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Interactive comment on "Accounting for model error in air-quality forecasts: an application of 4DEnVar to the assimilation of atmospheric composition using QG-Chem 1.0" *by* Emanuele Emili et al.

Anonymous Referee #1

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1 Main or general comments

This is a very interesting paper in at least two respects: use of a 2D low-model (as opposed to the 1D model of Haussaire and Bocquet (2016) named L95-GRS) and the introduction of an offline debiasing technique. Yet, the paper suffers from partially imbalanced assumptions: while it should get a bit more realistic than the L95-GRS model, QG-Chem is sometimes less. It also occasionally suffers from too strong and unsupported claims that should be mitigated. Moreover, it could also easily be shortened a bit.

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Discussion paper

Here are my main recommendations, followed by more detailed ones.

1. Some of the assumptions made for the model are rather imbalanced leading to very unrealistic conditions. In the one hand, you choose a detailed gaseous chemistry, which is fine. But on the other hand you neglect deposition which is very unrealistic to obtain an interesting dynamical equilibrium of the chemical species (typical of air pollution in the boundary layer), but which is not difficult to model.

2. At some point, advection is neglected. This assumption is really too strong since it leads to a collection of 0/1-D box/column-models, whereas the purpose of this paper is more on the 4D-EnVar aspects where advection is critical.

3. The claim of not localizing in time is actually partially wrong; that is only an approximate statement. The dynamics of a consistent space-localization operator within the time window of 4D-EnVar was explored in Bocquet (2016), from which it can be understood that in the absence of time-localization the localization operator satisfies a Liouville equation.

4. You are occulting the fact that the IEnKS has a fully nonlinear variational analysis which you don't have (this remark also applies to the current implementations of 4D-EnVar in meteorology). This is important because this could prove an asset when dealing with highly non-linear air quality models.

5. Actually 4D-EnVar should be compared to the EnKF. This is pretty obvious *for assimilators* using both ensemble filter and variational methods. Your standpoint looks like a biased one from specialists only used to variational methods. I do not encourage you to redo everything replacing 3D-Var with the EnKF. But several of your statements should be mitigated.

6. From my understanding, the bias removal technique that you propose is actually a parametrized one since you pick up the perturbations that you apply to the ensemble. This is just a stochastic variant of the parameter estimation technique. If I am correct, you should substantially mitigate your claim on this point.
7. To shorten the paper, I would suggestion to get rid of the first configuration. It is unrealistic and I believe a bit detrimental to the paper anyway.
8. Please number all your equations. Avoiding excessive numbering is usually reserve for books, not for articles especially meant for peer-reviews.

I would recommend minor revisions. Yet, they are substantial in numbers and several of them, if justified, are mandatory in my opinion.

2 Minor points or comments related to the main points

1. Page 1, line 2-3, “using a reduced-order chemical transport model based on quasi-geostrophic dynamics”: this statement is ambiguous since we do not understand whether it is a CCMM or a CTM. Please clarify.
2. Page 1, line 4: “to a generic software library for data assimilation”: which one? This meant to become a GMD paper. That type of info should be mentioned even in the abstract.
3. Page 1, line 12: “analysys” $\longrightarrow$ "analysis".
4. Page 1, line 12-13: “A comparison with results of 3D-Var, widely used in operational centers, shows that, for some species, analysys and next day forecast errors can be halved when model error is taken in account”: A similar result was obtained by Haussaire and Bocquet (2016). They showed that by using an

ensemble forecast of the meteorology, thus partially accounting for model error, the root-mean-square error of IEnKS (a nonlinear 4D-EnVar method) on the low-order online tracer model L95-T was improved by 25% to 50%.

5. Pages 3, line 6: “next day...” $\longrightarrow$ “Next day...”.

6. Page 3, line 13-14: Haussaire and Bocquet (2016) also did a similar experiment simultaneously estimating gaseous concentrations and fluxes using a nonlinear 4D-EnVar.

7. Page 3, line 15: “Results seems promising but still relies on the assumption that the model is perfect, i.e. that there are no additional sources of uncertainties in the model forecast other than the controlled variables (i.e. the initial state and the selected emissions)”: This is a rather biased statement. The model *per see* is not assumed perfect anymore, but only part of it, such as the dynamical part. This should be explained in a less biased way. If you estimate several parameters of the parametrization of a CTM, you are morally assuming that the model is imperfect. It is just that model error is parametrized.

