

First Comparison of TES Tropospheric Ozone and CO Retrievals with Results from a Global 3-D CTM

Qinbin Li¹, John Worden¹, Kevin W. Bowman¹, Susan S. Kulawik¹, Greg Osterman¹, Mingzhao Luo¹, Annmarie Eldering¹, Helen Worden¹, Reinhard Beer¹, Solene Turquety², Robert M. Yantosca², Paul I. Palmer², Shiliang Wu², Daniel J. Jacob², Dylan Jones³

¹Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109

²Harvard University, Division of Engineering and Applied Sciences, Cambridge, MA 02138

³University of Toronto, Department of Physics, Toronto, Canada, M5S 1A7



Introduction

The Tropospheric Emission Spectrometer (TES) is a high-resolution infrared imaging Fourier-transform spectrometer on a polar Sun-synchronous orbit aboard the Aura satellite [Beer *et al.*, 2001]. TES measures the spectral infrared radiances between 650 cm⁻¹ and 3050 cm⁻¹ in both nadir and limb modes. The observed IR radiance is imaged onto an array of 16 detectors, which have a combined horizontal footprint of 5.3 km × 8.4 km in the nadir viewing mode. The standard TES operating mode Global Survey consists of 16 orbits of nadir & limb observations repeated every other day. In its global survey mode, TES nadir observations are about 5° apart along the orbit track. Here TES retrieved tropospheric ozone and CO are compared with results from the GEOS-CHEM model for 20-22 September 2004. The TES retrievals are from the 16-orbit global survey data on 20-21 September and for two Step & Stare transects on 21 and 22 September. The Step & Stare TES special mode is such that TES repeats a cycle of pointing at nadir for 4 seconds during which the spacecraft has moved ~40 km. Comparisons were performed after applying the TES averaging kernels to GEOS-CHEM output to simulate the smoothing effect of the retrieval algorithm. Near-real-time (NRT) simulations are conducted with the GEOS-CHEM CTM v7.01.02 (<http://www-as.harvard.edu/chemistry/trop/geos>) [Bey *et al.*, 2001]. The model is driven by GEOS-4 assimilated meteorological observations from the NASA Global Modeling and Assimilation Office (GMAO). The GEOS-4 data have a temporal resolution of 6 hours (3 hours for mixing depths and surface quantities), a horizontal resolution of 1°×1.25°, and 55 layers in the vertical. We average them here over 2° latitude by 2.5° longitude grid and lumped the vertical grid into 30 layers for input to GEOS-CHEM. The NRT simulations use GMAO near real time "First-look" (FLK) data. These on-going NRT simulations are helpful for planning TES special observations such as Transects and Step & Stare for intensive targeted observations.

The TES Averaging Kernels

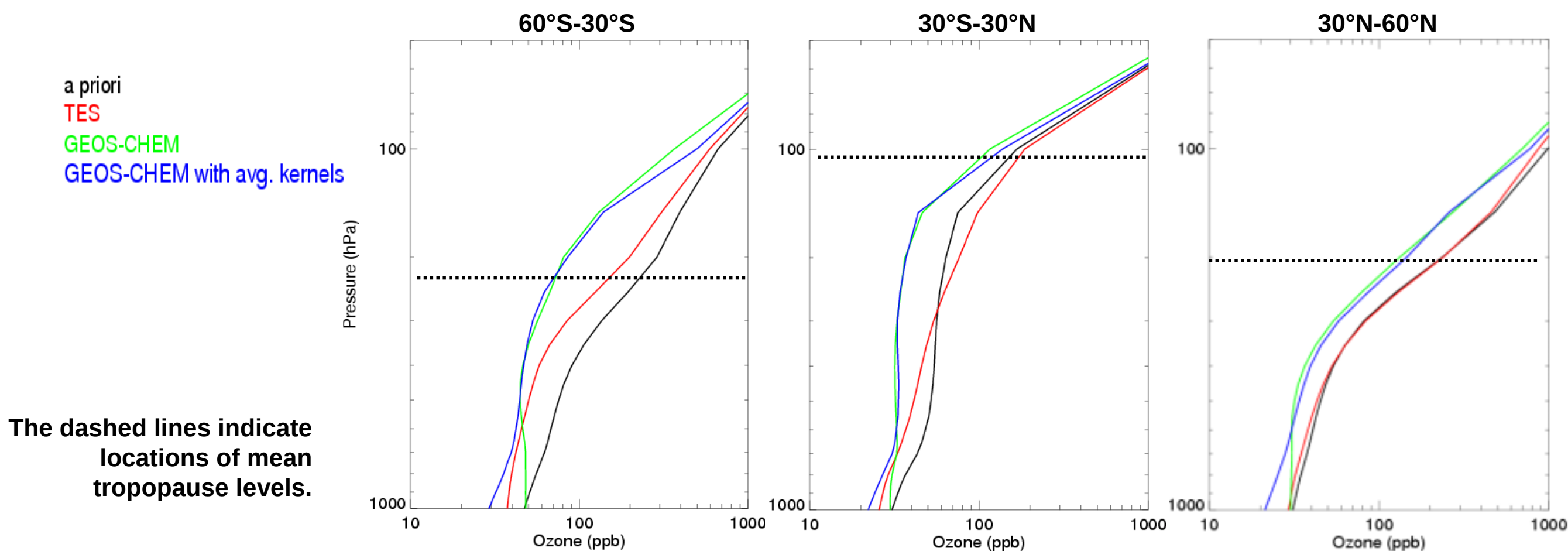
Explicit consideration of the TES averaging kernels is required to properly compare TES data with model results. First, GEOS-CHEM simulated vertical profiles of ozone and CO are resampled to TES retrieval pressure grid using linear interpolation in log space. Then the following transformation is applied to the resampled model profile:

