Comment on egusphere-2022-928
Annika Vogel (Referee)

Referee comment on "Toward a multivariate formulation of the PKF assimilation: application to a simplified chemical transport model" by Antoine Perrot et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-928-RC1, 2022

General comments:

The submitted manuscript "Toward a multivariate formulation of the PKF assimilation: application to a simplified chemical transport model" by Perrot et aline contributes to the developments of a parametric Kalman Filter (PKF) in which the error statistics of a geophysical system are represented in form of a few parameters of the statistics. Specifically, the main contribution of this paper is the extension of previously published PKF formulations to multivariate problems in which cross-covariances between the individual prognostic fields occur. This is a very important step towards the application to real problems like complex chemical transport models (CTMs) and makes the manuscript highly valuable to the scientific community.

The quality of the research and the way of its presentation is good, but the manuscript is too long and overloaded. It appears that the authors aimed at putting too much content into one manuscript. I would suggest division it into two (or even three) manuscripts, each specifically focusing on one aspect, eg:

- General aspects of multivariate PKF, including theoretical validation and limits (until end of Sect.2)
- Application to simplified chemistry, including proxy for cross-correlation function, contribution of individual terms and closure (mainly Sect.3 and maybe Sect.4)
- Maybe: application to more complex chemistry (Sect.4)

Besides that, some parts presented in the manuscript could be shortened significantly by referring to previous literature and focusing on the new aspects of this work (especially in Sec.2, see specific comments). The manuscript also contains a number of inconsistencies in the notation and some grammar/wording mistakes (see technical corrections) which
makes it sometimes difficult for the reader to follow the details.

Specific comments:

- Different quantities are used for error statistics in different equations and plots. Eg. in Sec. 2.3, variance $V$ and metric tensor $g$ are used in Equation (8) whereas standard deviation and length scale are used in Fig.2. Additionally, the aspect tensor $s$ is used in Equation (21) whereas the metric tensor is used in Equation (24). It would increase the readability significantly if the authors would stick to one quantity thought the manuscript were possible, or at least within the same evaluation (eg. to increase the consistency between Equation (21),(24) and (25) in Sec.3.3).
  - In addition, the correlation length scale (eg. in Fig.2 and LINE 247) was not defined and its connection to the other correlation quantities (metric and aspect tensor) remains unclear.

- Section 2: The main new scientific contribution of this section appears to be the comparison to the enKF with two different spatial resolutions showing that the PKF is able to produce reasonable statistics already at coarse resolutions. Thus, the section can be significantly shortened by focusing on the new aspects and the most essential information required for those:
  - The main content of Sec.2.2 and 2.3 was previously formulated in Pannekoucke2021. I suggest shortening the introduction of the PKF univariate equations by referring to this paper and just providing equations which are essential for the new aspect (i.e. numerical limits in Sec.2.4.3)
  - Section 2.4.2 seems to contain mainly results were already demonstrated in pervious publications. Eg. LINE 257: The ability of the PKF to produce high quality univariate forecasts of error statistics was already shown in Pannekoucke2016,2018,2021. Although the description presents the main aspects and advantages of the PKF in a well-formulated way, it appears to be more suitable for a review or textbook-like article than as part of a scientific manuscript. Here, the description can be shortened significantly, focusing on new aspects.
  - The main conclusion of Sec.2.4.3 is that the PKF is able to produce reasonable error statistics also for coarse spatial resolutions (LINE 302f, LINE 307f). No validation with true statistics is available for this setup and the conclusion is based on comparison of comparison of the low resolution PKF with high- and low resolution enKF. In this setup, the agreement between low resolution PKF and high resolution enKF does not necessarily proof good performance because both resolutions could be insufficient. The easiest way to indicate convergence of the methods, and thus the accuracy of the solution, would be to make sure that the solution of the PKF remains the same for high resolution simulations. This would indicate the convergence of the PKF to a solution which is well approximated by the low resolution simulation.
    Ideally, the convergence of the enKF to the same solution could also be indicated by performing even more high resolution simulations. But given the computational efforts, it might be sufficient to verify that the high resolution PKF solution agrees with the low resolution PKF and the high resolution enKF solutions.
  - Given the length of Section 2.4, I would suggest making it a new main Section (->Sec.3, if not significantly shortened according to other comments above. This comment is also related to the main general comment of dividing the manuscript.)
In addition, the title might be misleading, as it appears to include only the advection process as part of the forecast step and not the full PKF with forecast and analysis step. Maybe something like: “PKF for advection equation of passive tracer” would be a more appropriate section title.

