

Response to Reviewer 1 for Assimilating Compact Phase Space Retrievals of Atmospheric Composition with WRF-Chem/DART: A Regional Chemical Transport/Ensemble Kalman Filter Data Assimilation System

Response to the General Comments:

1. In my opinion, transforming $U_0^T E_m U_0$ instead at a later stage is an unnecessary complication. Furthermore, the authors apply to $U_0^T E_m U_0$ a SVD transform rather than an eigenvector decomposition. This makes me not so sure that the “final form of the observation error covariance” is the “truncated identity matrix” as stated in Section 5, as it becomes equal to $\Sigma^{1/2} \phi^T \phi \Sigma^{-1/2}$. And as far as I can see, $\phi^T \phi$ is different from the identity matrix. This problem would have been avoided if an eigenvector decomposition was used instead of an SVD.

The term $\phi^T \phi$ is a diagonal matrix equal to Σ (the diagonal matrix of singular values) because ϕ is a matrix composed of the left-singular vectors from the SVD of $U_0^T E_m U_0$. Consequently, $\Sigma^{1/2} \phi^T \phi \Sigma^{-1/2}$ is the identity matrix.

The final form of the observation error covariance is $\Sigma^{-1/2} \phi^T U_0^T E_m U_0 \phi \Sigma^{-1/2}$ (not $\Sigma^{1/2} \phi^T \phi \Sigma^{-1/2}$ as referenced in the review) where ϕ and Σ are as defined above. $U_0^T E_m U_0$ is a covariance matrix because: (i) E_m is a covariance matrix, and (ii) the U_0^T, U_0 are linear transforms of a covariance matrix. Therefore

$$\Sigma^{-1/2} \phi^T U_0^T E_m U_0 \phi \Sigma^{-1/2} = \Sigma^{-1/2} \Sigma \Sigma^{-1/2} = I_0$$

because $U_0^T E_m U_0$ has the number of non-zero singular values corresponding to the number of non-zero singular vectors in U_0 . Thus, its final form is the truncated identity matrix.

Finally, in this context the results of a SVD and an eigenvalue decomposition are the same because a covariance matrix is real, symmetric, and positive semi-definite.

2. Finally the compression approach used by the authors is conceptually equivalent to that in Eq. 24 of Migliorini et al. (2008) in the specific case when the considered forecast error covariance matrix is the identity matrix. This should be noted in the paper, as well that this simplification has the drawback that the compression is not based on a realistic estimate of the information content of the observations (as is the case of Eq. 24 of Migliorini et al. (2008)).

In Eq. 24 of Migliorini et al. (2008), they propose: (i) taking the eigenvalue decomposition of observation error covariance; (ii) transforming the system with the associated eigenvectors; (iii) scaling the system with the inverse square root of the associated eigenvalues; (iv) taking the eigenvalue decomposition of the ensemble forecast error covariance; and (v) neglecting those modes for which the eigenvalues from (iv) are smaller than unity – the scaled and transformed observation error

covariance (i.e., they neglect the modes for which the ensemble forecast error is smaller than the observation error). Our approach is different in that we propose: (i) taking the SVD of the averaging kernel (as discussed below in our Response to Comment 4, for this problem a SVD and eigenvalue decomposition are the same); (ii) transforming the system with the singular vectors that span the range of the averaging kernel; (iii) scaling the system with the inverse square root of the associated singular values; and (iv) taking the SVD of the scaled and transformed observation error covariance. The two approaches are different because our compression steps (i) and (ii) take advantage of the facts that the: (a) rank of the averaging kernel is much smaller than its dimension, and (b) left-singular vectors of the averaging kernel span its range. We do not rely on a comparison between the ensemble forecast and observation errors for compression. Our approach uses a realistic estimate of the information content of the retrieval because it is: (a) based on characteristics of the retrieval algorithm and tenets of linear algebra, and (b) directly related to the number of independent measurements made to better than observation error as discussed in Sec. 2.4.1 of Rodgers (2000).

Response to the Specific Comments:

1. *Introduction: The paper Migliorini, S. (2012), On the equivalence between radiance and retrieval assimilation, MWR should also be referenced as relevant to this paper.*

The paper will be modified to incorporate the Migliorini (2012) reference. At page 7689 after line 6 the following will be inserted: “A more recent paper, Migliorini (2012) shows that retrievals can be transformed to represent only the portion of the state that is well constrained by the original radiance measurements when two requirements are satisfied: (i) the radiance observation operator is approximately linear in a region of state space centered on the retrieval and with a radius on the order of the retrieval error, and (ii) the prior information used to constrain the retrieval does not underrepresent the variability of the state. Migliorini (2012) proves that when those conditions are met the assimilation of radiances is equivalent to the assimilation of retrievals. The Migliorini (2012) analysis shows that it is possible to use information from the retrieval algorithm to compress information in the transformed retrievals.”