$$\mathbf{x}' = \mathbf{x}_a + \mathbf{A} (\mathbf{x} - \mathbf{x}_a)$$

where $\mathbf{x}_a$ is the log of the *a priori*, $\mathbf{x}$ is the log of the resampled model profile, and $\mathbf{A}$ is the TES averaging kernel matrix. The quantity $\mathbf{x}'$ represents the result of applying a linear transformation (in log space) to the model profile in the same way that the TES retrieval process is believed to transform the true profile. The rows of the averaging kernel $\mathbf{A}$ describe the sensitivity of retrieved ozone and CO at a particular pressure level to perturbations to the *a priori* profile at different pressures. The figure to the right shows a sample set of TES averaging kernels for ozone retrieval. There are roughly two independent regions of information in the troposphere in the TES retrieved profile: one in the middle troposphere and one in the upper troposphere. Also shown in the figure are the vertical profiles of ozone concentrations illustrating the sensitivity of the TES retrieval to the vertical distribution of ozone. Since GEOS-CHEM has a parameterized stratospheric chemistry, we replaced the simulated stratospheric ozone vertical profile with the TES *a priori*.

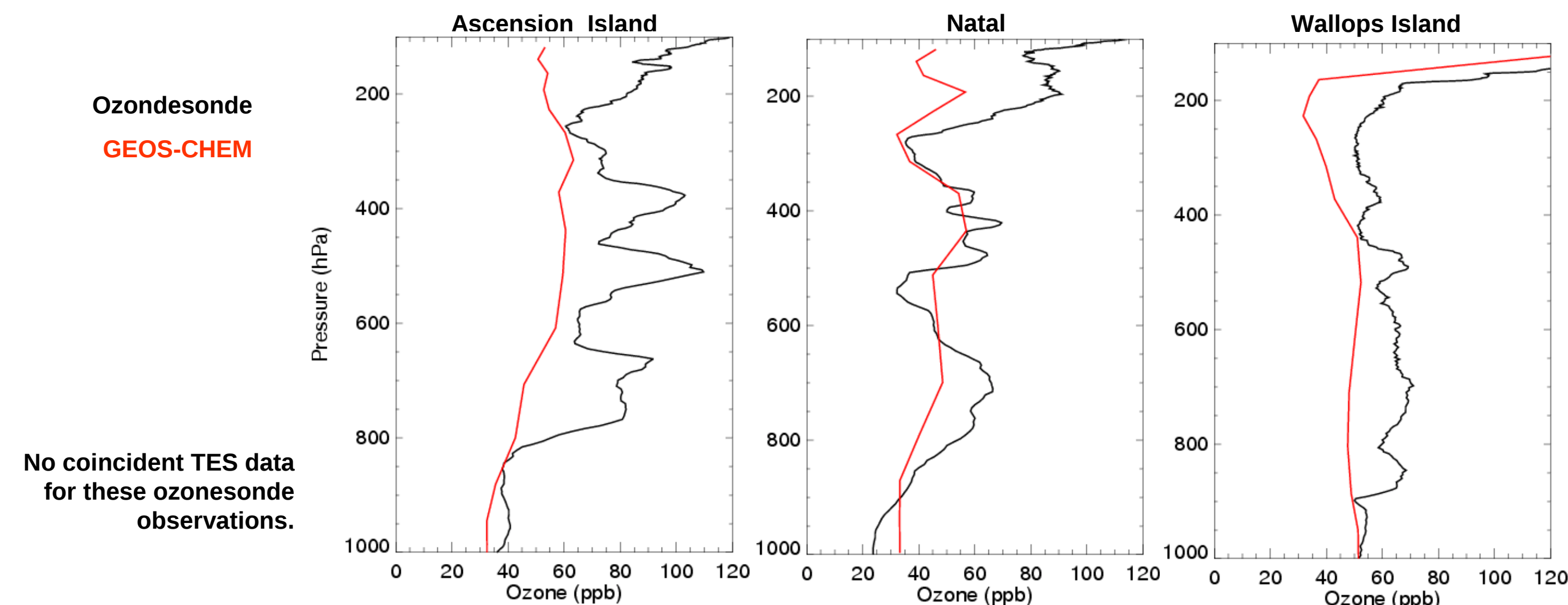
Vertical profiles of ozone

The figure below shows comparison of TES retrieved and GEOS-CHEM simulated vertical profiles of ozone averaged in three latitude bins (60°S-30°S, 30°S-30°N, 30°N-60°N) for the TES global survey on 20-21 September 2004. The dashed lines indicate the mean tropopause levels. Applying the TES averaging kernel on GEOS-CHEM output has smaller effect in the upper troposphere