The NOAA/EPA Air Quality Prediction System Update

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NOAA/NCEP
Environmental Modeling Center

Air Quality Forecasting
Experimental NE Configuration for 2004

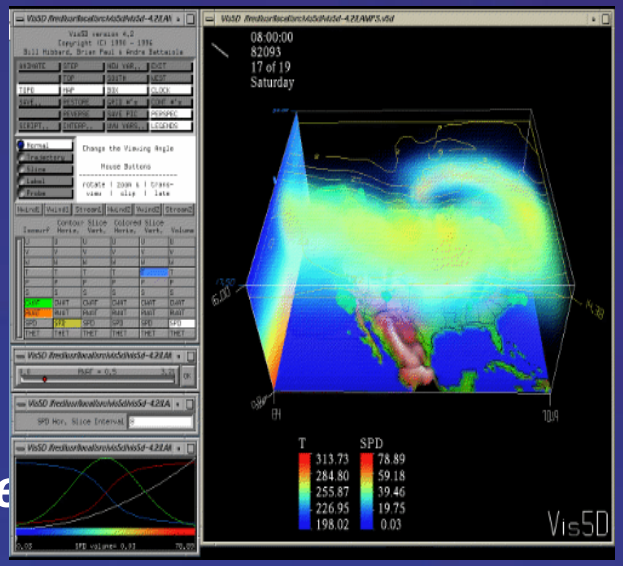
- ***NE Domain: 48 hour forecasts of ozone (O_3) : 06 and 12 UTC runs***
  - ***Eta-Post corrections to Land-Use, vertical temperature interp***
  - ***Updated emissions inventories:***
    - ***Project 2002 point and area source inventories for 2004***
    - ***Updated Mobile Emissions using MOBILE6 inventory***
      - **Simplified Temperature dependency on mobile emissions**
  - **Use of GFS ozone for upper Lateral Boundary Conditions**
    - ***" Cleaner" chemistry lateral boundary conditions below 400 mb***
  - **August 12-19, 2003 Retrospective runs completed and evaluated**
  - **6 hour cycling**
- ***Real-time Verification***
  - ***BUFR O3 and CMAQ output are now ingested into VSDB system***
  - ***PBL diagnosis from raobs, profilers***

Air Quality Forecasting
2004 Developmental Expanded Domain

- ***Eastern US : 48 hour forecasts of ozone (O_3) : 06 and 12 UTC runs***
  - ***Same system as operational except***
    - ***3x expanded domain***
    - ***Minimum Kz to reduce night-time mixing***
    - ***Transformed grid to reduce interpolation error bet. Eta, emissions processor and CMAQ***
    - ***Expanded emissions inventories***
    - ***Different GFS ozone as upper Lateral Boundary Conditions***
    - ***" Cleaner" chemistry lateral boundary conditions below 400 mb***
  - **August 12-19, 2003 Retrospective runs begun**
    - ***Need additional processors (~65)***
    - ***Available by 17:30 UTC***

PREMAQ-CMAQ

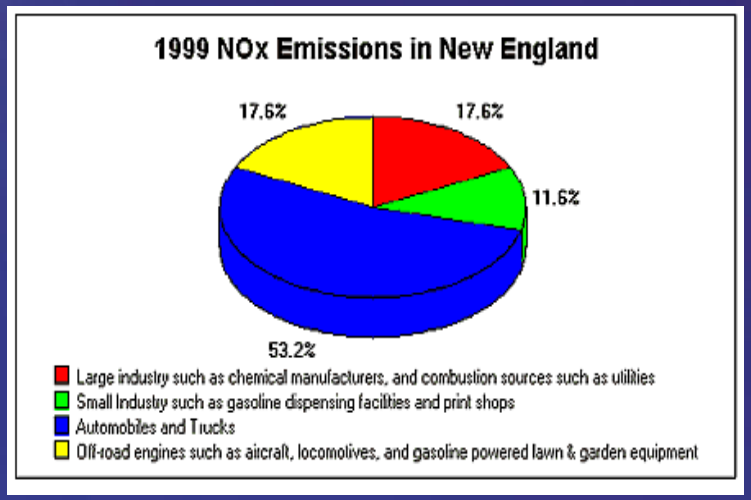
- ***EXPERIMENTAL NE Domain :***
  - *166x142 Lambert-Conformal Arakawa C grid*
  - *12 km grid spacing*
  - *22 sigma-P levels to 100 mb*
  - *CMAQ: 45 minutes for a 48 hour forecast (33 tasks)*
  - *PREMAQ: 30 minutes (not parallelized)*
  - *12z: 48 hr forecast*
  - *06z : 48 hr forecast*



- ***Multi-pollutant:***
  - *Ozone, Particulate Matter (PM), precurse*
  - *visibility, acid deposition, air toxics*

CMAQ
Primary Precursor Sources

- ***Volatile Organic Compounds (VOCs)***
  - *Biogenic (>50% of emissions)*
    - *Strong met. Dependence (T, PAR)*
  - *Mobile (~25% of inventory)*
    - *Large diurnal & day-of-week variations*
    - *Evaporative Emission ~ temperature*
  - *Other anthropogenic*
    - ***Assume no diurnal met influence***
- ***Nitric oxides (Nox)***
  - *Major fossil-fuel power plants (~35%)*
    - *Affected by temperature & maintenance schedules*
    - *Plume rise – Strong met. Dependence*
  - *Mobile (30%) - temp, speed dependence*
  - *Other anthropogenic (25%)*
  - *Soil (<10%) - affected by temperature, soil moisture*
  - *Lightning – **not modeled***



CMAQ

- ***Chemical Transport Mechanism***
  - *Advection: Piecewise Parabolic method (PPM)*
  - *Vertical Diffusion: Pleim-Xu PBL**
  - *Horizontal Diffusion: Eddy-diffusivity with grid size dependent*
- ***Cloud processes:***
  - *Aqueous chemistry & sub-grid clouds from RADM*
- ***Plume-in-Grid:***
  - *Subgrid Lagrangian plume effects: OFF*
- ***Dry Deposition:***
  - *M3dry: deposition velocities computed from the Pliem-Xu LSM*
- ***Gas-Phase Chemistry Mechanisms:***
  - *Smaller Carbon Bond 4 (CB4), limited species*
  - *Use Chemical steady states*
- ***Gas-phase Chemistry Solver:*** *Fast Hertel solver*

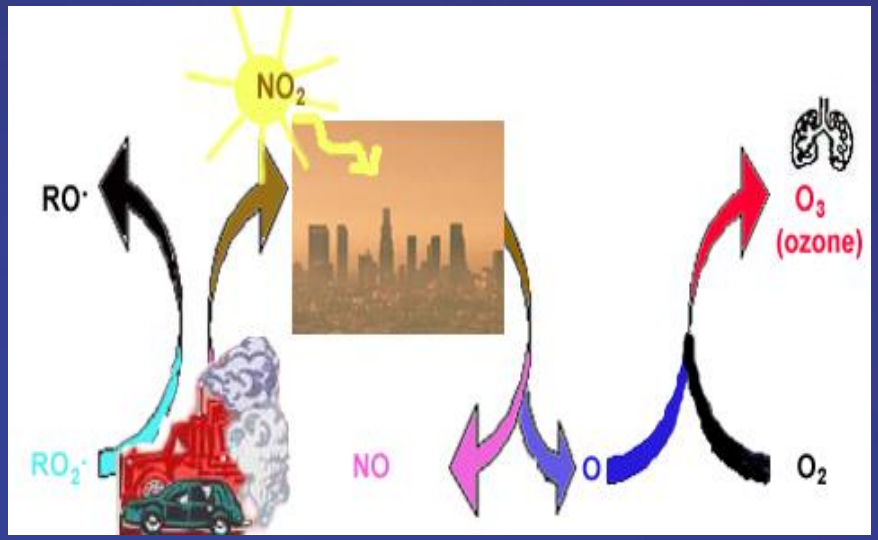
CMAQ

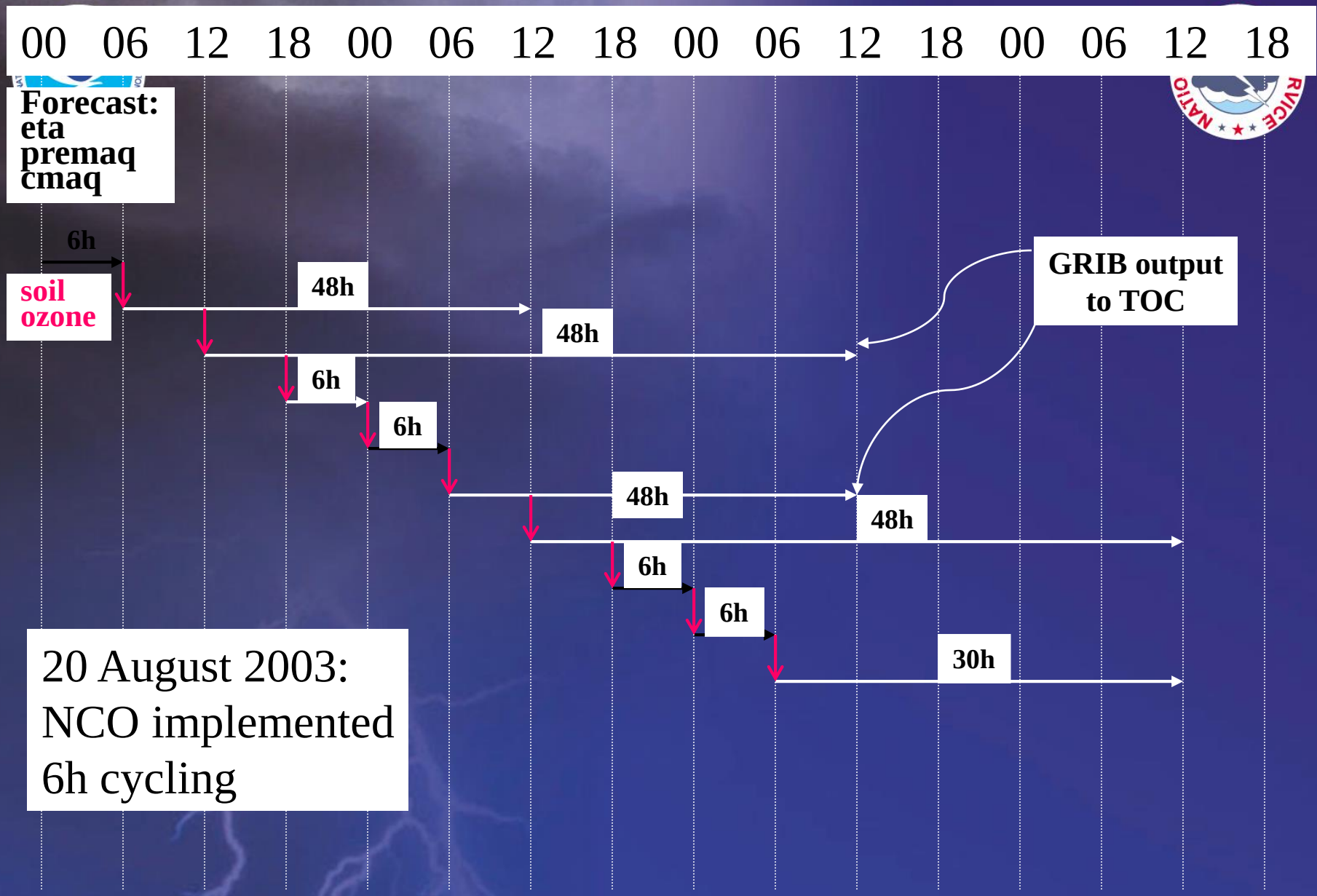
- ***Aerosols: OFF***
  - ***Inorganic, secondary anthropogenic***
  - ***Speciated primary emissions (Carbon, sulfate, nitrates)***

