Progress Report of ITR Project

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Presentation outline

- Methods
  - Background
  - Current 4D-Var
- Applications
  - Sensitivity tests
  - Identical twin tests
  - Assimilating Trace-P flight observations
  - ICARTT Forecasting
- Conclusions, and future work

Background

- Why do data assimilation?
  - Simply comparing the model results and observations is not enough
  - A systematic approach is needed to combine the model and observation together
    - Simply injecting observation into model will cause balance problem
    - Unconventional measurements are difficult to be included in the model, e.g. column data, NOy

Background

- What is needed for data assimilation?
  - To obtain the “optimal estimate” based on both numerical model and observations , we need
    - Background error statistics
    - Observation error statistics
    - Model error information

Background

- Some aspects of 4D-Var
  - 4D-Var operations at ECMRF shows positive effect of 4D-Var
  - Sensitivity analysis made easy
  - 4D-Var gives same result as KF, for a perfect, linear model
  - Adjoint model is needed

Basic idea of 4D-Var

- Define a cost functional

$$J(c^0) = \frac{1}{2}\left(c^0 - c^{\mathrm{b}}\right)^T B^{-1}\left(c^0 - c^{\mathrm{b}}\right) + \frac{1}{2}\sum_{k=0}^{N}\left(c^k - c^{k,\mathrm{obs}}\right)^T R_k^{-1}\left(c^k - c^{k,\mathrm{obs}}\right)$$

which measures the distance between model output and observations, as well as the deviation of the solution from the background state

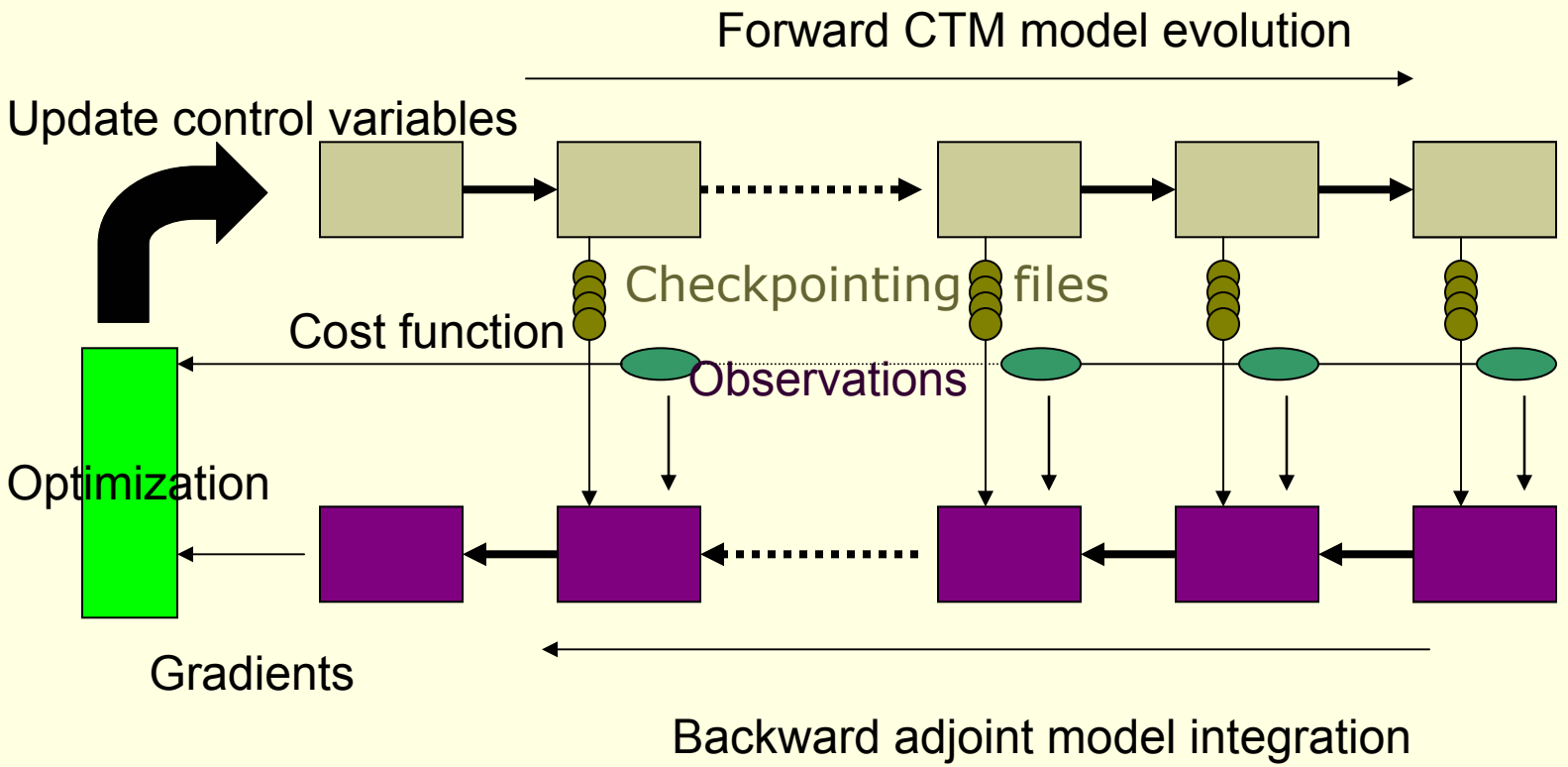
- Derive adjoint of tangent linear model

$$\frac{\partial \lambda_i}{\partial t} + \nabla\cdot(u\lambda_i) = -\nabla\cdot\left(\rho K \nabla \frac{\lambda_i}{\rho}\right) - \left(F^T(\rho c)\lambda\right)_i - \varphi_i$$

Where φ is the forcing term, which is chosen so that the adjoint variables are the sensitivities of the cost functional with respect to state variables (concentrations), i.e. $\lambda_i = \frac{\partial J}{\partial c_i}$

- Use adjoint variables for sensitivity analysis, as well as data assimilation

4D-Var application



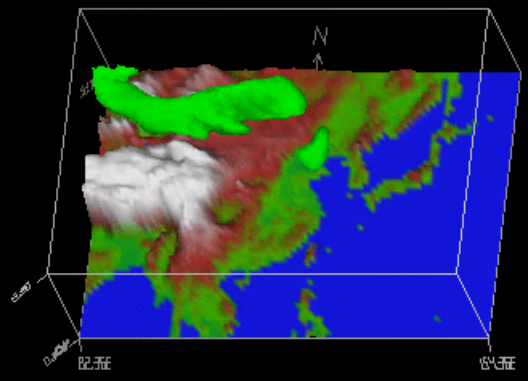
Sensitivity analysis

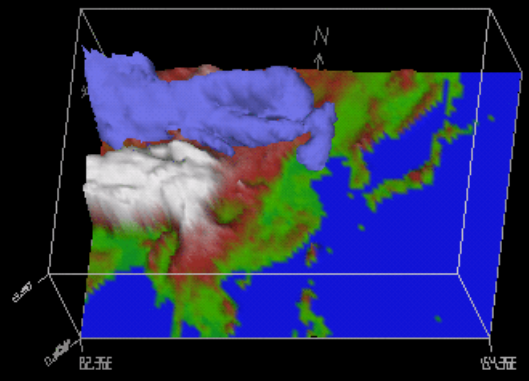
- In sensitivity analysis, the cost functional is chosen as

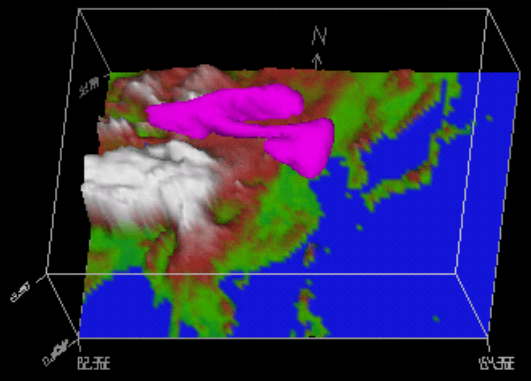
$$J = c_{O_3}(Cheju, t^{Final})$$

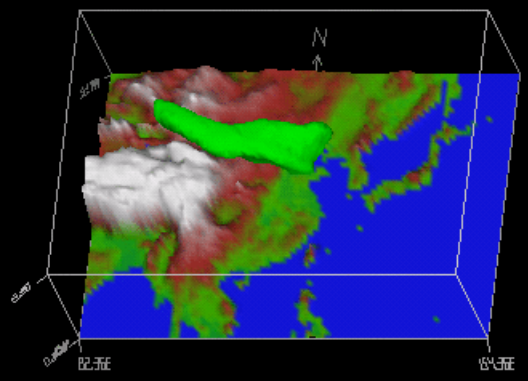
The adjoint variables then give the sensitivities of ozone concentration at Cheju at the final time step to different chemical species at different time steps,

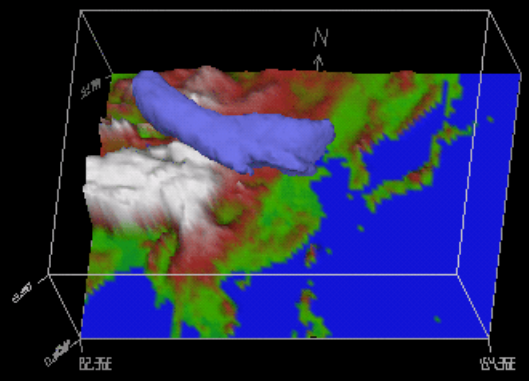
Influence functions (over Cheju O_3 concentration at 0:0:00 UT, 3/07/01) of O_3, NO_2, HCHO at -48, -24 hr