than in the lower troposphere, reflecting the different sensitivity TES has in these two altitude regions. The largest discrepancy is in the upper troposphere, where model ozone levels are lower than TES retrieved values by as much as 20 ppb or even larger. Validation with ozonesonde data shows that TES retrievals may overestimate upper tropospheric ozone due to 'contamination' by stratospheric influence through the averaging kernel.



The dashed lines indicate locations of mean tropopause levels.

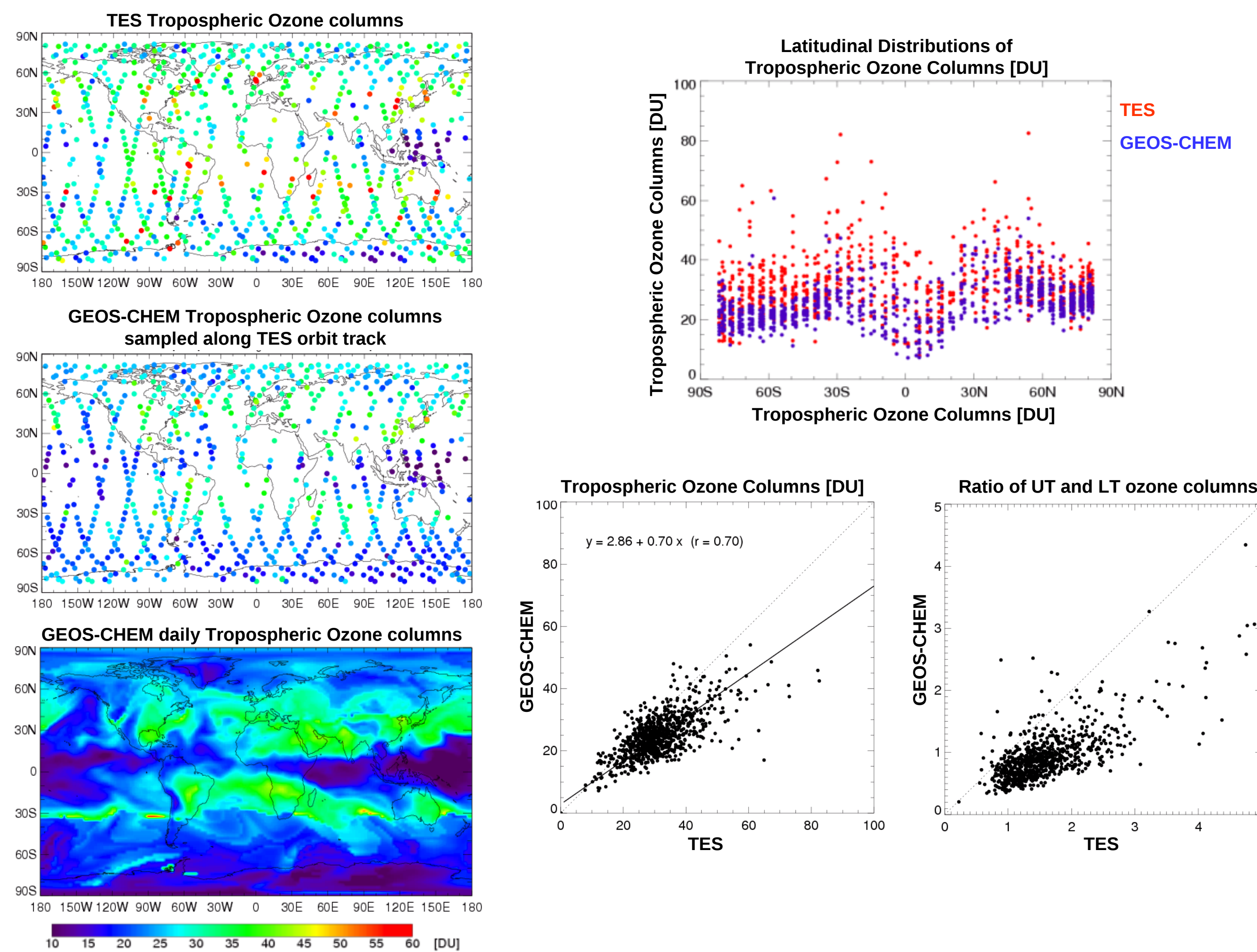
As part of TES validation, ozonesondes were launched at the Ascension Island (7.9°S, 14.4°W), Natal, Brazil (5.3°S, 35.2°W), and Wallops Island (37.9°N, 75.5°W). For the three sites on 20-21 September however there were no coincident TES retrievals. We nevertheless use the ozonesonde data to gauge the model performance. The figure below shows comparison of GEOS-CHEM simulated vertical profiles with ozonesonde data from the three sites on 20 (Natal) and 21 (Ascension and Wallops) September 2004. The vertical distributions of ozone at all three sites are broadly consistent between the model and the ozonesonde data. The model does not reproduce the enhanced ozone layers at Ascension Island. It appears that the model tends to underestimate ozone concentrations in the uppermost troposphere close to the tropopause region. This may be due to the difficulty of identifying the tropopause level in the model. The lack of vertical structure in the simulated profiles is not simply due to the coarse vertical model resolution as the model captures the ozone vertical structure at Natal very well.