- ***Initial Conditions: Cycles from 6 hour forecasts***

- ***Boundary Conditions : GFS ozone profiles blended with lower-level clean climatological profiles (below 400 mb)***

- ***Data Assimilation: None***





20 August 2003:
NCO implemented
6h cycling

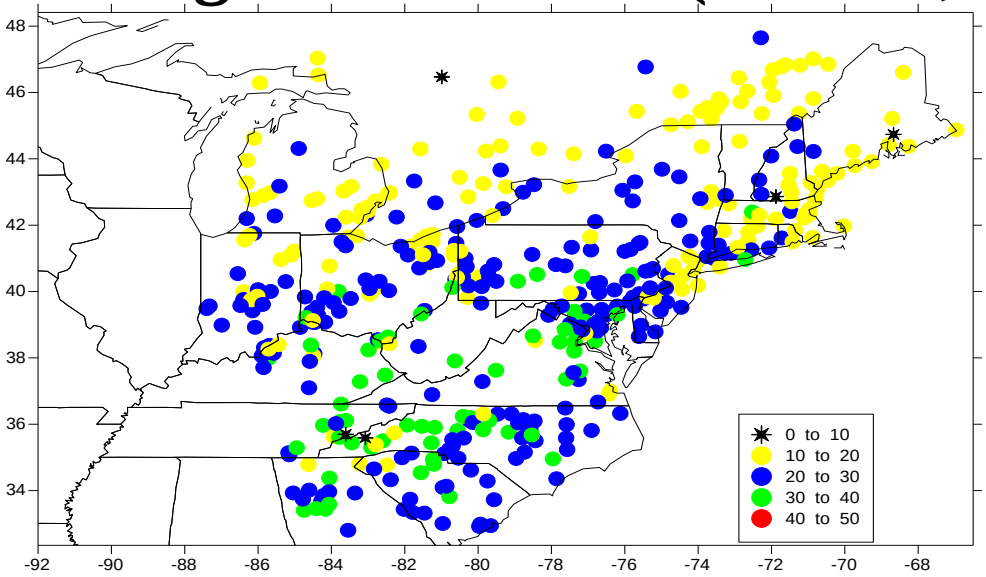
NE DOMAIN Evaluation

Maximum 1 Hr ozone Errors (Aug.12-19,2003)

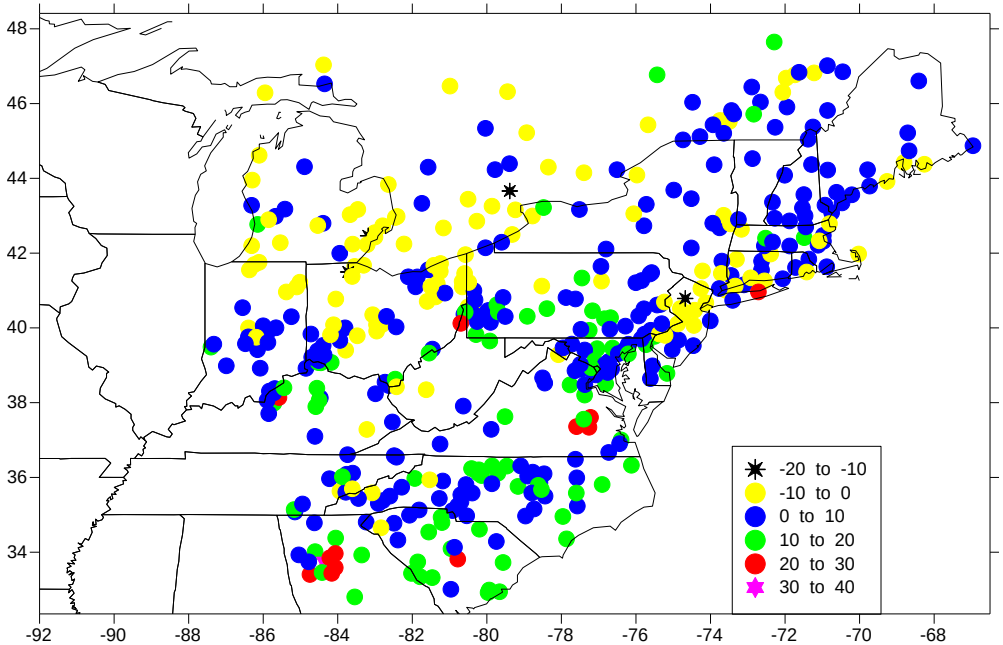
Runs	**RMSE (ppb)**	MAGE	MNGE	MNB	MFB	**MB**	**NMB**	**NME**	**R**
Ngfs	**15.37**	11.81	21.85	11.76	7.96	**4.88**	**8.15**	**19.71**	**0.64**
Gfs	**16.21**	12.59	23.45	14.00	9.75	**6.10**	**10.17**	**21.00**	**0.62**
GMb6nptar	**14.50**	11.19	21.00	11.91	8.36	**4.69**	**7.83**	**18.68**	**0.64**
LU_flawed	***22.84***					***16.04***	***26.76***	***30.88***	***0.62***
LU_corrected	***16.42***					***7.45***	***12.43***	***21.04***	***0.63***

NE DOMAIN Evaluation

1 Hr Avg ozone Errors (8/12-19, 2003)



RMSE



Mean Bias

Near-term projects

- **Expanded Domain Implementation**

- **Evaluation with NEAQS/ICARRT NE Study**
  - *8 aircraft, Ron-Brown, sfc super site – Full suite of chemical measurements*
  - *~ 10 Surface flux stations & profiler sites*

- **Test of CMAQ with Aerosol processes**

- **Improved coupling with Eta-x Cloud-radiation & land use processes**
  - Controls chemical transformation/photolysis, biogenic emissions

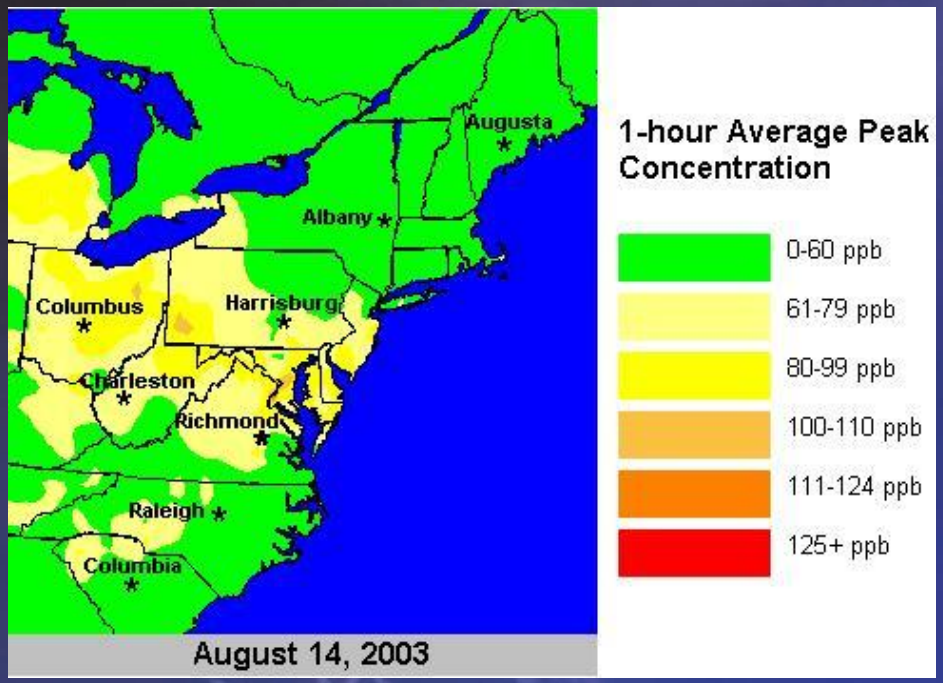
- *Real-time verification with additional field evaluation*

2004 Experiments Detailed Description

Experiment	Landuse/ Temp correct	LBC	Mixing	Emission
Base	X	Clean	CMAQ-Kh/ Eta PBL	1999
S1	X	GFS	CMAQ-Kh/ Eta PBL	1999
S2	X	GFS	Eta-Kh &PBL	1999
S3	X	GFS	CMAQ-Kh & PBL	1999
S4	X	GFS	CMAQ-Kh/Improved Eta PBL	1999
S5	X	GFS	Best	2002/Mobile 6

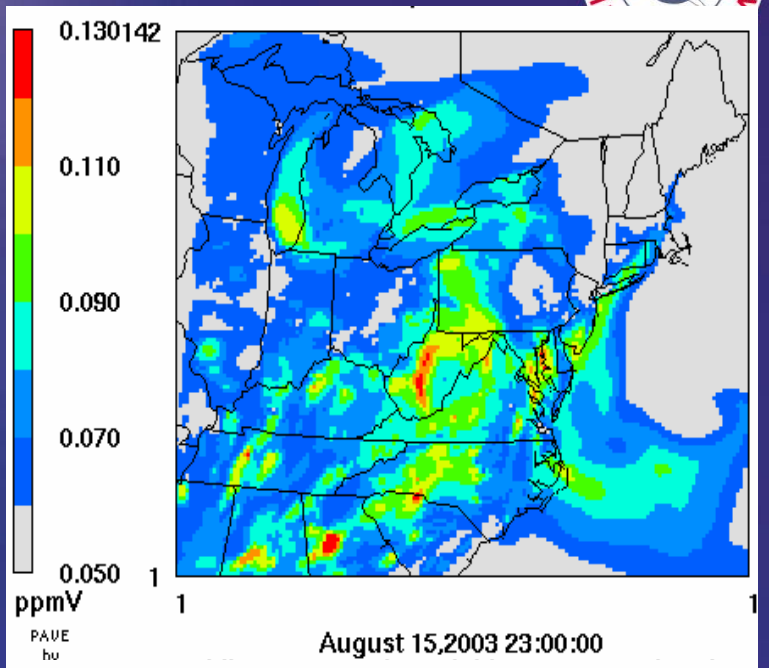
Land-use Coupling to Eta (Base)

