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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Effects of model chemistry and data biases on stratospheric ozone assimilation" *by* L. Coy et al.

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General Comments:

This article examines the impact of model chemistry on an ozone assimilation system. In particular, observation minus forecast residuals are shown to respond differently to the present of observation biases when model chemistry is included. Other issues such as bias of the reference chemistry state used in the parameterization, and the impact of the upper lid are also considered. Overall, the presentation is clear, thorough and effective. The figures aptly illustrate the points being made, and the issues explored are logically connected. The work is an important addition to the data assimilation literature because it clearly explains how and why including chemistry parameterization in an ozone assimilation system can be helpful. I recommend publication in ACP after

the authors consider the few minor comments below.

Specific Comments:

1. Section 2, p. 1071, para. 2: It is not clear why the dynamical state is a composite of 3 data sources, at the start of every 6-h cycle. It is clear that this must be done when starting a cycle, but after the first forecast, a dynamical state on the full model grid is available. Just as the GEOS-DAS is used for the ozone assimilation, the NAVDAS could have been used for the dynamical assimilation with NOGAPS-ALPHA. It is not clear why the forecast is discarded in place of the composite analysis. A little explanation here would be helpful.

2. Section 3.1.1: The results of this section can be understood from data assimilation theory as follows.

   Consider the usual analysis equation:

   $$\mathrm{x}_k^a = \mathrm{x}_k^f + \mathrm{W}_k(\mathrm{x}_k^{obs} - \mathrm{x}_k^f) \quad (1)$$

   where **x** is the model state (here it is ozone) and superscripts a, f and obs refer to the analysis, 6-h forecast and observations. The subscript k refers to the assimilation step k. **W** is a weight matrix which depends on specified background and observation error covariances. Note that the observations here are assumed to be at grid locations for simplicity (to avoid introducing the observation operator which maps the model state to observed variables and locations). This assumption does not affect the arguments below. To consider biases, simply subtract a true (but unknown) ozone state from both sides to get and take an ensemble mean to get:

   $$\mathrm{b}_k^a = \mathrm{b}_k^f + \mathrm{W}_k(\mathrm{b}_k^{obs} - \mathrm{b}_k^f) \quad (2)$$

   where **b** refers to the 3-D ozone bias.

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Now consider how the forecast is produced:

$$\mathrm{x}_k^f = \mathrm{M}_k \mathrm{x}_{k-1}^a \tag{3}$$

where **M** is the numerical model which advects ozone by dynamic fields. By subtracting the true state from both sides and taking an ensemble mean of the errors, we see that

$$\mathrm{b}_k^f = \mathrm{M}_k \mathrm{b}_{k-1}^a. \tag{4}$$

As noted by the authors (p. 1079 para. 2), the global mean ozone will not change through advection alone. Combining (2) and (4) yields a recursive equation for the evolution of bias:

$$\mathrm{b}_k^a = (\mathrm{I} - \mathrm{W}_k)\mathrm{M}_k \mathrm{b}_{k-1}^a + \mathrm{W}_k \mathrm{b}_k^{obs}. \tag{5}$$

In the case of a scalar state, one can avoid the matrix operations and complete the recursions to get

$$\mathrm{b}_k^a = (1 - \mathrm{W})^k \mathrm{M}^k \mathrm{b}_0^a + \sum_{i=0}^{k-1} (1 - \mathrm{W})^i \mathrm{M}^i \mathrm{W} \mathrm{b}^{obs}. \tag{6}$$

If full weight is given to the observation (W=1), the bias of the analysis is equal to the bias of the observation (since only the i=0 term of the summation remains). If no weight is given to the observation, of course nothing is known about the observation bias and the bias of the analysis is equal to the initial forecast bias. The usual case is for a weight between 0 and 1. In this case, as k goes to infinity, the first term gets very small and the last term can be summed to b^{obs}. Again, the analysis bias eventually picks up the observation bias. The speed at which this happens depends on the weight given to the observations (which depends on the relative accuracy of the forecast and observations). These results

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can be extended for the full matrix equations. Thus the results in Fig. 8b are understandable in that the analysis shows the observation bias.

Moreover, since the analysis bias picks up the observation bias (assuming no initial forecast bias), from (4), one can see that in a global mean sense, the forecast bias will also be identical to the observed bias. Then, because

$$< O - F >=< (\mathrm{x}^{obs} - \mathrm{x}^{t} + \mathrm{x}^{t} - \mathrm{x}^{f}) >= \mathrm{b}^{obs} - \mathrm{b}^{f} \tag{7}$$

the O-F residuals are zero. Thus, the results of Fig. 7b are understandable since the forecast eventually picks up the observed bias and the difference in observed and forecast bias goes to zero.