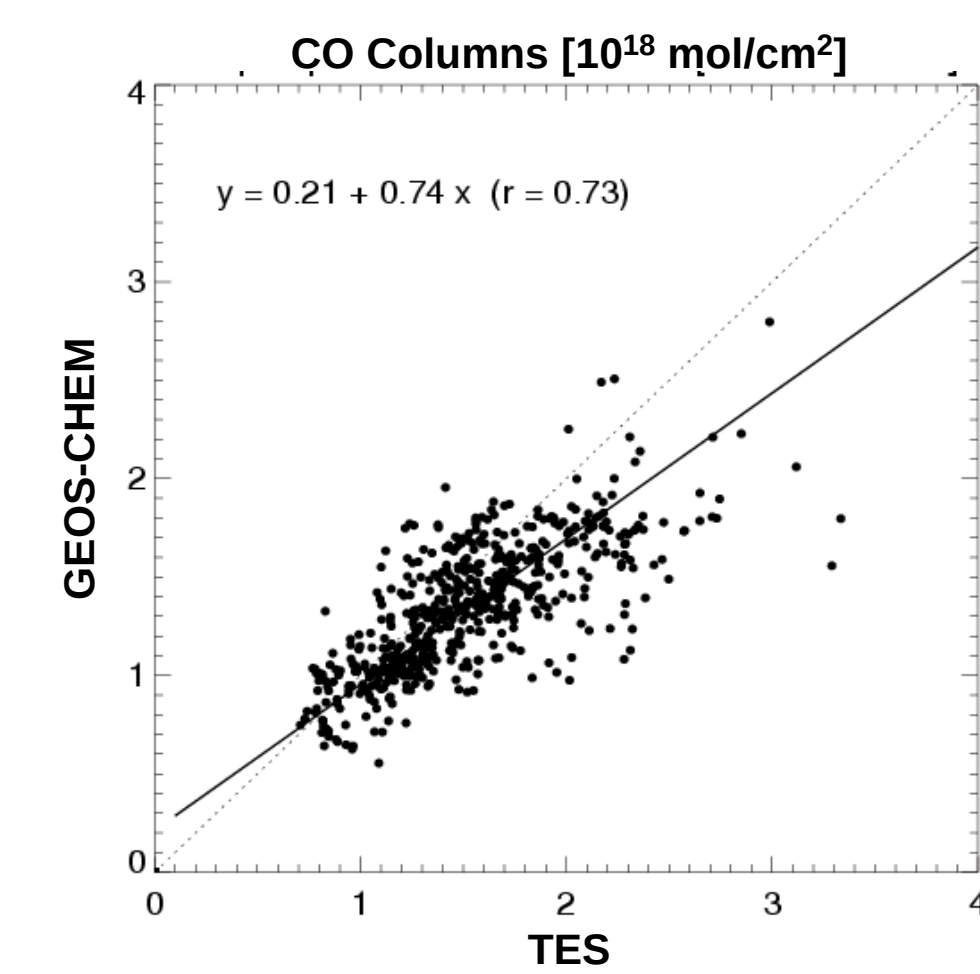
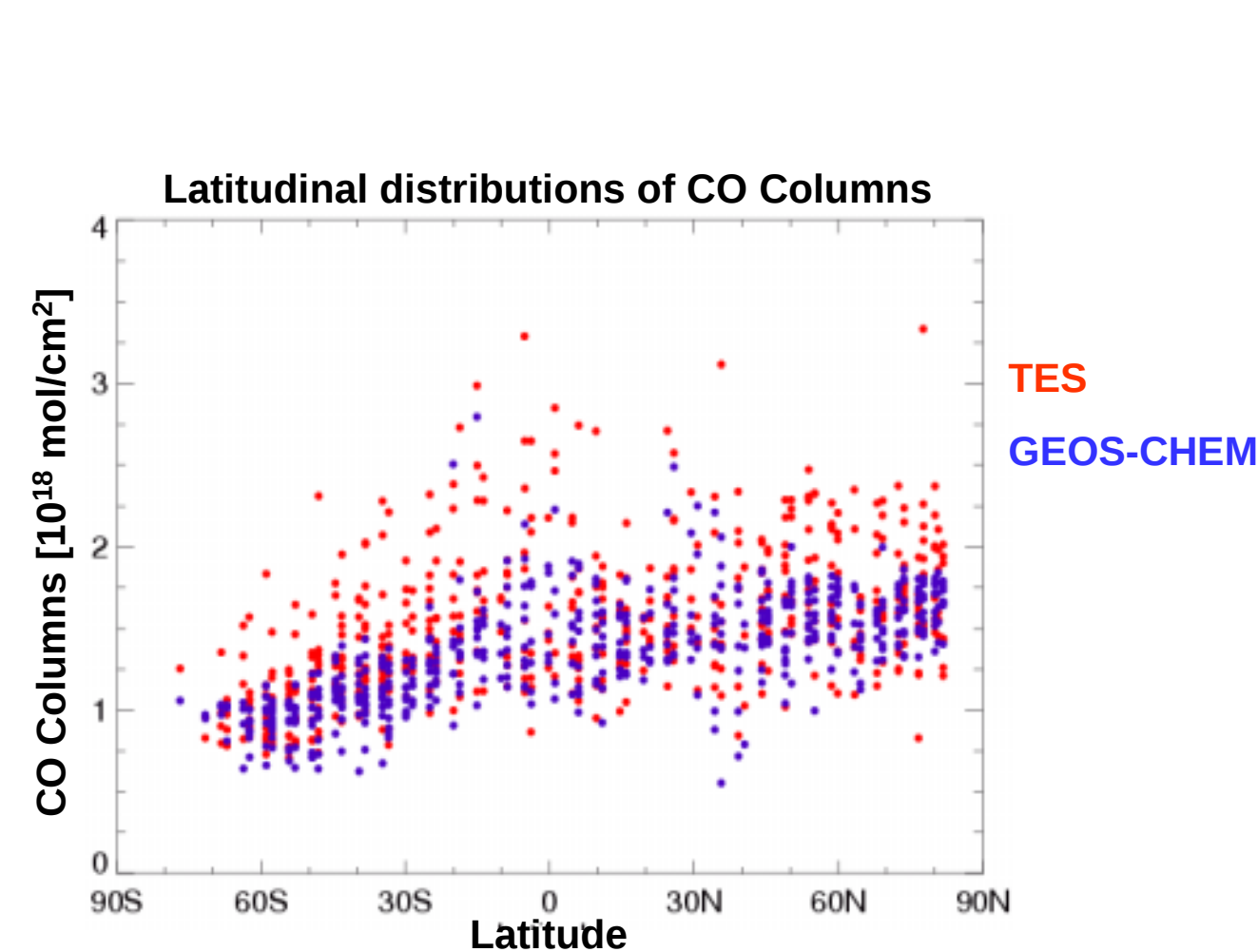
No coincident TES data for these ozonesonde observations.