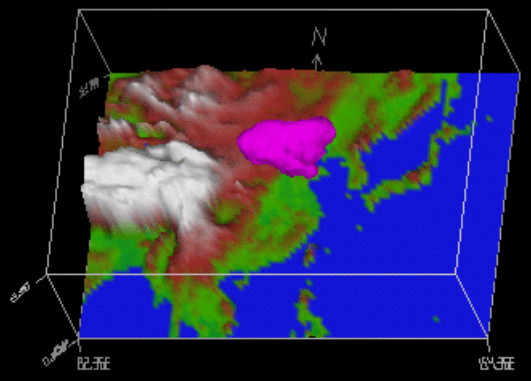








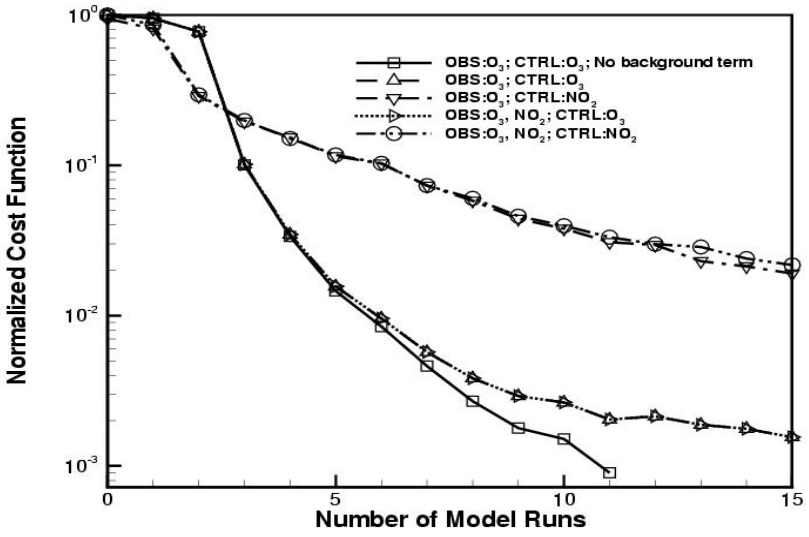


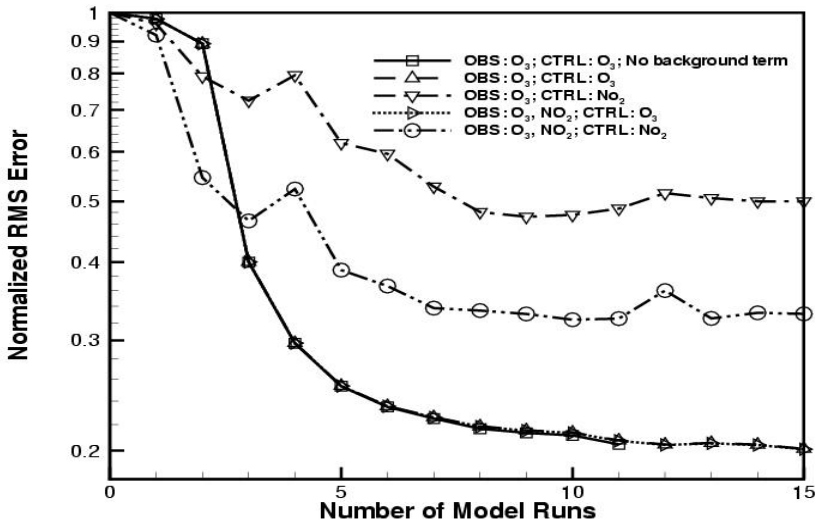


Data assimilation tests (ITE)

Assimilation window	*6 hours starting from 0:0:0 GMT on March 1st*
Observations	O3 and/or NO2 concentrations at the end of the assimilation window at all grid points from the reference run
Control variables	initial concentrations of O3 or NO2
Initial guess	reference initial values increased by 20%

Data assimilation results

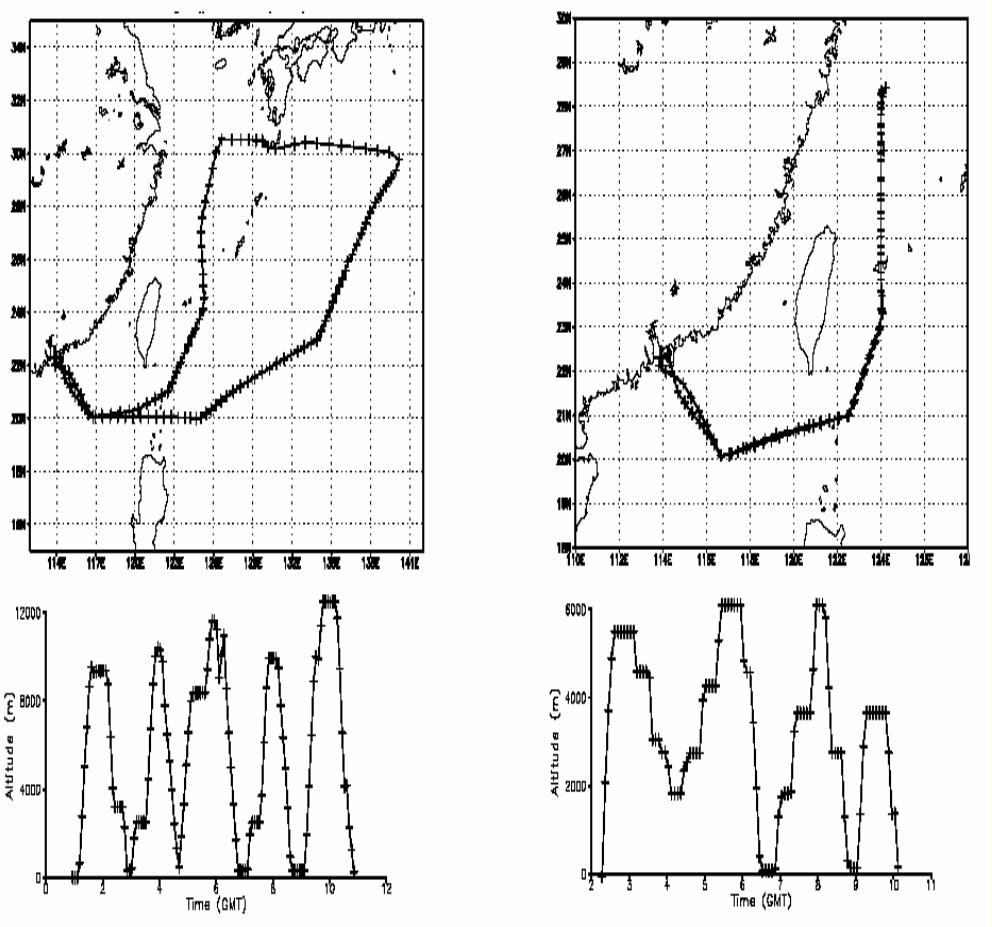




The evolutions of cost function and RMS error of the control variable during the optimization procedure. The results are normalized by their pre-assimilation values. Several tests are shown using different control (CTRL) and observed (OBS) variables.

