Assimilating tropospheric ozone data from TES

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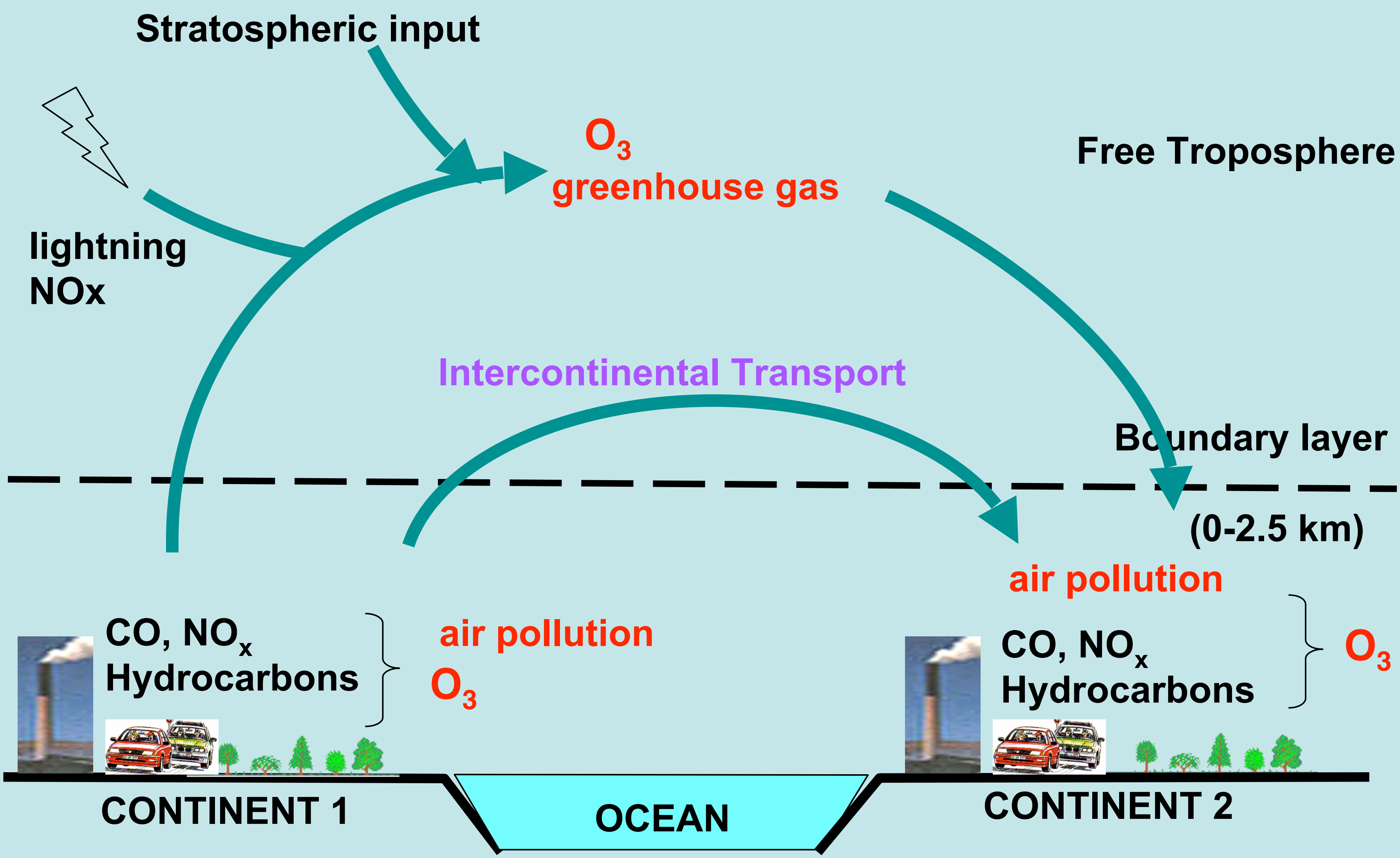
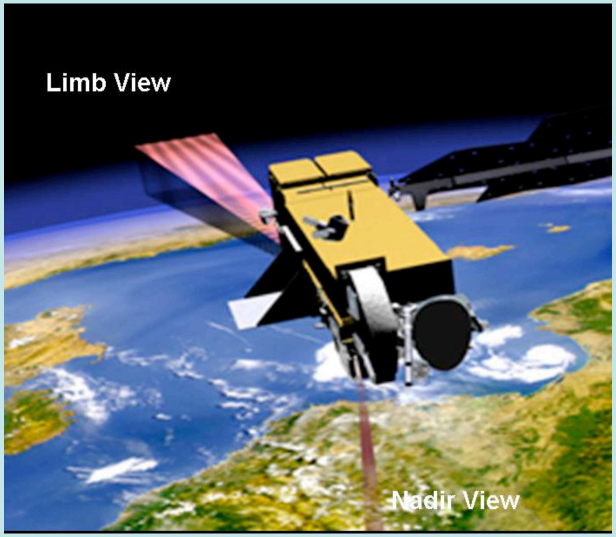
Processes Influencing the Global Distribution of Tropospheric O_3