First TES global maps of tropospheric ozone and CO: Large-scale features

The figure below shows tropospheric ozone columns for 20 September 2004. As the one-day data are fairly sparse, GEOS-CHEM daily results for 20 September 2004 are also shown in addition to TES retrievals and model results sampled along TES orbit track. The large-scale features are similar. In the northern hemisphere, high values are seen over the northern middle latitude polluted continental regions in east North America, Europe, and east Asia. High values are also seen from the Indian subcontinent to the Middle East, reflecting transport by the tropical upper troposphere easterly of ozone produced over south Asia [Li *et al.*, 2001]. Minimum values are seen over the warm pool region near Indonesia, both in the observation and in the model. In the southern hemisphere, high values are seen over the south Atlantic south of the equator to about 30°S, and over the biomass burning regions over the Amazon and southern Africa. High values over the Indian oceans are biomass burning outflows from southern Africa. The latitudinal distributions of the tropospheric ozone columns are very similar, with high values in the middle latitudes in both hemisphere and low values in the tropics. GEOS-CHEM simulated tropospheric ozone columns are generally lower than TES retrievals (see the first scatter plot). The lower model values reflect in part the lower levels of ozone concentrations in the upper troposphere in the model. This discrepancy is also illustrated by examining the ratio of upper troposphere (UT) ozone column (500 hPa to tropopause) to lower troposphere (LT) ozone column (surface to 500 hPa). The ratios are consistently smaller in the model than in the TES retrievals. The correlation between model and TES UT/LT ozone column ratios however indicates that the TES retrieved ozone has about two independent pieces of information.

