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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Implementation and testing of a simple data assimilation algorithm in the regional air pollution forecast model, DEOM" *by* J. Frydendall et al.

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Questions by the reviewer is highlighted with blue fonts and the answers from the authors are highlighted with red fonts to better distinction between the questions.

One of the main goals of air quality forecast models is to warn the public about potential exceedances of health-relevant pollutant thresholds. Therefore, the comparison of the reference run and the data assimilation runs should include categorical metrics such as false alarm rate, probability of detection, and critical success index for relevant ozone thresholds (e.g. 120, 180, and/or 240 micrograms per cubicmeter). This would provide additional evidence whether the data assimilation schemes investigated in this study can improve ozone forecasts. For a description of categorical metrics, please see Kang, D., B.K. Eder, A.F. Stein, G.A. Grell, S.E. Peckham, and J. McHenry, 2005: The New England air quality forecasting pilot program: development of an evaluation protocol and performance benchmark. J. Air Waste Manag. Assoc., 55, 1782-1796.

Answer to reviewer: The reviewer has a good point about testing the performance of the data assimilation algorithm with respect to the thresholds. However, the scope of this paper is to test different different configurations of a simple data assimilation algorithm against measurements, to carry out this performance test for a long time period (half a year) so that the statistical basis for the determination of the optimal setup is scientifically sound and to find the optimal configuration of the algorithm for operational use. To perform the performance tests with respect to the thresholds, would require another scope, namely the test of the forecast quality as function of forecast length with and without using the data assimilation algorithm. This will be carried out in a future paper.

In the introduction section, the authors may also want to include a discussion about postprocessing approaches (as opposed to data assimilation during model execution) that have been reported in the literature to account for model errors when issuing air quality forecasts. In these postprocessing approaches, model error often is estimated during a moving training period (e.g. the last seven days of forecasts) by comparing model output to observations. These bias estimates art then used to adjust the model forecasts for the current period after the model run is completed. For an example of such a postprocessing approach, please see Kang D., R. Mathur, S. T. Rao, S. Yu (2008), Bias adjustment techniques for improving ozone air quality forecasts, J. Geophys. Res., 113, D23308, doi:10.1029/2008JD010151.

Answer to reviewer: A full discussion of the the different methods for data assimilation and post processing algorithms is out of scope of this paper. However, the scientific area mentioned by the reviewer is very interesting. The following sentence has been included in the introduction: "An alternative to the direct use of data assimilation is postprocessing approaches. In these postprocessing approaches, a moving training window is assign to a fixed number of days where the model uncertainties are estimated from error residuals between model forcasts and observations. The model uncertainties estimates are used as bias corrections in the future forecast window. A nice example of such a postprocessing techniques is demonstraited in Kang et al., (2008)"

The data assimilation schemes described in this paper rely solely on updating ozone concentrations for the first layer with available surface ozone observations. Could the authors comment on the question how the lack of observations for other chemical species linked to ozone chemistry in the model as well as the lack of vertical data to adjust simulated vertical gradients affects the integrity and self-consistency of the modeled pollutant fields? This may be less of a concern when focusing only on the predicted ozone concentration but may become an issue when analyzing precursor species as well.

Answer to reviewer: The revirewer is correct that it would be very nice to be able to assimilate other species as well as vertical profiles. In the system described in

the paper, the ozone is assimilated during daytime in the whole mixing layer and not only in the first layer. It is very difficult to say something about the influence from the assimilation of other species, especially due to the fact that ozone is the only species available on hourly basis from the EMEP database used. Some hourly measurements from NO2 exists from monitoring networks, but are not collected and made available through international (meta)databases. Furthermore, the possible adjustment of the vertical profile in the model is also very interesting, but probably not within reach at the moment due to lack of data. Most studies on evaluation of modelled vertical profiles show that the spread within models and between modelled and measured profiles is large, so there is a great potential for improving model results if assimilating vertical profiles and of more species.

