Improving Air Quality Forecasting Using GEO-CAPE Observations: OSSE Framework and Initial Tests

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Motivation

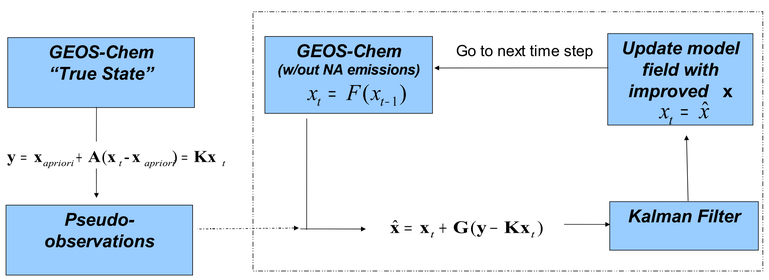
One major aim of current NASA mission planning is to improve air quality measurements over North America and from that to understand factors controlling and resulting from increasing anthropogenic sources of pollution. This improved understanding can then better inform policy on pollution control. This is a preliminary OSSE (Observing System Simulation Experiment) to explore the capability of current satellites such as TES (Tropospheric Emission Spectrometer) and future satellites such as GEO-CAPE (Geostationary Coastal And Pollution Events) to improve ozone air quality forecasts. In the OSSE framework we generate synthetic data to apply to a forecast model. We use an atmospheric chemical transport model (GEOS-Chem CTM) as both the forecast model and the source for pseudo-observations.

We use GEOS-Chem v8-01-01 (http://www-as.harvard.edu/chemisry/trop/geos) in a nested simulation of tropospheric ozone-NO_x-VOC-aerosol chemistry during summer 2001. The model has a horizontal resolution of 1° latitude x 1° longitude, 30 vertical levels, and a temporal resolution of 1 hour. Simulations were preceded by a 5-month global spin up at 4° x 5° resolution and a 1-month spin up at 1° x 1° for North America. See [5] for further model description. Data runs preformed for July and the displayed data are 12 hour daytime averages for 31 July, the final day of the assimilation period.

Three runs are compared in this test: the regular GEOS-Chem model to produce the pseudo-observations, the GEOS-Chem model without North American anthropogenic emissions as the *a priori*, and the GEOS-Chem model without these emissions but with TES-like observations assimilated once per day throughout the troposphere. The perturbation to emissions was begun 1 month prior to the assimilation period. To perform the data assimilation we apply a sub-optimal Kalman filter which corrects on average 45% of the difference between the a priori and the observations at 3 km and 26% of that difference in the boundary layer (below 1km).

To further examine the power of satellite observations to improve modelled surface ozone we used the GEOS-Chem ozone adjoint model to compute the relative sensitivity of surface concentrations to ozone produced at different vertical levels. Ozone produced below 2 km accounts for the bulk of ozone that is transported to the surface.

Kalman Filter process schematic (iterative):



Correction to Ozone Concentrations

Figure 1: 12-hour mean ozone mixing ratio at 700 hPa (3km)

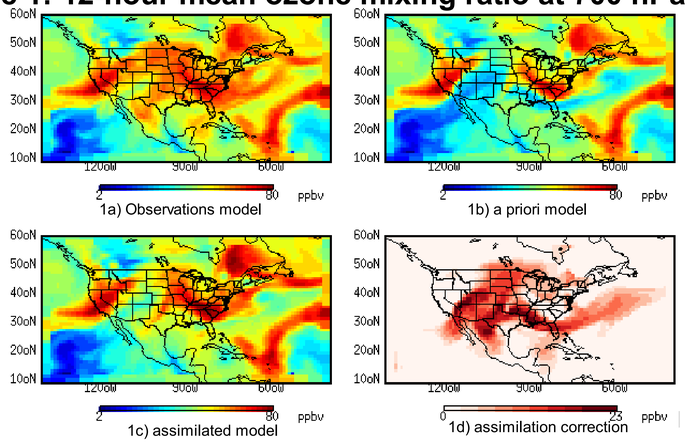


Figure 1 shows 12 hour daytime mean modelled ozone distribution on 31 July over North America at 3 km (1a, top-left), the model a priori (1b, top-right), the assimilated model (1c, bottom-left), and the correction to ozone by the assimilation (1d, bottom-left)

Since TES has good sensitivity to the free troposphere it is unsurprising to see a correction on the order of ~10-20 ppbv. This is of the same order as the correction seen in [3] using TES observations. On average 45% of the difference between the a priori and the observations is corrected by the filter. Note that the differences between the a priori and the assimilation models have a similar spatial structure to the a priori deviations from the observational data, showing the proper application of the filter.

