THE CMAQ PLUME-IN-GRID MODELING EFFORT : OVERVIEW , RESULTS, AND RESEARCH ACTIVITIES

Jim Godowitch*
Atmospheric Sciences Modeling Division
NOAA - Air Resources Laboratory
Research Triangle Park, NC

* On assignment to the National Exposure Research Laboratory, U.S. EPA.

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Key Objective of Plume-in-Grid (PinG) Effort :

*** Provide a realistic scientific sub-grid scale modeling treatment of the physical and chemical processes governing the pollutant concentrations contained in major point source plumes within regional Eulerian model domains.**

Key Aspects :

- Real-world plume growth is **gradual**
- Plumes initially considerably **smaller** than typical grid cell size
- **Excessive dilution** issue – impacts plume chemistry
  - Secondary species (O_3 , HNO_3) formation accelerated
- Improved boundary conditions needed for nested fine grid domains

Key Features and Developments of the CMAQ / PinG Model

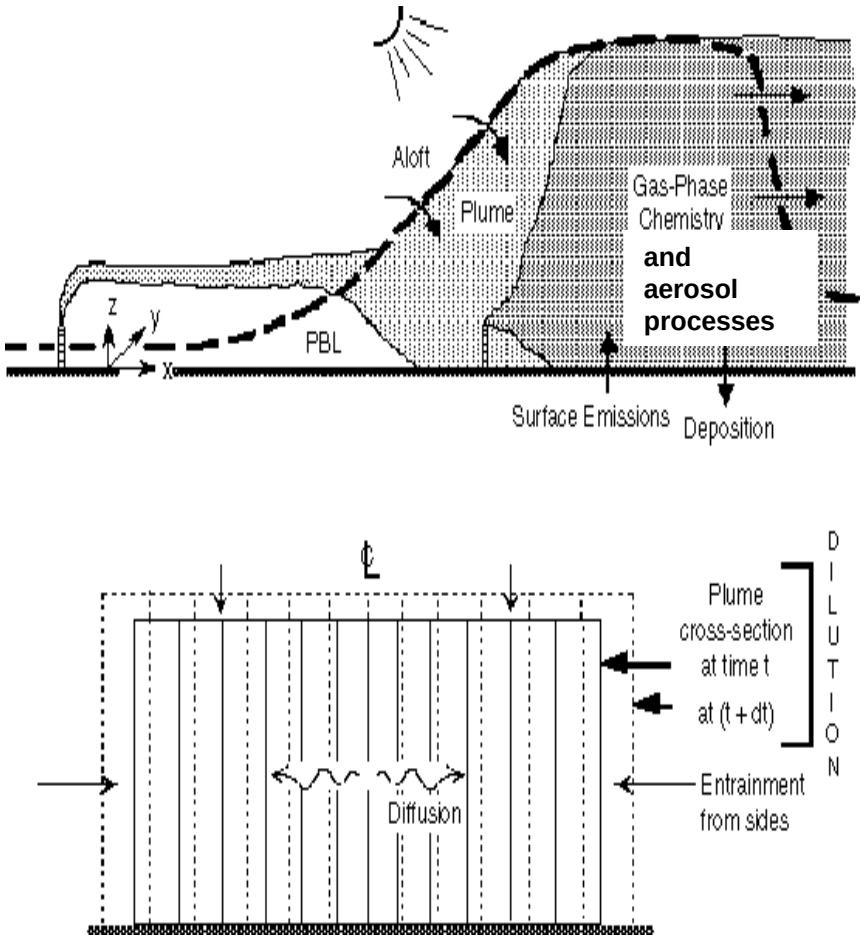
- Lagrangian plume module embedded in an Eulerian grid
- Hourly releases from multiple sources over diurnal cycle

- PinG-specific chemical solvers – QSSA, Gear, MEBI
- Continuation / restart capability
- PinG code upgrade for parallel processing (challenging)
- Include aerosol processes – AE3 modal approach

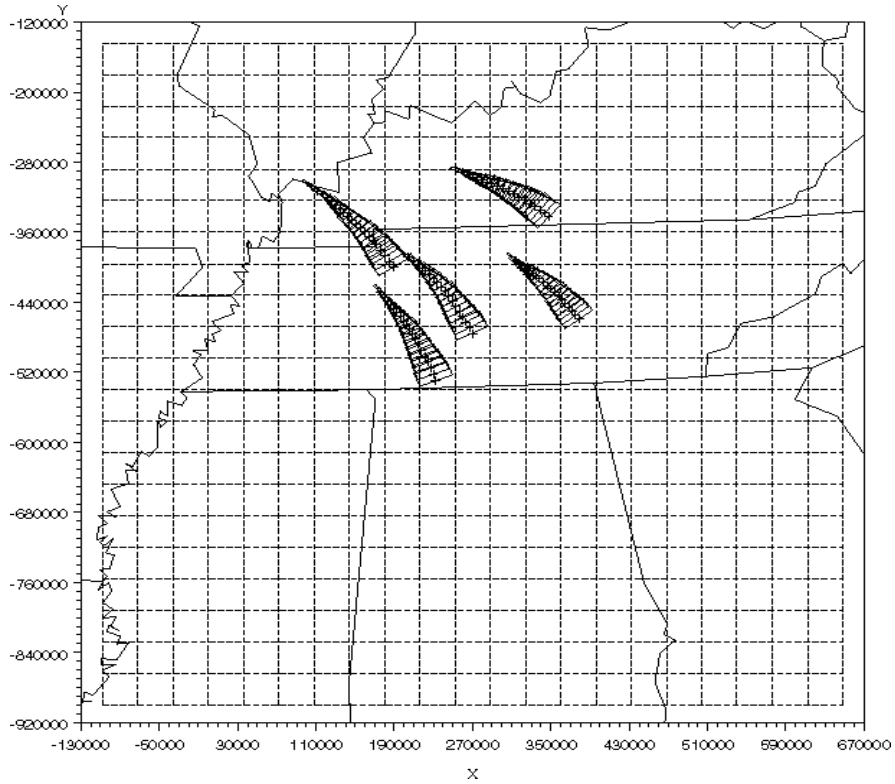
CMAQ Plume-in-Grid Modeling Effort Activities

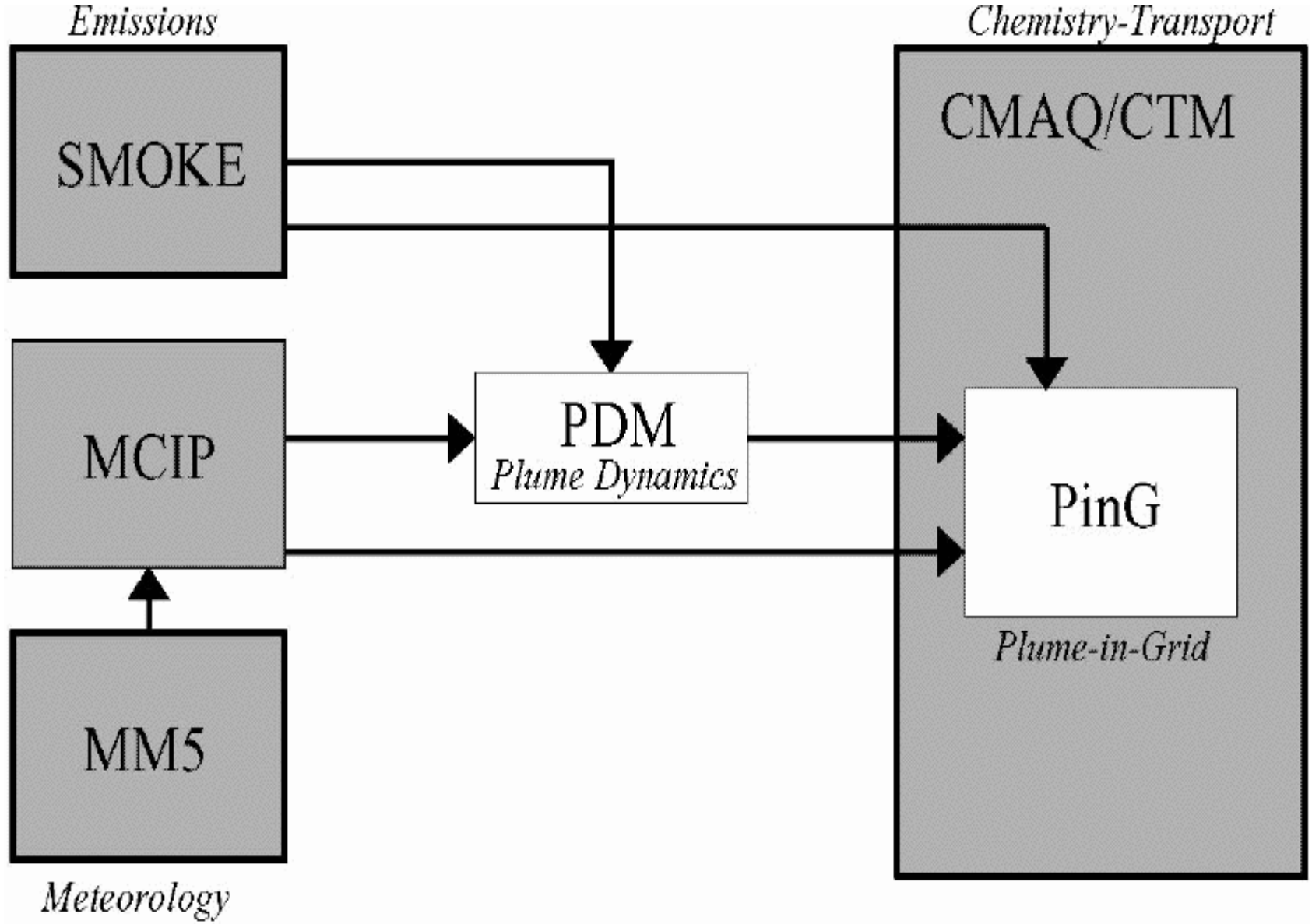
- Code revisions/upgrades and numerous test simulations
  - common domain and common case study dataset
  - different computer platforms
- Sensitivity test simulations
  - different chemical mechanisms , different chemical solvers
- Applications and evaluation activities
  - 36 km and 12 km domains (with /without PinG treatment)
  - PinG concentrations vs plume data (airborne platforms)
- Analyses techniques – statistical, graphics (SAS, PAVE), visualization (Data Explorer)