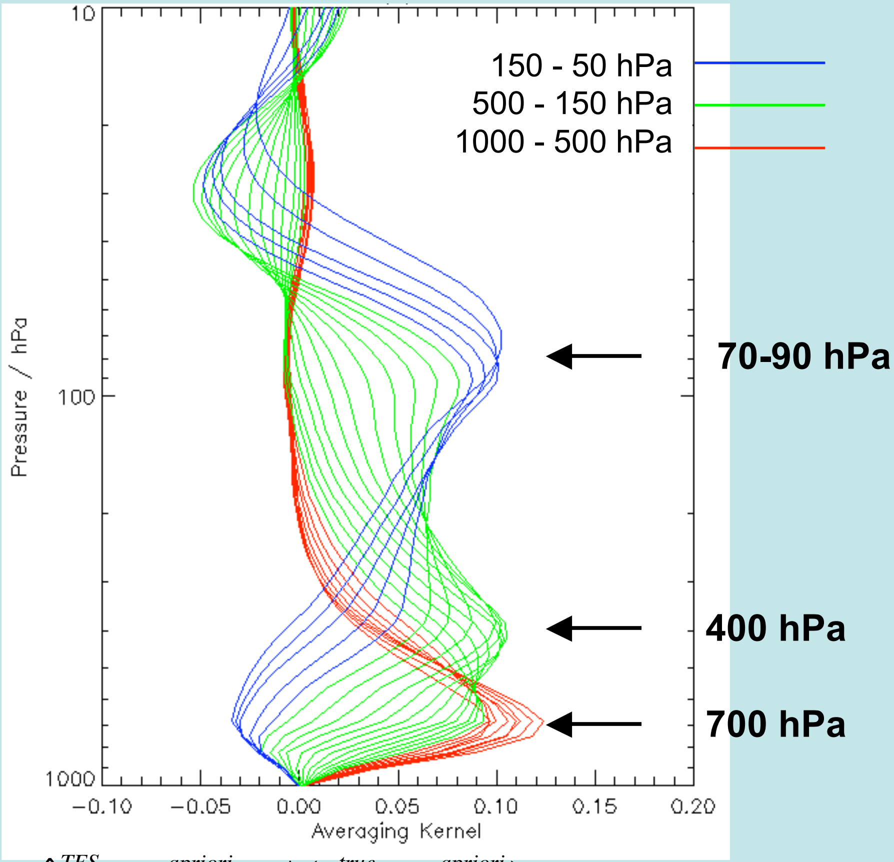
Improved understanding of the processes influencing the global distribution of tropospheric O_3 is needed for better prediction of air quality and for quantifying climate change.

Tropospheric Emission Spectrometer (TES)



- One of four instruments on the NASA Aura spacecraft (launched July 2004)
- Infrared Fourier transform spectrometer (3.3 - 15.4 μm)
- Nadir footprint = 8 km x 5 km
- Orbit repeats every 16 days
- Observations spaced about 2º along orbit track
- Data products include O_3, CO, H_2O, and HDO

Averaging kernels for retrieval at 30°N, 87°W



$$\hat{\mathbf{x}}^{TES} = \mathbf{x}^{apriori} + \mathbf{A}(\mathbf{x}^{true} - \mathbf{x}^{apriori})$$

$$\mathbf{A} = \frac{\partial \hat{\mathbf{x}}^{TES}}{\partial \mathbf{x}^{true}} = \text{averaging kernel}$$

Tropospheric O_3 retrievals have with maximum sensitivity at 700 and 400 hPa

Chemical Data Assimilation Methodology

Sequential sub-optimal Kalman filter

$$\hat{\mathbf{x}}^a = \mathbf{x}^f + \mathbf{K}[\mathbf{y}^{\mathrm{obs}} - \mathbf{H}\mathbf{x}^f]$$

Kalman Gain Matrix: $\mathbf{K} = \mathbf{P}^f\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}$

