

Comparison of National and State Emissions Inventories used for Houston Ozone Simulations

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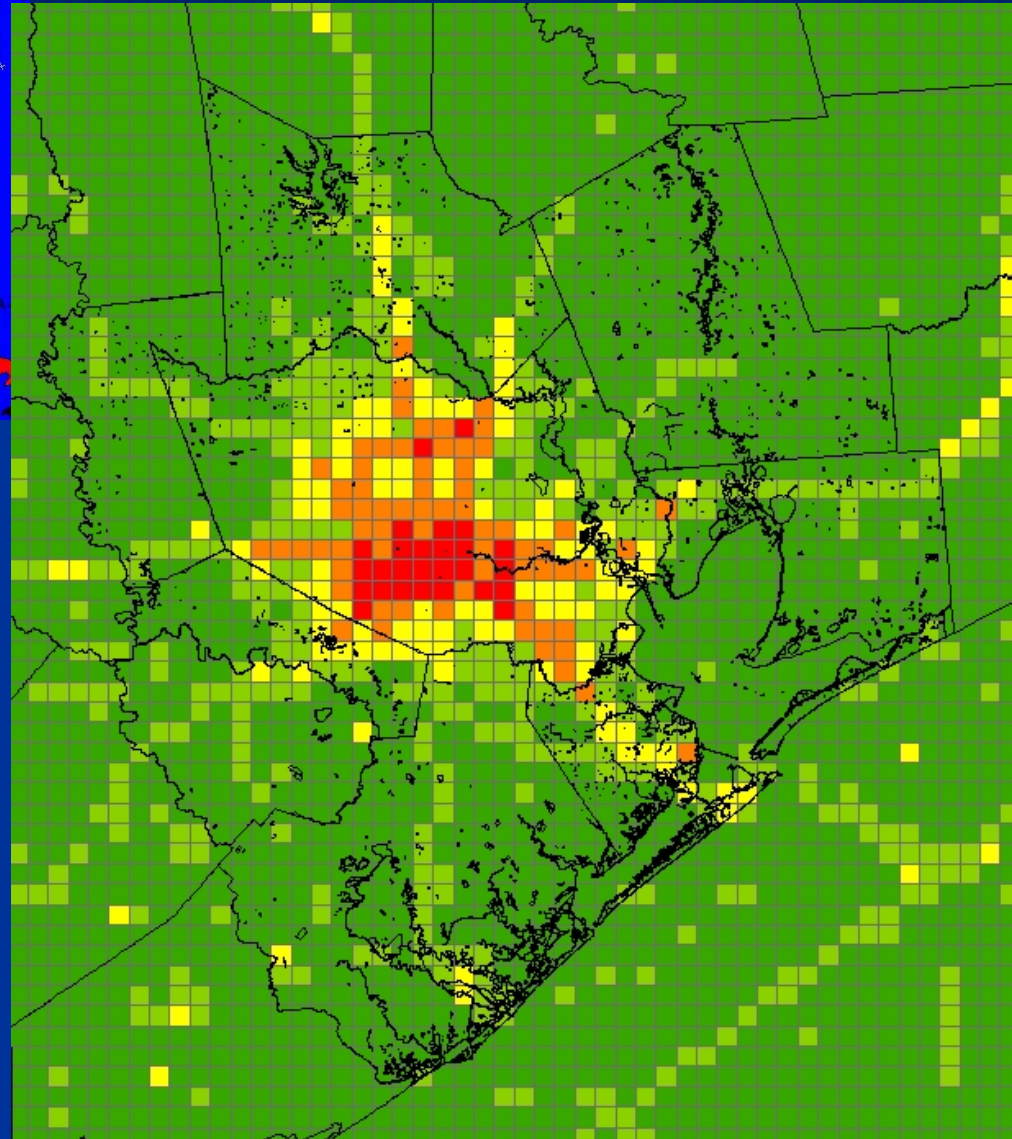
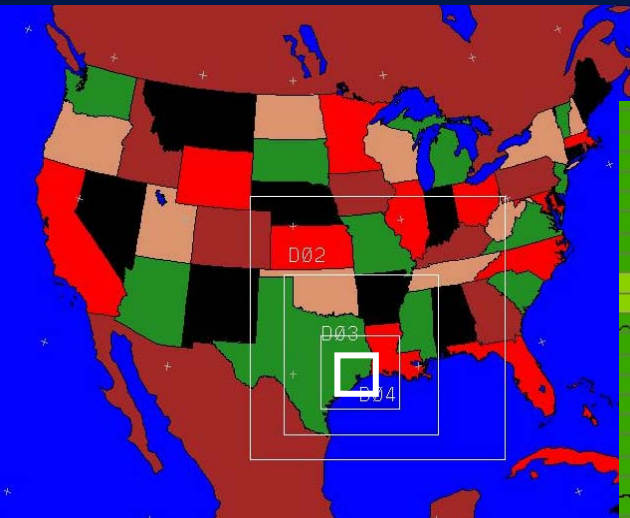
Institute for Multidimensional Air Quality Studies
University of Houston, Houston, TX

Outline

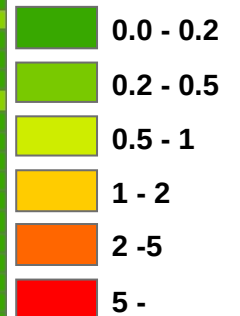
- Introduction: Overview of Houston-Galveston area
- Objectives of this study
- Comparison of Emissions inventories: National vs. State
- Ozone simulations with CMAQ
- Comparisons of CMAQ results to observations
- Conclusions

NO emissions

At a resolution of 4 km



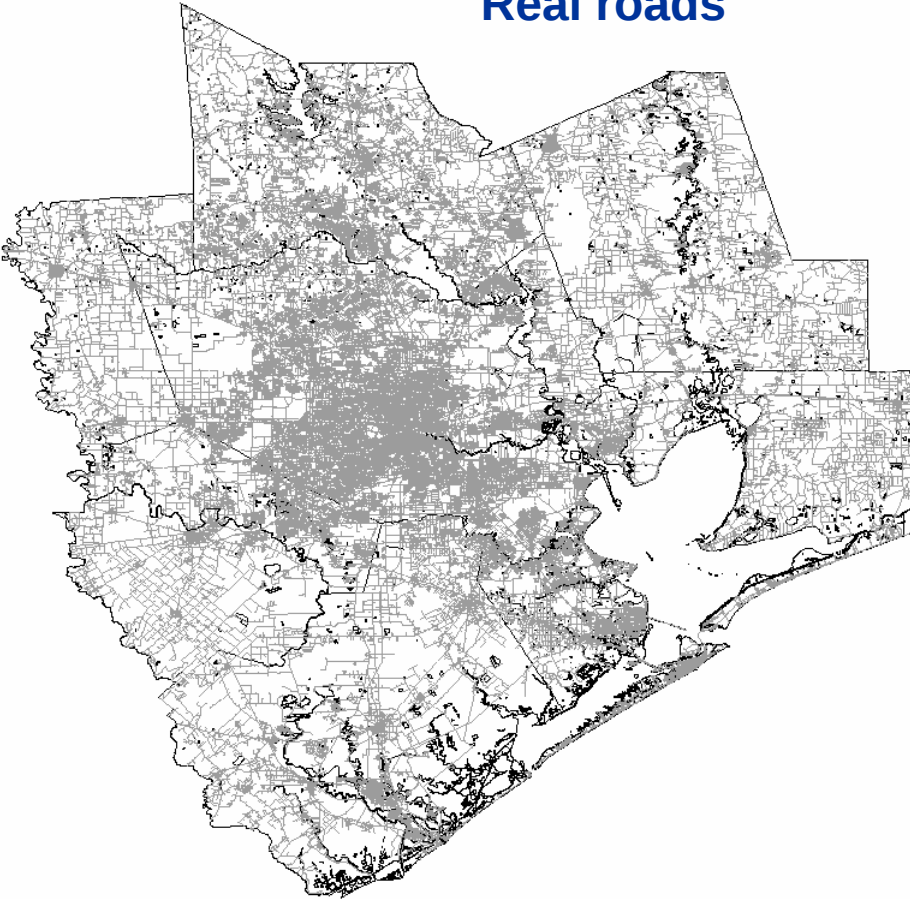
NO (moles/s)



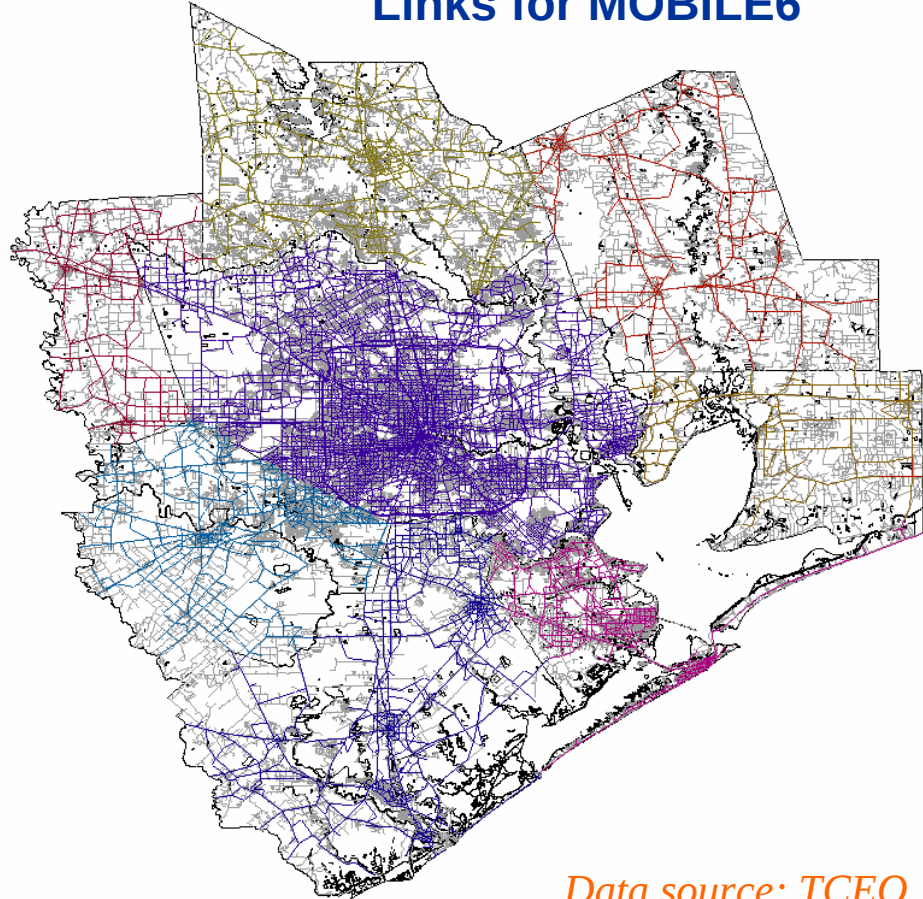
From all the sources

Houston Road Network

Real roads



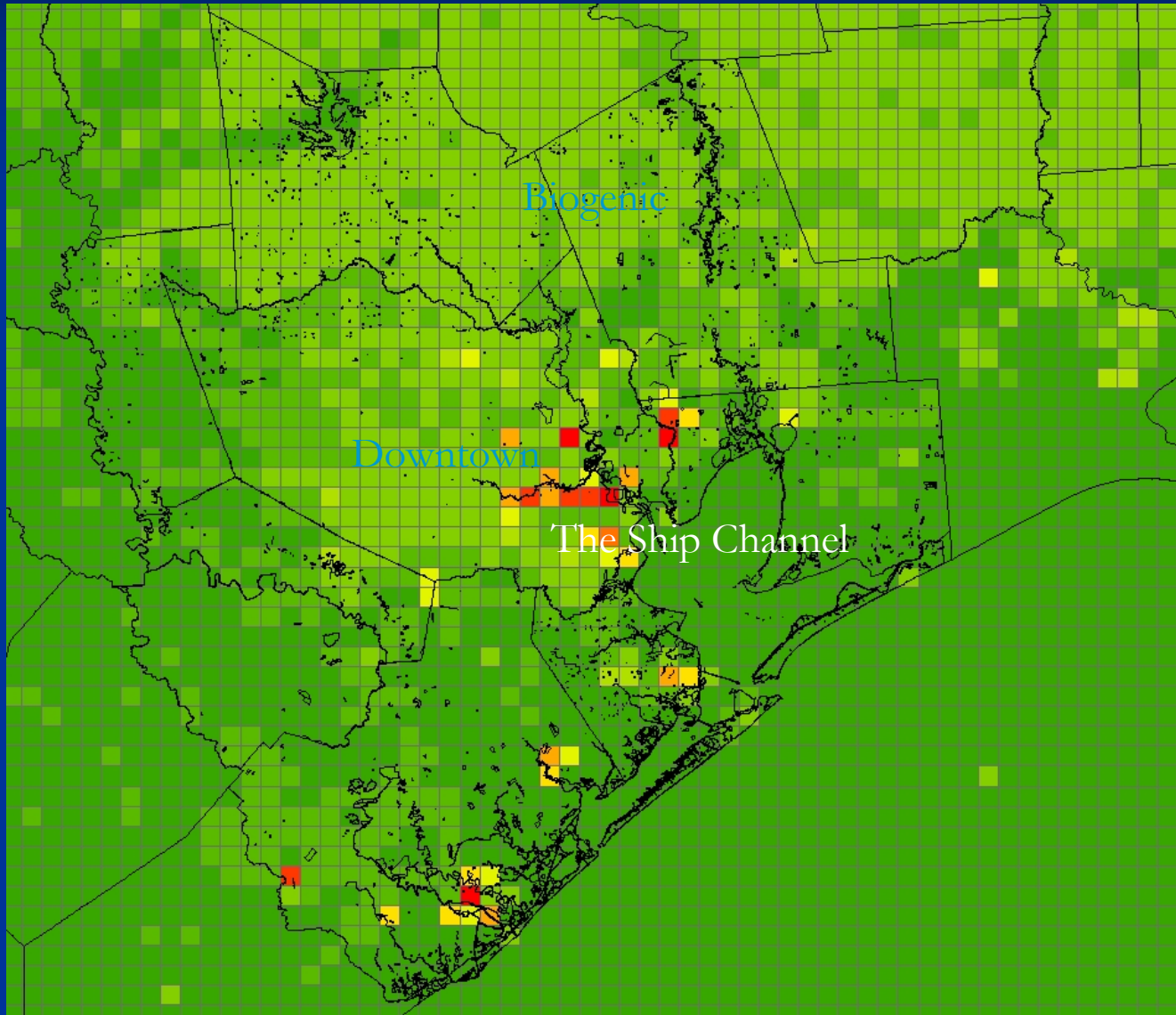
Links for MOBILE6



Data source: TCEQ

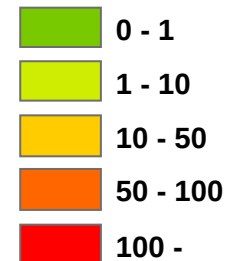
VOC emissions

Ethene (ETH) emissions for CB4
gridded at a resolution of 4 km



From all the sources

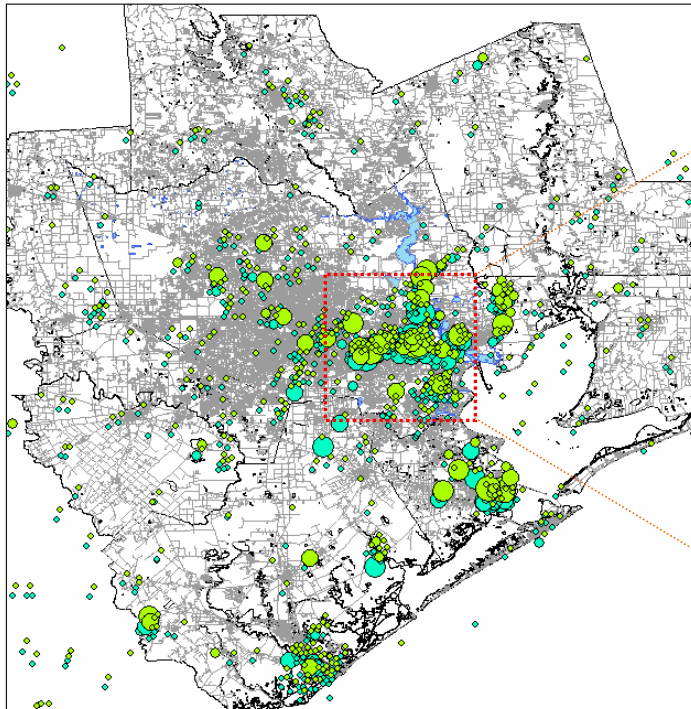
ETH (Kmole/d)



Point Source along the Ship Channel

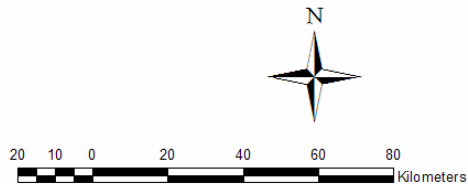
VOC

The Houston Ship Channel

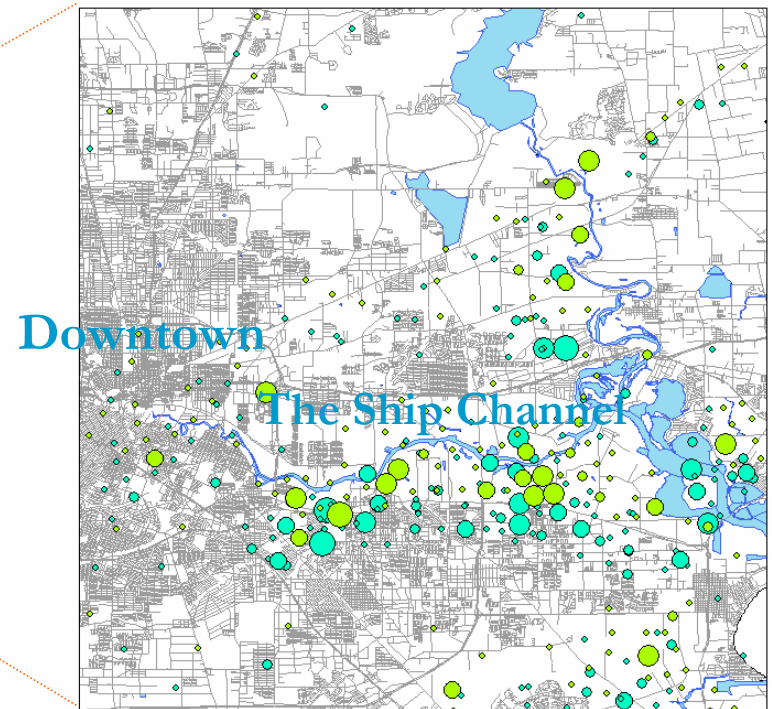


VOC_DY (tons/day)

- 0.0000 - 0.5000
- 0.5001 - 1.0000
- 1.0001 - 2.0000
- 2.0001 - 5.0000
- 5.0001 - 10.0000

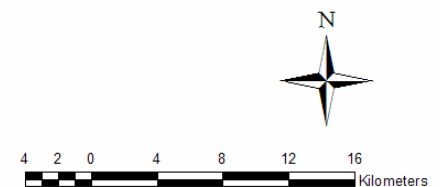


The Houston Ship Channel



VOC_DY (tons/day)

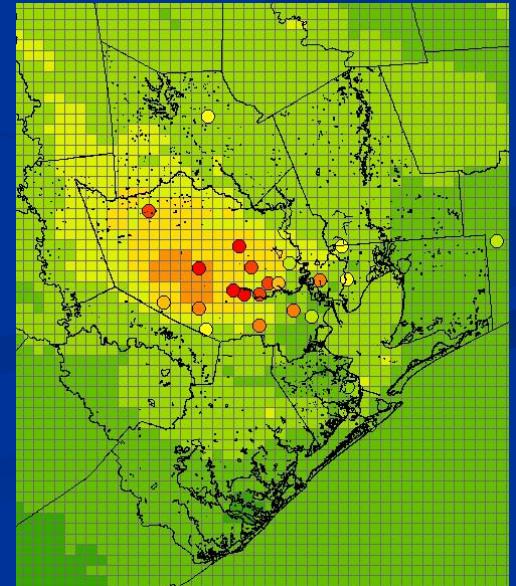
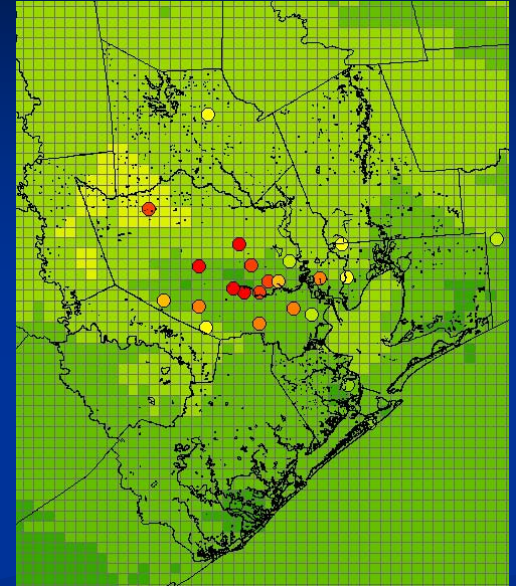
- 0.0000 - 0.5000
- 0.5001 - 1.0000
- 1.0001 - 2.0000
- 2.0001 - 5.0000
- 5.0001 - 10.0000



Emissions Inventory

For Ozone simulations

- National EI for 1999 (NEI)
 - U.S. EPA
 - NEI 1999 final version 3
 - Annual/Peak ozone day
- State EI from TCEQ (TEI)
 - Texas Commission on Environmental Quality
 - TexAQS 2000
 - Hourly or Peak ozone day
 - Regular and imputed



Objectives

- To see how national and state EIs are different for the Houston-Galveston area
- To answer how different simulation results we could have when those EIs are used for air quality simulations under a given condition
- To better understand several issues;
 - Which emission source has more uncertainties and how it could be improved.
 - Why it is difficult to get high ozone concentrations observed.
 - EI for air quality forecast for the region.

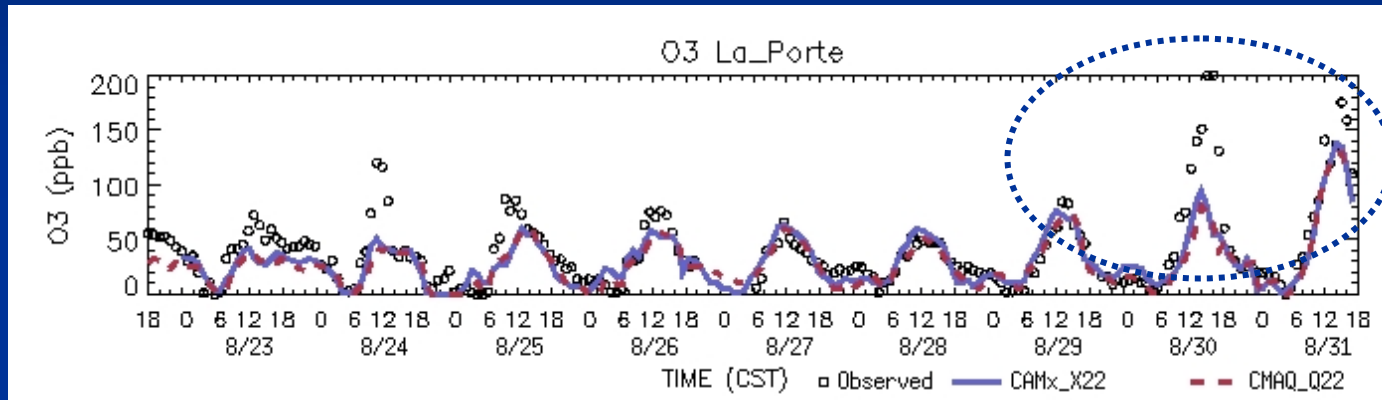
TEI: VOC Imputation

- TEI has two types of EIs; regular and imputed.
- Regular EI includes all the anthropogenic emission sources; area, non-road, mobile, and point sources.
- Imputed EI = Regular EI + additional VOC emissions to adjust
- Targeted NEGU point sources only
- Based on surface and airborne measurements, and CAMx simulations

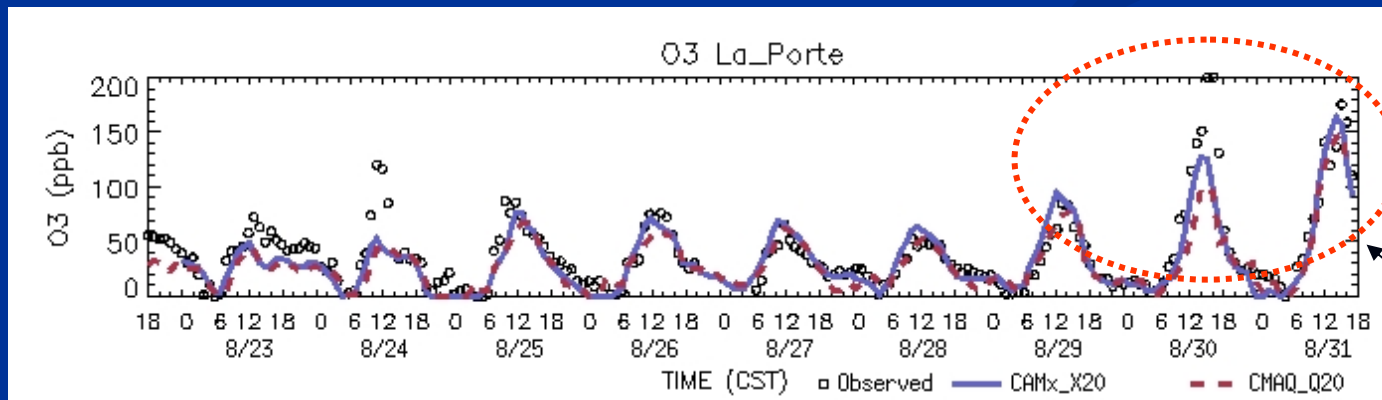
Simulated O3 Concentrations: Regular vs. Imputed

Previous simulations
CAMx & CMAQ
CB4 mechanism

Regular



Imputed

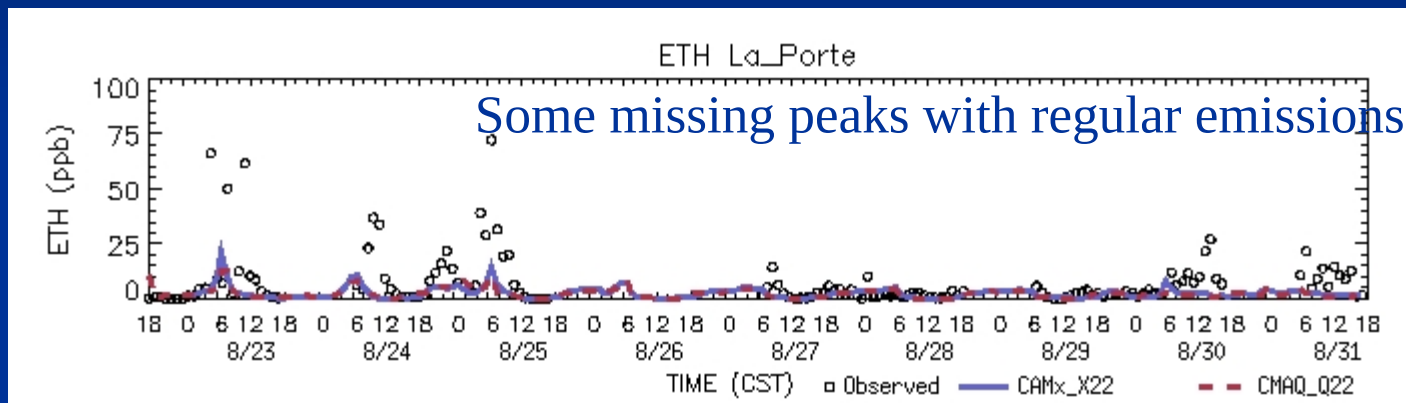


Improvements on
high ozone days

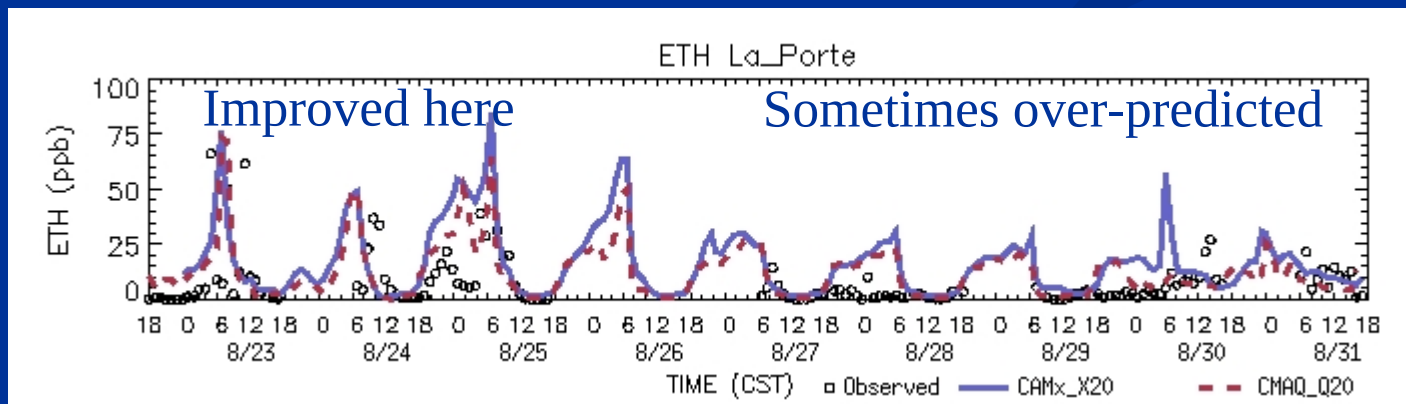
La Porte site for August 22 ~ August 31, 2000