Figure 2: Change to 12 hour mean ozone below 1 km

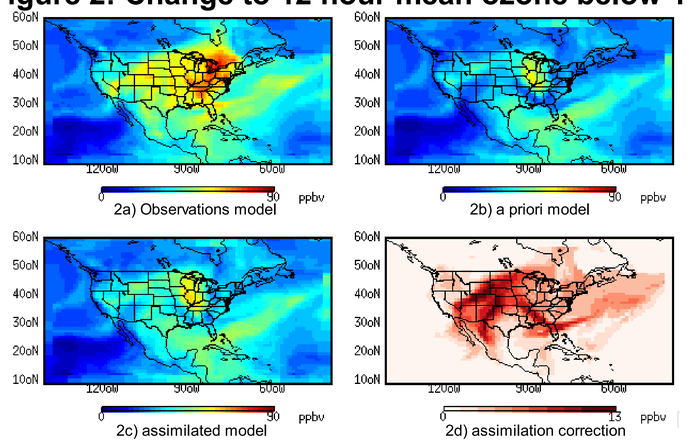


Figure 2 shows 12 hour daytime mean modelled ozone distribution on 31 July in the boundary layer (2a, top-left), the model a priori (2b, top-right), the assimilated model (2c, bottom-left), and the correction by the assimilation (2d, bottom-left)

We see that assimilation corrects surface ozone levels by up to 13 ppbv and this correction removes 26% of the difference between the "true state" and the a priori. Since TES has lower sensitivity to the boundary layer it is not surprising the correction here is less than at 3 km. Further tests need to be performed to examine if this boundary layer correction is robust to forms of model error other than emissions.

Vertical Sensitivity of Surface Ozone

To evaluate the necessary vertical sensitivity of ozone retrievals to improve surface ozone forecasts it is necessary to know the sensitivity of surface ozone to ozone production at different vertical levels. We use the ozone adjoint simulation for GEOS-Chem v6-02-05 with stored ozone production and loss rates from a ozone-NO_x-VOC-aerosol chemistry simulation. The resolution is 2.5° x 2.5° with 30 vertical levels and 15 minute transport time steps. The adjoint was run for a two-week period and accumulated sensitivity over the entire run was integrated over all latitude and longitude to give relative vertical sensitivity. Results over two urban centers (LA, left and Boston, right) are displayed below. We see that most of the sensitivity is below 2 km for both locations, and thus improved satellite sensitivity to ozone below 2 km will be desirable for future air quality forecasting.

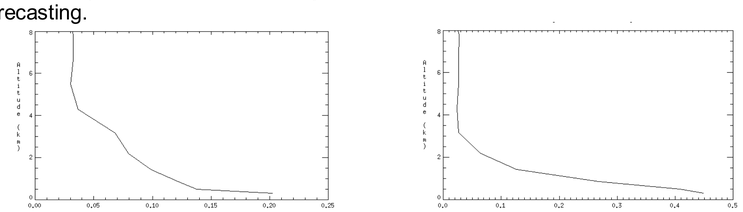


Figure 3: Accumulated relative sensitivity of surface ozone to ozone produced at different heights for two sites (arbitrary units)

Implications and Future Work

- A working Kalman Filter has been implemented in GEOS-Chem to perform data assimilation from satellite observations
- Initial testing shows a significant correction to model fields at 3 km, resulting in a perturbation to the ozone mixing ratio in the boundary layer
- This data is an initial test and more work needs to be done to determine how much influence TES-like observations can have on forecasting
- Since we are primarily concerned with surface concentrations, what additional information is required to improve corrections?
- Adjoint analysis shows ozone at surface primarily sensitive to ozone produced below 2km, implying need for improved vertical sensitivity
- Can acquire additional information by including effect from GEO-CAPE observation of ozone precursors (NO_x, HCHO)
- Model to be improved by consideration of spatial correlation and time evolution of model error covariance
- Measure sensitivity of results to different averaging kernels (e.g. from OMI or combined UV-TIR-VIS)
- Generate pseudo-observations using ozone fields from MOZART and CMAQ to test robustness to complexity of model error

Kalman Filter Algorithm

The Kalman filter allows the assimilation of satellite data (y) into our CTM to correct a modelled concentration for a given chemical species (x). For this study the assimilated data was pseudo-observations generated by running the base model and applying a generic TES averaging kernel [2]:

$$\mathbf{y} = \mathbf{x}_{apriori} + \mathbf{A}(\mathbf{x}_t - \mathbf{x}_{apriori}) = \mathbf{K}\mathbf{x}_t$$

We then can update the model concentration for ozone by application of the Kalman filter:

$$\hat{\mathbf{x}} = \mathbf{x}_t + \mathbf{G}(\mathbf{y} - \mathbf{K}\mathbf{x}_t)$$

$$\mathbf{G} = \mathbf{S}_a\mathbf{K}^T(\mathbf{K}\mathbf{S}_a\mathbf{K}^T + \mathbf{S}_e)^{-1}$$

This assimilation is performed once per day at 1700 GMT for each tropospheric ozone column over North America except when the scene is cloudy. The Kalman gain matrix depends on $\mathbf{S}_a$ and $\mathbf{S}_e$, the model and observational error covariance matrices respectively, both of which are assumed to be diagonal (i.e. spatial correlation of error is neglected) and has a fixed variance, as in [3]. The percent errors considered to calculate $\mathbf{S}_a$ and $\mathbf{S}_e$ are 40% in the model [3] and 10% in the pseudo-observations [2]. Note that since the satellite retrieval only appears in the innovation term, significant effects from the a priori are removed.

References

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[5] Wang et al. (2008) *Atmos. Environ.* submitted.
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Acknowledgements

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