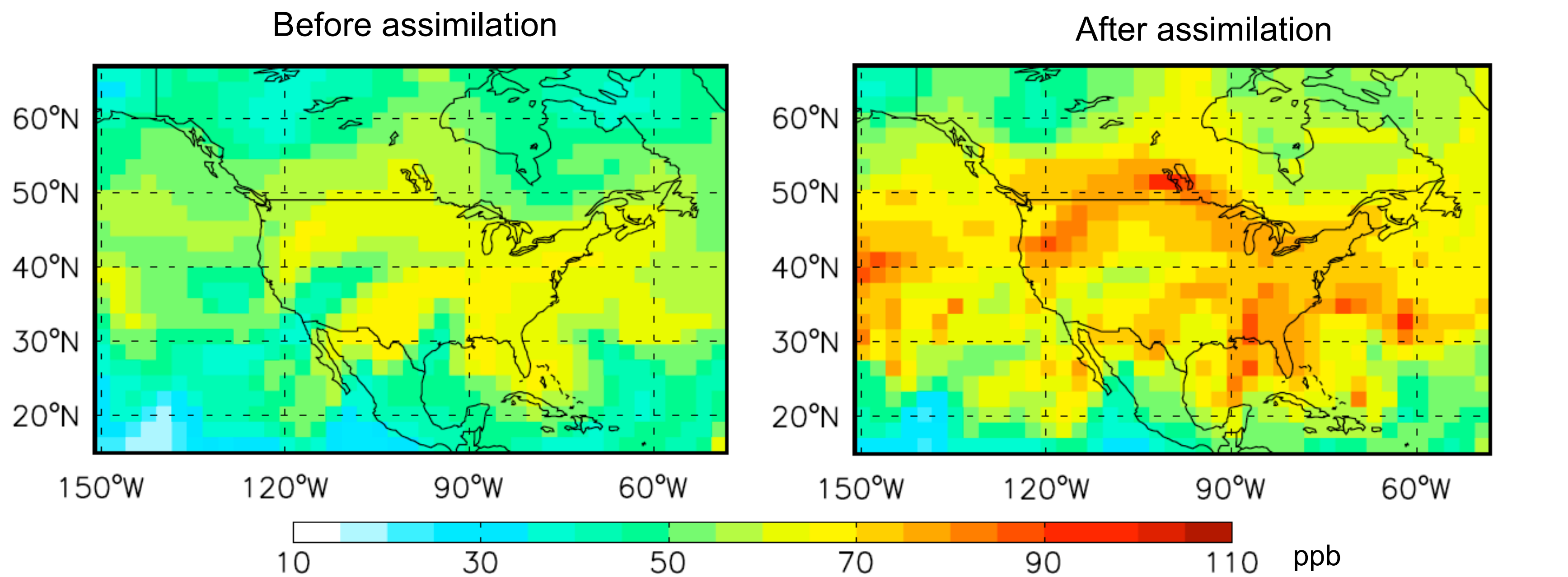
Analysis Error Cov. Matrix: $\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^f$

- Observation operator (H) accounts for TES averaging kernels and a priori profiles
- Analysis error variance transported as a passive tracer

Model

- GEOS-Chem model with full nonlinear tropospheric chemistry
- Linearized (LINOZ) O_3 chemistry in the stratosphere
- Model transport driven by assimilated meteorological fields from NASA GMAO (at a resolution of 2° x 2.5° or 4° x 5°)
- O_3 and CO profile retrievals from TES are assimilated from 1 Jul. - 31 Aug. 2006
- 6-hour analysis cycle
- Assumed forecast error of 50% for CO and O_3
- Neglected horizontal correlations in forecast and observation error covariance matrices

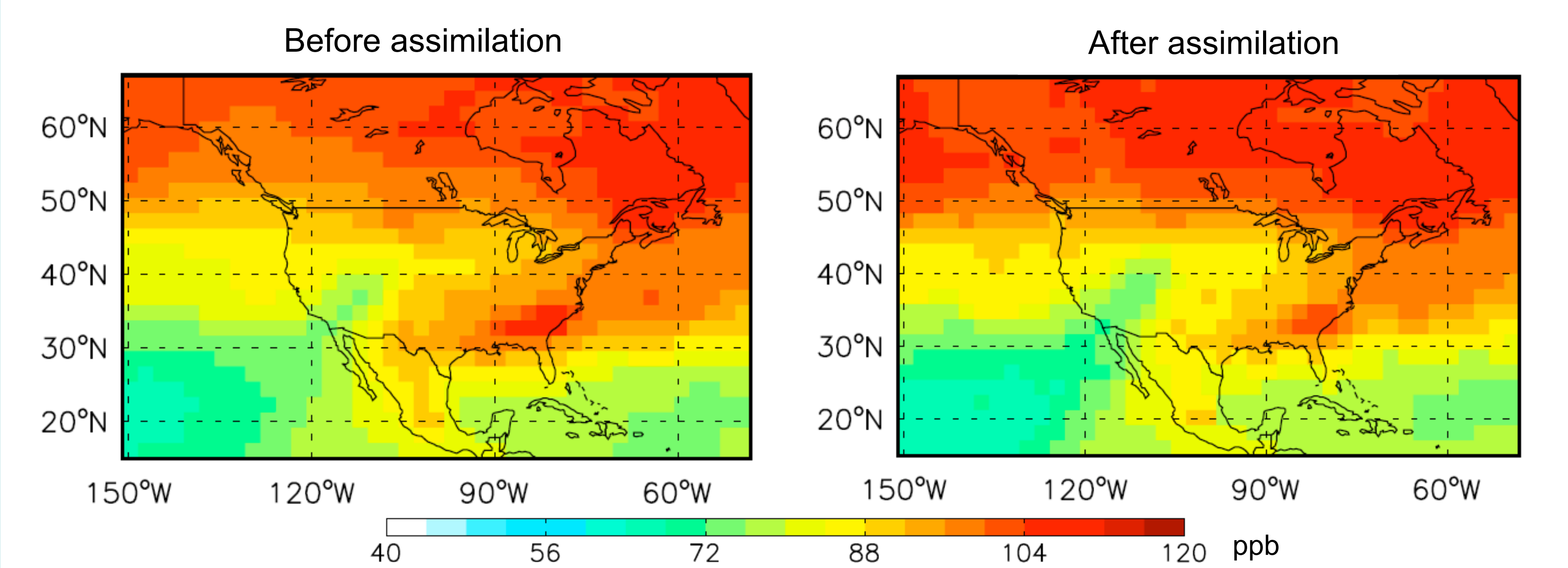
Ozone Analysis Over North America (at 5 km on 15 August 2006)