Simulated ETH Concentrations: Regular vs. Imputed

Previous simulations
CAMx & CMAQ
CB4 mechanism



Regular

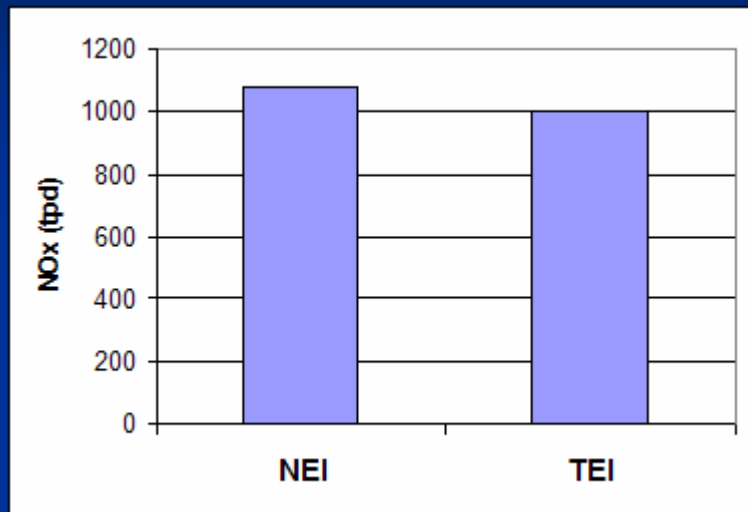


Imputed

La Porte site for August 22 ~ August 31, 2000

Overall NO_x & VOC Emissions

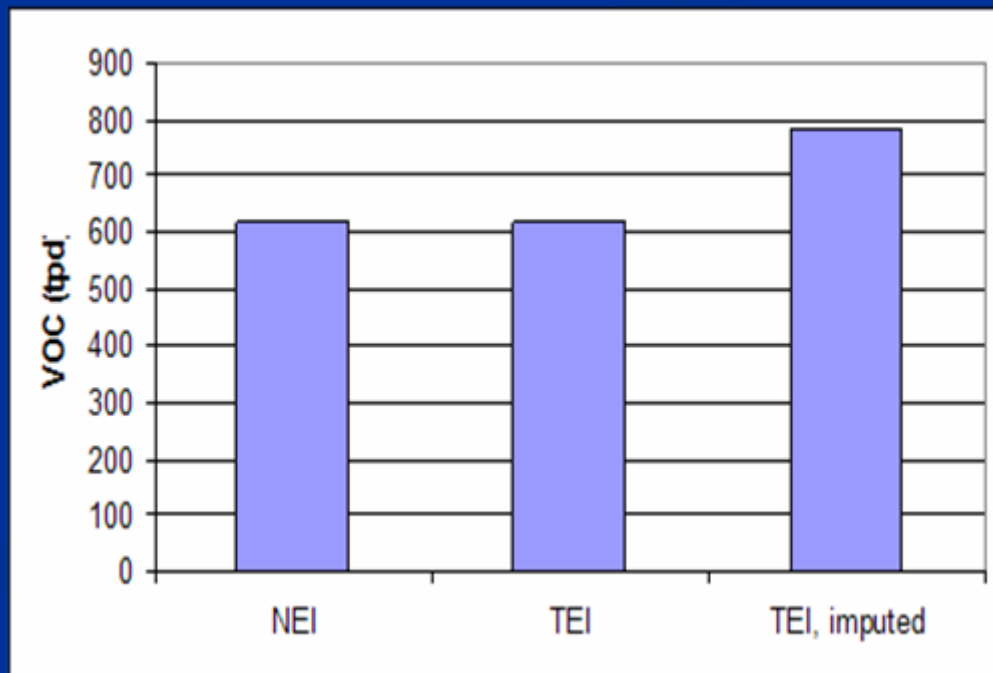
*From all the anthropogenic sources
inside the HG 8 counties*



For NO_x, NEI 5 ~ 10 % higher than TEI

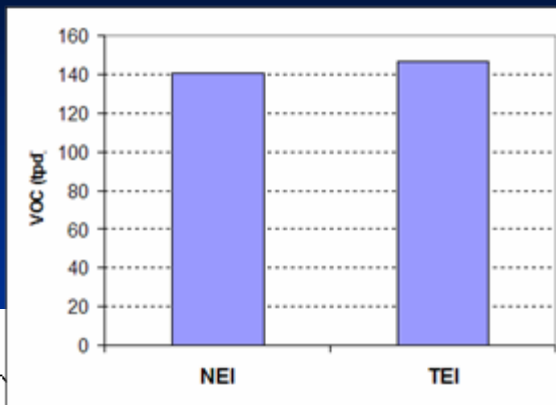
Before VOC imputation, NEI and TEI are comparable in the emissions rates.

After the imputation, TEI shows 20 ~ 25 % higher VOC emissions for HG 8 counties



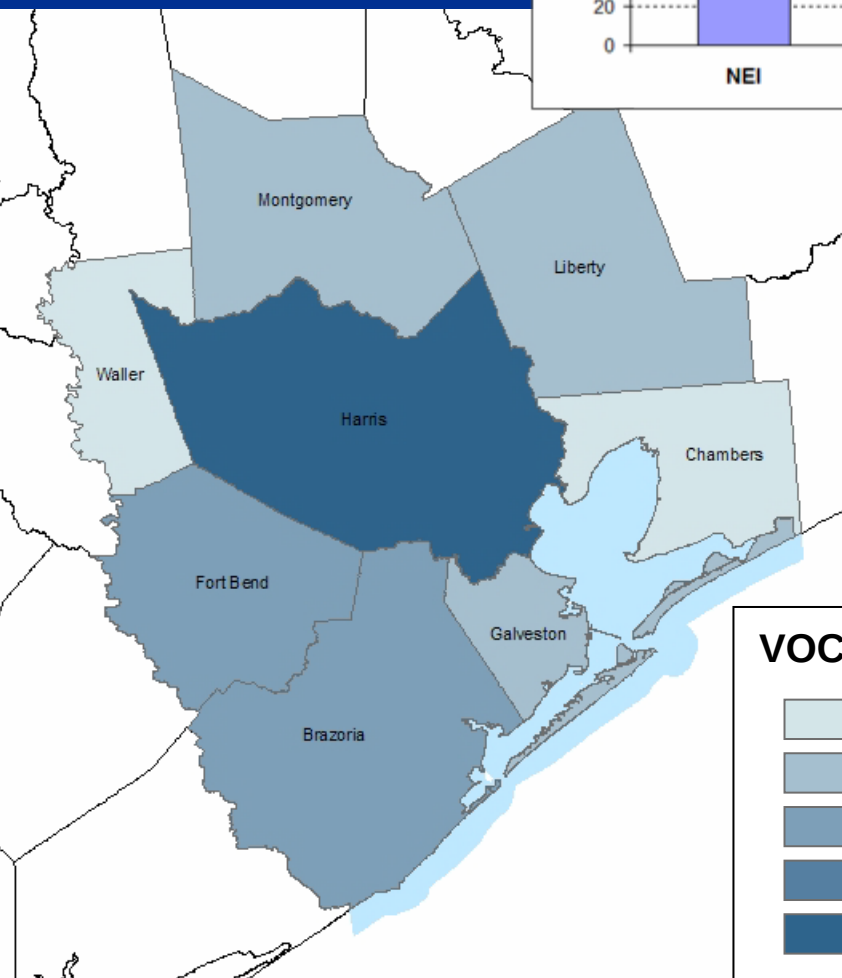
VOC Emissions from Area Sources

NEI

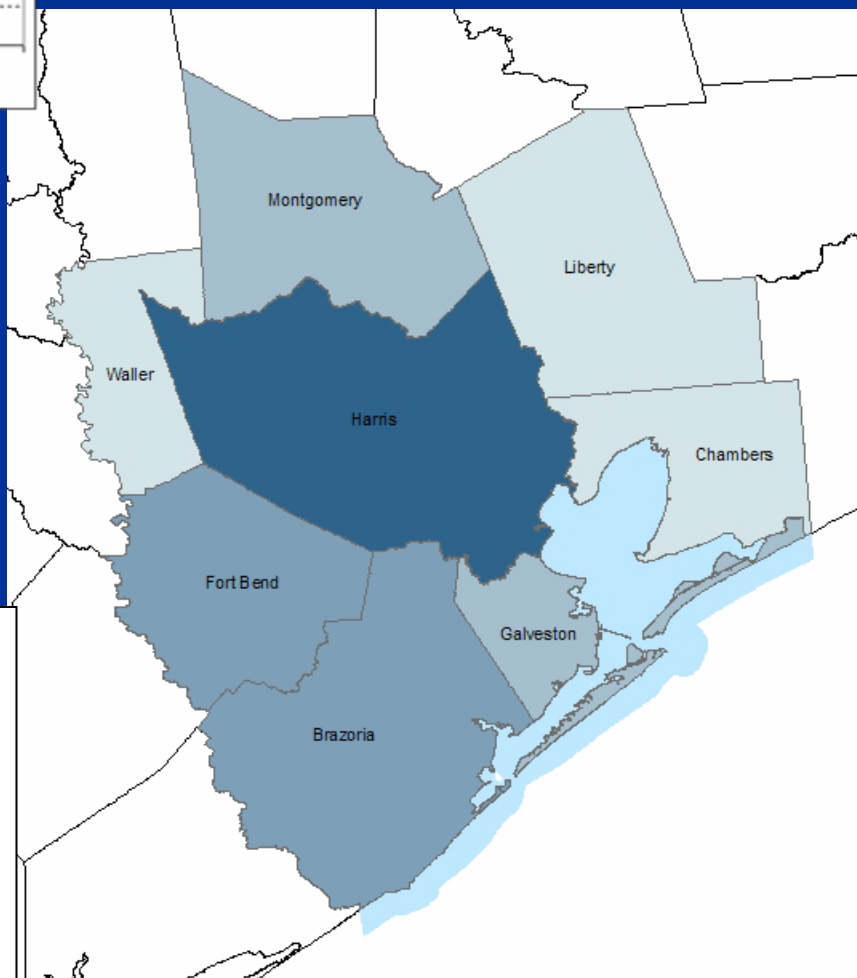
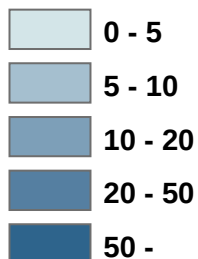


VOC emissions from area sources explain 20 ~ 25 % of total VOC emissions in two EIs.

TEI



VOC (tons/day)

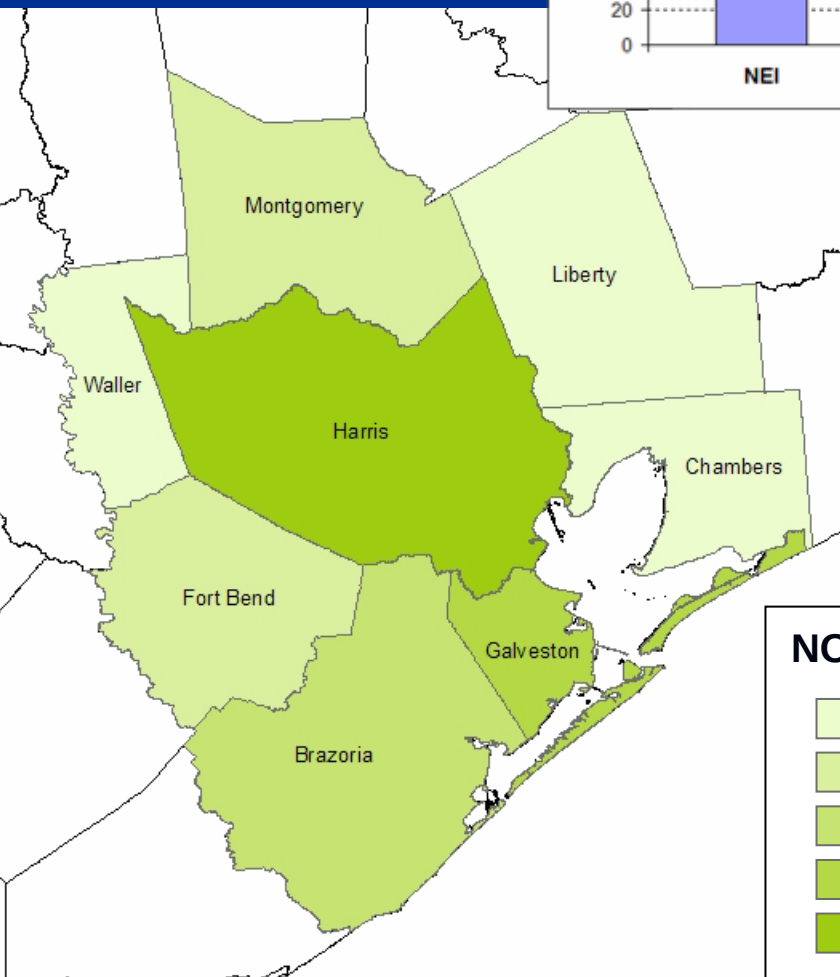
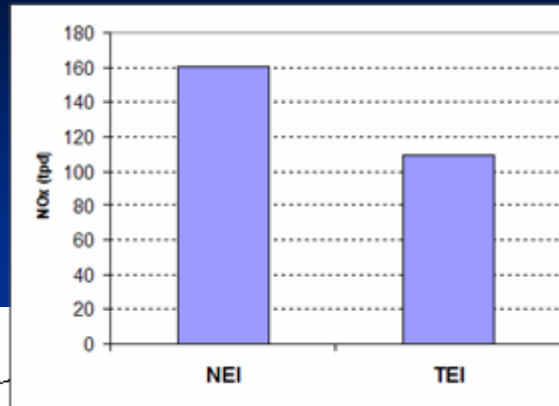


Non-road NOx Emissions

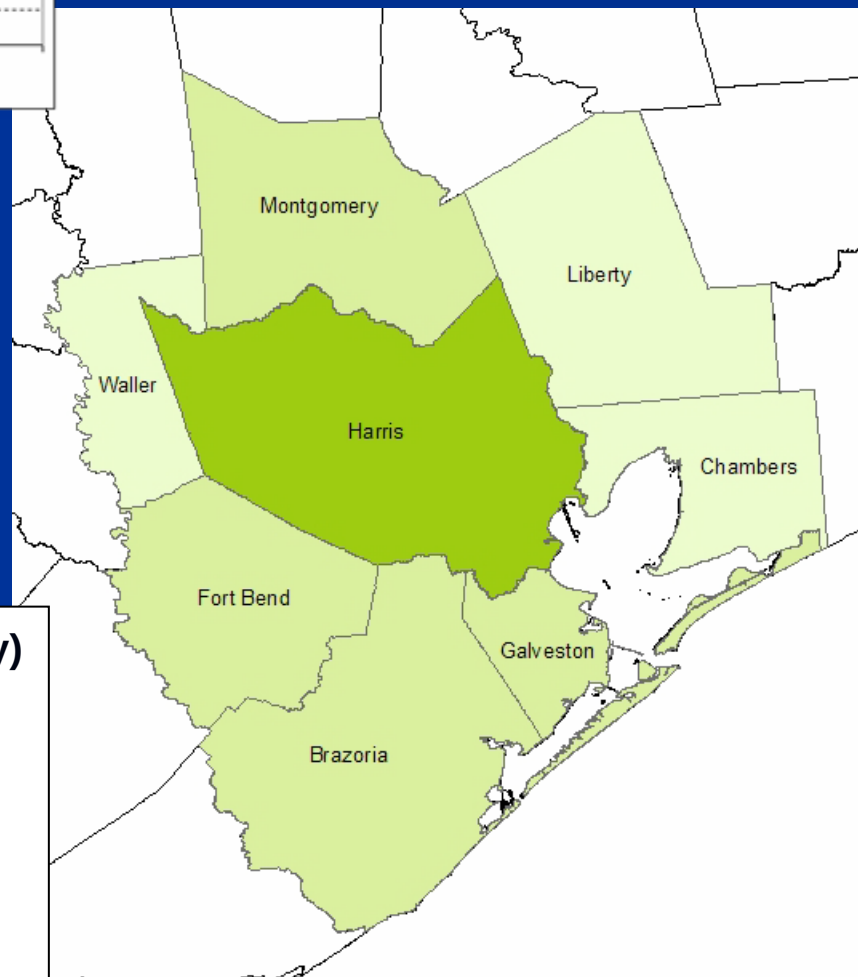
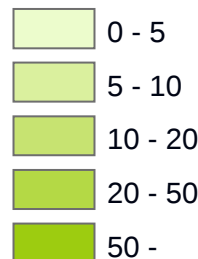
NOx emissions from non-road mobile sources take ~ 15 % and 11 % of total NOx emissions in NEI and TEI, respectively.

NEI

TEI



NOX (tons/day)

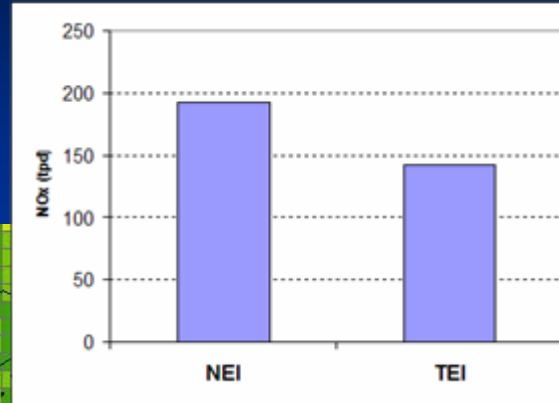


Area & Non-road NO emissions

Different surrogates for spatial allocation were used.

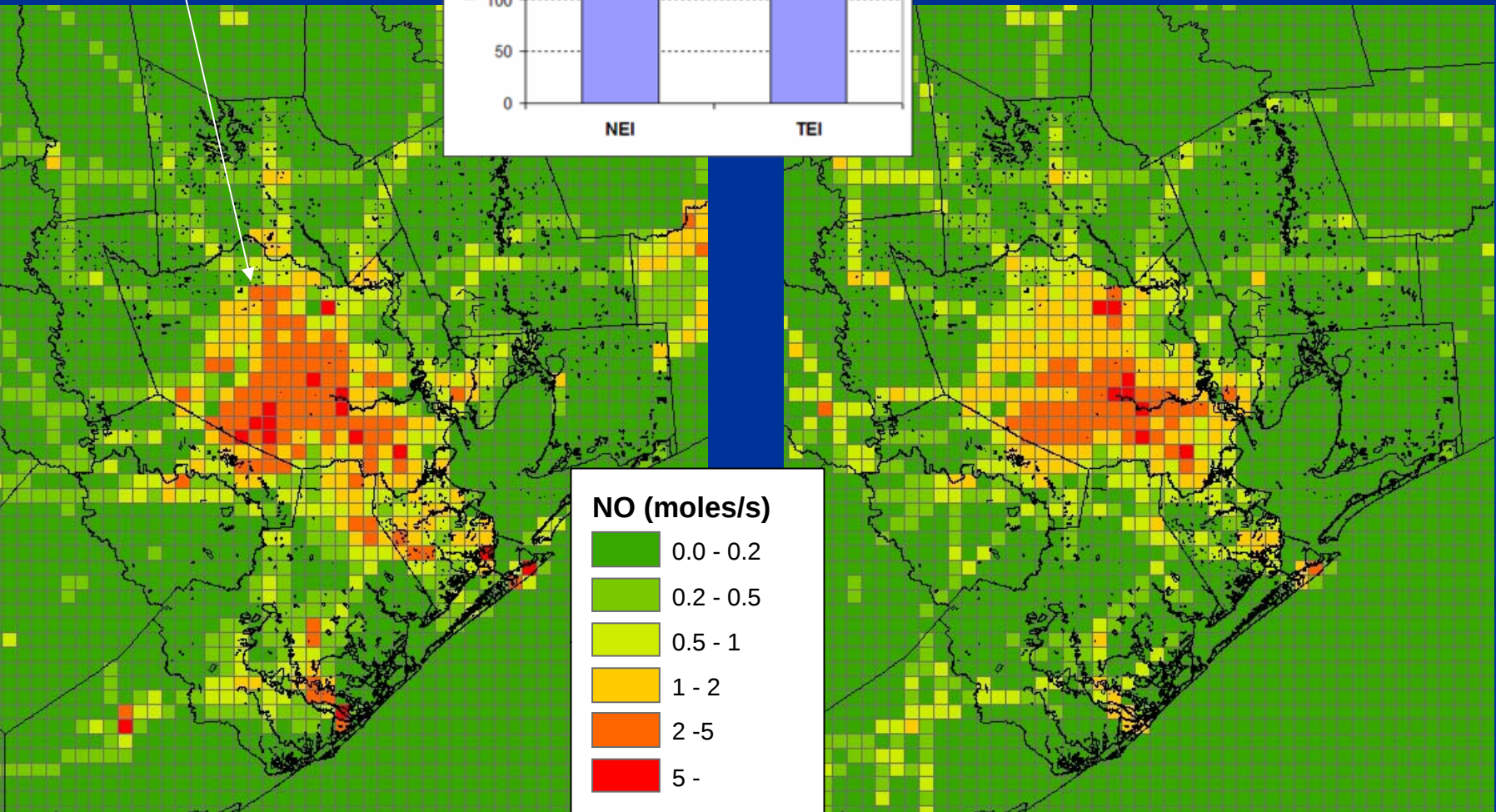
Higher NO emissions
downtown Houston

NEI



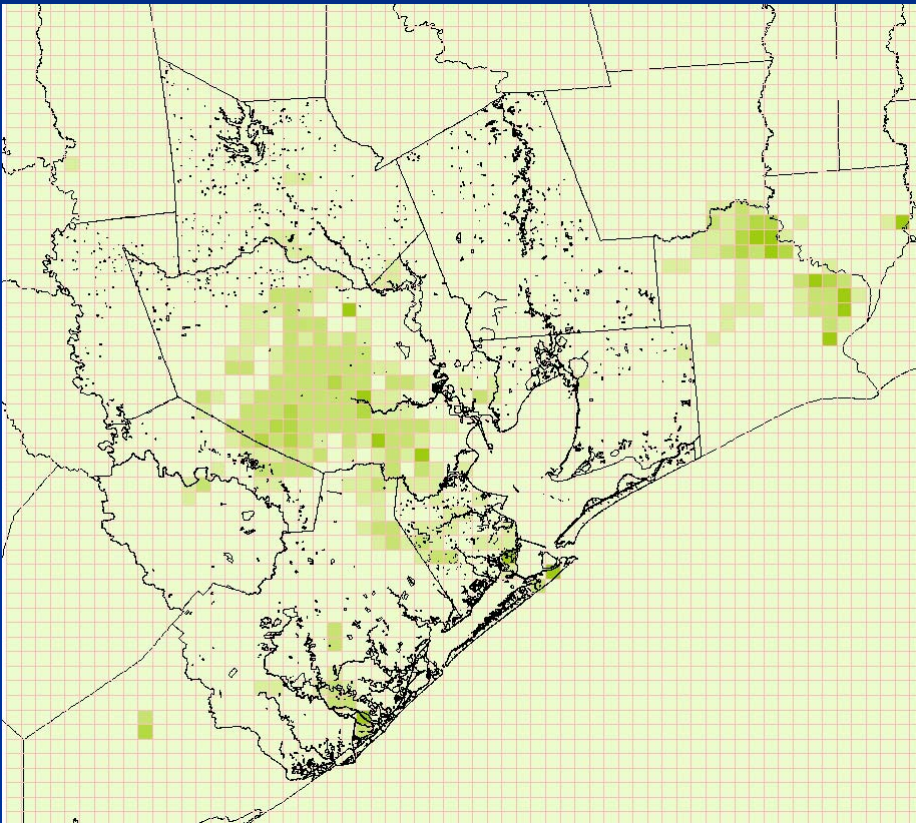
NEI shows ~ 50 tpd higher
NOx emissions for area & non-
road sources than TEI.