Also on page 7689, lines 7 and 8, should be modified as follows:

“In this paper, we propose an approach that achieves results similar to: (i) Migliorini et al. (2008) without needing to approximate the covariance of A_{y_i} , and (ii) Migliorini et al. (2012) without needing information about the retrieval algorithm.”

Also on page 7698, line 19, following “compress the system” insert the following: “It differs from Migliorini (2012) in that it does not require information about the retrieval algorithm.” And change “As with Migliorini et al. (2008)” to “As in Migliorini et al. (2008)”.

2. *Eq (3) and later: it is not clear what is the benefit of Eq 3 that is not already in Eq 1, given that the retrieval error is unknown. Practically the only quantity that can be*

calculated is the left term of Eq 1, not that of Eq. 3.

We agree with the reviewer's comment that the retrieval error is unknown. The point of Eq. 3 is to explicitly recognize that the left singular vectors of the averaging kernel span a range that includes the impact of the unknown retrieval error. The distinction between Eq. 1 and Eq. 3 is subtle but forms the basis for the compression transformation proposed in this paper. Whether one calculates the left side of Eq. 1 or Eq. 3 is not material because both yield a result that includes the retrieval error.

3. *Typo in the SVD decomposition of $U_0^T E_m U_0$ above Eq 5: Psi should have a transpose sign.*

Typo will be fixed. On page 7689, line 12 change " $\phi\Sigma\psi$ " to " $\phi^T\Sigma\psi$ ".

4. *P7699 L20 "The result should be an identity matrix": This is only the case if an eigen-decomposition is used in place of the SVD.*

As explained in our Response to the General Comments, in this context the SVD and eigenvalue decomposition yield the same result.

5. *Section 4: replace "vertical grid points" with "vertical levels".*

Text will be changed. On page 7701, line 7 change "34 vertical grid points" to "34 vertical levels" and at line 8 change "15 grid points" to "15 levels". Also at line 13, change "50 grid points" to "50 levels".

6. *Section 4 "vertical localization": This concept is introduced here but more information should be given about the chosen radius of horizontal and vertical localization (and the reader should also be referred to section 7.5)*

More information will be given. On page 7701, at line 17 insert the following at the end of the paragraph: "For our experiments we used a three-dimensional Gaspari-Cohn type localization with a localization radius half-width of 3000 km in the horizontal and 800 m in the vertical. We conducted sensitivity experiments to determine the appropriate localization settings. Results from the horizontal tests are not discussed. Results from selected vertical localization tests are discussed briefly in Sec. 7.5."

Also on page 7703, modify line 25 as follows:

"For all experiments we used: (i) DART horizontal and vertical localization – Gaspari Cohn localization with a localization radius half-width of 3000 km in the horizontal and 800m in the vertical,"

7. *End of section 4: It is not clear what was done in terms of vertical error correlations of emission perturbations. Did you take those into account? Note that MOPITT retrievals may have done so (actually it would be good to know about that too).*

Text will be changed to indicate that no vertical error correlations were considered for the emissions. On page 7702, modify line 12 as follows: “so we set the horizontal and vertical correlation lengths to zero.”

8. Section 5: It would be good to have more information on the specific flavour of the DA system used within DART for the experiments in this paper.

More information will be given. On page 7702, at line 15, change “DART” to “the DART Ensemble Adjustment Kalman Filter (EAKF)”

9. End of section 5: it is not clear what C_m is, as the “measurement error in retrieval space” or retrieval noise is given by $K C_a K^T$, not by C_m . Also there must be a typo in the definition of C_m , given that $I + (A - I)^T$ is equal to A^T .

At the end of Sec. 5, C_m refers to the measurement error in retrieval space. We think the expression is correct as written and can be derived from Rodgers (2000) as follows: Eq. 4.44 from Rodgers (2000) is

$$\hat{S} = (I - GK)S_a(I - GK)^T + GS_\varepsilon G^T \quad (a)$$

where $A = GK$, $C_a = S_a$, $C_r = \hat{S}$, and $C_m = GS_\varepsilon G^T$. We can rewrite (a) as

$$C_m = C_r - (I - A)C_a(I - A)^T. \quad (b)$$

From Rodgers (2000) Eq. 4.45 we have $C_r = (I - A)C_a$. Substitute that definition into (b) and rearrange to get

$$C_m = (I - A)C_a(I - (I - A)^T) \text{ or } C_m = (I - A)C_a(I + (A - I)^T).$$

10. Section 6: “DART horizontal localization”. Please provide more details (see above)

More information will be given. See changes in response to Comment 6 above.