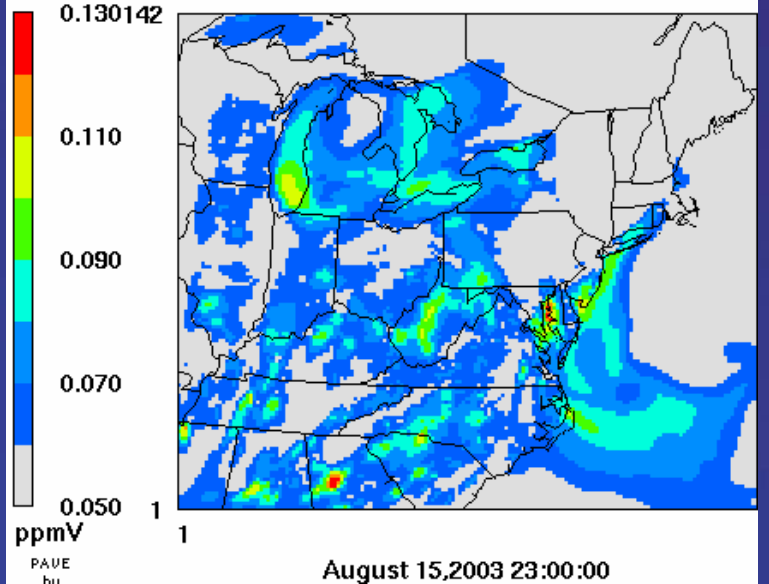
With wrong land-use→



AIRNOW Ozone obs

With correct land-use→



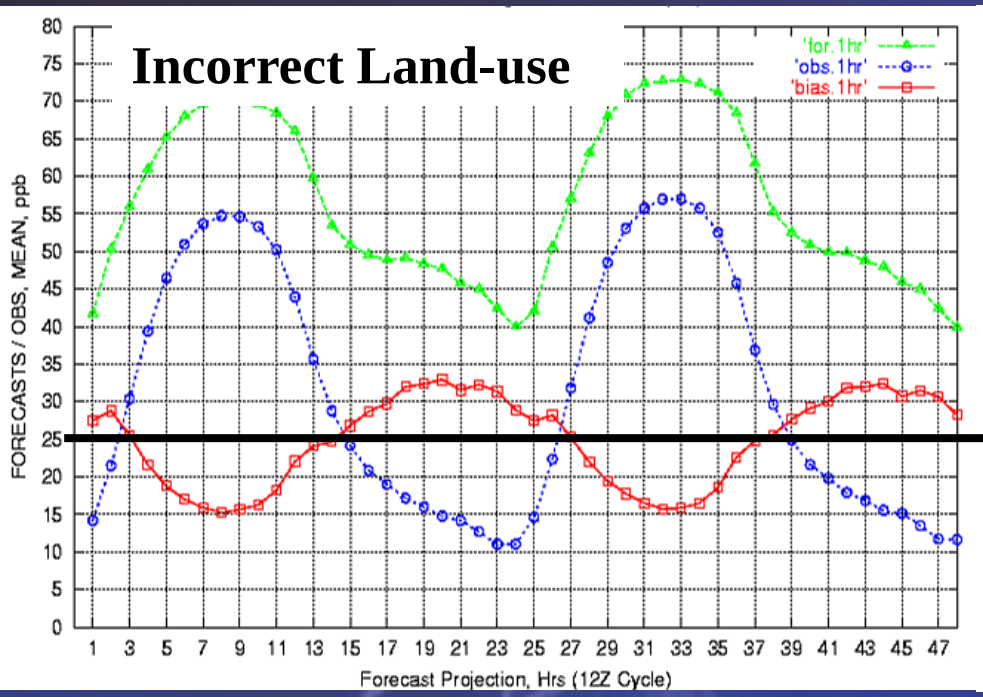


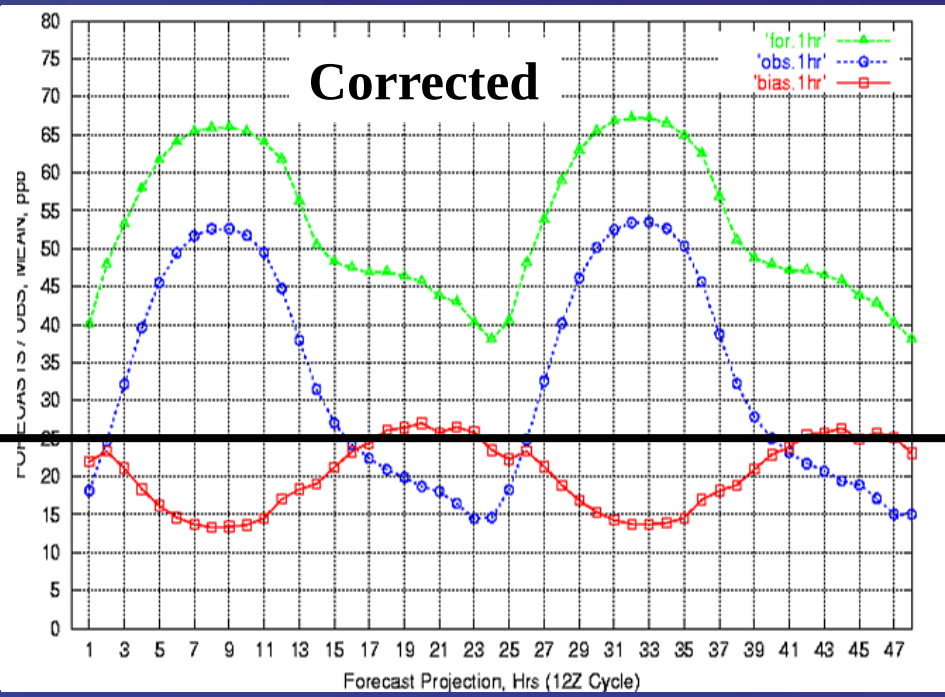
1 hr Averaged Ozone Error

Land-use specification error impact

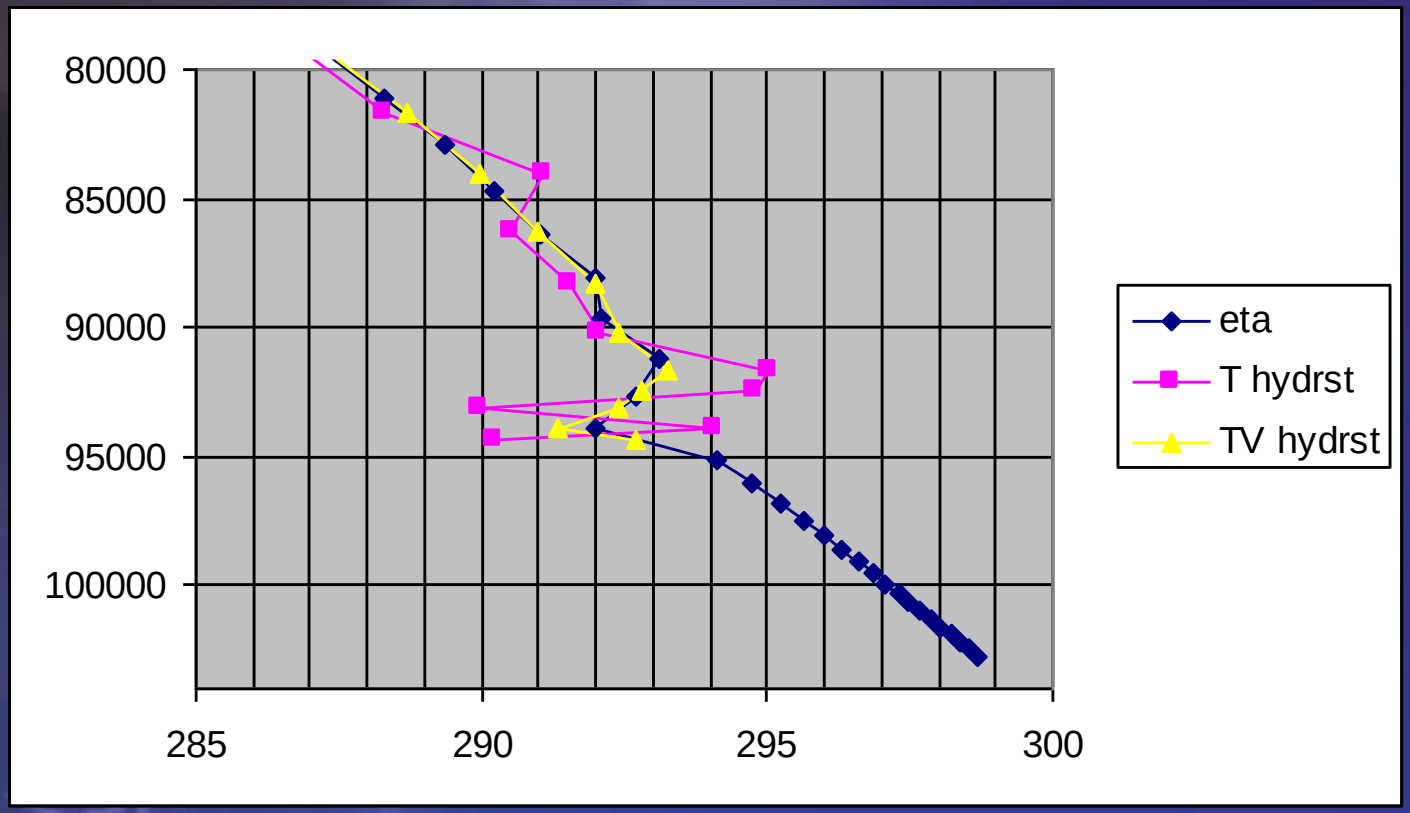
1 hr avg (ppb) Forecast(green), obs(blue), bias(red)

