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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Using 3DVAR data assimilation system to improve ozone simulations in the Mexico City basin" *by* N. Bei et al.

N. Bei et al.

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We are grateful to the reviewer's thoughtful comments and suggestions for the manuscripts. Below are the replies to the reviewer's comments.

Reply to the major comments:

1)The paper lacks significant discusssion of several issues related to data assimilation. A discussion section is needed (probably just before the conclusion section) that addresses the following issues:

A discussion section regarding data assimilation has been added on page 12543 before the conclusion section:

5. Discussions

As the essential inputs for air-quality models, meteorological fields control or strongly influence the evolution of emissions, chemical species, and aerosols through many atmospheric processes, including horizontal and vertical transport, turbulent mixing, convection and lightning-induced generation of nitrogen oxides (NOx), and both dry and wet deposition to the surface. The rates at which secondary species form and certain chemical reactions take place are affected directly by the relative humidity, solar energy, temperature and the presence of liquid water (clouds) (Seaman 2000). Data assimilation aims at accurate re-analysis, estimation and prediction of an unknown, true state by merging observed information into a model. The goal of using data assimilation in numerical weather prediction is to improve the simulated wind transport by improving the model initial conditions. 3DVAR has been extensively used in the meteorological community, but seldom in air quality modeling. Overall, the meteorological simulations have been improved using the 3DVAR data assimilation system in the present study. However, simulations are still occasionally unsuccessful compared with observations. One of the possible reasons is the use of static background errors in the 3DVAR system, which does not reflect the flow-dependent background error covariance. An ensemble-based background error covariance will be employed in our next study. Additionally, the intrinsic predictability of the numerical weather prediction might also contribute to the failure of the improvement for meteorological simulations. The initial error and model error inevitably bring about uncertainties in meteorological simulations and the initial error growth is also strongly nonlinear. Recent studies (Bei and Zhang, 2007; Tribbia and Baumhefner, 2004) on predictability suggest that, while there is significant room to improve forecast skill by improving forecast models and initial conditions, both mesoscale and large scale predictability are inherently limited. Nevertheless, the ensemble forecast approach can provide a probabilistic guidance for reducing uncertainties in meteorological simulations. Independent verification is an effective way to examine a data assimilation system. We did not have sufficient data to carry out a complete data withholding experiment, but comparisons of the mixing layer heights with tethersonde observations (Velasco et al., 2008) have provided an

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independent evaluation of model improvement in terms of a variable that is important for air quality simulations.

2) Why does the paper focus only on ozone? While ozone is important in terms of impacts to human health, ozone precursors should be examined as well. For example, it would be useful to quantify changes in CO and other primary emissions. Do other chemical species show similar improvements as ozone?

In order to further provide a more comprehensive understanding about the improvement of chemistry simulation caused by the 3DVAR system, we have included an additional figure for ozone precursors (CO and NOx) as the referee suggested (Fig. 9) and the corresponding description on page 12540: Fig. 9 shows the observed and simulated time evolution of NOx and CO during the same period. They are both improved through using 3DVAR data assimilation, which is consistent with the result of the ozone simulation.

3)Since the performance of 3DVAR will depend significantly on the prescribed errors for the observations and background information, please describe in more detail why the NMC method (page 12535, line 11) and its 1-month data set would be applicable to the present study. Also include the possible impact of the assumption on the results in this study. The possible impact of the error covariance is only briefly mentioned in the conclusions.

The following paragraph has been added after page 12535, line 12:

The NMC method is the common way to produce the background error covariance in 3DVAR system. However, the background error covariance derived using the NMC method is stationary and isotropic, which does not reflect the flow dependent error information. This will affect the analysis results because the real background error covariance should be flow dependent. Future work will focus on the role of background error covariance formation in 3DVAR system and the possibility of obtaining them from ensemble forecasts.

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Interactive Comment

Reply to the minor comments:

Page 12531, line 18: Please include a few sentences describing the differences between 3D and 4D variational approaches and what the advantages of 3DVAR are.