- Section 3: This section is much too long. Following the general comments (above), I would suggest taking this section as a paper on its own, which would be of appropriate length (17 pages + introduction, conclusions etc). In any way, Sec.3.3+3.4 as well as Sec.3.5 could be separate sections each, i.e dividing Sec.3 into three sections, eg: 1) Sec.3.1+3.2, 2) Sec.3.3+3.4, 3) Sec.3.5.
- In Sec.3.3.2 and Sec.3.5.2 it remains unclear how much the results can be generalized are subject to the specific setup of the experiments. For example, it would be interesting to see if the advection terms remain dominant under different conditions like weaker wind or accelerated chemistry. This becomes also important for verifying the neglection of chemistry part in the anisotropy for the GRC CTM in Sec.4.2.
- Section 5: The discussion section only partly includes an actual discussion.
  - The first paragraph of the discussion refers only to a specific part of the study, not to the complete work. I suggest moving it to the referring Sec.3.2.2 (maybe as new subsection if necessary).
  - The rest of the section is a conclusion rather than a discussion and should be moved to the conclusion section.
- Appendix D: This appendix provides no added value for this paper because the equation is not used and can be found in Pannekoucke2021 for reference. Remove appendix and refer only to the equation in Pannekoucke2021 paper in Sect. 3.5.2 (LINE 638)

Technical corrections:

General technical corrections (at multiple locations in the manuscript):

- Suggest replacing “modelized” by “modelled” and “modelizes” by eg “models” or similar (LINE 2, LINE 239)
- Inconsistent typing w.r.t. hyphen. The manuscript composition guidelines suggest the form without hyphen (eg. “auto correlations” and “cross correlations” in LINE 21, “forecast error” in LINE 117, “length scale” in LINE 247,...)
- Replace “validated from” eg with “validated by” or “validated w.r.t.” (LINE 66, LINE 188)
- The formulation “so to” should be replaced eg by “to” or “in order to” (LINE 74, LINE 148, LINE 356, LINE 436, LINE 449, LINE 452, LINE 458, LINE 698)
- There are inconsistent indications of locations in different variables. Eg. subscript like V_x vs. in brackets like g(x) in Equation (7) whereas V(x) was used in LINE 118 (same in LINE 191 vs LINE 195, and Equation (20)). Suggest sticking to common indication (either as subscript or in brackets) for all variables, or to point out specifically the difference between the two types of variables (eg. discrete vs continuous?)
- Suggest avoiding double use of brackets, if possible (eg. P(V,s)(x,y) in Equation (7) and rho(g^f) (x_L,x) in LINE 169)
- Figure captions need to be extended in order to describe the figure sufficiently, that it
can be understood independent of the text.

- 1: missing information that this is a predefined and stationary wind field and description of axes incline normalization.
- 6: missing description of individual lines, unclear: cross-correlations to which species at which location x=0.5?
- 14: analog to Fig.1 for wind field and emissions inventory mask
- (Related to point 7): Label sizes need to be increased, especially for axes and legends (all figures).
- (Related to point 7): Purely technical figure descriptions should be removed from the text, and put in the figure caption instead (eg. LINE 306 “cyan dash-dotted lines”, LINE 379, LINE 398, ... including LINE 623-624, LINE 713-715, LINE 716f).
- Often, subsections are finished by a sentence introducing the following subsection. This hinders the flow of reading. I would suggest removing these sentences and, were necessary, motivating/introducing the new subsection in its beginning (LINE 242-243, LINE 275f, LINE 309f, LINE 446f, LINE 509f, LINE 552, LINE 563, LINE 577, LINE 645f, LINE 675, LINE 688, LINE 739)
- When referring to figures in the text, the authors often only indicate the subplot panel and not the actual Figure number, eg "(panel a)". Although the Figure number was mentioned before in the text, it is standard to refer to subfigures by eg "(Fig.1a)" (compare also manuscript preparation guidelines) which also makes it easier for the reader to follow the argumentation. (LINE 245, LINE 247, and many more...)
- The word “paragraph” should be replaced by “Sect.” according to the manuscript preparation guidelines (LINE 257, LINE 439, LINE 449, LINE 452, LINE 457, LINE 529, LINE 534)
- The naming convention of (cross)(co)variances is sometimes confusion. I would suggest using different names or at least clearly highlighting the differences, eg V_A(x) (variances (between same species, same location =diagonal elements of P_A)), P_A(x,y) (auto-)covariances (same species, different locations), V_AB(x) cross-variances (different species, same location =diagonal elements of P_AB), P_AB(x,y) cross-covariance (different species, different locations), or similar. Eg. in LINE 351, V_AB(x) is named cross-covariance without mentioning that is refers to the same location, and in LINE 440, V_AB is named covariance although is refers to different species.
- The two species indicators are sometimes written as lower and sometimes as upper index, eg. V_AB vs V^AB in LINE 351 vs LINE 353. Again if these are different quantitates, it should be clarified in the text, if not, please check the whole document for a consistent notation.
- Replace “independant” by “independent” and “independance” by “independence” (LINE 441, LINE 591, LINE 831, LINE 855)