TEI

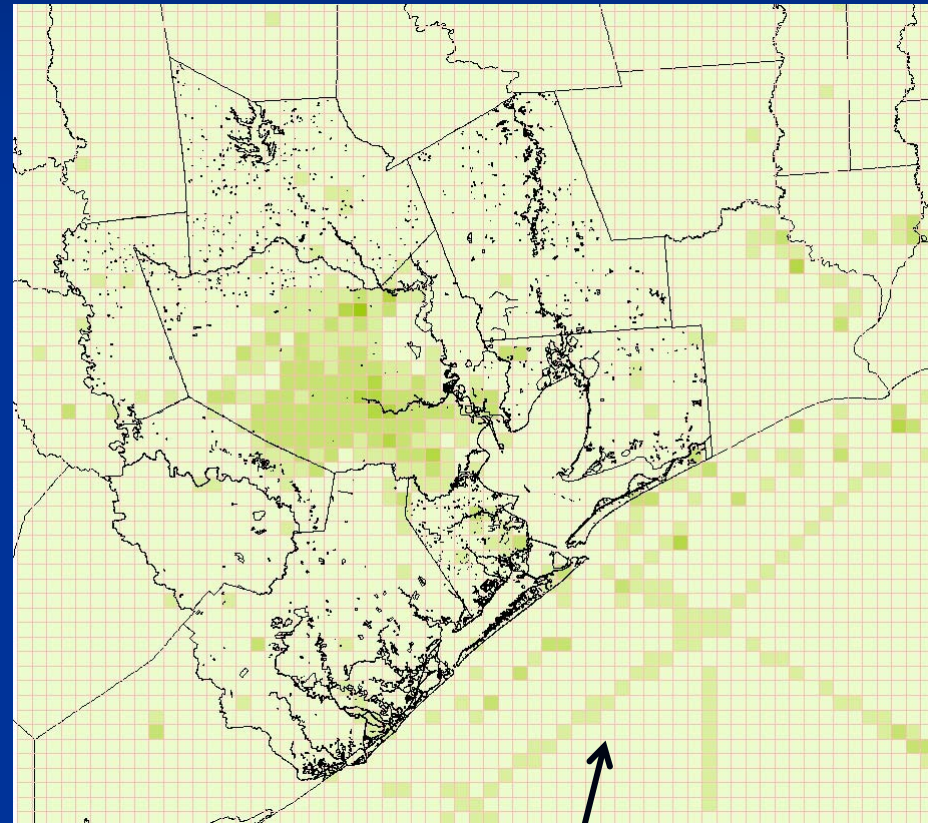


Area & Non-road Emissions

NEI



TEI



Onshore and offshore emissions

Mobile Emissions

■ NEI

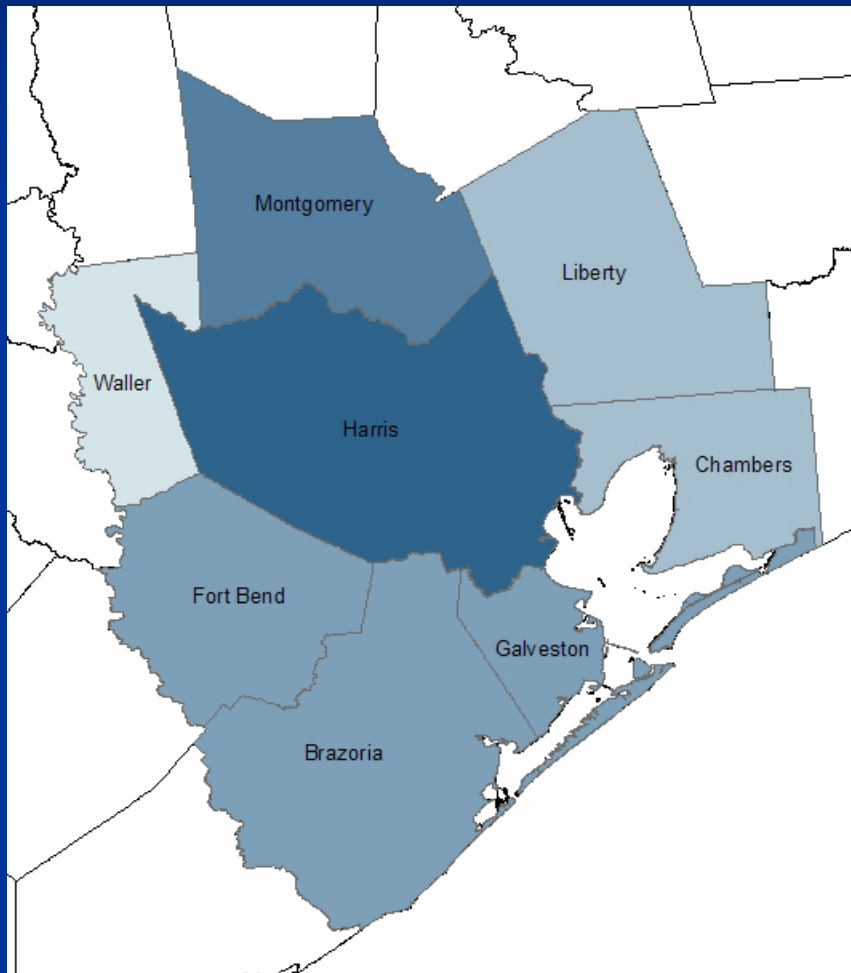
- County-based: Surrogates used for spatial allocation
- Monthly EI: Temporal profiles needed.

■ TEI

- MOBILE6 (outside SMOKE)
- Link-based (for HG 8 counties): No needs for surrogates
- Hourly emissions: No temporal profiles required
- Hourly temperature and relative humidity for each county provided.

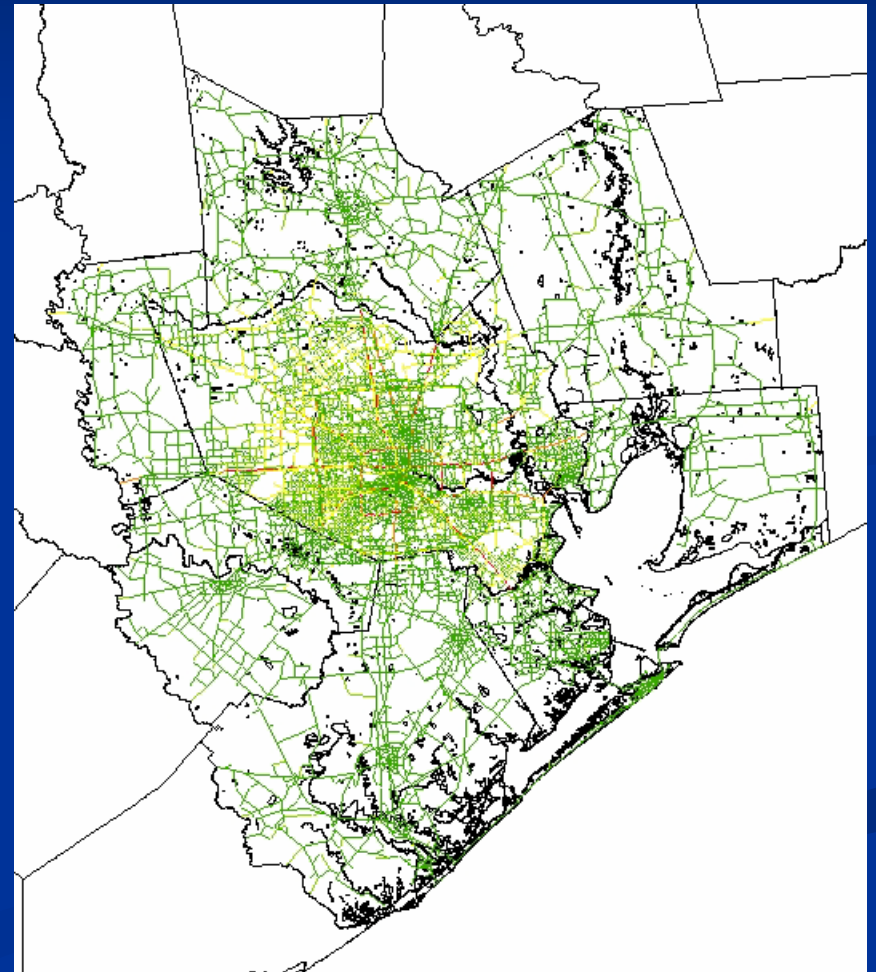
Mobile Emissions

NEI



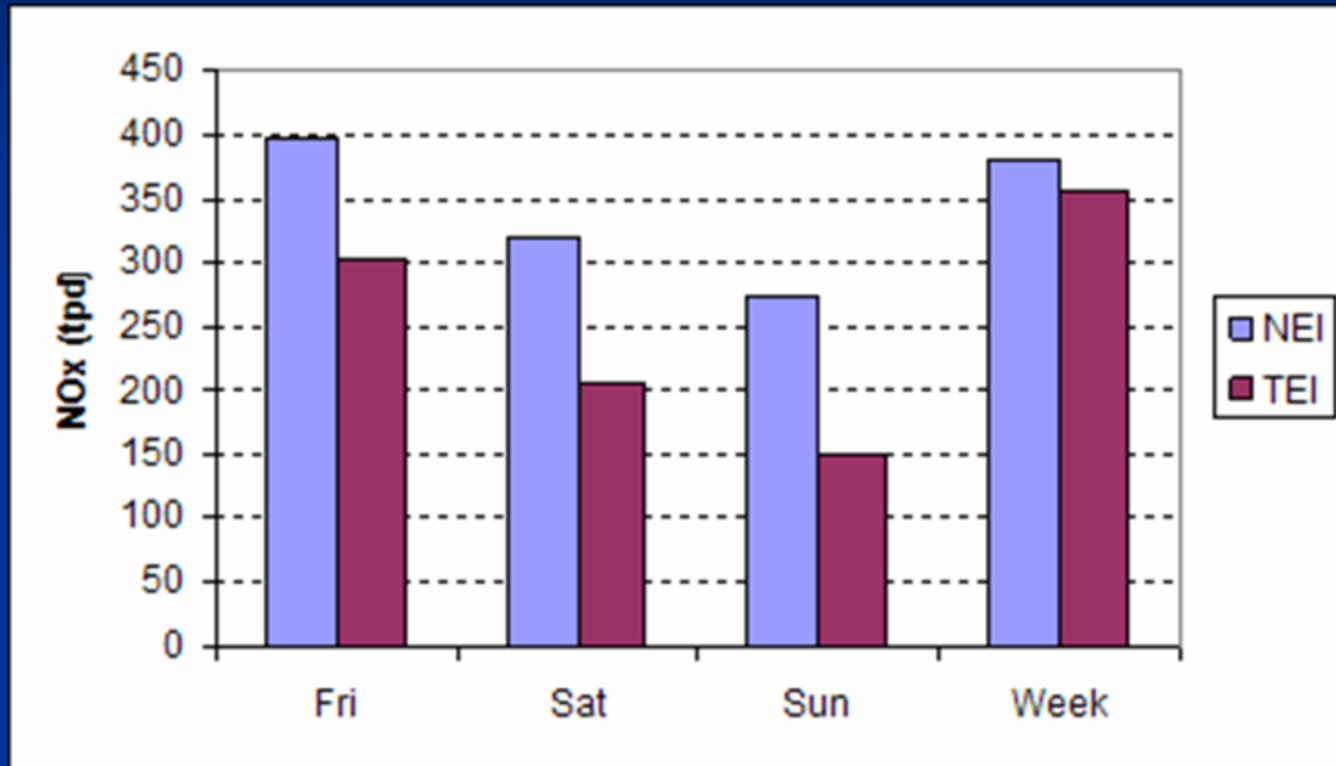
County-based emissions

TEI



Link-based emissions

Mobile Emissions

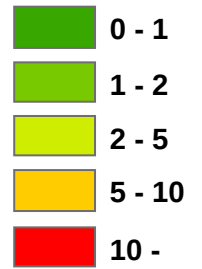


NOx emissions from on-road mobile sources explains ~ 35 % of total NOx emissions on a week day.

NEI shows ~ 20 tpd higher NOx emissions on a week day and ~ 120 tpd on a Sunday than TEI.

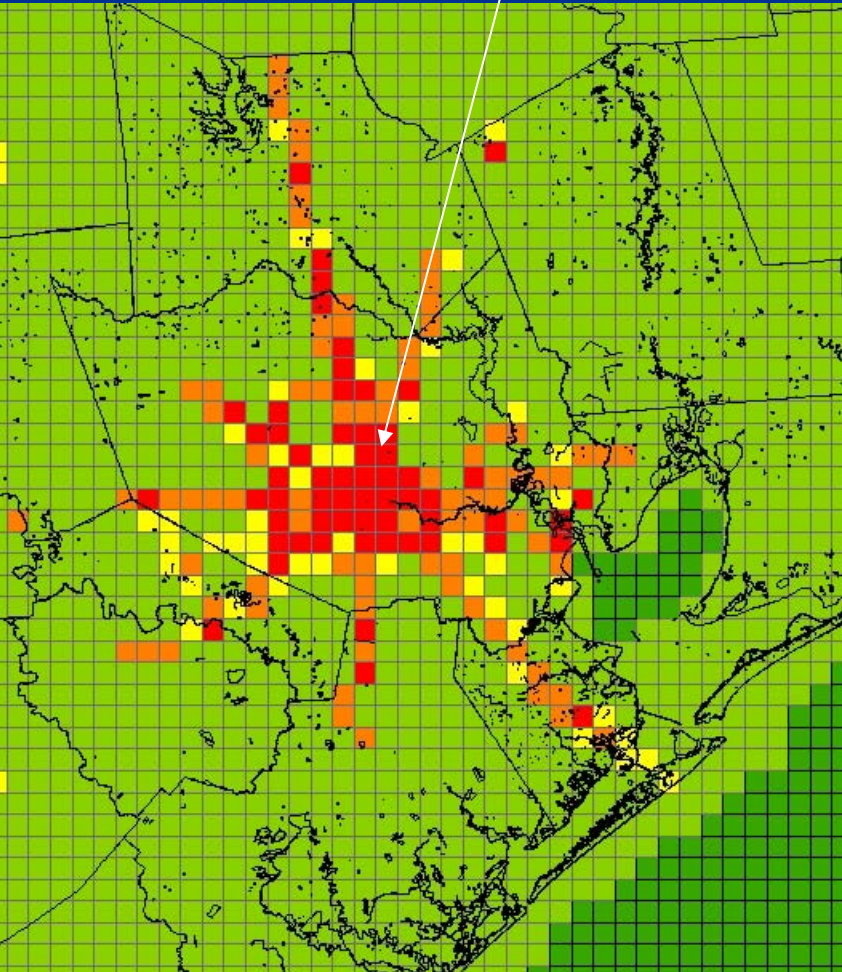
Mobile NO emissions

NO (moles/s)

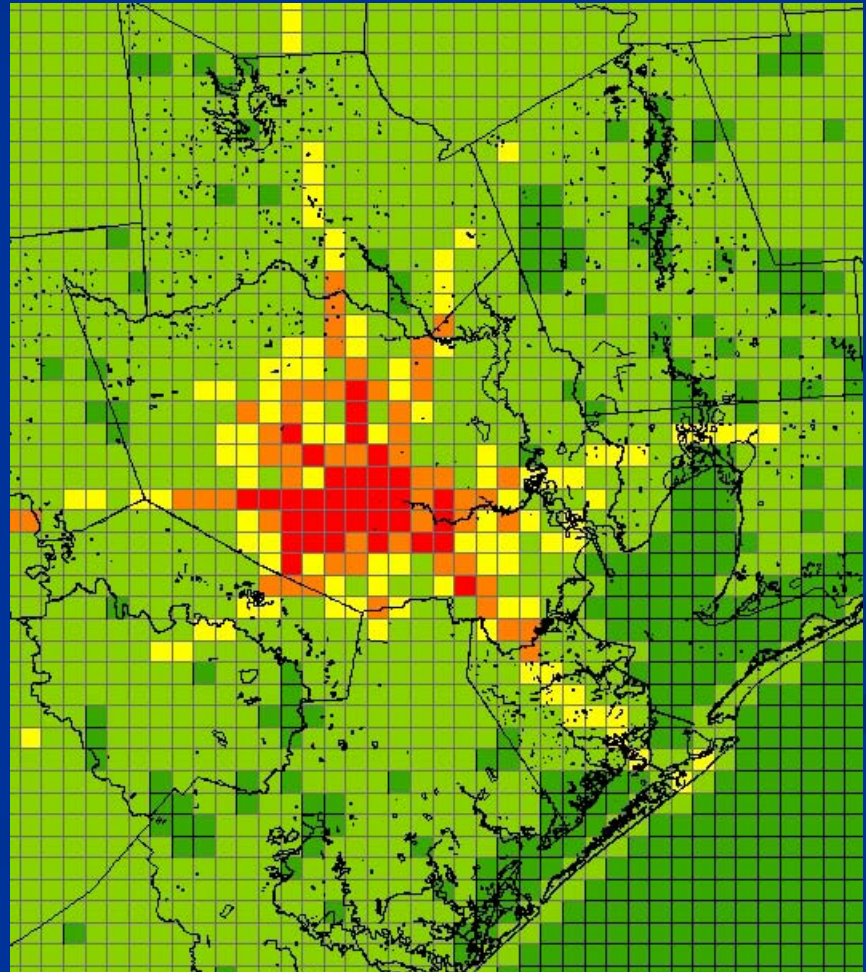


Higher NO emissions
downtown Houston

NEI



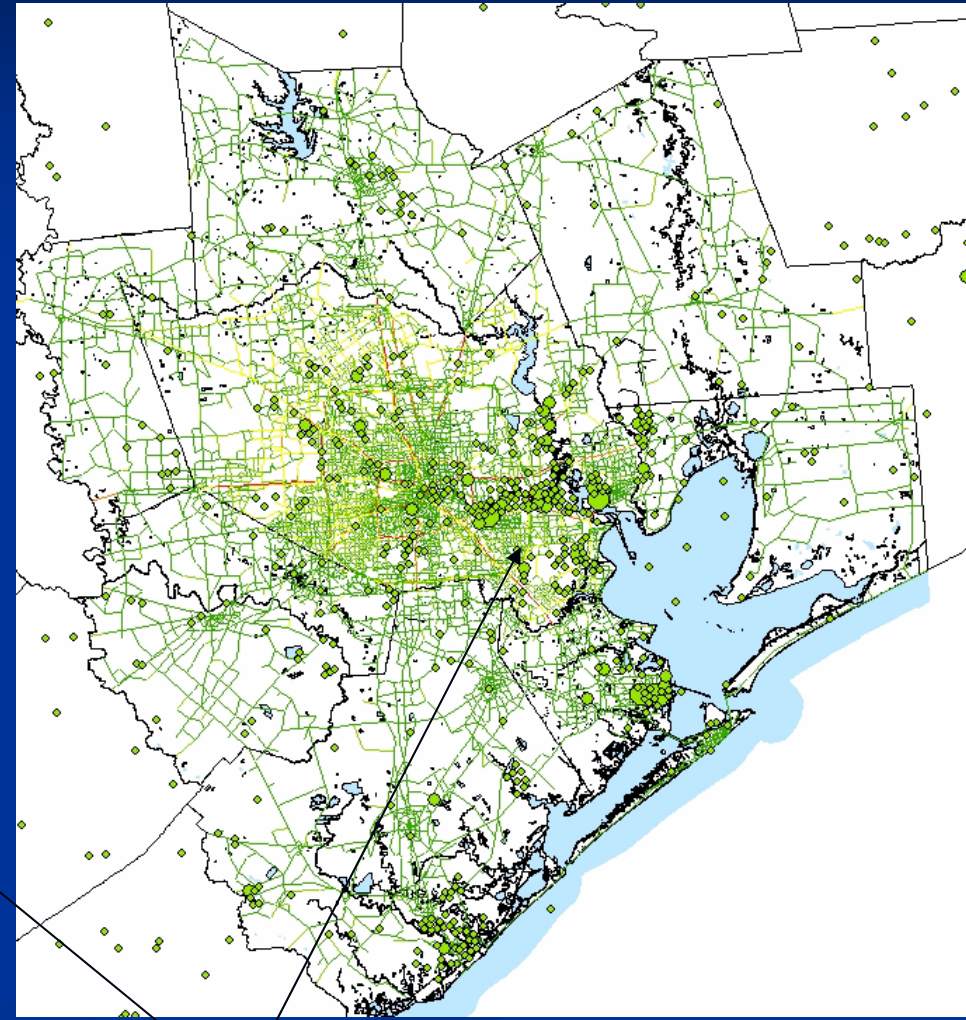
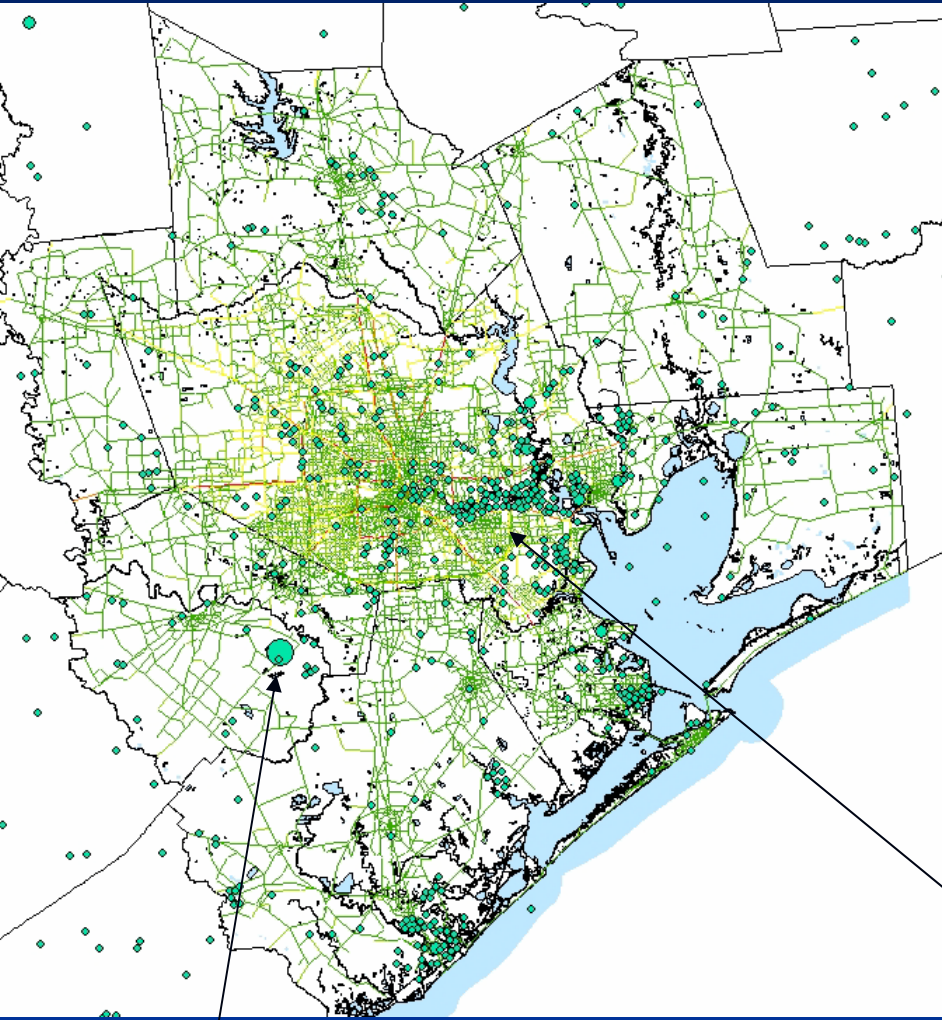
TEI



