Sensitivity analysis of tropospheric ozone at middle and high latitudes to precursor emissions

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Outline

- Adjoint provids an efficient means of calculating sensitivities of the model state
- Examples where the adjoint model provides supplemental insights:
  (1) Ozone transport to Arctic sites
  (2) Surface ozone in eastern North America
  (3) Midlatitude lightning NOx emissions constraint

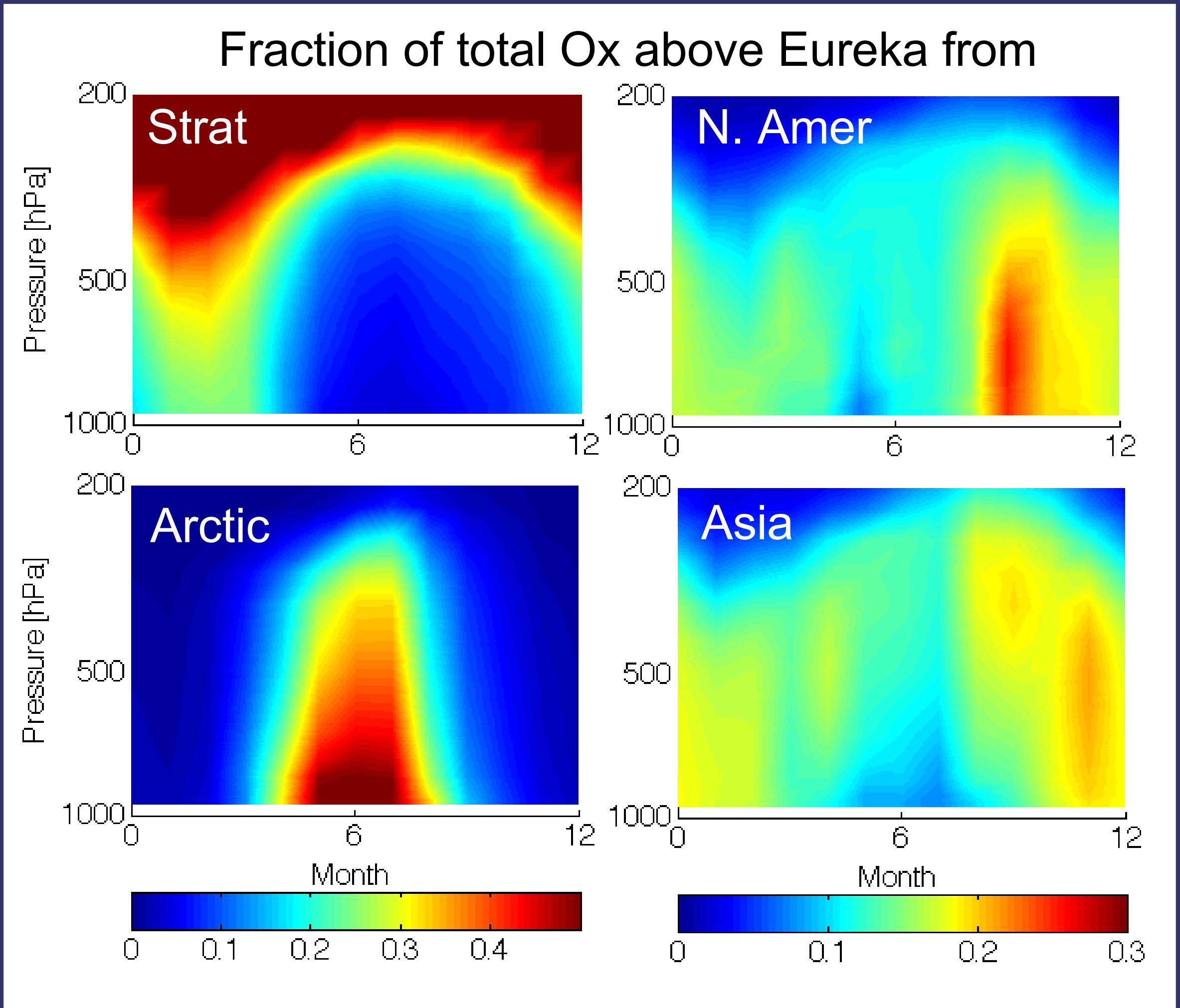
Given a small perturbation to the model inputs, the tangent linear model (TLM) can calculate the change in the model state

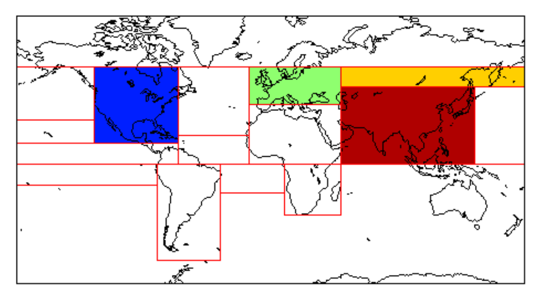
$$\Delta y = TLM(\Delta x)$$

Likewise, given a perturbed model state, the adjoint model (transpose of TLM) can calculate the required change in inputs