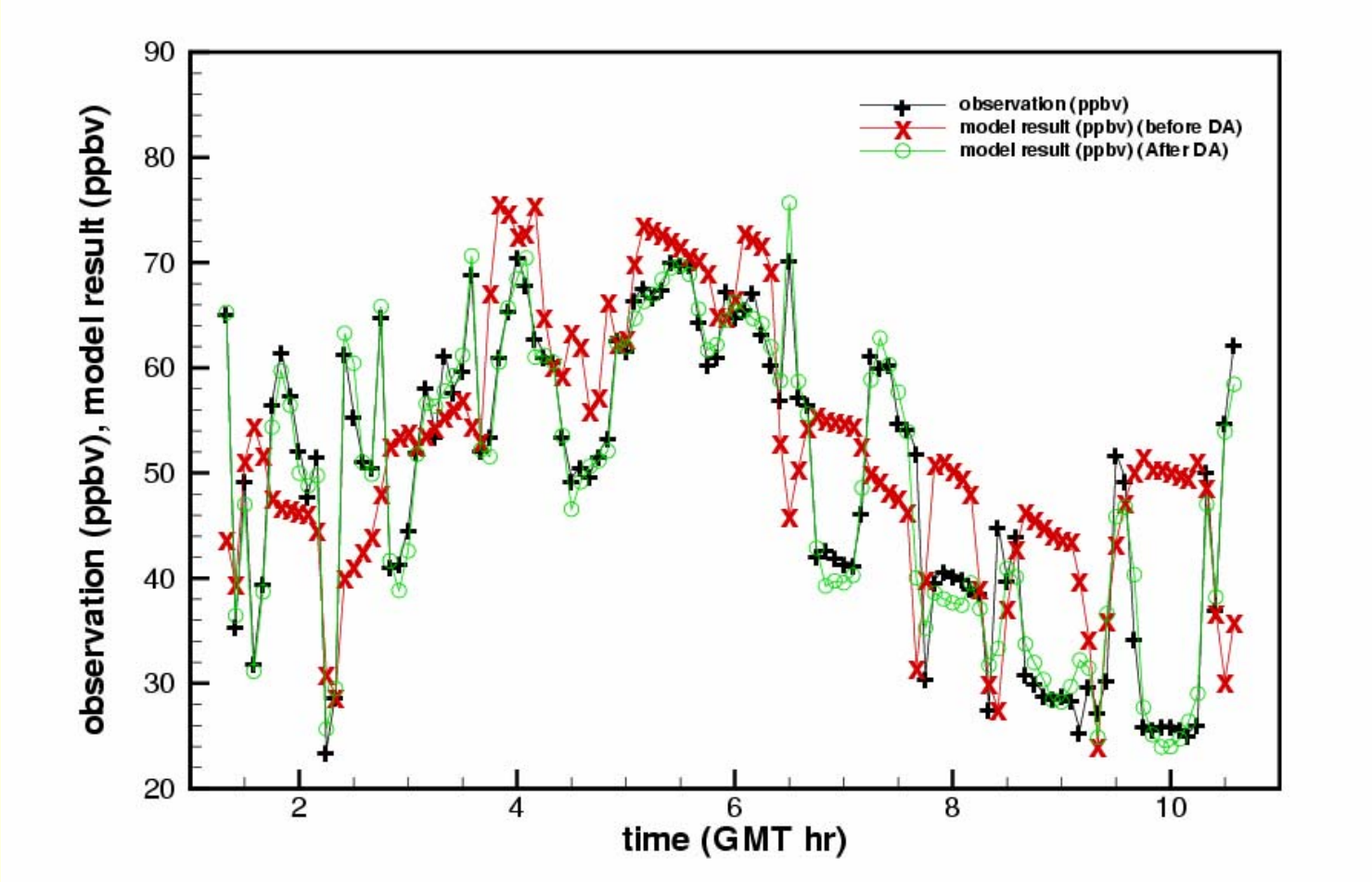
- Timing : Assimilation/Forward = 2.2

Trace-P DC-8 and P3-B flights on 3/7/2001



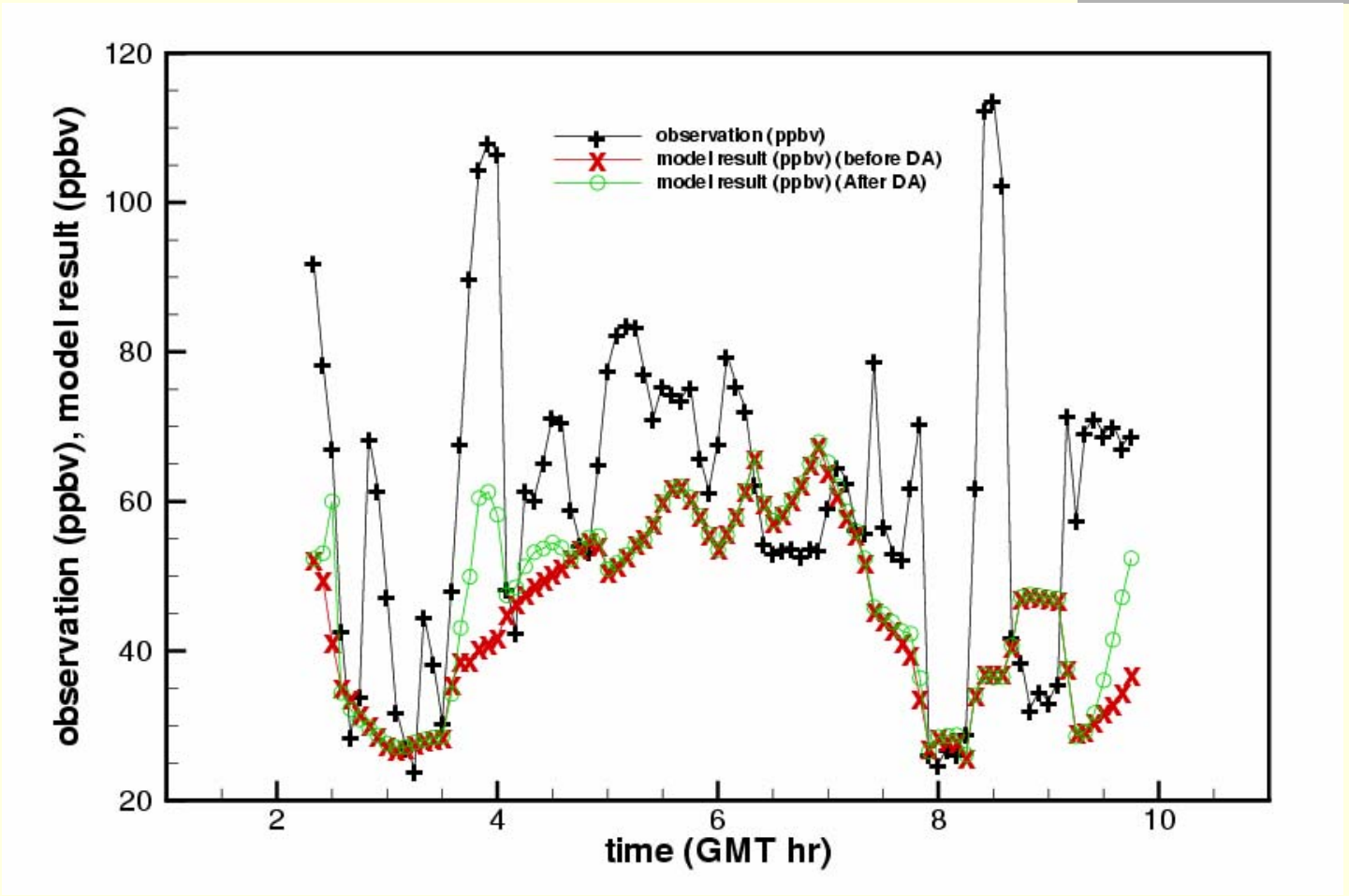
- Simulated region: East Asia
- Simulated time interval: 12 hours (starting at 0:00:00 GMT 3/7/01)
- Meteorological fields: given by RAMS
- Grid size: 90 × 60 × 18
- Horizontal resolution: 80 Km × 80 Km
- Control parameters: initial concentration
- Optimization algorithm: L-BFGS-B

Assimilating DC-8



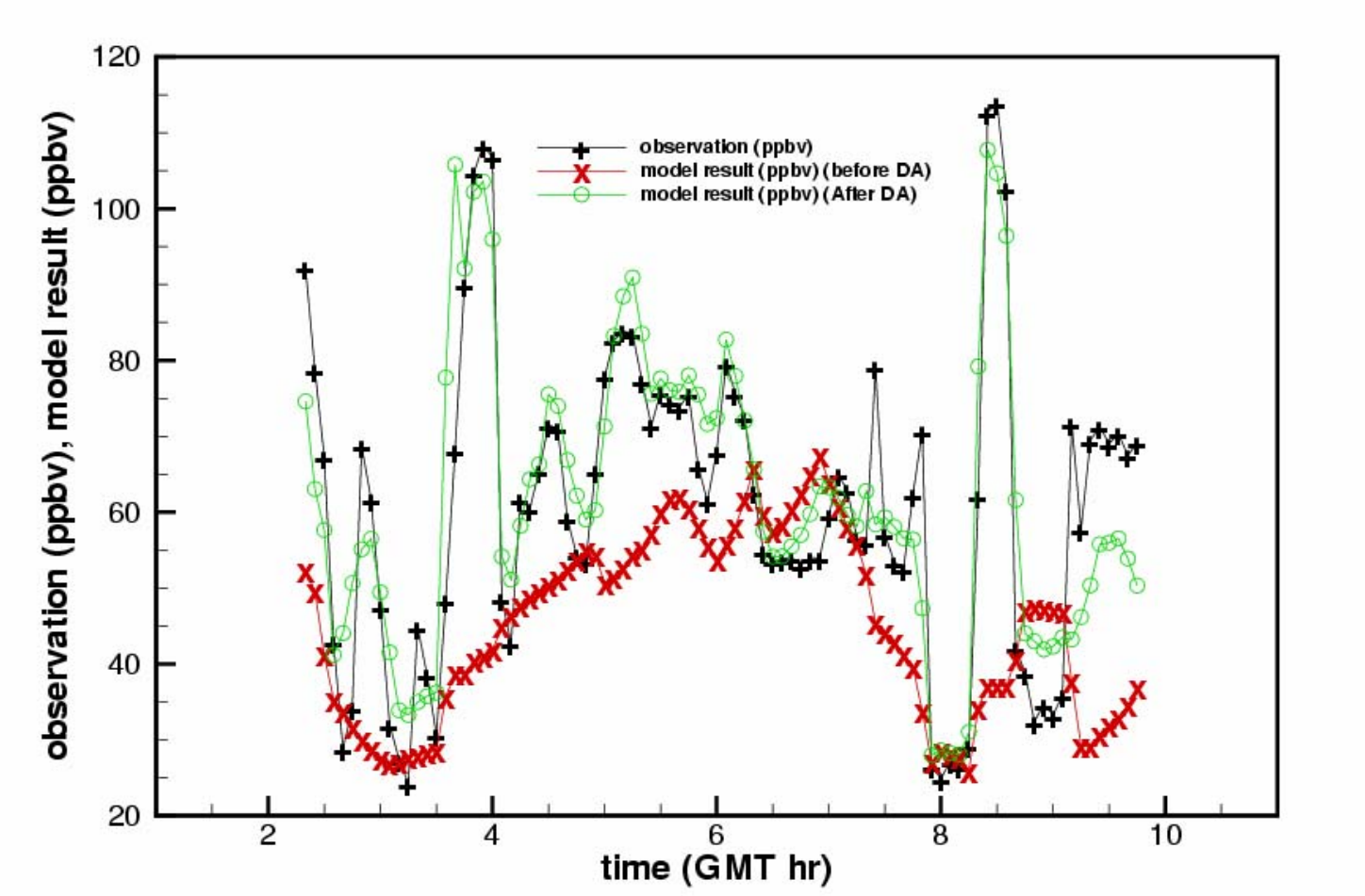
Observations from DC-8 and their model counterparts