Schematic of processes treated in the CMAQ PinG model



Paths and plume growth of plume releases at 15 UTC on July 7, 1995 (Domain with 36 km grid cell size)

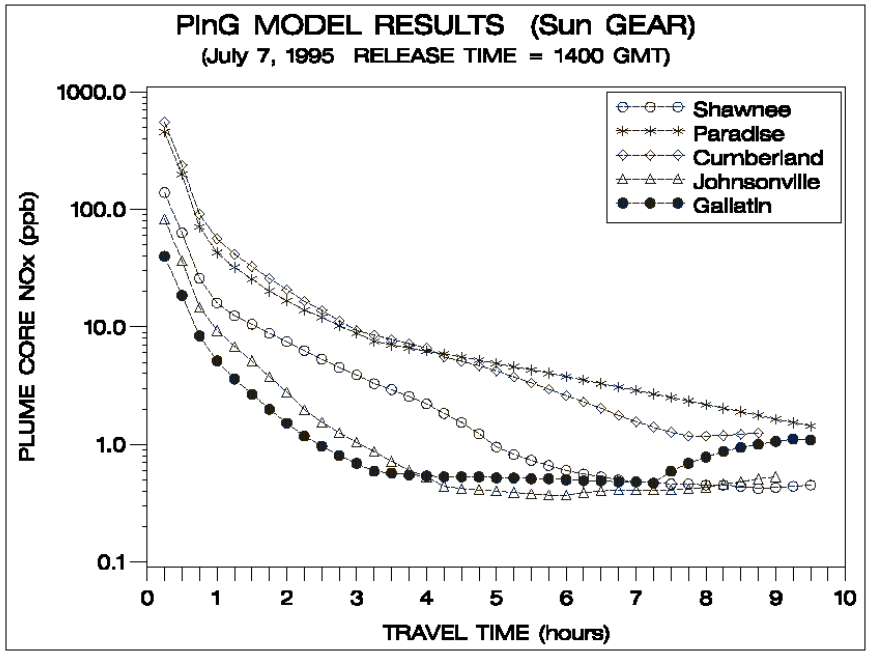



Emissions
Chemistry-Transport
SMOKE
CMAQ/CTM
MCIP
PDM
Plume Dynamics
PinG
Plume-in-Grid
MM5
Meteorology

SELECTED POWER PLANT EMISSIONS

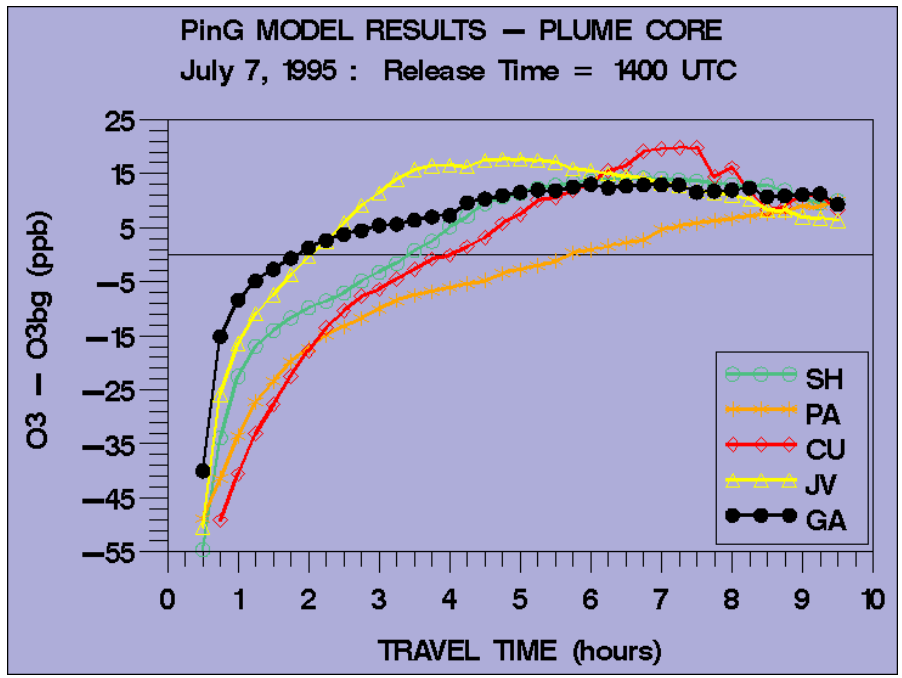
(July 7, 1995)

Source	NOx/NOx(GA)	SO_2 / NOx	$PM_{2.5}$ (Tns/day)	PM_{10} (Tns/day)
GA	1	7.3	0.6	1.7
JV	2	6.0	2.7	17.0
SH	2.9	2.3	4.6	32.1
CU	14.8	0.13	1.4	4.2
PA	14.9	1.7	0.0	0.4

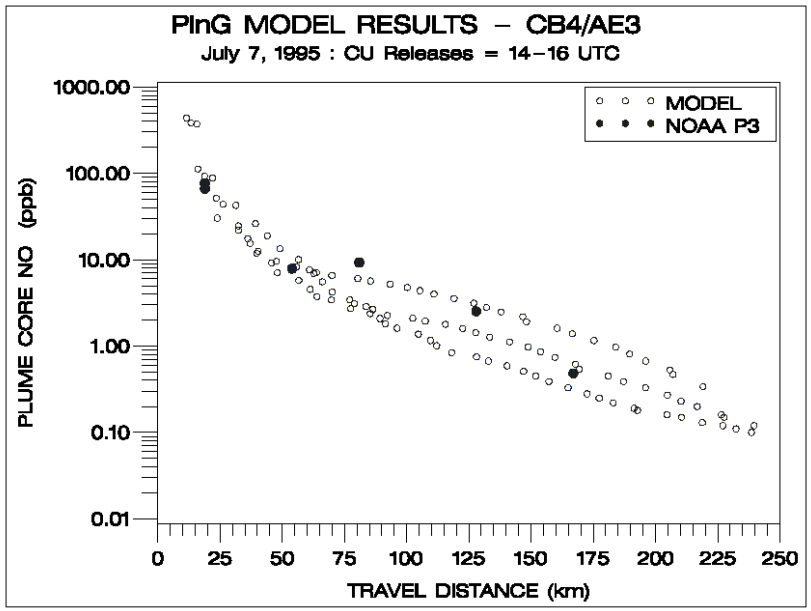


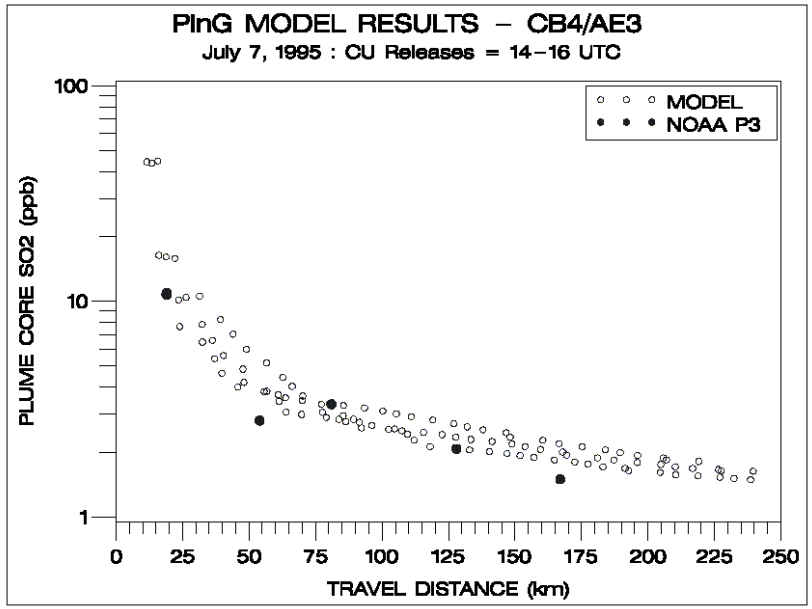
← Rate of NOx oxidation in plumes varies inversely with NOx emission rate