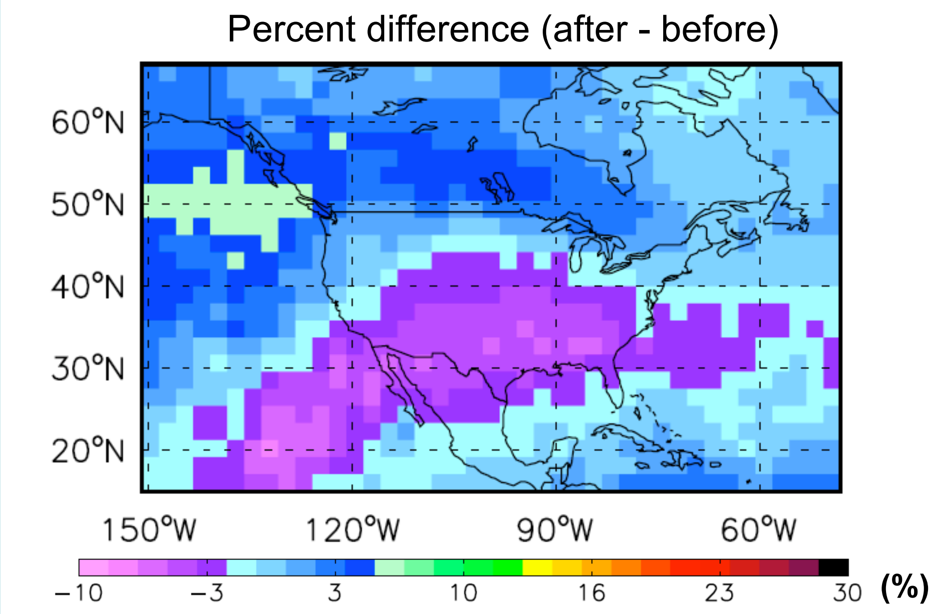


[Parrington et al., JGR, 2008]

- Assimilation of TES data (1 Jul. - 31 Aug.) increased O_3 across North America by 0 - 40%
- Large increases in O_3 in the eastern Pacific, in the vicinity of a stratospheric intrusion, and across Canada, linked the stratosphere-troposphere exchange
- The summertime O_3 maximum over the southeast is more pronounced after assimilation

Impact of Assimilation on Atmospheric CO (5 km on 15 August 2006)





- The assimilation increased CO by about 5% at high latitudes and reduced it by 5-10% over southern North America

- Decrease in assimilated CO over southern North America suggests that the negative bias in O_3 in the model is not due to an underestimate of the hydrocarbon precursors of O_3 in the model

[Parrington et al., JGR, 2008]

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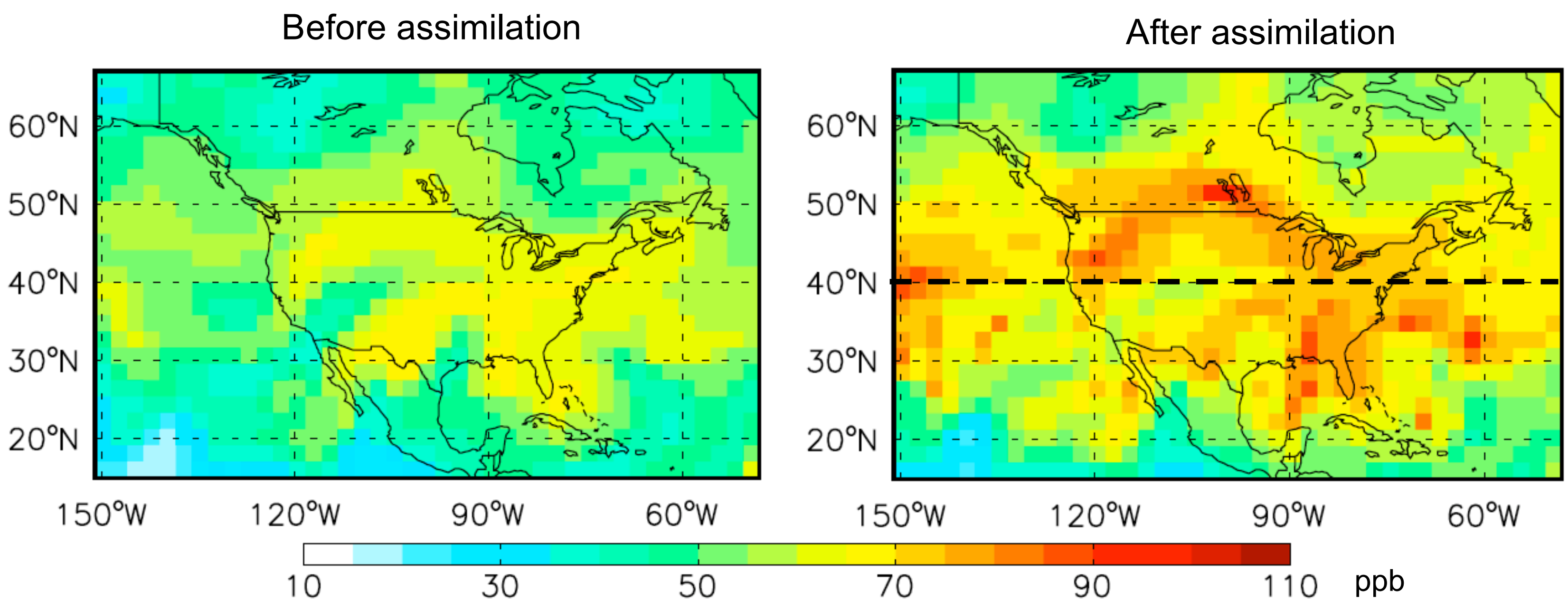