The following paragraph has been added after Page 12532 line 4:

The main reason for using 3DVAR rather than 4DVAR is that it is computationally cheaper to run because it does not require the tangent linear (TL) or the adjoint of the forecast model. 4DVAR can provide an improved analysis under certain situation, but 3DVAR can achieve similar goal by using a rapidly updating cycle. Another benefit of 4DVAR is the use of flow-dependent background error covariances, which may also be approximated in 3DVAR through grid transformations, anisotropic recursive filters and/or the use of ensemble information. The 3DVAR system provides an efficient training ground for crucial aspects of the data assimilation system because many of the algorithms used in 4DVAR are found in the much less computationally expensive 3DVAR system. These include observation operators, minimization, preconditioning, multivariate background error specification and data assimilation diagnostics. 3DVAR has been widely used in operational weather forecasting, but has not been used in air quality study.

Page 12532, line 3: It would be useful to include any references that have used 3DVAR for air quality applications. If there are none, the authors should state so.

We did not find any literature reference that has used 3DVAR for air quality applications. This has been mentioned after line 3 on page 12532.

Page 12535, line 6: It would be useful to include a table listing the specific observations that are assimilated into the model results that depends on the domain.

A table describing the specific observations used for each domain has been included.

Page 12536, lines 16-21: Unless, the VOC and Nox regimnes are examined again with and without data assimilation, this paragraph is irrelevant to the present work and can

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be deleted.

The paragraph has been deleted.

Page 12537, line: Mark the positions of the high pressures systems in Figure 2 that are discussed in the text.

The positions of the high pressures systems in Figure 2 have been marked.

Page 12537, line 7: It is difficult to see significant differences in the profiles presented in Fig. 3. Perhaps the differences could be quantified better by plotting the observed profile in one panel and differences between the observed and simulated profiles in other panels.

Figure 3 has been revised as suggested by the reviewer.

Page 12538, line 3: I assume that the tethersonde observations were not assimilated into the model results, and thus present an independent data set to evaluate 3DVAR. The authors should include some text pointing this out.

The tethersonde observations present an independent data set to evaluate 3DVAR. This has been pointed out in the text.

Page 12538, line 3: Please state why the mixed layer depths were changed significantly when assimilation was used. For example, was the surface tempmerature during the entire day too cool? Probably not, since the surface temperatures in Fig. 6 do not change much. Or was the stability changed that encouraged more vigorous boundary layer growth? Or was it something else?

We have added the following sentence on page 12538 line 3: The surface temperature increased during the daytime (see Fig. 5) when 3DVAR assimilation was used, which contributes to the increase in height of the mixing layer. The increase of horizontal convergence inside the basin also leads to the increase of vertical motion and mixing layer heights (see the analysis in Section 4.3).

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Page 12538, lines 16-17: Even the 3DVAR simulations didn't capture the winds in the northwest part of the basin. Presumably they were assimilated into the model. Please comment on why 3DVAR failed to improve the model in the region.

The available surface wind observation is very limited at 8:00 CDT. The model does not assimilate the data at 8:00 CDT. We assimilate observations every 6-h in 3DV6h and every 3-h in 3DV3h. The 3DVAR modeling failed to improve the winds simulation in this region might be caused by the deficiency in initial background field.

Page 12543, line 25: Improvements to humidity is mentioned, but humidity is not described in the text.

Humidity is described in Figure 3 using the difference between temperature and dew-point temperature. And the improvement to humidity has been described on page 12537 line 12.

Page 12549: The black squares in the right panel are not defined. What are they used for?

The black squares in the right panel have been defined in the legend of Figure 1b.

Page 12550: The coast of Mexico and the boxes need to have thicker lines to be legible.

The coast of Mexico and the boxes have thicker lines in Figure 2.

Page 12553: Move labels from inside the panels to outside the panels to be more legible. I t might be useful to draw in convergence lines at 20 LT so the reader can more quickly see the differences in the position of the convergence zone.

The labels have been moved from inside the panels to outside the panels in Figure 5. The convergence lines at 20 LT have also been included.

Page 12554: Gray shading has not been defined or discussed. Either describe or remove.

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Gray shading has been defined in Figure 6 caption.

Page 12556: Gray shading has not been defined or discussed. Either describe or remove.

Gray shading has been defined in Figure 8 caption.

Page 12557: A 20 ppb contour increment seems too big for this time period. Suggest raising the minimum value to about 30 ppb and decreasing the interval to better illustrate the differences between the observations and predictions.

Figure 10 has been re-plotted as the reviewer suggested.

Page 12558: Include labels for the colors in the figure as well.

The labels for the color have been included in Figure 11.

Page 12550: The arrows are far too small.

The arrows in Figure 2 have been enlarged.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 12529, 2008.