August 12-19, 2003



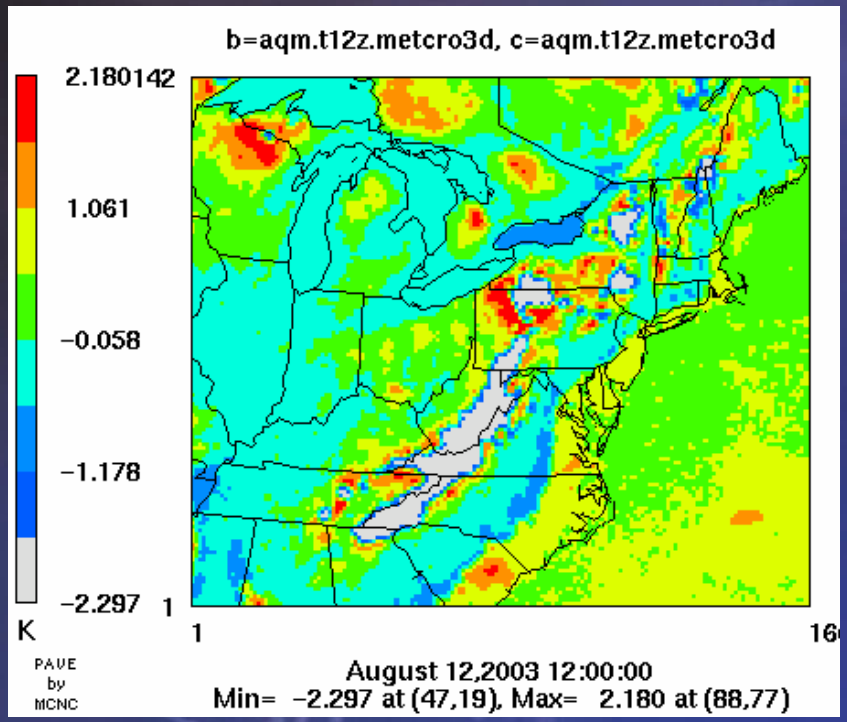


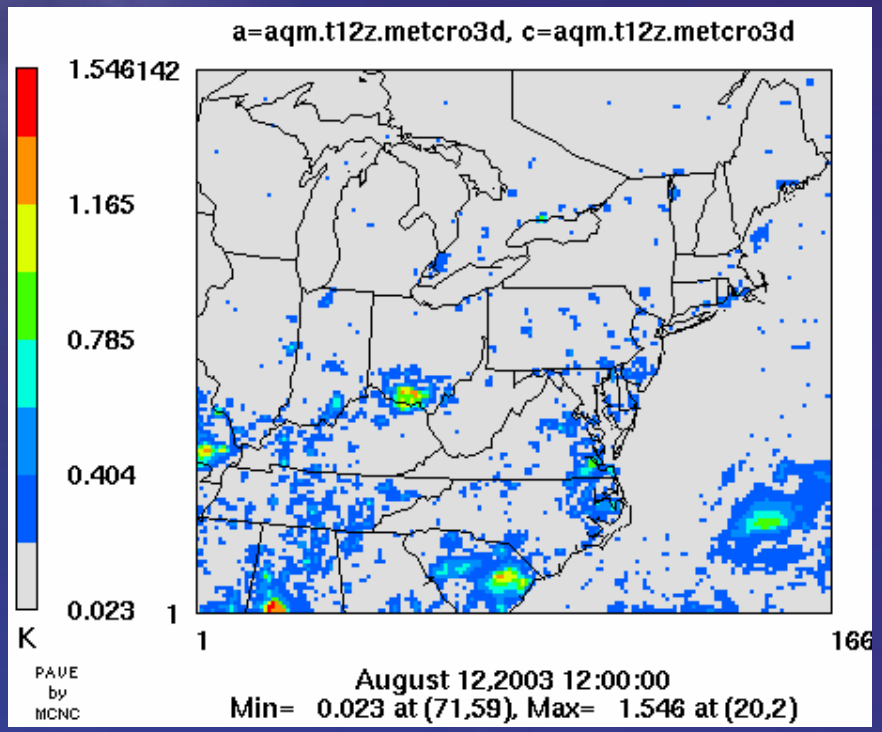
Eta-Post Temperature Interpolation Error (Base)



Eta-Post Temperature Interpolation Error

Maximum lowest layer Temperature Differences





Max T difference: Vertical Interpolation Error

Max T difference: Eta-X: 10/31/03 Vs Eta-X:current

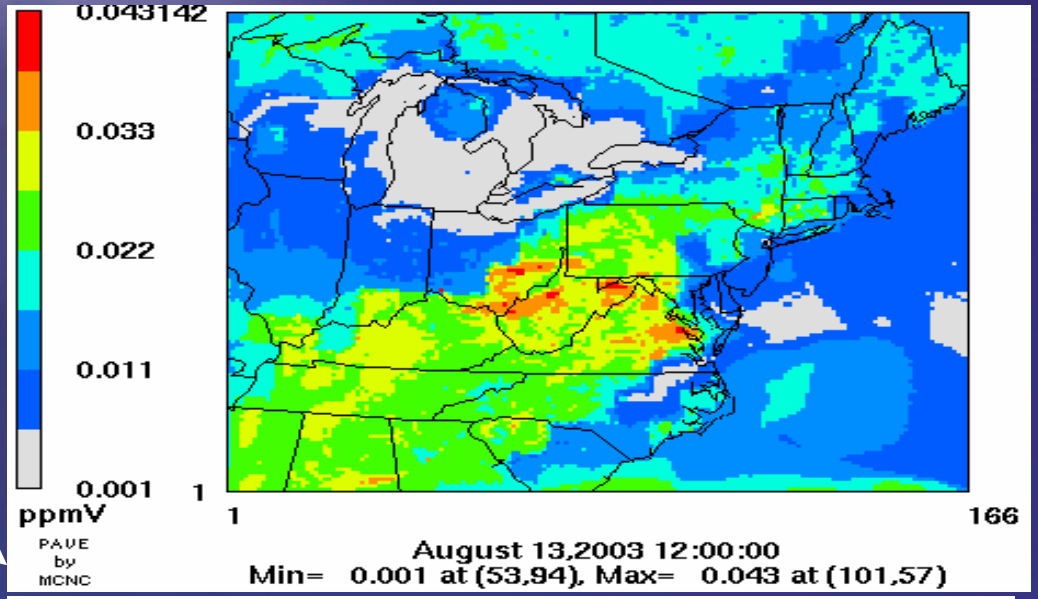
1 hr Averaged Ozone Error

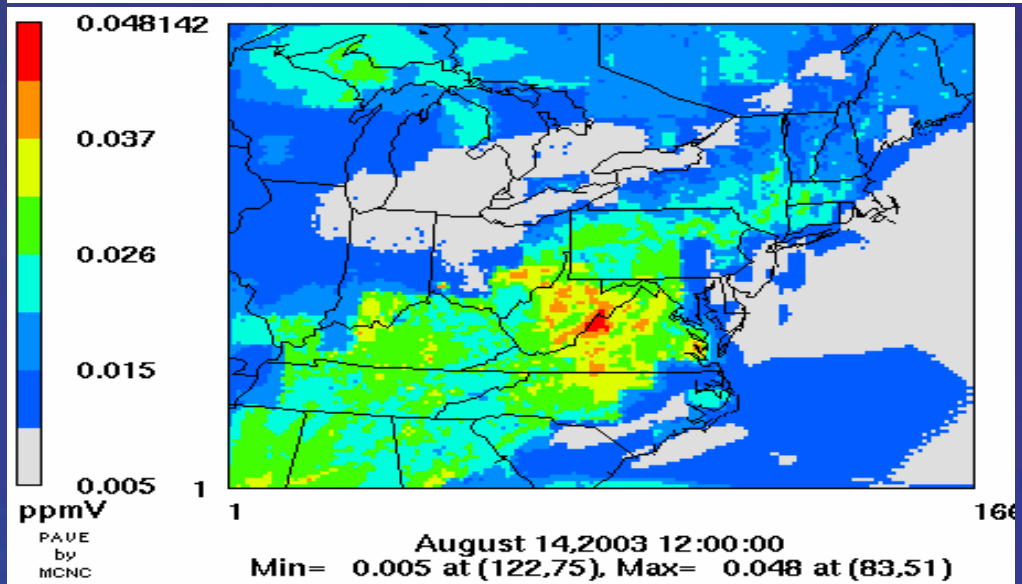
Vertical Temperature Profile Correction (Base)

Max Differences w and w/o Landuse & temp. corrections

Vertical Temperature profile error

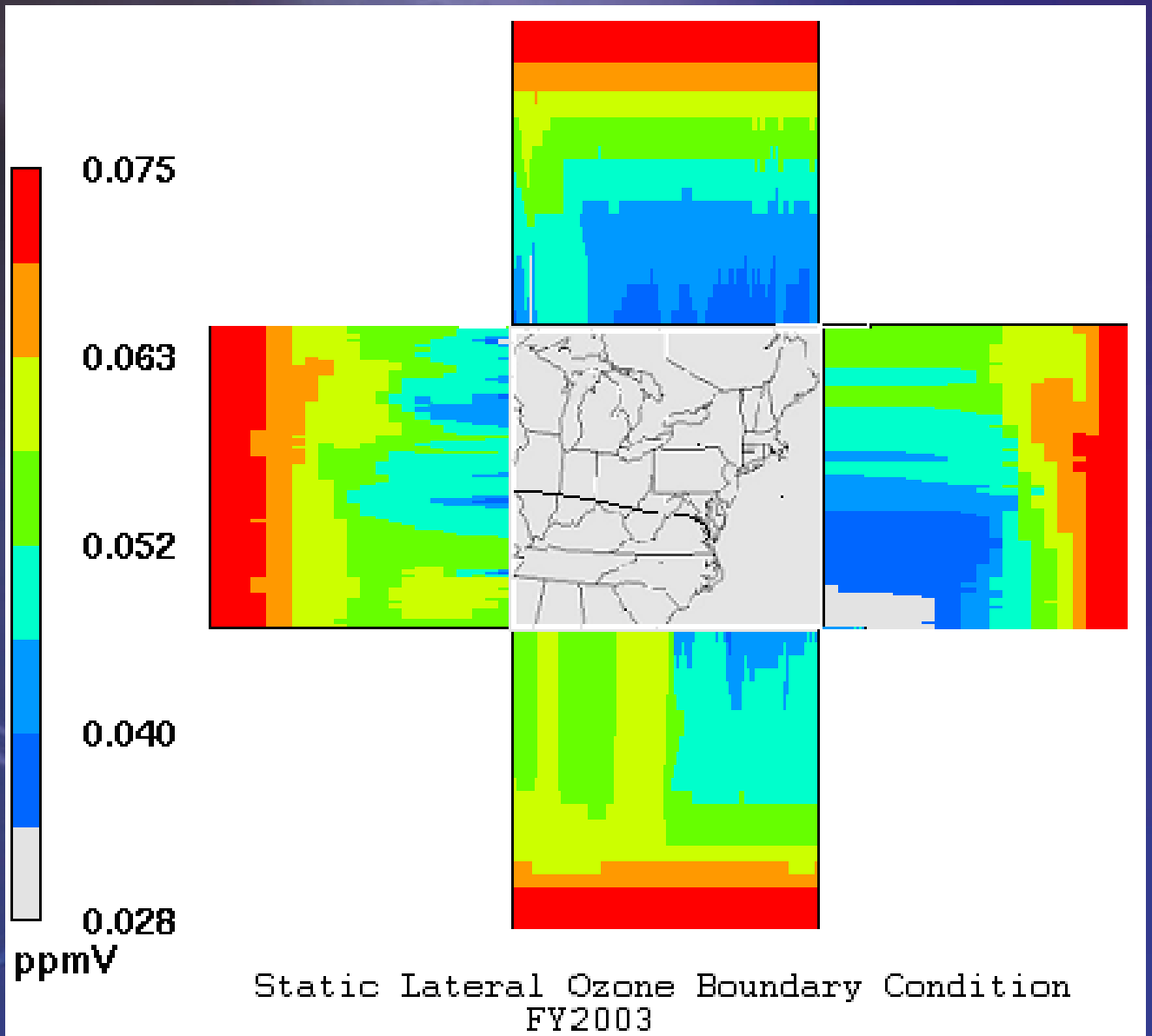
- Error interpolating from Eta to CMAQ Sigma surfaces
- Corrected with improved hydrostatic reduction





