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IMPACT OF COVARIANCE MODELING AND DATA SELECTION ON ASSIMILATED OZONE

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1. INTRODUCTION

The ozone distribution in the upper troposphere and lower stratosphere is needed in many geophysical applications. For example, it is needed in quantification of cross-tropopause fluxes, tropospheric ozone, and radiative transfer calculations. Accurate estimates of ozone fields in the lower-most stratosphere and troposphere can provide better first guess profiles for retrievals of ozone from remote sensing instruments, and thus, improve our ability to extract information from satellite observations.

Global three-dimensional ozone fields are produced at NASA/Goddard Data Assimilation Office (DAO) by assimilating the Total Ozone Mapping Spectrometer (TOMS) and the Solar Backscatter Ultraviolet (SBUV) instrument observations into an ozone transport model (Riishojgaard *et al.* 2000, Stajner *et al.* 2001). Satellite instrument ozone observations, including those by TOMS and SBUV instruments, have low vertical resolution in the upper troposphere and lower stratosphere. Therefore, vertical structure is largely provided by the assimilation model. We investigate the sensitivity of the assimilated ozone in this region to changes in specification of error covariances and to data selection, which change the balance between the amount of information from the observations and the model.

2. TOMS ERROR COVARIANCE MODELING

Differences between incoming observations and the model forecast of the same variables, so called observed-minus-forecast (O-F) residuals, are a very useful byproduct of the assimilation process. More rigorously, the O-F residuals are the differences

$$\mathbf{w}^o - H\mathbf{w}^f,$$

where $\mathbf{w}^o$ is the vector of observed values, $\mathbf{w}^f$ is the vector of forecast values, and H is the matrix of the observation operator mapping model variables to observed variables. Information about observation errors and model errors is contained in the O-F residuals. They can be used to evaluate the performance of the assimilation system, tune the error models, or indicate a change in the observation errors, like a change in the instrument calibration.

The errors in observations made by satellite borne sensors are likely to be spatially correlated. The TOMS measurements are made by the same sensor at all locations. Furthermore, the retrieval algorithms rely on the same climatological first guess values for nearby points. The same cloud height climatology is used in retrievals of ozone values at nearby points. Consider a departure of any geophysical field needed in the TOMS retrievals. If the spatial scale of this departure is larger than the distance between neighboring TOMS measurement locations, it will introduce correlated errors in the retrieved total column ozone.

The current assimilation system (Riishojgaard *et al.* 2000, Stajner *et al.* 2001) is implemented using uncorrelated TOMS errors. However, maximum likelihood estimation of the parameters of error covariance models using TOMS O-F residuals indicates that there is no uncorrelated part in TOMS errors. We will compare the current assimilation system with a system in which TOMS error correlations are modeled by

$$\rho(r) = \exp(-r/L_o),$$

where r is the chordal distance between observation locations in kilometers and $L_o = 150$ km.

With the correlated TOMS error model the global mean and root-mean-square of TOMS and SBUV O-F residuals are larger, indicating increased disagreement between the short term model forecasts and the incoming observations. This was expected, because the correlated model for TOMS errors implies that a smaller weight is given to TOMS observations in calculation of assimilated ozone fields, which are subsequently advected to provide the short term forecast. Although the O-F residuals are larger, we show below that the χ^2 related statistics indicate a better agreement of the error covariance models with the realizations of O-F residuals. The agreement of assimilated ozone with high quality independent data also improved.

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The χ^2 related statistics were used to evaluate how consistent the error covariance models are with the realizations of the O-F residuals. Each of these comparisons was in favor of the assimilation systems using correlated model for TOMS errors. For example, the normalized mean of χ^2 statistics should be 1 if all the assumptions used are indeed true. This normalized mean in the experiment with uncorrelated TOMS errors for all the O-F data in 10 months was 1.45. The use of correlated TOMS error model reduced this normalized mean to 1.19. Given this positive impact on the χ^2 related statistics, we next examined the impact of the change in the TOMS error model to the assimilated ozone fields.

The assimilated ozone fields were compared with independent ozone observations from ozone sondes and the Halogen Occultation Experiment (HALOE). Regionally the largest impact of the changes was found at high latitudes. Globally, the impact on assimilated fields was the strongest at the pressure level of 150 hPa. In both cases, the correlated TOMS error model resulted in generally closer agreement with independent sonde and HALOE ozone data.

3. SBUV DATA SELECTION

The usual configuration of the DAO's ozone assimilation system (Štajner *et al.* 2001) includes assimilation of SBUV partial ozone columns in 10 Umkehr layers 3-12 that cover ozone profile at pressures smaller than 126 hPa. We investigated the impact of withholding ozone observations from the lower-most of these SBUV layers, which is layer 3 between 63 and 126 hPa. Despite their large uncertainty, the assimilation of these data usually improves the comparison of the lower stratospheric assimilated ozone with HALOE observations. For example, the mean difference between assimilated and HALOE ozone decreases from about 0.35 to about 0.15 ppmv at 100 hPa in southern midlatitudes in July 1998 when SBUV layer 3 data are used. The comparison is degraded in the northern midlatitudes, where the mean difference between assimilated and HALOE ozone increases from about 0.25 to about 0.35 ppmv at 100 hPa. As expected, the largest impact on the assimilated fields is seen locally, around 100 hPa.

The result is consistent with a finding by Balok and Fishman (2001) of regional differences in SBUV layer 3 ozone biases relative to ozone sondes. Our comparison provides a global perspective, valid also away from sparse ozone sonde locations. We found that despite of the uncertainty in the layer 3 ozone, the use of SBUV data typically improves assimilated ozone, likely due to a good SBUV spatial coverage.

4. CONCLUSIONS AND FUTURE WORK

We have shown that the lower stratospheric assimilated ozone from the DAO's ozone data assimilation system is sensitive to the covariance modeling assumptions and data selection. Changes can improve the comparisons with high quality independent ozone data. Further research in error covariance modeling and data selection may yield significant improvements in the quality of the lower stratospheric assimilated ozone.

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