribution method has an important effect on estimating the transport time between uptake and rainout (Fig. 9c). With the random attribution method, you have much more "old uptakes" and therefore you have more long-range transport and remote sources (Fig. 10). This is very interesting and most likely an important result of this study (see also your discussion in lines 672-682). My problem is just that I didn't understand the random method (see my point C above) and that I don't find physical reasons in the paper why the random method has these effects compared to the linear attribution method. Again (see my point E above), a case study with a few trajectories might be very helpful for explaining what is going on.

<u>We will add a more detailed explanation and a figure to clarify the random attribution concept.</u>

G) How sensitive are your main conclusions with respect to the total number of parcels calculated with FLEXPART? I don't ask you to redo a certain analysis with more parcels (this might be too time consuming), but it might be interesting to look at the effects of reducing the number of parcels.

We thank the reviewer for this question, which is indeed interesting. It is, unfortunately, true that an additional analysis with more parcels would be very time consuming. An (artificial) reduction of parcels would be feasible, but we do not really see the benefit of doing that for two reasons. First, we believe that the current setup with 2 million parcels globally represents a reasonable minimum number, as it approximates on average 30 parcels per 1°x1° grid cell and resembles at least ~half of the vertical layers from the driving reanalysis (61 layers in ERA-Interim). Considering the vertical distribution of these parcels, less than half of them remain in the ABL and for our evaluation. Further, this setup with 2 million parcels globally remains a common setup used in other studies recently published (e.g., Algarra et al., 2020; Braz et al., 2021; Drumond et al., 2019; Nieto et al., 2019; Vicente-Serrano et al., 2018) and hence provides a state-of-the-art reference. Second, technically, we are already reducing the number of parcels that we are evaluating, e.g., through a minimum threshold of Delta(q) in the SOD08 criterion or through a maximum threshold of Delta(RH) in the RH-20 criterion for the detection of E. Hence, these criteria mimic an (artificial) reduction of the number of parcels. There are, nonetheless, other studies that investigated the impact of the number of parcels on the uncertainty of moisture source regions (e.g. Tuinenburg and Staal, 2020) and could be used as a rough indication. We note, however, that the approach in those studies is different.

Finally, we wish to highlight that our study evaluates the uncertainty inherent in the *evaluation* of Lagrangian simulations. By changing the number of parcels that are being tracked, we would assess additional uncertainties arising from the simulations directly — which could and should entail other uncertainties, e.g. arising from the convection scheme (see Sodemann, 2020) as well. We hope that the reviewer agrees that this is beyond the scope of this study.

Minor comments

1) Line 18: “synergistic impacts” on what? And what is meant by “a cohesive assessment”, maybe “coherent assessment”?

What we mean is: without the bias correction, the approaches presented in this study yield large uncertainties. However, this uncertainty is significantly reduced if (source- and sink-) bias-correction is employed. We will revise this sentence.

2) Line 28: here reference to Sodemann et al. (2008) would be more appropriate than Sprenger and Wernli (2015).

Thanks. The referencing here was meant to encompass the broad range of models that exist. We will also include a reference to Sodemann et al. (2008).

3) Line 33 and in other places: I think references should be listed in chronological order.

According to the GMD guidelines, “the order can be based on relevance, as well as chronological or alphabetical listing, depending on the author’s preference” (https://www.geoscientific-model-development.net/submission.html). We will update the reference list to chronological order where we believe that a chronological order is more appropriate.

4) Lines 36-74: I appreciate this nice summary of Lagrangian approaches to identify moisture sources. What may be missing is a remark that Lagrangian approaches suffer from accuracy errors of trajectory computations, which can be substantial for trajectory integrations over several days. These errors stem from limitations of the numerical schemes, and most likely more substantially from the limited temporal resolution of wind fields available for offline trajectory computation.

We thank the reviewer for this remark. It is indeed true that errors in the trajectory computation are another source of uncertainty for such analyses. We will add a corresponding sentence/paragraph, that highlights additional uncertainties, to the manuscript.

5) Line 88: “A myriad” seems a bit exaggerated.