$$\Delta x = TLM^T(\Delta y)$$

Ozone Transport to Arctic Sites



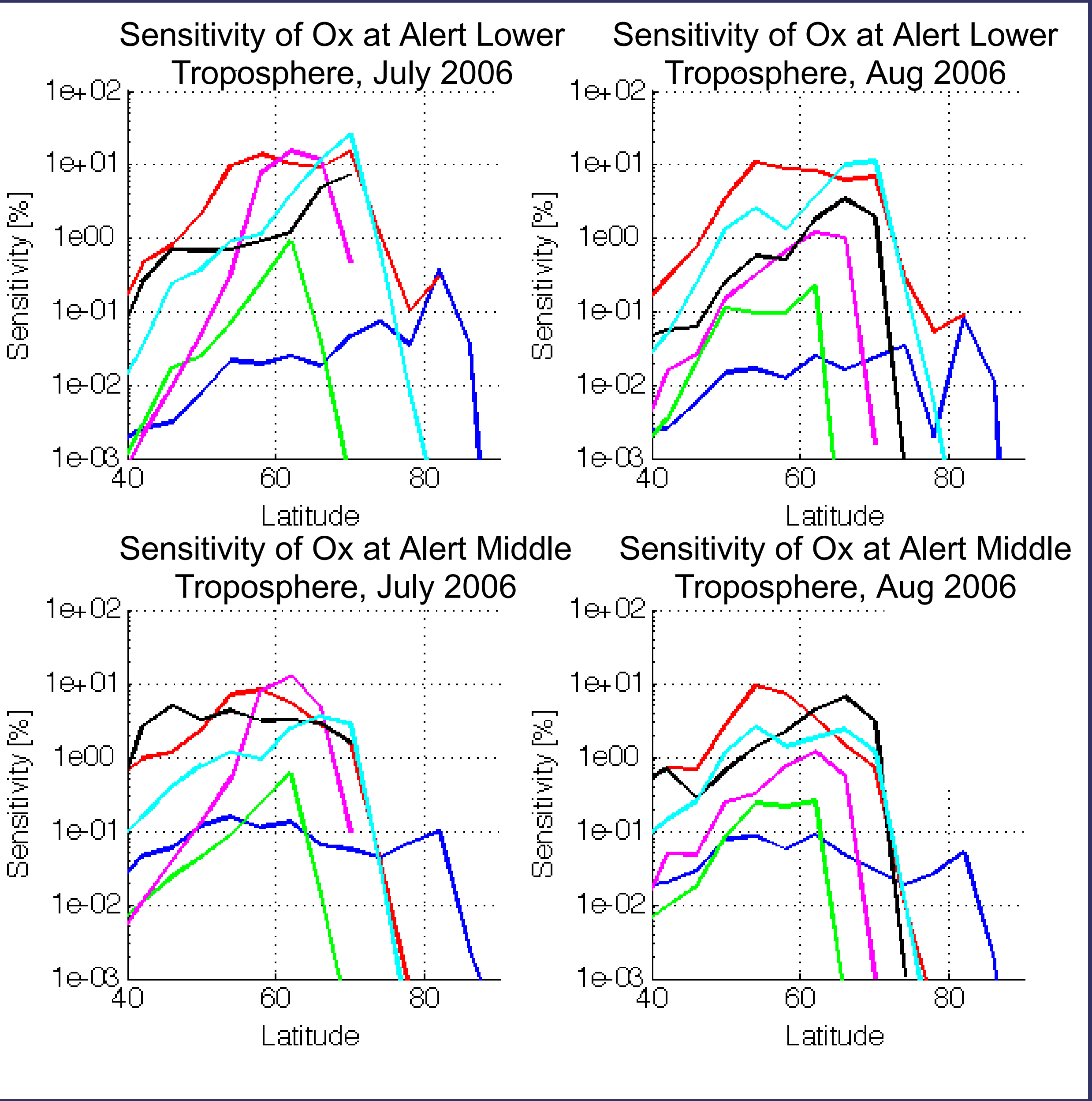


- One year of vertical profiles of tagged Ox tracers above Eureka, NU (80.0N, 86.2W)
- Stratospheric descent in spring; local influence inside “polar dome” in summer
- Transport from midlatitude source regions contribute 15-20% in spring and fall

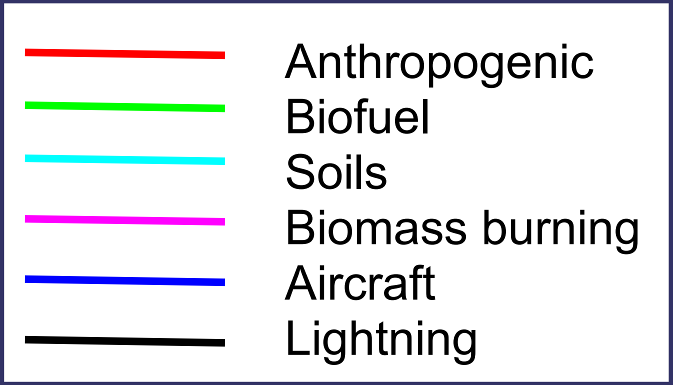
... WHAT'S MISSING?

- No separation of precursor source types (how much from anthropogenic, biomass burning, etc...)
- “Traditional approach” - numerous forward simulations to isolate each source individually

Ozone Transport to Arctic Sites

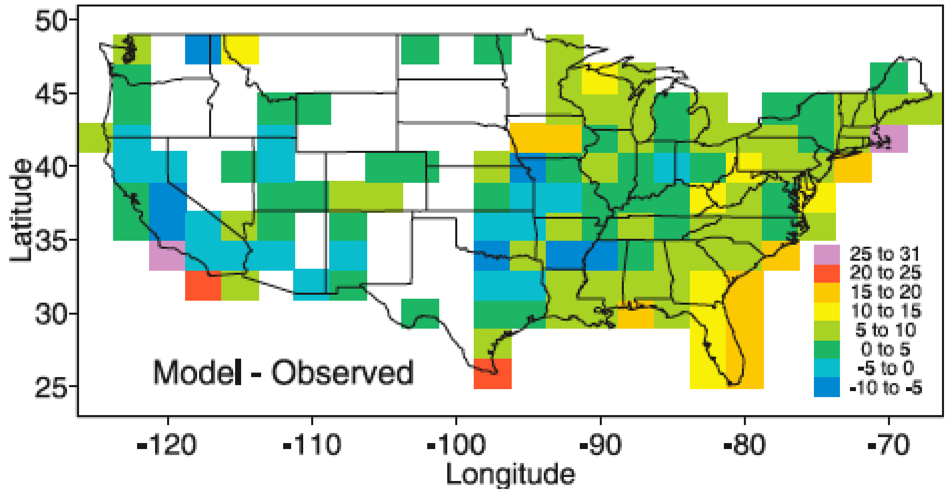


- Single adjoint model run calculates sensitivity of ozone at the Arctic site to different NOx emissions sources
- Sensitivity is calculated for every grid box
- Strongest sensitivities are to anthropogenic (red), soils (cyan), lightning (black), and biomass burning (magenta)