Section 4.1, covariance determination: How sensitive is the determination of the correlation length and error covariances to the period used in the analysis (April – September in this study 1999)? Do the estimates for these parameters vary by month and/or for different years? If the analysis were to be performed for different regions of the do- main, would there be sub-regional differences in the estimates, e.g. Southern Europe vs. Central Europe? How sensitive are the results of the data assimilation experiments described in Section 5 to the time period(s) and/or sub-region(s) used for estimation of the error covariances?

Answer to reviewer: The following has been inserted into the section 4 to clarify the method. The estimated covariances from the analysis will vary over the seasons and over the local regions i.e. Southern and Northern Europe. The ideal correlation function should be adapted to the fit the local regions and be varied over different seasons. However, in this implementation the basic correlation function will only be tested to determind the effects of the error covariance in the data assimilation routine. Experiments with finding proper correlation functions have been carried out by Houtekamer et al. (1998); Hamill et al. (2001) for the EnKF. Finding better error covariances is a investigation in itself and is beyond the scope of this paper.

Page 7,656, lines 15-17: Please provide a reference for this statement. What is the typical spatial separation of the observation stations – is it equivalent to the typical transport distance corresponding to the temporal separation between assimilation time and evaluation time, i.e. approx. 4-6 hours? Why did the authors not consider an analy- sis approach that includes both spatial and temporal separation between observations used in the assimilation scheme and the observations used for evaluation?

Answer to reviewer: The typical spatial separation of observation stations is a couple of hundreds of km. Assuming typical wind speed of e.g. 5-10 m/s, this would correspond to transport distance equivalent to the separation of the stations during the 4-6 hours. Concerning the question about including both a temporal and spatial separation between observations used for assimilation and validation, we chosed to make the temporal separation only in order to have as many stations for validation and assimilation as possible and due to the fact that we are testing a forecasting system where the temporal development of the air pollutants is very important at specific locations rather than the spatial distribution at large scale. To make the spatial separation, the number of measurement stations for assimilation as well as for validation would be aound 45. Since we are evaluating the system for the whole of Europe with relatively large gradients in the oxone levels, we concluded that we preferred the temporal separation only.

Page 7,658, lines 5-6: Please clarify the design of experiment 6. In my understanding, experiments 4 and 5 use different correlation functions, so which correlation function was used in experiment 6?

Answer to reviewer: The orignal formulation of experiment 6 was not clear enorgh therefore the following formulation of the experiment 6 is replacing the orignal formulation: "Experiment 6: Combination of experiments 4 and 5 with both the anisotropic and the density of observations correlation function. The assimilation routine is activated once per day at 12 UTC."

Page 7,657, last paragraph: It might also be instructive to include maps of model performance as measured by bias, RMSE, etc. for the different experiments.

Answer to reviewer: The reviewer is correct, that it would be very interesting to map the spatial distribution of the statistical measures for the different experiments. However, we have chosen not to do this for two reasons - first, the number of maps would be 30 if all should be included for consistency, Secondly, the overall conclusions of the experiments for finding the optimal configuration of the algorithm would not be changed including the spatial distributions of the metrics.

Page 7,658, lines 13-15: Was the ranking performed by month? The tables provide results by month but the description of the ranking system does not specify if the ranking was performed separately for each month.

Answer to reviewer: To clearify the on the comment from the reviewer the following has been added to the text: "The ranking was performed for each month, April to September, and one ranking for the entire period."

Page 7,659, lines 4-6: How can continuous data assimilation be performed in a forecastsetting where future observations are not available? For simulating historic periods, this statement is relevant, but I do not see how it is relevant for the forecast system analyzed in this study.

Answer to reviewer: To minimized the forecast error sequential data assimilation is preferred. This is due to the model will be corrected on a short time interval and thereby will the model solution not drift to far away from the observations at next time step. This will result in smaller forecast errors which is also evident from the experiment in the text. To clarify, the sentence has been rephrased to: "This suggests that doing sequential assimilation like from the Ensemble Kalman filter or 4D variational assimilation would enhance the model performance significantly by updating the model at every observations time."