Ozone recovery slower and peak further downwind in → higher NOx plumes

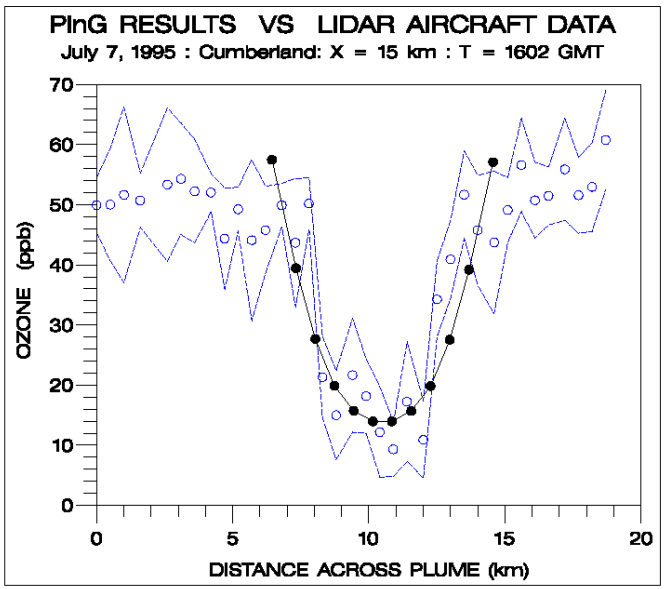


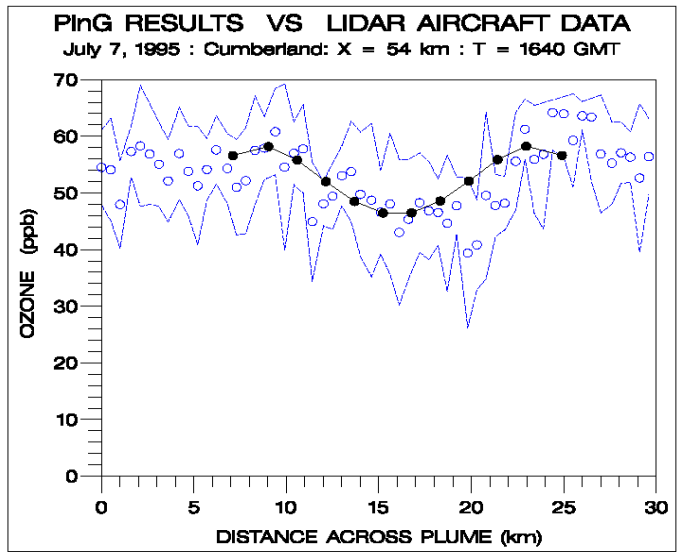
Modeled and Observed Values – Primary Pollutant Species



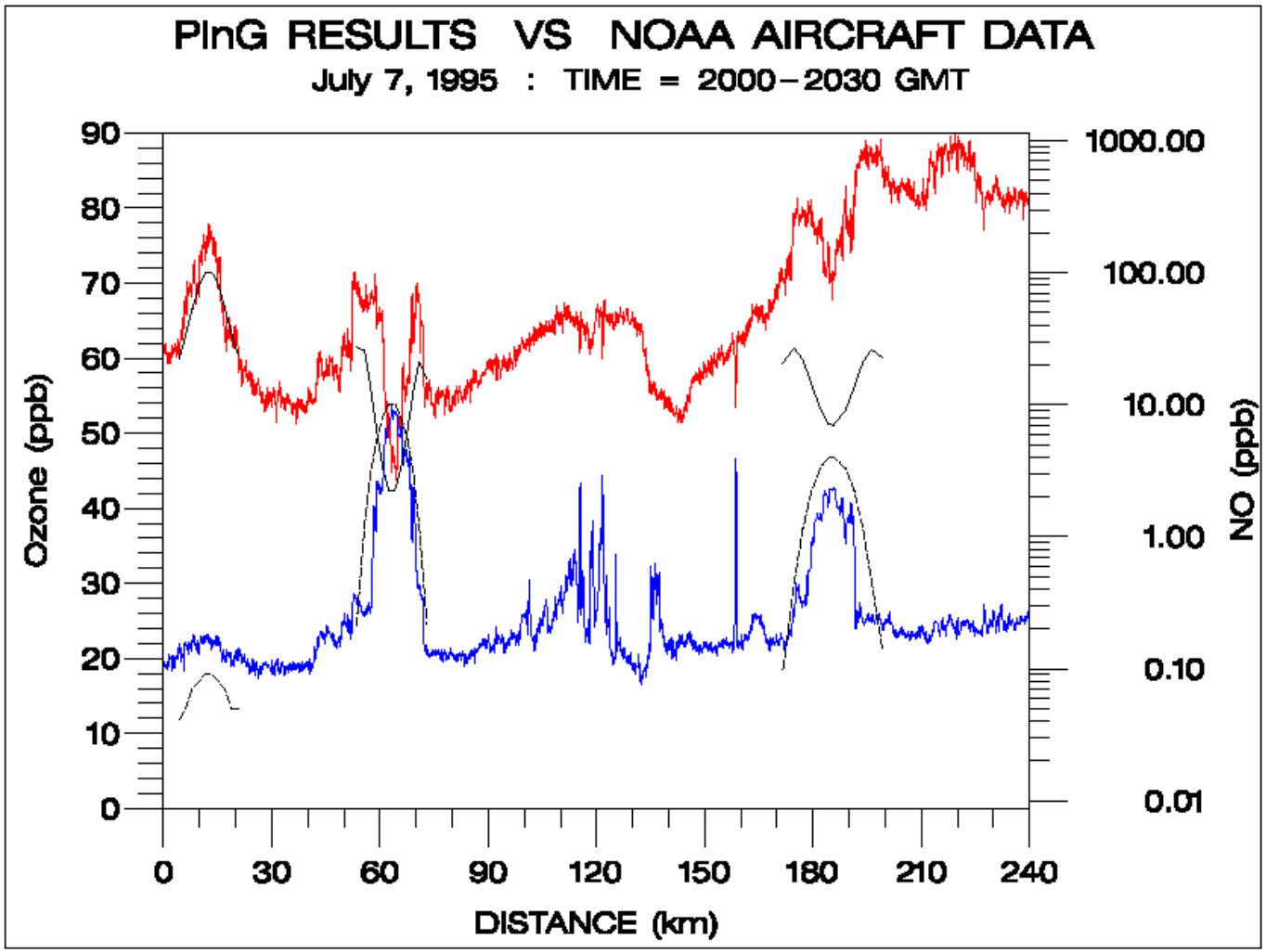


Comparisons of PinG Plume Ozone to NOAA Casa Aircraft Averaged Ozone (✂ 1 Std Dev) from Vertical Profiles