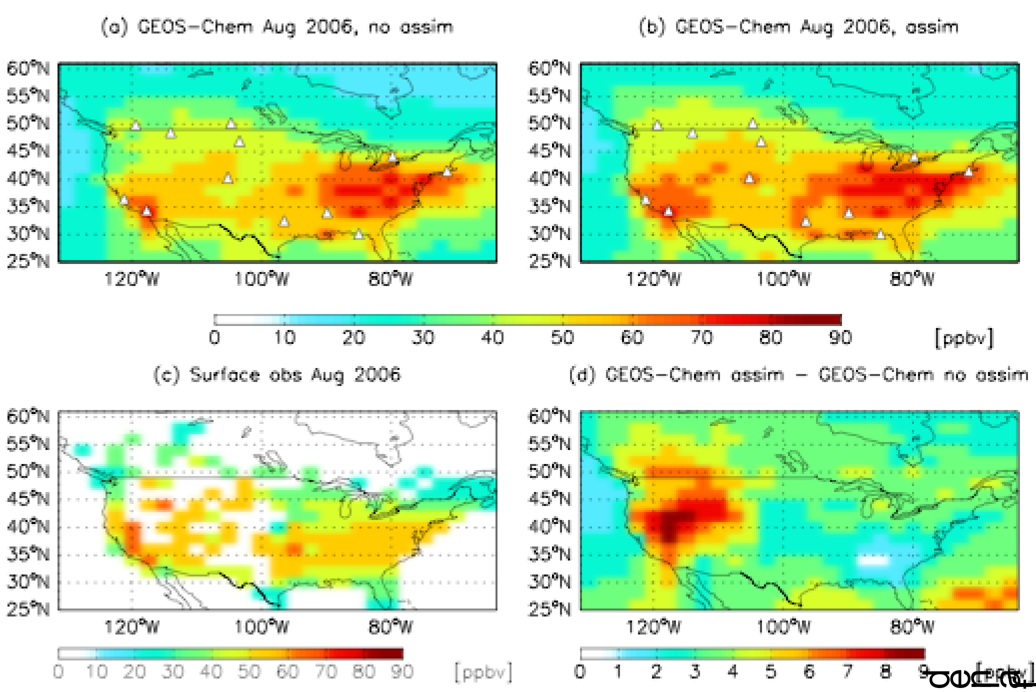


Watch for this in: Walker et al., (in prep.) *Impacts of midlatitude precursor emissions and local photochemistry on ozone abundances in the Arctic*