Assimilating DC-8



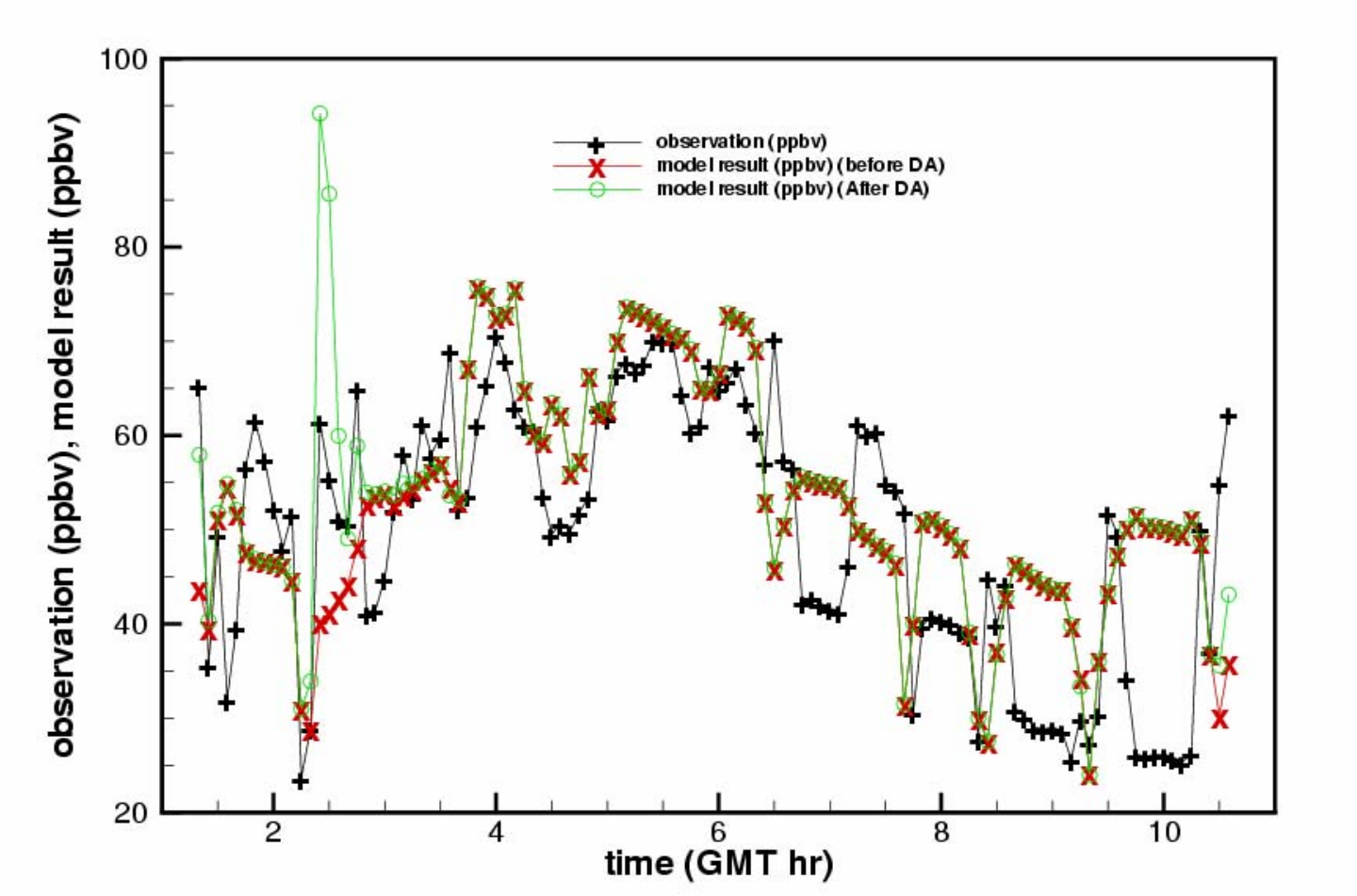
Observations from P3-B and their model counterparts

Assimilating P3-B



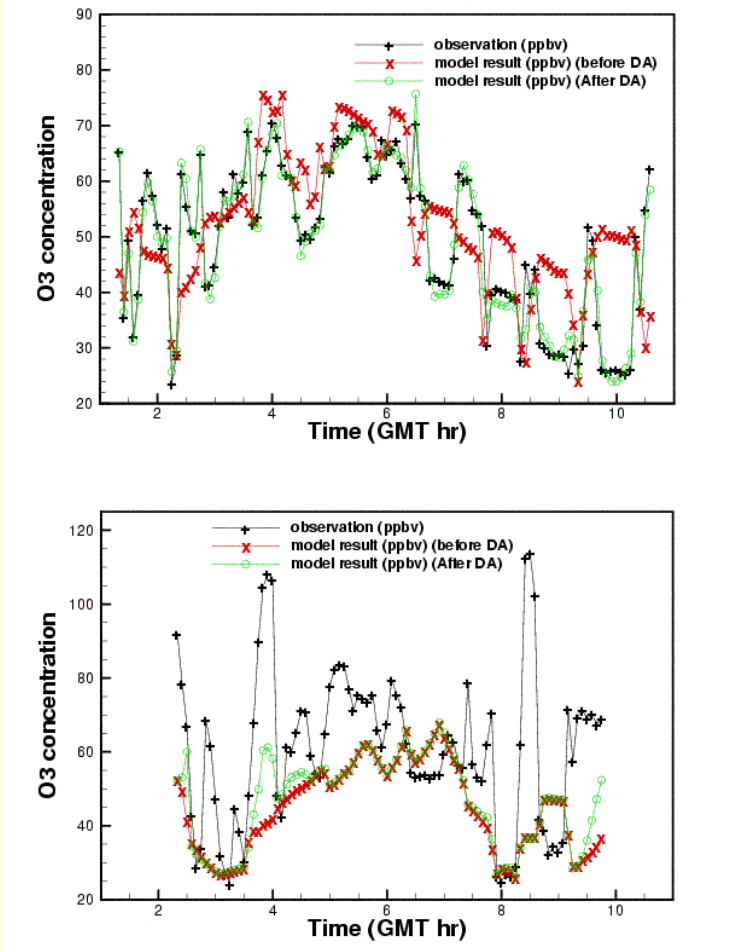
Observations from P3-B and their model counterparts

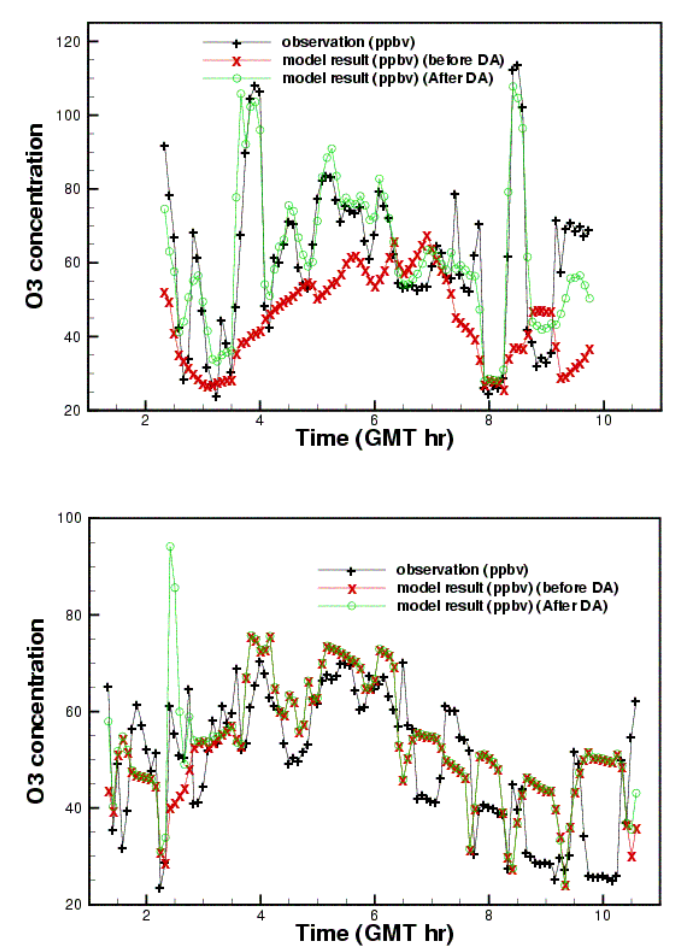
Assimilating P3-B



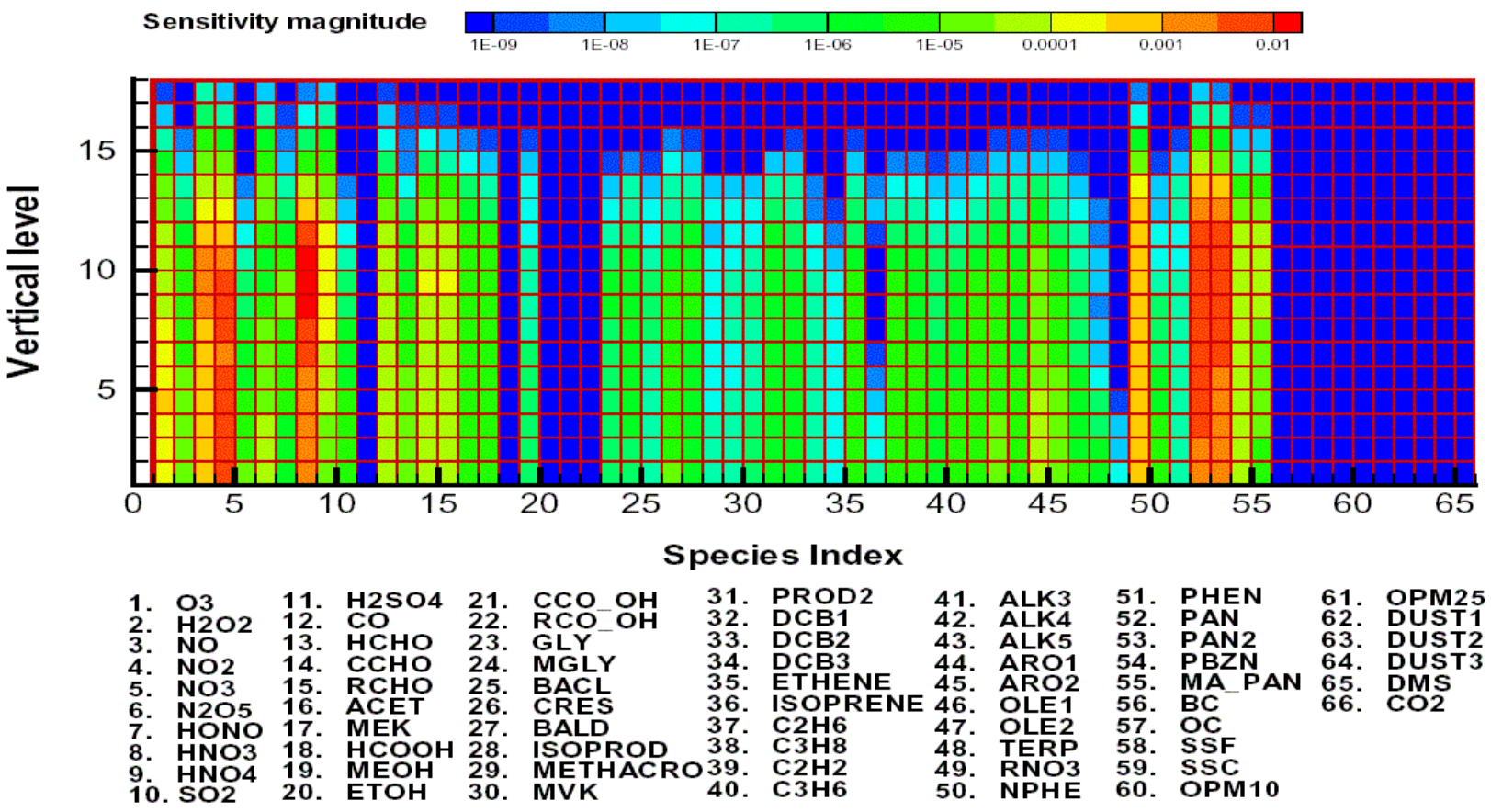
Observations from DC-8 and their model counterparts