Point Sources: NEI

NO_x

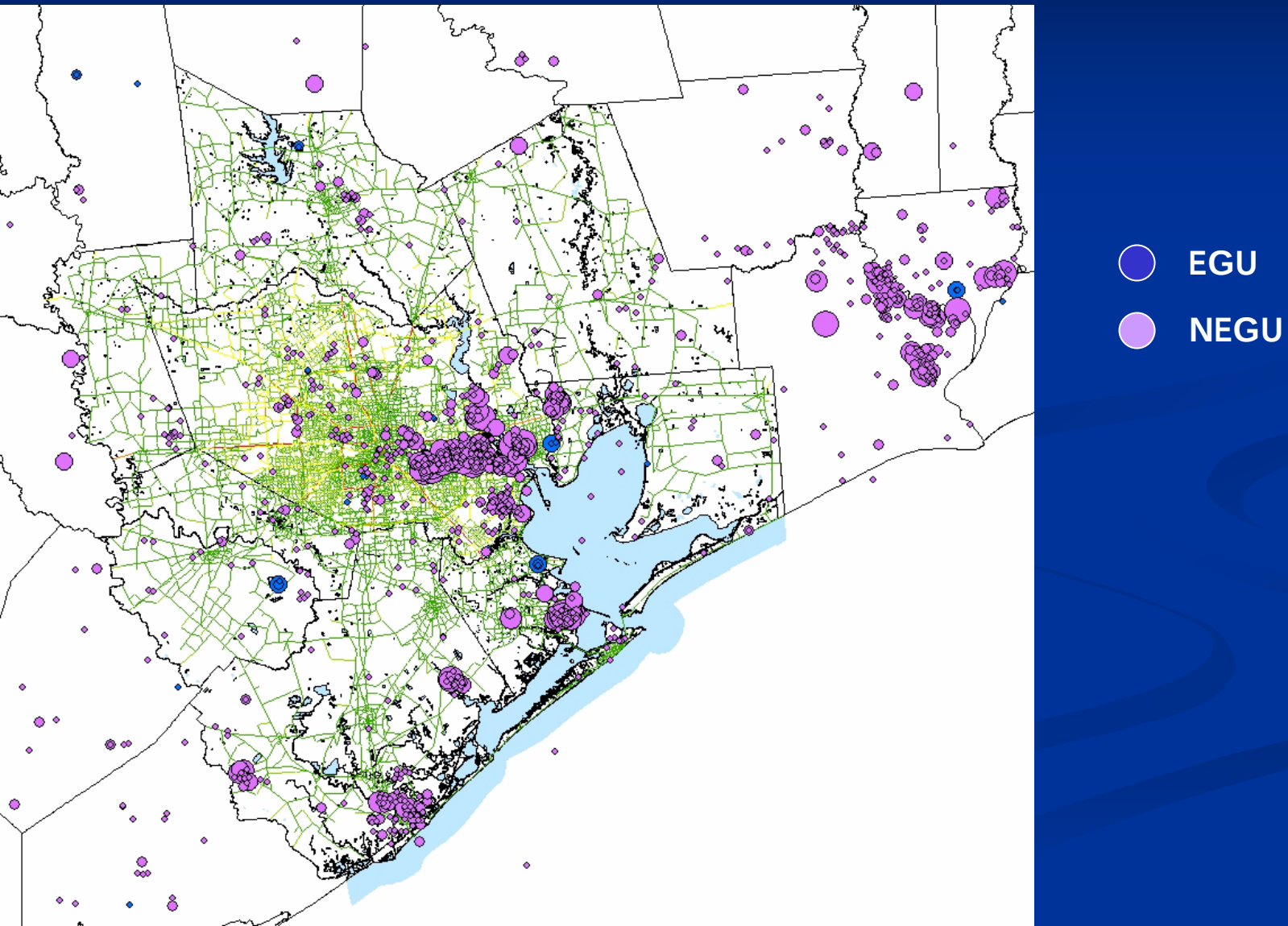
VOC



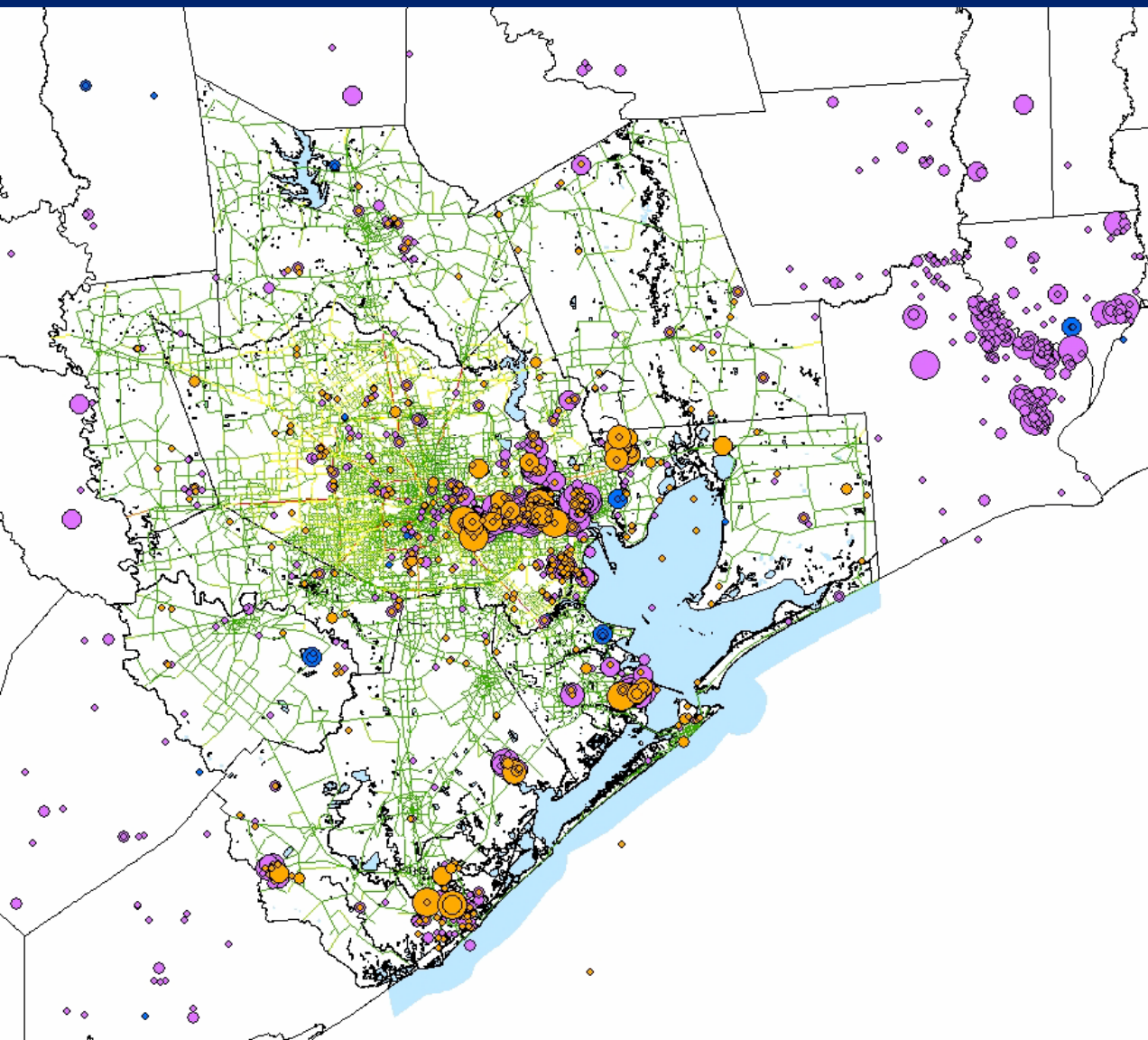
A power plant

The Ship Channel

Point Sources: TEI

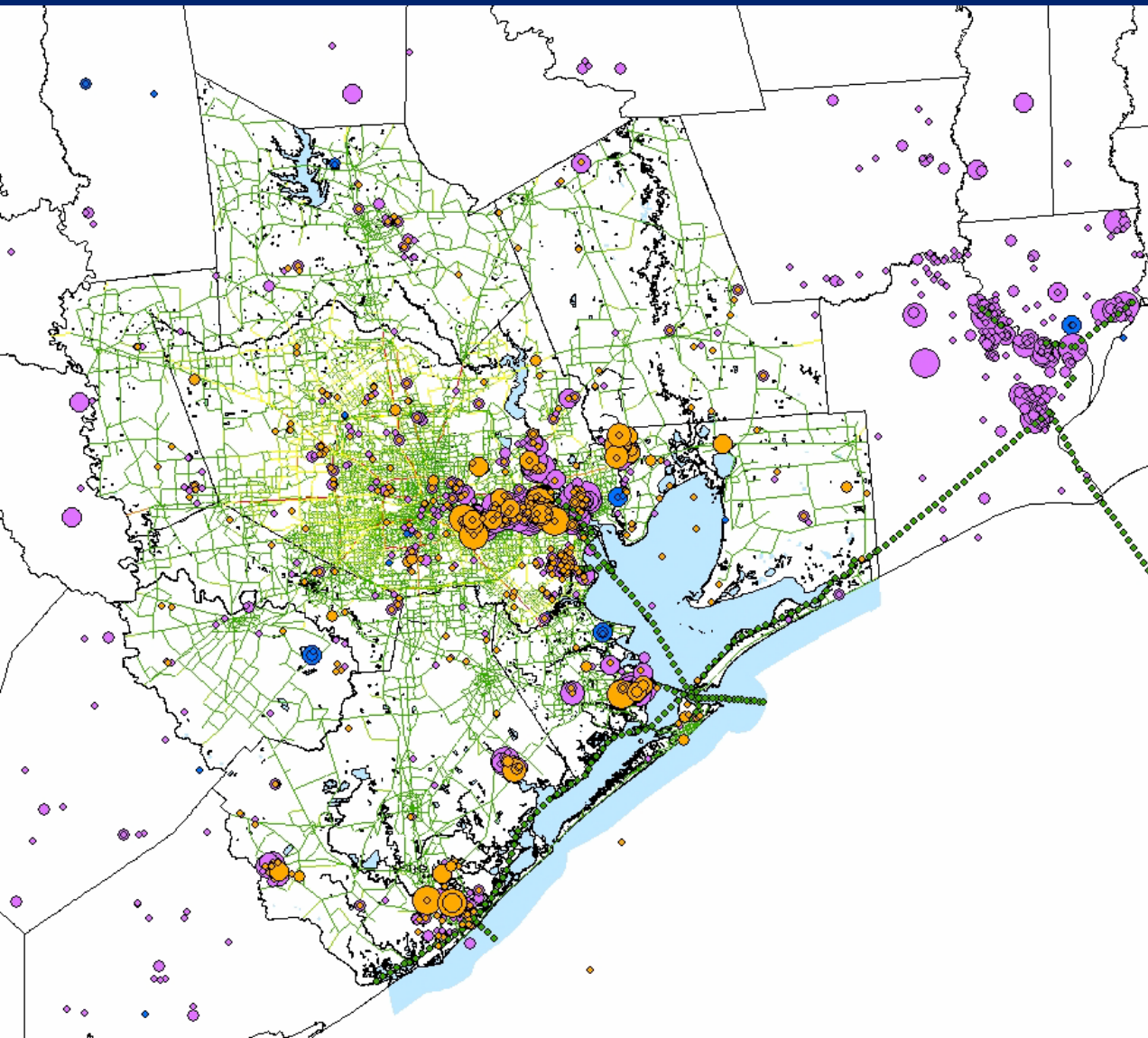


Point Sources: TEI



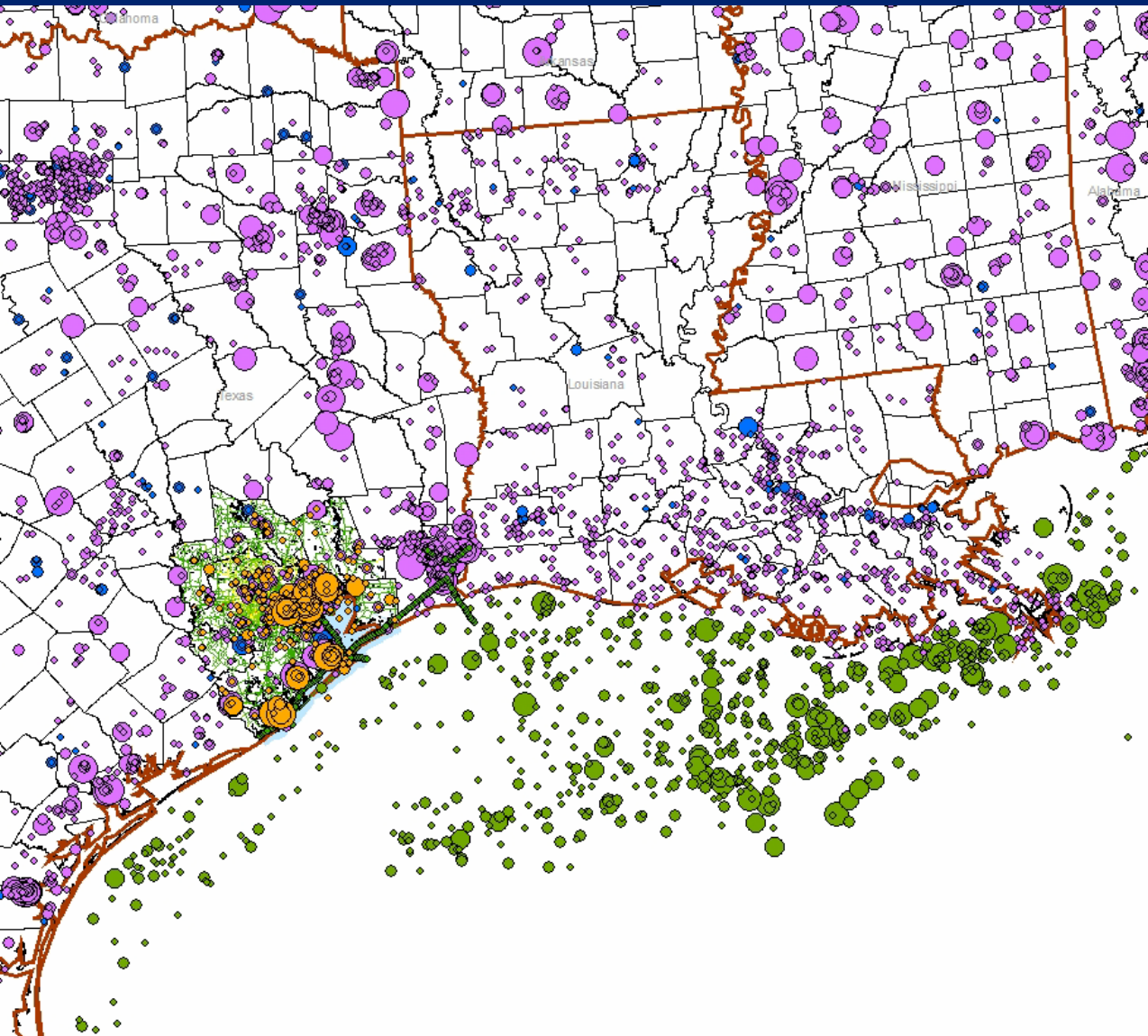
- EGU
- NEGU
- Additional VOC for imputation

Point Sources: TEI



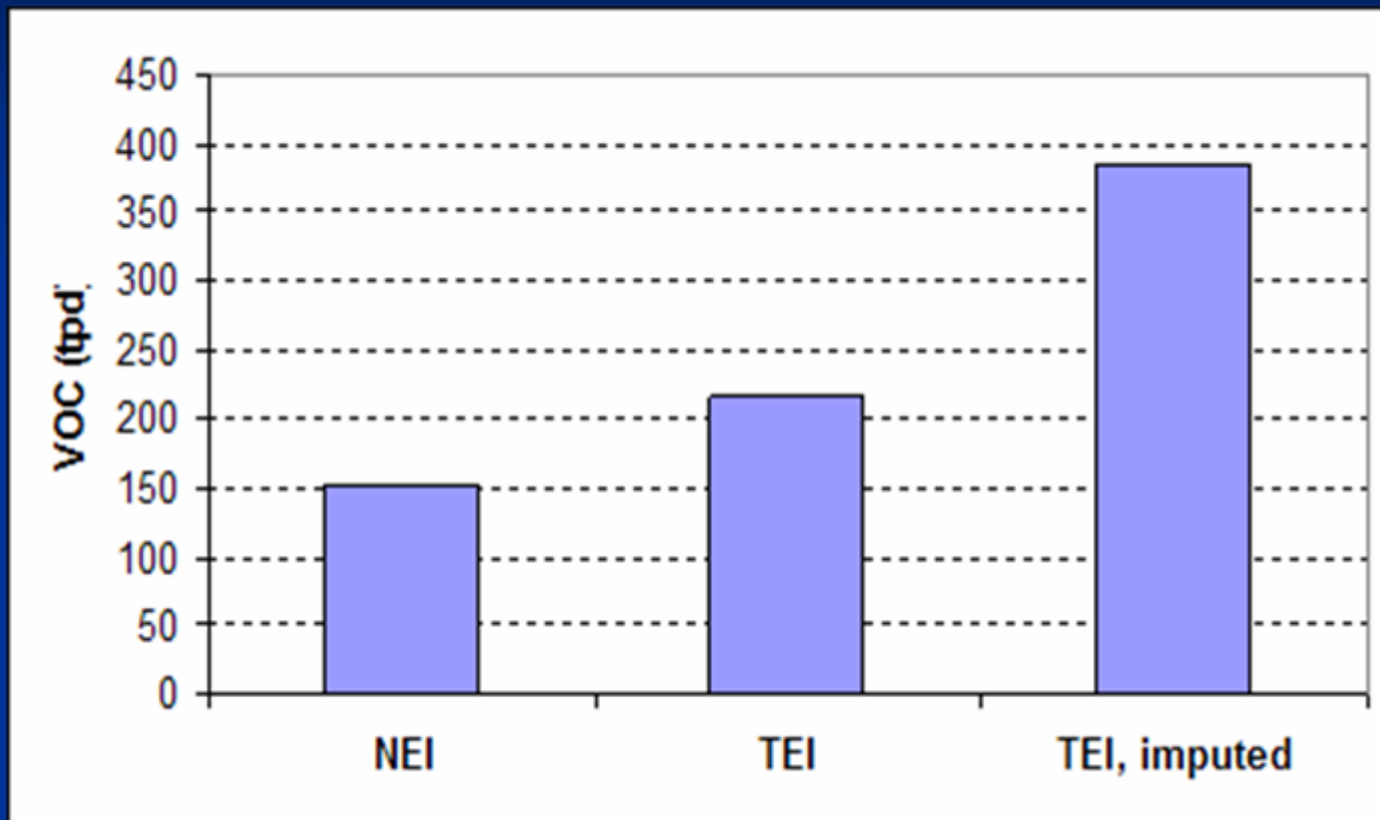
- EGU
- NEGU
- Additional VOC for imputation
- Elevated ship emissions (area)

Point Sources: TEI



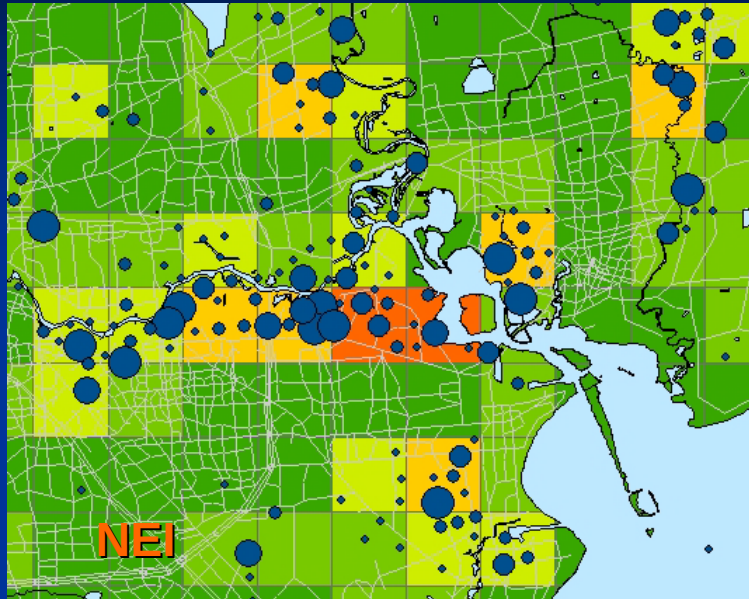
- EGU
- NEGU
- Additional VOC for imputation
- Elevated ship emissions
- Offshore point

Point Emissions

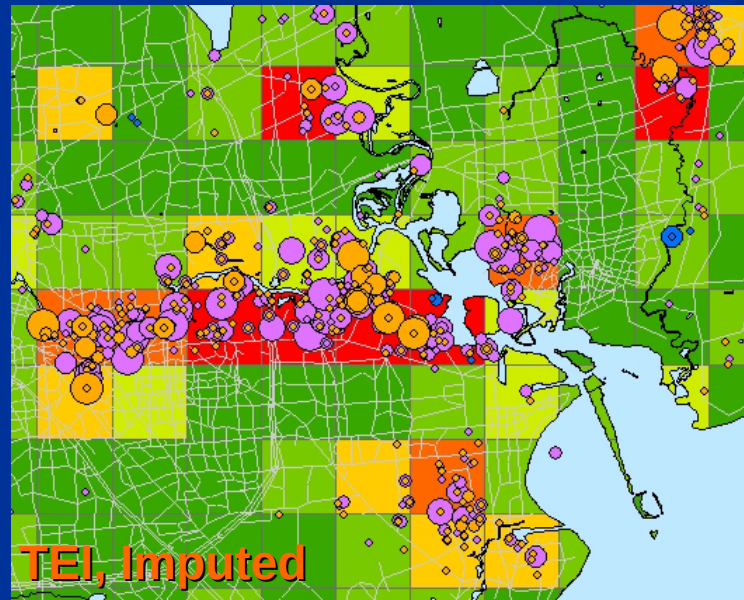
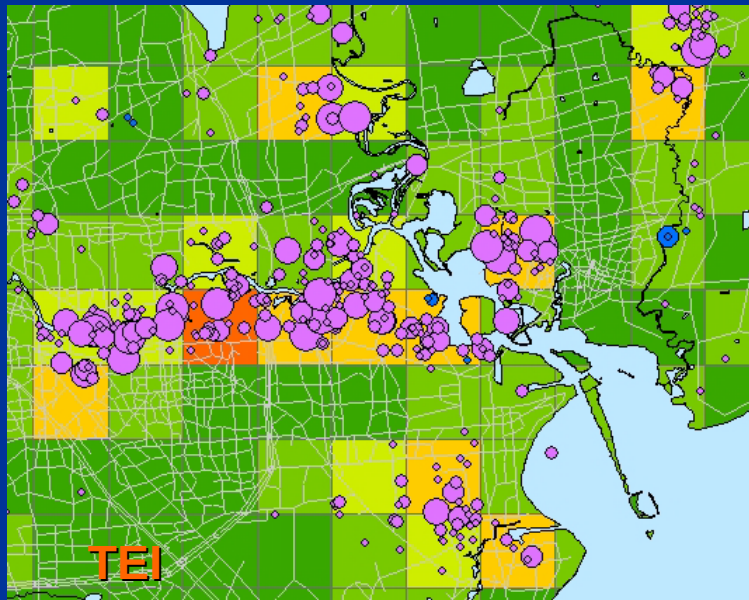


VOC emissions from point sources explain ~ 25 % and 35 % of total VOC emissions in NEI and TEI (regular), respectively.

VOC emissions



- NEI Point VOC emissions
- TEI Point VOC emissions
- Additional VOC emissions for TEI imputation
- Gridded & speciated ETH emissions at a resolution of 4 km for CB4 mechanism



VOC (tons/day)

tx_negu_pa_00

VOC_DY

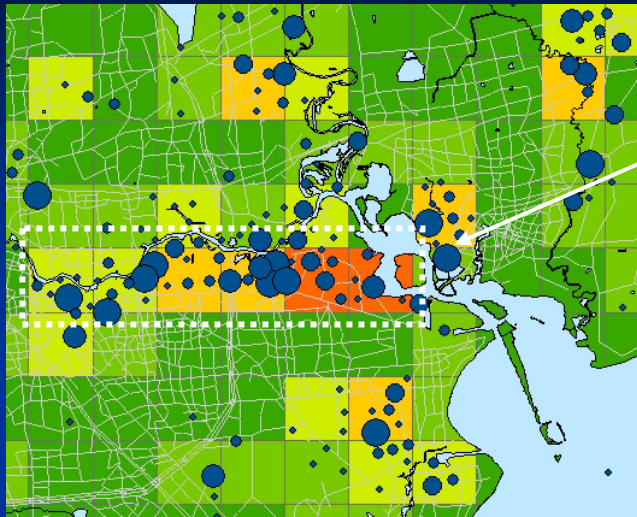
- 0.00 - 0.10
- 0.10 - 0.50
- 0.50 - 1.00
- 1.00 - 2.00
- 2.00 -

ETH (Kmole/d)

- 0 - 1
- 1 - 10
- 10 - 50
- 50 - 100
- 100 -

VOC emissions

After plume rise

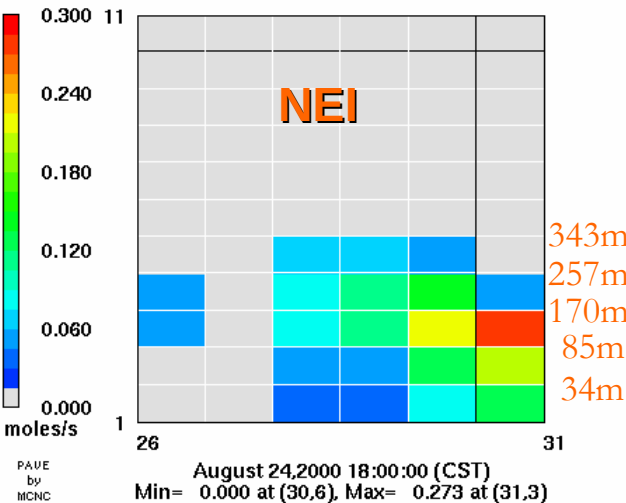


Vertical structures of cells along the Ship Channel

- Stack heights
- Stack diameters
- Exhausting gas temperatures
- Exhausting gas velocities

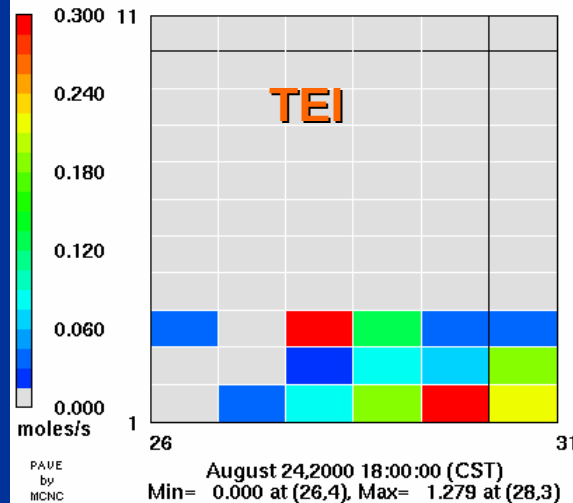
(a) NEI

ETH, Vertical view
Along the Ship Channel



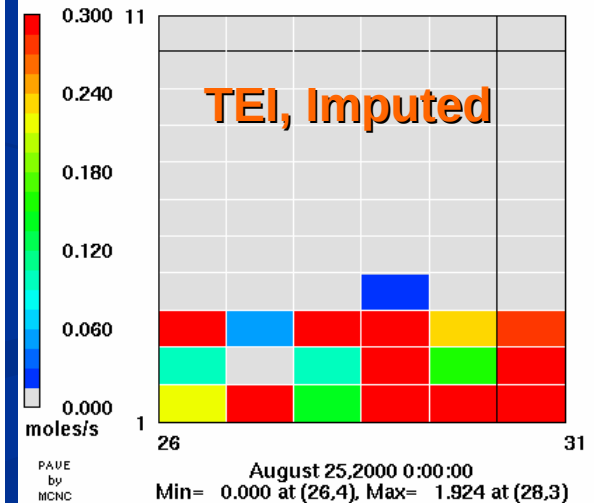
(b) TEI

ETH, Vertical view
Along the Ship Channel



(c) TEI imputed

ETH, Vertical view
Along the Ship Channel



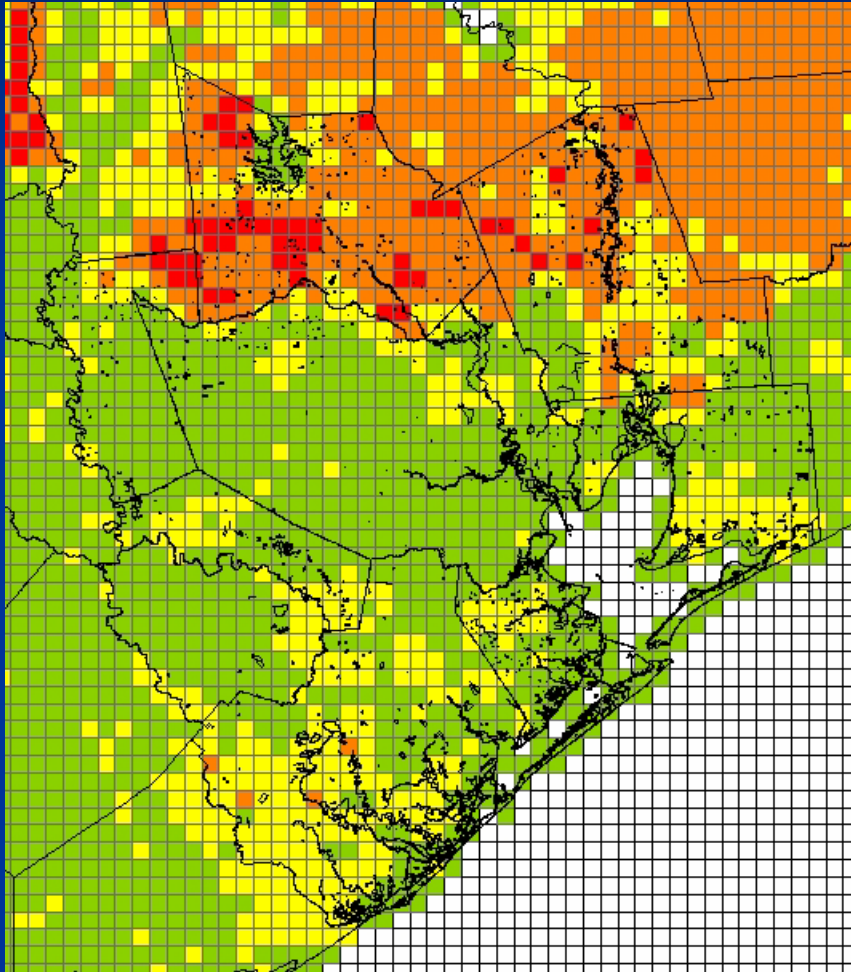
August 24th, 2000 at 18 CST

Biogenic Emissions

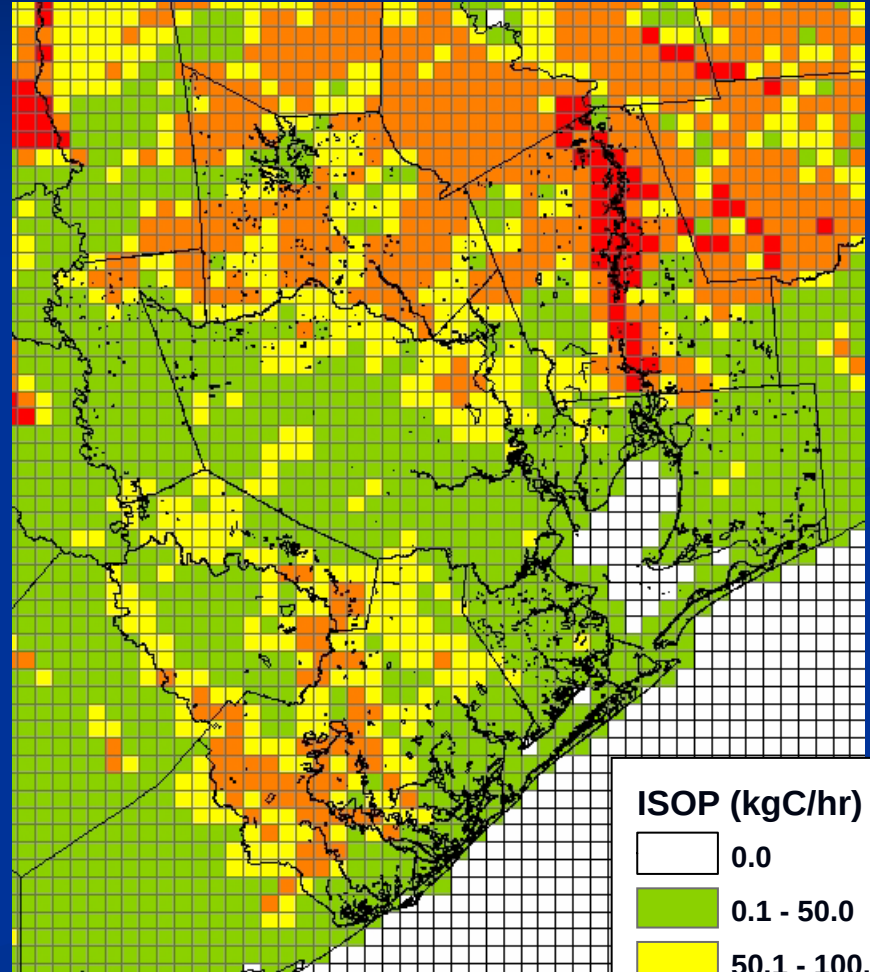
- Processors
 - NEI: BEIS version 3.12
 - TEI: GloBEIS version 3.1
- LULC data
 - NEI: BELD3
 - TEI: TCEQ LULC for biogenic emissions
- PASR (Photo-synthetically Active Solar Radiation)
 - NEI: Calculated with RGRND from MM5-MCIP
 - TEI: Derived from GOES satellite data
- Temperature
 - NEI: 10-m temperature from MM5-MCIP
 - TEI: temperature field based on observations