Surface Ozone in Eastern North America

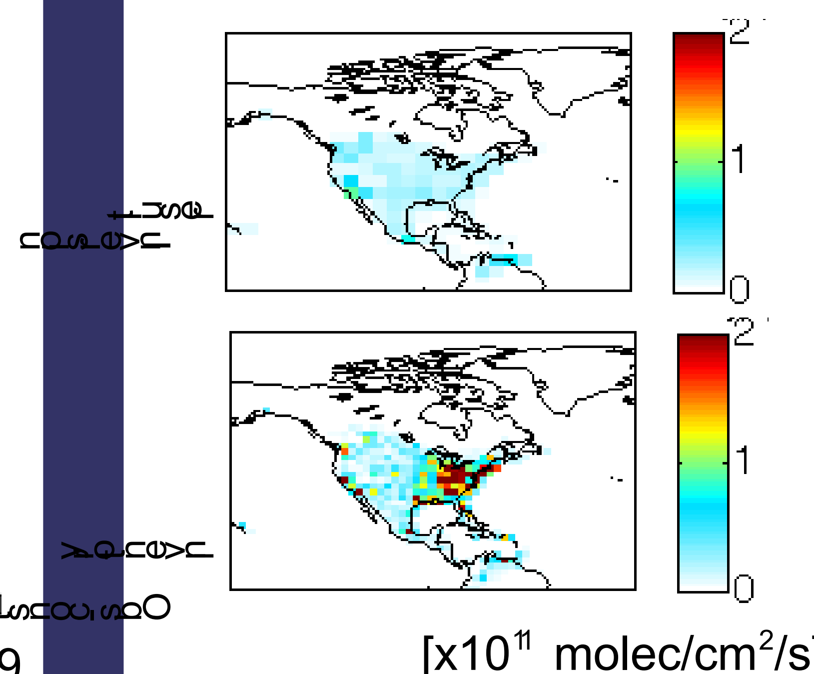


Fiore et al. 2002

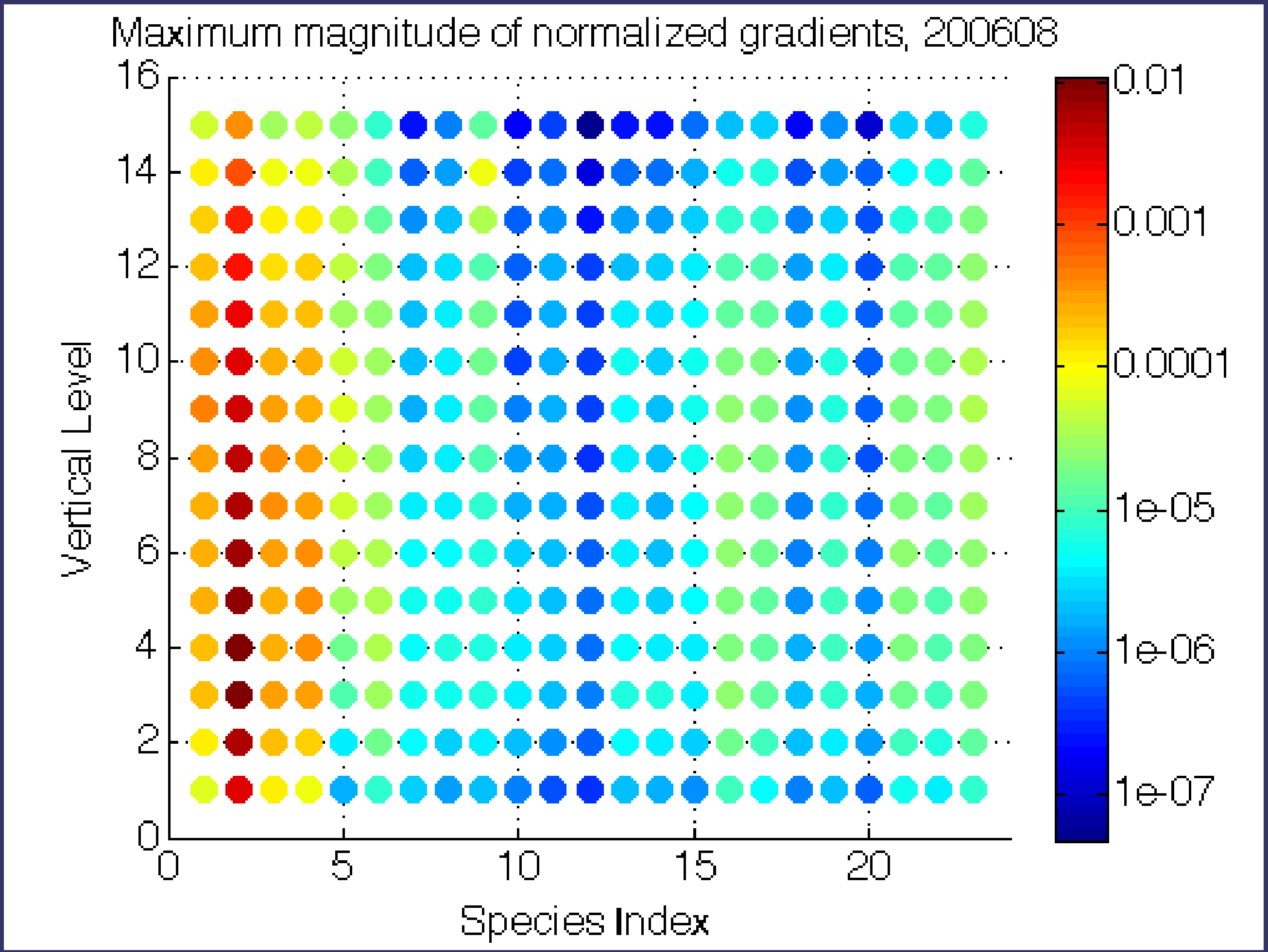


Parrington et al. 2009

- GEOS-Chem has trouble reproducing surface ozone observations in some regions
- Constraining background tropospheric ozone with assimilated observations does not correct
- An inversion for NOx emissions using surface ozone observations imposes an unrealistic constraint



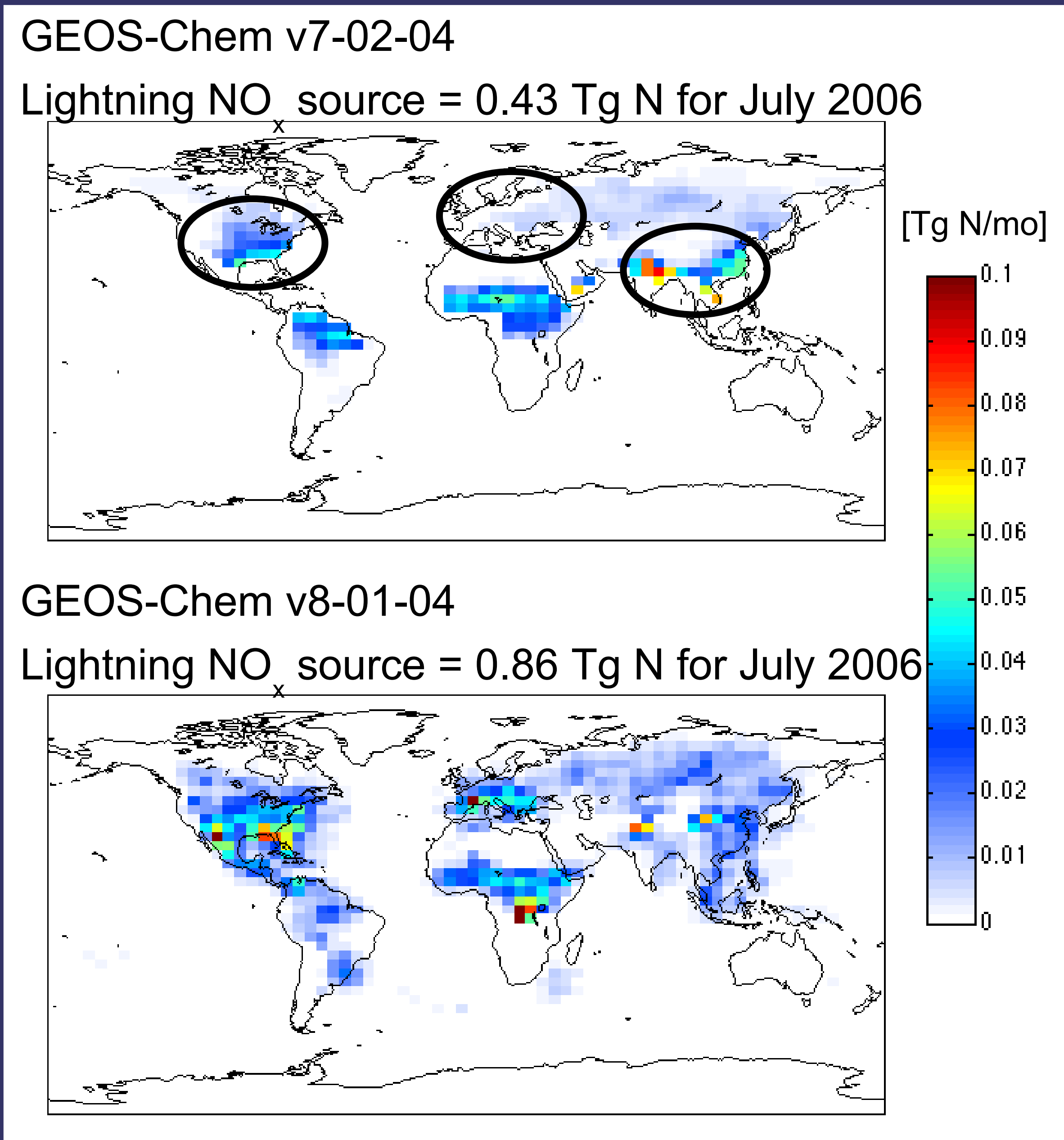
Surface Ozone in Eastern North America



1 – NOx
2 – Ox
3 – PAN
4 – CO
5 – HNO3
6 – ACET
7 – ALD2
8 – ALK4
9 – ISOP
10 – H2O2
11 – MEK
12 – RCHO
13 – MVK
14 – MACR
15 – PMN
16 – PPN
17 – R4N2
18 – PRPE
19 – C3H8
20 – CH2O
21 – C2H6
22 – N2O5
23 – HNO4

