Air Quality Forecasting system and its application

Southeast Texas Photochemical Modeling Technical Committee meeting

March 26, 2013

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Department of Earth and Atmospheric Sciences

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Regional CTMs

- Regional chEmical trAnsport Model, REAM for the first presentation [Choi et al., 2005, 2008a, 2008b, 2009, 2010]
  - developed for capturing transient features such as soil emissions, convection, lightning, and convective outflow
- WRF-CMAQ 4.7.1 for the second presentation [Choi et al., 2012 and preparations for the submission]
- WRF-CMAQ 5.0.1 and WRF-Chem 3.4.1
  - for establishing two different air quality forecasting systems and evaluating historical modeling for Southeast Texas
  - 200 CPU MPI system at UH modeling group

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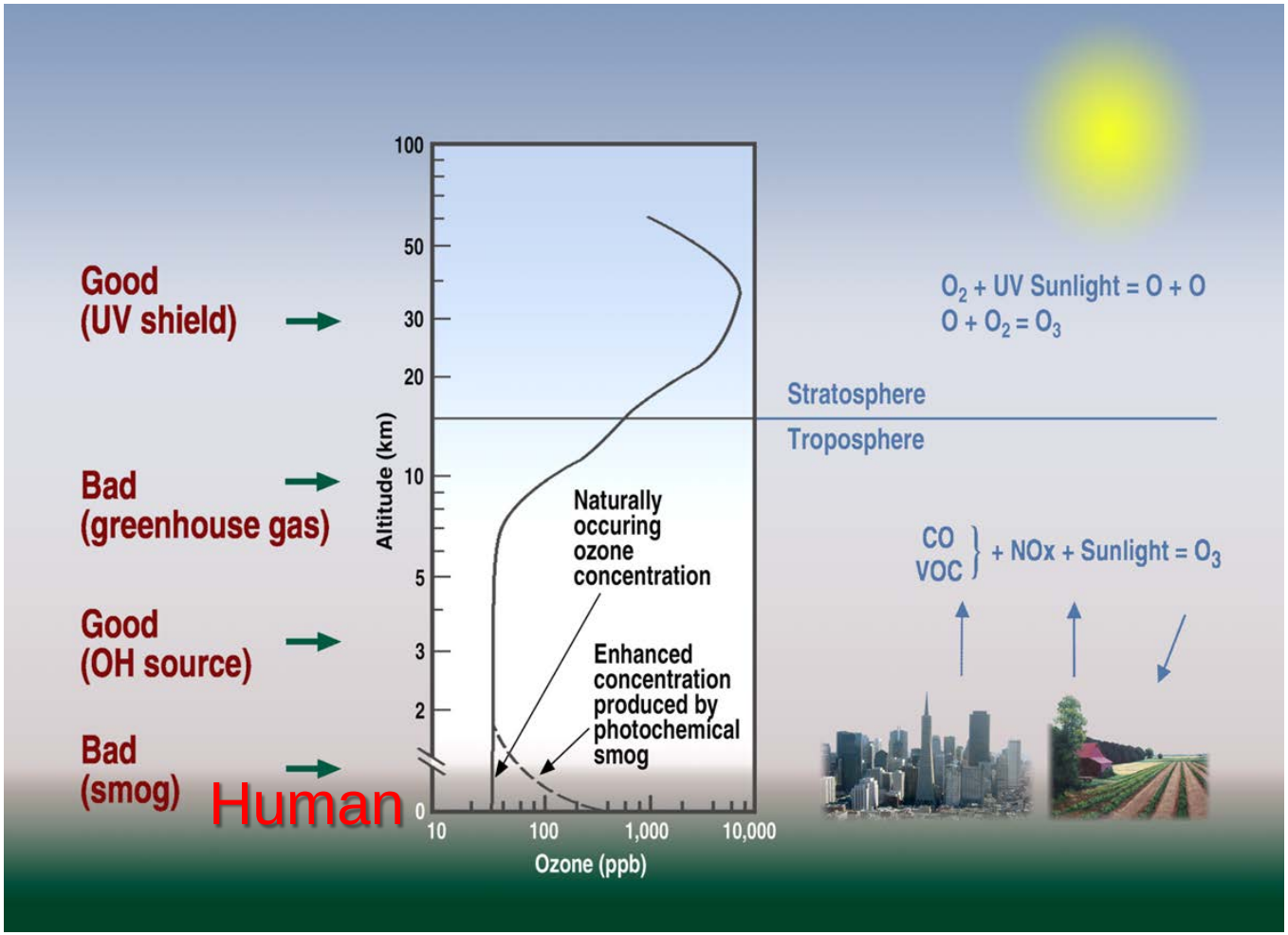
Human-derived O_3



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Houston is a Smog Capital

PAGE 6A Laredo Morning Times Thursday, October 28, 1999

MEXICO/STATE

Houston tops Los Angeles as smog capital

BY MEGAN K. STACK
Associated Press Writer

HOUSTON — It was probably just a chemical belch this month at one of the factories on the edge of town.

But it was enough to send this sprawling industrial mecca sailing by Los Angeles to claim a dubious distinction: smoggiest city in the United States.

"The day that will live in infamy," Houston health department spokesperson Kathy Barton said. "Really."

Houston and Los Angeles were running neck-and-neck in the national air pollution race until Oct. 7, when Texas' largest city surpassed California's largest by notching its 44th smog day this year. As of Wednesday, the Houston count had reached 46.

Just what caused the ozone overflow remains a mystery.

Researchers pinned down the nature of the leak — large clouds of ethylene and propylene billowed over east Houston Oct. 7, Texas Natural Resource Conservation Commission spokesman Patrick Crimmins said.

Those gases likely were the product of one of the industrial plants on the edge of the nation's fourth-largest city.

But which one?

Factories are required to report any accidental spills. A few plants admitted to leakage, but none of the reported slip-ups singularly could have accounted for the magnitude of the ozone leap.

Ozone levels climbed to 251 parts per billion that day — more than twice the Environmental Protection Agency's standard. It was the most lung-irritating ozone to hang over Houston in years, researchers said.

"There was an aberration, a spike," Crimmins said.

Researchers have narrowed their search for a culprit to 25 factories, all clustered around the Houston Ship Channel southeast of the city and home of the nation's largest concentration of petrochemical plants.

In the meantime, Texas is staring at an EPA ultimatum. The state has until next month to come up with a plan to clean its skies by 2007.

The federal government has threatened to snatch away money for Texas highway construction if the state doesn't start making progress soon.

But clearing Houston's air is no small task.

"These reductions are going to have to be extremely steep," TNRCC executive director Jeff Saitas said. "It's going to press the limits of cooperation."

Oil refineries and industries tend to release heavy amounts of chemicals that thicken into ozone above the city.

And then there are the grandfathered plants — factories that were already running when the Clean Air Act was penned. Those older plants were not required to meet the emissions standards outlined in the 1970s legislation.

"The thought at the time was that, soon enough, these guys wouldn't be operational anyway," Barton said.

But almost three decades later, an estimated 800 grandfathered plants continue to blow dirty air into Texas skies. According to a 1998 state study, those factories accounted for 36 percent of all industrial air pollution in Texas.

And almost a quarter of the state's dirtiest grandfathered plants are clustered around Houston.

Smog broods over the skyline and glimmers from a distance. Ozone is scratching the throats, eyes and lungs of the elderly and the very young, Ms. Barton said.

"It will eventually compromise your respiratory system," Ms. Barton said. "It speaks to the quality of your life as you age."

Critics claim smog-spitting industry represents campaign cash for Texas governor and presidential hopeful George W. Bush and that Bush stopped short of forcing the plants to clean up emissions because he was collecting campaign contributions from employees and lobbyists.

"Rather than clear the air, Gov. Bush has ceded to the demands of some of his biggest donors," Tom Smith, director of the consumer group Public Citizen, said. "He's given them a walk on their responsibilities."

Bush officials dismiss the barbs, contending the governor has reduced industrial pollution and toxic waste in Texas.

"Gov. Bush makes his decisions based on what's right for Texas," Bush campaign spokesman Scott McClellan said Wednesday.

http://airwolf.lmtonline.com/news/archive/1028/pagea6.pdf

Photo from http://texasvox.files.wordpress.com/2010/02/hou-smog.jpg

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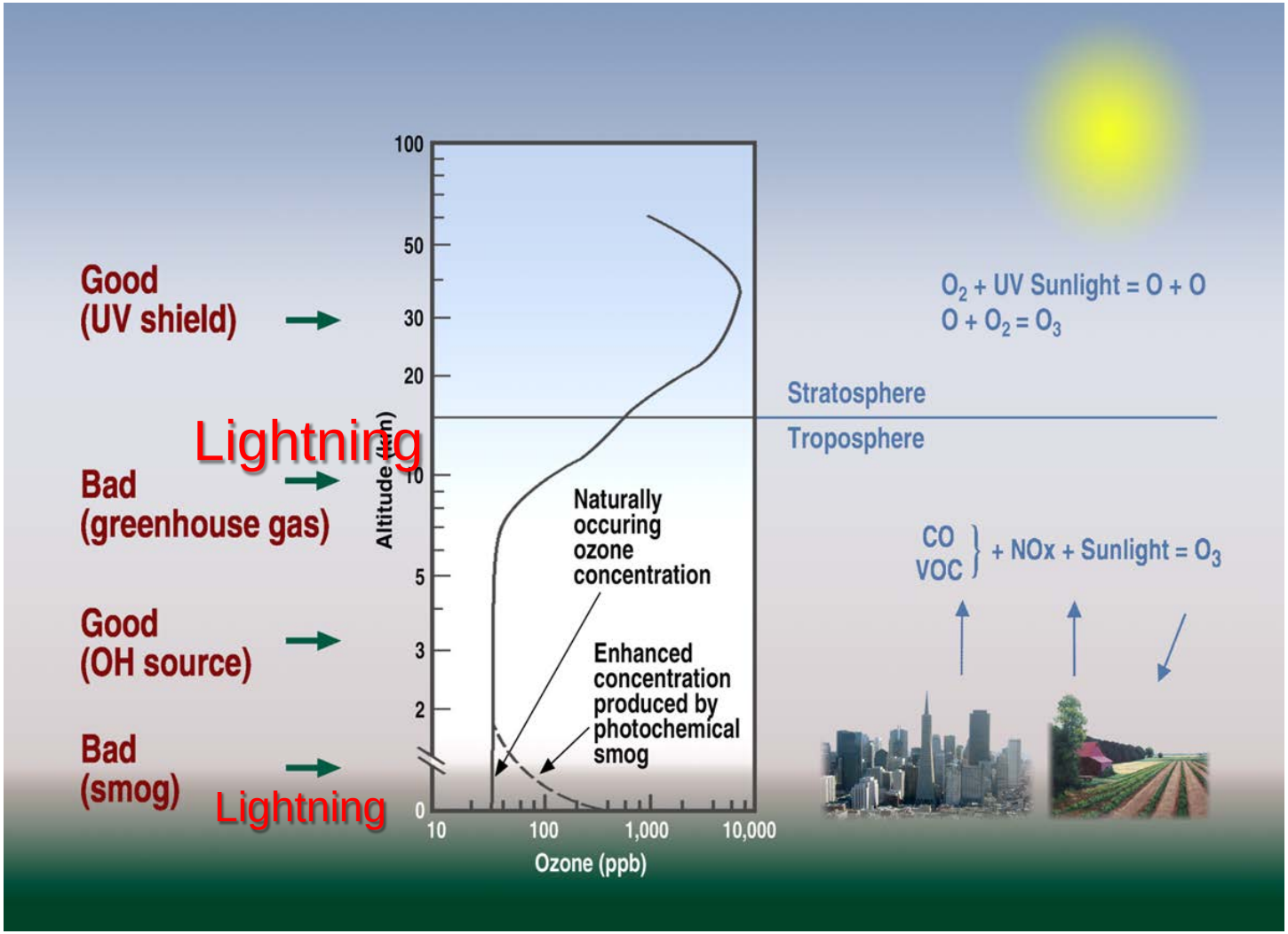
Lightning-derived O_3