Content-related technical corrections:

- LINE 137: Add reference to Weaver&Courtier2001: https://doi.org/10.1002/qj.49712757518
- LINE 3: suggest adding “has previously been” to make clear that this is not part of the present work
LINE 18-19: state-of-the-art CTMs are much more complex than transport and chemical reactions (eg. diffusion, emissions, deposition, interaction with clouds, ...). I suggest reformulating the sentence to make clear that transport and chemistry are some of multiple processes, which are however considered dominant for most applications.

LINE 39ff: The sentence beginning with “In air quality,...” makes a jump in the chronology of the text. Based on the previous sentence, it is not clear to what the word “them” is referring. Please reformulate.

LINE 44: The context of the word “but” is not clear in this sentence. Suggest replacing by something like “…a numerical model, which are often computed in parallel at lower resolution.”, if this fits the statement.

LINE 85: Sparse observations and modelling errors are not the only reasons for the unknown true state. I would suggest reformulating, for example adding that all available information (observations and model forecasts) contain errors.

LINE 87: The formulation “estimation of X^t_q coming from the past” is unclear and unspecific. Does it refer to the forecast state?

LINE 94: The Kalman Filer also assumes independent errors between observations and forecast.

LINE 118: The definition of eps^f (x) is inconsistent with Sec.2.1 were it was a discrete vector. If a continuous formulation is used here, this should be introduced accordingly. If not, the transposed notation should also be used here.

Equation (4)+Equation (7): The norm is not defined. Suggest a short note on the norm and the meaning of its lower index, maybe with reference to literature if needed.

LINE 122+130: Suggest adding “at each grid location x” to make clear that g is a tensor at each location.

Equation (5): A note on the meaning of x_i and x_j (indication of derivatives into two directions?) is missing.

LINE 137-139: This sentence is too long and repetitive. Suggest reformulating, eg. something like: "This covariance model is used in variation DA to generate heterogeneous covariances were correlation functions vary between grid points."

LINE 147: formulation remains unclear: "leads to sum up the statistical content into a set of parameters”. Reformulate for clarification.

LINE 165+Equation (8): Although it is referred to a single observation here, I would suggest adding the indication of the observation location for the observation variance “V^o(x_L)" to be consistent to the other quantities at observation location (eg. "V^f(x_L)”).

LINE 169: Suggest adding "is the correlation function between the observation location and each model gridpoint x”.

LINE 186: The formulation “to predict the uncertainty dynamics, the latter being estimated from an ensemble method introduced to provide a reference.” is quite complicated and long. Suggest reformulation, eg something like “to predict the uncertainty dynamics compared to a reference ensemble estimation (enKF)."

LINE 291-292: The reasoning of the statement “the dispersive term influences both, the variance and the length scale” remains unclear because Equation (13) only refers to the mean state. Maybe is could be described a bit more how the authors come to this statement.

LINE 296ff: The statement of the sentence starting with “Therefore, as with the PKF...” remains unclear. How does the fact that error statistics are forecasts equivalently to state forecasts in the PKF relate to the sensitivity of the enKF to model errors? This seems to be two different aspects. Please reformulate or clarify.