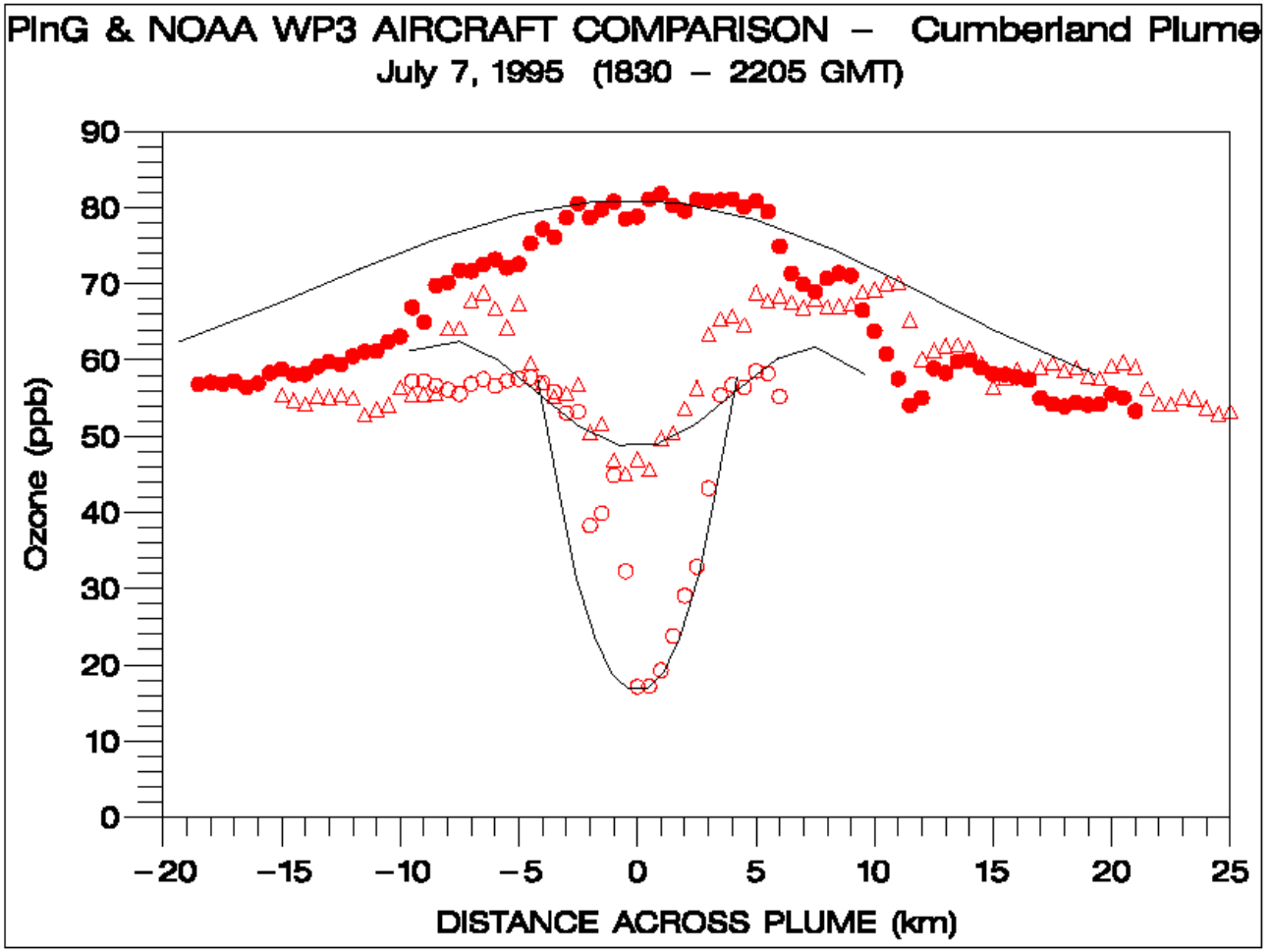




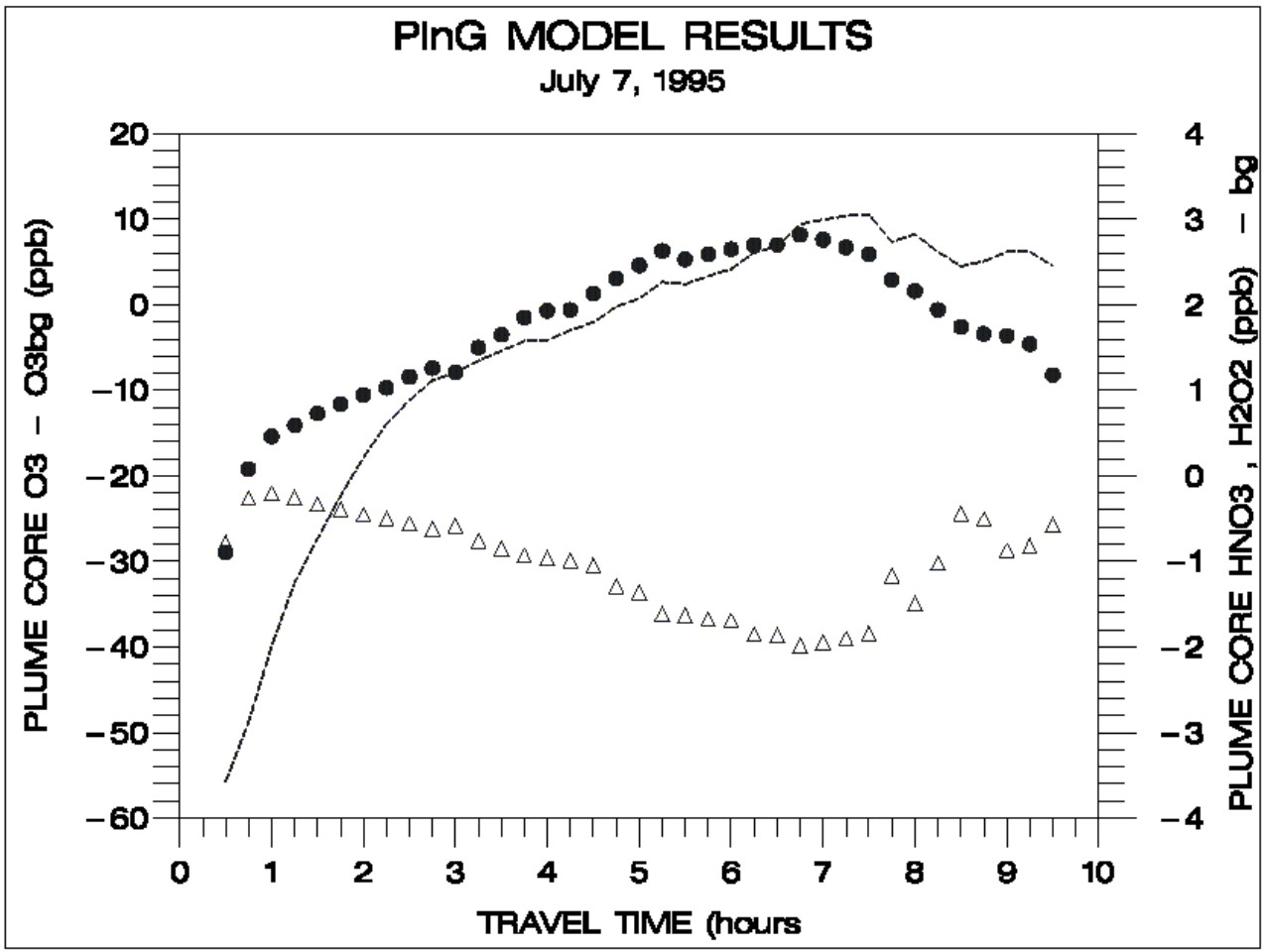
Modeled Plume Concentrations Superimposed on the Horizontal Flight Data Traversing 3 Plumes – JV, CU and PA (left to right)



PLUME OZONE AT 20 , 80, 160 KM DOWNWIND (MODEL AND DATA)



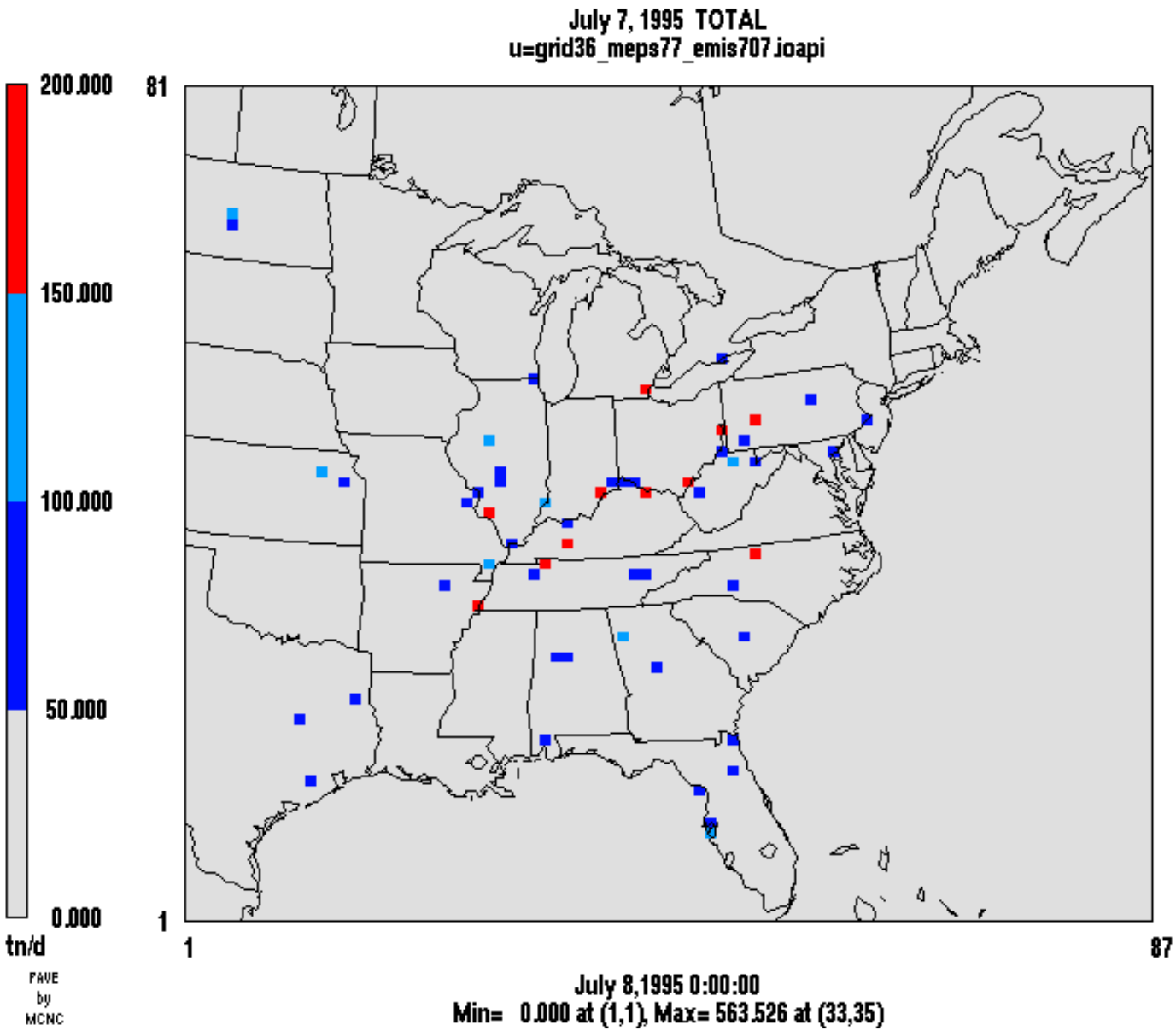
SIGNATURE OF A HIGH NOx POINT SOURCE PLUME : excess O_3 (---) and HNO_3 (•••) , H_2O_2 (◔◔◔) deficit downwind



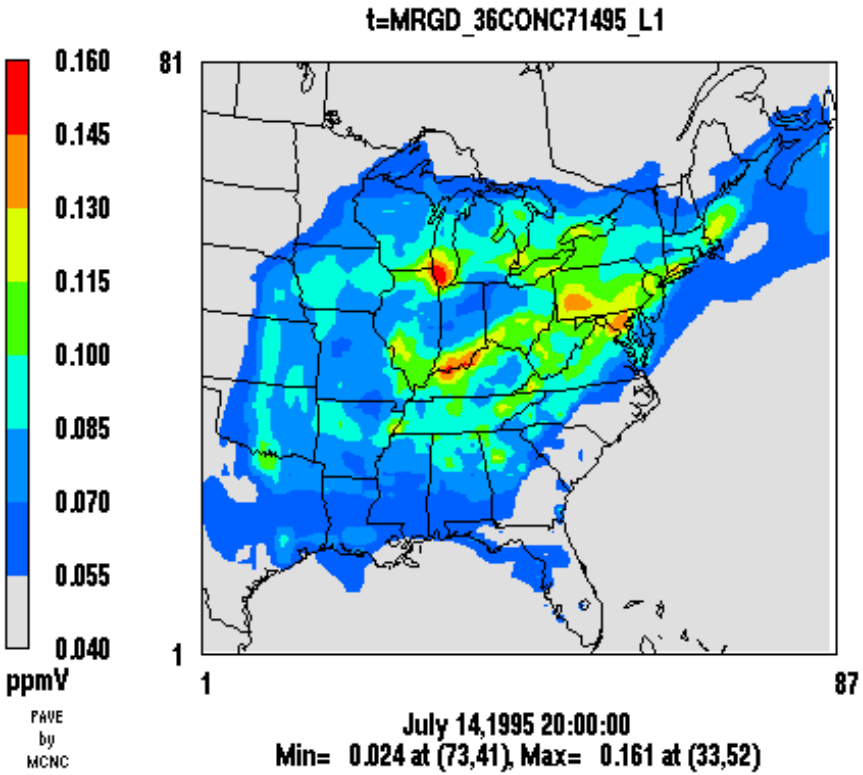
MODEL SIMULATION DETAILS

- Applied CTM / PinG and CTM without PinG (NoPinG)
- Simulation period - July 1-16, 1995
- Domains : 36 km eastern domain, 12 km SOS domain
- Chemistry – CB4 , RADM2 with GEAR solver
- 1995 Emissions ; CEM data for major point sources
- PinG treatment applied to 77 and 45 pt. sources in the 36 km and 12 km domains, respectively ($\mathbf{Q_{NOx}}$ > 75 tons/d)