Houston is a Lightning Capital

- **Houston is called as Lightning Capital of Texas [White and Orville, July 15, 2002]**

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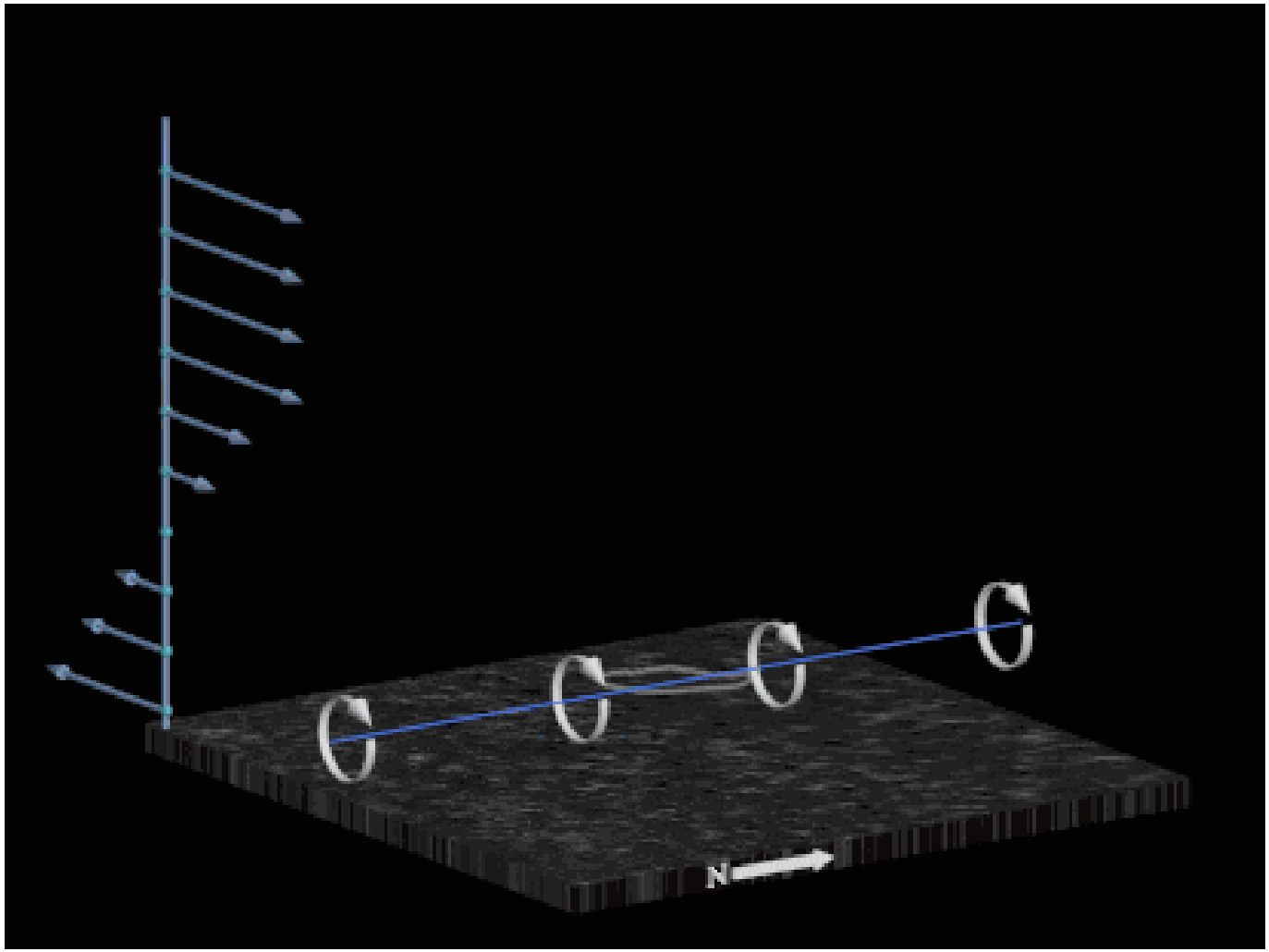
Convection



COMET

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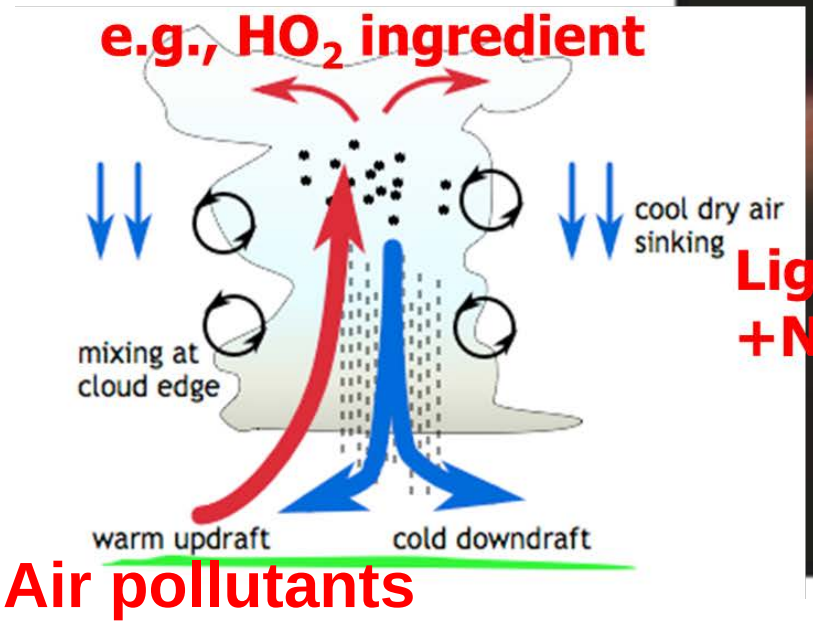
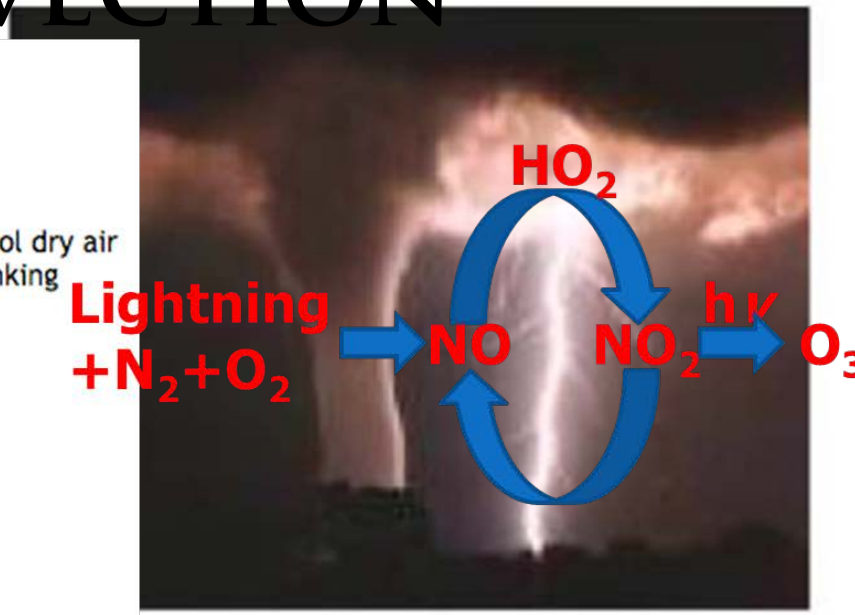
Lightning and Convection



http://www.cmmap.org/learn/clouds/cloudCloud1.htm



From Leet Software

- Convection transports HO_x sources and lightning enhances nitric oxide (NO) to the upper troposphere
- CTM includes detailed updraft and downdraft of tracers and their scavenging inside of cloud [Choi et al., 2005]

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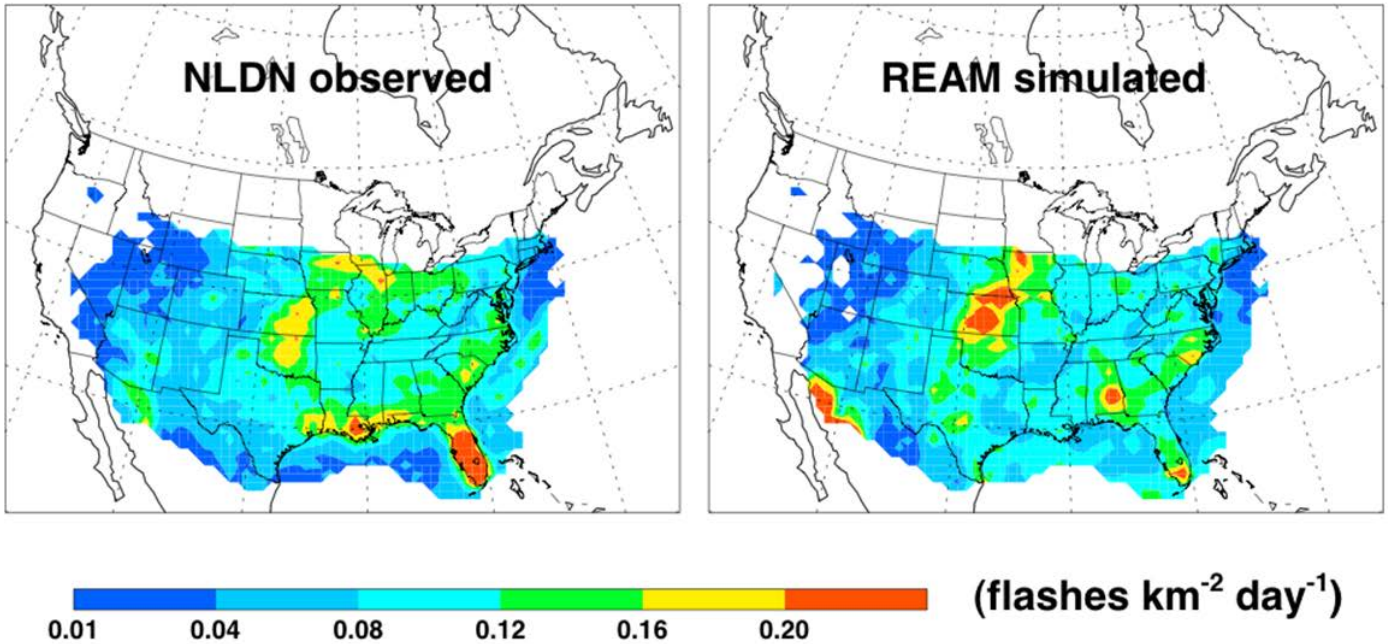
Lightning Flashes



- **Difficult to capture lightning occurrences in model**
- **Dependence of lightning occurrence on CAPE and cloud mass flux with higher-order (4th order) [Choi et al., 2005, GRL].**