[Parrington et al., JGR, 2008]

- Assimilation increased O_3 across North America by 0 - 40%
- Large increases in O_3 in the eastern Pacific, in the vicinity of a stratospheric intrusion, and across Canada, which may be linked the stratosphere-troposphere exchange
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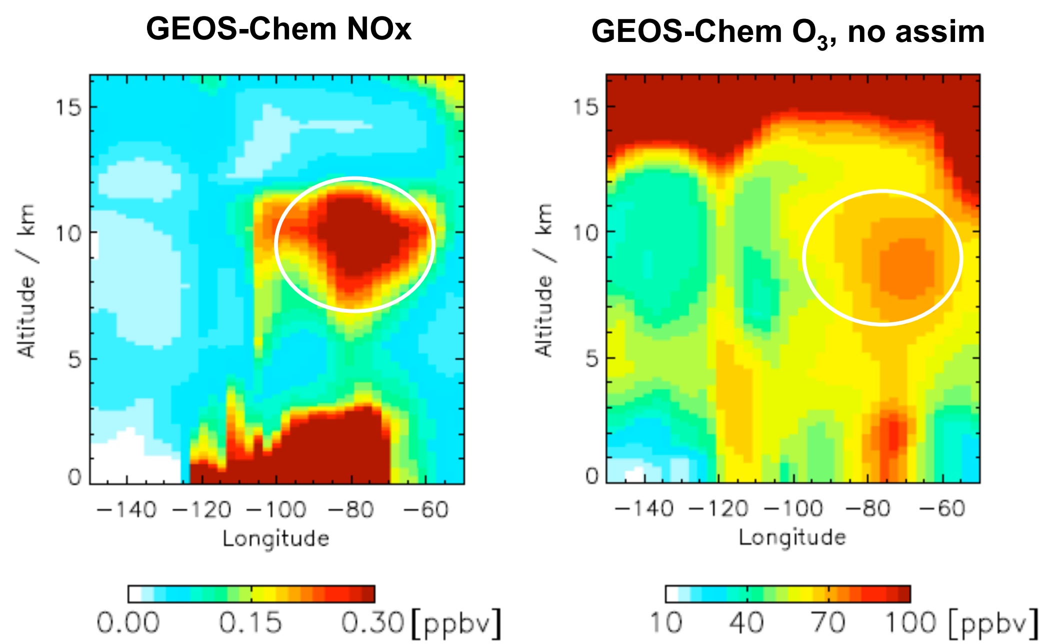
Modelled O_3 Over North America along 40°N



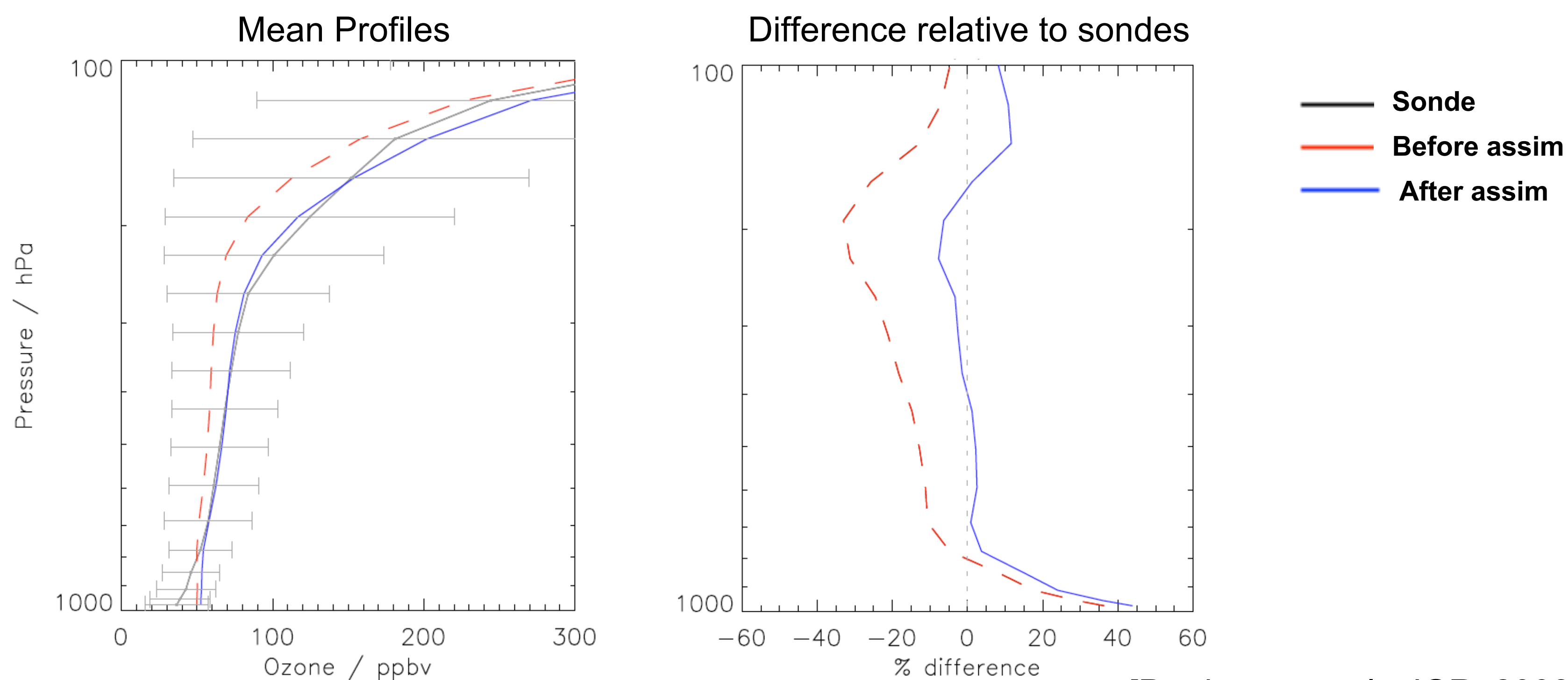
[Parrington et al., JGR, 2008]

