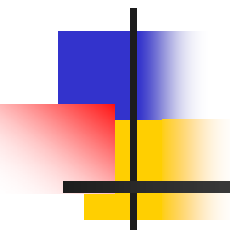


NSF ITR/AP&IM 0205198
**Development of a General Computational
Framework for the Optimal Integration
of Atmospheric Chemical Transport Models
and Measurements Using Adjoint**



G.R. Carmichael: *University of Iowa*

A. Sandu: *Virginia Tech*

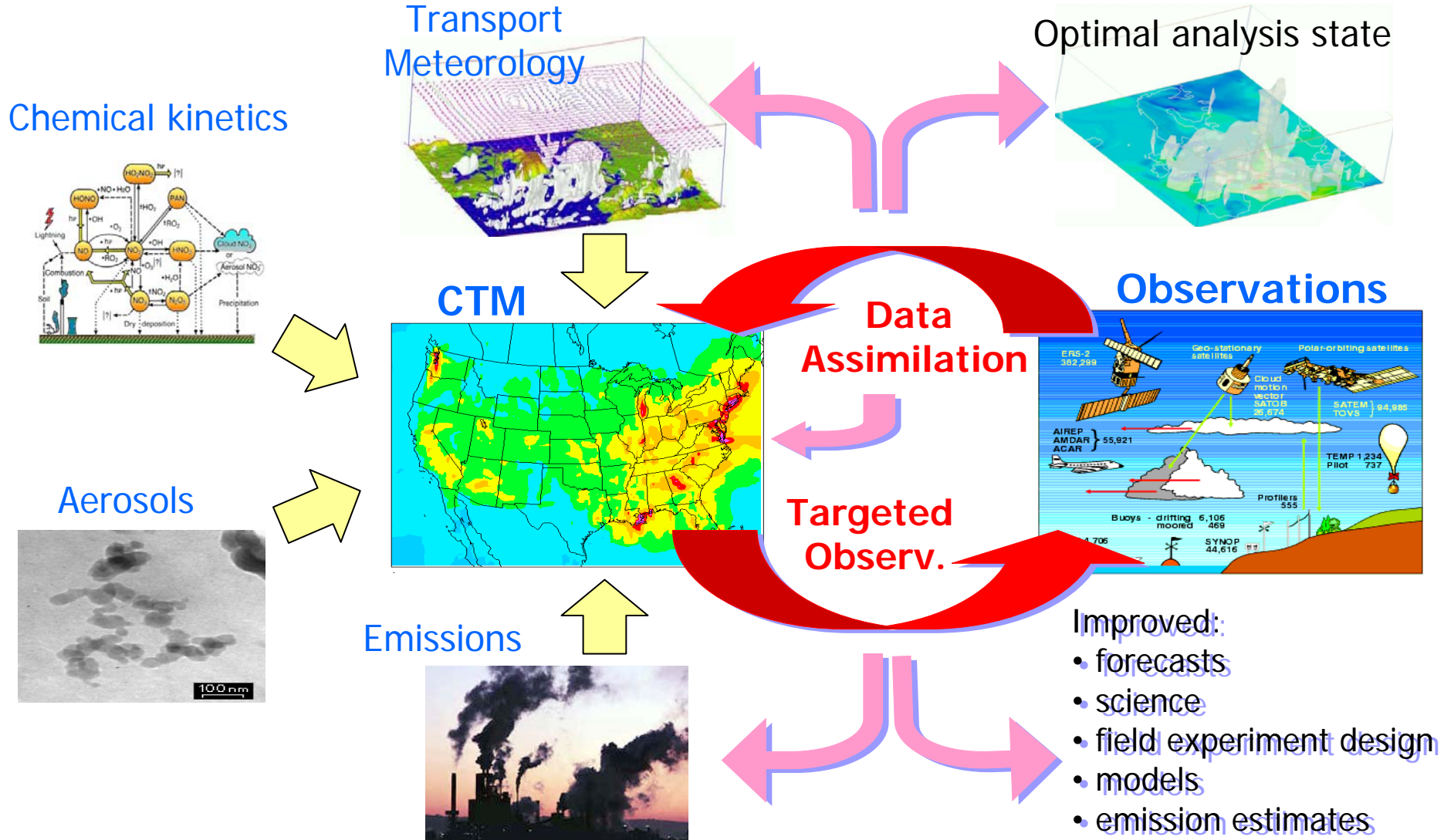
J.H. Seinfeld: *Caltech*

D. Daescu: *Portland State University*