We will substitute ‘a myriad’ with ‘a multitude’. However, we have noticed the recent development of additional models and tools to track moisture and estimate the origins of precipitation. Just to name a few examples (which are also cited in our introduction): Tuinenburg and Staal (2020) just developed a new Lagrangian model that tracks moisture (UTrack) — but that is not set up to track heat (yet). The Water Accounting Model (WAM-2layers, van der Ent et al., 2014) is the base for many moisture tracking studies — but remains restricted to water. And 2L-DRM (Dominguez et al., 2020) and WRF-WVT (Insua-Costa and Miguez-Macho, 2018) are just two more examples of models that have recently been developed for the purpose of tracking moisture — and that are not readily available for the tracking of heat. And this development of models is in addition to the analytical tools already available (see introduction). Hence, we believe that the statement is not exaggerated.

6) Line 98: maybe this summary of recent Lagrangian heat wave studies should also include the one by Zschenderlein et al. (2019): Zschenderlein, P., A. H. Fink, S. Pfahl, and H. Wernli, 2019. Processes determining heat waves across different European climates. Quart. J. Roy. Meteorol. Soc., 145, 2973–2989.

We thank the reviewer for the reference and will add this reference to the text.

7) Line 159: I think that the notation Delta_q(t0 – t-1) is not ideal. Delta_q does not so much depend on the time difference but rather on the two times themselves. I therefore suggest that Delta_q(t0; t-1) would be more appropriate, or maybe even Delta_q(t-1; t0).

We wanted to emphasize the direction of this 'backward time axis' — as similar analyses could be performed in a forward manner. Thus, the sign of this difference is important here. However, we will reconsider our choice here in the context of the aforementioned changes to the methods section.

8) Line 174 and elsewhere: units should not be in italics.

We thank the reviewer for noticing. We will adjust the format of units in equations in the revised version.

9) Line 181: I was first confused and thought that *z* is a function of *m*, but your m is the unit of z. I don't think that you need to mention units in the text, or you write "*z* (in m)".

We wish to mention units in the text for the sake of completeness. We will consider rephrasing some sentences where appropriate.

10) Line 190: either "applied" or "used"

Thank you for noticing. We will delete 'used'.

11) Line 198: is Delta q_i the absolute change? I assume that Delta q_i is negative if mixing with free tropospheric air occurs and then the Delta q_i condition is trivially fulfilled and does not help to exclude mixing with dry tropospheric air. Please clarify.

We thank the reviewer for noticing this mistake: there is an 'absolute' missing in this equation. The correct criteria reads as follows: abs(Delta(q) / q) < 10%. We will fix the equation in the revised version of the manuscript. So, while some negative Delta(q) changes are accounted for, also these are restricted. In addition, the height criterion was introduced to filter for mixing processes with tropospheric air. Hence, mixing is (at least partially) excluded.

12) Lines 213/215: I am not sure that I understand these RH criteria. Evaporation is particularly intense for dry air, and so why shouldn't intense (ocean) evaporation not lead to a strong increase in RH? And for the heat flux H, I assume that H leads to warming and therefore to a reduction of RH, so Delta RH should be negative, meaning that the criterion Delta RH < 10% is trivially fulfilled(?). Please clarifiy.

In essence, we argue as follows:

1) The absolute change in RH is not only dependent on evaporation, but is further determined by the temperature (change).

2) Large relative humidity changes are often indicative of mixing processes with free tropospheric air — which we wish to filter out. This is especially true for the detection of H using RH changes.
3) The RH criteria were designed to complement the existing criteria as a means to gauge the uncertainty arising from these detection criteria.

We will elaborate on each aspect below.

First, in general, we agree with the reviewer that intense evaporation can lead to a strong increase in humidity in an air parcel. However, it needs to be emphasized that relative humidity is a function of specific humidity and temperature; the (absolute) relative humidity change in an air parcel is thus a result of both specific humidity changes (e.g., through evaporation) and temperature changes (e.g., through heating from the land surface). Further, both changes are subject to the time step employed — 6 hours in our case. Due to the strong diurnal cycle of all variables affecting RH (e.g., E, H, T; see e.g. Betts and Tawfik, 2016), we often encounter that a moistening of an air parcel is accompanied by warming — which counteracts the relative humidity increase through the specific humidity increase. Further feedback processes, such as the growth of the ABL via heating from the land surface (e.g., van Heerwaarden et al., 2009; Huang et al., 2011), need to be taken into account and affect the relative humidity.