- The upper tropospheric ozone maximum is linked to NOx emissions from lightning, which are 0.068 Tg N for North America (in August), a factor of 4 lower than recommended by Hudman et al. [JGR, 2007] based on comparisons of the model with aircraft data.

- Assimilation increased upper tropospheric ozone over the southeast by 11 ppb, in agreement with the estimate of 10 ppb from Hudman et al. [JGR, 2007] for the enhancement in upper troposphere ozone due to lightning NOx.

Comparison with IONS-06 Ozonesondes Over North America

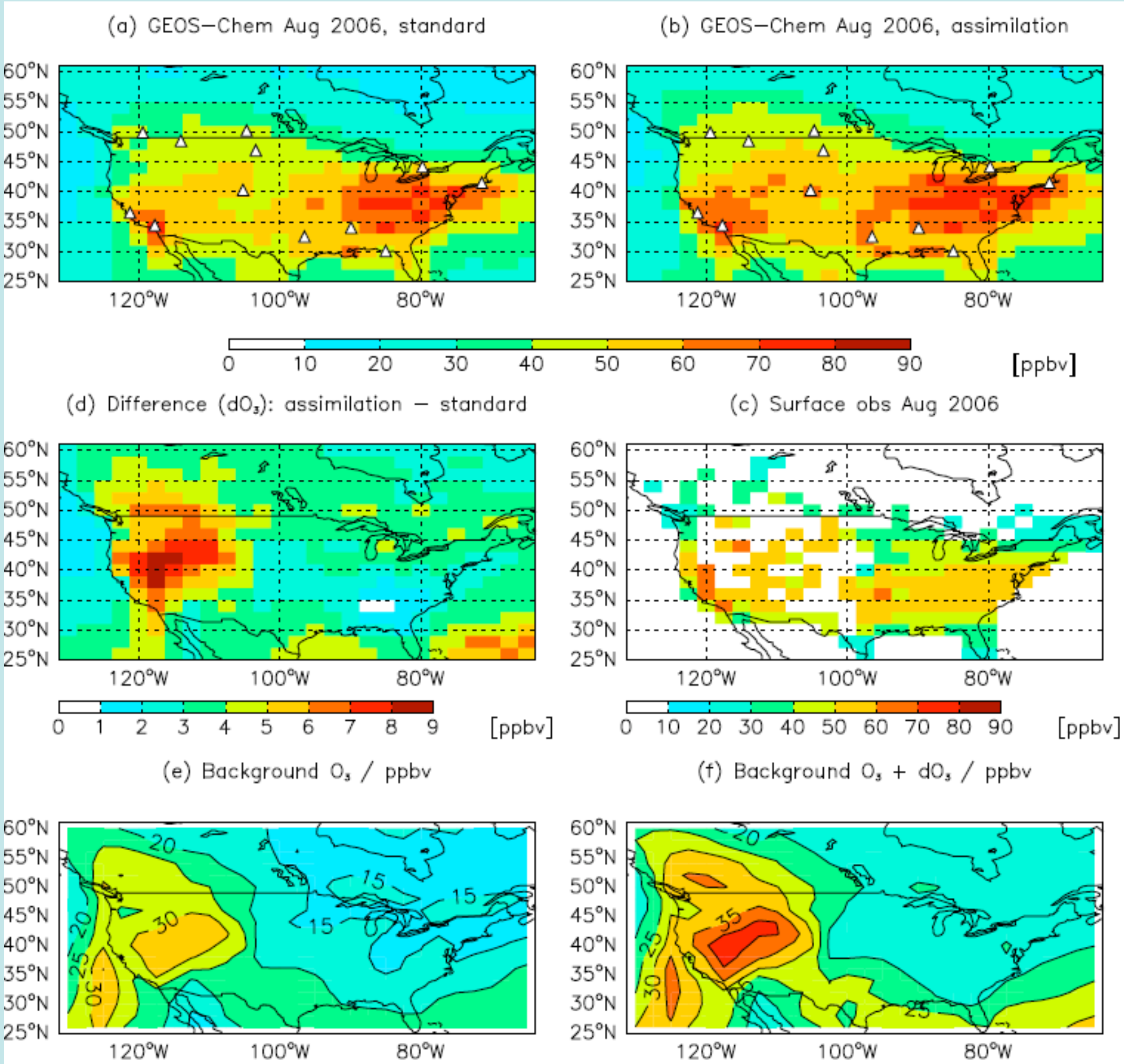
Mean (August 2006) O_3 profile over North America (model sampled at the ozonesonde observation time and location)