The equations shown thus far are standard and can be found in any data assimilation text such as Daley (1991). What is more interesting, are the results shown for the case with chemistry. The model chemistry is given by:

$$\frac{dr}{dt} = (P-L)_o + \left.\frac{\partial(P-O)}{\partial r}\right|_o (r-r_o) + \left.\frac{\partial(P-O)}{\partial T}\right|_o (T-T_o) + \left.\frac{\partial(P-O)}{\partial \Sigma}\right|_o (\Sigma-\Sigma_o) \tag{8}$$

The true evolution of the chemistry can also be written in a similar form, but instead of linearizing about a reference state, one must linearize about the truth:

$$\frac{dr^t}{dt} = (P-L)_t + \left.\frac{\partial(P-O)}{\partial r}\right|_t (r-r_t) + \left.\frac{\partial(P-O)}{\partial T}\right|_t (T-T_t) + \left.\frac{\partial(P-O)}{\partial \Sigma}\right|_t (\Sigma-\Sigma_t) + missing\,terms \tag{9}$$

where the missing terms include higher order terms as well as derivatives with respect to other variables besides ozone, temperature and column ozone. Now we can compute the forecast bias due to the chemistry model by subtracting (9) from (8) and taking an ensemble mean.

$$\frac{db^r}{dt} = < (P-L)_o - (P-L)_t > - \left.\frac{\partial(P-O)}{\partial r}\right|_o < (r_o - r_t) >$$

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$$- \left.\frac{\partial(P-O)}{\partial T}\right|_o < (T_o - T_t) > - \left.\frac{\partial(P-O)}{\partial \Sigma}\right|_o < (\Sigma_o - \Sigma_t) >$$
$$- \left(\left.\frac{\partial(P-O)}{\partial r}\right|_t - \left.\frac{\partial(P-O)}{\partial r}\right|_o\right) b^r - \left(\left.\frac{\partial(P-O)}{\partial T}\right|_t - \left.\frac{\partial(P-O)}{\partial T}\right|_o\right) b^T$$
$$- \left(\left.\frac{\partial(P-O)}{\partial \Sigma}\right|_t - \left.\frac{\partial(P-O)}{\partial \Sigma}\right|_o\right) b^\Sigma - < missing\, terms > . \quad (10)$$

If, as assumed in section 3.1, the reference chemistry state (subscript o) is unbiased, the first 4 terms are negligible. Of the remaining terms, the 5th one dominates and it reflects a damping of the ozone bias. The rate at which the damping occurs is proportional to the error of the coefficient (inverse time scale). Thus the damping of the ozone bias is strongest where the lifetime is shortest. We can represent the effect of the chemistry on the forecast bias by

$$\mathrm{b}_k^f = (\mathrm{M}_k - \mathrm{D}_k)\mathrm{b}_k^a \quad (11)$$

where D_k represents the damping due to chemistry. While **M** represents advection and cannot affect the global mean, certainly **D** can affect the global mean bias. If the damping is strong enough, the analysis bias can be effectively eliminated (Fig. 8a is consistent with this assumption). Then, according to (7), the O-F bias becomes the observation bias. This is what is seen in Fig. 7a. If the data is unbiased, so too are the O-F's.

Figs. 9a,b show that the damping effect is strongest in the upper stratosphere and higher. Thus the forecast bias is removed and the O-F bias reflects the data bias at these levels. At lower levels where the damping of the bias is not strong, the O-F scores are similar whether or not chemistry is modeled (Fig. 9a,b).

(10) shows that if the reference chemistry is biased, this will affect the forecast bias. However, some of this bias will also be in the form of damping terms. Thus bias due to reference chemistry, forecast and observations will be all mixed together.

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The authors have identified a very interesting impact of using a highly damped chemistry model on data assimilation diagnostics. In particular, where the model is highly damping, (in the upper stratosphere and higher), analysis biases are also damped so O-F biases reflect observation biases. This could be a very powerful tool for monitoring chemistry measurements in the upper stratosphere. Because the conclusions are based on one particular form of chemistry model, it is useful to question the generality of the result. The data assimilation result (above) depends on the highly damping nature of the second term of (8). In models which use a full chemistry such parameterization does not occur. However, if the importance of this damping is realistic (when compared to full chemistry models), then the result should hold for the full chemistry model. Consultation with chemistry modelers suggests to me that this is the case, and the results are general. However, the authors may wish to comment on the generality of the result in the discussion section.

3. Section 3.2: In this section, adaptive photochemistry is considered. This means that in (10), the terms with subscript "o" will be replaced by functions of the state. Thus these terms too will be functions of the bias of the analysed temperature, ozone and column ozone. In this case, the first 4 terms of (10) will depend on the bias of these terms in the analysis and may not be zero. Thus, like the case with no chemistry, the forecast bias is related (but not identical) to the analysis bias and some cancellation in the O-F bias will occur. But like the case with non-adaptive chemistry, the global forecast bias is damped. Thus, the result of Fig. 14 makes sense. Like the case with no chemistry, some reduction of the bias is seen. Unlike the case with nonadaptive chemistry, the bias is only partly diagnosed. (10) shows that there is some advantage to choosing unbiased reference states (as the authors point out in this section) since the first 4 terms are then neglible.

4. Section 4, p. 1089 para.3 (continues on next page): A warning is given here about

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the misleading nature of O-F. However, it is well understood in data assimilation community that O-F does not provide independent information about measurement bias. The analysis draws to the measurements so if the latter is biased, so too is the analysis (and forecast). The general solution is use independent measurements to identify observation bias.

5. Section 5, points 1 and 2: You may wish to qualify these statements to indicate that the impact of the OPP on mean analyses and O-F is limited to regions where lifetimes are short.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 1067, 2007.