- Sensitivities to species concentrations can guide future studies (eg. Chai et al. (2006))
- Looking to develop sensitivities to more control parameters to offer more insights

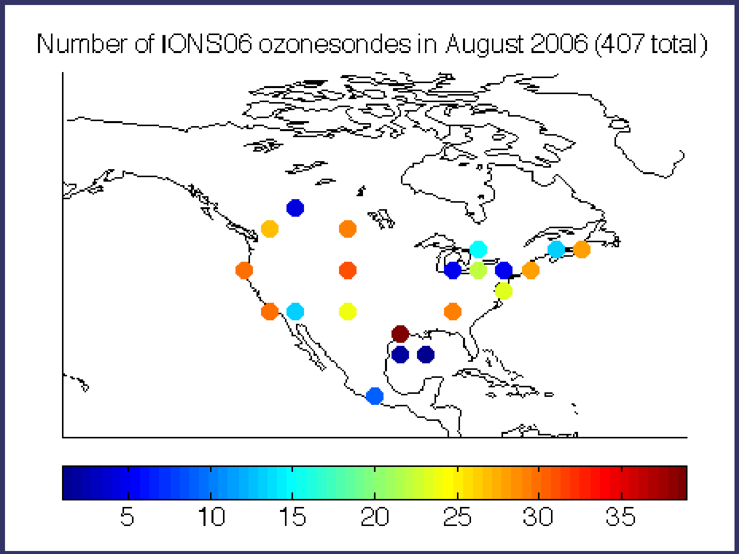
Midlatitude Lightning NOx Emissions Constraint



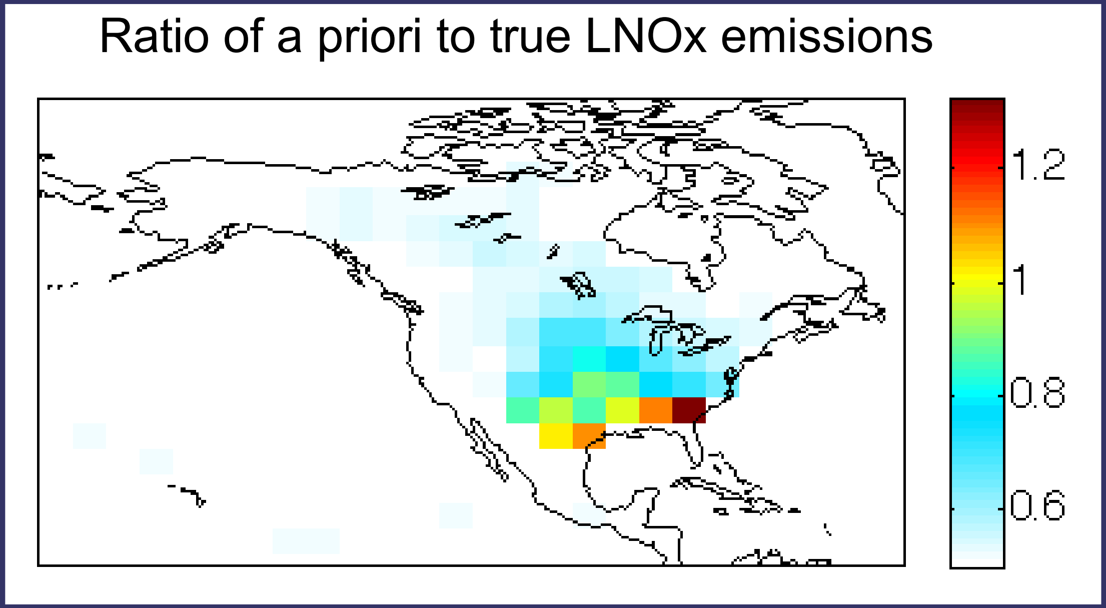
- Global lightning NOx emissions in v7-02-04 and earlier follow Price & Rind (1992)
- Emissions in v8-01-04 and later are rescaled to match OTD-LIS climatology (Lee Murray)
- Rescaling produces a more realistic midlatitude ozone distribution

... CAN WE DO BETTER?

Midlatitude Lightning NOx Emissions Constraint



- Let the model be the "true" state of the atmosphere, but start with a bad guess (2x the true lightning NO_x emissions)
- We take pseudo-observations of the "true" state at times and locations of IONS06 observations
- Then, let the adjoint assimilate the pseudo-observations and try to converge back to the "true" state from our bad first guess
- Gives confidence that an inversion using these observations will provide a constraint



... NEXT:

- Perform inversions using real IONS06 observations
- Assess and compare different a priori inventories (Price & Rind, OTD-LIS, WWLLN)

Watch for this in: Ok, this is a work in progress and has no title yet, but it will soon!

Conclusions

(1) Ozone transport to Arctic sites

- Midlatitude sources contribute 25-30% of ozone in the Arctic middle and upper troposphere in the summer
- Adjoint provides complementary detailed source-specific information

(2) Surface ozone in eastern North America

- Adjoint sensitivities can guide further studies into model biases

(3) Midlatitude lightning NOx emissions constraint

- Simulation experiment shows ozonesonde data can provide a constraint on midlatitude NOx emissions

Thank you for listening!

EXTRAS

Adjoint Model Methodology

We are concerned with the model misfit to observations, expressed as a quadratic cost function J:

$$J = \frac{1}{2} < M(x) - y^{obs}, M(x) - y^{obs} >$$

Performing a linear expansion about some background set of parameters x_o,

$$J(x) = J(x_o) + < \nabla_x J(x_o), x - x_o >$$

$$\delta J = < \nabla_x J(x_o), \delta x_o >$$

If M is sufficiently regular, then given a small perturbation δx, the Jacobian L(x) can be used to calculate the perturbation to the state δy:

$$\delta y = L(x_o)\delta x$$

However, using a forward sensitivity study (eg. experimenting with different variations δx) requires an integration of this tangent linear model for each grid point, time interval, iteration ~(46 x 72 x 55 x ...)