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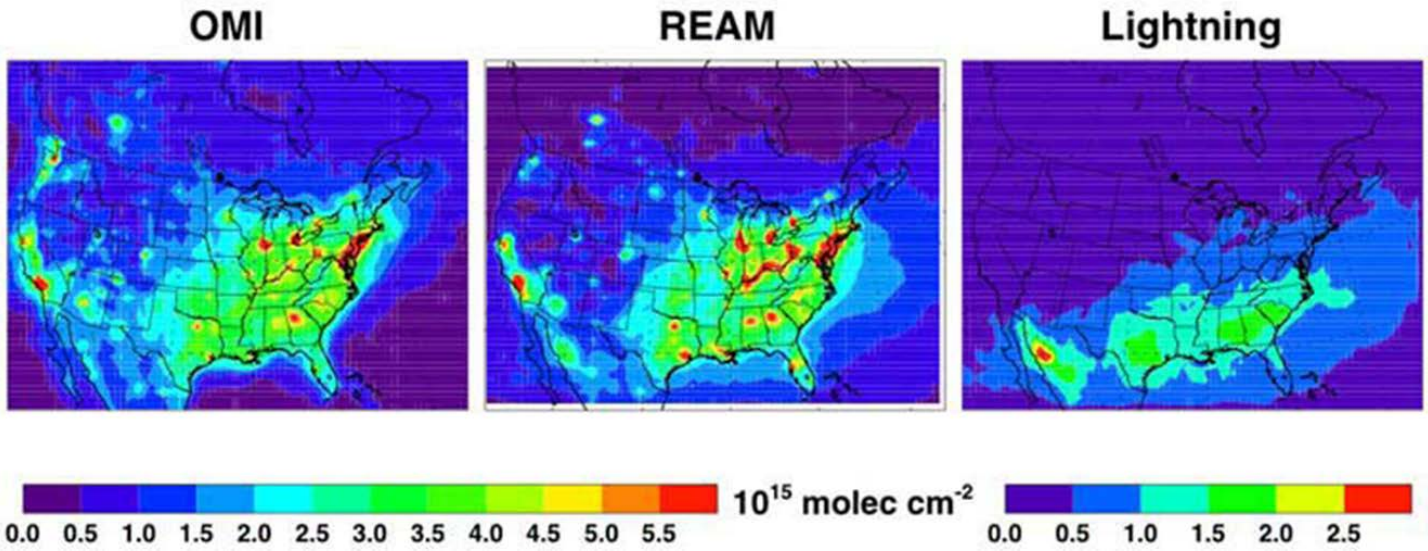
Lightning: OMI NO_2



[Choi et al. 2008, GRL]

- Tropospheric NO_2 for May-Aug 2005 from OMI (first), model (second), and lightning contribution (third).
- Summertime lightning NO is important (≈17%).

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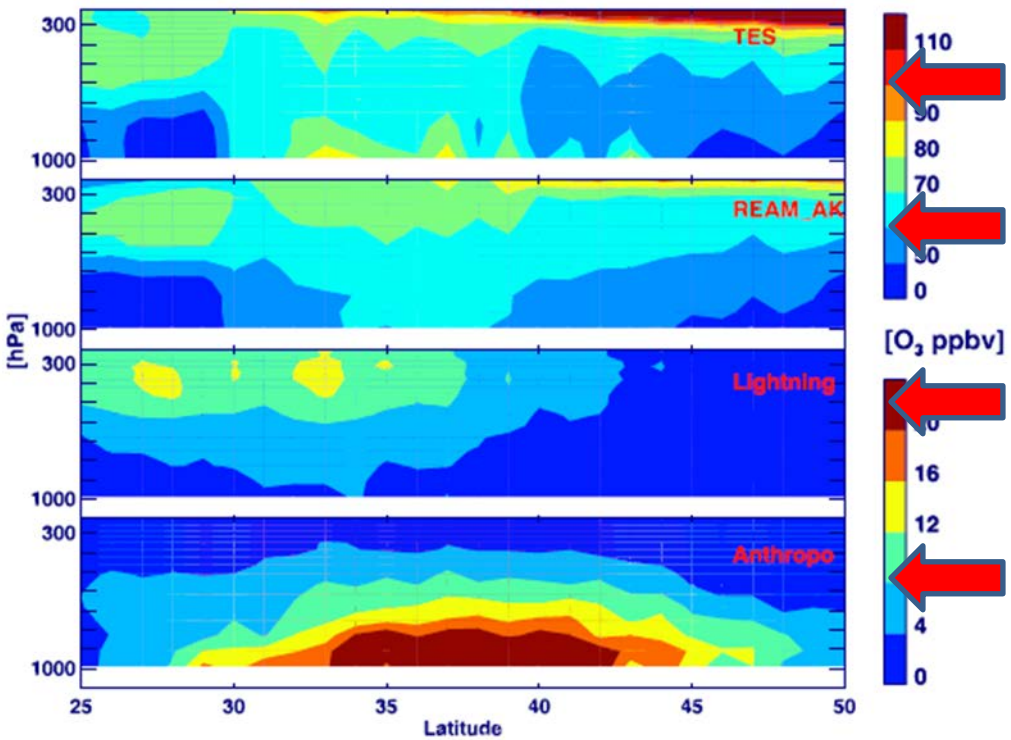
TES O_3 vertical profile



Satellite

Model

Lightning's contribution

Human's contribution

- Zonal O_3 over NA for Jul 2005 from TES (first), model (second), and lightning (third) and anthropogenic (last) contribution.
- Anthropogenic and lightning NOs are important for the lower and upper tropospheric O_3.

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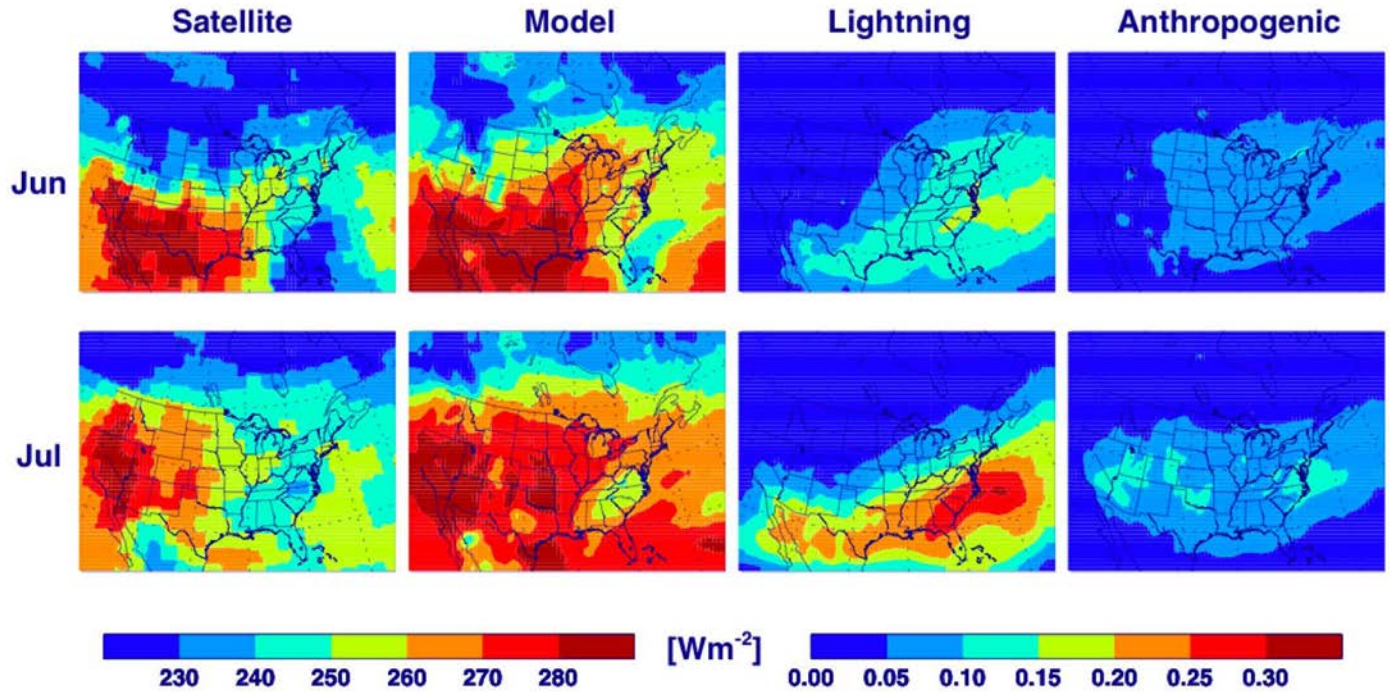
Outgoing Longwave Radiation



[Choi et al. 2009, GRL]

- OLR for Jun-Jul 2005 from NOAA-16 (first), model (second), and OLR reduction by lightning (third) and anthropogenic NO-derived O_3 increase (last)
- Lightning exerts a larger impact by their large radiative sensitivity.

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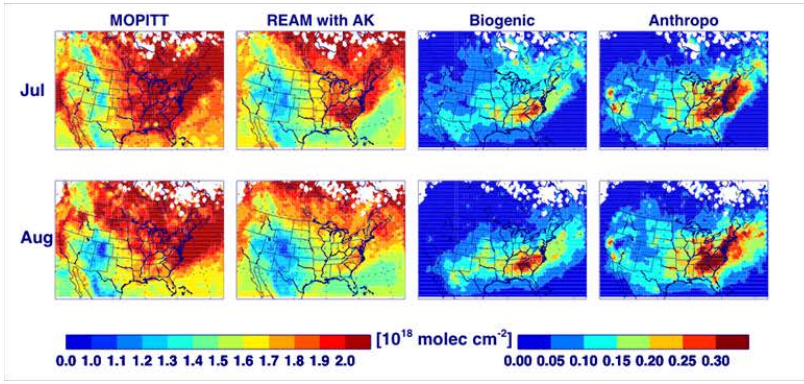
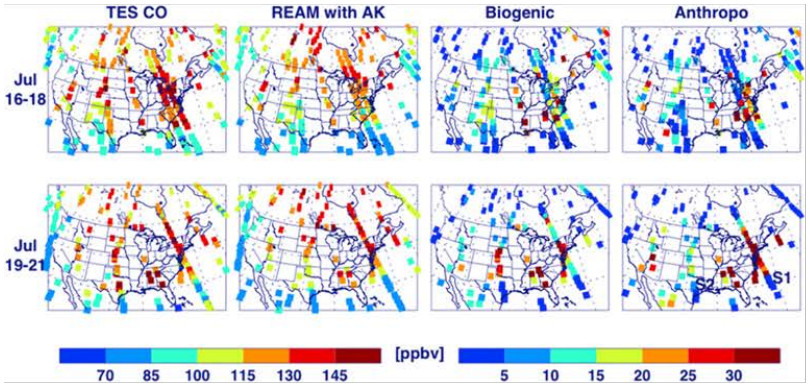
Heat wave impact on CO

MOPITT CO column for 2006



Anthropogenic sources are larger than biogenic.

TES CO at 800 hPa for 2006



For very warm days, biogenic sources produce as much as CO from anthropogenic.