O3 Boundary Conditions

Summer 2003: Static

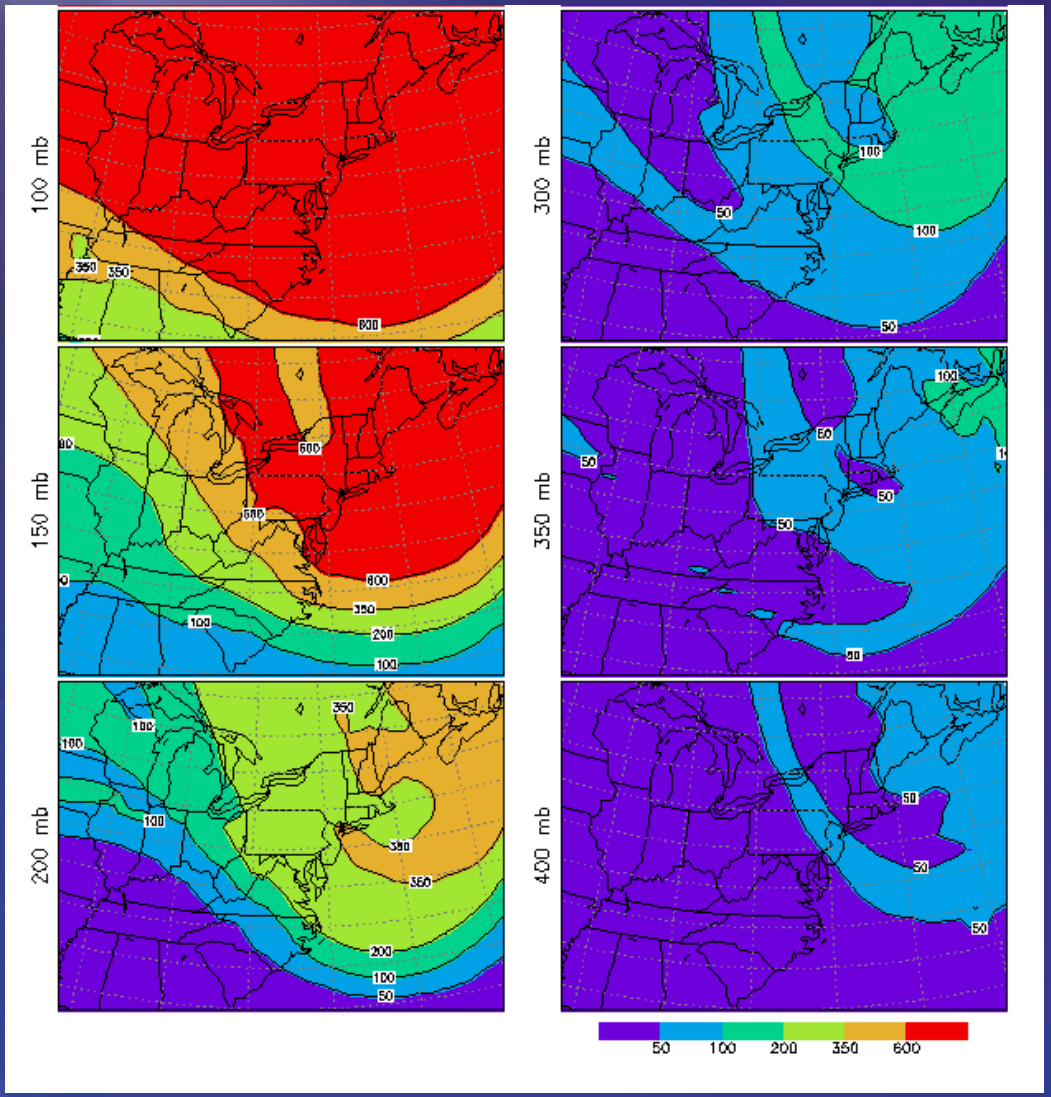


O3 Boundary Conditions

2004: Couple to GFS Ozone (S1)

GFS O3 (ppb) from 100-400 mb:

- More accurate near & above tropopause
- Blend climatological profiles below trop.

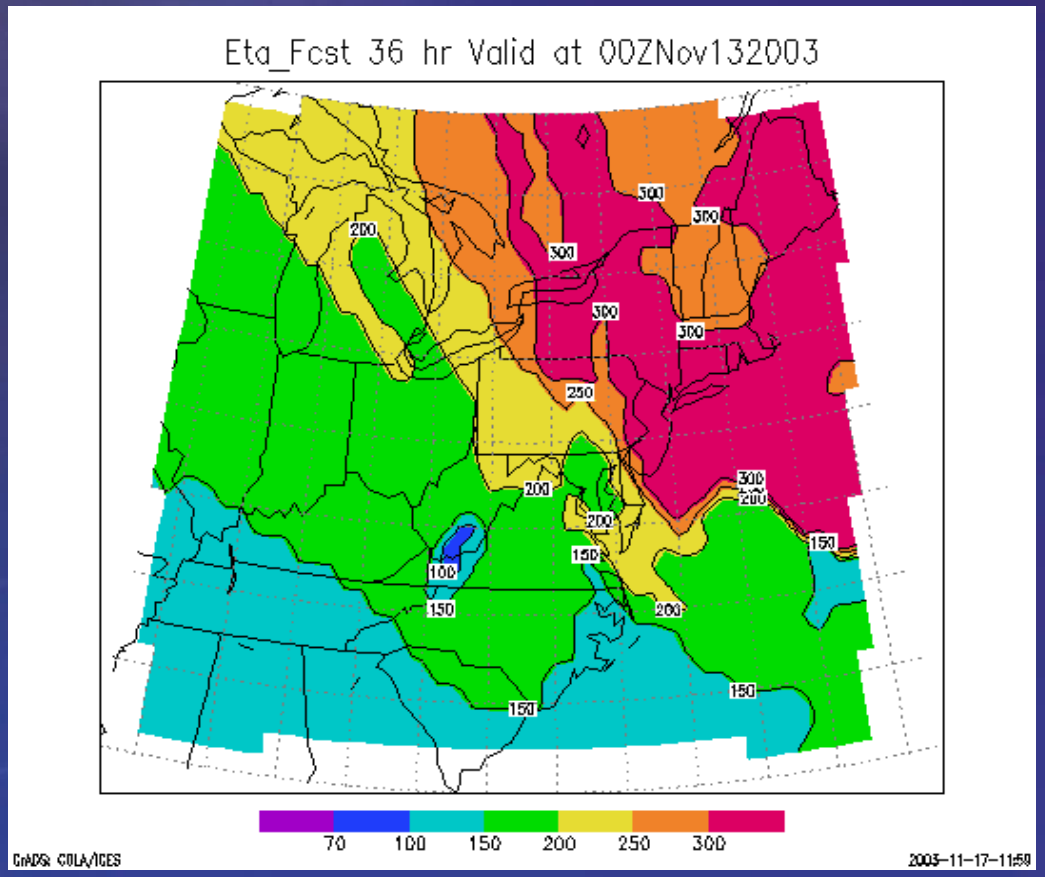


O3 Boundary Conditions

2004: Eta Tropopause Heights (mb)

GFS O3:

- consistency with GFS and Eta trop. heights
- Preliminary results show good consistency