Adjoint Model Methodology

Instead, we define the adjoint model L*:

$$< v, Lw > = < L^* v, w >$$

Then, from the derivative of the cost function,

$$\delta J = < M(x_o) - y^{obs}, L(x_o)\delta x >$$

$$\delta J = < L^*(x_o)(M(x_o) - y^{obs}), \delta x >$$

$$\nabla_x J(x_o) = L^*(x_o)(M(x_o) - y^{obs})$$

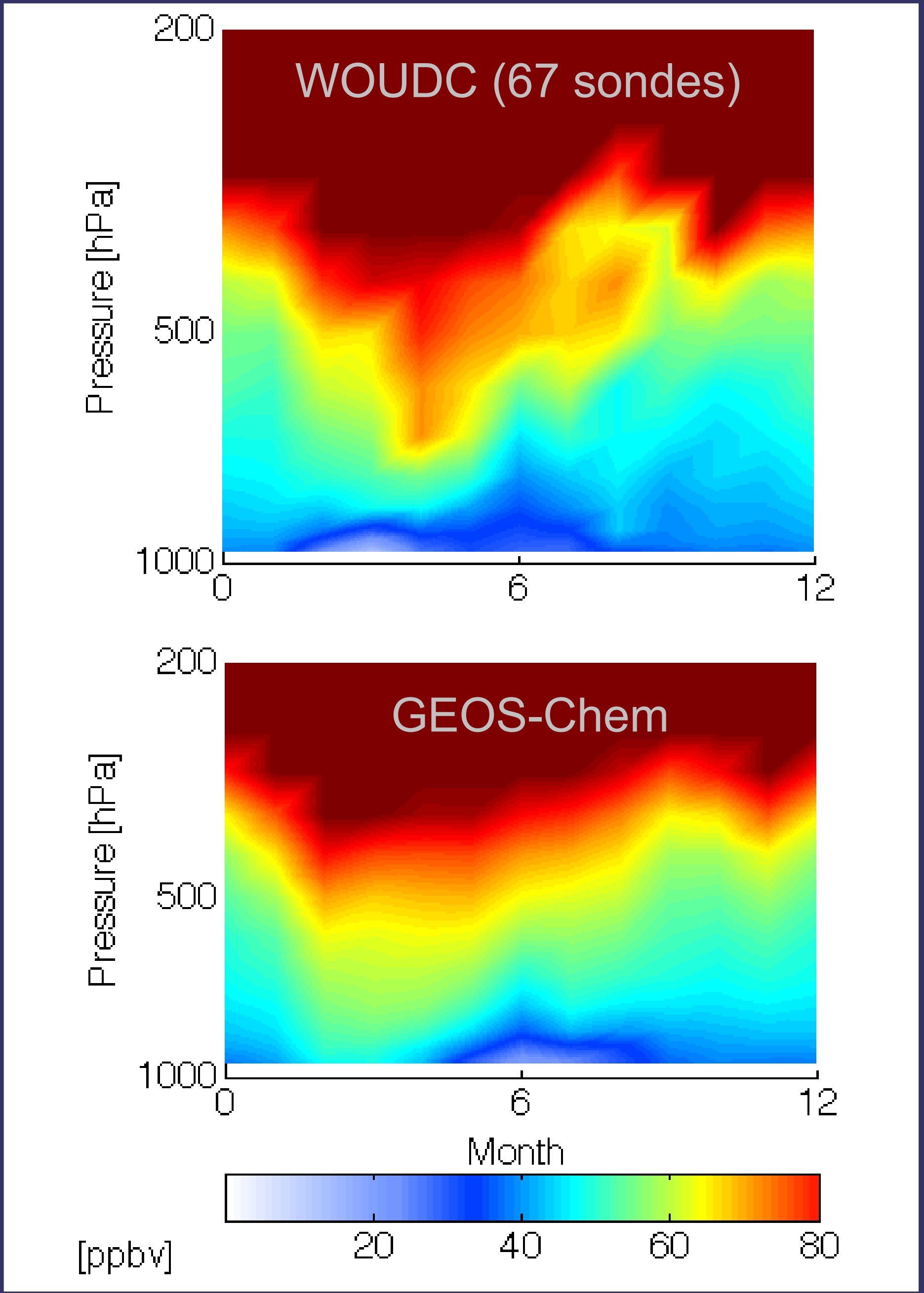
The gradient can be used to minimize J by iteratively correcting parameter values. Also, a single calculation of the adjoint model provides sensitivity of model outputs to model inputs:

$$\delta x^* = L^*(x_o)\delta y^*$$

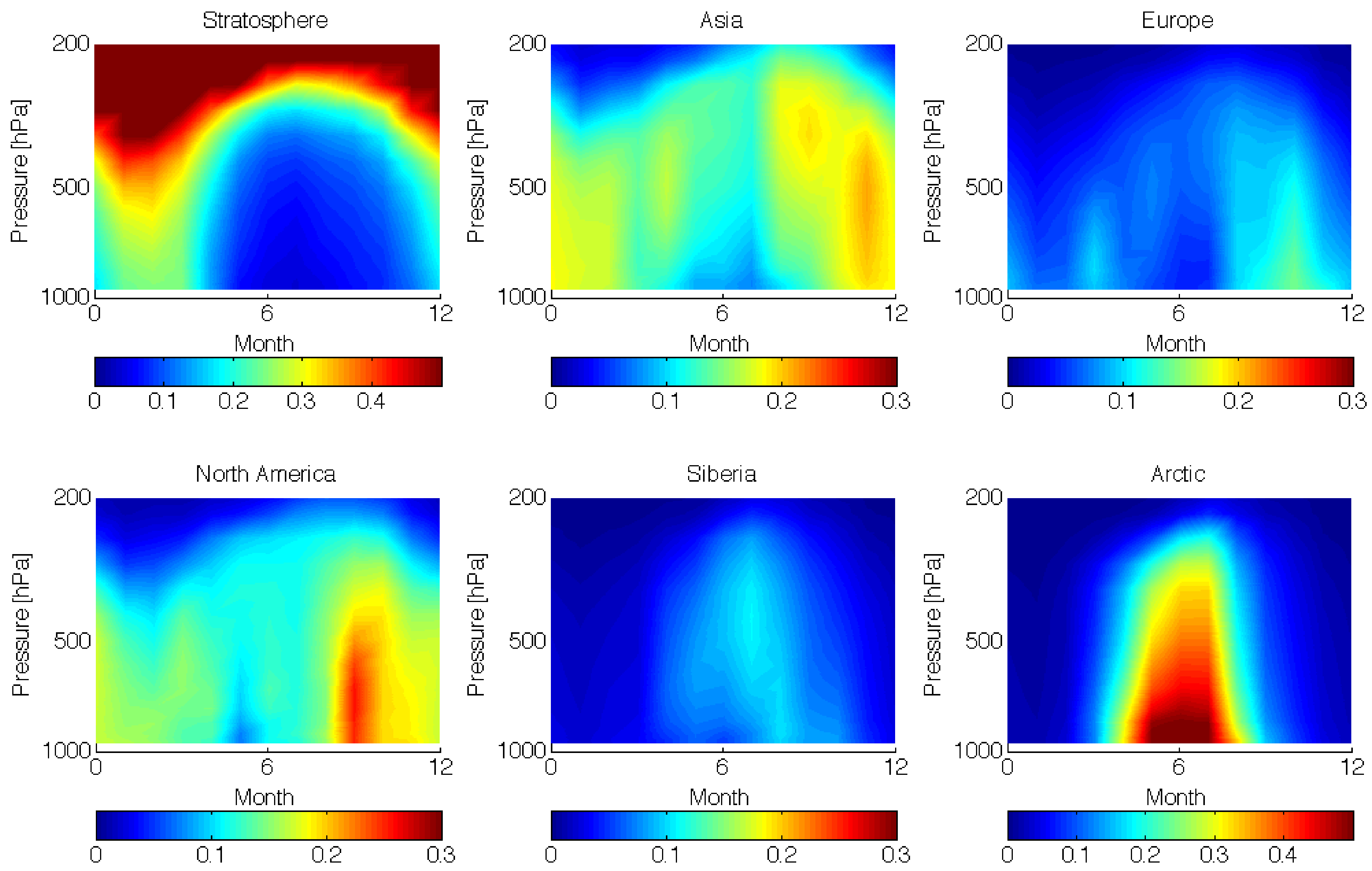
Here, we will plot fully normalized sensitivities: $\frac{\delta y}{\delta x}\frac{x}{y}$

Total Ozone Profiles above Eureka, 2006

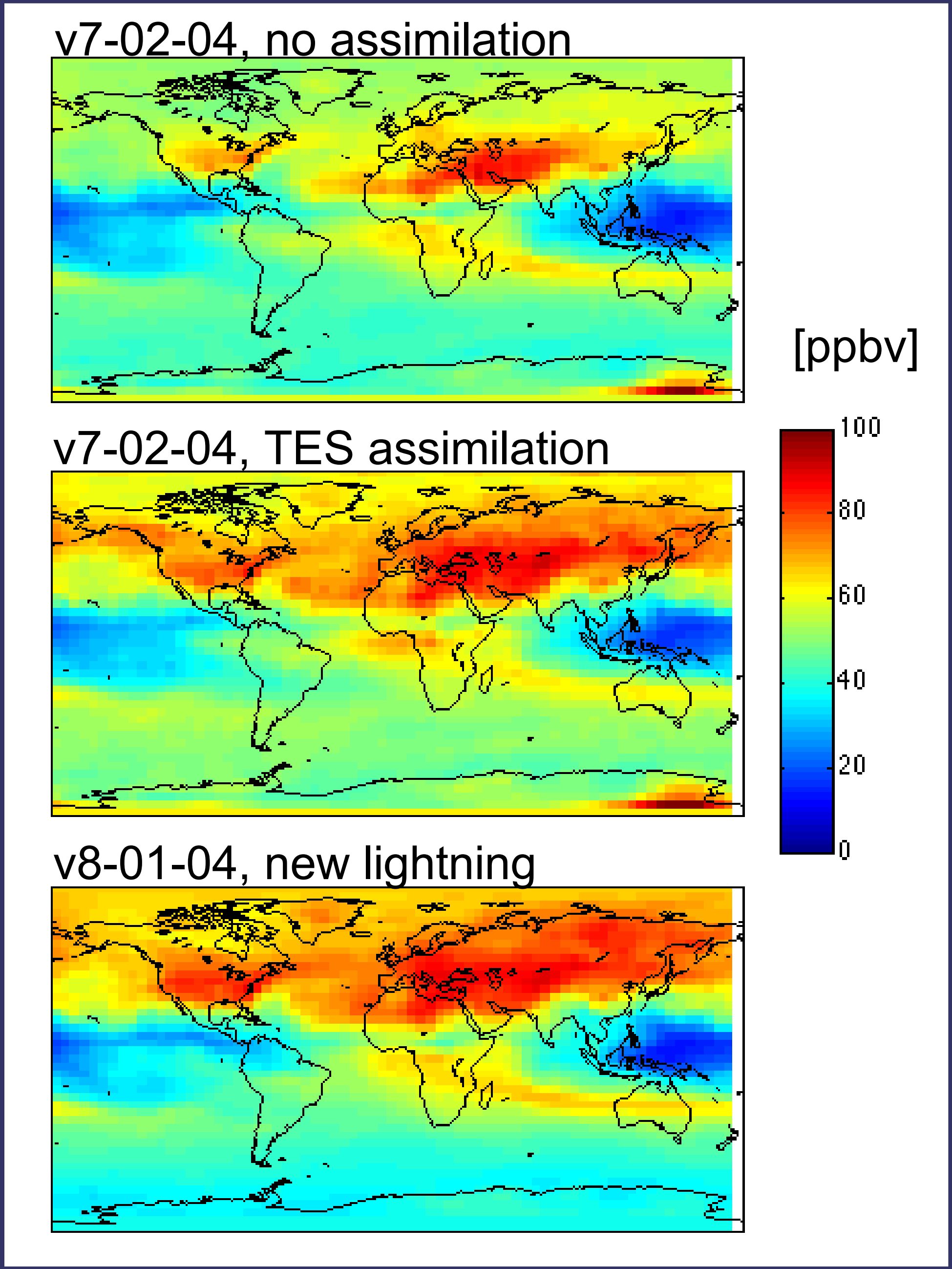
- model agreement with ozonesondes is good except for a ~10 ppbv underestimate in the upper troposphere in summer
- spring ozone maximum appears earlier in model than in observations