[Choi et al. 2010, AE]

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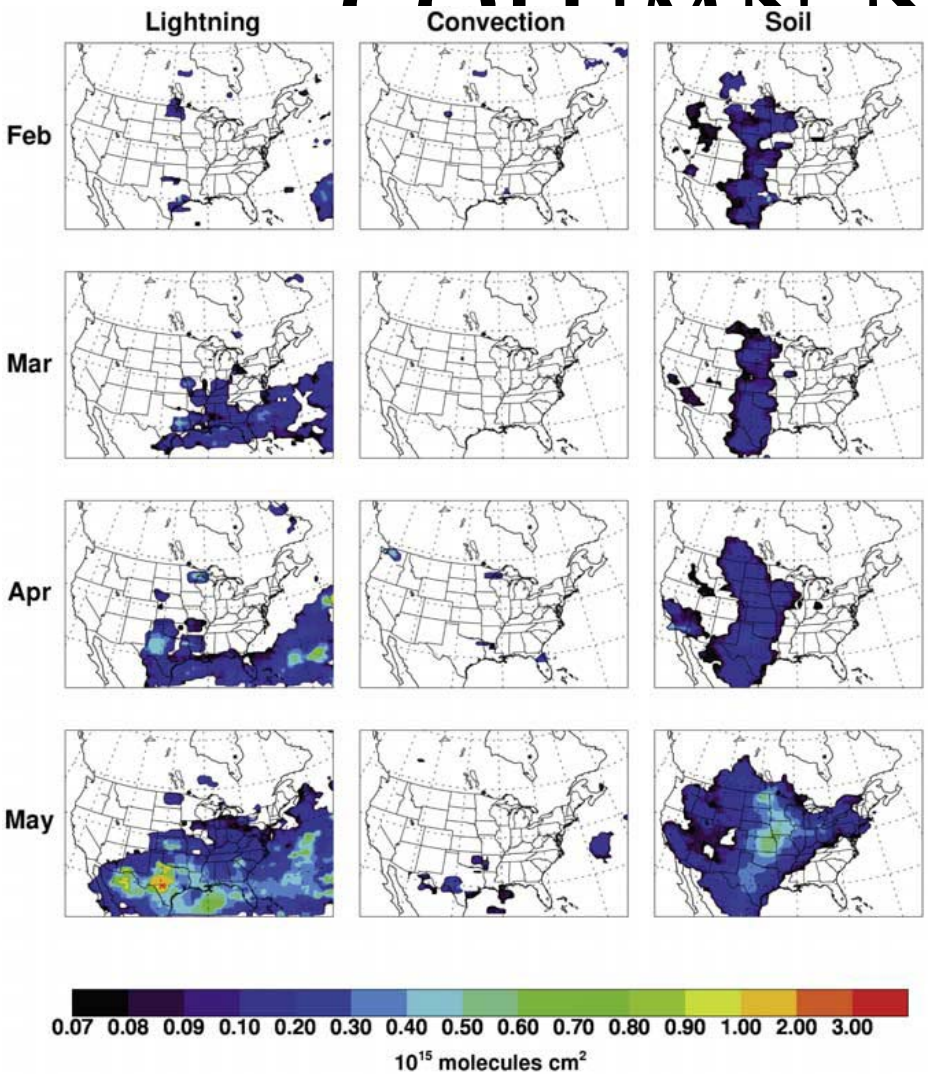
Source impact on column NO_2



Monthly mean contributions of lightning, convection and soil emissions to NO_2 columns for Feb-May 2000.

Choi et al. [2008, JGR]

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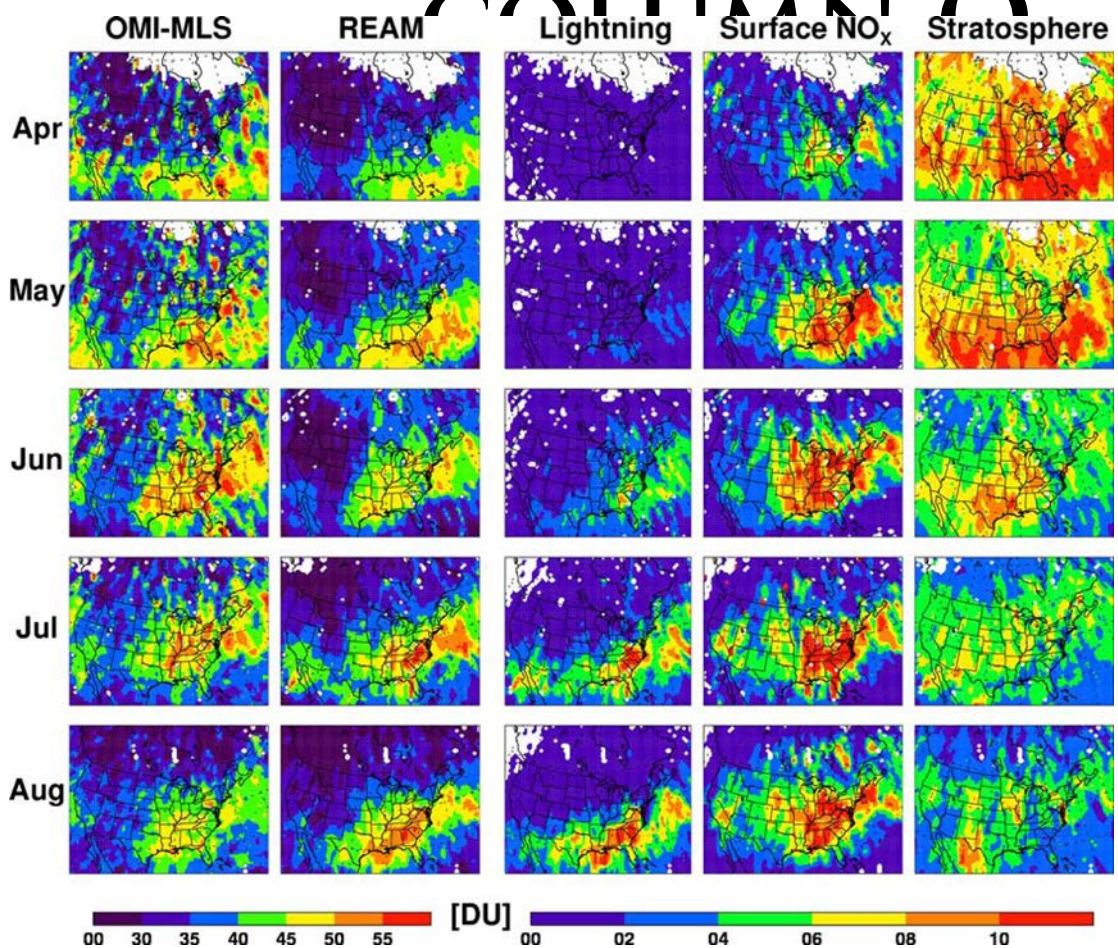
Source impact on column O



[Choi et al. 2008, GRL]

Northward migration for Apr-Aug 2005 is by seasonal shifts of O_3 from stratosphere to surface and lightning NO sources.

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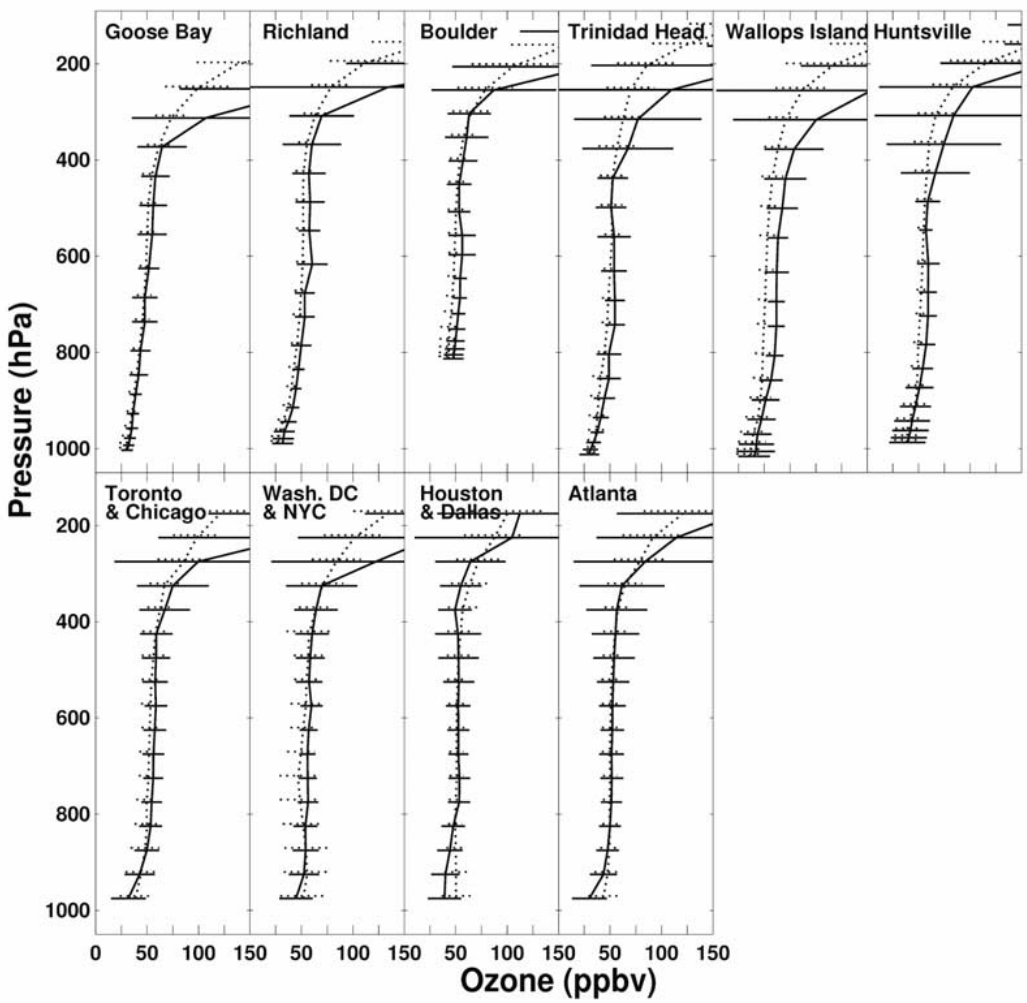
Springtime O_3 profile



[Choi et al. 2008, JGR]

Observed(solid lines) and simulated(dotted lines) mean O3 for Feb-May 2000, showing ozonesonde (top) and MOZAIC aircraft (bottom)

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Conclusion

- **Fossil NO_x emission is a major source for tropospheric NO_x and O_3. Lightning NO_x effectively enhance upper tropospheric O_3.**

- **Due to the large radiative sensitivity of upper tropospheric O_3, the lightning NO_x contribution to OLR via its O_3 production is significantly larger than anthropogenic.**

- **O_3 enhancement over the NA migrates northward from spring to summer due to seasonal shifts of the O_3 from stratosphere to surface and lightning productions.**

- **For very warm days, biogenic sources produce as much as CO from anthropogenic.**

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Surface Air pollution

Marion E. Lent makes her way to work as smog dims City Hall in this 1953 photo (from Los Angeles Times)