Normalized Isoprene Emissions

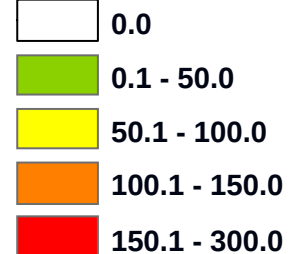
BEIS/BELD3



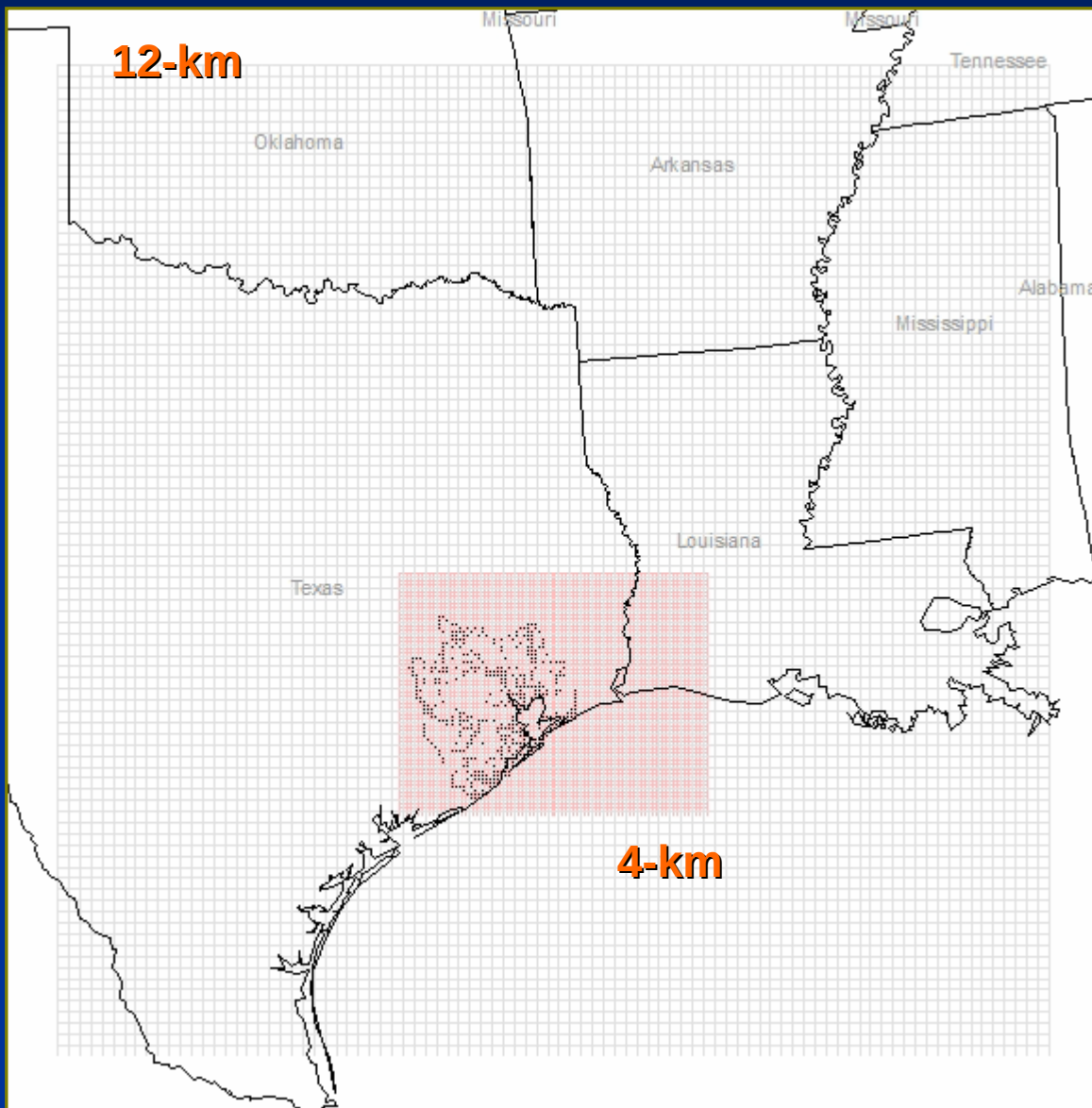
GloBEIS/TCEQ



ISOP (kgC/hr)



CMAQ Simulations

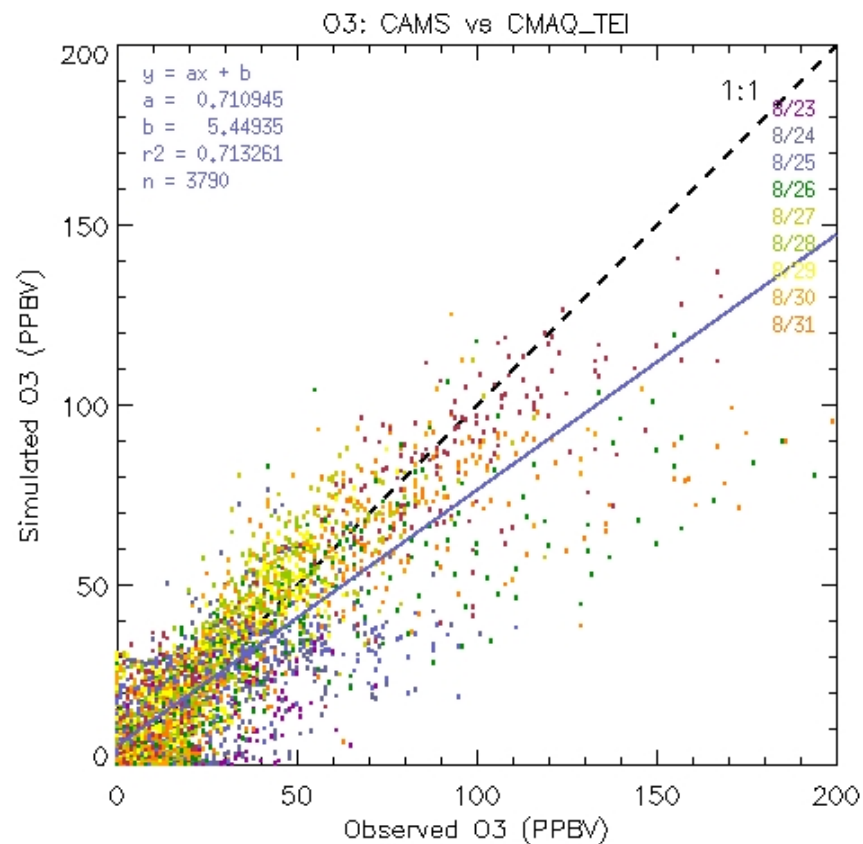
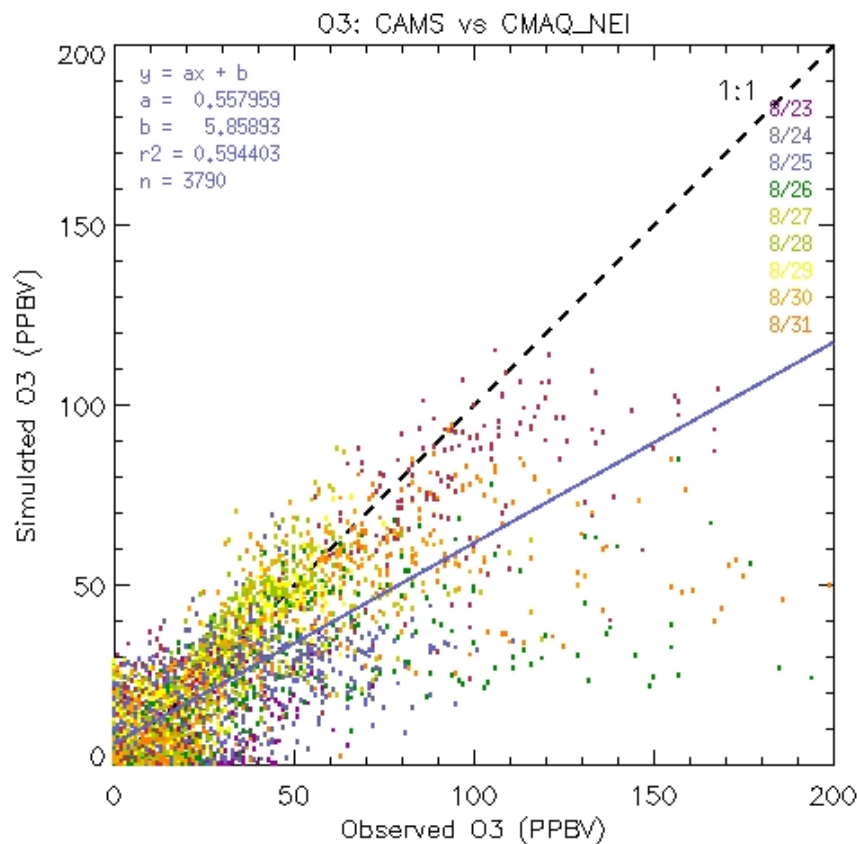


- ✓ CMAQ version 4.4
- ✓ CB4 mechanism
- ✓ TAMU MM5
- ✓ MCIP version 2.3
- ✓ 36 km, 12 km, and 4 km
- ✓ August 23 ~ 31, 2000
- ✓ TexAQS 2000
- ✓ NEI vs. TEI imputed