Assimilating different flights





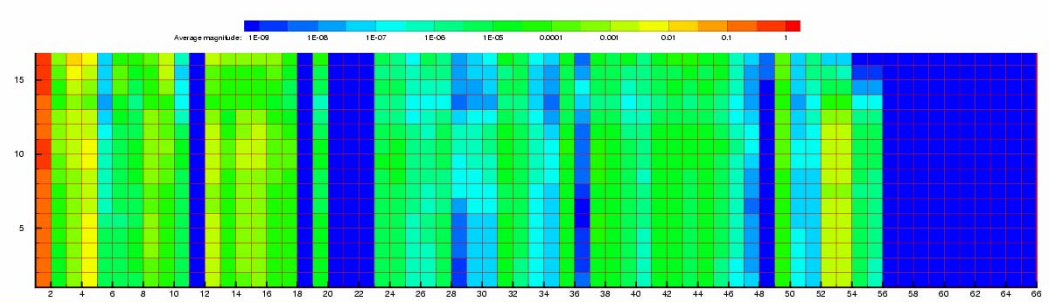
Sensitivity Analysis



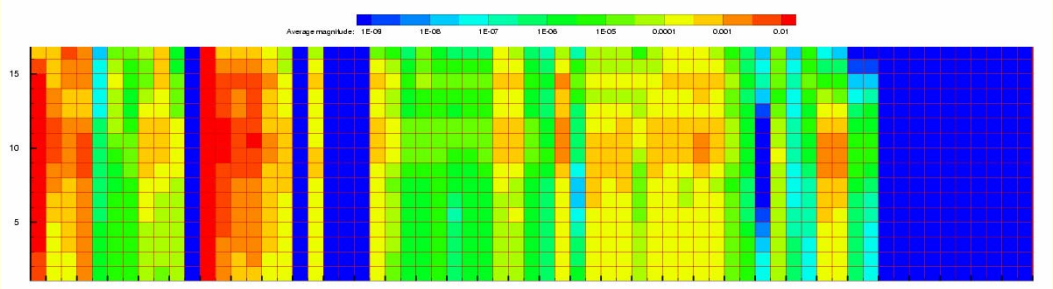
Adjoint sensitivities identify key species affecting model predictions (NOy of P3-B).

