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Interactive Comment

Interactive comment on "Development and application of the WRFPLUS-Chem online chemistry adjoint and WRFDA-Chem assimilation system" *by* J. J. Guerrette and D. K. Henze

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This paper is clearly work in progress, and describes in large detail the development of a 4DVAR system for WRF-Chem. The final aim is clearly outlined: chemistry will be an integral part of the WRF model, and will influence the dynamics of the model. Aerosols may lead to atmospheric heating, and to shading of the surface, influencing the surface energy balance. Therefore, I was a bit disappointed to read that the coupling to radiation has not yet been implemented in the adjoint model. The authors are quite elaborate in their description, which is somehow good, but also makes the paper lengthy. An interesting section is the weighting scheme for observations. The authors argue that the

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normal Bayesian scheme puts too much weight on the observations that are within 2σ of the model. Therefore, they propose an additional weighting scheme. Although you can argue about the necessity, the approach is interesting and well documented. Some remarks about it you will find below. The implemented scheme is applied to observations of BC, both from the surface and from aircraft. Although the emissions are not optimized, clear indications are found for too high anthropogenic emissions, and too low biomass burning emissions. Also, shifts in emission diurnal patters are predicted. All in all, the paper is a very valuable contribution and well written. I have some minor remarks, which I list below.

1 Link to other work

In the introduction, no reference is made to the pioneering work of Elbern et al. with the EURAD model, who worked on 4D-VAR chemical data assimilation for more than two decades. In general, it would be interesting to compare the approach described here to other approaches. For instance, some 4DVAR approaches (e.g. Bergamaschi, P., Frankenberg, C., Meirink, J. F., Krol, M., Villani, M. G., Houweling, S., et al. (2009). Inverse modeling of global and regional CH 4emissions using SCIAMACHY satellite retrievals. Journal of Geophysical Research, 114(D22), D22301. doi:10.1029/2009JD012287) use a two-step inversion. Observations that are not fitted within 3σ after the first optimization are left out with an argument that the model is not able to reproduce these observations. In the current study, some of the high aircraft observations may be due to specific layered outflow from a specific convection event, which is not (and might never be) adequately resolved by the model. Nevertheless, the advanced estimation of model error with the different settings in WRF is impressive. Without a true inversion, however, it is not possible to assess how well the observations finally will be matched. My main point here is that a discussion of this work in the context of existing techniques would be of added value.

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2 Comments

I do not see why the summation is split in eq. 2a and does not simply run to *n*. Please explain.

Page 2321, line 2: “earliest emission time”: up to now “x” was a general variable, that is now linked suddenly to emissions. Please explain this better.

Page 2331, line 17: “nonlinear to a quadratic form”. I see what you mean, but strictly speaking quadratic is also nonlinear.

Page 2325: “some cost function at location p and time step f with”. Up to now, the cost function was introduced as a global variable (eq. 1). Defining it here as a space and time dependent variable is confusing.

Page 2325: Comparing the results of eqs. 5 and 6 is known as the gradient test (see e.g. ECMWF documentation). Normally, you take *dx* that approaches zero and the finite difference gradient will approach the true gradient until numerical rounding errors become important. To my experience, for double precision calculations, derivatives can be approximated within 10^{-7} before rounding errors kick in. In my applications there is convergence until *dx* is about 10^{-6}. I do not see why one has to fiddle around with different values of dx (0.1, 1, 10%, i.e. relatively large values) to see what value performs best. In the paper (page 2326) it is written: “A range of finite difference perturbations dx is used for U, T , and Q_v control variables in order to find a value of XNL with the best compromise between truncation and roundoff error.” Another problem might be that perturbations to *U* in the forward model perturb the physics (atmospheric flow is normally defined in vorticity and divergence), and that this violates some mass-conservation constraints. This might be the reason for the strange behavior presented later in figure 5, which look rather suspect in my opinion. The sensitivities for something linear as emissions (figure 5, first panel) look perfectly fine and what would be expected.

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Page 2326: The adjoint test presented is figure 2 was compromised by some errors, as mentioned later in the paper (page 2328). So it seems logical to replace figure 2 by a corrected one.

Page 2326, line 5: Q_v has not been introduced in the paper.

Page 2328, line 26: "BC concentrations respond linearly to a 1% perturbation of emissions for at least 48 h". Is there any reason that a non-linear response can be expected when coupling with BC and radiation is turned off?

Page 2331, line 28: reference missing

Page 2332: I am a bit worried that you use two different measurement techniques for BC. BC is particularly tricky to measure and LAC and TOR might have different biases. For sure, BC and EC cannot be compared directly, because they are defined differently. Using ARCTAS and IMPROVE data in the same inversion might have to deal with a bias of one method to the other. Maybe it is important to highlight how comparable the data are. There is a wealth of literature available on bias correction of particular data streams (e.g. satellite data).

Page 2335, eq. 16: Sure you divide by L^2?. Anyhow, it would be better to have the non-summed part before the summation sign for clarity. Also for eqs. 17, 20, 24.

Page 2838. In the discussion of the model-data mismatches and associated adjoint forcings, I miss a discussion of the role of the adjoint model. The H^T operator projects the mismatches to dJ/dc_k and indicates how sensitive a particular observation is for a particular emission change. By only discussion the adjoint forcings and their magnitudes, I cannot see how you can defend the need for a w_k scaling in the covariance matrix. In my opinion, the need of this scaling only appears after a full inversion, and I would like to hear the authors' opinion about this.

Page 2341, discussion figure 11. Figure is unclear to me. Results are shown for anthropogenic (red?) and biomass burning (blue?) BC emissions. I understand that

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the black markers highlight boxes with biomass burning, but how do I see where the anthropogenic emissions are and how this relates to the blue and red colors?

Page 2343, page 21. The authors write: "The increased burning sensitivity magnitude indicate the weighting scheme is successful at generating a cost function that is more robustly sensitive to emission perturbations." I think this is not a valid reasoning. It is not surprising that the inversion is somewhat sensitive to the settings of the physical model parameters, simply because the boundary layer scheme determines how emissions are transported in the atmosphere and how the simulated observations look like. By using a different weighting these sensitivities become more alike, but this is not a proof that the new weighting scheme is better or worse: it simply gives different results because outliers receive more weight compared to better simulated observations. Like stated before: it is unclear why the authors felt the need to deviate from Bayesian statistics. Only after a true inversion and calculation of the associated statistics (e.g. χ^2 values) one might conclude that the weighting scheme gives more favorable results.

Interactive comment on Geosci. Model Dev. Discuss., 8, 2313, 2015.