Surface 1-hour O₃ concentrations

NEI

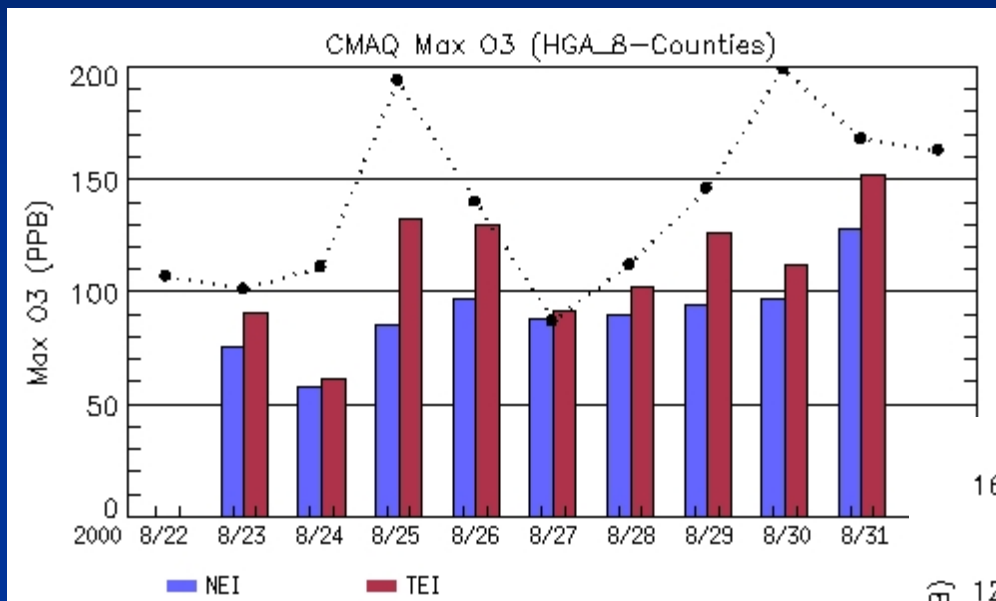
TEI



CMAQ simulations compared to CAMS sties for August 23rd ~ August 31st, 2000

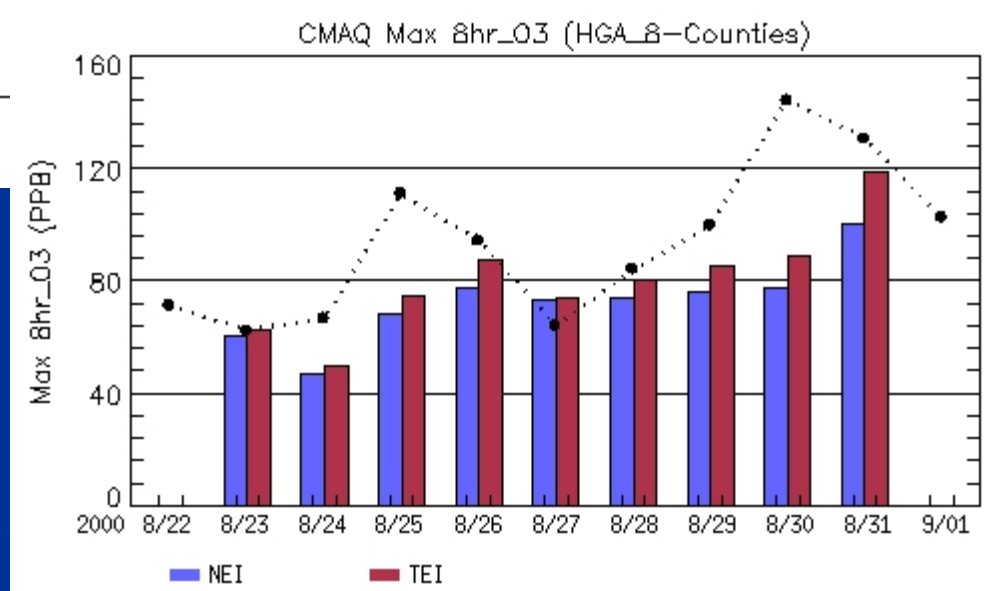
Daily Maximum O3 concentrations

1-hr



- For HG 8 counties only
- Spatially unpaired

8-hr



CMAQ simulations compared to CAMS sties for August 23rd ~ August 31st, 2000

Surface O₃ concentrations

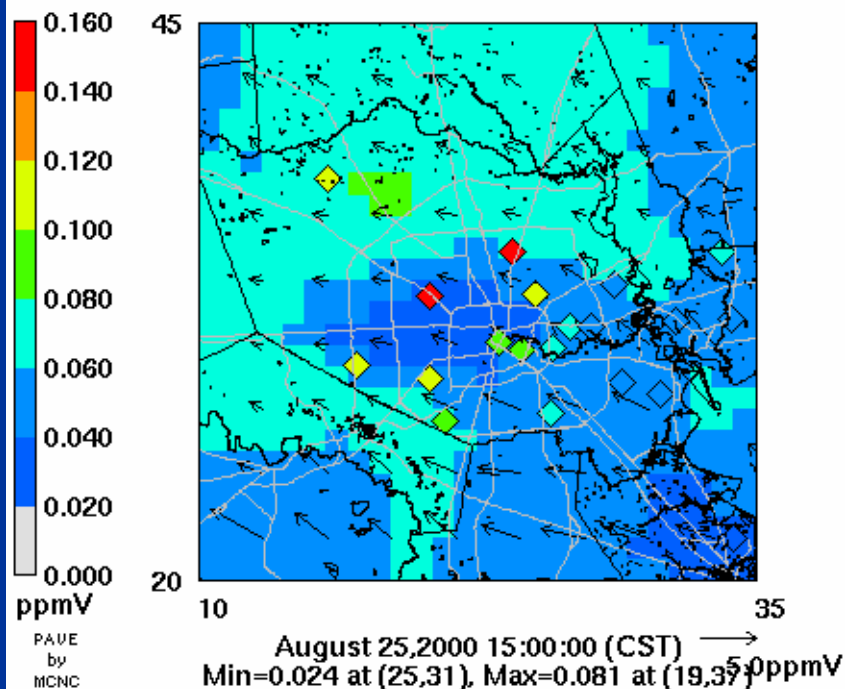
August 25th, 2000 at 15 CST

NEI

TEI

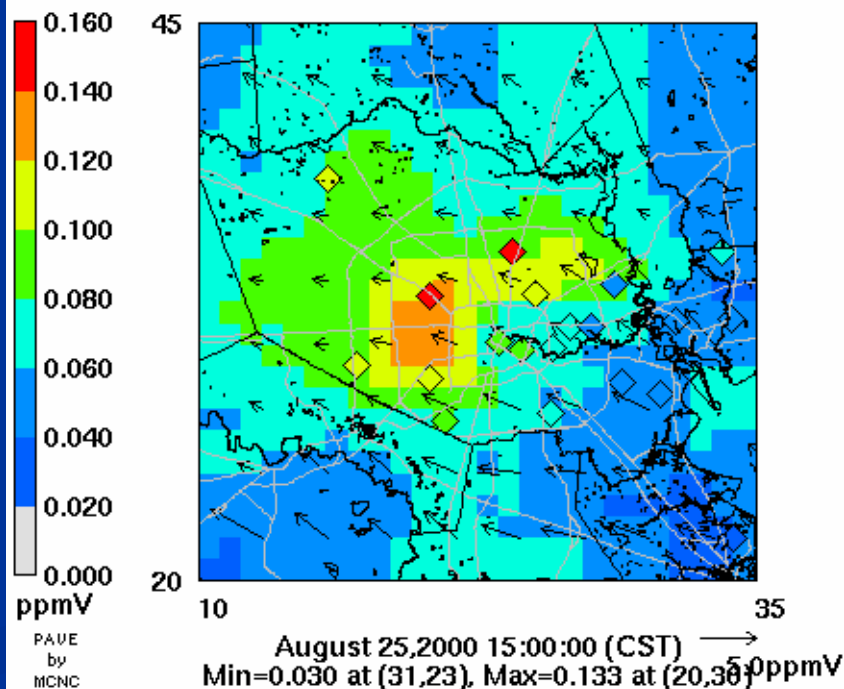
(a) NEI

Layer 1, O₃



(b) TEI

Layer 1, O₃



Surface NO_x concentrations

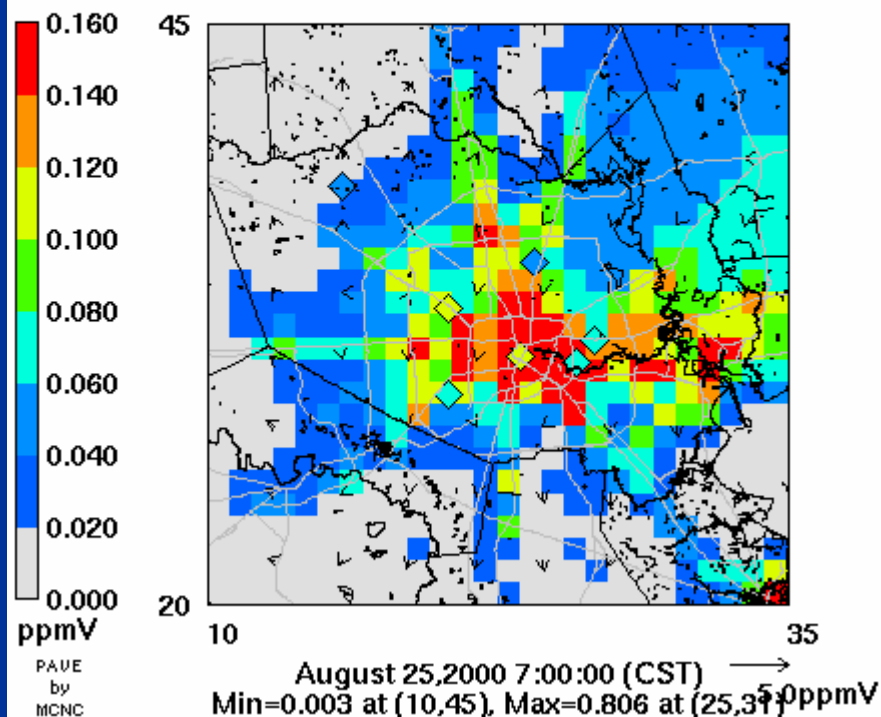
August 25th, 2000 at 07CST

NEI

TEI

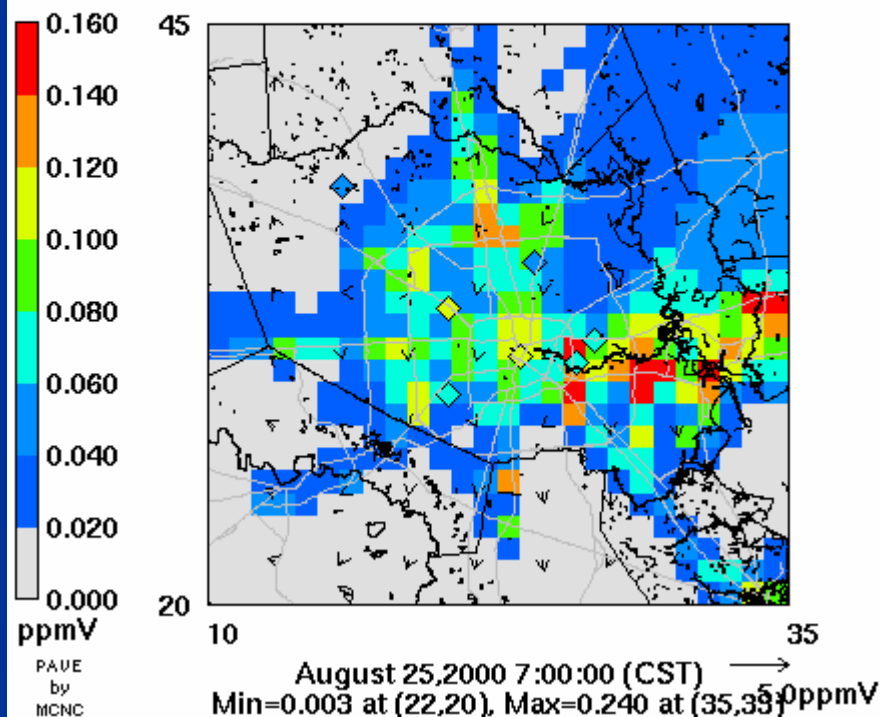
(a) NEI

Layer 1, NO + NO₂



(b) TEI

Layer 1, NO + NO₂



Surface NO_x concentrations

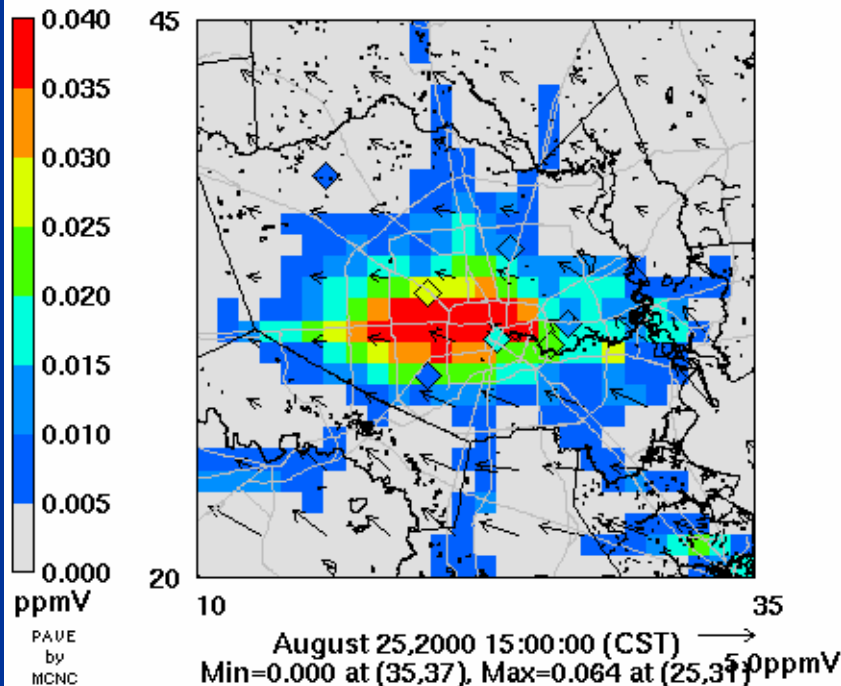
August 25th, 2000 at 15 CST

NEI

TEI

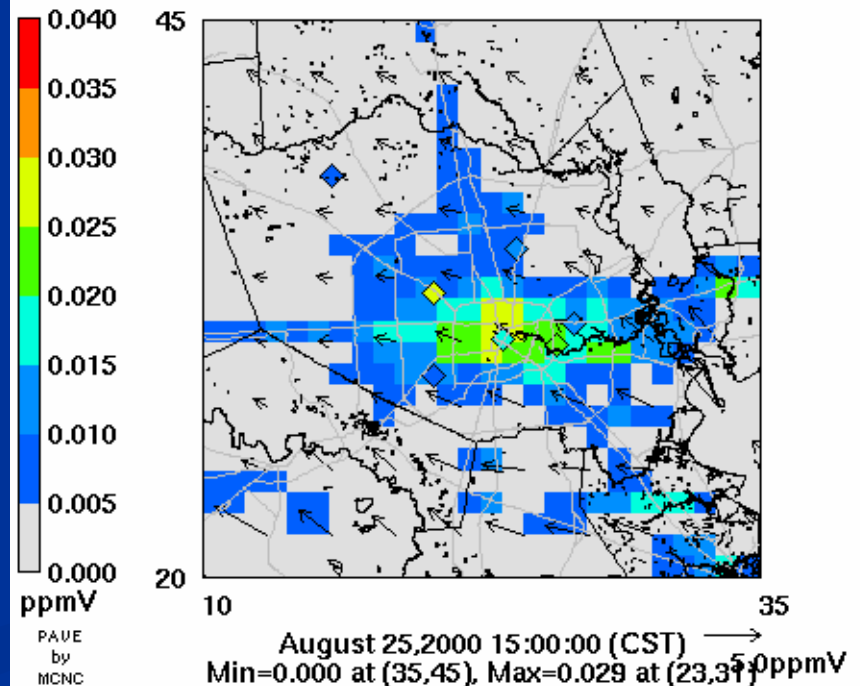
(a) NEI

Layer 1, NO + NO₂



(b) TEI

Layer 1, NO + NO₂



Surface ETH concentrations

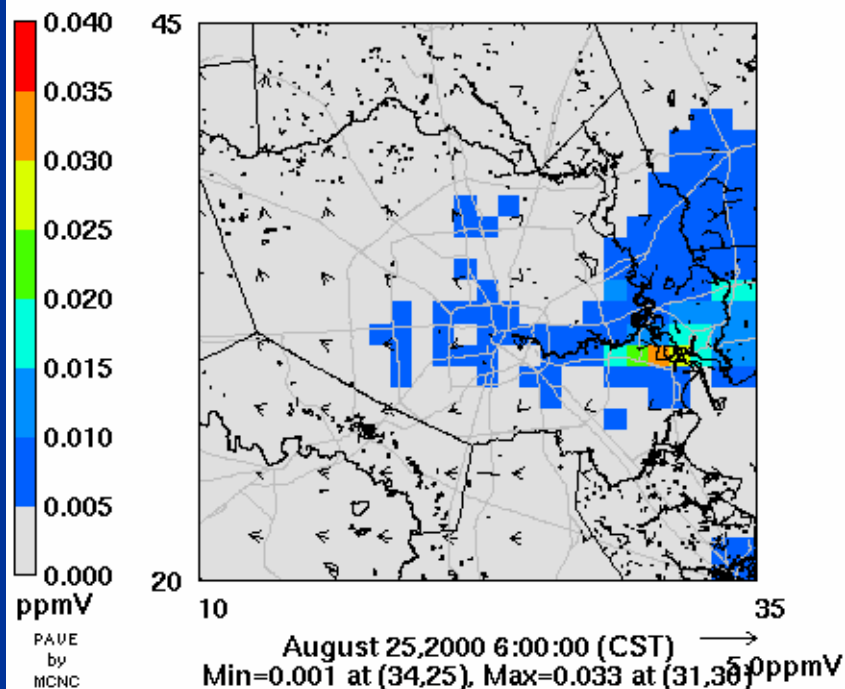
August 25th, 2000 at 06 CST

NEI

TEI

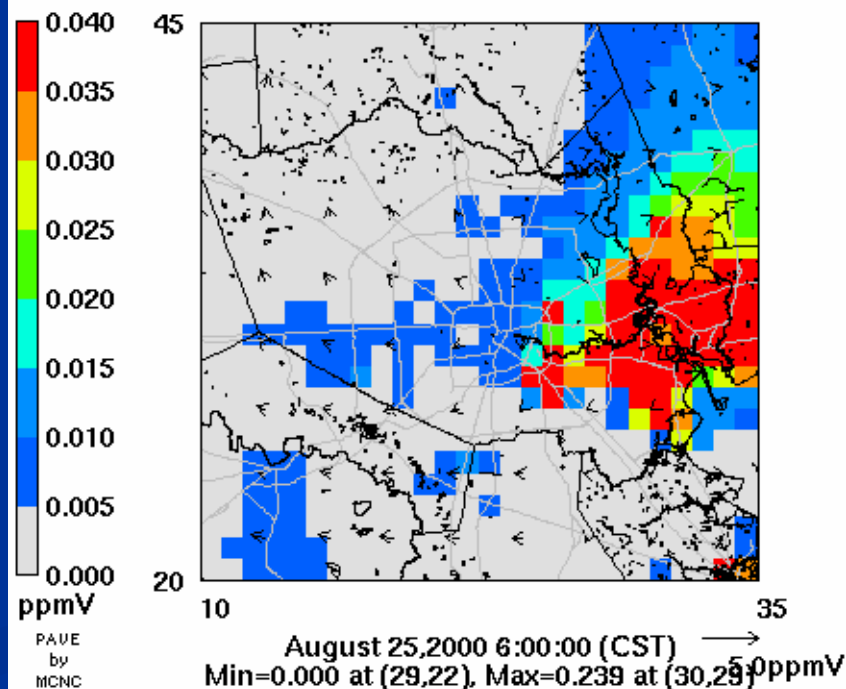
(a) NEI

Layer 1, ETH



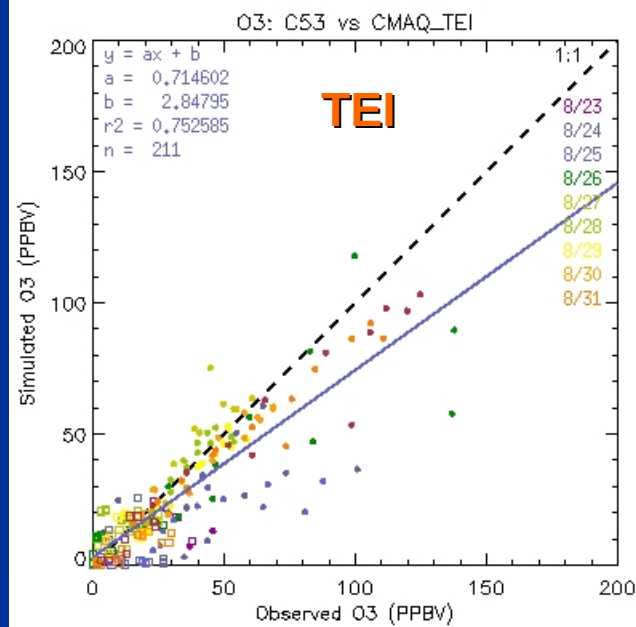
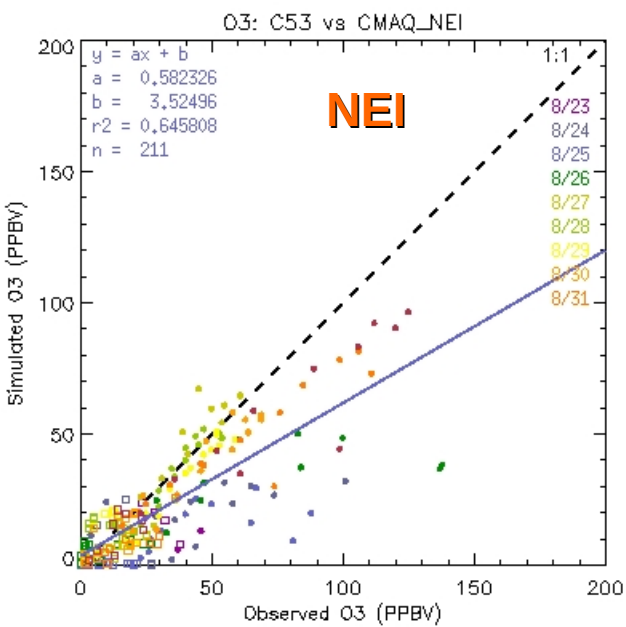
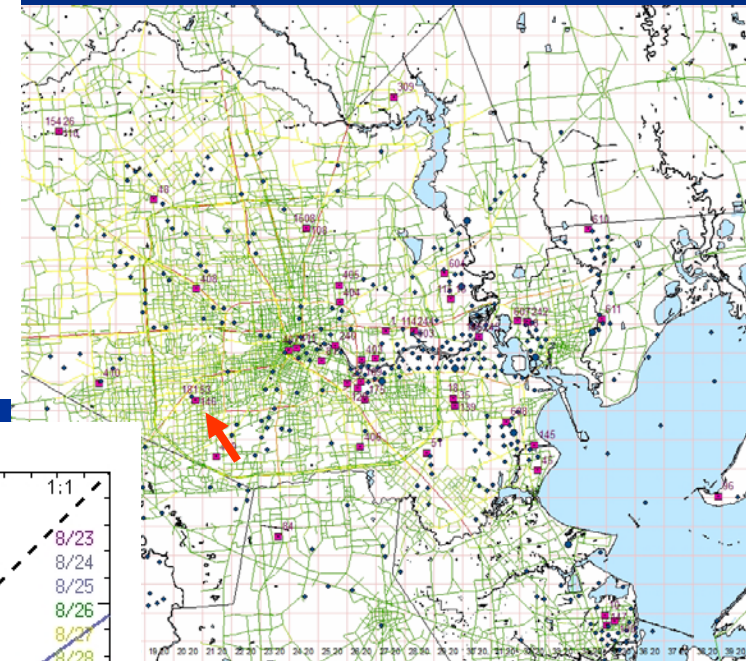
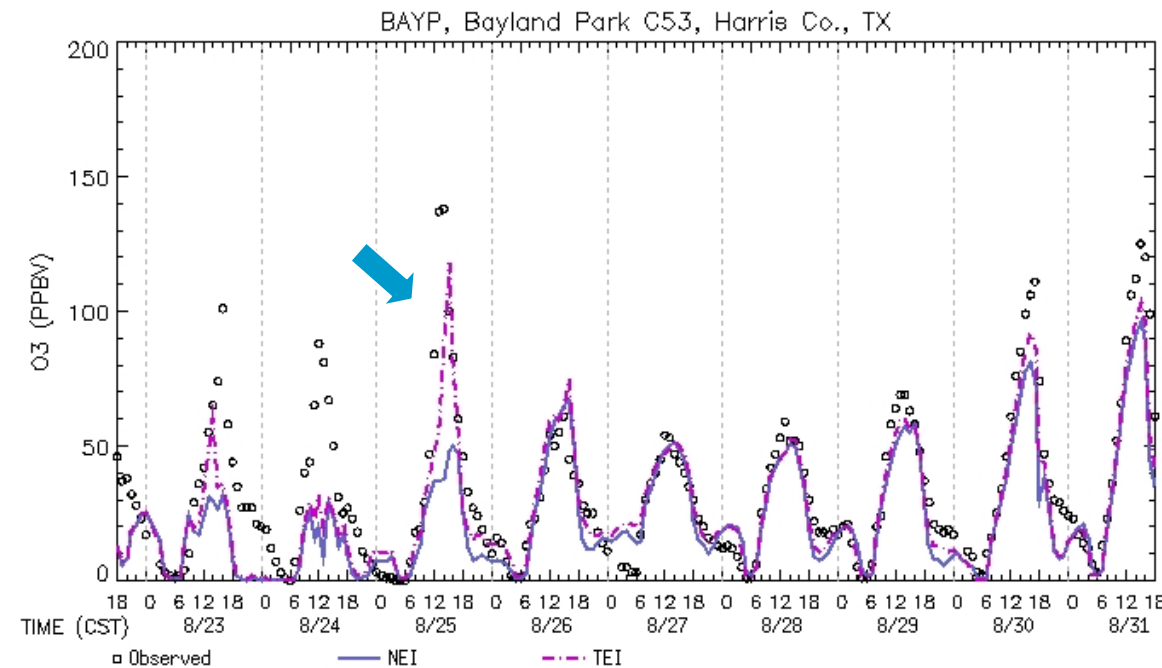
(b) TEI

Layer 1, ETH



Surface O3

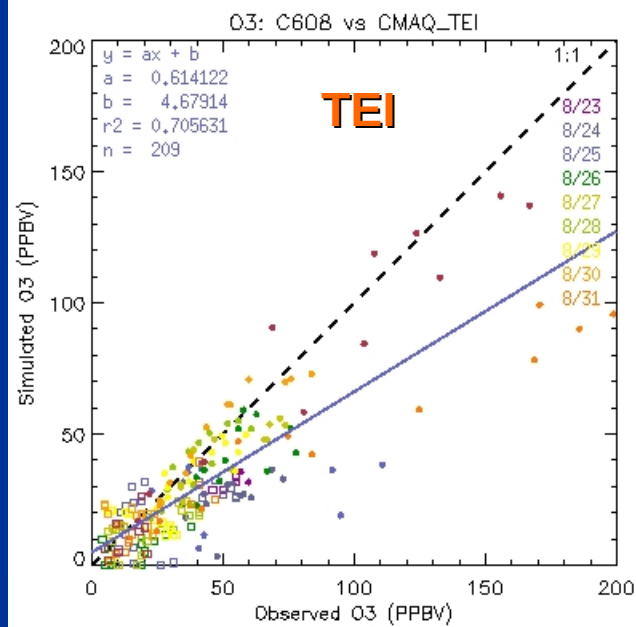
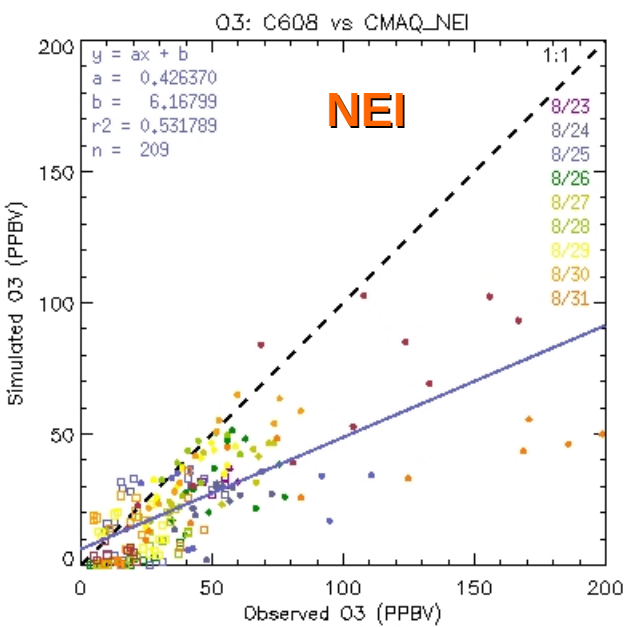
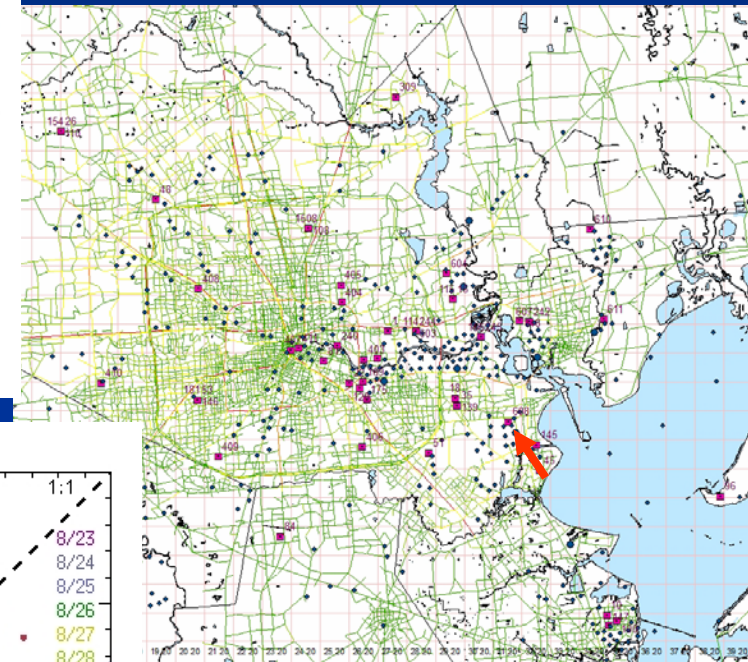
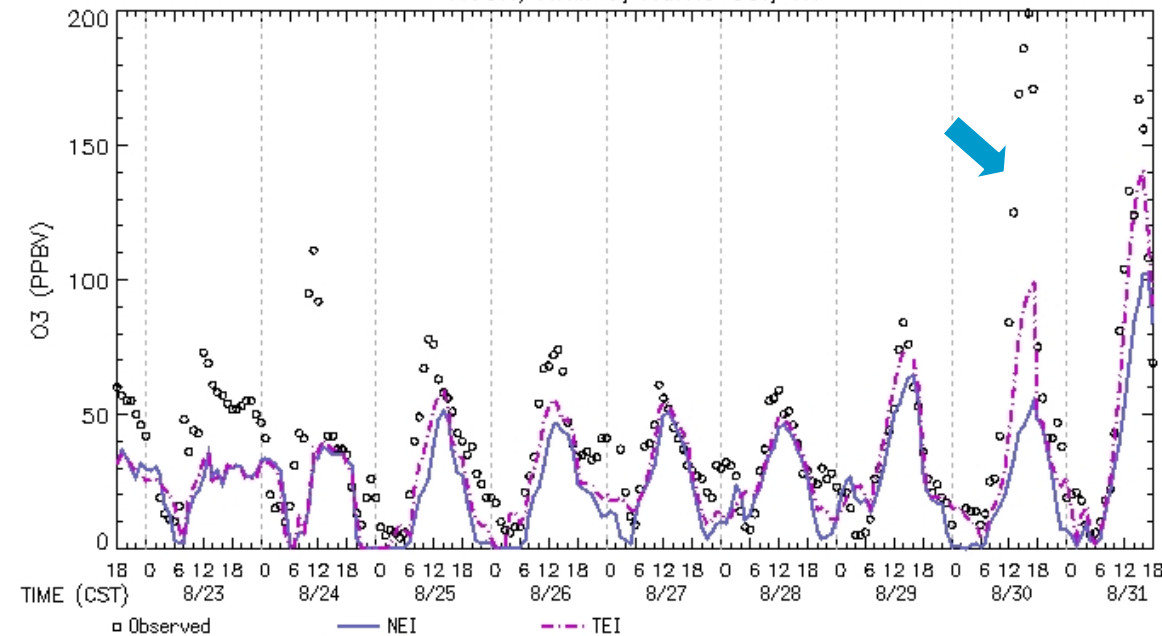
Bayland Park



Surface O3

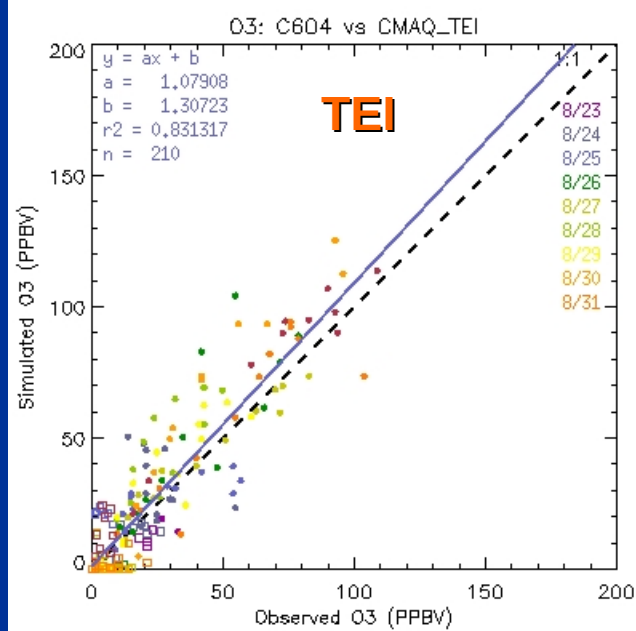
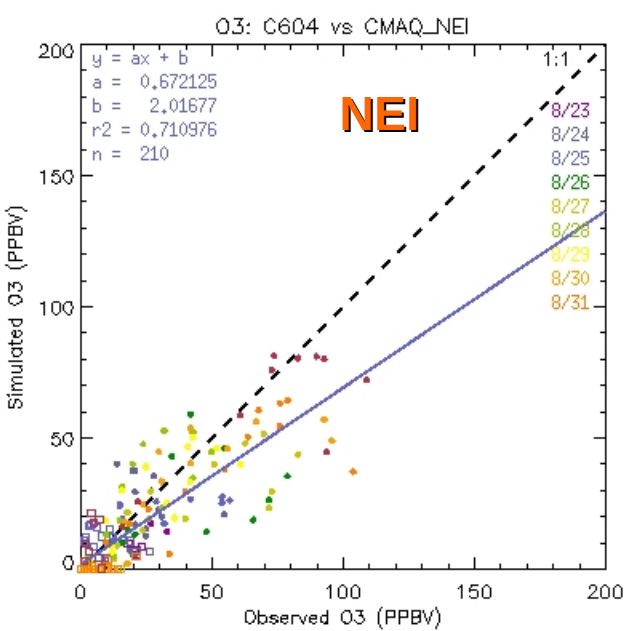
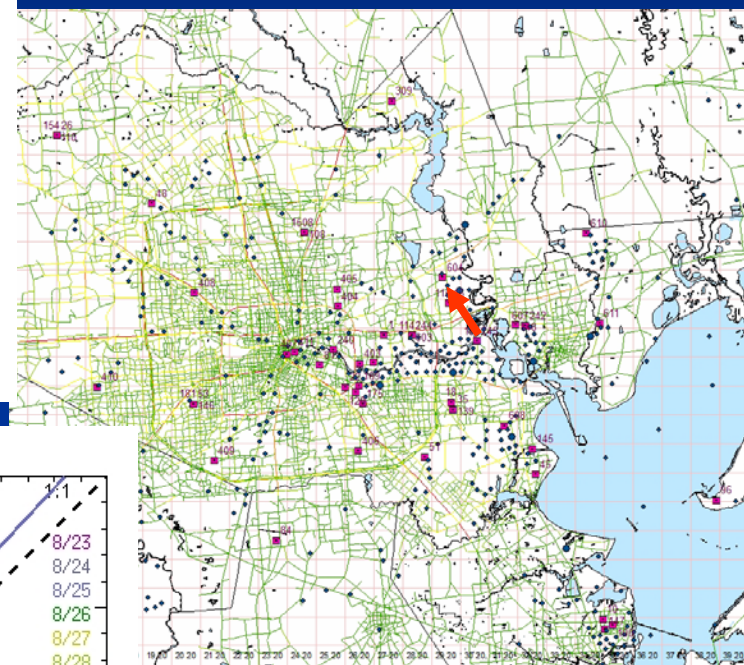
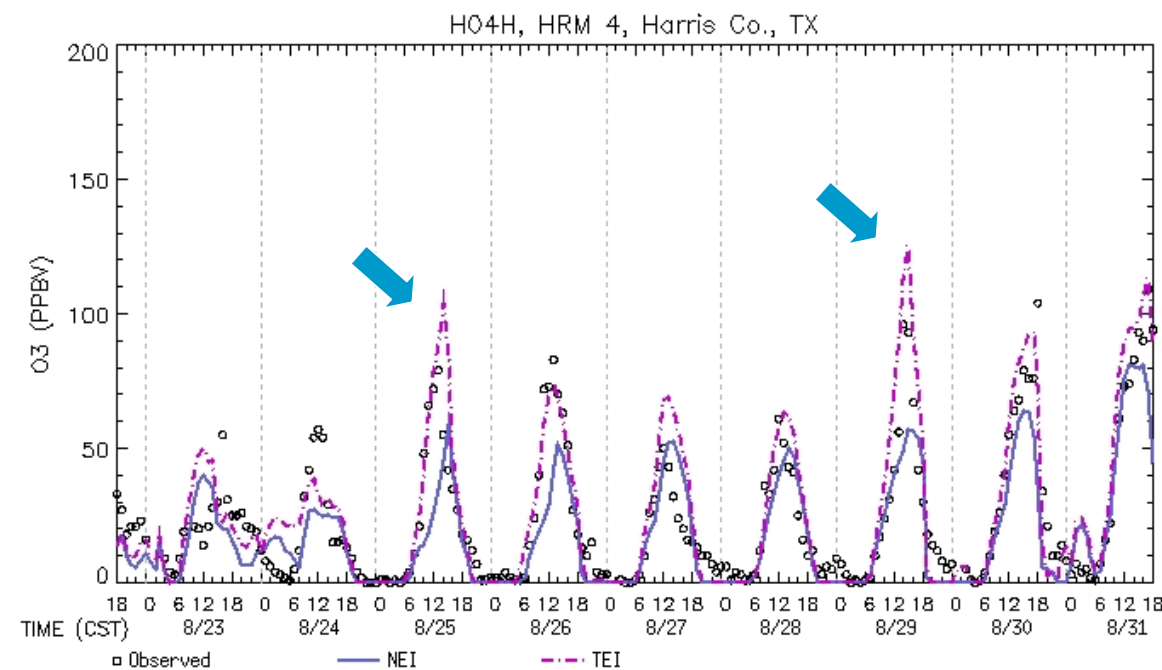
HRM 8