Page 7,659, lines 15-20: How sensitive is the conclusion that the optimal weights approach performs better than the equal weights approach to the training time period and/or spatial training domain used to determine the weights?

Answer to reviewer: The reviewer is right in addressing this statement. It is clear that the data assimilation routine will performed better with the optimal weights since is the weights are regressed over the training period. However, in the test under investigation we did not perform more sensitivity test other then the equal and optimal weights test. This question will have to be open until addressed in later experiments.

Page 7,659, line 25 – Page 7,660, line 2, Figure 2: Which hours are used for the analysis of daily mean values? In particular, do these hours include model values, pre- and post-assimilation periods, and the assimilated observations themselves during the 10:00 – 12:00 time period? In other words, there is a clear separation in time between assimilation period and analysis period for the daily maximum values, but it is not clear if there is also a separation for the analysis of the daily mean values

Answer to reviewer: The reviewer is correct that when considering the daily mean values, there is not a clear separation between the assimilation period and the validation period. The daily mean values was, however, still included since they gives some indications on whether the signal from the assimilation is changing the model is a positive direction for more than just the first 4-6 hours. Furthermore, there is another purpose of assimilating observation data into a model than performing better forecasts - namely to make the best possible "analysed fields" - meaning the most realistic (or precise) fields of air concentrations combining both measurements and model results (analogous to the analysed fields in meteorology). Analysed air pollution fields, can be used for more precise assessment of e.g. exceedances of critical levels and loads or for the best possible assessment of impatcs from air pollution on e.g. human health or eco-systems. The analysed fields should of course also be evaluated - meaning that it is partly compared to data included also in constructing the fields.

Page 7,662, lines 12-13: Please specify how this different combination of experiments could be performed. In addition, this was not shown or discussed in Section 5 so probably this statement does not belong in the conclusion section.

Answer to reviewer: The sentence was to loose formulated and has been removed.

Page 7,662, lines 24-26: What are the conclusions from this examination? Please specify.

Answer to reviewer: The conclusion from this experiment was to clarify that the data assimilation routine did not shock the model in the updating step. If the model solution did not predicted any ozone concentrations in an area where there is measured large ozone concentration. This could introduce a large gradient in the model solution in the update. The data assimilation routine could introduce artifacts into the model solution. The easiest way of testing this by a visual representation of the test. The two test were chosen where there was to known ozone episodes to see if there were any artifacts in the model solution. The following sentence has been added to clarify: "It was concluded from this experiment that the data assimilation routine did not introduced any sharp gradients into the model which could lead to artificial model solutions."

Pages 7,679 – 7,680, Figures 9-10: Suggest including an additional panel showing the observed values.

Answer to reviewer: The reviewer is correct in stateting the additional panel with the observed values might help the readers for better understanding of the figures. Unfortunately we cannot comply to this request because the software that we have used to visualize the figures does not have this option in the software.

Editorial comments:

Answer to reviewer: All the editorial comments have been implemented into the text.

Pages 7,673 – 7,680, Figures 3 – 10: Please change “upper”/”lower” to “left”/”right” to reflect the arrangements of the panels.

Answer to reviewer: the mauscript is optimized towards the ACP format and therefore the figures are aligned in the rigth “upper”/”lower” format.

References

Thomas M. Hamill, Jeffrey, S. Whitaker, and Chris Snyder. Distance-dependent filtering of background error covariance estimates in an ensemble kalman filter. *2776 MONTHLY WEATHER REVIEW VOLUME 129 Monthly Weather Review*, 129(11):2776ï£¡ @ S2790, 2001.

P. L. Houtekamer, Mitchell, and L. Herschel. Data assimilation using an ensemble kalman filter technique. *Monthly Weather Review*, 126(3):796ï£¡ @ S811, 1998.