Equation (16),(17): The notation is confusion w.r.t. P_AB(x,y) and V_AB(x,y). Both are defined in the text as “two-point cross covariance.” If the same quantity is meant, the same variable should be used, if not, the different should be made clearer.

LINE 398: Generation of “ensemble estimated cross-correlation” unclear. Is the cross-correlation model applied to each ensemble realization?

LINE 470,Fig.8: How is the open term calculated? Eg. from the truth or the ensemble
mean?

- **LINE 482**: For clarification, I would suggest noting that these are analytical expressions, eg “evolution of the statistics analytically” or “an analytical evolution of the statistics”

- **Equation (24f)**: Inconsistent notation. Up to now the overbar was used to indicate the expectation, whereas the $E[. ]$ notation was used here. Please stick to one notation for the entire manuscript.

- **Equation (26),(27),Fig.10**: The different normalization of the weights by term in Equation (26) and by process in Equation (27) might lead to confusion when looking at Fig.10. For example, the relative contribution of the two advection terms seems to be only slightly higher than the chemistry terms in Fig.10a (~55% vs 45%), but advection is highly dominant in Fig.10c (~80% vs 20%). I would suggest noticing the different normalization in the text or maybe even consider using a common normalization for both, if that makes sense.

- **LINE 546ff**: The discussion of different approaches for closure is split into Sec.3.3.2 (LINE 546-551) and Sec.3.3.3. I would suggest moving LINE 546-551 into Sec.3.3.3 and renaming this section eg “closure of the PKF dynamics”.

- **LINE 568**: The formulation beginning with “the subscript I must be ...” is slightly confusing. Suggest reformulation for clarification. $x$: element w.r.t. any species at any location, $x_L$: observation of a species $Z_L$ at observation location?

- **LINE 573**: Is there a reason for having the second species index $Z_1$ as superscript in $\rho$ whereas it is written as subscript for all other variables? I would suggest putting it as subscript for consistency reasons.

- **Algorithm 1**: Inconsistent syntax for loops. Eg. line 1 should be “for each observation I do” to be consistent with the other (or the other way around)

- **LINE 595**: Is each observation sampled independently for each time or are they temporally correlated? In addition to describing in the text, it might be useful to add the time index to make this clear in the equation.

- **LINE 623**: It remains unclear if only one assimilation of the four observations is performed at time $t=t_{\text{max}}$ or if several assimilation cycles are performed during the simulation. Please add this information.

- **LINE 686ff**: Was any investigation done if the dominating impact of dynamics vs chemistry also holds for the GRS-CTM? (compare specific comment 5a)

- **LINE 722**: Context, the description in the previous sentences appears to describe the general behavior. A conclusion of the performance of the PKF requires mentioning the fact that the PKF is able to reproduce all features described above. It also remains unclear if this statement only refer to chemistry or also to transport. I would suggest adding a related sentence and moving into the next paragraph (eg LINE 725ff), if that fits the content, and reformulating accordingly.

- **LINE 728, Fig.15**: It looks like the PKF produces the same length-scales for all species. It this is the case, it would be interesting to mention and explain.

- **LINE 734**: Suggest replacing the word “Indirectly” by a more specific formulation. Does this refer to the other cross-correlations, which are also well captured by the PKF but not shown here?

- **LINE 759ff**: I don’t see a connection of this statement to the content of the paper. While not being wrong, it seems to appear without any explanation. Therefore, I would suggest removing it here.

- **LINE 762**: Sec.6 also includes a short summary (first part of this section). Therefore, I would rename the section “Summary and conclusions”

- **LINE 767-773**: The paragraph deals with the first experiment with simplified chemistry (eg the evaluation of transport vs chemistry). This needs to be mentioned in order to put the conclusions into context. I would suggest reformulating the sentence in LINE 774-777 accordingly and moving it to the beginning of this paragraph.