H08H, HRM 8, Harris Co., TX



Surface O3

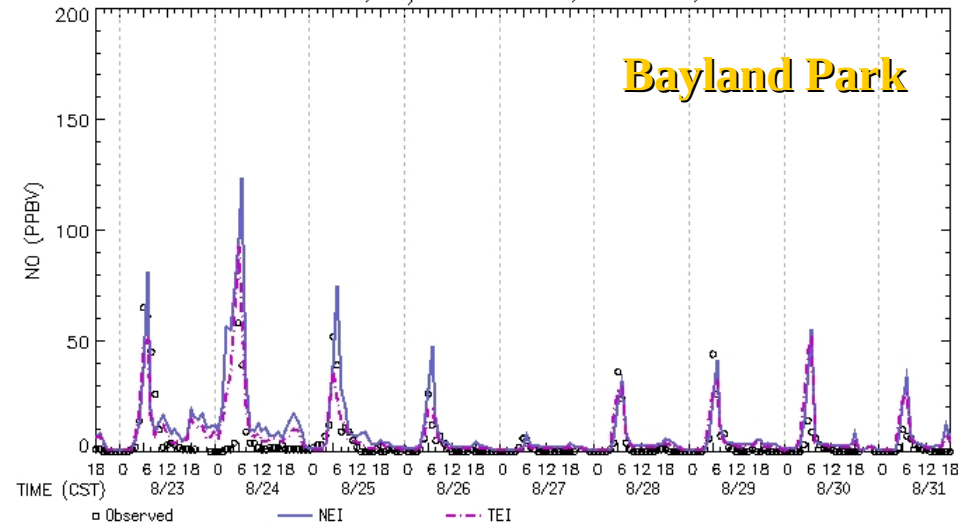
HRM 4



Surface NO

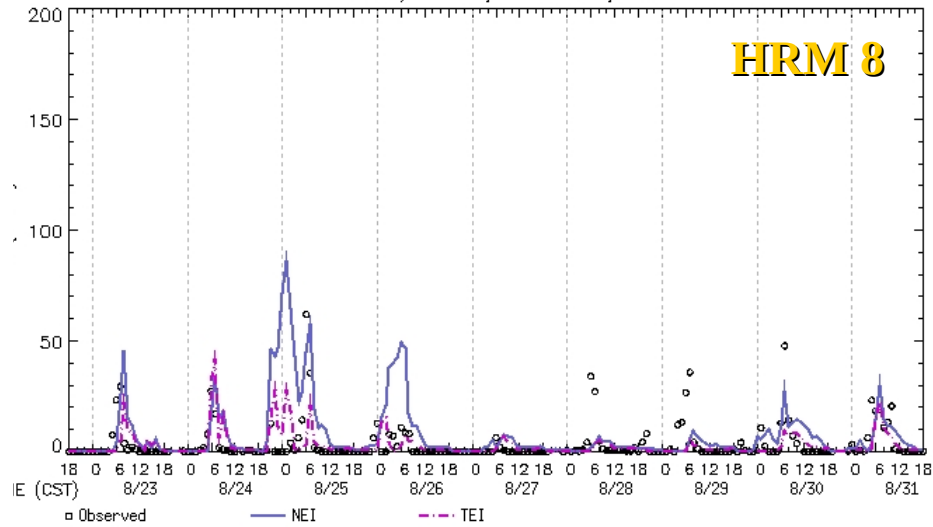
BAYP, Bayland Park C53, Harris Co., TX

Bayland Park



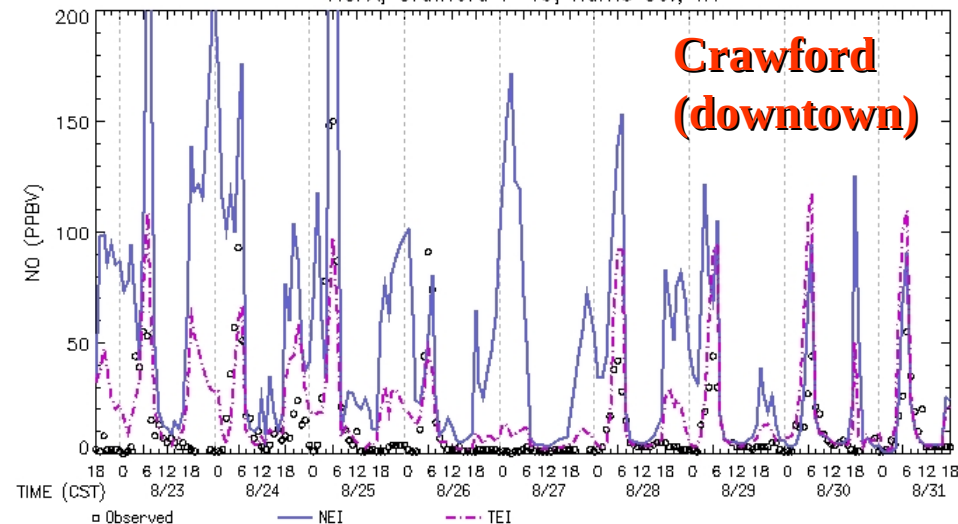
H08H, HRM 8, Harris Co., TX

HRM 8



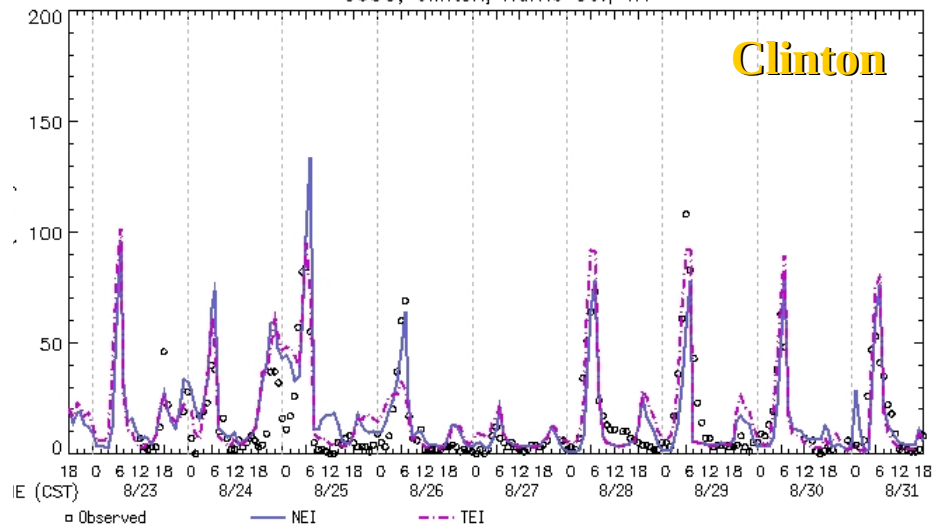
HCFA, Crawford T-19, Harris Co., TX

**Crawford
(downtown)**



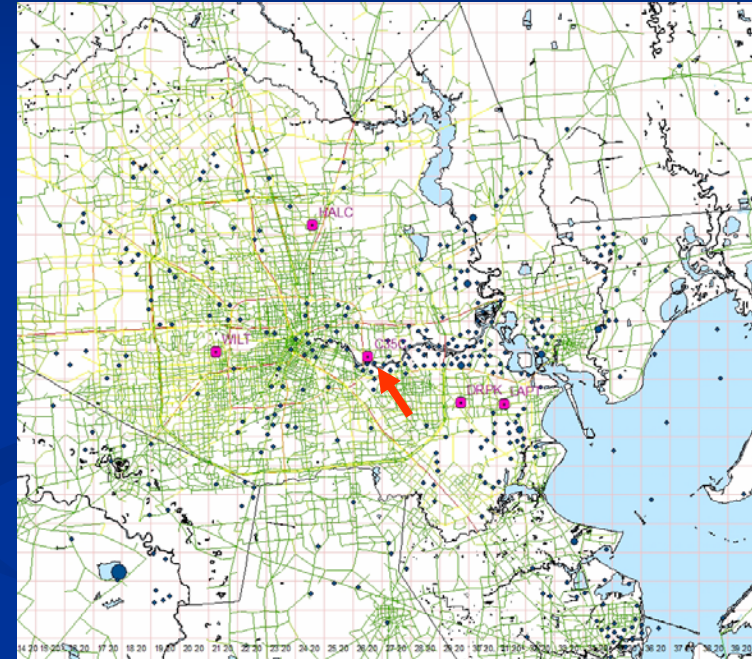
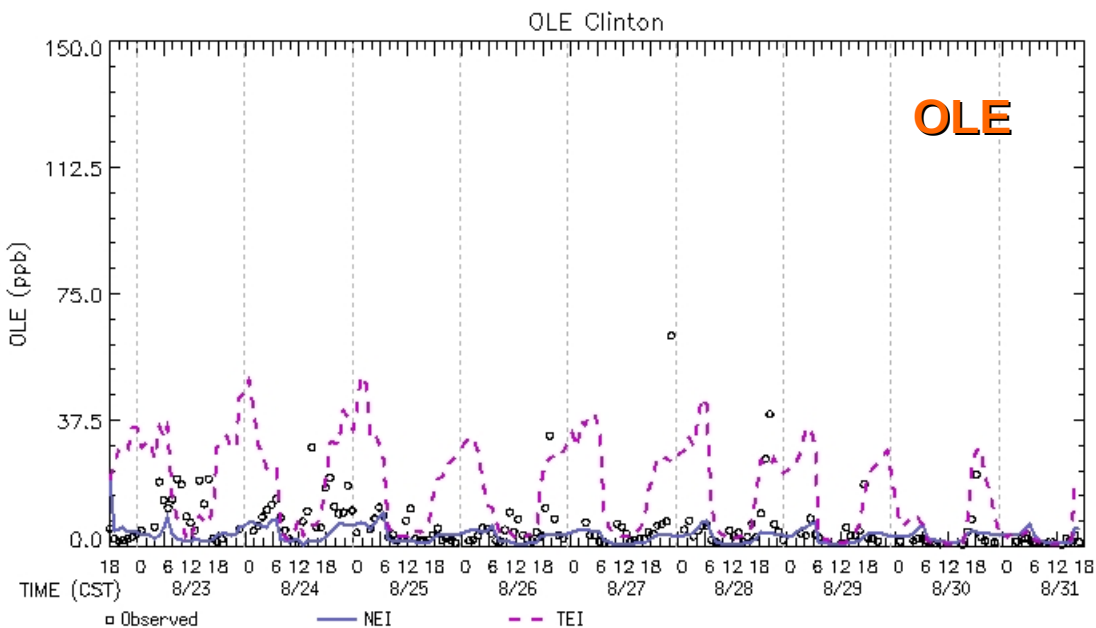
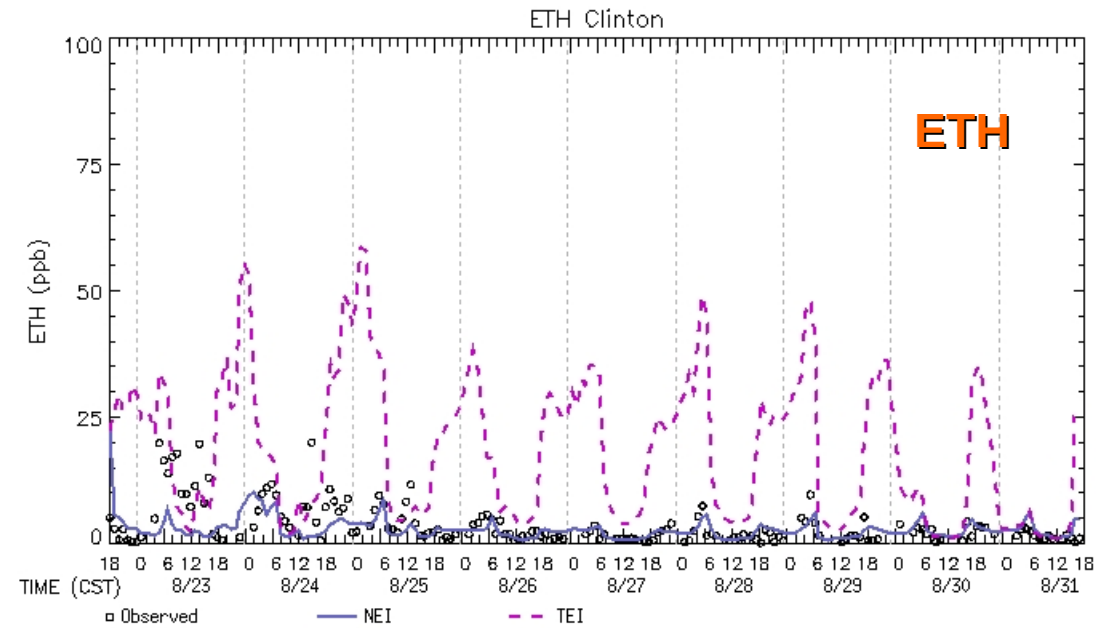
C35C, Clinton, Harris Co., TX

Clinton



ETH & OLE

Clinton

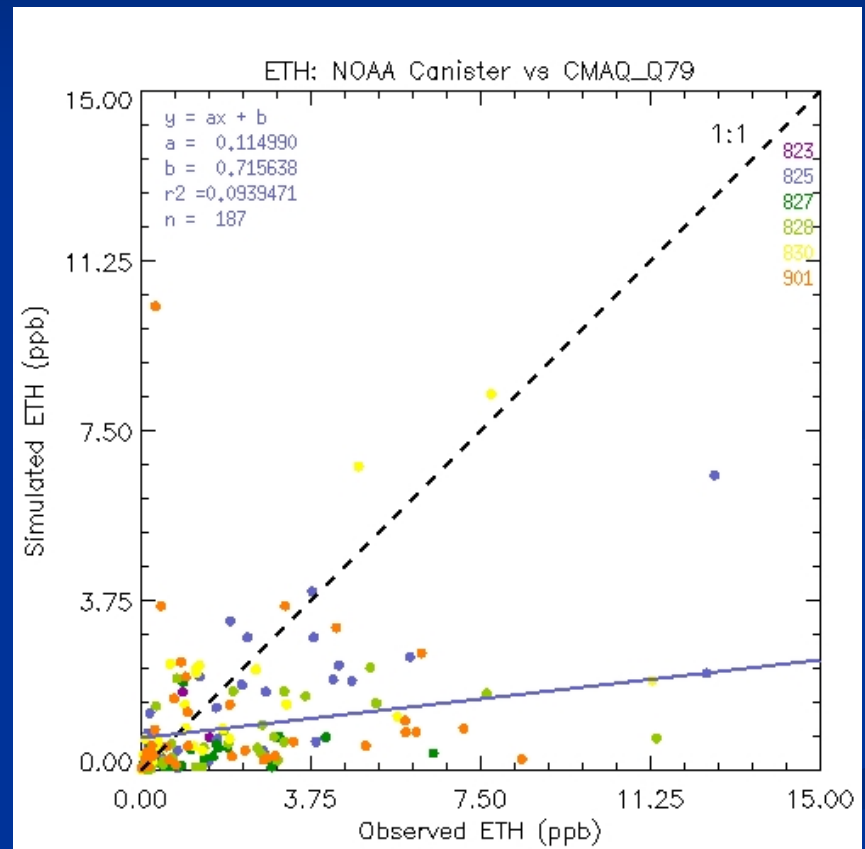
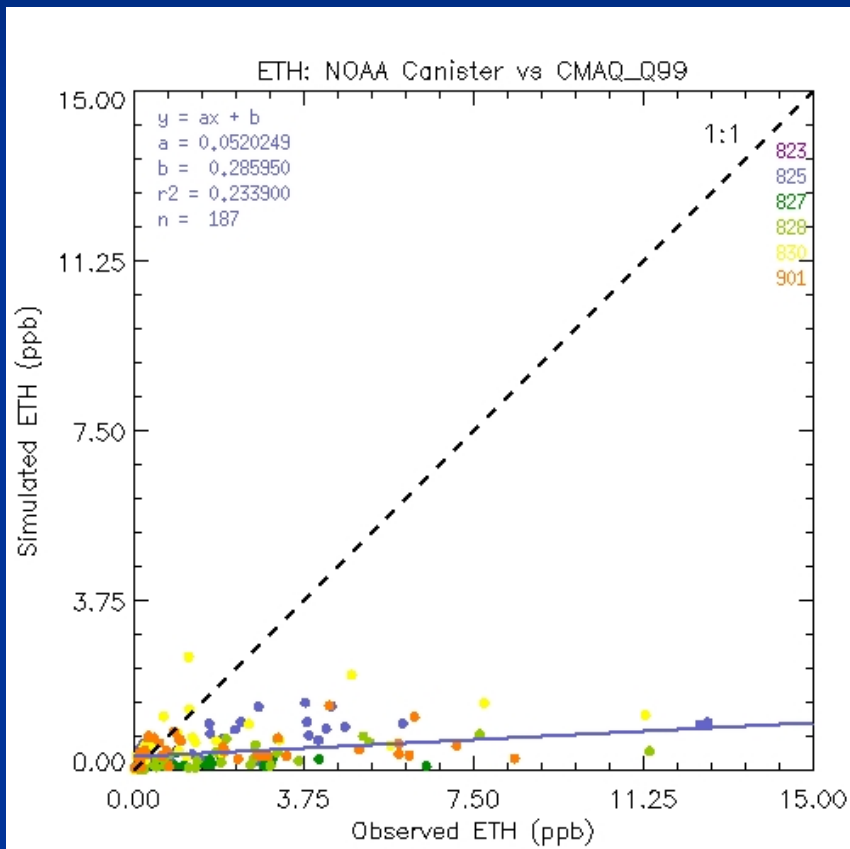


Canister ETH concentrations

August 25th, 2000 at 06 CST

NEI

TEI

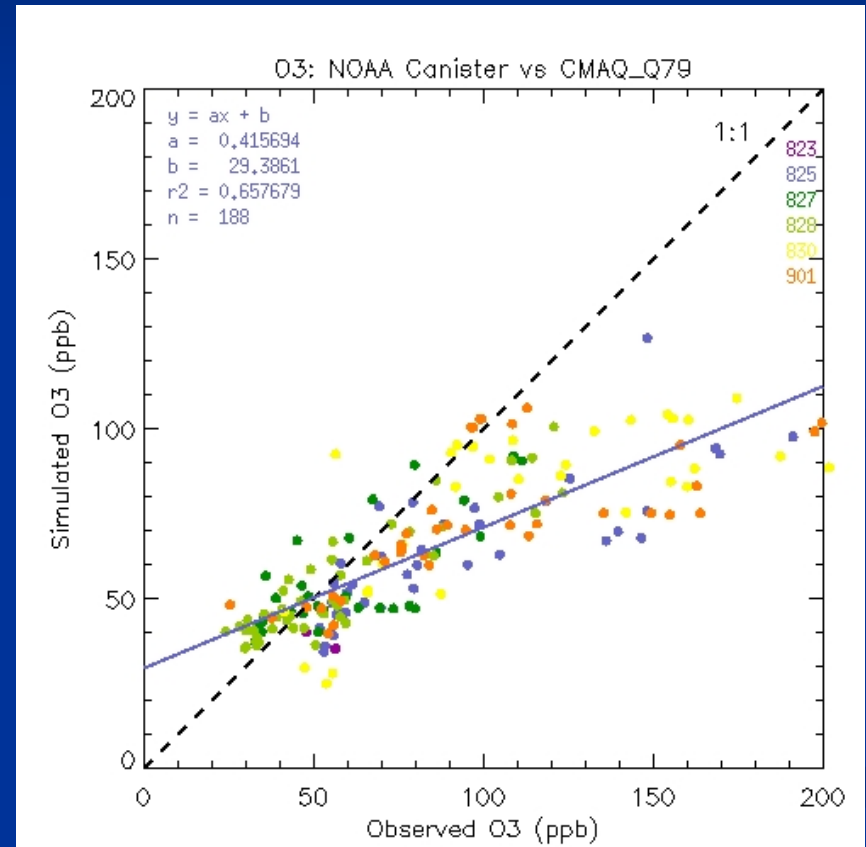
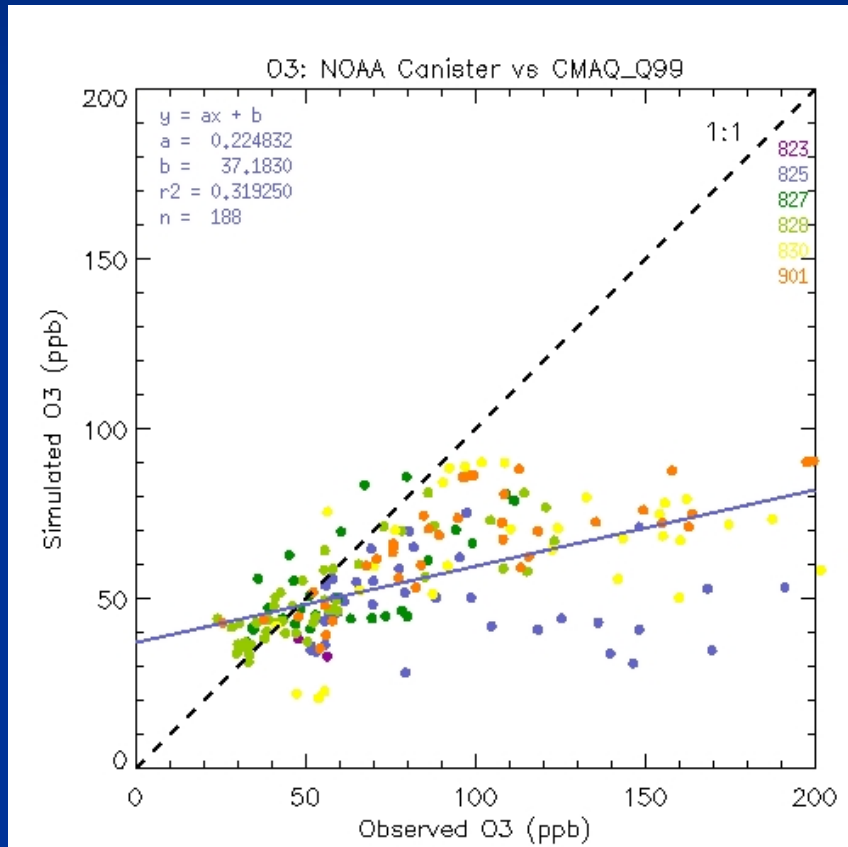


Canister O3 concentrations

August 25th, 2000 at 06 CST

NEI

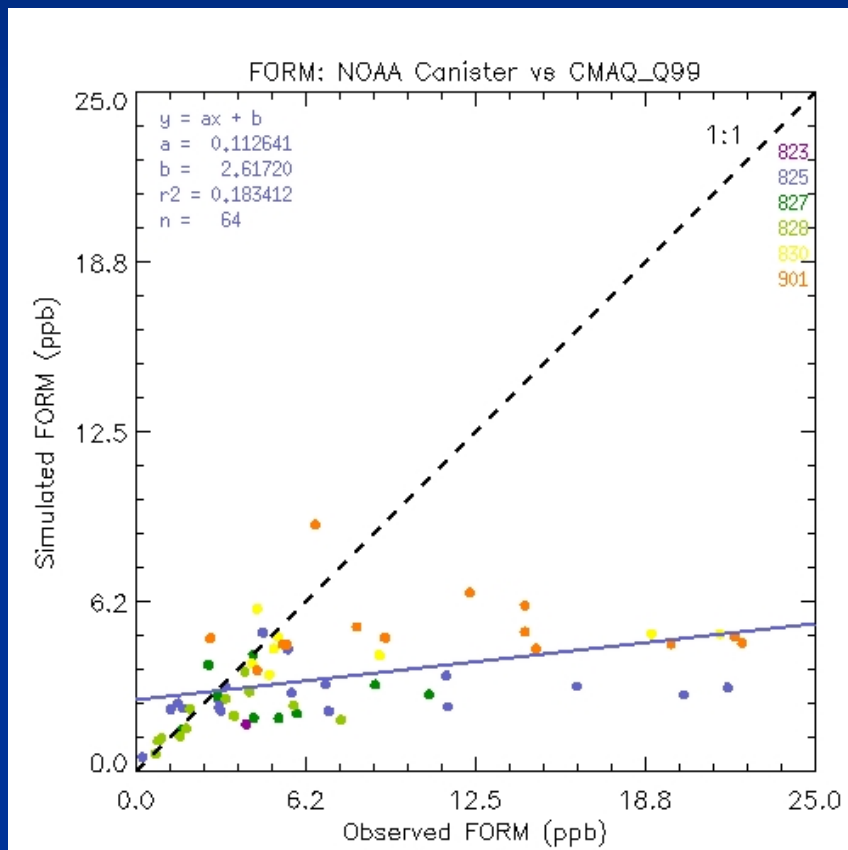
TEI



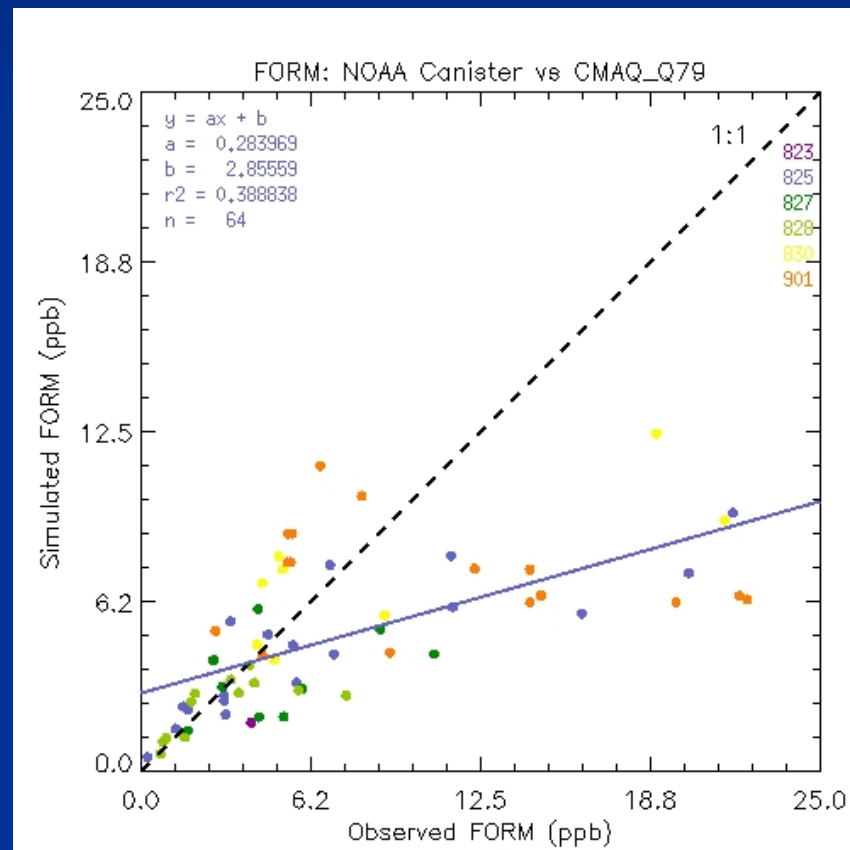
Canister FORM concentrations

August 25th, 2000 at 06 CST

NEI



TEI

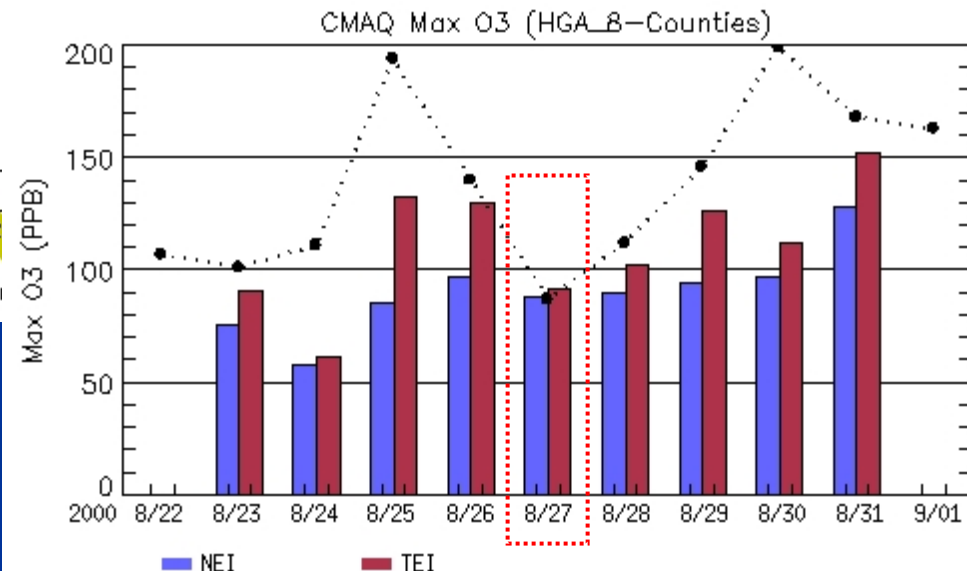
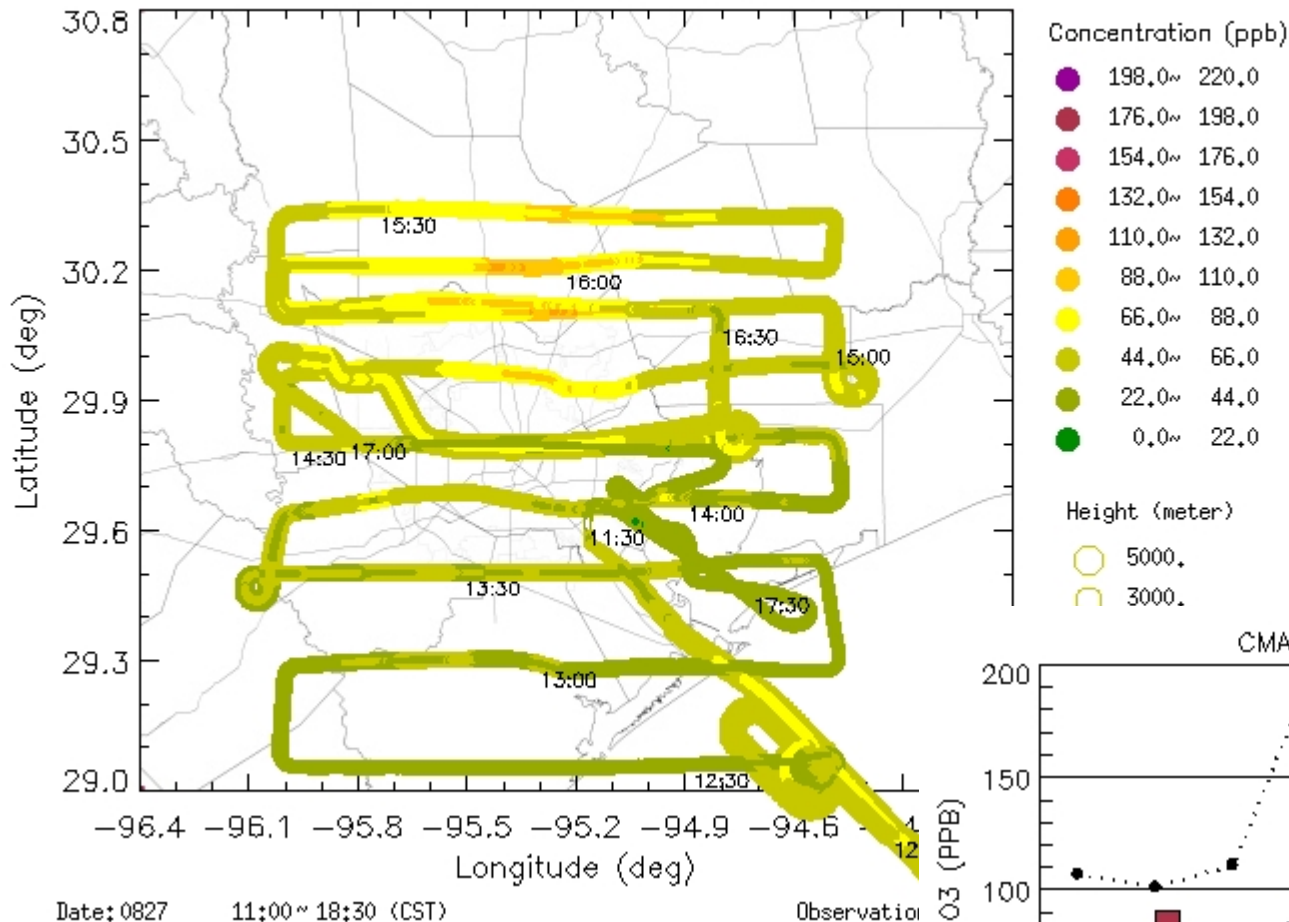


NOAA AL aircraft flight path

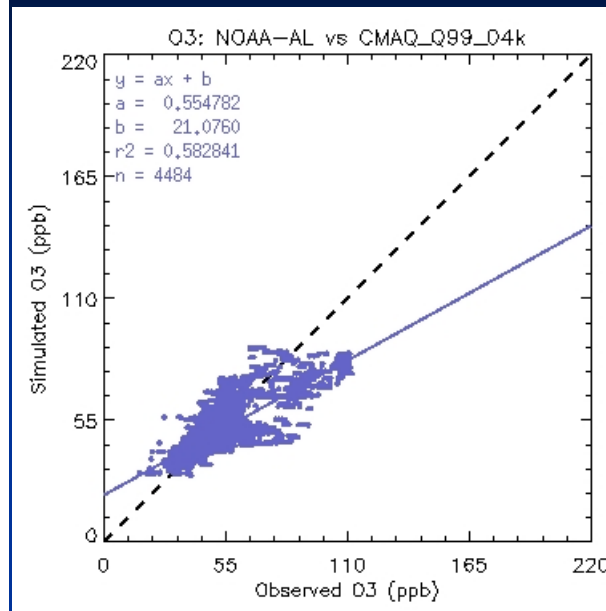
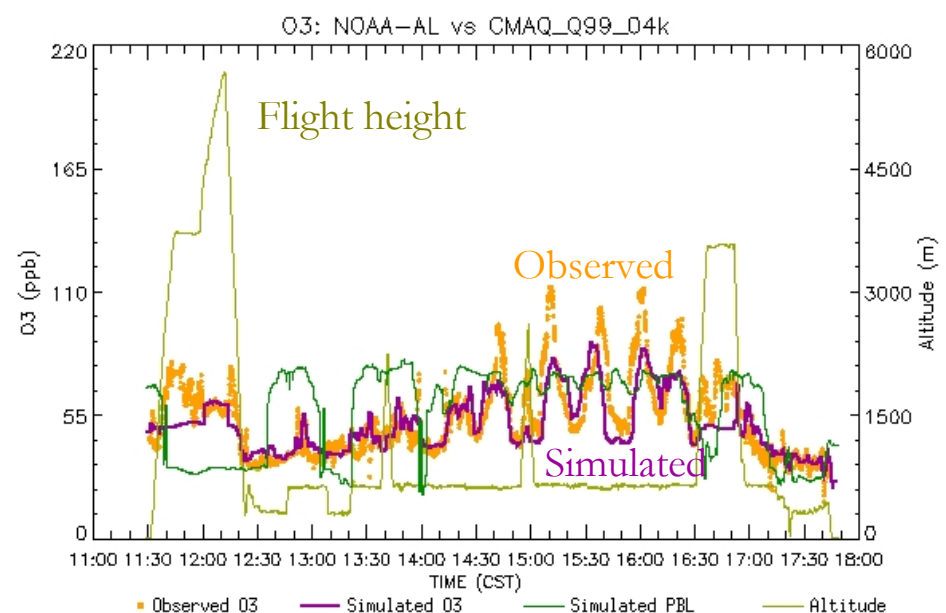
August 27th, 2000

Southerly was predominant during the flight.