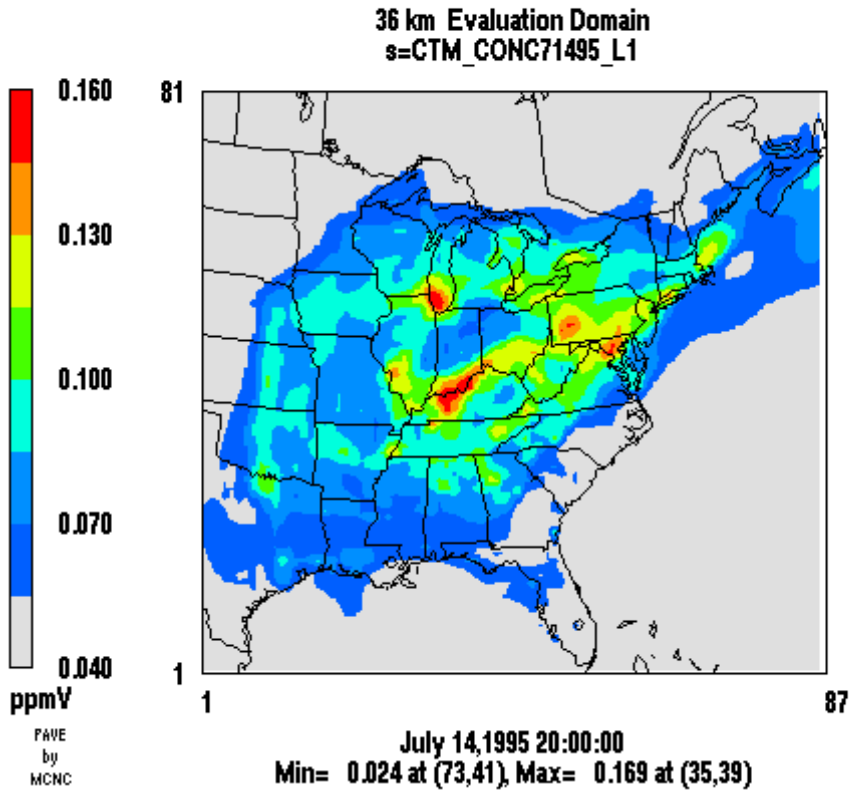
PinG SOURCE NOx EMISSIONS



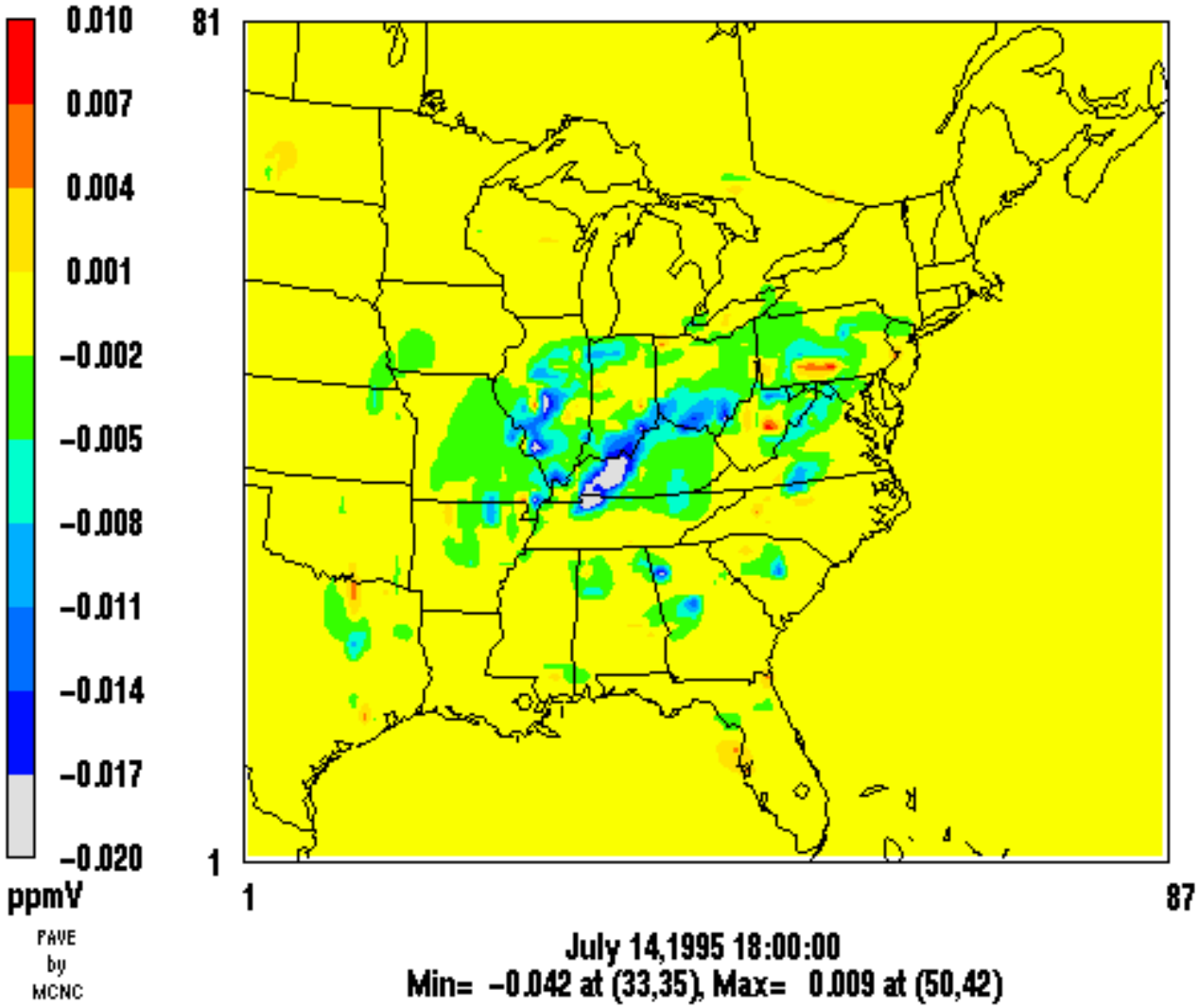
CMAQ PinG Results – Ozone



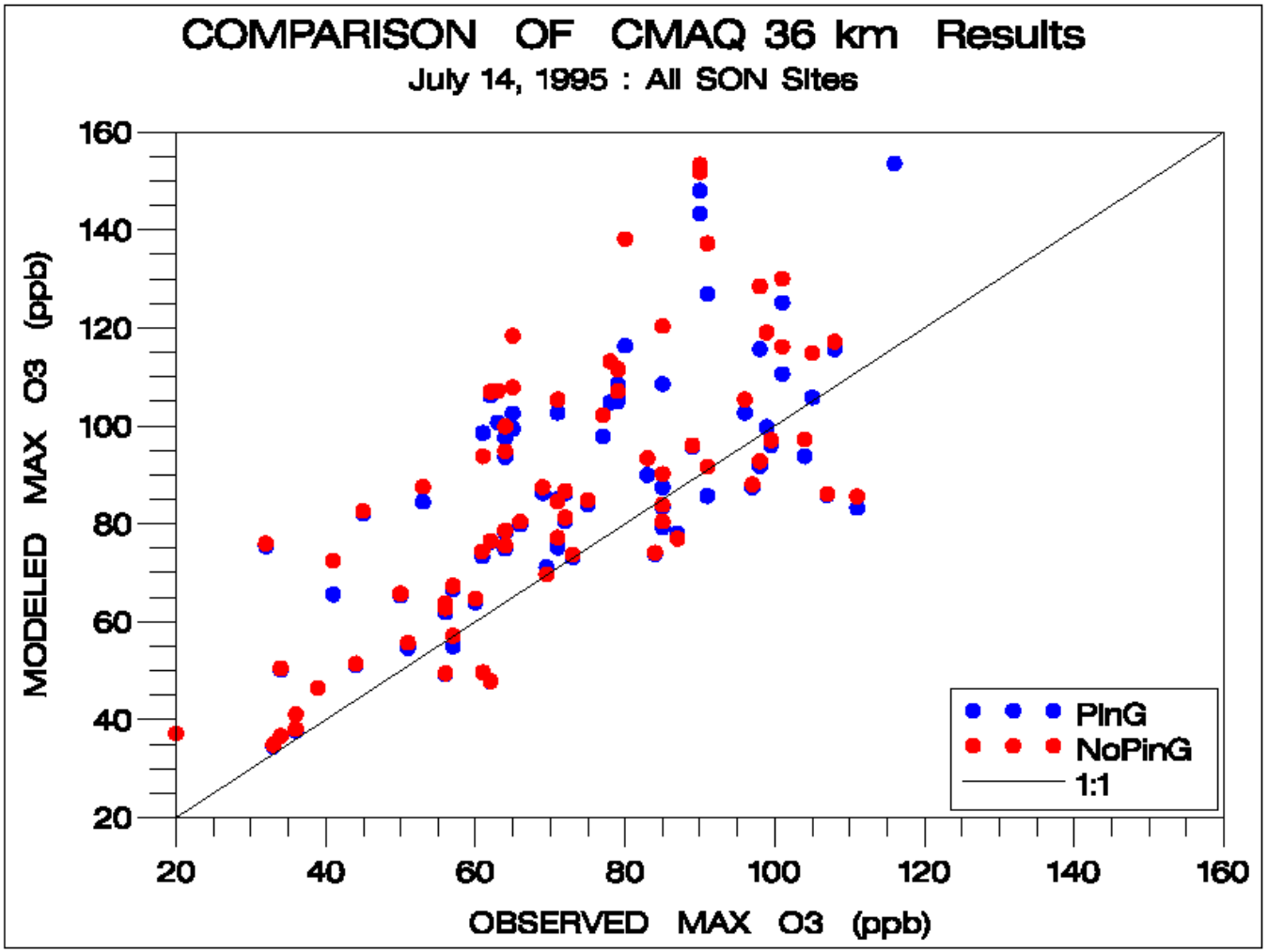
CMAQ NoPinG Results – Ozone



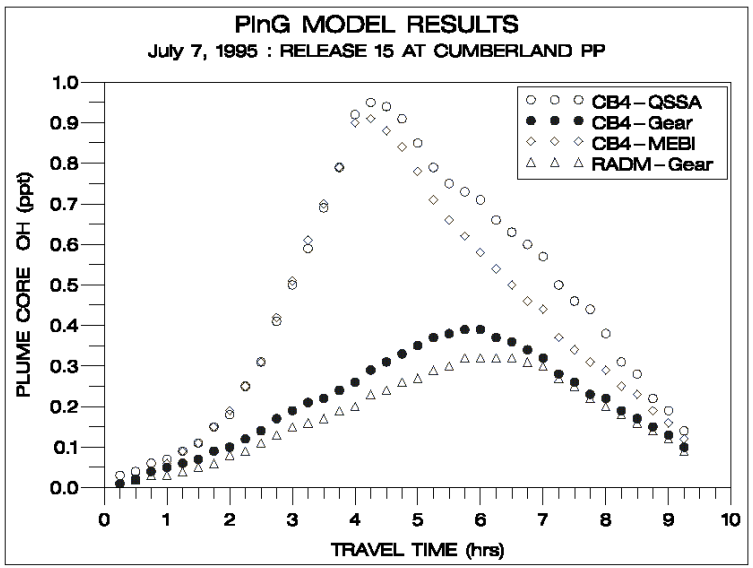
OZONE DIFFERENCE

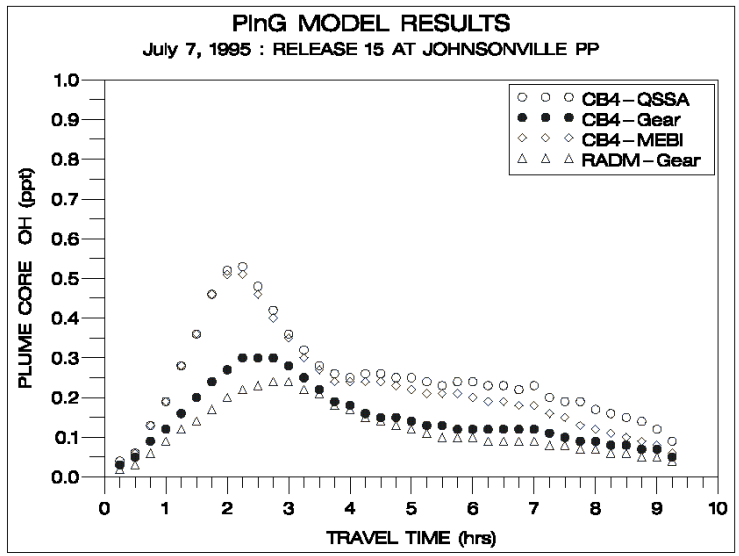


CMAQ/CTM PinG and NoPinG vs Obs Maximum 1-hr Ozone Concentrations