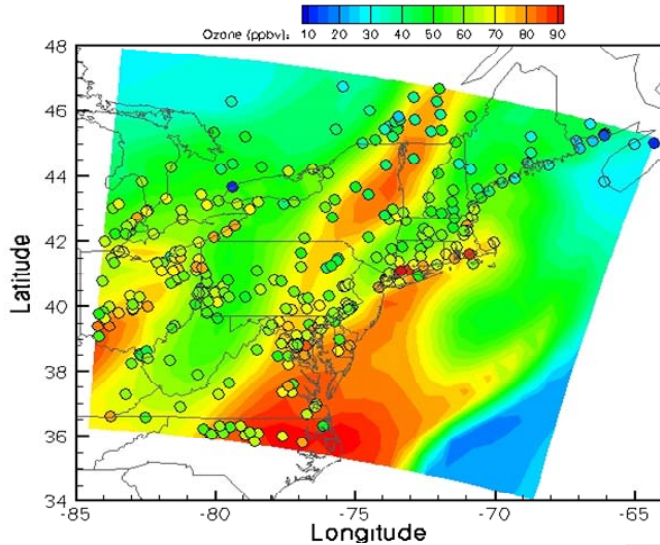
P. Hess: NCAR

T. Anderson: University of Washington

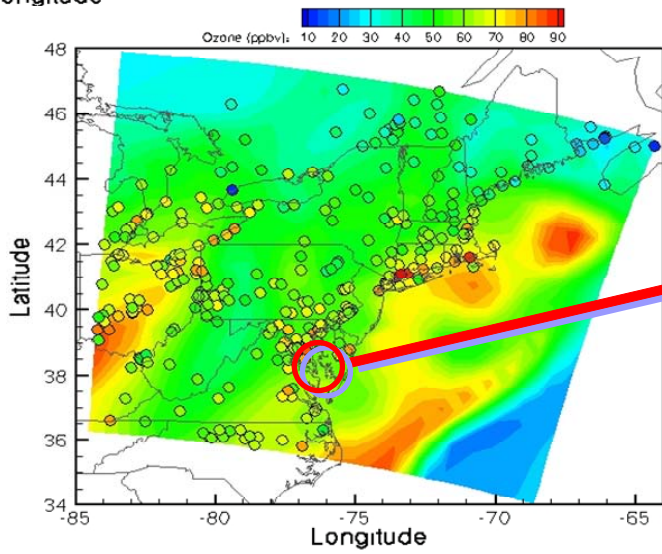
Goal: develop tools for assimilation of atmos. chemical/optical measurements in models



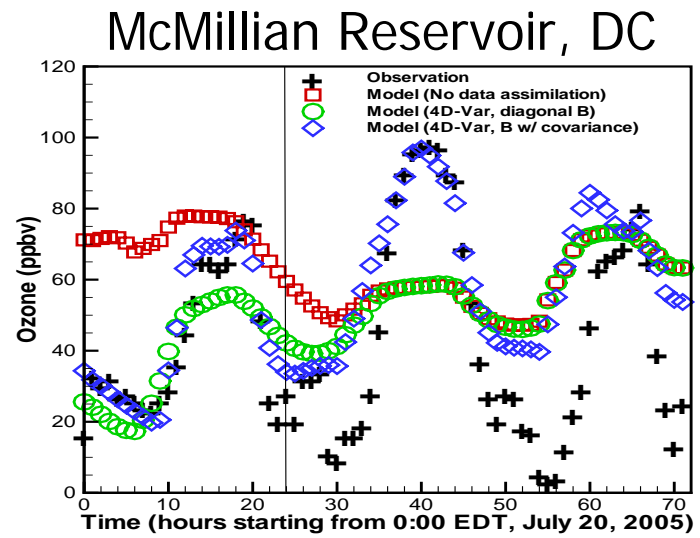
Better air quality analyses and forecasts



Forecast O₃
and AirNow
surface obs.
July 20, 2004



Analysis O₃
and obs.