Second, the detection criteria were chosen as a means to ensure that the sampled air parcel's evolution of humidity and (potential) temperature is mainly indicative of ABL processes. Strong changes in RH are often the consequence of additional processes, notably entraining/detraining air parcels mixing with ambient air (and thereby typically experiencing strong specific humidity in/decreases, and potential temperature de-/increases). For the detection of H, it is indeed the case that in the absence of other processes (e.g., evaporation, mixing, fog dissolution), we would expect RH to decrease. Whenever H is strong, however, this implies ABL growth and a subsequent shrinking towards the evening — then, many air parcels previously part of the ABL mix with free tropospheric air, whose potential temperature tends to be higher (and relative humidity is often markedly different). To limit the detection of such events, and thus the overestimation of H, it is useful to sample only potential temperature increases associated with a moderate (absolute) change in relative humidity.

Finally, the RH criteria were designed to complement the existing criteria. In this context, we wish to mention: there are downsides to all of the proposed criteria. From a moisture perspective, the SOD08 criteria use a minimum Delta(q), and one could also argue that small increases in Delta(q) may still be associated with evaporation and should not be neglected. Or in case of the ALL-ABL criteria, one could argue that not all humidity changes are associated with surface evaporation. With the comparison of the three criteria (SOD08, RH-20, ALL-ABL), we wanted to compare the impact of three criteria that filter for opposites: one that counts small increases (RH-20), one that only evaluates sufficiently large increases (SOD08) and one that counts just everything (ALL-ABL). Further, as pointed out in the manuscript, we employed all thresholds globally and did not calibrate any thresholds. And as our results show: the impact of those criteria on the estimation of the source regions is considerably small — if the detected source region fluxes are bias-corrected.

<u>We will add a comment on the advantages and disadvantages of all criteria to the manuscript.</u>

13) Line 235: I expect the opposite: with 6-hourly data we estimate the diurnal cycle of the ABL height poorly and therefore the ABL height criterion might be important. If we had hourly data (e.g., with ERA5) then there should be less sensitivity with respect to the design of the height criterion.

We agree with the reviewer that the accuracy of the simulated ABL heights — and the parcel heights — should get better as the temporal resolution increases. As time steps get smaller, the differences between the ABL heights become smaller as well. We assumed that it would make sense to filter 'more strictly' (i.e., require both occurrences to be within the ABL) for the detection of surface fluxes in that case, because mixing with tropospheric air could be better detected. However, we agree that this is speculative and, in the context in which it is presented, misleading. We will remove this sentence.

14) Line 260: "for E for P" should read "for E and P".

Thank you for noticing. We will replace 'for' with 'and'.

15) Line 274: Strange formulation "Due to the consideration ..., mass and energy are conserved ...". I think mass and energy conservation is valid independent of what is considered by the algorithm(?).

We thank the reviewer for highlighting this sentence. We will rewrite this sentence. For the sake of completeness, we wish to clarify this issue in our response here too: The Lagrangian simulations are mass and energy-conserving. However, the way the analysis of the output is conducted is not necessarily mass- and energy conserving. Consider, for example, the following trajectory that extends 7 timesteps into the past:

Time	**t-7**	**t-6**	**t-5**	**t-4**	**t-3**	**t-2**	**t-1**	**t0**
Specific humidity ($g\ kg^{-1}$)	1	2	5	2	3	4	5	1
Change in specific humidity ($g\ kg^{-1}$)		+1	+3	-3	+1	+1	+1	-4

Some approaches consider +4 $g\ kg^{-1}$ between t-7 and t-5 for the estimation of source regions of the precipitation event at t0. However, this is not mass-conserving as the moisture loss *en route* (at t-4) is not considered. And in this particular case, the parcel contained less specific humidity at t-4 than it gained before — the corresponding sources thus depict qualitative source regions but do not facilitate a quantitative assessment. Consequently, if the sinks of moisture along individual trajectories are not considered (e.g. through linear discounting and attribution), the approach is not mass-conserving.