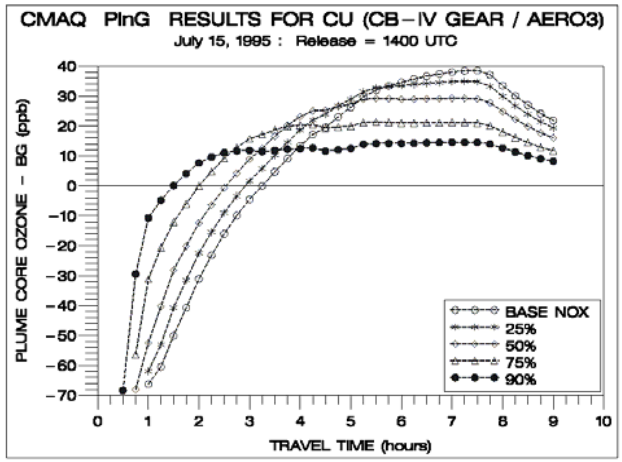


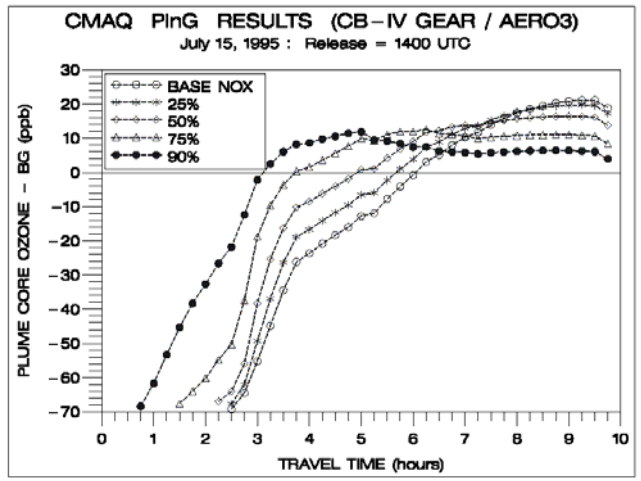
SENSITIVITY OF MODELED OH CONCENTRATION TO CHEMICAL MECHANISM AND SOLVER

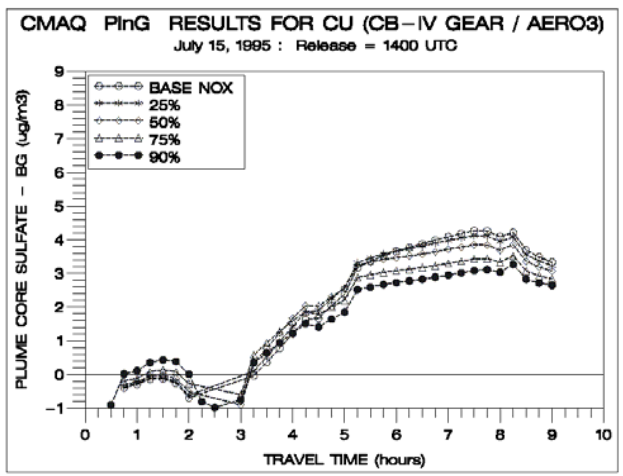


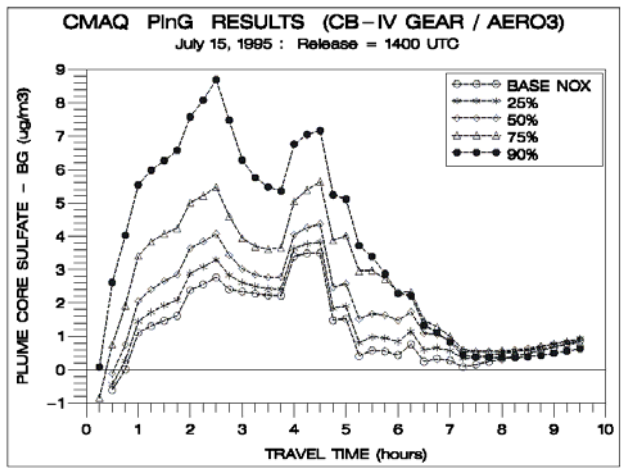


IMPACT OF NOx EMISSION REDUCTIONS ON PLUME CORE O_3 AND SULFATE LEVELS : (LOW AND HIGH SO_2 EMISSION SOURCES)