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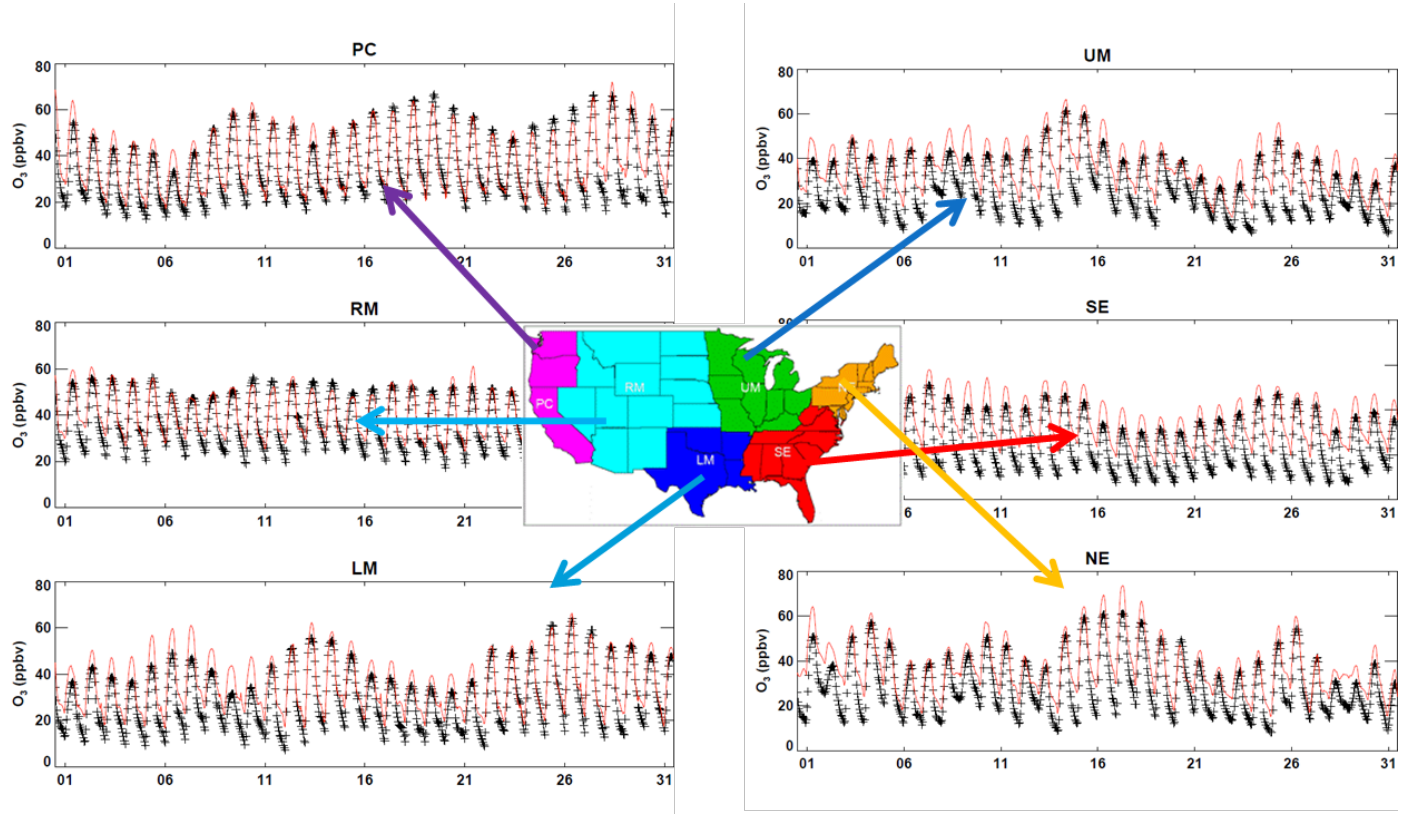
Surface O_3 overprediction



CMAQ model over-predicts surface O_3 over the eastern US during Summer.

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Surface O_3 overprediction

- **Geological regions are categorized into chemical regimes**

NO_x sensitive regime

NO_x saturated regime

- **Chemical regimes are from chemical environments**

NO_x sensitive regime: VOC >> NO_x → O_3 decreases as NO_x decreases

NO_x saturated regime: VOC << NO_x → O_3 increases as NO_x decreases

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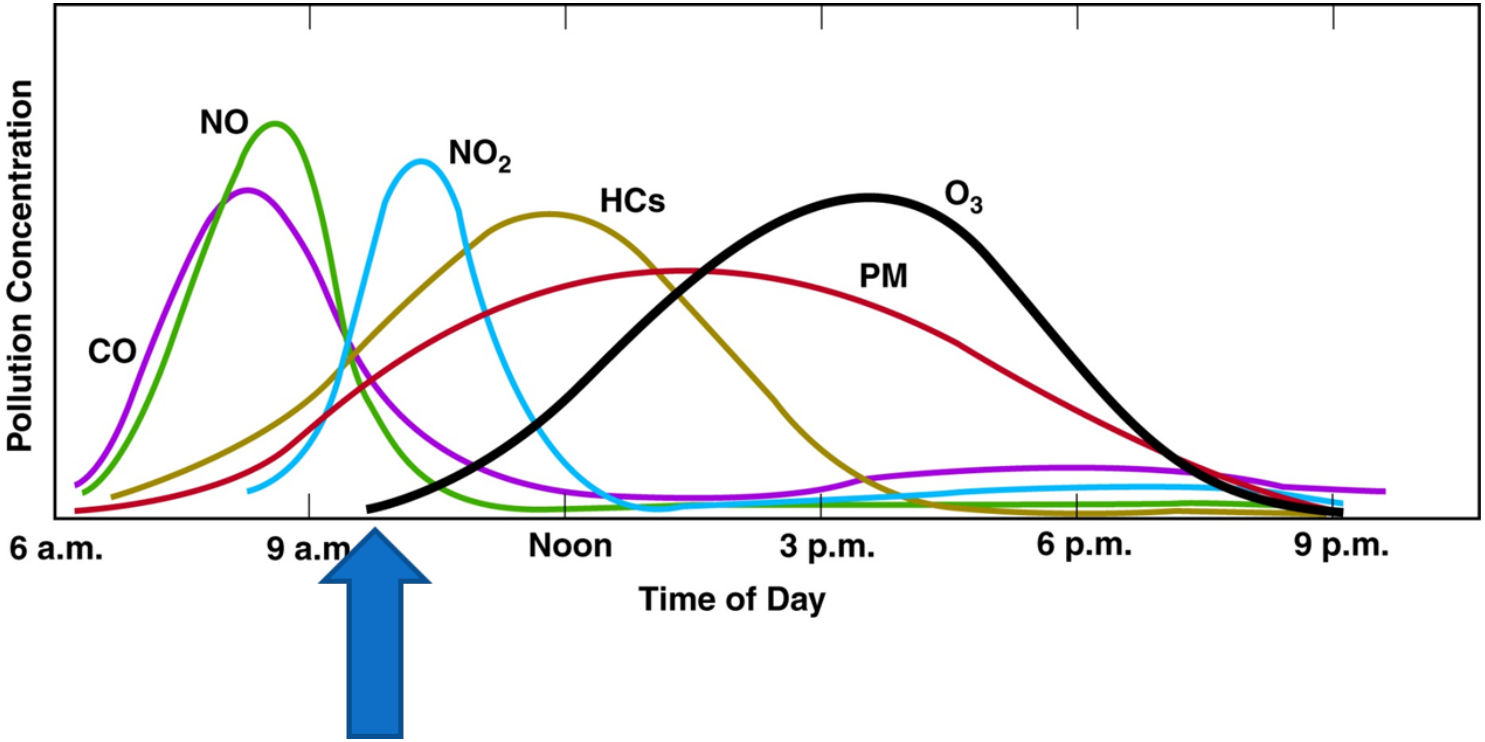
Satellite: Chemical Environment



GOME-2 captures light reflected from the Earth's surface.

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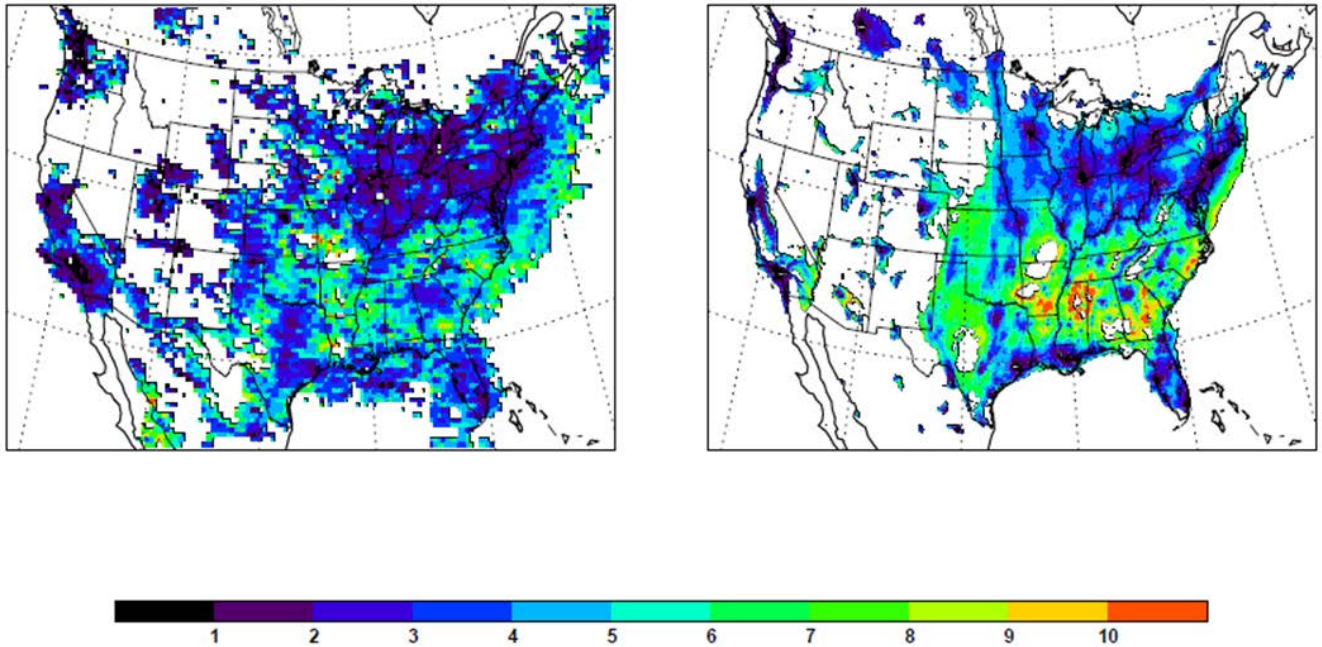
VOC/NO_x~GOME-2 HCHO/NO_2

GOME2 and CMAQ HCHO/NO_2 (unitless)



Ratio of HCHO/NO_2 is a proxy for VOCs/NO_x emissions or concentrations

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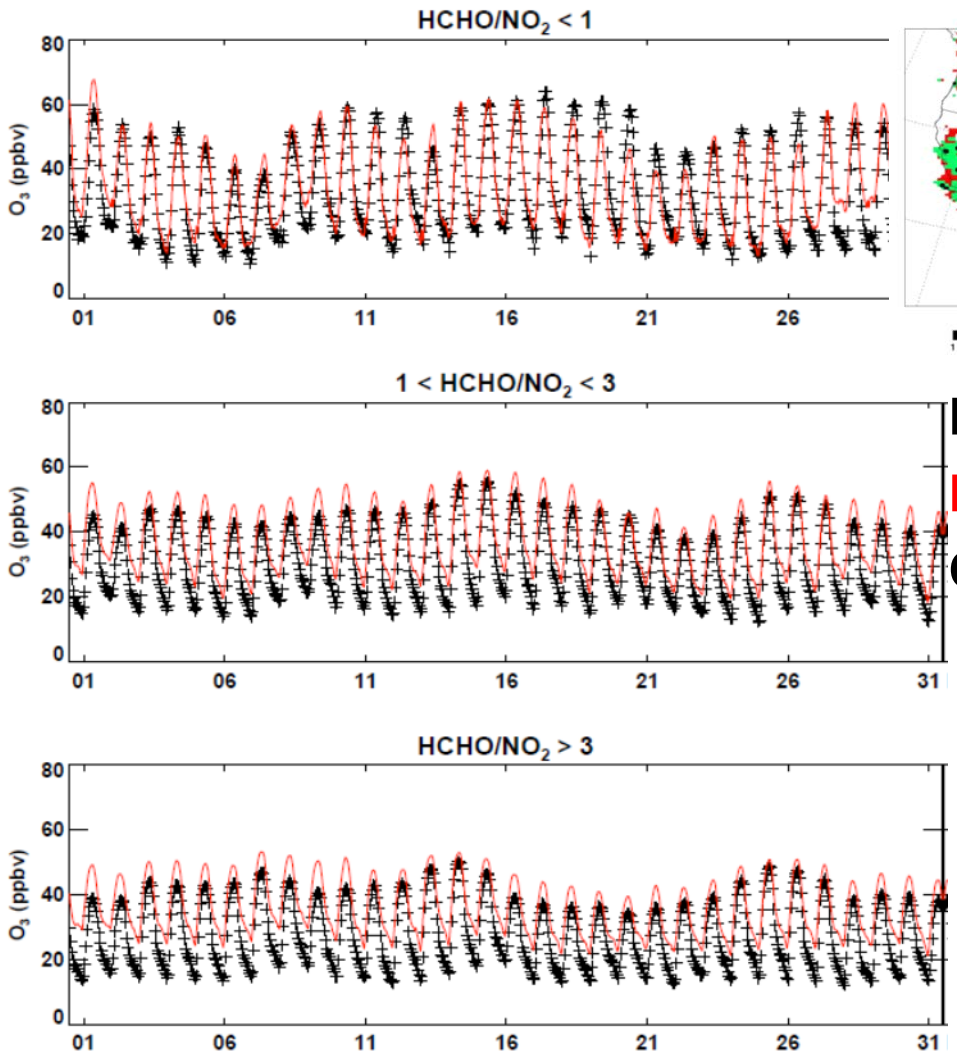
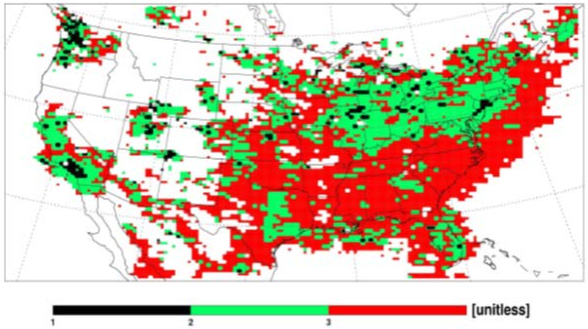
O_3 from EPA AQS and CMAQ