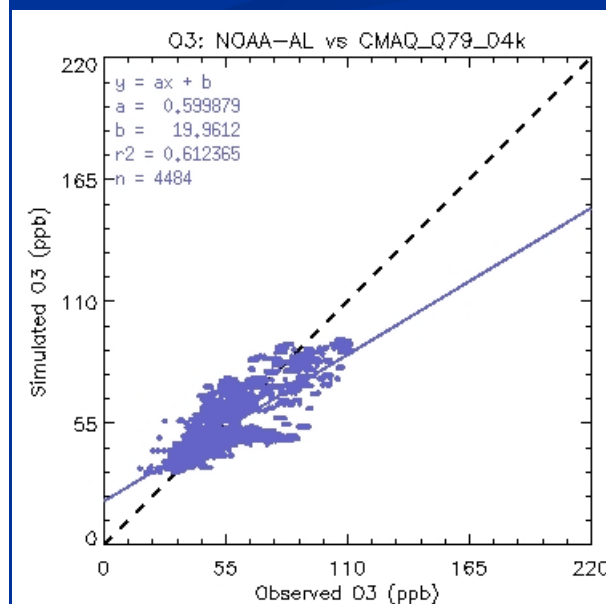
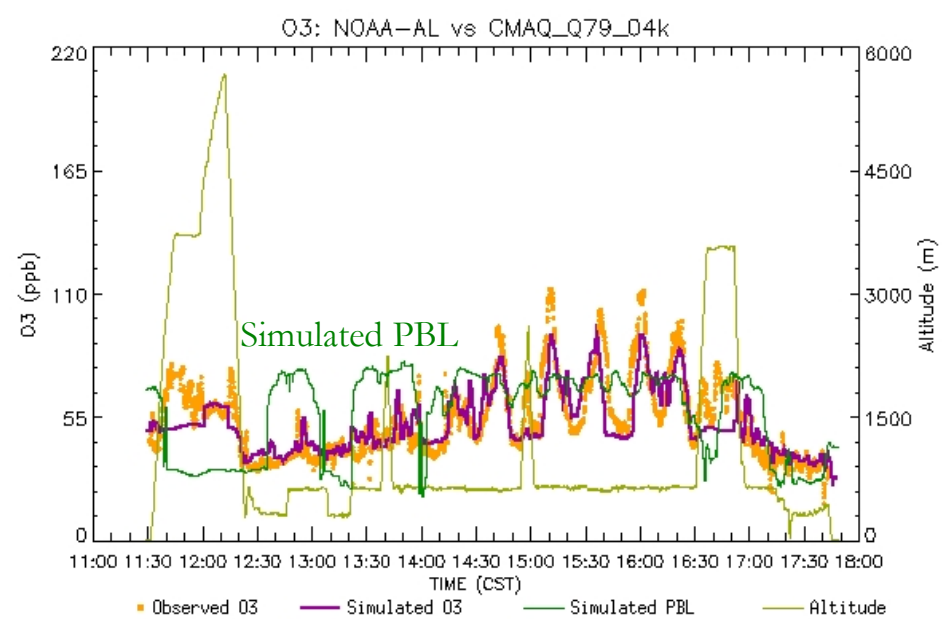
O3: NOAA-AL vs CMAQ_Q79_04k



NOAA AL O3 concentrations

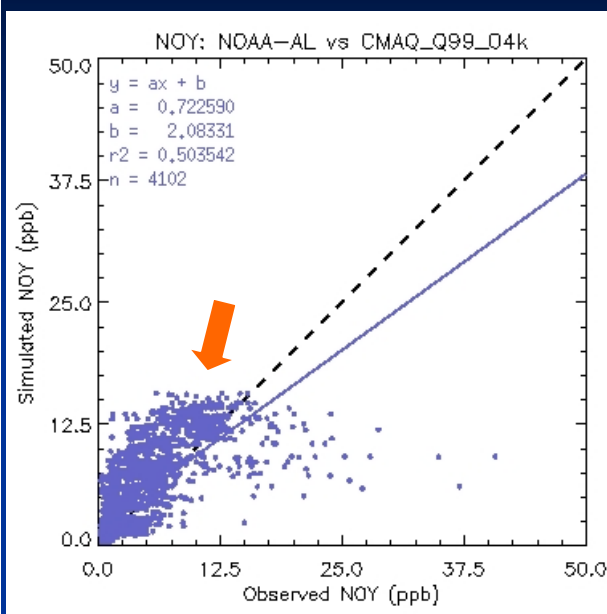
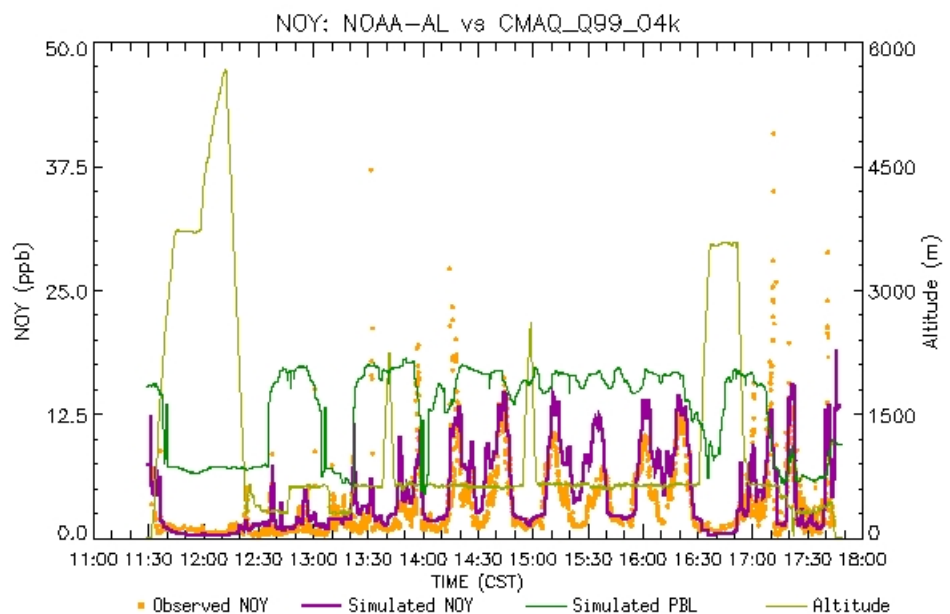


NEI

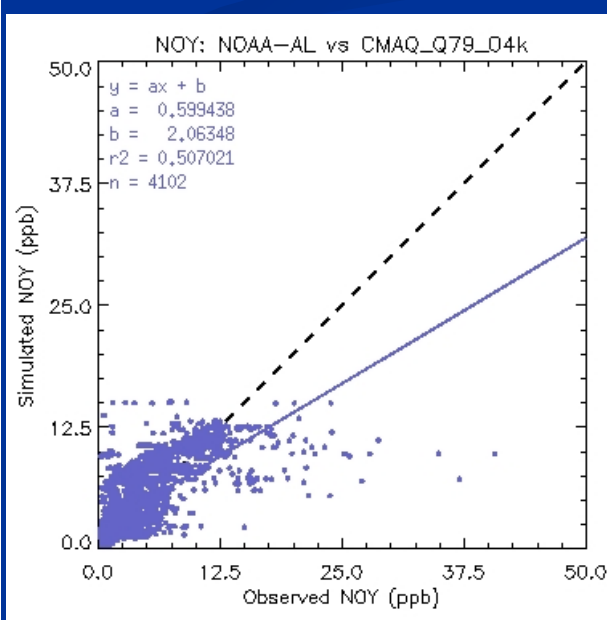
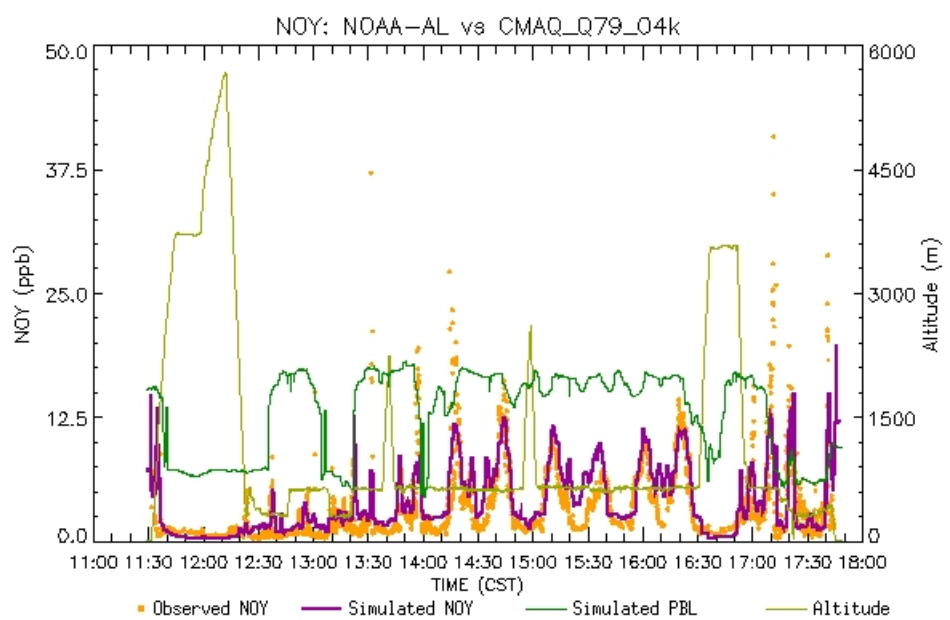


TEI

NOAA AL NO_y concentrations

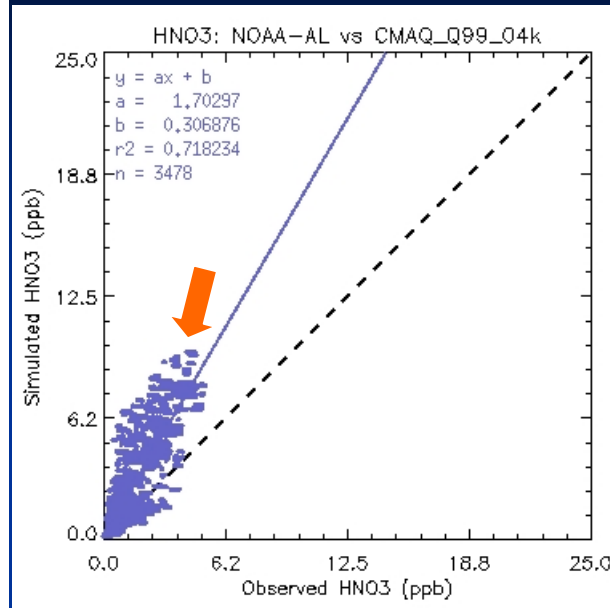
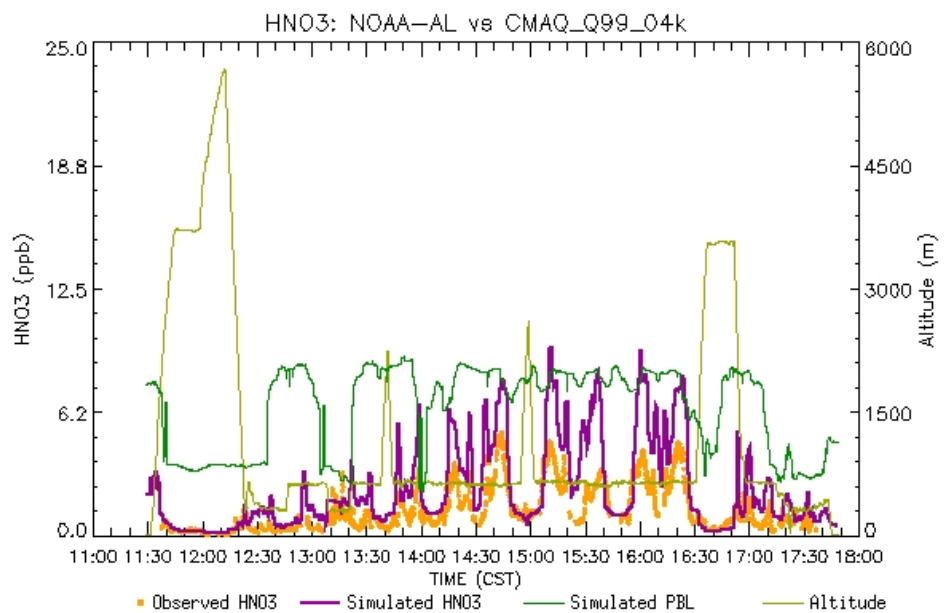


NEI

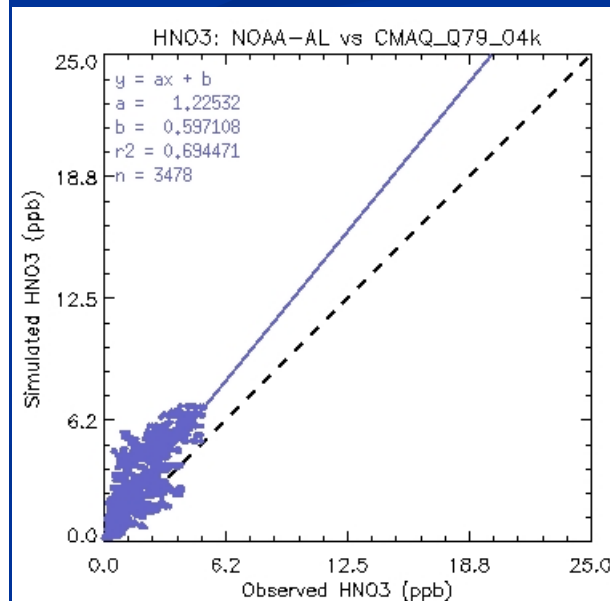
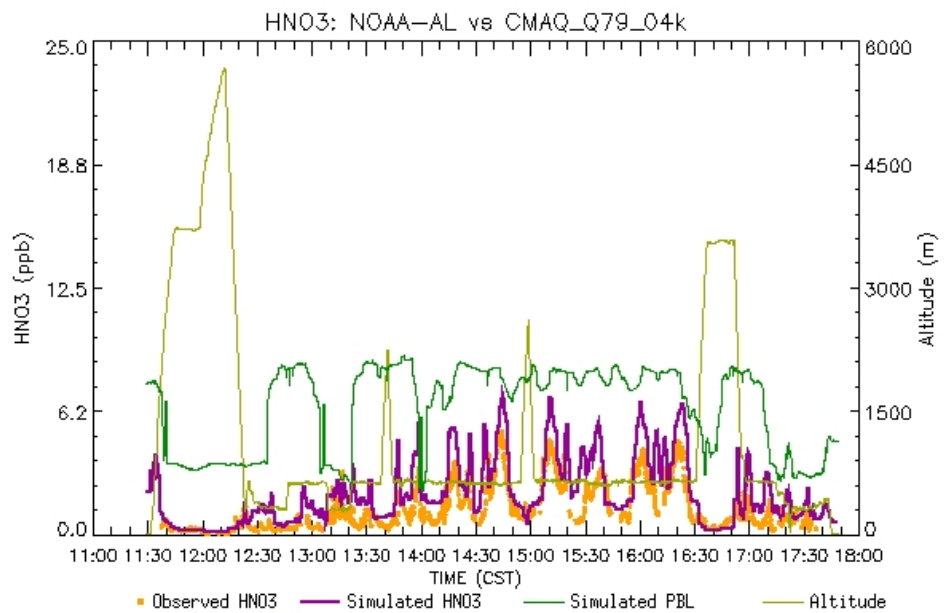


TEI

NOAA AL HNO₃ concentrations



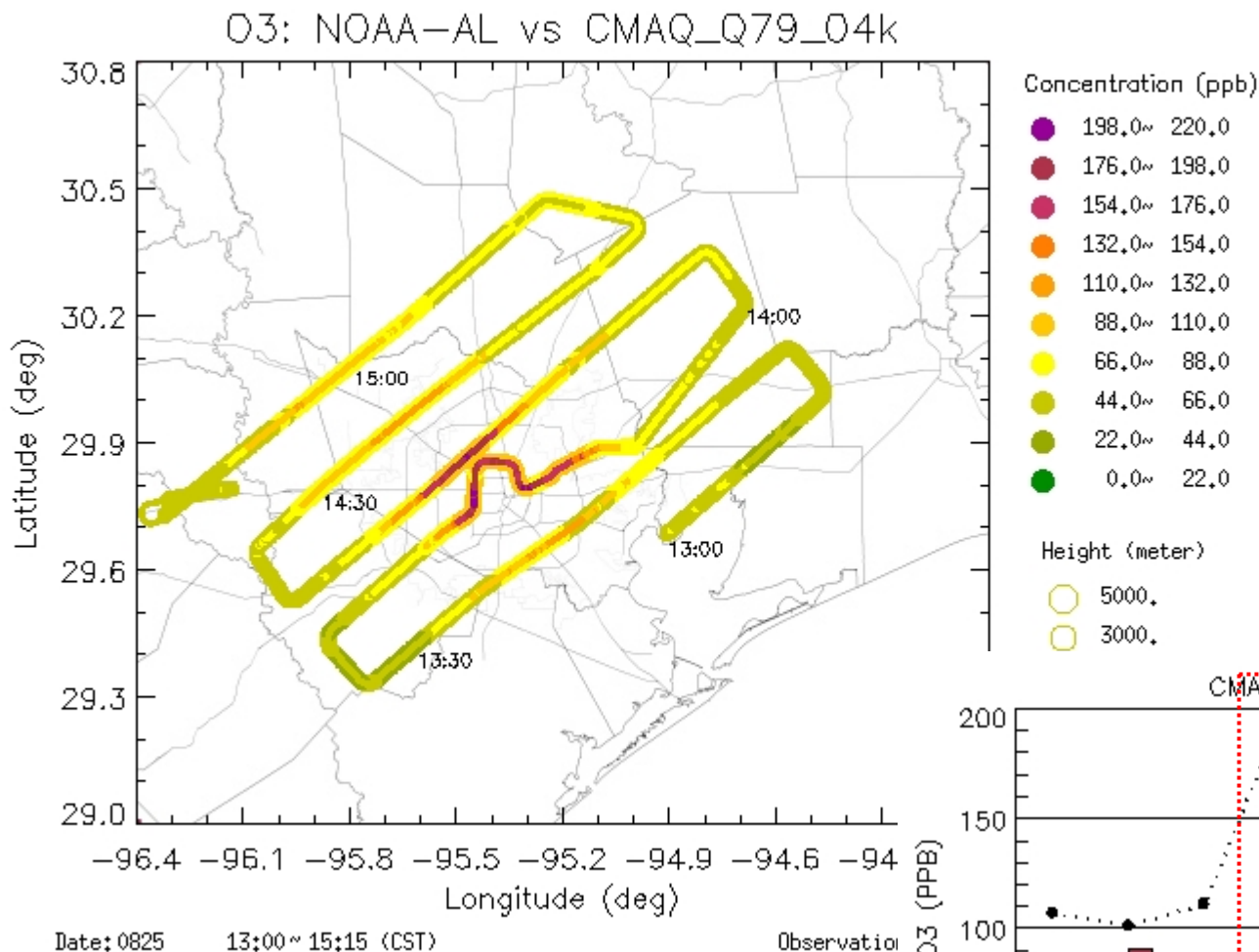
NEI



TEI

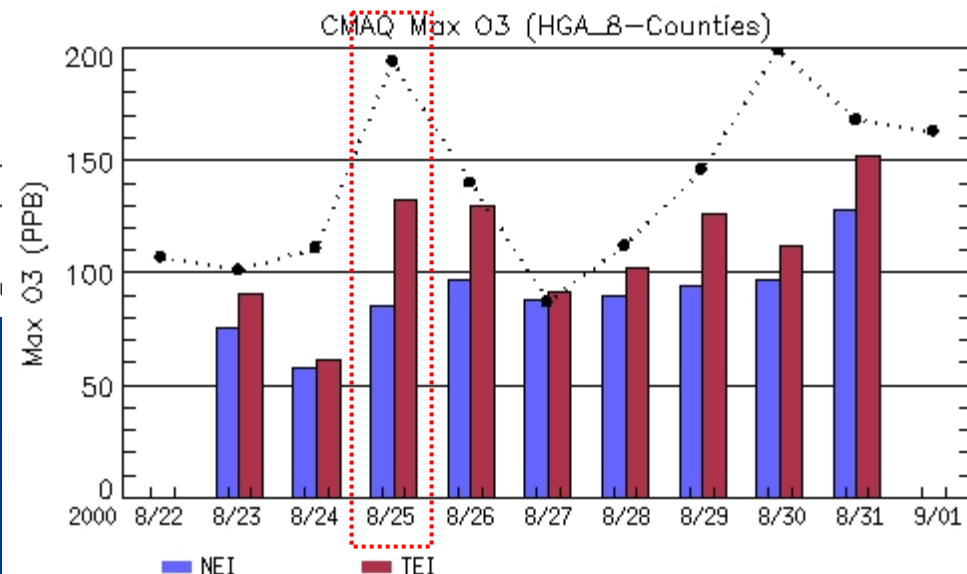
NOAA AL aircraft flight path

August 25th, 2000

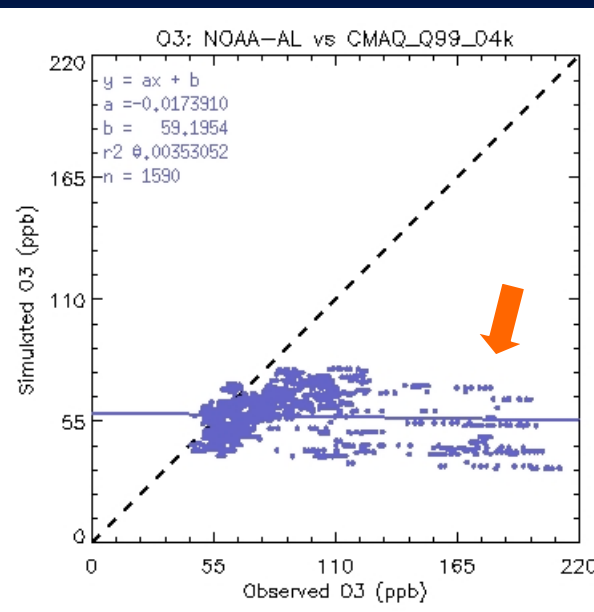
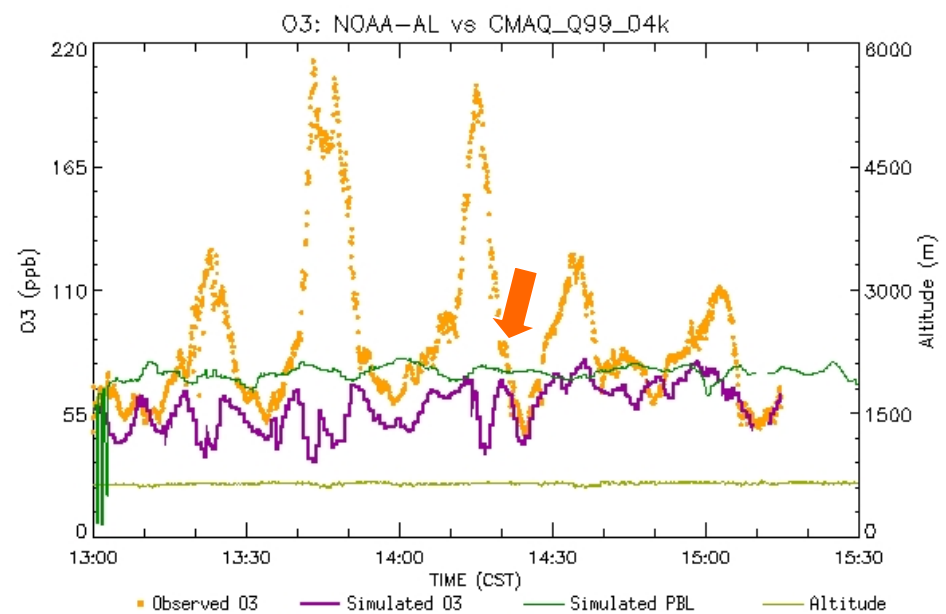


Plume moved from the Ship Channel to downtown during the flight.

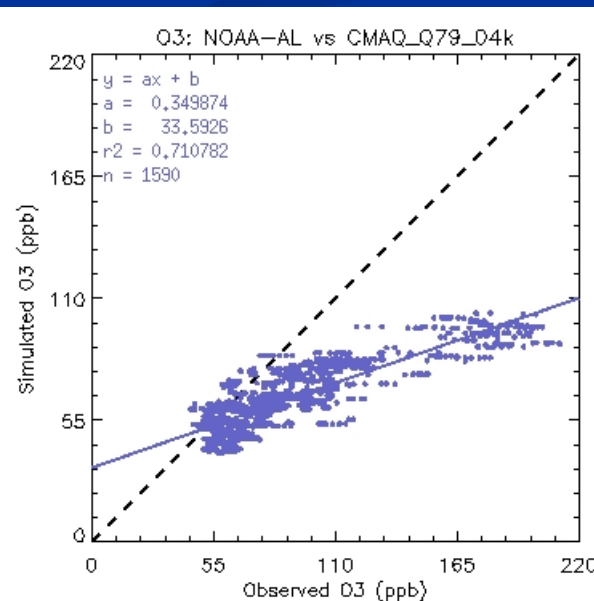
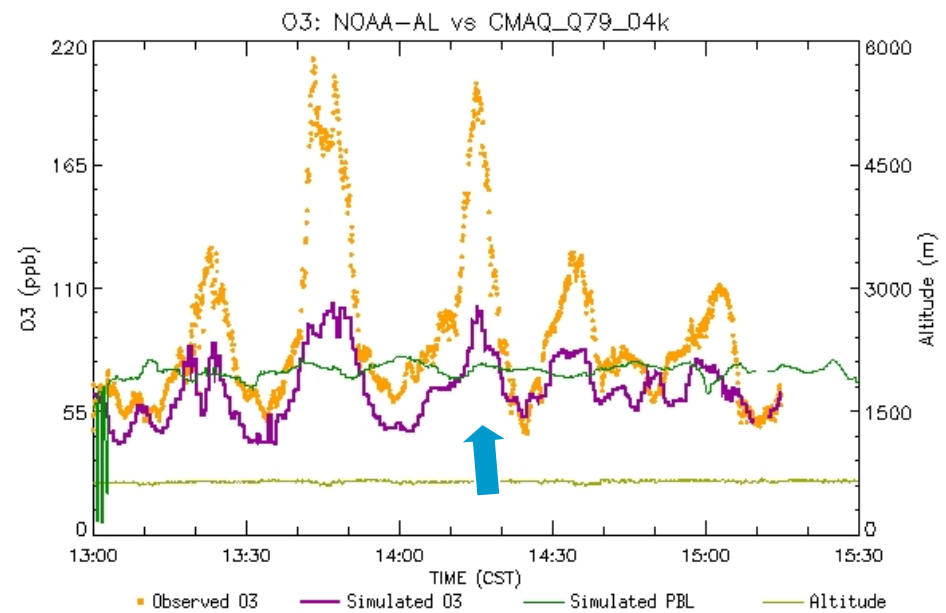
High ozone concentrations (up to ~210 ppb) were observed over downtown Houston.



NOAA AL O3 concentrations



NEI



TEI

Summary

- With NEI, the CMAQ simulation shows a coefficient of determination (r^2) = 0.5944 and the slope of linear regression (a) = 0.5580. The CMAQ simulation with TEI shows r^2 = 0.7133 and a = 0.7109, indicating that the overall performance of the simulation with TEI better predicted than that with NEI.
- Within the 10 days of the simulation, the largest difference was observed on August 25, 2000, by about 50 ppb of O₃ concentrations predicted for the Houston-Galveston 8-County area.
- It is supposed that too high NO_x emissions downtown and relatively low VOC emissions over the Ship Channel in NEI caused more under-predictions in high O₃ concentrations observed.
- When compared to the airborne canister measurements from the NOAA Aeronomy Laboratory aircraft, simulations with both emissions inventories were difficult to have those high concentrations observed. However, CMAQ with TEI showed 3 ~ 5 times higher airborne ETH concentrations than that with NEI.