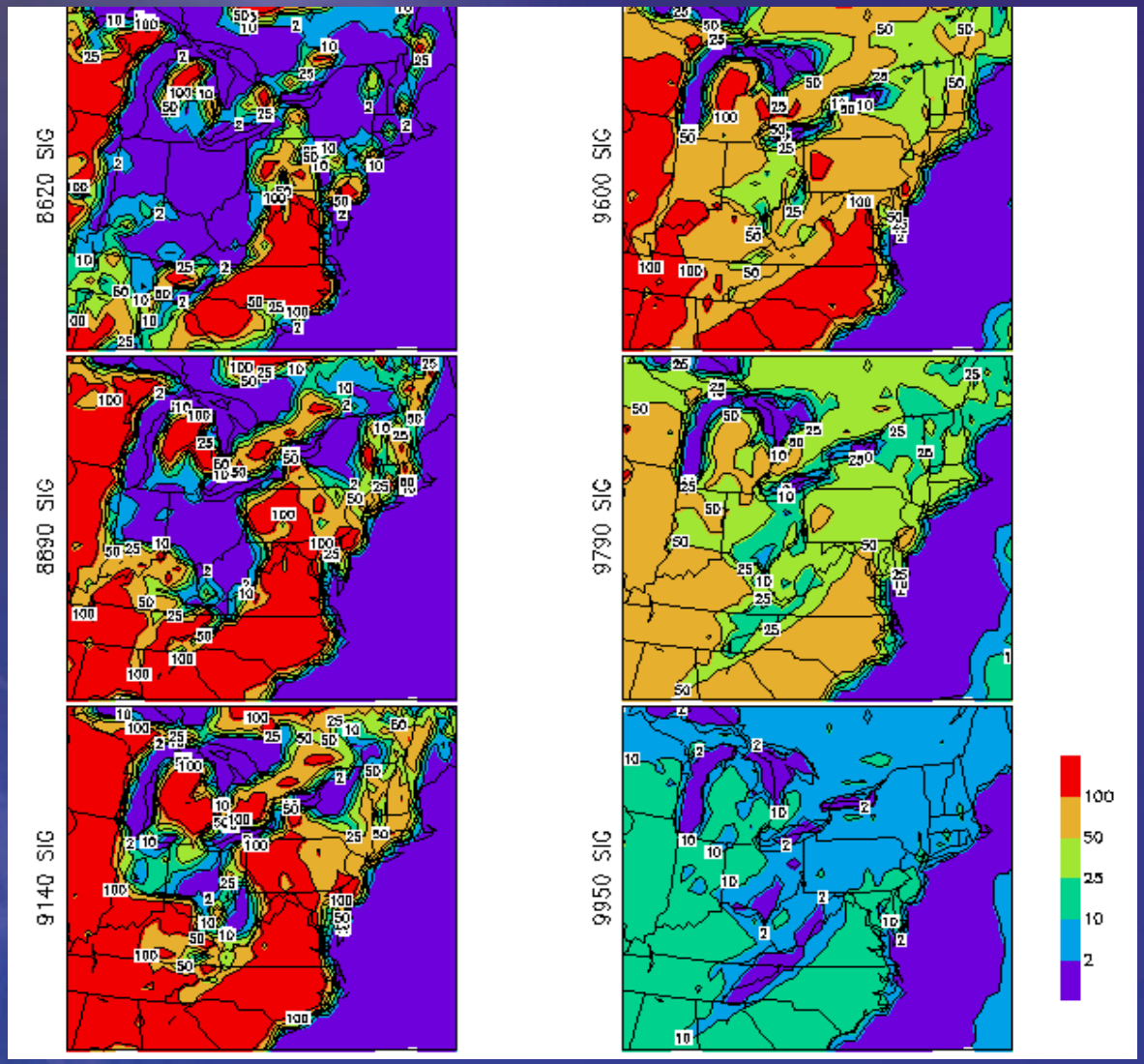


PBL Mixing (S2)

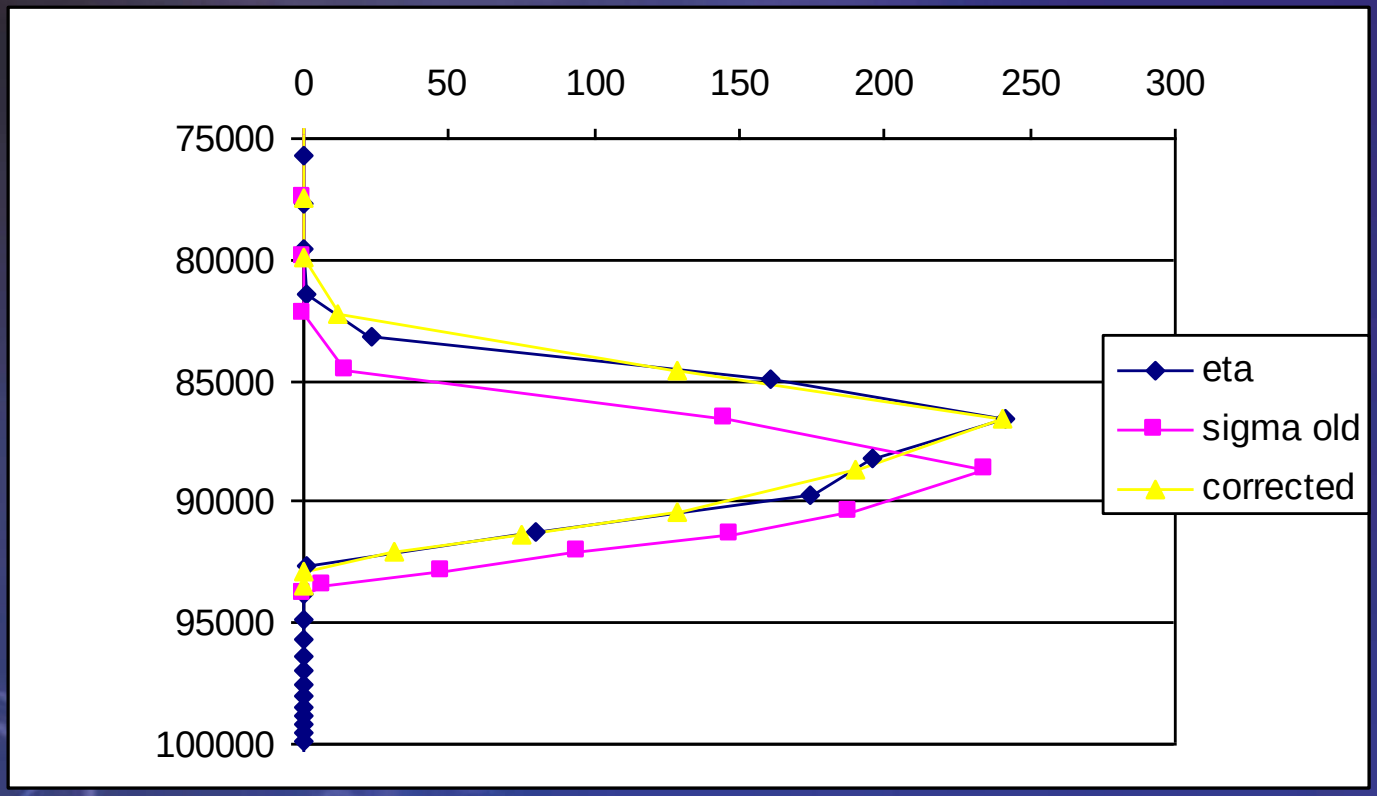
Test coupling to Eta TKE Kh (m2/s)

Couple Eta Eddy heat diffusivities from Mellor-Yamada TKE scheme

- use to drive CMAQ pbl mixing
- ? Eta Kh does not include effects of shallow convection near pbl top

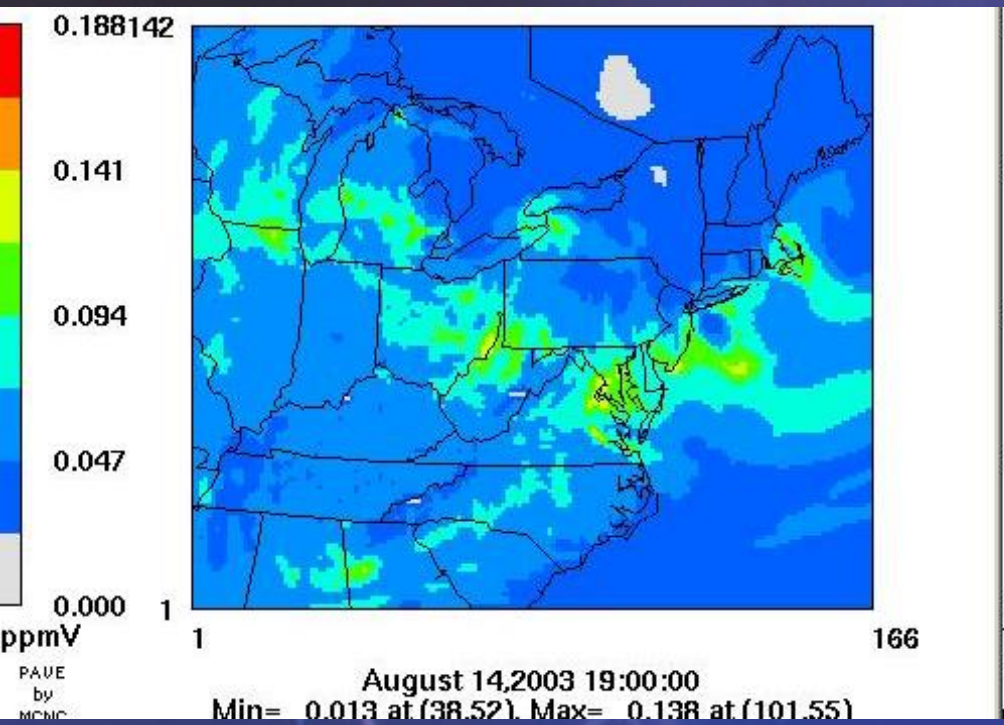


Eta Kh profile differences:
Mid-layer vs layer top

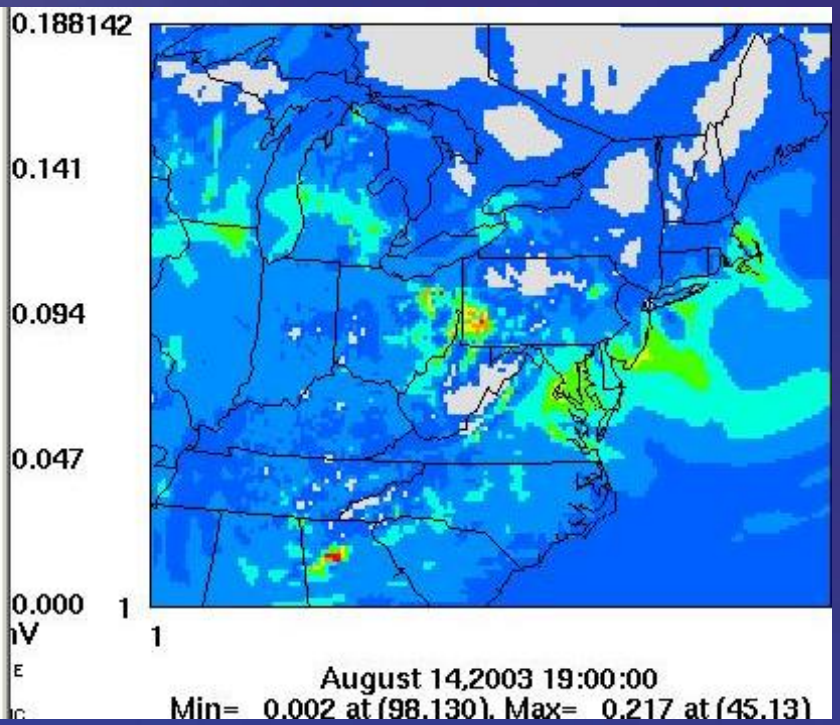


CMAQ coupled w/ Eta Turbulence Parameterization (S2)