[Parrington et al., JGR, 2008]

Significant improvement in fee tropospheric O_3 (300 - 800 hPa) after assimilation.
The bias was reduced from a maximum of -35% to less than 5% (between 300-800 hPa).

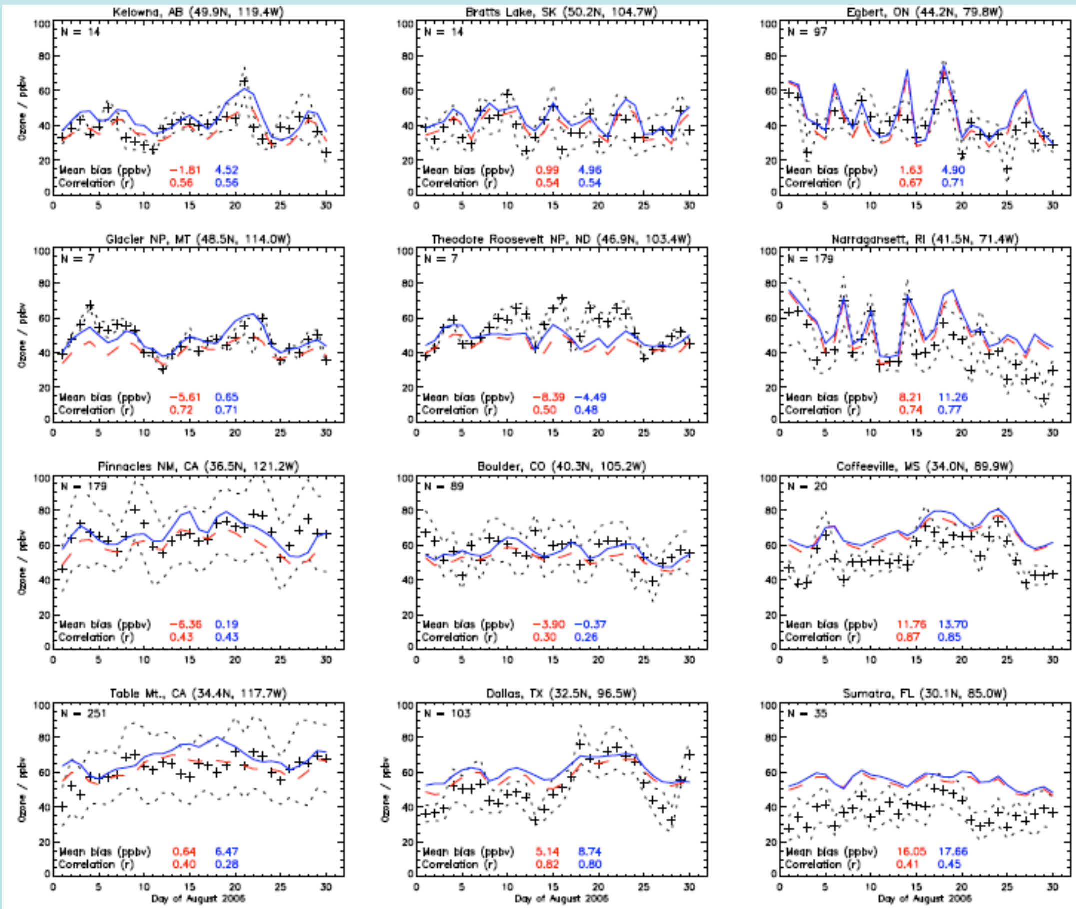
Impact of Assimilation on Surface Ozone



- The model overestimates surface ozone in the east and underestimates it in the west
- Assimilation increases surface O_3 by as much as 9 ppb, with the largest increase in western North America
- TES-based estimates of background O_3 are 20-40 ppb

[Parrington et al., GRL, 2008]