- **LINE 779**: Formulation “feeds the reflection on” is unclear. Does it mean that this work is an important step in extending the univariate implementation to complex operational CTMs like MOCAGE? Reformulate.
- LINE 780: Sentence starting with “In particular” seems to refer to a different aspect, which is actually a drawback of the method. This should be made more clear in this sentence.
- Equation (B3),(B4): The expectations of $\varepsilon_A^2$, $\varepsilon_B^2$ and $\varepsilon_A\varepsilon_B$ denote the boundary condition at time $t$ for $x=0$. Instead, it should be the initial condition $\varepsilon_A^0 = E[\varepsilon_A^2](0,x)$ were $\varepsilon_A(0,x) = \varepsilon_A^0$, right?
- Equation (B5b): If I’m not mistaken, there is a square root missing for $V_A$ in the second term of the numerator: “$-\varepsilon_A \frac{d}{dx} \sqrt{V_A}$”
- LINE 830: The assumption of homogeneous initial fields remains unclear here. Doesn’t $E[(d_x \varepsilon_A^0)^2] = V_A^0$ follow directly from Equation (B6a) evaluated at $t=0$ ??
- Equation (B8b): The homogenous assumption is used in this step.

Individual purely technical corrections:

- LINE 14: put reference in brackets “(Kalman, 1960)”
- LINE 18: put reference in brackets: “(Josse et aline , 2004)”
- LINE 20: suggest replacing “features” eg. by “contains” or “includes” (if this fits the statement)
- LINE 24: remove final “s” from “others”
- LINE 35: “On the other hand” should only be used when following “On the one hand”. Suggest replacing eg. by “At the same time” or “But”, “However”, ...
- LINE 38: suggest replacing “needs to introduce” eg. by “requires the introduction of”
- LINE 54: replace the word “leveraged”. Meaning unclear.
- LINE 55: “an other” -> “another”
- LINE 71: grammar, replace “before to conclude” with eg. “before concluding remarks” or similar
- LINE 90+104: wrong symbol for $X^{\alpha}_q$
- LINE 116: wording, replace “recalled here for the forecast-errors covariance matrix” eg by “applied to forecast-error covariance matrices” or “used for the description of the forecast-error covariance matrix”, or similar.
- LINE 112: remove “,” before “that”
- LINE 158: wording “sketch”, replace eg with “In practice, this step consists…” if fitting the statement.
- LINE 175: Suggest less metaphoric formulation replacing “To put some flesh on the bone”
- LINE 185: grammar, replace “In what follows” eg with “In the following”
- LINE 240: inconsistent units for $\tau_{adv}$ [s] vs $1/u$ [s/m].
- 2 caption: “low resolution forecast” might be confusing here because the different resolutions were not mentioned yet. Suggest putting it into brackets here.
- LINE 264-265: The explanation of correlation anisotropy beginning with “e.g. in panel (e) were the…” is unnecessary. Suggest removing it.
- LINE 266: wording, suggest replacing “covariance error” by eg “(main parameters of the) error covariance” to avoid confusion with the uncertainty of the covariance estimate.
- LINE 269: bracket “(with O being … “proportional to”)” unnecessary, suggest removing.
- LINE 278: referring to the general technical correction 10, Sect.2.4.3 could be
introduced eg by something like “As described in Sect.2.4.2, the experiments show a

gap between ...” (just a suggestion)

- LINE 299: Connection to previous sentence unclear (may be due to unclear statement,
  see content comment-related technical comment about previous sentence). Suggest
  reformulating, maybe eg “This is demonstrated by comparing the PKF statistics to a
  high resolution forecast of the EnKF, ...”

- LINE 323: Formulation “non-linearly” unclear. Is something like "non-linear reactive
  chemical species" or "non-linearly reacting chemical species" meant? Suggest
  rewording.

- 5 caption: complicated formulation “with one orbit by level of purple transparency
  magnitude”. Maybe it can be replaced by something like “purple curves with different
  transparencies”.

- LINE 351: typo, replace “Morover” by “Moreover”

- LINE 354: it might be useful to note that all parameters are a function of model space
  (not only V_AB)

- LINE 372: I guess, “computation of the cross-covariance” refers to the enKF. If so, I
  would suggest replacing eg. by "ensemble cross-covariance" or "sample cross-
  covariance" to emphasis the calculation from enKF.

- LINE 388: “as function of”

- LINE 289: “an interpolation”

- 7: Suggest y-axis ranging from 0% to 100% to avoid the visual impression that the
  relative error almost vanished to zero at certain times.