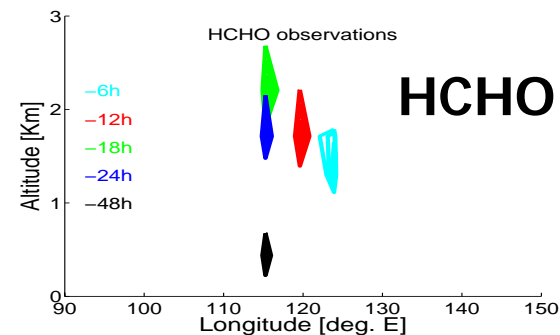
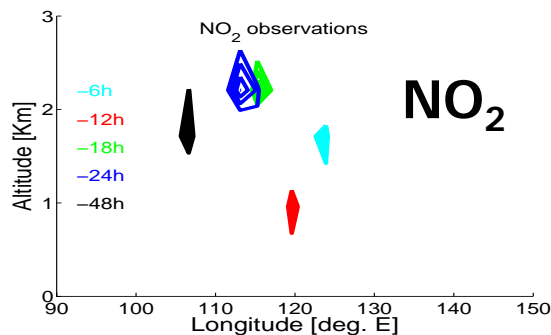
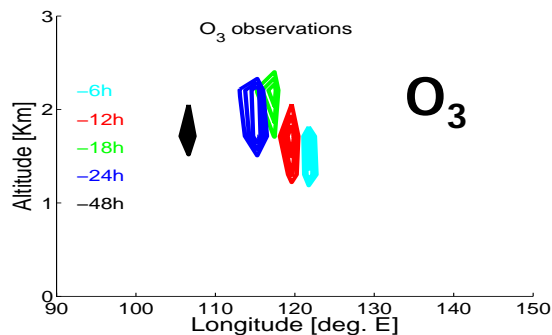
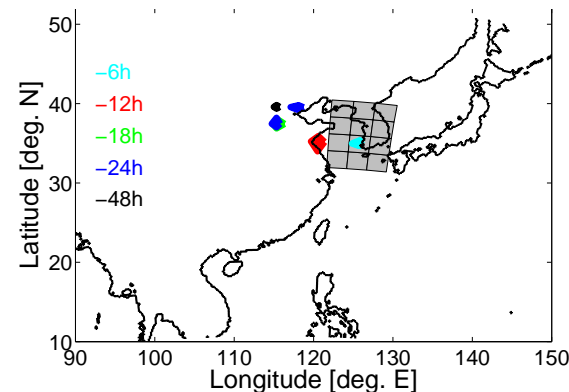
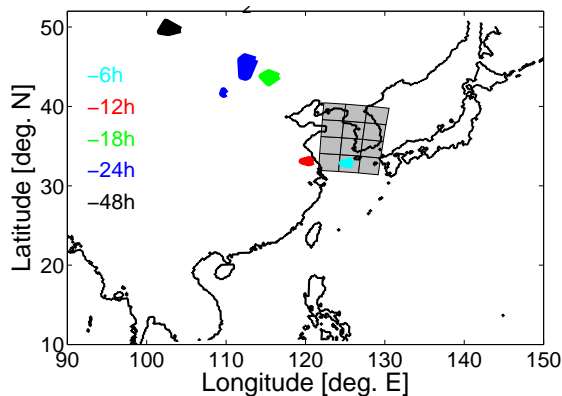
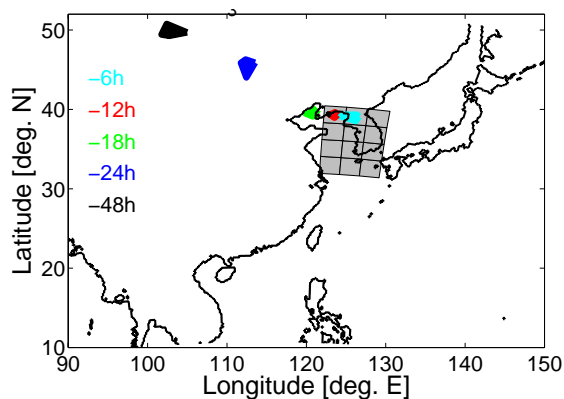