8. Page 4, line 4-5: “The IEnKS (Bocquet and Sakov, 2014) is a fixed-lag ensemble Kalman smoother formulated under perfect model assumptions, which can also be used to estimate erroneous model parameters through an augmented state formalism (Haussaire and Bocquet, 2016).” No! the IEnKS is an *iterative* ensemble Kalman smoother. This is quite different from the standard “fixed-lag ensemble Kalman smoother”! It is better described as a nonlinear 4D-EnVar method. Please correct. For instance: “The iterative ensemble Kalman smoother (IEnKS, Bocquet and Sakov, 2014) is a nonlinear 4D-EnVar formulated under perfect model assumptions, which can also be used to estimate erroneous model parameters through an augmented state formalism (Haussaire and Bocquet, 2016).”

   Moreover, the augmented state formalism applied to the IEnKS was first demonstrated in Bocquet and Sakov (2013).

9. Page 4, line 8-10: “These type of approaches are generally referred in the literature as ensemble-variational EnVar (Lorenc, 2013), as opposed to “hybrid” methods, which make use of ensembles only to specify error covariances matrices in variational algorithms (Belo Pereira and Berre, 2006).”

   - Instead of “These types of approaches...” it would be much better to write “These approaches”, to avoid any ambiguity in the rightful claim that the IEnKS, the 4D-Var-EnKS and the 4D-EnVar are ensemble variational techniques.

   - What you call the “hybrid” methods are in fact called EDA standing for *ensemble of data assimilation* methods.

10. Page 4, line 18: “the need in IEnKS to select a number of model parameters among all the possible erroneous parameters in complex CTMs”: yes, but the EnKS and the IEnKS can account for stochastic perturbations in the integration step of the ensemble as already demonstrated in Haussaire and Bocquet (2016), section 3.2, configuration Offline 2. Please amend your statement.

11. Page 4, line 23-25: “To the knowledge of the authors, EnVar type methods have not yet been implemented in air-quality or atmospheric chemistry models and no previous study has already examined the potential of 4DEnVar for chemical DA”: Without any ambiguity, they have been tested in Haussaire and Bocquet (2016). I do not see any problem in recognizing that fact. Please correct.

12. Page 4, line 26: “Then” $\longrightarrow$ “Than”.

13. Page 5, line 6: “This allow” $\longrightarrow$ “This allows”.

14. Page 5, line 14: “under a generic library for data assimilation”: Again, which one? Please be specific.

15. Page 6, line 18-19: “For all the experiments presented in this study a coarse resolution of 16x8 grid points has been used.”: That is quite a low resolution and

in contradiction with one of the early promises: “This choice permits to examine the behavior of DA in presence of complex gradients of wind fields and vorticity”. Please revise or tune down your promises.

16. Page 6, line 21-22: “The only desired property is to obtain wind fields that exhibit typical patterns of the complex atmospheric circulation.” which you don’t have with such a resolution. I am not criticizing your choice but the claims that are not matched by what you present. Please rephrase.

17. Page 7, line 5: “(Cariolle D, personal communication)”: Daniel Cariolle is the third author. Remove this or give more details.

18. Page 7, line 6: “which has a special treatment of the Jacobian matrix”. This is too vague. Please be more specific.

19. Page 7, line 13: “The meridional boundary conditions for chemical species are set to climatological values.”: Ok, but what type of numerical boundary conditions? That’s important.

20. Page 7, line 14-15: “Moreover, no physical removal process for the chemical species has been included in the model so far.”: This is both problematic (because this a key process of air pollution modeling) and odd (because it is not so really difficult to implement). Actually accounting for removal processes here is as important as having a fine, realistic meteorology. This is quite a weakness of your paper. The budget of all species is strongly affected. This also leads to an unbalanced photochemistry (induced by a wrong ratio of precursors).

21. Page 7, line 21: How does this configuration relate to regional air pollution modeling? Please elaborate.

22. Page 8, Fig. 1: Did you show the grid? If not, could you please do so. That would help.

23. Page 10, table 3: Please give the extended name of each species in a another column.

24. Page 12, Figure 2: Haussaire and Bocquet (2016) have more realistic values of ozone for regional air pollution with a simplified CCMM than with your model! Please discuss this. Besides, the absence of a clear daily cycle for ozone is worrying and cast doubts.