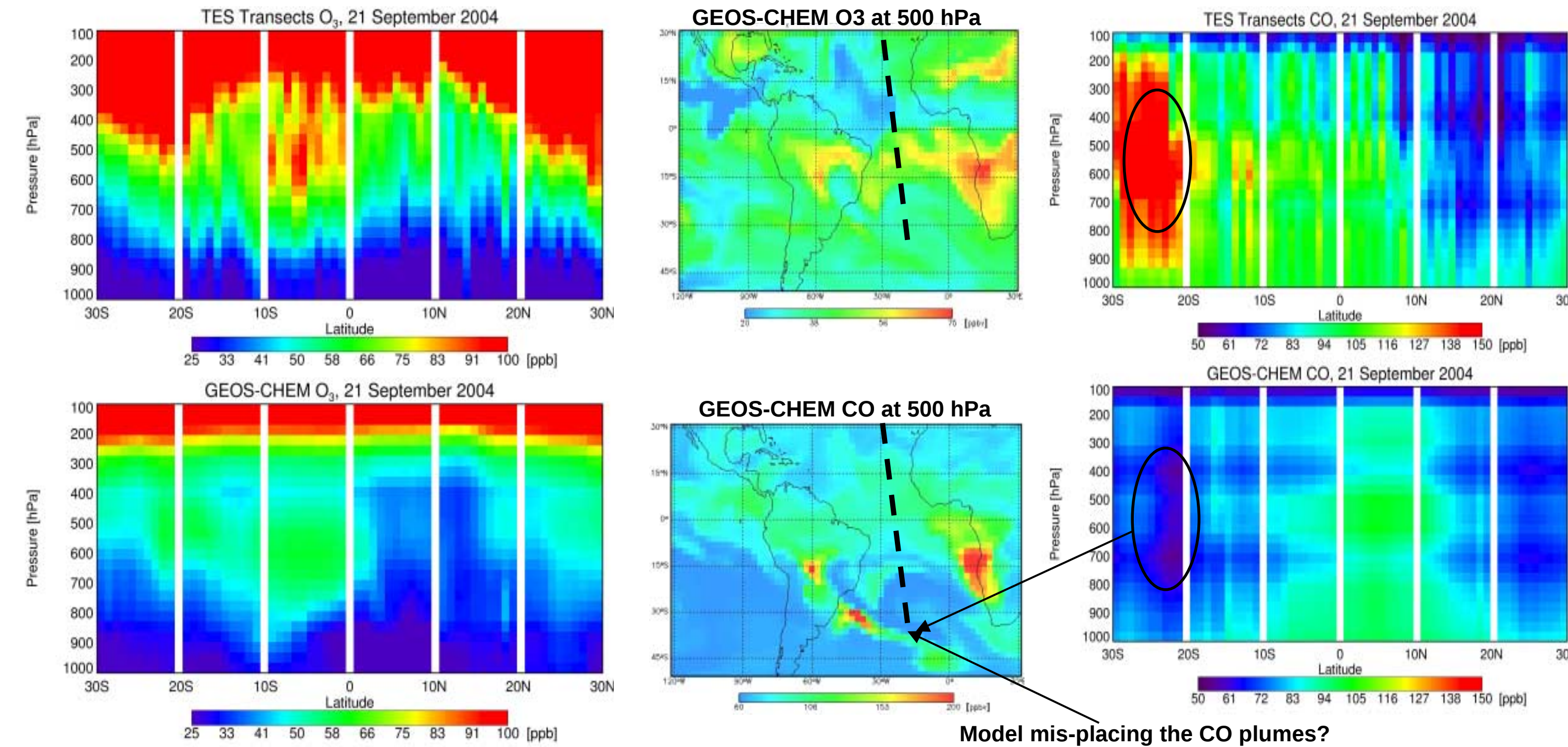


The figure below shows CO columns from the same global survey on 20-21 September 2004. In the southern hemisphere, the high values are outflows from the biomass burning in south America and southern Africa. The latitudinal gradients of the CO columns are consistent. Model CO column values show better agreement with TES retrieved values than ozone (see the scatter plot).