As mentioned before, we will add similar examples to the supplementary material to highlight the differences.

16) Line 285: "time step (t)" should read "time step *t*" (italics).

Indeed, we will adjust the sentence.

17) Line 288: I don't see the need to introduce a new notation 1_Delta Phi ... for this function. This is the Heaviside step function, which in this case could be written as H(–Delta Phi_j).

Yes, it could. We will use the Heaviside function in the revised version of the manuscript.

18) Lines 285-299: please clarify whether everything here is identical to SOD08, or whether you introduced some modifications.

This is identical to the approach introduced in Sodemann et al. (2008) — just written down differently. We decided to use our own formulation as we found the description in Sodemann et al. (2008) more difficult to follow. We will add a sentence clarifying that this is identical to Sodemann et al. (2008) but follows a different notation.

19) Lines 300-307: I don't understand why this explained here after the linear discounting, appears a bit out of place.

This part is needed to aggregate the contribution of sources along individual trajectories to coherent source regions, as displayed in Figs. 4, 7, and 8. While it appeared logical to us to add it to this section, analogous to the upscaling of the fluxes in Equations 2–8, it is true that a similar step is needed for the random attribution. We will thus consider adding a subsection "2.3.3 Source region aggregation" (or similar) that explains this step with a bit more detail for both attribution schemes.

20) Line 358: I again struggle with the notation: is x here an index? If yes, why then do you write it as a superscript of S_LM? I realize that at this point of the paper I cannot really follow any further, mainly because of confusing notation. What are indices, what are coordinates, what are just subscripts/superscripts ...? Does "LM" mean "Lagrangian model" or something else?

The notation S_LM(x) was introduced earlier already (Eq. 16–17) as the source region contribution as estimated from a Lagrangian Model — the "x" here refers to the conditioning of the flux at a specific point x (in space and time). I.e. for every source grid cell only a subset of all parcels over that grid cell are evaluated using the multi-day backward trajectories. In contrast, the unconditional S_LM version evaluates all parcels over that grid cell. As we do have four coordinates (longitude, latitude, time, backward time) we were hoping to avoid an explicit referencing of those throughout the paper. The "x" thus simply refers to the conditional evaluation for a specific receptor region. However, we do understand that this notation is not ideal and will try to harmonize it in the revised version.

21) Line 497: typo in "heat"

We will remove this typo.

22) Fig. 6: I cannot find the information how you define "local"; does this "local region" have the same size for all cities?

Yes, 'local' refers to the 3°x3° grid cells around the center of each city. This is defined in l. 408: "Unless otherwise noted, a 3°x3° box around each city center is used as a receptor area.". We will specify this in the text and repeat the information in the captions of Figs. 6 and 10.

23) Figs. 7 and 8: I find it very difficult to see something in these many panels, except that they all look very similar. I think the smooth blue-only color bar does not help. Can you find an alternative way of visualizing the results that is more insightful for the reader and that makes the differences more apparent? Maybe by showing difference fields from a “reference setup”.

It is true that these are quite similar and that differences are difficult to spot. However, we decided to show the absolute source regions for two reasons. First, it is consistent with the source region illustration of heat (Fig. 4), but displays much more similar source regions. This underlines the minor impacts of the detection criteria for the estimation of precipitation source regions compared to heat source regions. Second, we do not want to single out **one** criterion as ‘the’ reference. Displaying differences would make much more sense if the ground truth was known and/or a ‘best’ criterion could be highlighted following a validation exercise. This is, however, not the case here as observations for the latter are missing. We thus wish to refrain from showing differences here. We have published the data along with the manuscript, which allows any reader to analyze differences on their own. However, we may adjust the color scale.

24) Line 661: why are the new criteria better to assess global warming trends?

If the air is becoming drier under global warming, this will be reflected in the specific humidity of air parcels as simulated with, e.g., FLEXPART. A static specific humidity threshold might thus impact the assessment of trends from such models. Around l. 661, we simply wanted to note that a relative humidity threshold could be used instead and could eliminate these issues. We will revisit this sentence/discussion.

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