25. Page 13, Figure 3: The magnitude and variation of ozone concentration is not realistic. I would have thought it should for such a toy-model.

26. Page 13, “by the variance:”: You mean by the covariance matrix?

27. Page 14, lines 3-9: What is the point in using the diffusion equation trick to obtain $\mathbf{C}_x$ for such toy-model and such 1D-correlation function? And why not for $\mathbf{C}_y$?

28. Page 14, lines 3-9: Why did you use a 2D correlation function $\mathbf{C}_{x,y}$? There, using the diffusion equation would have been more meaningful(?).

29. Page 14, line 25: “The 4DEnVar algorithm is meant to solve the main drawbacks of 3D-Var”: Of course that is not its primary purpose. Please replace “is meant to” with “can”.

30. Page 7, line 28: “written as :” $\longrightarrow$ “written as:”

31. Page 14, 31-32: “The cost function is computed for an assimilation window that can span several hours or days”: How long is the data assimilation window in your study? That is a key value that must be mentioned and discussed, including in the paper at this point.

32. Page 15, line 10: “an hybrid 3D-Var”: What is an hybrid 3D-Var for you? What you have described does not look like what is usually understood as an hybrid algorithm.

33. Page 15, line 29: “...no time localization is applied and the same 3D (and multivariate) correlation operator C is used for all 4DEnVar sub-windows”: As I explained, this is not really a “no localization” condition. Please mention this.
34. Page 15, line 32: “Hence, for the experiments presented in this study, we could use the covariance operator described in (6) by setting the variance terms to one.”: The sentence is confusing. I would write “Hence, in order to specify $\mathbf{C}$, we could use the covariance operator described in (6) by setting the variance terms to one.”
35. Page 16, line 1: “is an ongoing research topic (Bocquet et al., 2015)” should be “is an ongoing research topic (Bocquet, 2016)”
36. Page 16, lines 19-23: There is an approximation here. These are not strict inequalities. You should use at least one $\simeq$ symbol.
37. Page 16, line 26: Again, you should use the $\simeq$ symbol here.
38. Page 17, before section 4: How are the perturbations generated? This is a critical part of the EnVar schemes, rigorously derived in the IEnKS (Bocquet and Sakov, 2014), and approximately so in other EnVar systems (so far).
39. Page 18, line 1: “and by adding a normally distributed error”: What did you do with the negative measurements?
40. Page 18, line 5-6: “The meteorology is never observed neither perturbed.”: so this is a CTM-like experiment. This should be emphasized since this is critical.
41. Page 18, line 22: “gaussian” $\longrightarrow$ "Gaussian".
42. Page 18, line 22: 1 in the Gaussian distribution should actually be the identity matrix.

43. Page 19, line 1: “ensemble localization” $\longrightarrow$ “localization of covariances”.
44. Page 19, Table 4: That would be good to have the relative value of the stds, *i.e.* divided by a standard concentration value.
45. Page 19, line 5: “All vertical terms of the covariance or localization matrix are always set to zero in this study, since only the bottom layer of the QG-Chem model is considered”: I do not understand the justification. Could you please clarify?
46. Page 19, line 11: “Fig. 4 “ $\longrightarrow$ “Figure 4”.
47. Page 19, line 20-21: “The memory of the initial condition is rapidly lost for O3, as it was also demonstrated within regional air-quality models (Jaumouillé et al., 2012).”: I doubt Jaumouillé et al. (2012) were the first to show/discuss this. Please give an earlier reference in addition to yours unless I am mistaken.
48. Page 20, line 4: “...which stays...”: what is “which” referring to? Please clarify.
49. Page 21, line 1: “Fig. 5 a,d Fig. 7“ $\longrightarrow$ “Figures 4 and 7”.
50. Page 21, line 5: This definition is a bit confusion since Eq.(17) has a normalization and Eq.(18) has not. Please clarify or use non-confusing notations.
51. Page 24, line 10: “satisfactory” is inappropriate. Be more specific. *Per se* the RMSE do not mean much because of what you wrote. Only the comparison of the RMSEs between the 3D-Var and 4D-EnVar is relevant. This comparison yields satisfactory results.
52. Page 25, line 25: “If this is not the case, a larger ensemble size allows in principle less severe localization (Ménétrier et al., 2015).”: The reference to Ménétrier et al., 2015 is inappropriate here (fully justified later on). This is very well known in

ensemble data assimilation (especially for the EnKF) for 15 years. Cite an EnKF paper instead, or nothing since this is common knowledge.