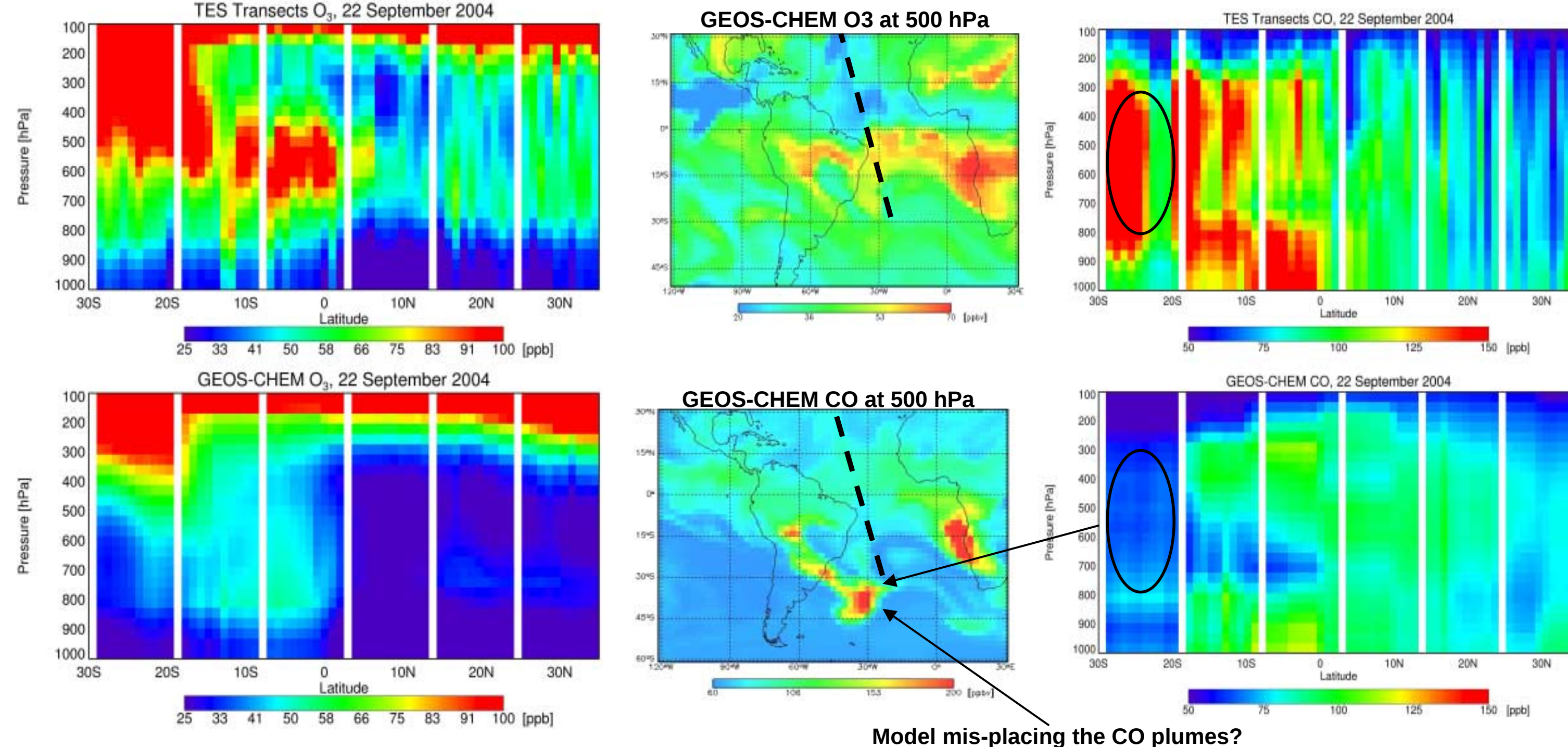


Ozone maximum over the South Atlantic

The TES special operating mode – Step & Stare is designed for targeted intensive measurements. On 21 and 22 September 2004, TES made two Step & Stare special transects over the south Atlantic, one passing the Ascension Island, the other over Natal. These transects were intended to probe the ozone maximum over the south Atlantic associated with the biomass burning season in southern Africa and the Amazon. Both transects indicate enhanced ozone in the middle and upper troposphere south of the equator to 30°S. Model results show strong outflows from biomass burning regions in both south Africa and the Amazon. GEOS-CHEM ozone results are broadly consistent with the observed features with large discrepancy in the peak values in the middle and upper troposphere. The CO results show very large difference in terms of the peak values and the locations of these maxima. The enhanced CO values south of 20°S in both transects are completely missing in the model, which may be due to a displacement in the model of the biomass burning plumes from south America. This displacement may be corrected in model simulations with GMAO "Late-Look" (LLK) data, which have a two-week lag and are the best possible analysis. The lack of clear correlations between ozone and CO in the middle and upper troposphere indicate that in addition to convective outflow from biomass burning regions in southern Africa and the Amazon, other sources of ozone such as lightning and stratospheric intrusion also have large contributions to the ozone maximum. Back-trajectory analyses (not shown here) for the peak ozone regions in the middle troposphere show consistent subsidence.



The dashed lines indicate the location of the TES step & stare transects.



Conclusions