Black: EPA AQS

Red: CMAQ model

CMAQ over-predicts O_3 at EPA AQS stations over NO_x-sensitive regime ($HCHO/NO_2 > 3$).

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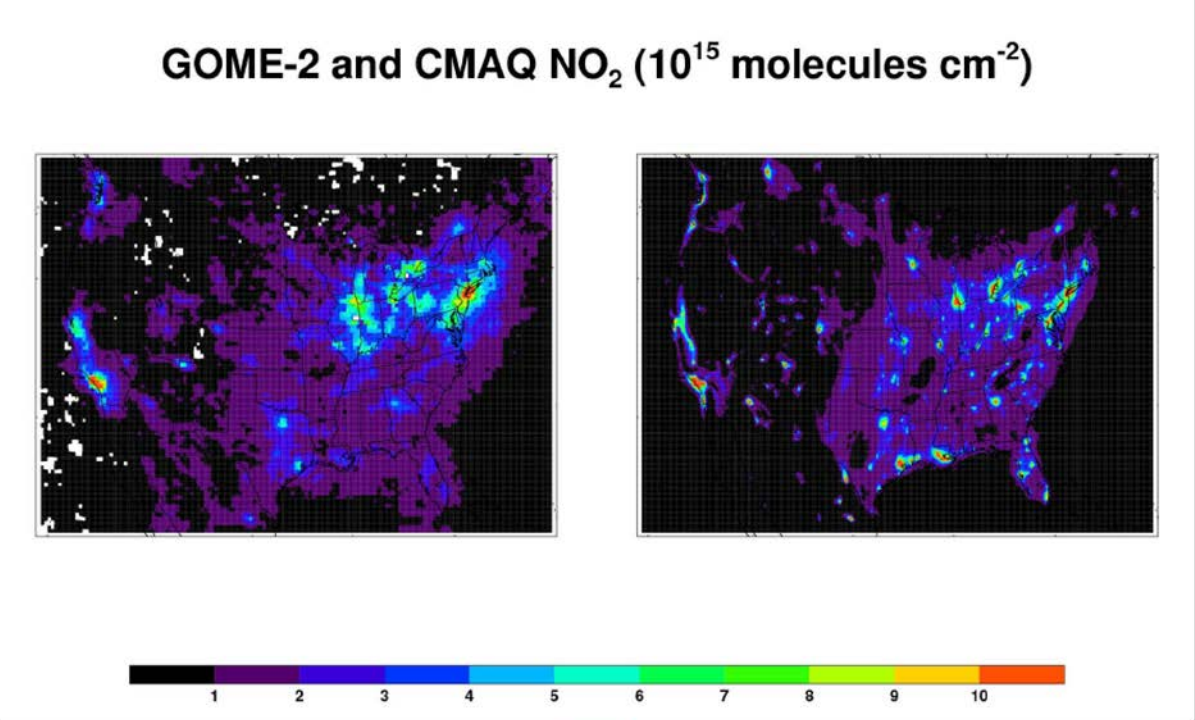
Uncertainty of NO_x



Uncertainty of NO_x emission inventory?

Which region has the largest uncertainty?

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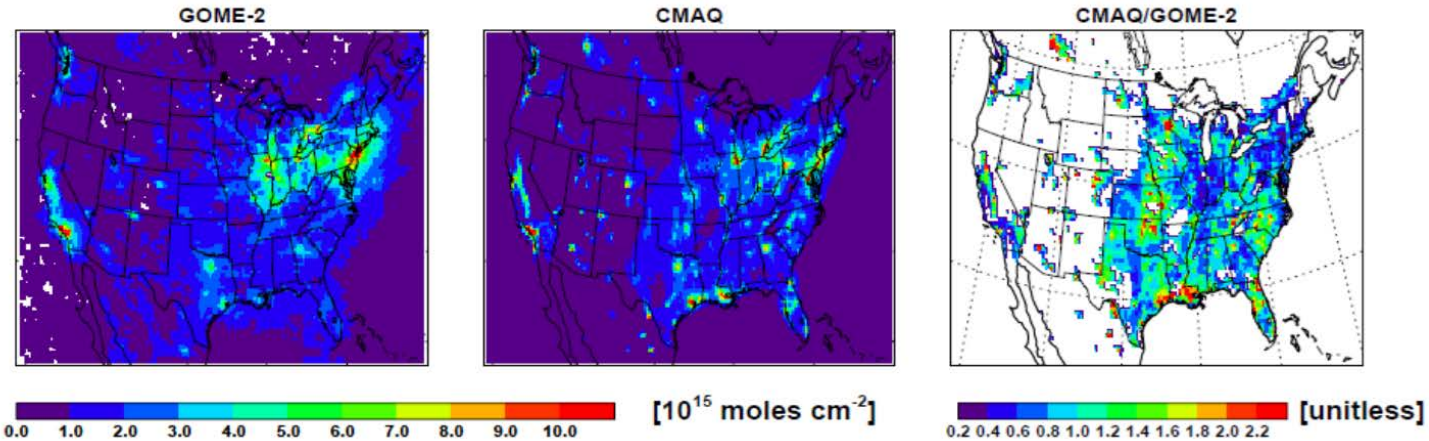
NO_2 from GOME-2 and CMAQ



[Choi et al. 2012, ACP]

CMAQ generally over-predicts NO_2 columns particularly over the urban areas of the Low Middle US, but under-predicts over some urban and rural areas.

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Satellite-adjusted NO_x emissions

- **Assuming that NO_x concentrations are proportional to NO_x emissions.**
- **NO_x emissions are scaled by comparing satellite and CMAQ NO_2 columns.**

New emission = emission X Ω(GOME-2)/Ω(CMAQ)

National Emission Inventory (NEI) 2005 → Modified emission inventory

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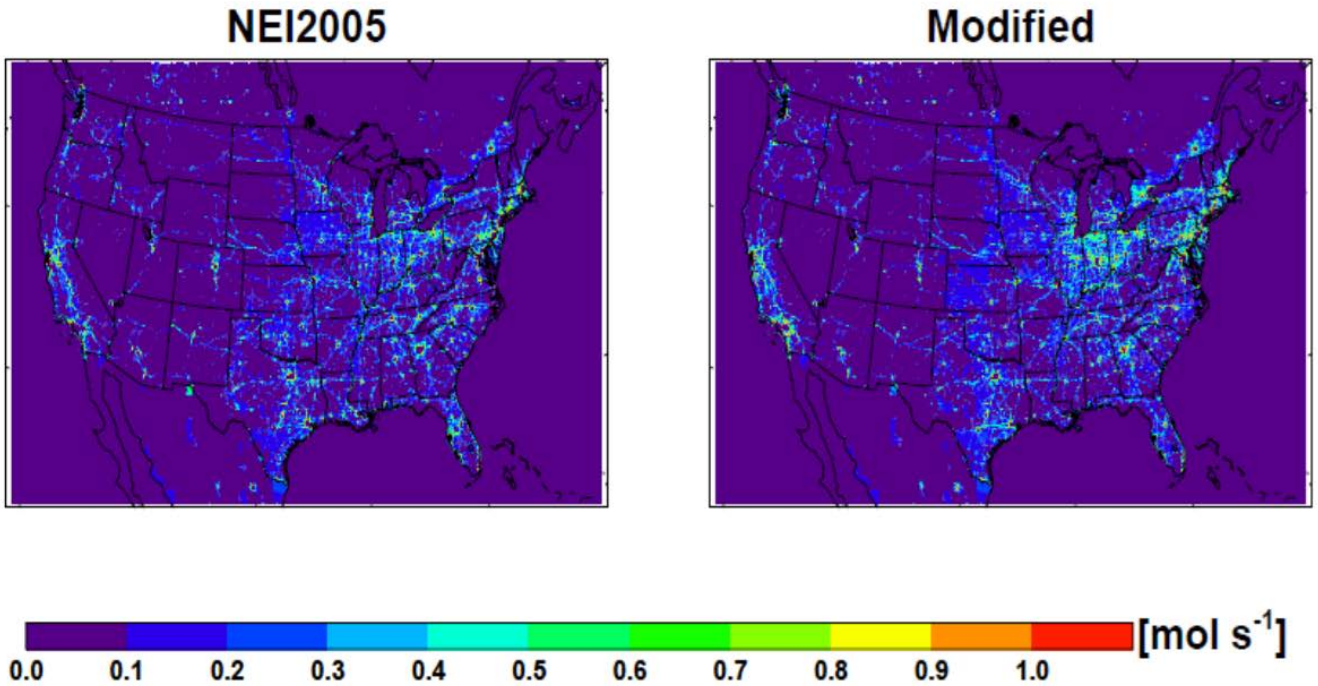
NEI2005 and Adjusted Emissions



NO emissions generally decrease over urban areas, but increase over some urban areas of Indiana, Illinois, and Pennsylvania and rural areas.