53. Page 25, line 33: “The ensemble size is the main limiting factor in operational forecast centers...”: This is not always true. For instance in Meteorology Environment and Climate Change Canada is using large ensembles, an option that they prefer (to better deal with inflation and localization).

54. Page 26, line 16: “In few cases...” $\longrightarrow$ “In a few cases...”.

55. Page 26, line 21-22: “We remind that the objective of this study is to demonstrate the applicability of a DA algorithm that outperforms currently implemented methods in operational centers...” A biased statement since other ensemble-based methods are ignored.

56. Page 27, Fig. 8: Unfortunately the average RMSE of case 2, which I consider as the most enlightening indicator in this figure cannot be seen very easily because of the larger bars of the maximum. I suggest that you multiply by 5 the average values or, alternatively, provide a second y-axis on the right.

57. Page 28, line 4: “...i.e. a case that cannot be addressed using 3D-Var or strong constraint 4D-Var.” Indeed, but you could address it with an EnKF, and it has already been. Please mitigate your statement.

58. Page 29, line 4: “A multiplicative factor of 2.35 has been sampled for the NO emissions of the forecast simulation...”: I do not understand “has been sampled”; please clarify.

59. Page 29, line 5-6: “The advection has been deactivated in this set of experiments to better focus on the impact of emissions uncertainty on chemistry.”: This seems too strong an assumption to me! the model becoming 1D on the vertical. Some of

your conclusions are based on these experiments which have a limited scope because of this assumption. Advection is of course critical for qualitatively realistic atmospheric chemistry modeling.

60. Page 32, line 12: “during night” $\longrightarrow$ “during the night”.
61. Page 33, Fig. 13: the useful subtitles of each panel, as seen in Fig. 11, have disappeared. Please add them.
62. Page 33, line 3: “This difficulty could be overcome by introducing external loops within 4DEnVar”: this has been partly addressed in Haussaire and Bocquet (2016). Please mention it.
63. Page 36, line 1: The title of section 4.3 “Validation on multiple DA cycles” is very misleading, since you are not cycling the scheme, but only repeating one-cycle experiment, i.e. gathering statistics. Please rephrase.
64. Page 38, line 6: “The justification of using an ensemble method for operational air-quality DA, which is significantly more costly than 3DVar, has been demonstrated when model errors were introduced”: This has been demonstrated long before by many teams using RRSQRT, EnKF for air quality. Please rephrase.
65. Page 38, line 7-16: Many of the statements there should be mitigated: systematically recall that these results have been obtained in the context of a simplified model (with unrealistic features). Generalized statements for 4D-EnVar cannot be made.
66. Page 38, line 15: “...on multiple cycles of DA...”: this is very misleading, as discussed before! Strictly speaking this is wrong. Please remove this statement.
67. Page 38, line 18: “We conclude that 4DEnVar provides a practical and powerful algorithm for chemical DA.”: Again, you have to mitigate this statement. “In the context of a low-order/simplified model, we conclude”. Also powerful is too much.

68. Page 38, line 26: “QG-Chem will represent a useful tool for this type of studies.” $\longrightarrow$ “QG-Chem could represent a useful tool for this type of studies.”

References

Bocquet, M.: Localization and the iterative ensemble Kalman smoother, Q. J. R. Meteorol. Soc., 142, 1075–1089, doi:10.1002/qj.2711, 2016.

Bocquet, M. and Sakov, P.: Joint state and parameter estimation with an iterative ensemble Kalman smoother, Nonlin. Processes Geophys., 20, 803–818, doi:10.5194/npg-20-803-2013, 2013.

Bocquet, M. and Sakov, P.: An iterative ensemble Kalman smoother, Q. J. R. Meteorol. Soc., 140, 1521–1535, doi:10.1002/qj.2236, 2014.

Haussaire, J.-M. and Bocquet, M.: A low-order coupled chemistry meteorology model for testing online and offline data assimilation schemes: L95-GRS (v1.0), Geosci. Model Dev., 9, 393–412, doi:10.5194/gmd-9-393-2016, 2016.

Jaumouillé, E., Massart, S., Piacentini, A., Cariolle, D., and Peuch, V.-H.: Impact of a time-dependent background error covariance matrix on air quality analysis, Geosci. Model Dev., 5, 1075–1090, 2012.