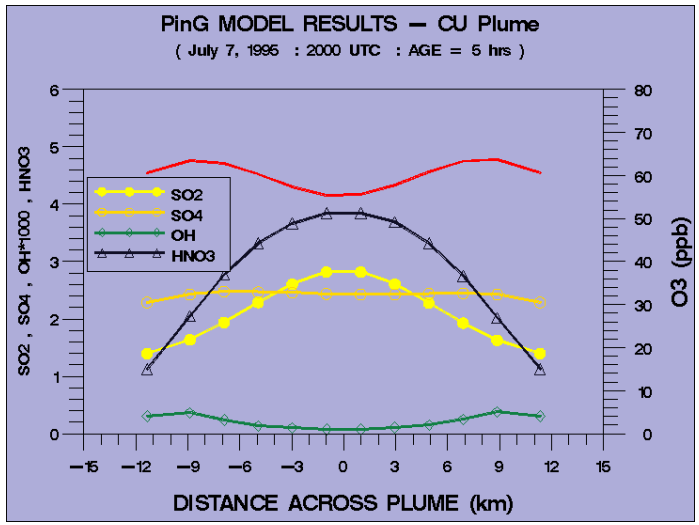


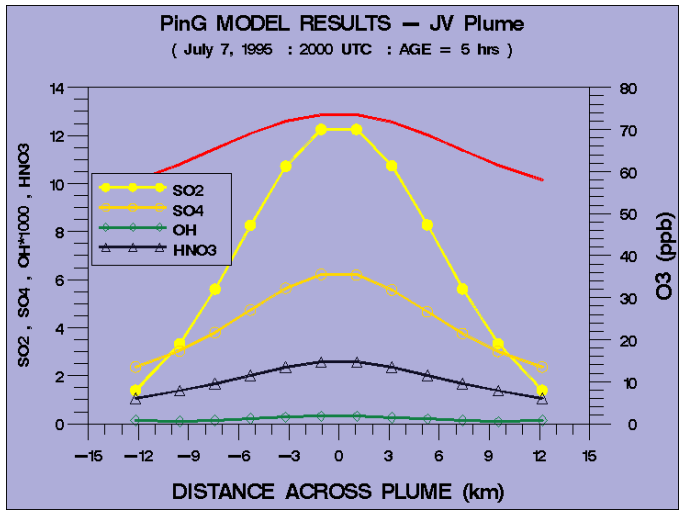




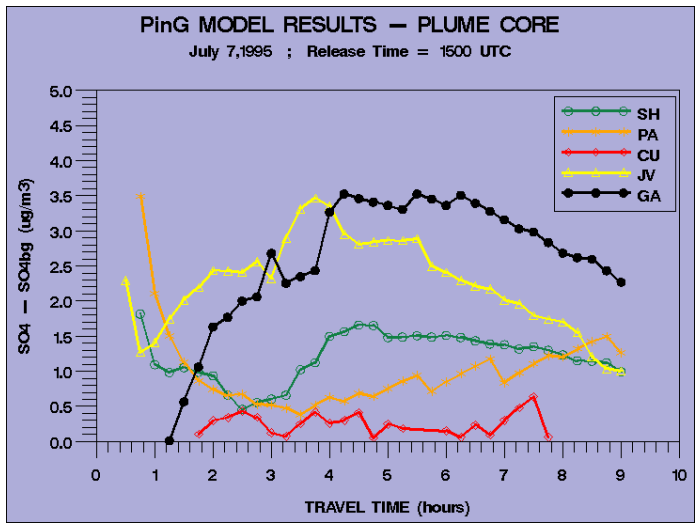


Impact of Different Mixtures of NO_x and SO_2 on Plume Aerosol Sulfate Formation

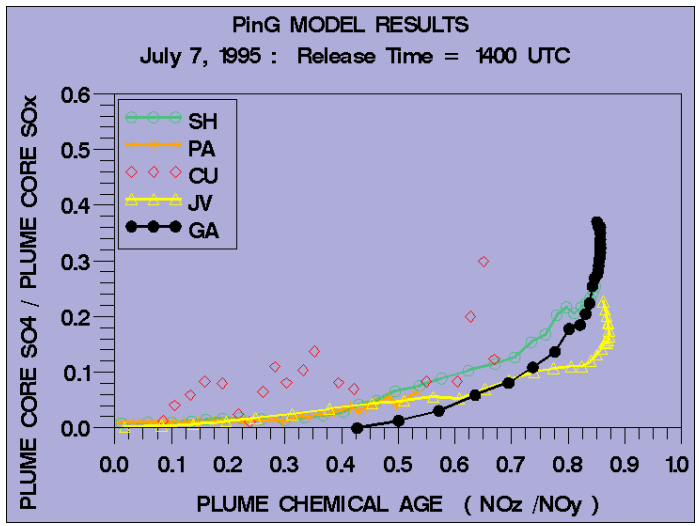




Less SO_4 in higher NO_x plumes

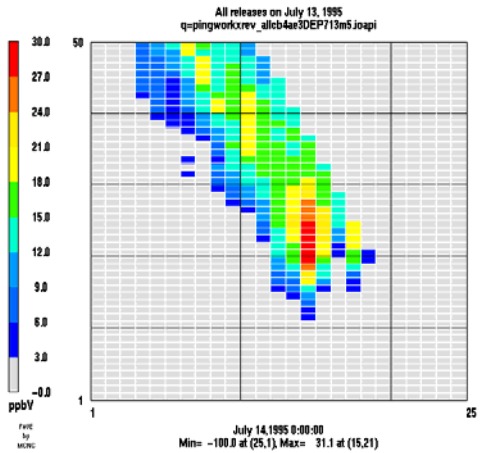


SO_4 / SO_x vs chemical age

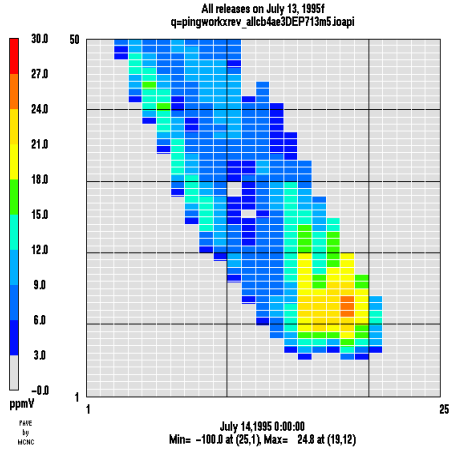


EFFECT OF TIME OF RELEASE ON PLUME CORE O_3 AND SULFATE EVOLUTION FOR CU AND JV

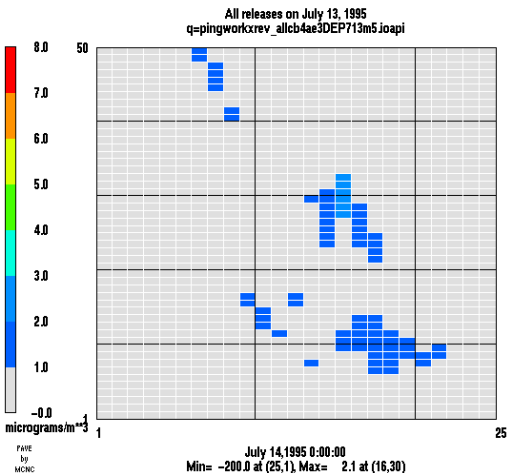
Plume Core O3 – O3bg



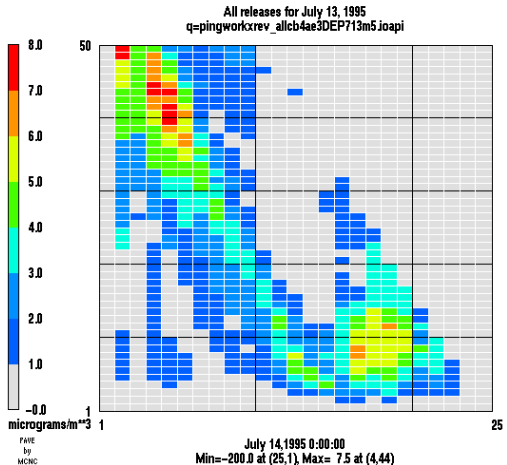
JV Plume Core O3 – O3bg



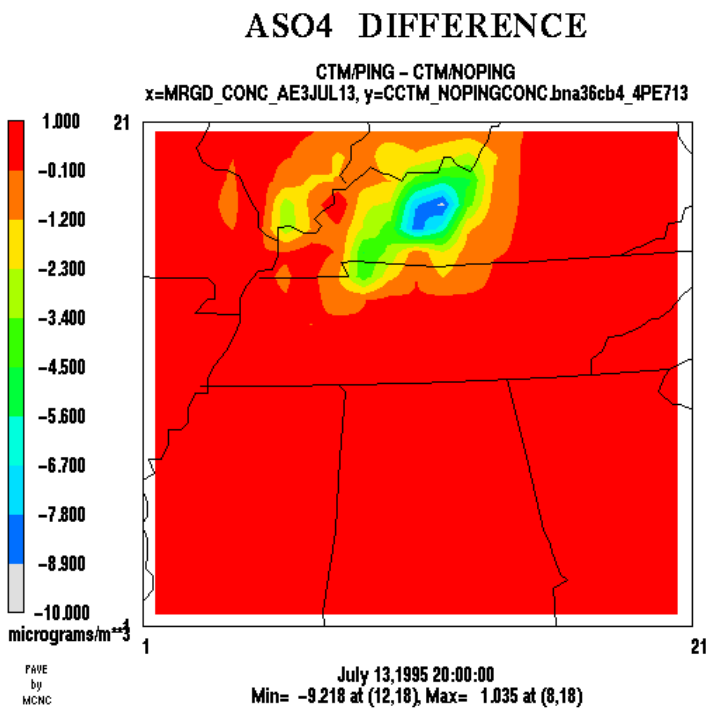
CU Plume Core ASO4 – ASO4bg

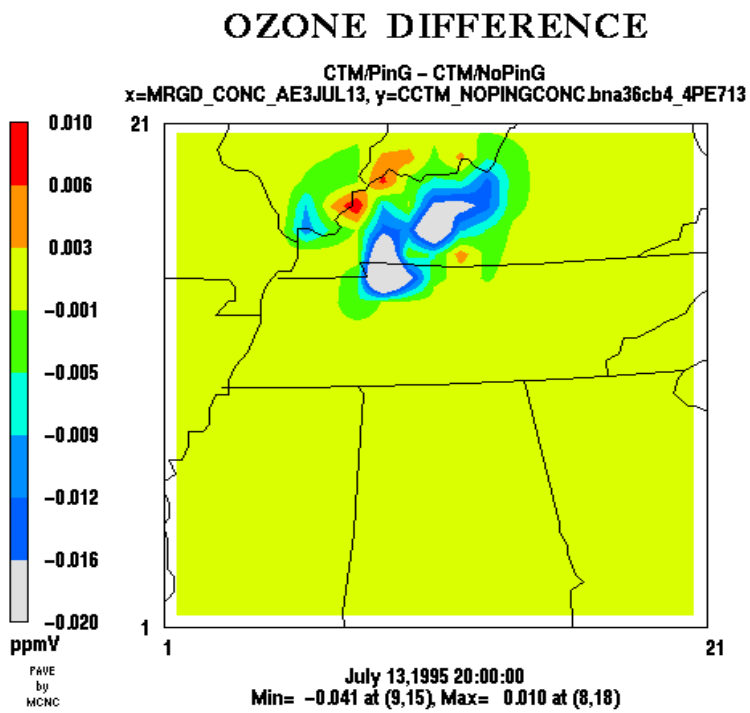


JV Plume Core ASO4 – ASO4bg



INITIAL TEST RESULTS USING AE3 WITH CTM/PinG - CTM/No PinG (Note : Lower SO4 and O3 with PinG)