Comparisons of TES tropospheric ozone and CO retrievals with results from the GEOS-CHEM CTM show qualitative agreement in some regions and disagreement in others. In particular, large-scale distributions of ozone and CO are consistent between TES retrievals and model results. The latitudinal gradients in tropospheric ozone and CO columns are consistent. GEOS-CHEM simulated ozone concentrations in the upper troposphere are systematic lower than the TES retrieved values, leading to lower model values of tropospheric columns. The displacement of the CO plumes during the two south Atlantic transects may result from model simulation using "First-Look" meteorological data. We expect model simulations using "Late-Look" meteorological data to reduce the discrepancy. Further detailed analyses of both TES data and model results in conjunction with other satellite and in-situ observations should help explain the discrepancies. Resolving these differences should ultimately improve both the TES products and the GEOS-CHEM model.

Acknowledgements

This work was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with NASA. The GEOS-CHEM model is managed by the Atmospheric Chemistry Modeling Group at Harvard University with support from the NASA Atmospheric Chemistry Modeling and Analysis Program.

References

- Beer, R., T.A. Glavich, and D.M. Rider, Tropospheric emission spectrometer for the Earth Observing System's Aura satellite, *Appl. Opt.*, 40(15), 2356-2367, 2001.
- Bey, I., D.J. Jacob, R.M. Yantosca, J.A. Logan, B.D. Field, A.M. Fiore, Q.B. Li, H. Liu, L.J. Mickley, and M.G. Schultz, Global modeling of tropospheric chemistry with assimilated meteorology: Model description and evaluation, *J. Geophys. Res.*, 106, 23,073-23,095, 2001.
- Li, Q.B., D.J. Jacob, J.A. Logan, I. Bey, R.M. Yantosca, H. Liu, R.V. Martin, A.M. Fiore, B.D. Field, B.N. Duncan, and V. Thouret, A tropospheric ozone maximum over the Middle East, *Geophys. Res. Lett.*, 28, 3235-3238, 2001.
- Rodgers, C.D., *Inverse Methods for Atmospheric Sounding, Theory and Practice*, World Scientific, 2000.