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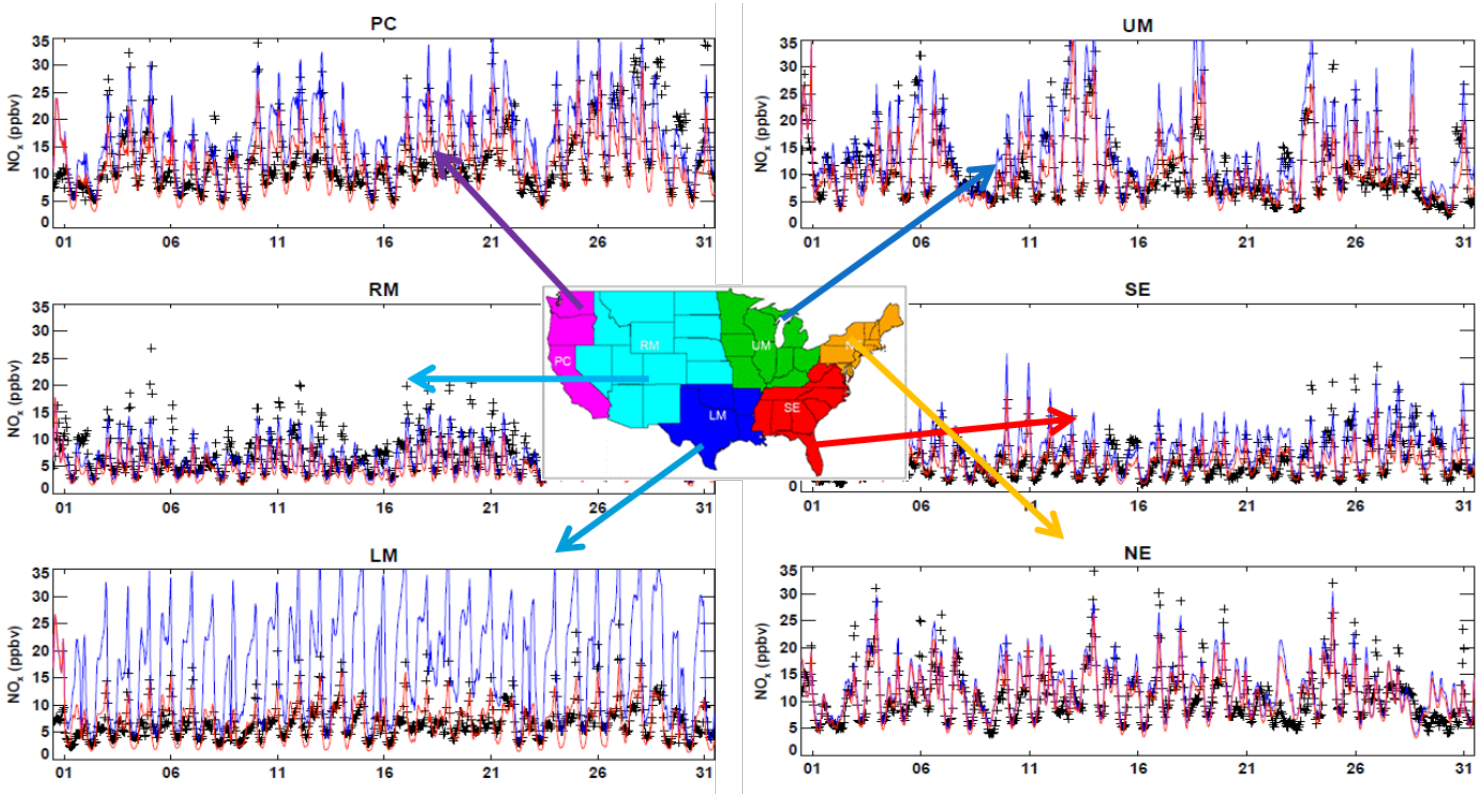
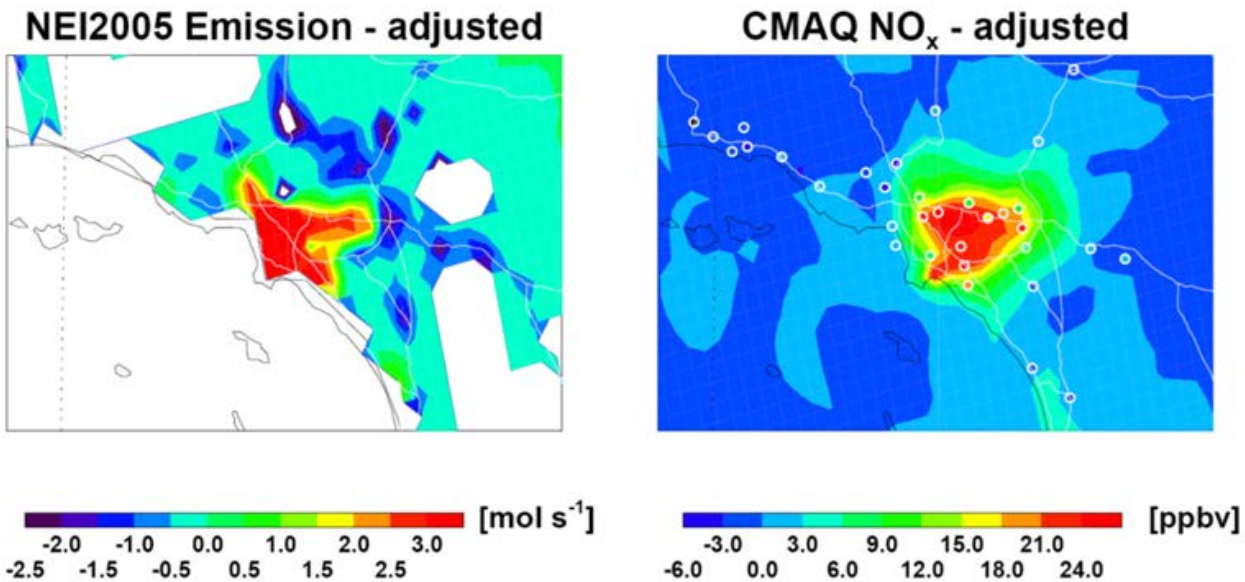
NEI2005 and Adjusted Emissions



NO_x emissions from NEI2005 over Low Middle US are high biased.

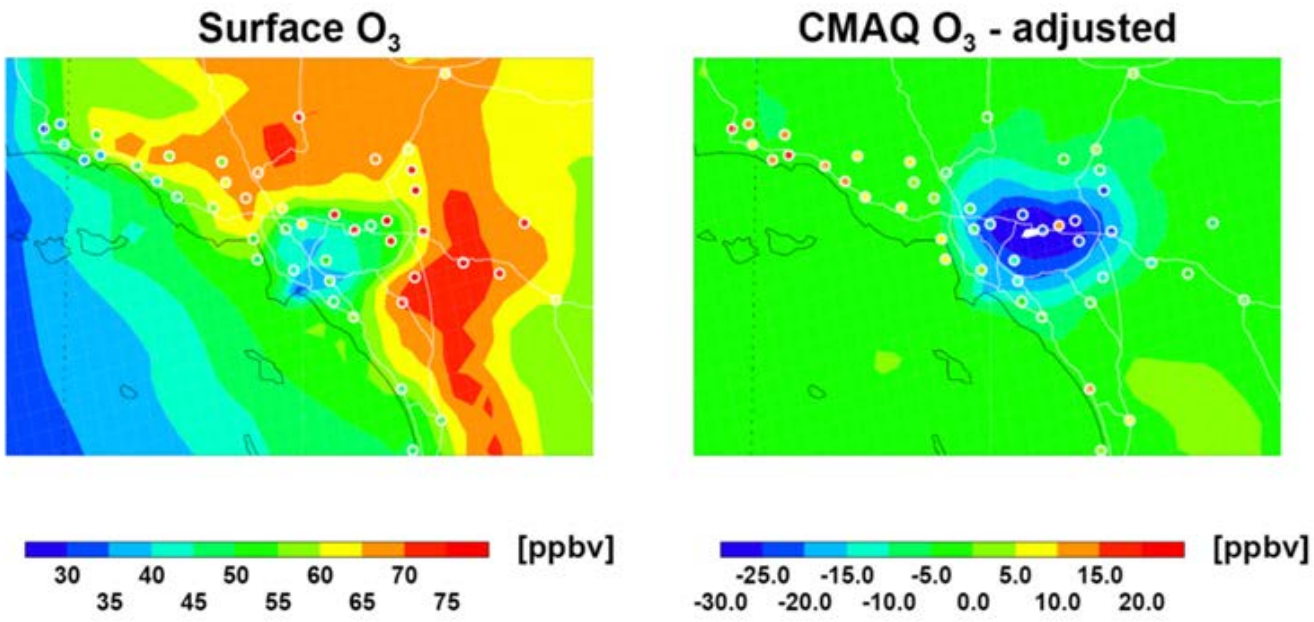
Case 1: NO_x study over Los Angeles



Circle: CMAQ – EPA NO_x observation

NO_x emission reduction mitigate the discrepancy between simulated and observed NO_x concentrations

Case 1: O_3 study over Los Angeles

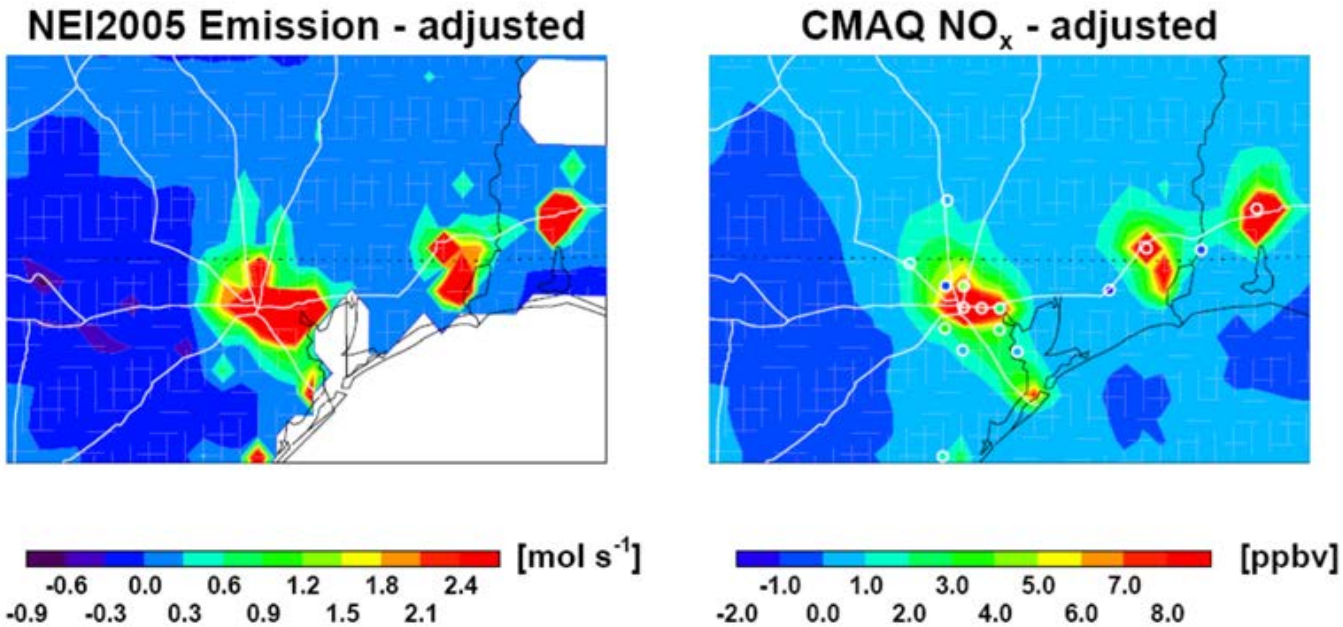


Circle: EPA O_3 observation

Circle: CMAQ – EPA O_3 observation

NO_x emission reduction mitigate the discrepancy between simulated and observed O_3 concentrations