Sensitivities

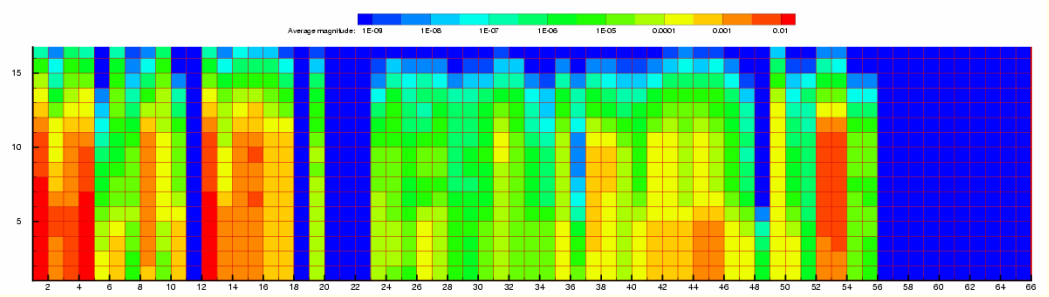
O_3



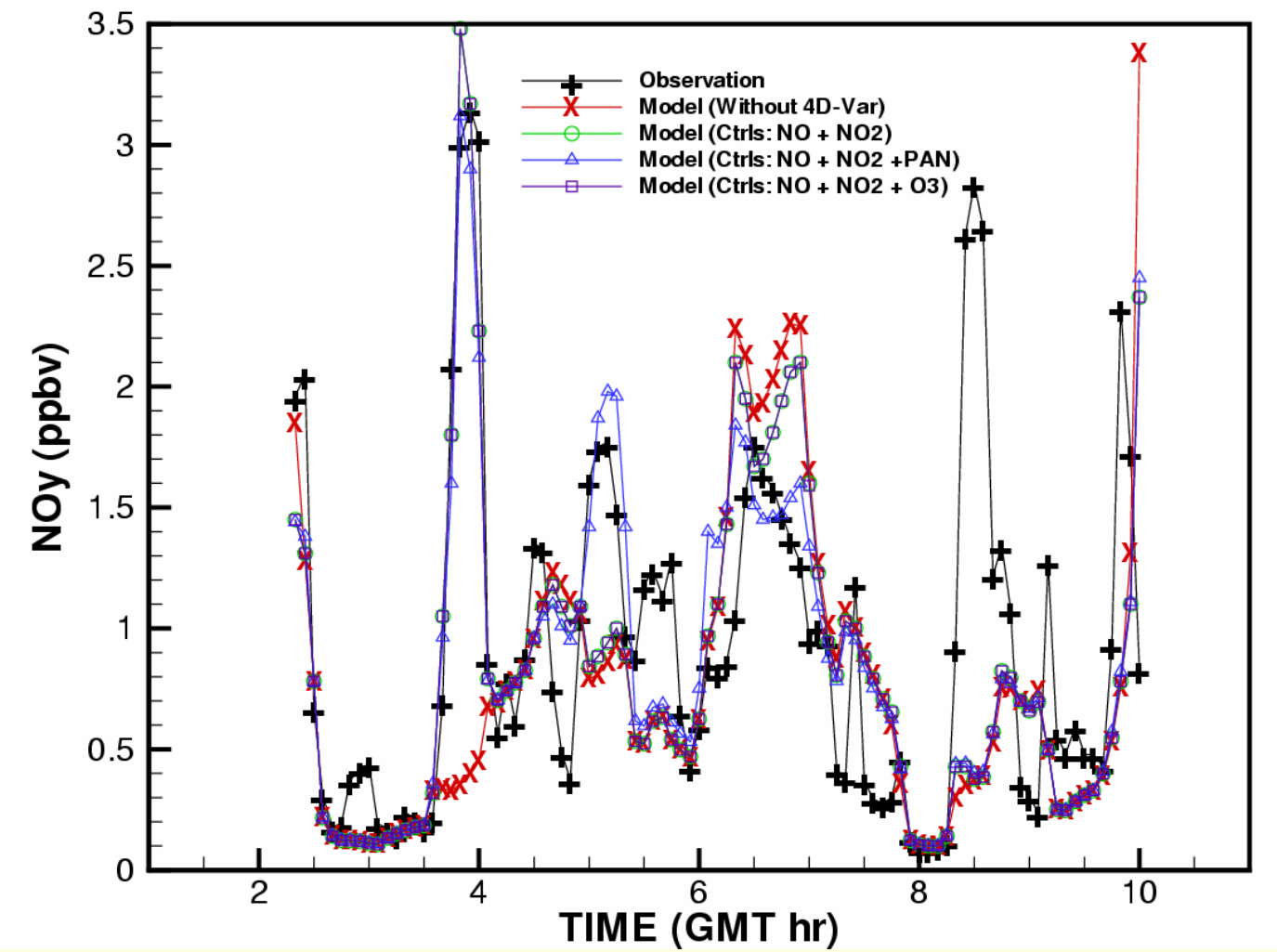
CO



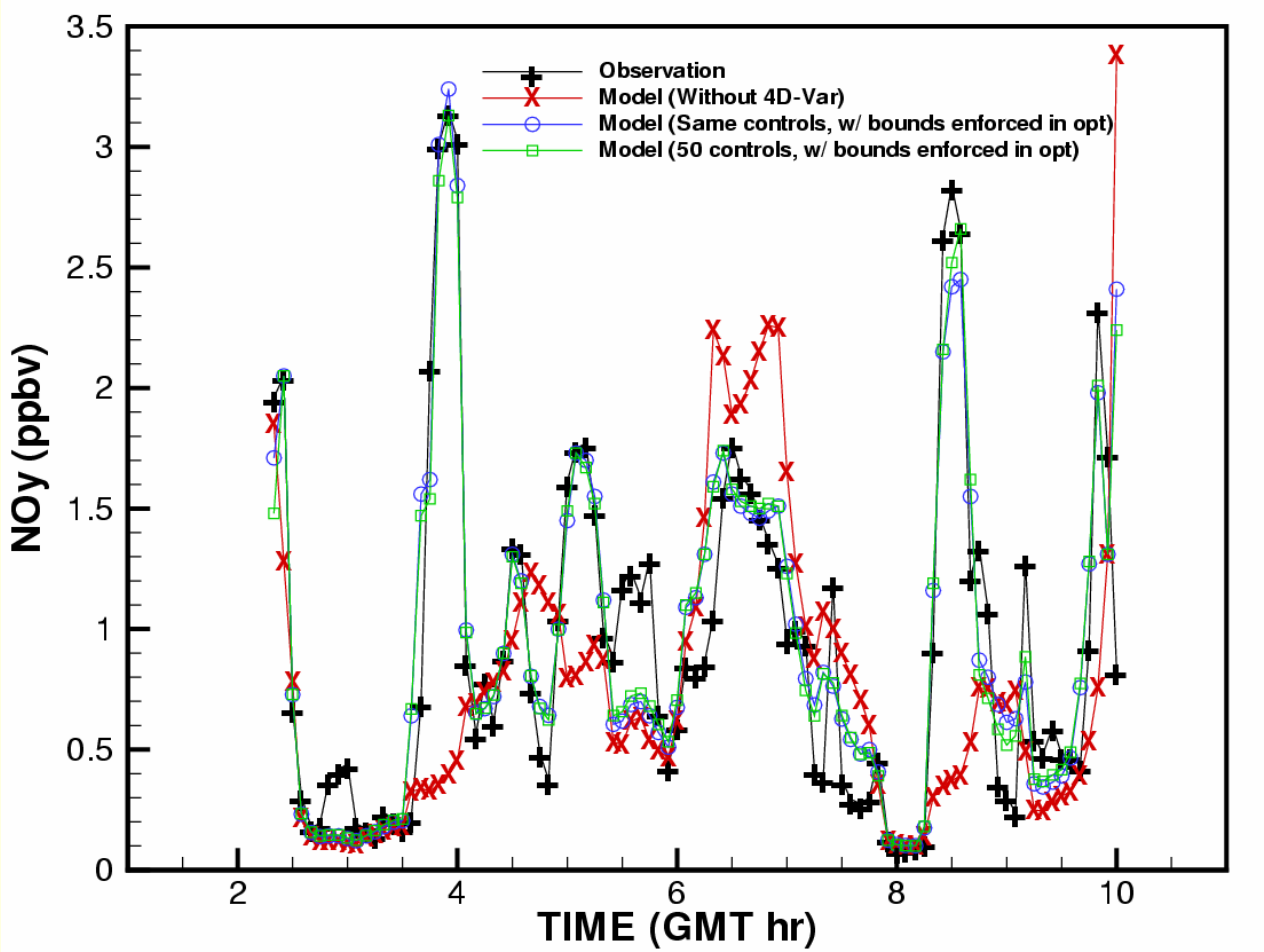
NO_2



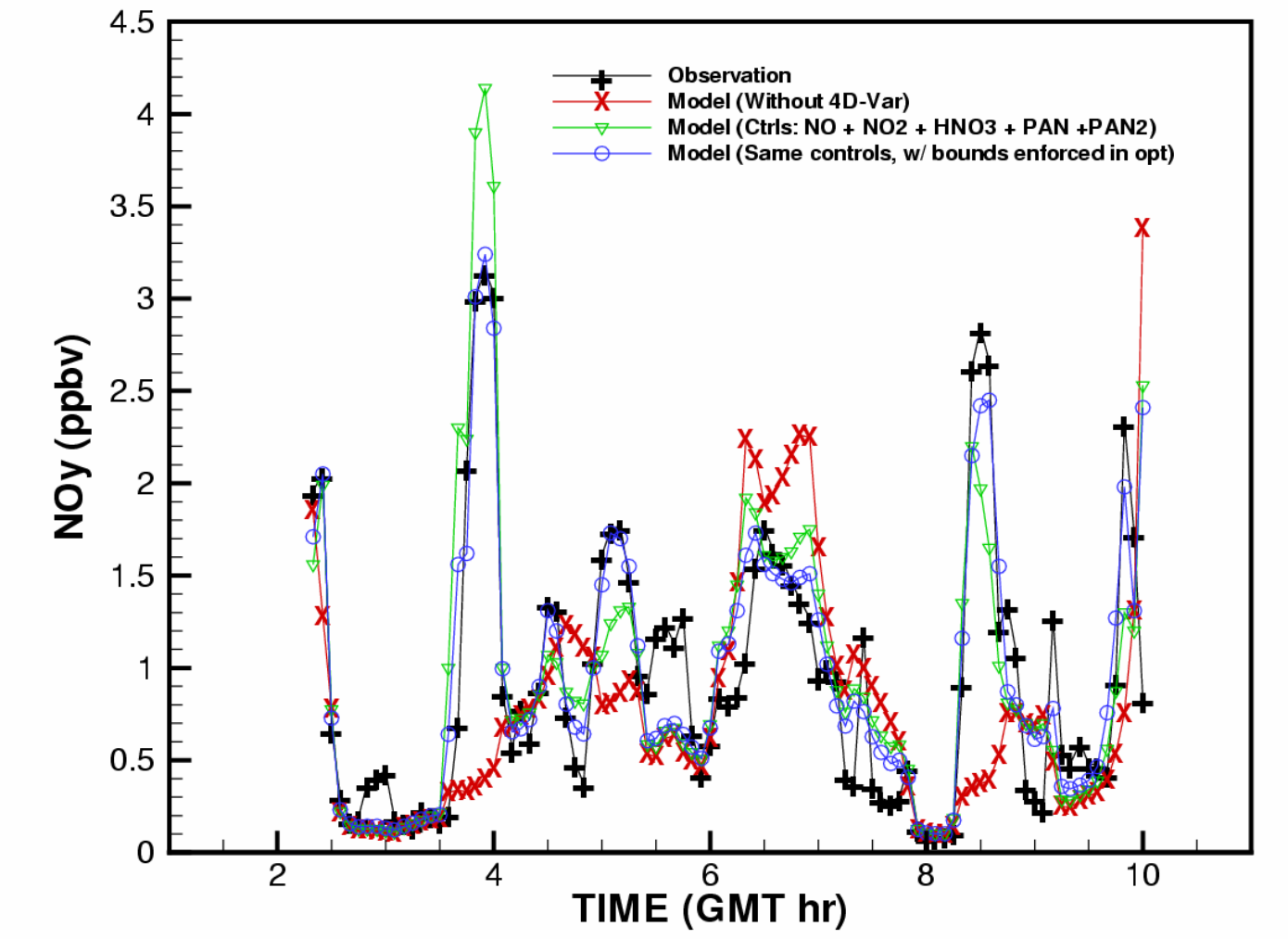
Choice of control variables



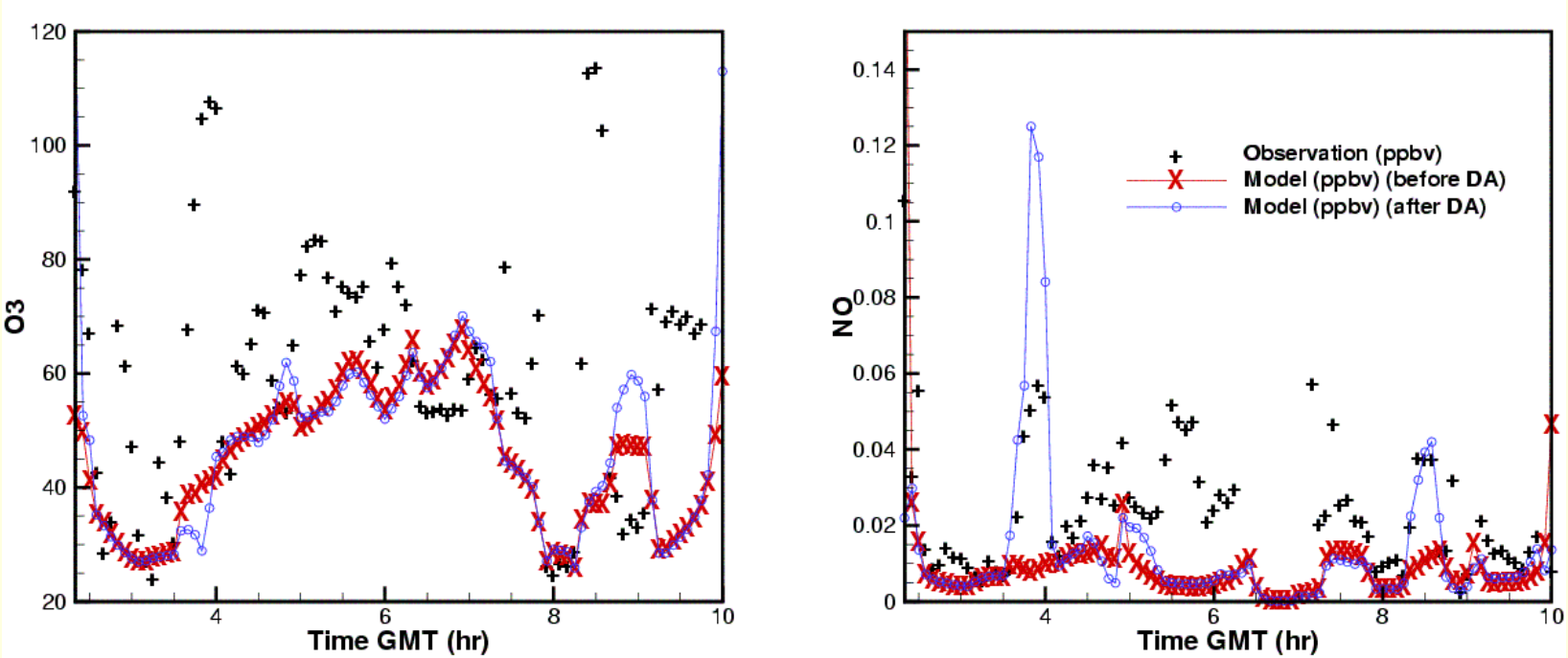
Choice of control variables (continued)



Effect of "B" in l-BFGS-B



Assimilating NOy (P3)