Better design of field experiments

$$T = \sum_{k \geq 1} \frac{\sigma_k^2}{\sigma_{\max}^2} s_k^2$$

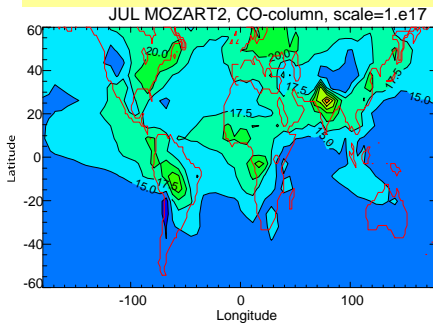
(criterion based on SVs)

Verification:
Korea, ground O₃
0 GMT, Mar/4/2001

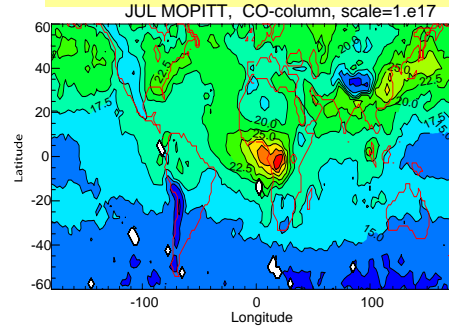


Better estimates of emission inventories

MOZART Modeled CO



MOPITT Observed CO



Inversion of multiyear
CO observations
Apr. 2000 – Dec. 2003

A priori CO emissions

North of 14°N

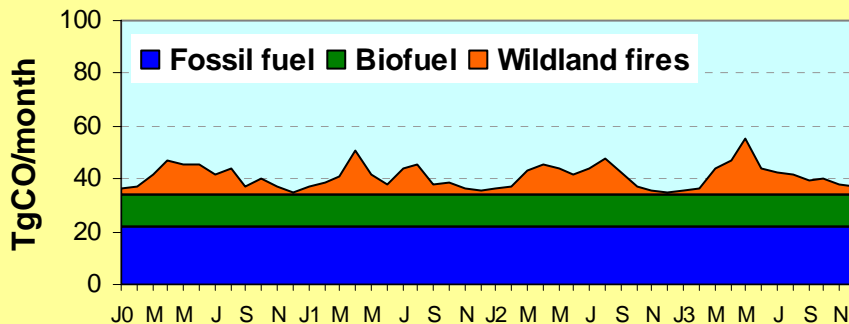


Figure 2

Optimized CO emissions

North of 14°N

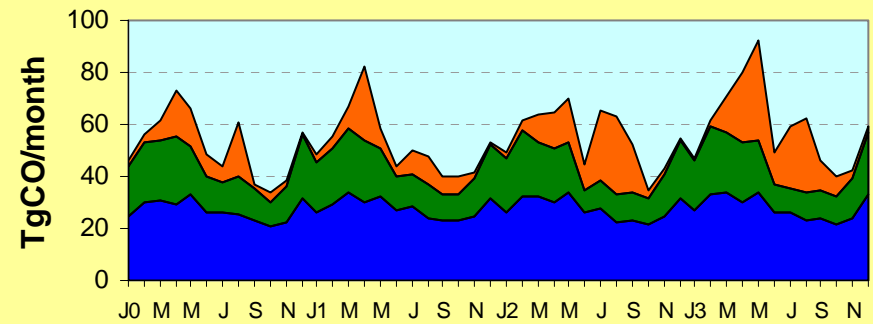
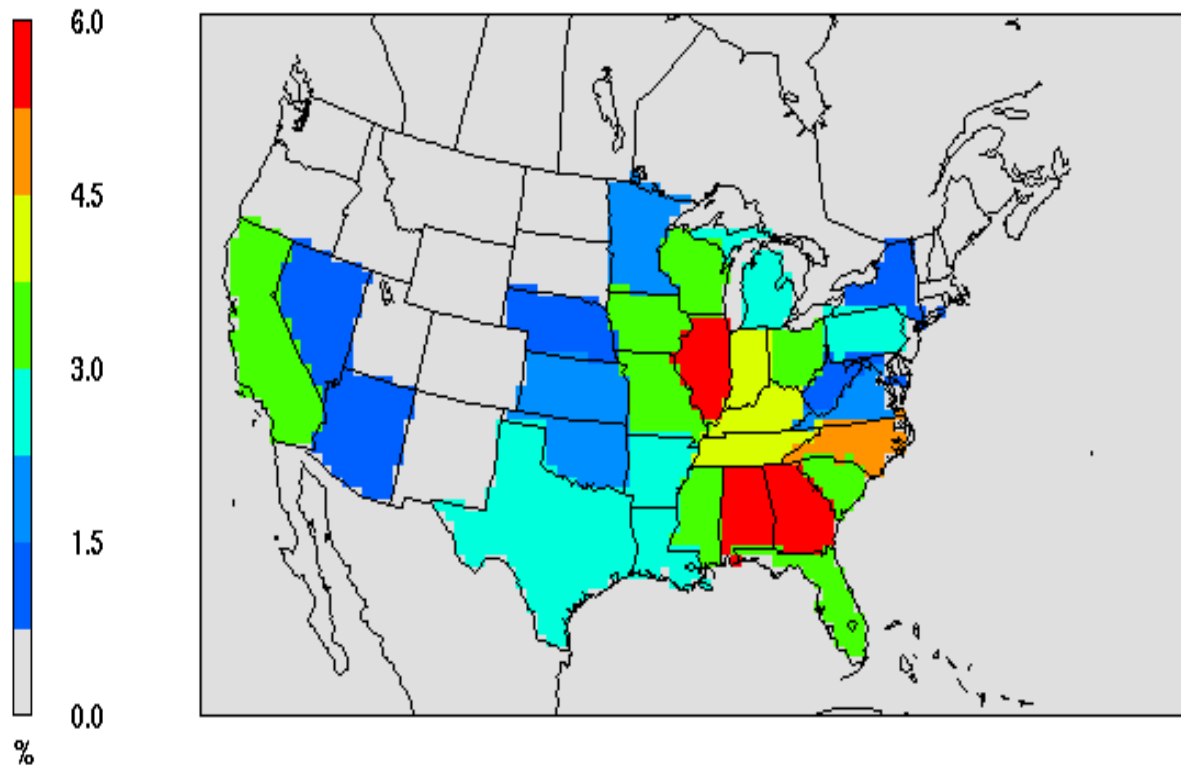


Figure 3

Better policy decisions



**State contributions
to violating U.S.
ozone National
Ambient Air
Quality Standard
in July 2004**

Broader impact of the project

Tools are being adopted by:

EPA (CMAQ), JPL (GEOS-Chem), NCAR and NOAA (WRF-Chem), Canadian Meteorological Centre, Max Planck Institute Germany (MESSY), University of Koeln (EURAD - EUROpean Air Pollution Dispersion)

Representative journal publications (20)

- Z. Liu and A. Sandu: "Analysis of Discrete Adjoint of Numerical Methods for the Advection Equation". *SIAM J. NA*, in review.
- A. Sandu and R. Sander: "Simulating Chemical Kinetic Systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1". *Atmospheric Chemistry and Physics*, 2006.
- W. Liao, A. Sandu, G.R. Carmichael and T. Chai: "Singular Vector Analysis for Atmospheric Chemical Transport Models". *Monthly Weather Review*, 2006.
- T. Chai, G.R. Carmichael, A. Sandu, Y. Tang, and D.N. Daescu: "Chemical Data Assimilation with TRACE-P Flight Measurements". *Journal of Geophysical Research*, 2006.
- A. Hakami, D.K. Henze, J.H. Seinfeld, T. Chai, Y. Tang, G.R. Carmichael, and A. Sandu: "Adjoint Inverse Modeling of Black Carbon During ACE-Asia". *Journal of Geophysical Research*, Vol. 110, No. D14, D14301, doi:10.1029/2004JD005671, 2005.
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- A. Sandu, W. Liao, G.R. Carmichael, D.K. Henze, and J.H. Seinfeld: "Inverse Modeling of Aerosol Dynamics using Adjoint - Theoretical and Numerical Considerations", *Aerosol Science and Technology*, Vol. 39, p. 1-18, DOI:10.1080/02786820500182289, 2005.
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