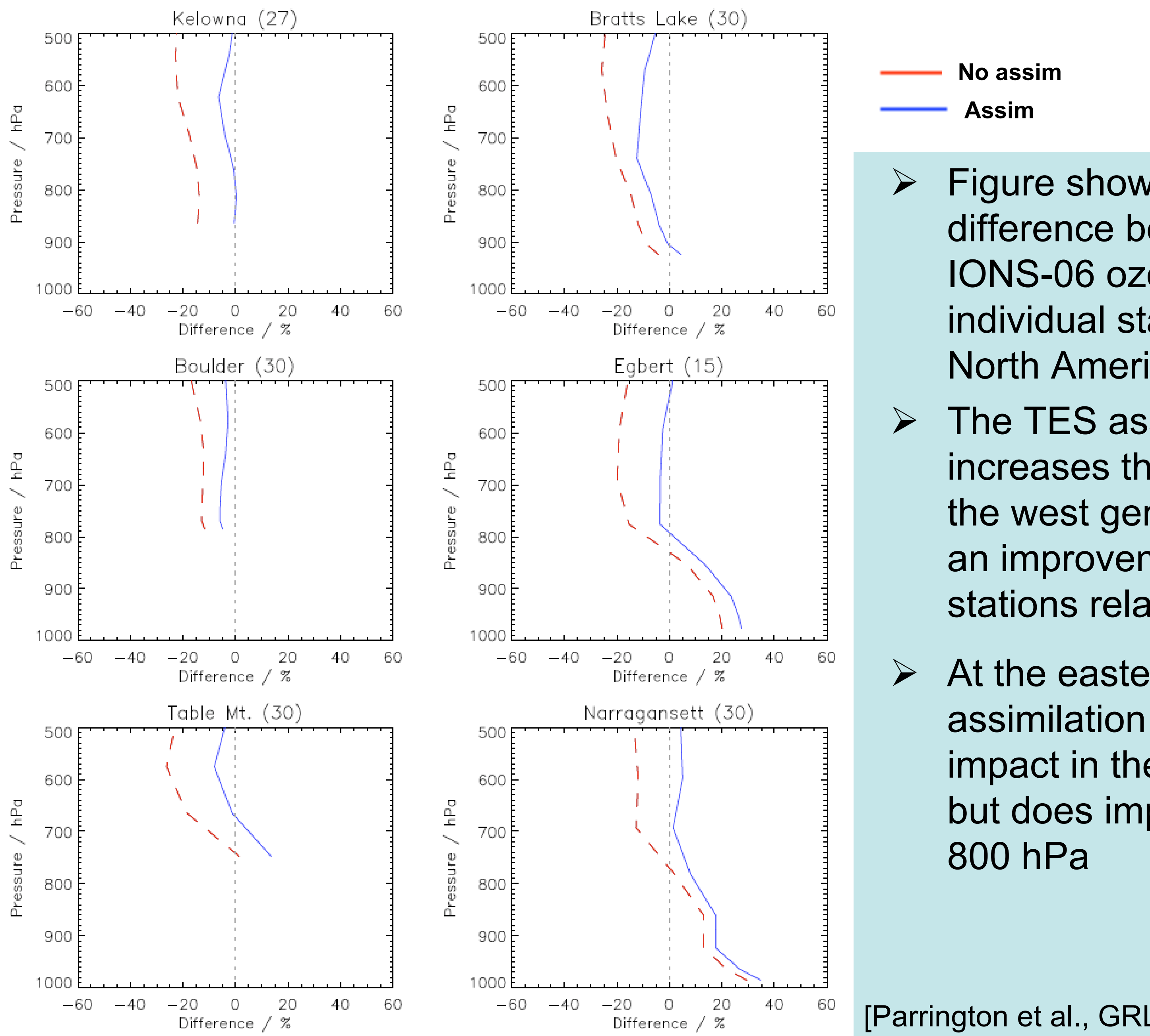
Comparison with AQS and NAPS Ozone Data



Location	Mean bias before (ppb)	Mean bias after
Kelowna, AB	-1.81	4.52
Bratt’s Lake, SK	0.99	4.96
Glacier NP, MT	-5.61	0.65
Pinnacles NM, CA	-6.36	0.19
Theodore Roosevelt NP, ND	-8.39	-4.49
Boulder, CO	-3.90	-0.37
Table Mt., CA	0.64	6.47
Dallas, TX	5.14	8.74
Egbert, ON	1.63	4.90
Narragansett, RI	8.21	11.26
Coffeeville, MS	11.76	13.70
Sumatra, FL	16.05	17.66

- Assimilation reduced the bias at the western sites, but increased it in the east
- The increase in the bias in surface O_3 despite the good agreement with ozonesonde data in the free troposphere, indicates the presence of model errors in the O_3 sources or sinks, or in the simulation of the PBL mixing depths.

Comparison to ozonesonde data



- Figure shows monthly mean % difference between model and IONS-06 ozonesondes at individual stations across North America.
- The TES assimilation increases the model ozone in the west generally leading to an improvement at those stations relative to the sondes
- At the eastern stations, the assimilation has a smaller impact in the boundary layer but does improve ozone above 800 hPa

[Parrington et al., GRL, 2008]

Summary

- Assimilating TES data reduces the negative bias in the modelled free tropospheric ozone, enhancing the flux of background ozone into the boundary layer.
- The resulting increase in modeled surface ozone is greatest in western North America (as much as 9 ppbv) and smallest over the southeastern USA (less than 2 ppbv).
- TES assimilation is providing best estimate of North American background ozone of 20-40 ppbv.
- Despite the good agreement between the assimilation and ozonesonde measurements in the free troposphere, comparisons with surface measurements show that the assimilation exacerbates the bias in surface ozone, suggesting a potential model bias in the ozone sources and sinks or in the downward transport of ozone into the boundary layer.
- Model errors associated with ozone precursor emissions are currently being evaluated through integrating top-down emissions estimates of NO_x and isoprene, derived from SCIMACHY NO_2 and OMI formaldehyde respectively, and GEOS-Chem adjoint model simulations for North America.