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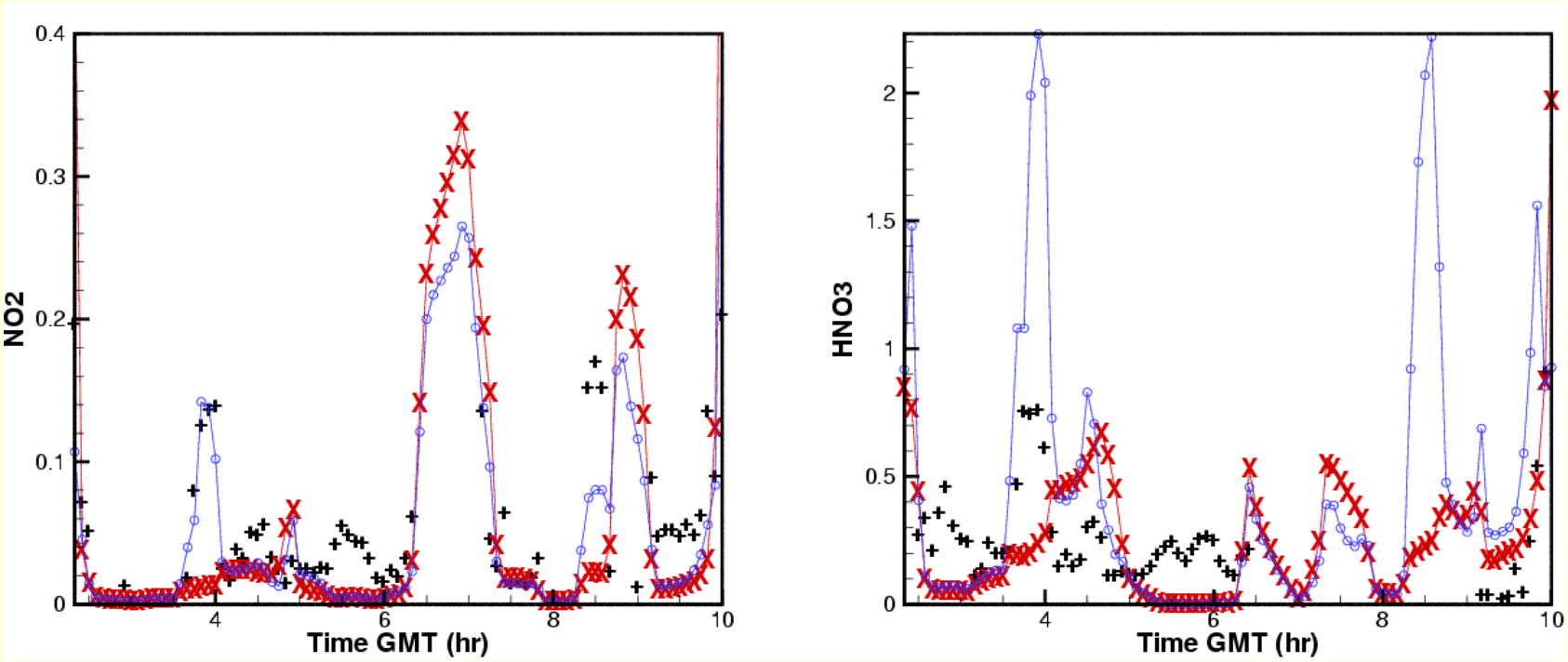

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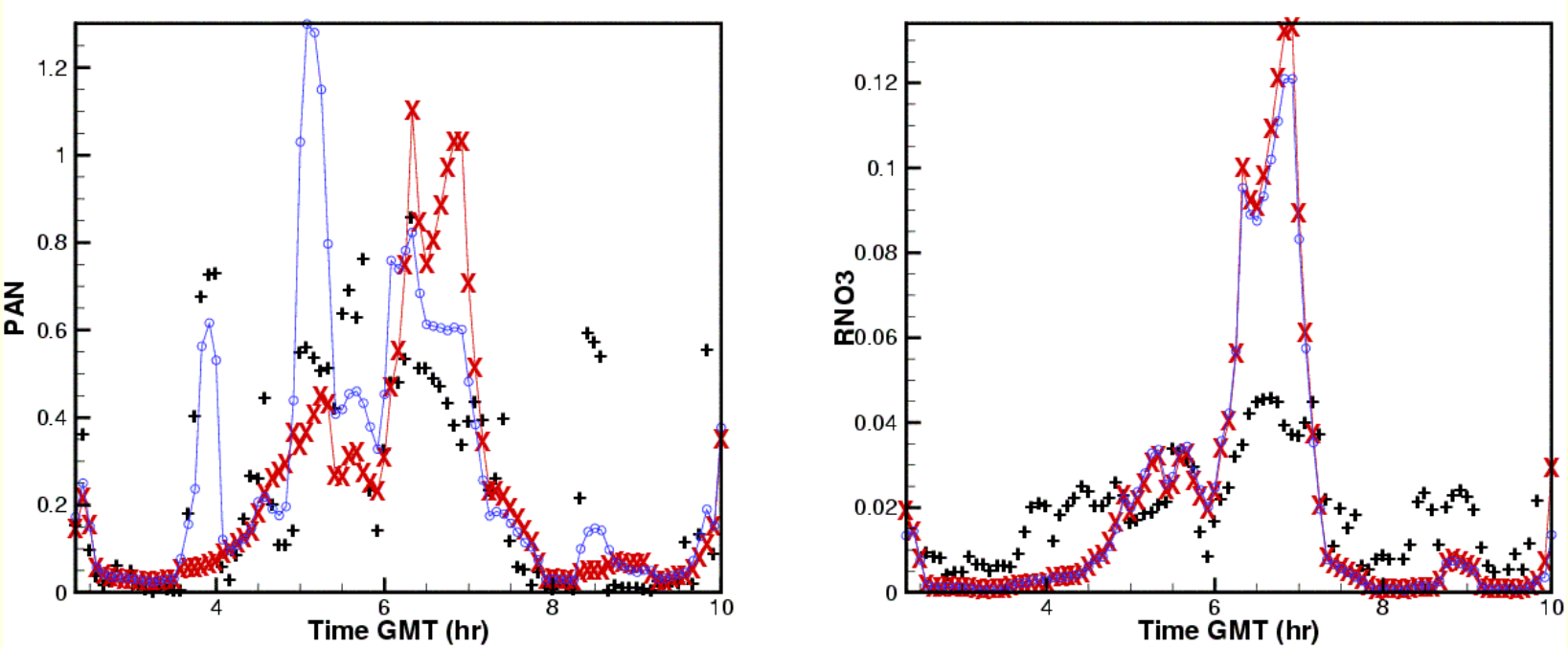
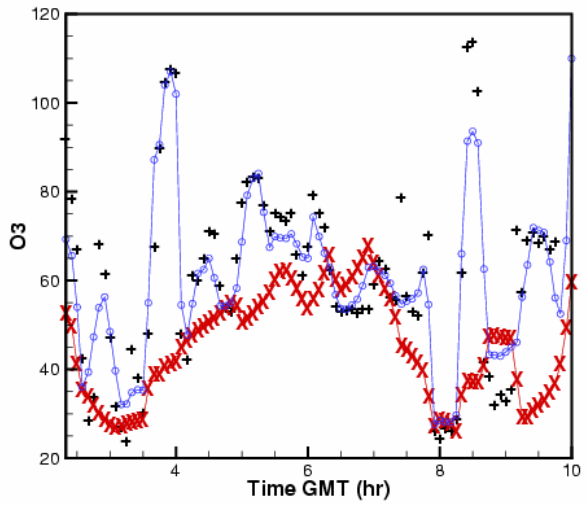
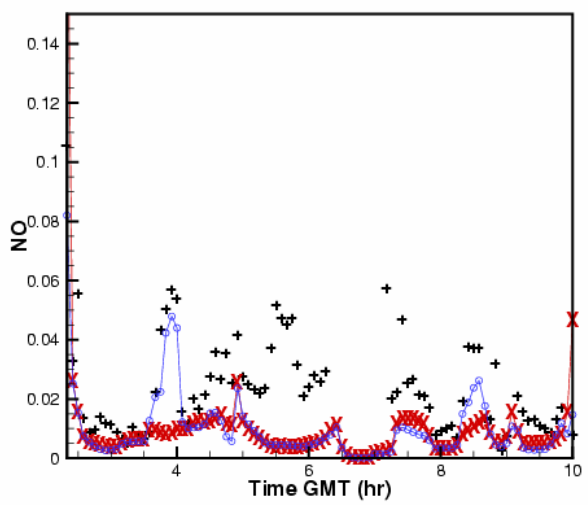
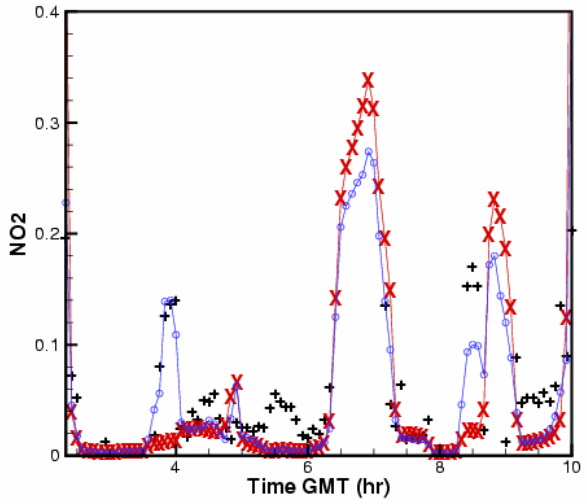
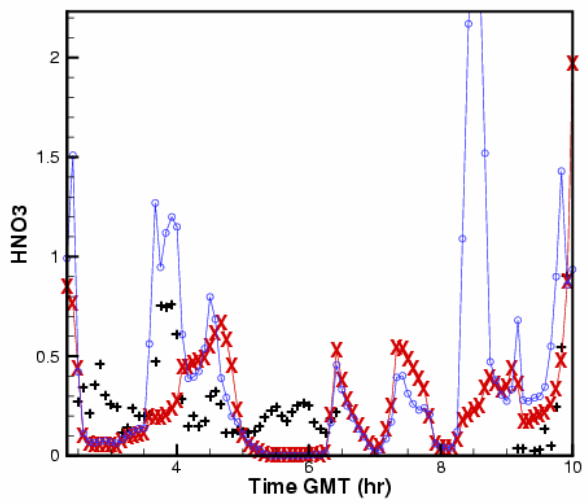