Upcoming Plans for the PinG Modeling Effort

- Continue testing PinG with AE3 improvements
- Test code for different plume release intervals (sub-hourly)
- 'Freeze' code in preparation for public release
- Plume process analysis
- Simulations with CTM/PinG
  - July 1995 SOS field study period
  - Summer 2001 , Winter 2002 periods
  - July 1999 SOS field study period
  - Texas 2000 - Houston study period

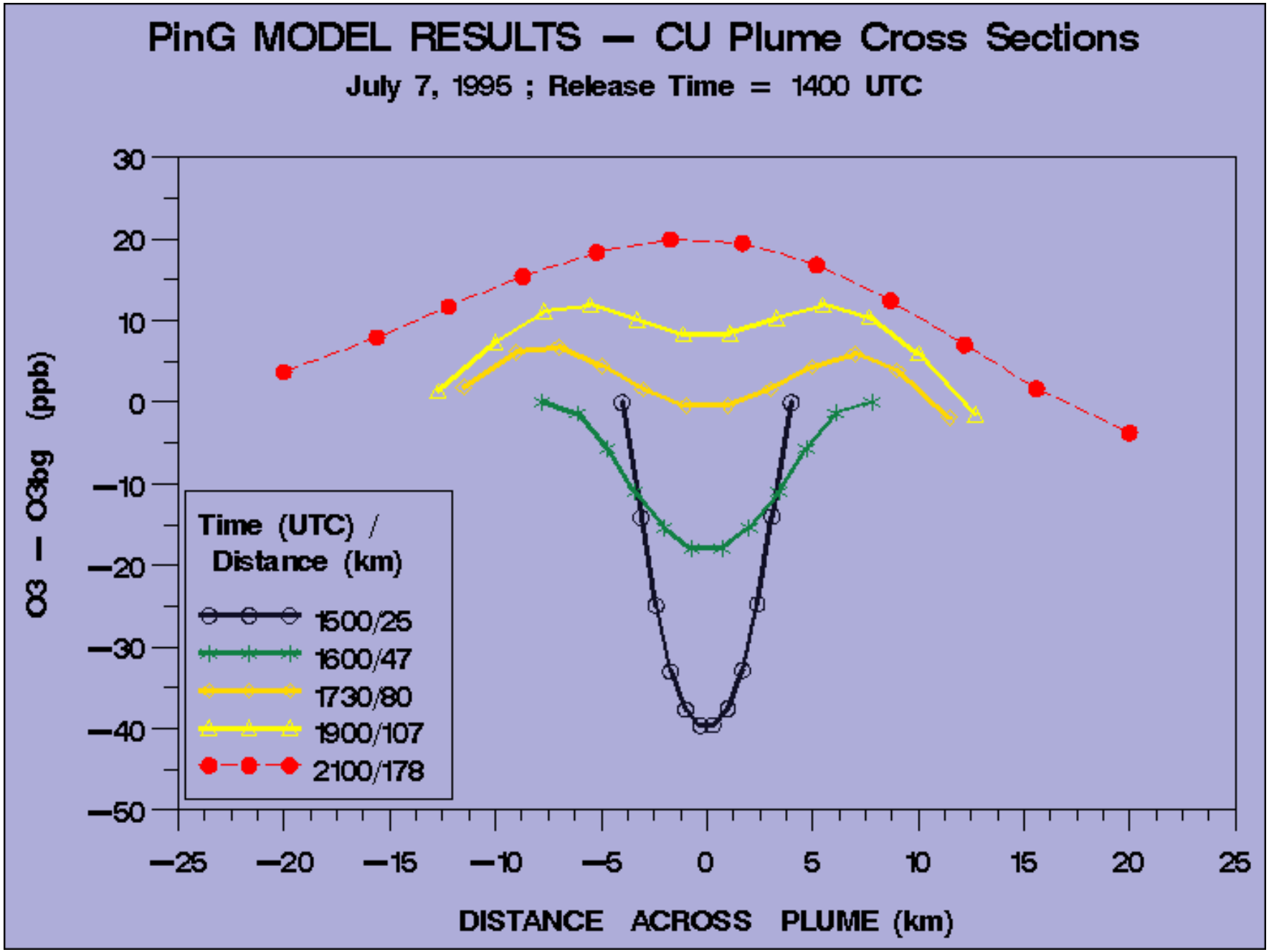
SUMMARY OF MODEL RESULTS with / without PinG Treatment

- Higher O_3 without PinG treatment in the 36 km and 12 km domains

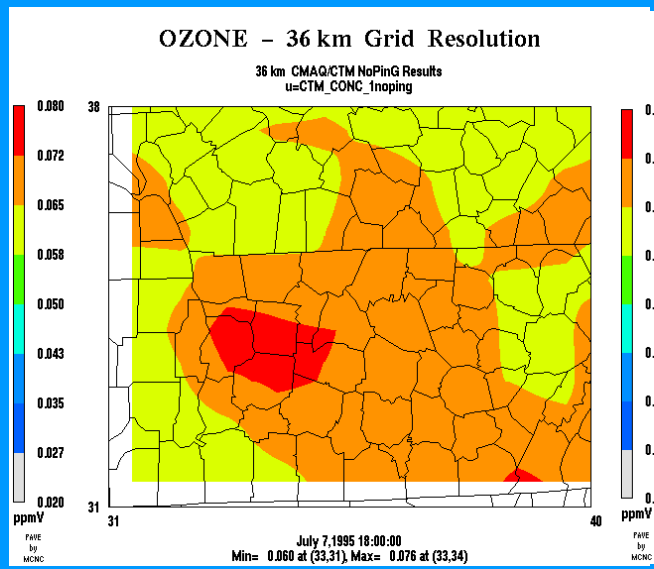
  (Greatest differences in high NOx point source grid cells and downwind vicinity)

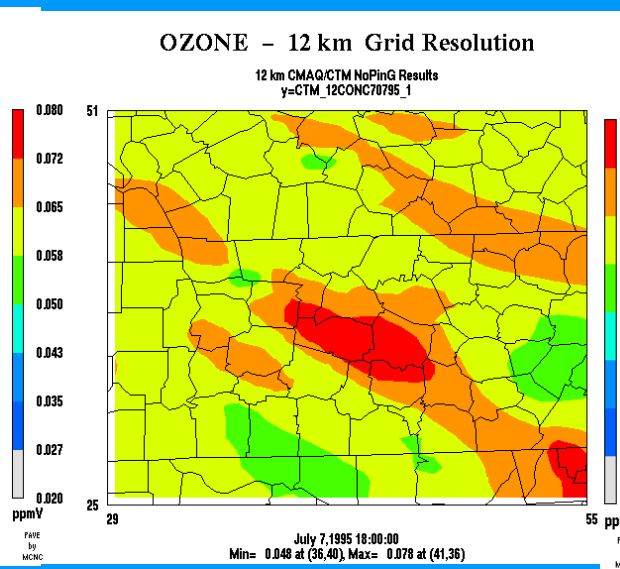
- Better agreement between CTM/PinG results and observed ozone than NoPing results on the 36 km domain ; comparable results found for the 12 km domain

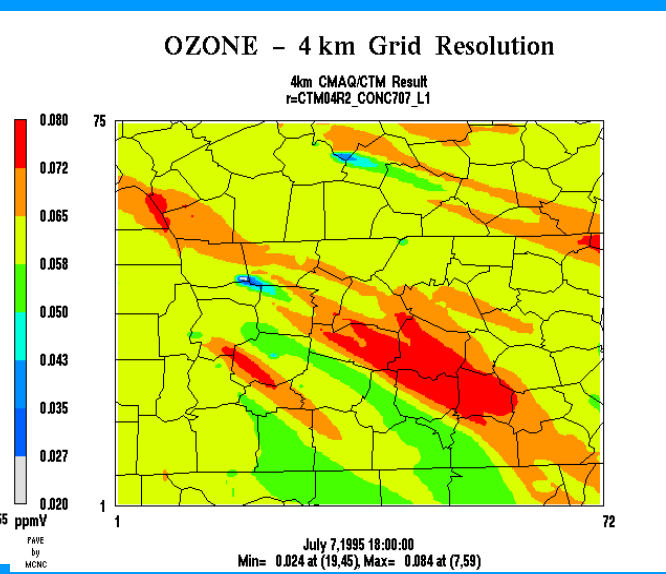
- Model results also differed for other species (ex. HNO3 …)


PinG MODEL RESULTS — CU Plume Cross Sections
July 7, 1995 ; Release Time = 1400 UTC
O3 − O3bg (ppb)
30
20
10
0
−10
−20
−30
−40
−50
−25
−20
−15
−10
−5
0
5
10
15
20
25
DISTANCE ACROSS PLUME (km)
Time (UTC) / Distance (km)
1500/25
1600/47
1730/80
1900/107
2100/178

Spatial Resolution Issue for Point Source Emissions Released Into an Eulerian Grid







REALISTIC PLUME GROWTH NEEDED FOR PROPER PLUME CHEMICAL EVOLUTION