- LINE 410: “are excluded”

- LINE 412: Complicated and unclear formulation. What is meant with “the true value of
  the averages”? Is “by an amount of 8 points of percent” equivalent to just writing “by
  8%”?

- LINE 414: Unscientific formulation, suggest reformulation (assuming that sufficient
  literature search has been performed): eg “According to our/the authors knowledge, no
  proxy of cross-correlations similar to Equation (20) has been introduced up to now.”

- LINE 736-738: This paragraph is a conclusion which should be moved to the conclusion
  section.

- Equation (21): The order of terms is inconsistent between the individual subequations.
  In Equation (21a)-(21e), the transport term is on the left hand side, while the T_adv
  are on the right hand side in Equation (21f)-(21g). Suggest putting on the same side
  for all subequations.

- LINE 436-438: Sentence about the notation of terms starting with “Hence, each term...”
  is unnecessary. Suggest removing.

- LINE 441: remove “s” from “fields”

- LINE 450: remove “,” after “dynamics”

- LINE 453: suggest adding “in Sec.3.3.3”, eg something like “simplified dynamics of the
  anisotropy are used in Sec.3.3.3 to close the PKF dynamics”

- LINE 457-458: remove the two “,” after T_adv and T_chem, respectively.

- LINE 460: “dynamics in Equation (21)”

- LINE 460: remove “,” after “transport”

- LINE 492: Suggest replacing “at the opposite” with eg “in contrast”


- LINE 508: Unclear formulation “along each specie”. Meaning a different magnitude of
  uncertainty (=stdev?) for each of the two species?

- LINE 512: Formulation, replace "What follows aim" eg by something like "The following
  section aims at..." or "In the following, we aim at..."

- LINE 513: Wording, suggest replacing “among” with eg “with respect to”

- LINE 537f: Suggest adding “can be neglected compared to the advection part
  (Fig.10c,d)” and “by W_chem-1 and W_chem-2 (Fig.10b,d)” to support the relation
  between statement and plot.

- Equation (28), LINE 540: Suggest removing Equation (28) and referring to Equation
  (25) instead of writing the same equation again.
"Equation (21g), which leads to a closure of the PKF dynamics"
"Equation (8) presented in 2"
typo: “location x_L of the chemical species”
suggest “is the forecast cross-correlation function”
suggest replacing “settings” by “setup”
I would suggest replacing “Fig.12 are now discussed” by eg “are shown in Fig.12”.
Wording, suggest replacing “With less exactitude” eg with “While being less accurate”
Removing “The last two panels (f) and (g) which correspond to” and adding reference to figure in brackets “of the length scales (Fig.12f,g) show a general…” would increase the readability of the sentence.
For readability, it is most important to name the field rather than the subplot in the text. Add name of field and refer to subplot in brackets, eg "For instance, the standard deviation of species A (Fig.13c) shows important …"
similarly to above, I would suggest adding “specie B (Fig.13d) for which …” and remove last part of sentence “as panel (d) shows”.
"which has been detailed in paragraphs 3.3.1-3.3.3” could be shortened to “(compare Sec.3.3)” – just a suggestion.
"terms”
replace “set as” by “by setting as” or “defined to be”
remove “one” -> “for each of the six”
suggest removing “of the six ones” because it provides no additional information.
"appears”. The rather long sentence could also be shortened significantly eg to something like “The impact of chemistry leads to non-zero cross-correlations between all pairs of species (Fig.15, right column, except the autocorrelation in Fig.15p)."
the word “roughness” is quite unspecific. Suggest replacing by eg “small-scale spatial variation” if that fits the content.
remove additional bracket “)” after “Sec.3.5.2”
remove final “s” from “describes”
missing “s” in “reduces”
replace “study” by eg “studied” or “investigated”
typo, “We consider four chemical species, …”
meaning of “(that is in excess)” unclear. Reformulate or remove.
double use of word “initial”. Remove.
remove additional “)"
empty subequation. Remove.
remove final “s” in “tensors”
replace “X^f+eps_f” with “X^f = X^t + eps_f”?
remove double “a” -> “Equation (8a)”
V^o is the observation error variance. Reformulate, eg. “observation and forecast error variances V_ZL^o (x_L) = ..... , V_ZL^f (x_L) + ...” or similar.