Tagged Ox Profiles above Eureka, 2006

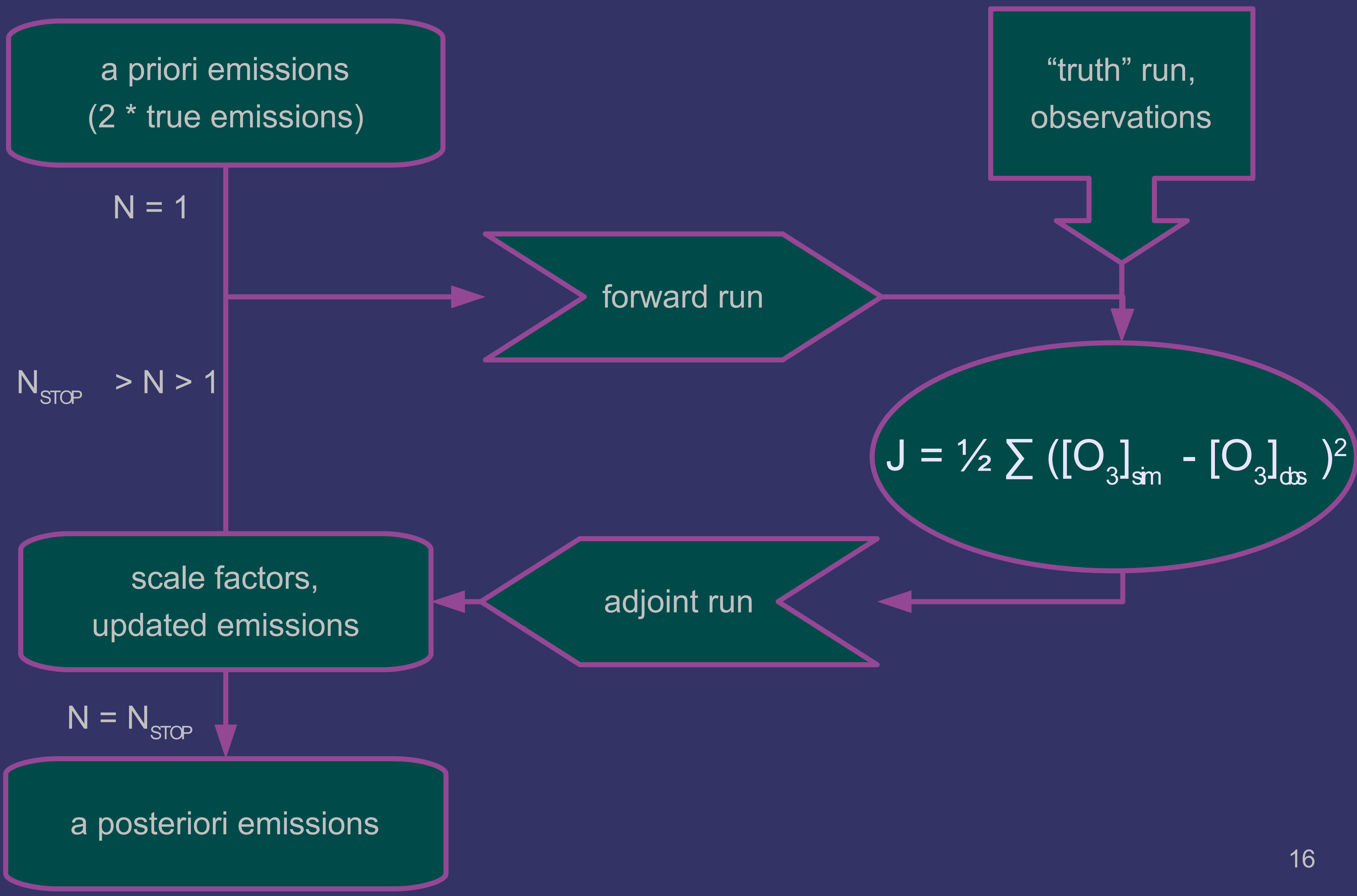


New LNOx Emissions Produce More Realistic Ozone Distribution



- Ozone concentrations at 6km
- Relative to N. American ozonesondes, TES assimilation reduces bias from a maximum of -35% to less than 5% between 300-800 hPa
- Relative to the TES assimilation, the new lightning NO_x source reduces the mean bias in the middle troposphere from -7 ppbv to 2 ppbv
- This better representation of midlatitude ozone provides an improved boundary condition for transport into the Arctic

OSSE Evaluation Diagram



References

- Fiore, A. M. et al. (2002) Background ozone over the United States in summer: Origin, trend, and contribution to pollution episodes. JGR, 107 (D15) 10.1029/2001JD000982
- Parrington, M. et al. (2009) Impact of the assimilation of ozone from the Tropospheric Emission Spectrometer on surface ozone across North America. GRL, 36 (L04802) 10.1029/2008GL036935
- Henze, D. K., A. Hakami and J. H. Seinfeld (2007) Development of the adjoint of GEOS-Chem. ACP, 7, 2413-2433
- Price, C. and Rind, D. (1992), A simple lightning parametrization for calculating global lightning distributions, JGR, 97, 9919-9933
- Chai, T. et al. (2006) Chemical data assimilation of Transport and Chemical Evolution over the Pacific (TRACE-P) aircraft measurements. JGR, 111 (D02301) 10.1029/2005JD005883