Assimilating multiple species









Measurement uncertainties:

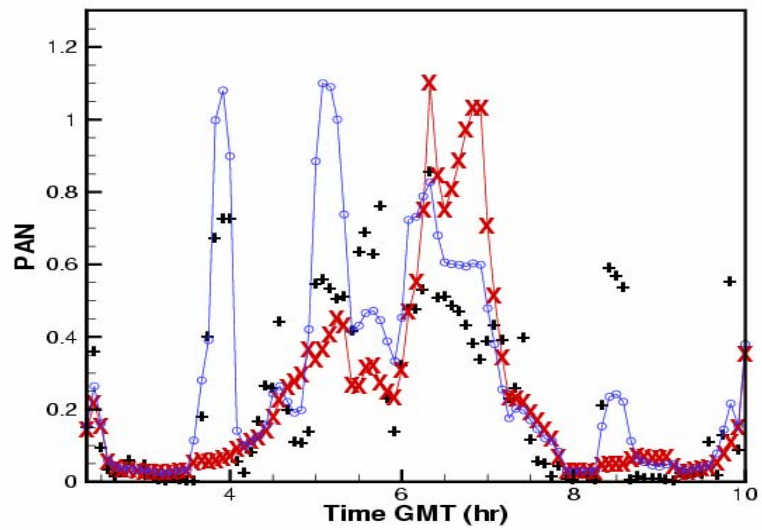
O3:	8%
NO:	20%
NO2:	20%
HNO3:	100%
PAN:	100%
RNO3:	100%

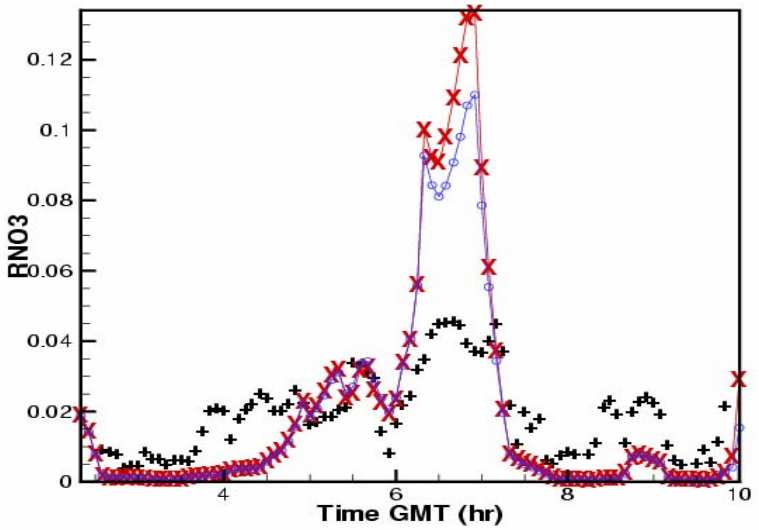
Conclusions

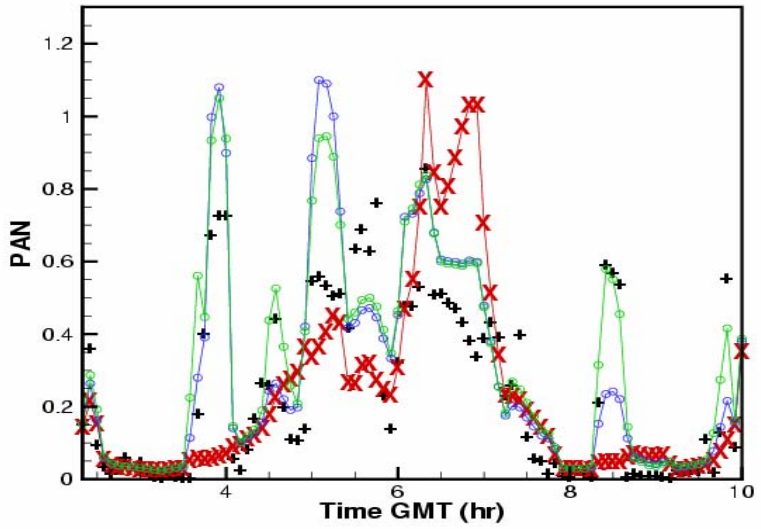
- The current 4D-Var system is able to perform general data assimilation tasks (observations can be multiple, indirect, at any time, any location)
- Adjoint sensitivity analysis is computationally efficient, and gives valuable information
- By only adjusting initial concentrations, 4D-Var assimilation tests are able to match observations
- Assimilating observations help to improve some model predictions, but the impact is not significant for 1-D flight observations
- 4D-Var is time consuming

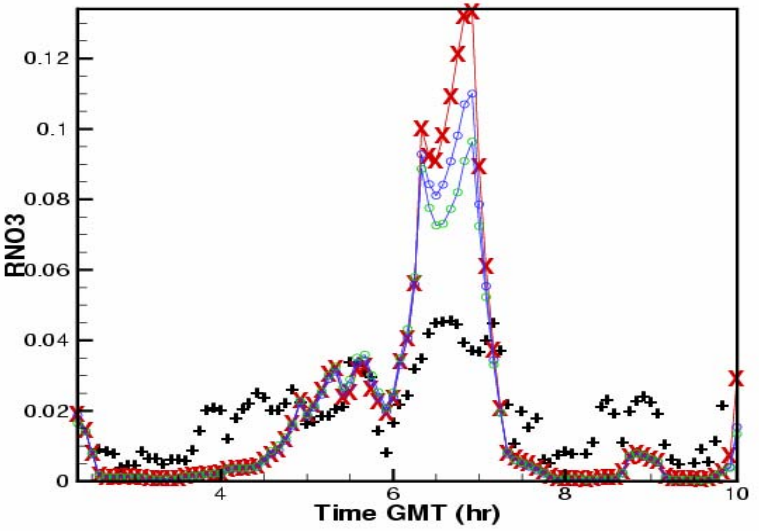
Assimilating multiple species

(In lower panels, green lines shows the effect of more iterations)

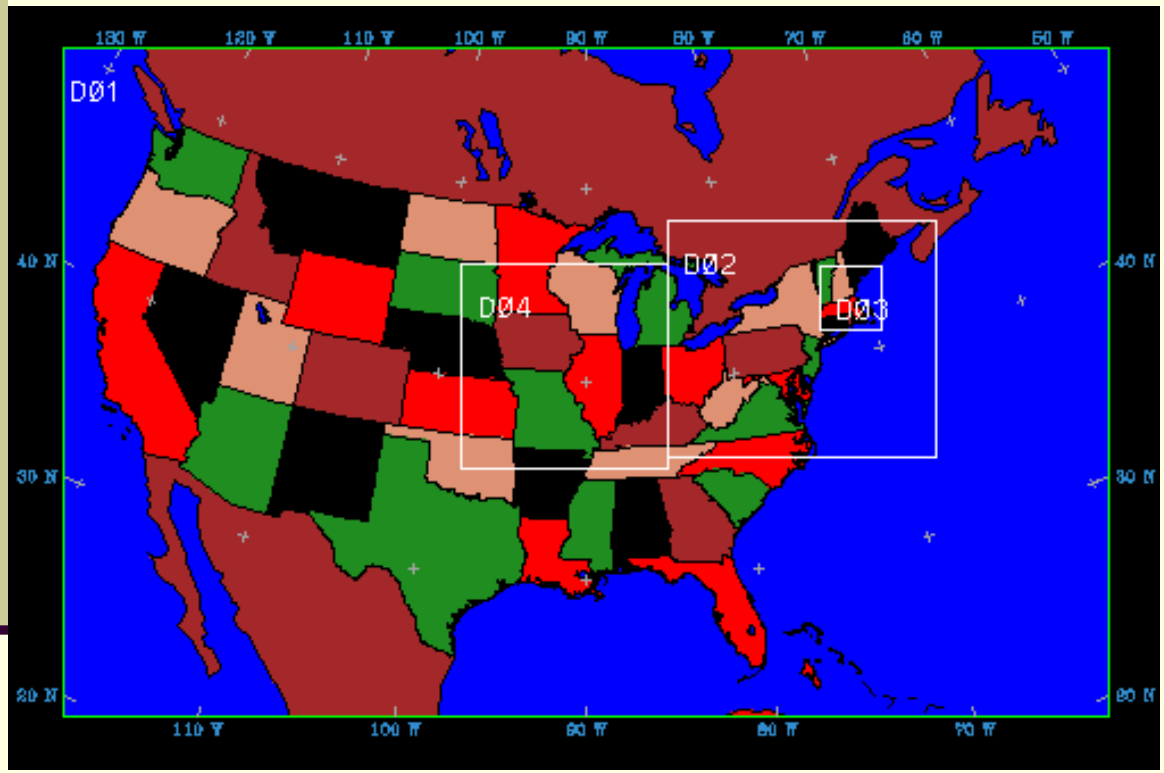








ICARTT forecasting (ongoing)



Hourly O_3 measurements at ~1500 surface stations.

Domain:
D02
(~300 stations)

Grid size:
25 × 22 × 20
(60km × 60km)

DA window:
24 hrs
(0~23 EDT)

Forecasting:
72 hrs
(easy to change)

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- Adjoint sensitivity analysis is computationally efficient, and gives valuable information
- By only adjusting initial concentrations, 4D-Var assimilation tests are able to match observations
- Assimilating observations help to improve some model predictions, but the impact is not significant for 1-D flight observations
- 4D-Var is time consuming

Future work

- Background error statistics need to be considered, e.g. using NMC method or ensemble methods
- Emissions can be estimated in the 4D-Var frame work, and possibly lateral boundary conditions for regional models
- For operational forecasting, the 4D-Var can be simplified to run faster (incremental 4D-Var)
- Model error and parameter uncertainty can be studied and calibrated
- It is possible to have a hybrid method, combining the benefit of EnKF, which explicitly gives the error propagation

Thank you!