11. Section 6 “DART clamping”: just a minimum threshold?

Clamping will be clarified in the text. On page 7704, at line 2, insert the following after “clamping”: “(the imposition of a minimum threshold)”.

12. Section 7.1: replace “assimilation sparse observations” with “assimilation of sparse..”

Text will be corrected. On page 7705, at line 3, change “assimilation sparse” to “assimilation of sparse”.

13. Section 7.1 L10 “the results are consistent with Fig 1”: this is difficult to say at this stage, before the explanations given later.

Text will be changed. On page 7705, at line 13, change the text as follows: “As discussed below, those results are consistent with Fig. 1”

14. Section 7.1 L5: *It is not so evident to me that IC/BC effects can be ruled out completely.*

Text will be clarified. On page 7706, at line 10, following “too much CO destruction.” insert the following: “We reach the conclusion regarding model error versus IC/BC error because Fig. 3 shows that the bias reduction in the lower troposphere is greater for the analyses than it is for the forecasts. That suggests the following the assimilation MOPITT CO in MOP QOR the CO IC/BCs have improved relative to MET DA. Then during the course of model integration the bias increases. Thus, we conclude that model error is a more likely cause of that bias.”

15. Section 7.2 L5: *I believe $c_r U_0$ should instead be written as $U_0 c_r$, for dimensional reasons.*

Text will be corrected. On page 7707, line 8 and 9, change the text as follows: “(e.g., $\hat{y}_r = U_0 c_r$ is the truncated retrieval – denoted MOP-Trc and $\hat{y}_{qor} = U_0 c_{qpr}$ is the truncated QOR – denoted QOR-Trc)”

16. Section 7.2 L20 “*that can also indicate a contribution..but not always*”: *It seems to me that this is always the case for QOR residuals*

Text will be clarified. On page 7707, at line 22, insert the following after “but not always”: “(Note: that is always the case for the QOR residuals but not always the case for the retrieval residuals)”.

17. Section 7.2 L20: “*When components of the retrieval...*”: *I don’t quite understand this statement, as I believe QOR removes precisely the components of the prior that lie in the range of A (I guess except in the limiting case when $A = I$). Please clarify.*

Text will be clarified. On page 7707, at lines 21 to 22 change “That can indicate . . . but not always” to the following: “That always indicates a contribution from the retrieval prior term $((A - I)y_p$. However a zero residual does not always indicate that the contribution from the retrieval prior term has been completely removed.”

18. Section 7.2 L25: “*This analysis shows...*” *I don’t think the sentence is justified by the discussion above (see my previous comments).*

With the clarifications in the response to Comment 17, this sentence should be supported.

19. Section 7.4 “zeroing of the cross-correlations”: *In Migliorini et al. (2008) a scaled inverse transform on the observation error was used (their Eq. 23) rather than zeroing of the cross-correlations.*

Text will be clarified. On page 7711, at lines 3 and 4, change “(Migliorini et al., 2008)” to “(see the Introduction to Migliorini et al., 2008)”.

20. Section 7.5 L5 “transformed averaging kernel”: *please clarify what you mean by transformed here.*

Text will be clarified. On page 7712, at line 1, after “the transformed averaging kernel” insert “i.e., the transformed averaging kernel is the averaging kernel after the compression and diagonalization transforms discussed in Sec. 2.”

21. Figure 1 caption: *add “domain” to “represents the WRF-Chem”.*

Text will be corrected. On page 7718, at line 4 of the caption, change “WRF-Chem” to “WRF-Chem domain”.

22. Figure 2. *I believe the solid lines in both panels represent the same data. Consider explaining that in the caption.*

Text will be clarified. On page 7719, replace the caption to Fig. 2 with the following: “Time series of the domain average CO from the MOP QOR and MET DA experiments. The red and magenta dots show the domain average CO in retrieval space for the MOP QOR and MET DA analyses denoted in the legend by “A.” The blue and black dots show the domain average CO in retrieval space for the MOP QOR and MET DA forecasts denoted in the legend by “F.” The green dots show the domain average MOPITT CO retrievals and are the same in both panels. The solid lines show the domain average CO in model space with the same color scheme as used for the analyses and forecasts in retrieval space. The solid lines are the same in both panels.”