W/ Eta ½ layer Kh profiles



W/ Eta full layer Kh profiles



Summary

- ***Summer O3 NE US 48 hour prediction capability***
  - **Over-prediction primarily due to:**
    - ***Incorrect land-use specification***
    - ***Eta temperature interpolation to CMAQ Sigma surfaces***
    - ***Incorrect Precip coupling***
- ***FY04: Complete experiments & implement***
  - ***Improved O3 boundary conditions (GFS predictions)***
  - ***Improved Coupling to Eta PBL mixing***
  - **Expanded parallel domain on development machine**
  - **Improved Emissions (Mobile 6)**
  - **Improved Eta cloud & radiation routine**
  - **Additional products for AIRMAP/ICARRT**
  - **FVS Evaluation (O3, pbl hgt…)**

National Air Quality Forecast Capability
Beyond IOC: Goals/Targets to FY 12

- Near-Term: Initial Operating Capability (IOC)
- Mid-Term (YR 5): Initiate nationwide forecasting
- Longer-term (YR 10): Enhanced capabilities

Proposed Products	*2-year Target*	*5-year Target*	*10-year Target*
Ozone forecasts	IOC 1-day forecasts: Northeast US	1-day forecasts for the Nation	Extend to day 2 and beyond
PM	R&D	1-day forecasts: Northeast US	1-day forecasts for the Nation
Extend to other pollutants		R&D	1-day forecasts

BACKUPS FOLLOW

National Air Quality Forecasting
Vision and Strategy

Vision

National Air Quality Forecast System which provides the US with ozone, particulate matter and other pollutant forecasts with enough accuracy and advance notice to take action to prevent or reduce adverse effects

Strategy

Work with EPA, State and Local Air Quality agencies and private sector to develop end-to-end air quality forecast capability for the Nation

Historical Background

- **Developed 1) Software Design Requirements, 2) Initial Operating Capability, 3) Software Development Plan and 4) Target Minimum Accuracy Goals**

- **CMAQ typically driven by MM5 and not easily adapted to Eta grid structure:**
  - ***Eta post-processor to generate sigma levels like MM5***
  - ***EMC's product generator to be adapted to generate the horizontal MM5 look-alike grid***
- **EMC generates test datasets for 20 September case**
  - ***Extra fields required***
  - ***Hourly frequency***
  - ***Complicates "Spring Bundle"***

Ozone Depletion Mechanism:

Day Time

$O_3 + NO_2 \rightarrow NO_3 + O_2$

$O_3 + N_2 \rightarrow NO + N + O_2$

$O_3 + NO \rightarrow NO_2 + O_2$

$OH + O_3 \rightarrow HNO_2 + O_2$

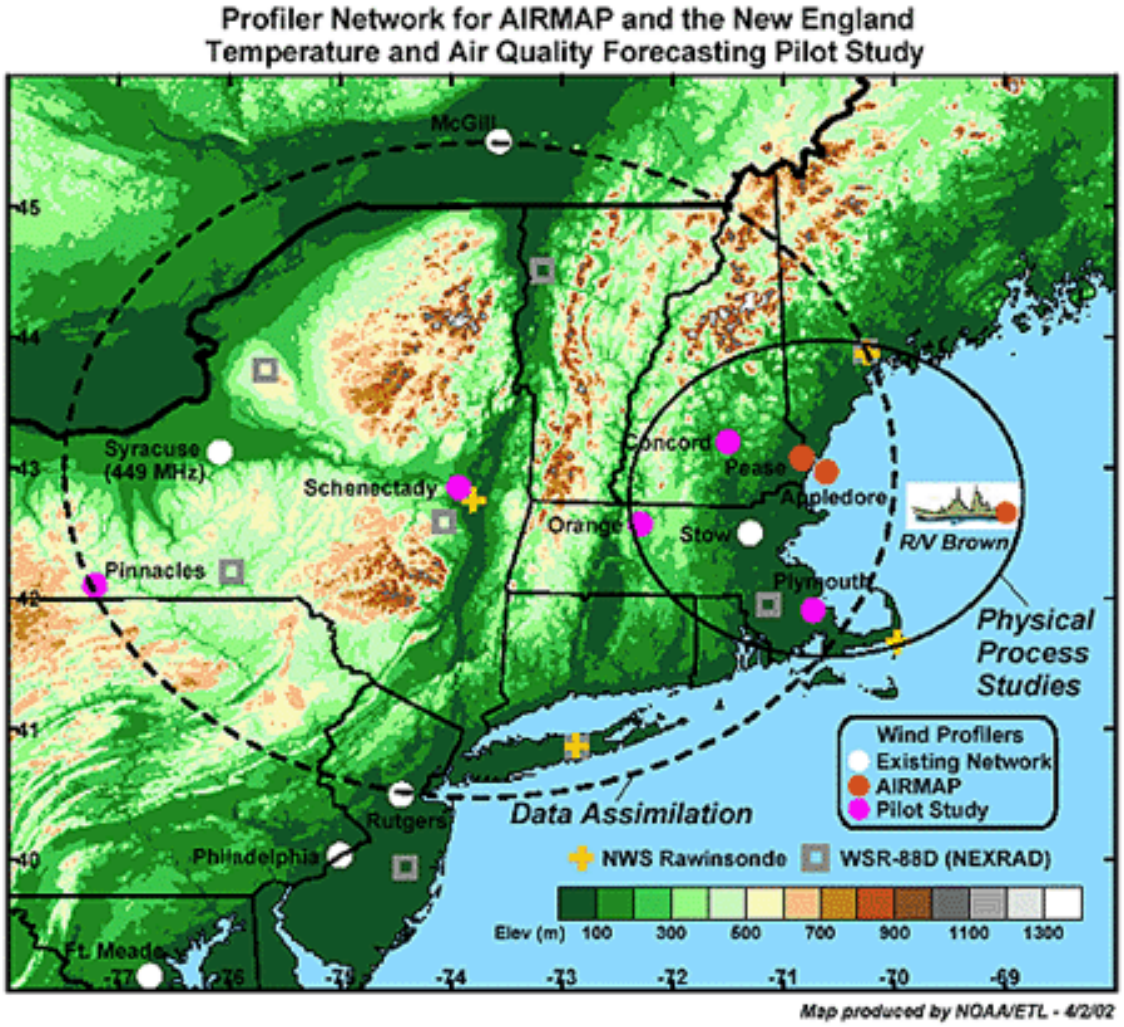
$VOC + O_3 \rightarrow$ hydrocarbons + [inorganic oxides]

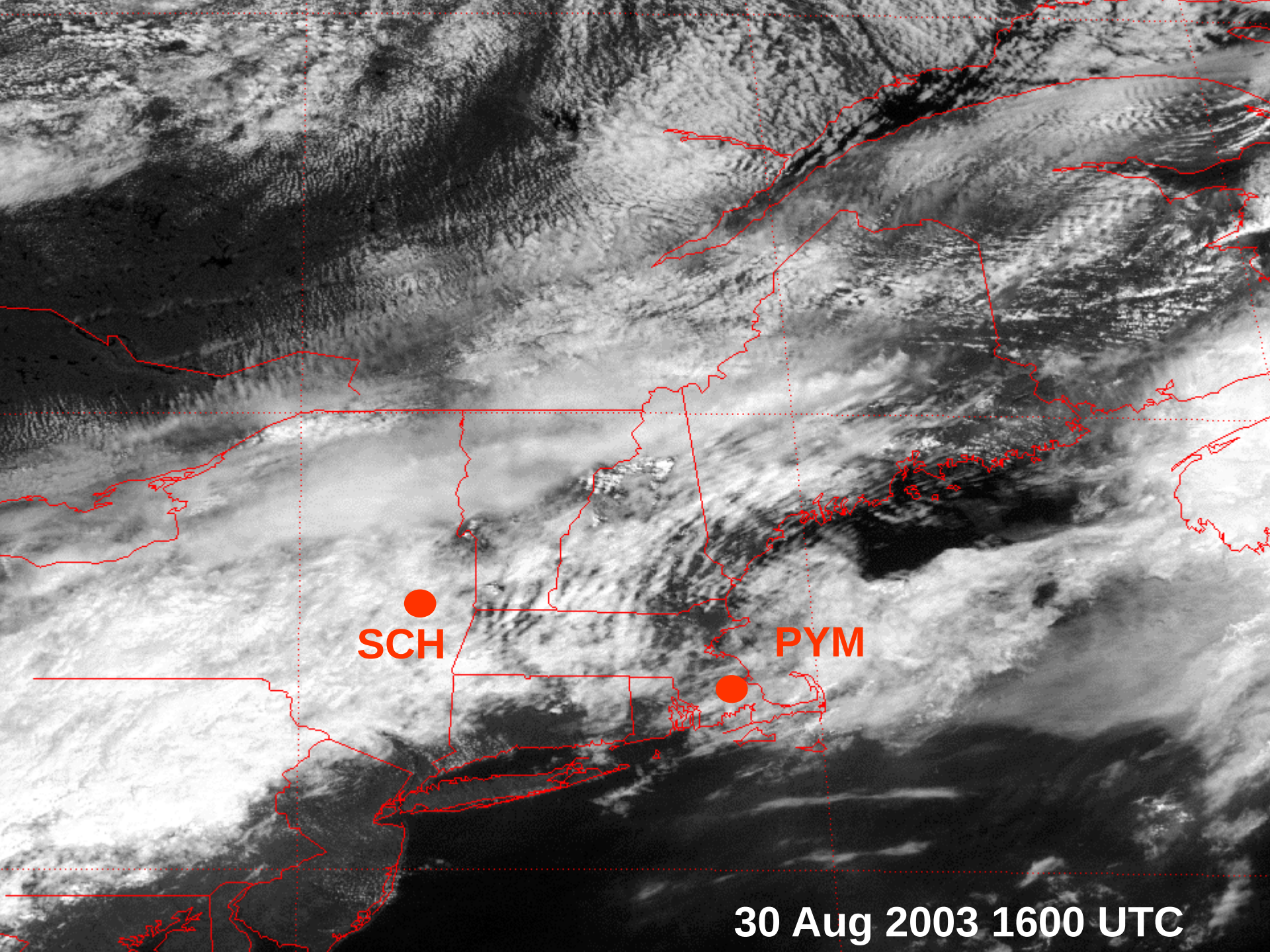
Night Time:

$O_3 + NO \rightarrow NO_2 + O_2$

North East High Res.Temperature Program

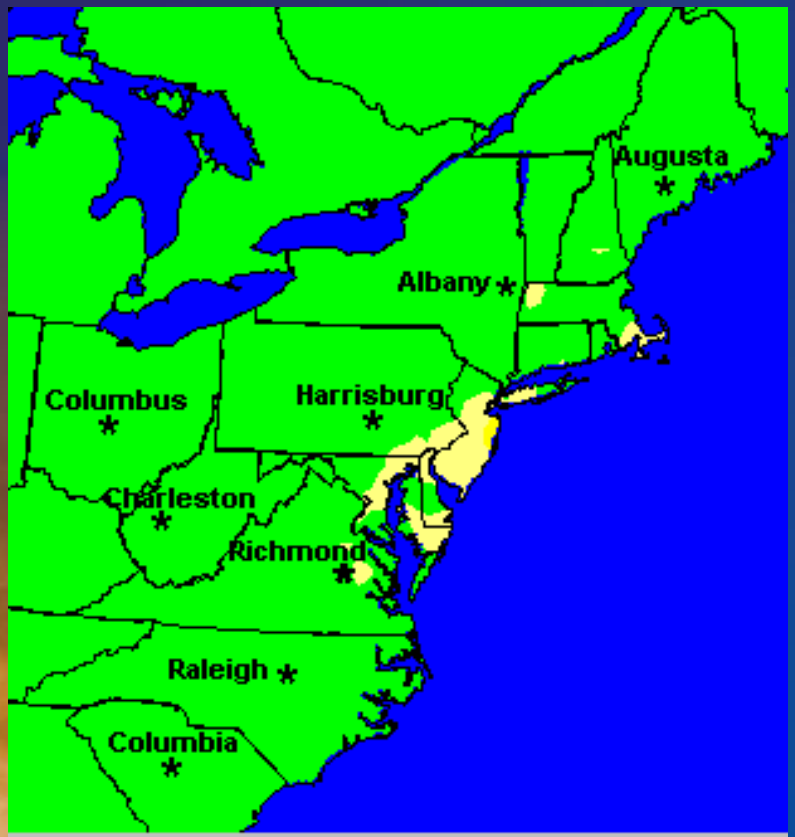
Air Quality Evaluation




SCH
PYM
30 Aug 2003 1600 UTC

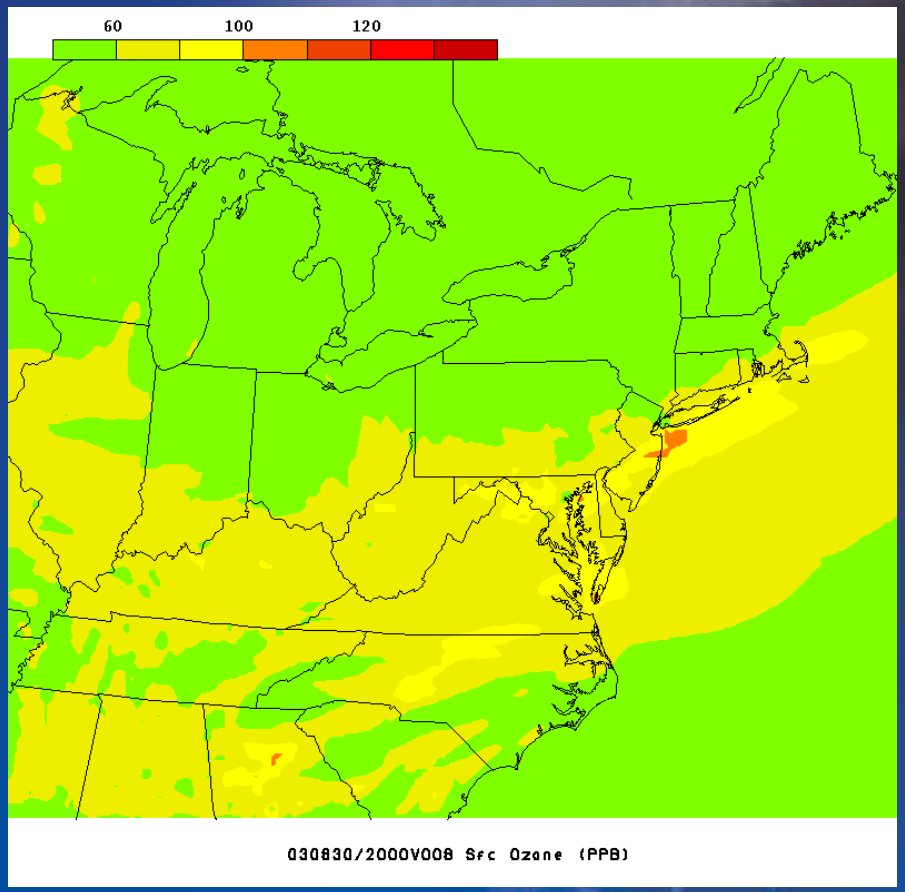
Retrospective Test Results:

Predicted Surface Ozone Concentrations



August 30, 2003

16:00 EDT



Eta-Post: Land-Surface Fields Added

Parameter Name	GRIB No.	GRIB Table(s)
Snow depth	066	130 (or 2)
Maximum snow albedo	159	130
Liquid volumetric soil moisture	160	130
Snow-free albedo	170	130
Number soil layers in root zone	171	130
Canopy conductance	181	130
Minimal stomatal resistance	203	130
Wilting point (volumetric soil moisture)	219	130
Planetary boundary layer height	221	130 (or 2)
Surface slope type	222	130
Soil type	224	130
Vegetation type	225	130 (or 2)
Transpiration stress-onset (vol. soil mst.)	230	130 (or 2)
Direct evaporation cease (vol. soil moist)	231	130
Snow cover	238	130 (or 2)
Soil porosity (vol. soil moisture)	240	130
Solar parameter in canopy conductance	246	130
Temperature parameter in canopy cond.	247	130
Humidity parameter in canopy cond.	248	130
Soil moisture parameter in canopy cond.	249	130

Eta-Post: Coupling w/ CMAQ

Hourly fields on CMAQ sigma levels to 48 hours

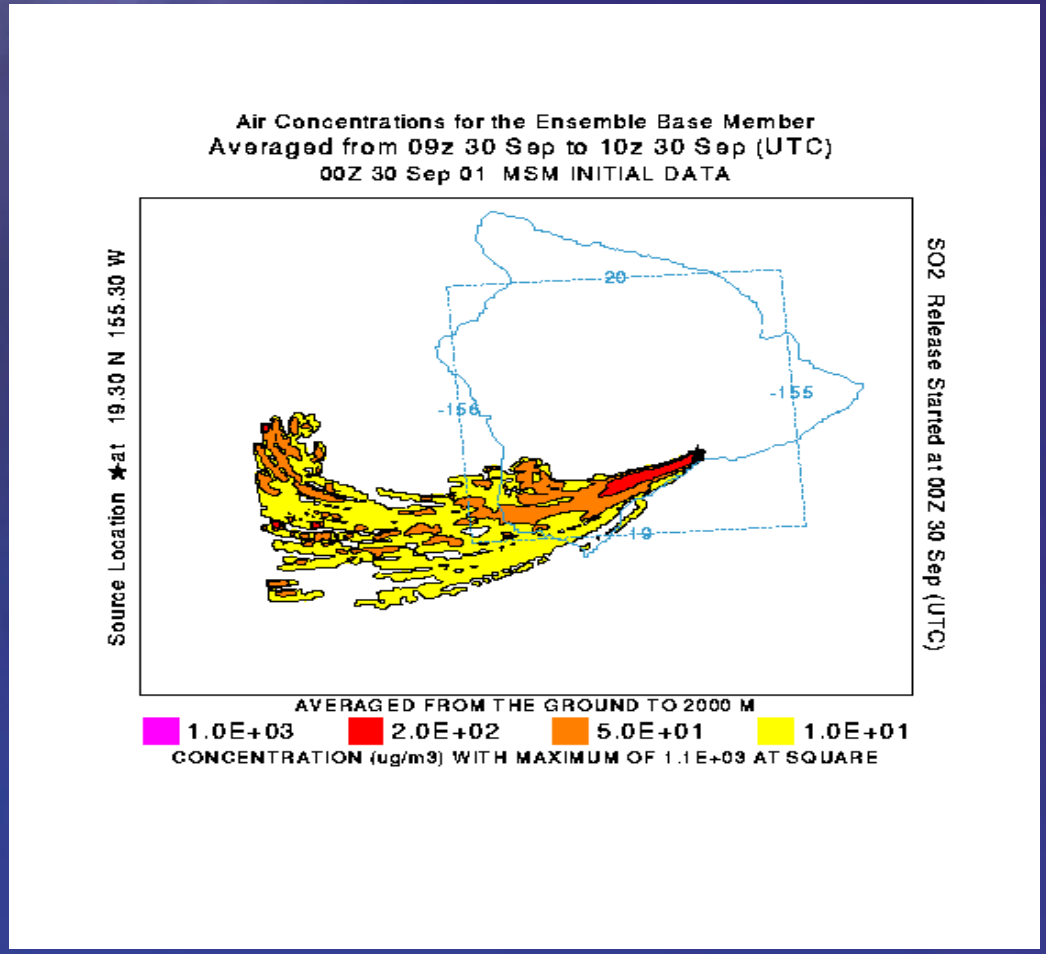
- *3-D pressure* - *3-D vertical velocity*
- *3-D temperature* - *3-D TKE*
- *3-D specific humidity* - *3-D cloud water mixing ratio*
- *3-D u-component wind* - *3-D cloud ice mixing ratio*
- *3-D v-component wind* - *3-D total cloud cover*
- *3-D geopotential* - *3-D total condensate*

• Hourly fields to 48 hours

- *terrain height* - *vegetation* - *latitude*
- *2-m temperature* - *land cover* - *longitude*
- *10-m u-component wind* - *ice cover* - *albedo*
- *10-m v-component wind* - *net latent heat flux*
- *accumulated convective precip* - *net sensible heat flux*
- *upward shortwave radiation flux* - *surface roughness*
- *upward longwave radiation flux* - *friction velocity*
- *accumulated non-convective precip* - *drag coefficient*
- *Blackadar mixing length* - *surface pressure*
- *soil temperature (all four layers)* - *soil moisture (all four layers)*

Short-range Mesoscale Ensembles

- Link SREF to dispersion modules:
  - perturb initial conds
  - perturb physics
- Perturb emissions & source term modules
- Variational assimilation to determine ensembles



Need for Improved Physical Parameterizations

Limitations to Similarity Theory

- ***MO Similarity theory:*** *Express a turbulence length scale to relate fluxes to vertical gradients (V, T, Q)*

  - ***Limitations:***
    - ***Spatial homogeneity, time stationarity, short vegetation***
    - ***Stable conditions: fluxes controlled by regional-scale***

- ***Hypotheses should be relaxed to fit real-world data***