Case 2: NO_x study over Houston



Circle: CMAQ – EPA NO_x observation

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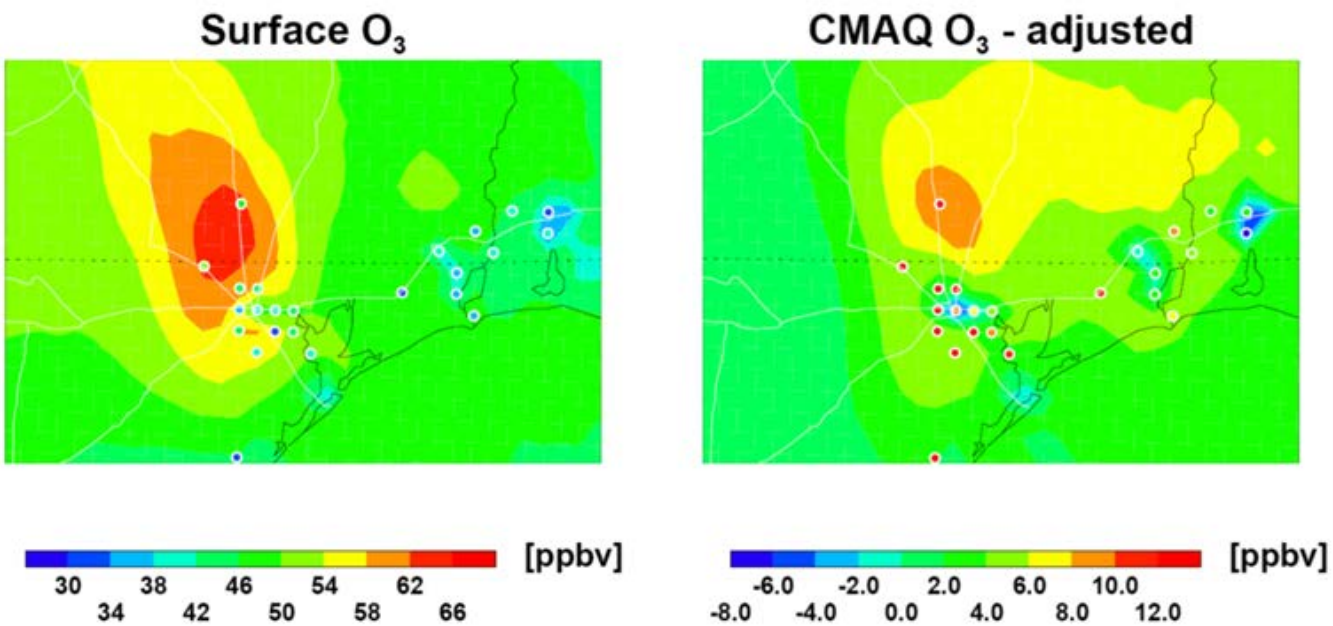
Case 2: O_3 study over Houston



Circle: EPA O_3 observation

Circle: CMAQ – EPA O_3 observation

NO_x emission reduction worsen the discrepancy between simulated and observed O_3 concentrations

Conclusion

- **The summer largest O_3 biased region is characterized as NO_x-sensitive regime.**
- **Uncertainty of EPA NEI 2005 is largest over the low middle US.**
- **CMAQ with GOME-2 derived NO_x emissions better captures in-situ observed NO_x and daytime O_3. However, we need to find another major cause for the O_3 bias.**

Star Trek Spock to UH spock.geosc.uh.edu

From www.startrek.com/database_article/spock

- **Affiliation: UHfleet Choi Government**
- **First name: Spock**
- **Posting: Air Quality Forecasting officer/first officer**
- **Rank: Main Node Commander**

- **Spock is helping UH modeling group for managing air quality forecasting system**

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Spock
192 processors
2 TB of system memory
60 TB of storage space
~ 200 k
Uses specialized (Xeon) processors. (e5-4640)
Uses about 40 Amps of power
~ 500 GFLOPS
Very dense, same space as about 3-4 pcs

To boldly go where no atmospheric chemist has gone before….

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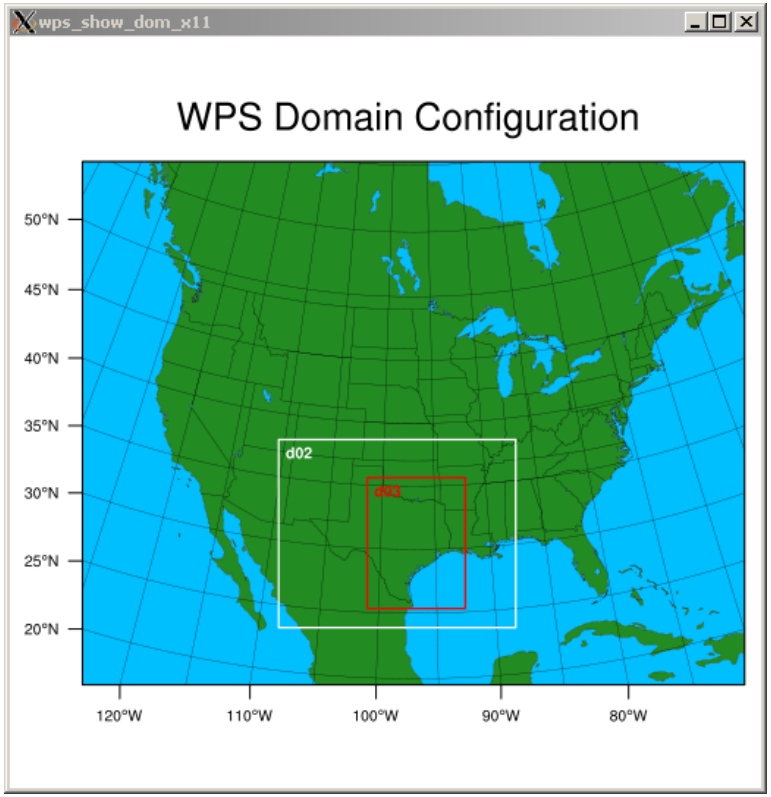
UH Air Quality Forecasting System



- **Forecasting domains based on WRF-CMAQ (Beata Czader) and WRF-Chem (Lijun Diao) (36-12-4km) and having a plan to go further (12-4-1.3km)**
- **If available, data assimilation is utilized using in-situ observed chemicals and lightning**

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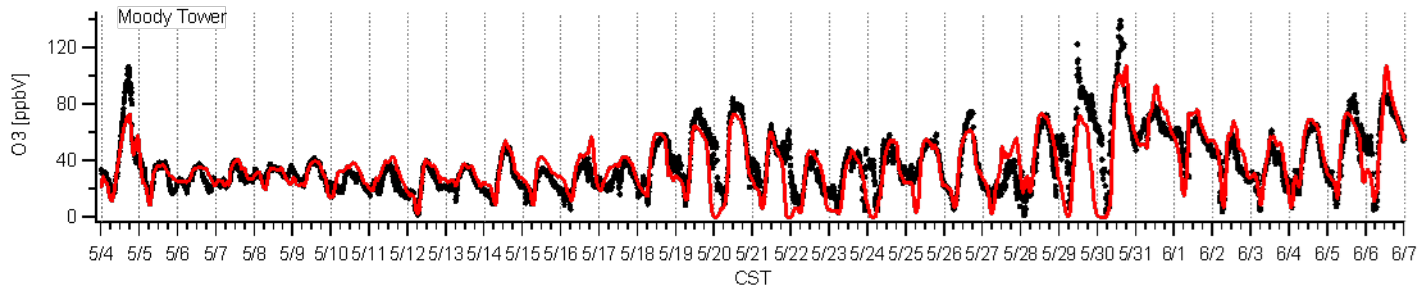
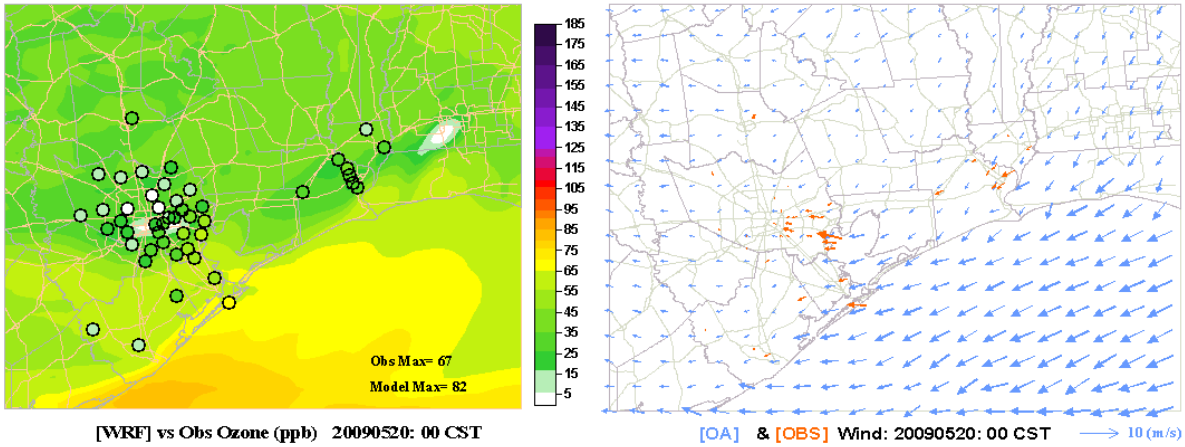
WRF-CMAQ FORECASTING SYSTEM





[Czader et al., preparation for publication]

- Beata Czader is performing QA/QC process of the WRF-CMAQ modeling system on 2000, 2006 and/or 2009 field campaigns and will do for 2013 DISCOVER-AQ
- Have a plan to implement TCEQ emissions over Texas

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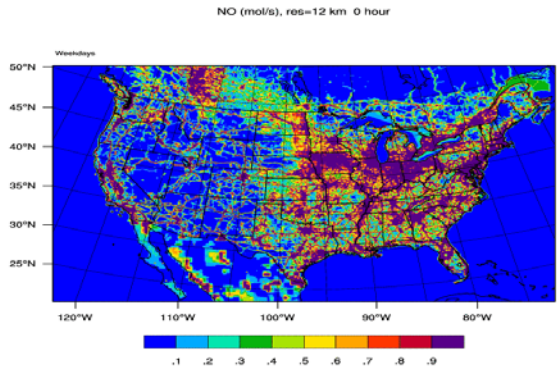
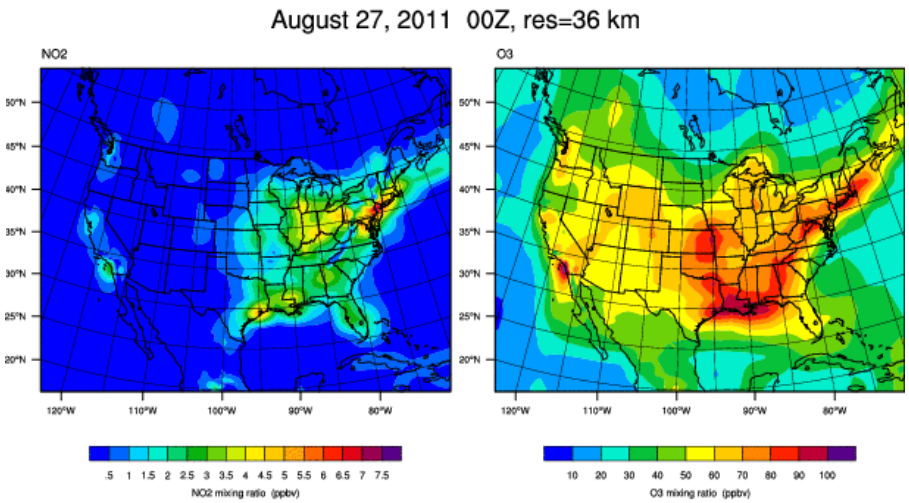
WRF-Chem forecasting system





- **Lijun Diao is performing QA/QC process of the WRF-Chem forecasting system on a big wildfire event over Texas (September-October, 2011) and will do for 2013 DISCOVER-AQ**
- **Have a plan to implement TCEQ emission over Texas**

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Air Quality Climate Forecasting System

NCAR WACCM Whole Atmosphere Community Climate Model

UH Chemical Transport Model
(troposphere [Choi et al., 2005] + greenhouse gases + stratosphere + mesosphere)

- **See the impact of climate change on atmospheric chemicals and vice versa**
- **TCEQ emissions will be used in UH CTM over Texas**

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From Wikipedia

Kirk/Spock collaboration makes miracles.

We are looking for collaborators like you.

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