Plume Chemistry Modeling with SCICHEM and CMAQ: Cumberland Power Plant on 6 July 1999

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Motivation

- A need exists for single-source modeling that accurately simulates secondary $PM_{2.5}$ and ozone formation
- The SCICHEM reactive plume model could potentially play a role in single-source applications for secondary pollutants
- However, tools for processing SCICHEM inputs/outputs must be developed and predictions thoroughly evaluated
- This study is a preliminary evaluation of a “pre-release” version of SCICHEM using in-plume observations
  - Information presented here is considered preliminary by the U.S. EPA and is provided to describe and illustrate potential approaches
  - Results could change due to improvements in the modeling tools through our ongoing development work

SCICHEM: Second-order Closure Integrated puff model with CHEMistry

- Plume represented by numerous puffs that are advected and dispersed independently according to local meteorology
- Second-order closure for integrating turbulent diffusion equation
  - Dispersion rate is related to velocity fluctuation statistics
- Puff merging/splitting to represent inhomogeneous meteorology
  - Puffs split when grow to value related to grid resolution
  - Puffs merge when overlap is significant
- Simulates chemical processes in gas, aerosol, and aqueous phases

TVA Cumberland Power Plant

Source: Steven Greenwood (Feb 2004)

- Located ~80 km NW of Nashville
  - Lat: 36°23'29" N, Lon: 87°39'17" W
- Consumes ~20,000 tons of coal per day
- Two coal-fired generating units with summer net capability of 2,386 MW
- Observations available from helicopter plume transects in July 1999
- Emissions (tons):

Species	1999	2010
NO_x	80,900	4,890
SO_2	15,920	11,430

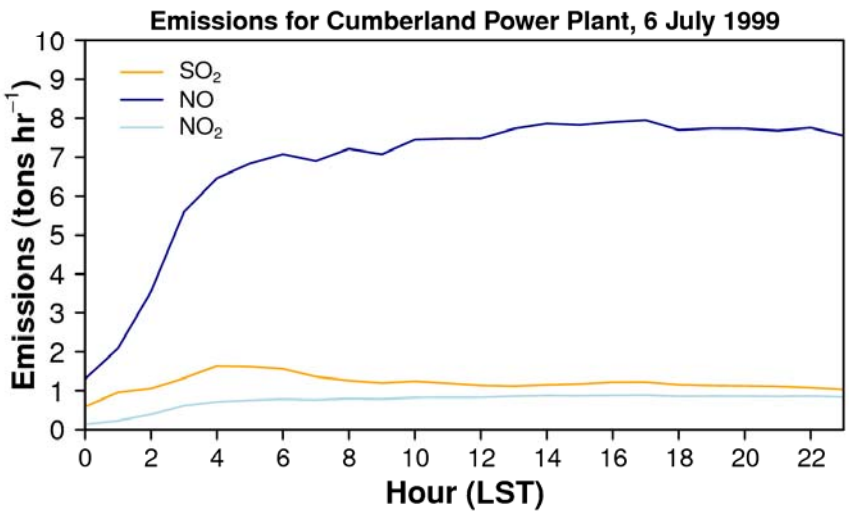
Source: http://www.tva.com/environment/air/cumb.htm

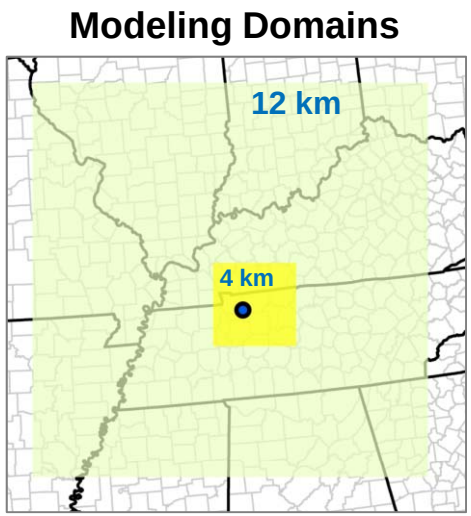
SCICHEM Modeling

- SCICHEMv2.1 configuration
  - Carbon Bond-IV gas-phase chemistry
  - MADRID aerosols w/ ISORROPIA inorganic thermodynamics
- Period
  - 1999 Nashville/Middle Tennessee Southern Oxidants Study
  - 6 July 1999 for hour 0-18 LST
- Cases
  1) **SCICHEM-WRF**
     - Meteorology: WRFv3.3 output converted to MEDOC format with MMIFv2.1
     - Background concentration: Time-varying based on CMAQ output
  2) **SCICHEM-DIAG**
     - Meteorology: Interpolated field based on observations from four stations provided in SCICHEM "pre-release" test-case files
     - Background concentration: Constant values from SCICHEM "pre-release" test-case files with O_3=60 ppb and SO_2=0.5 ppb
- Emissions
  - Hourly emissions of NO, NO_2, SO_2, etc. based on CEM data (see next slide)

CMAQ Modeling

- Community Multiscale Air Quality (CMAQ) model version 4.7.1
- 2001 National Emissions Inventory anthropogenic emissions
- 1999 hour-specific biogenic emissions estimated with BEIS model
- 1999 hour-specific CEM data for TVA Cumberland plant emissions
  - http://camddataandmaps.epa.gov/gdm/index.cfm?fuseaction=emissions.wizard

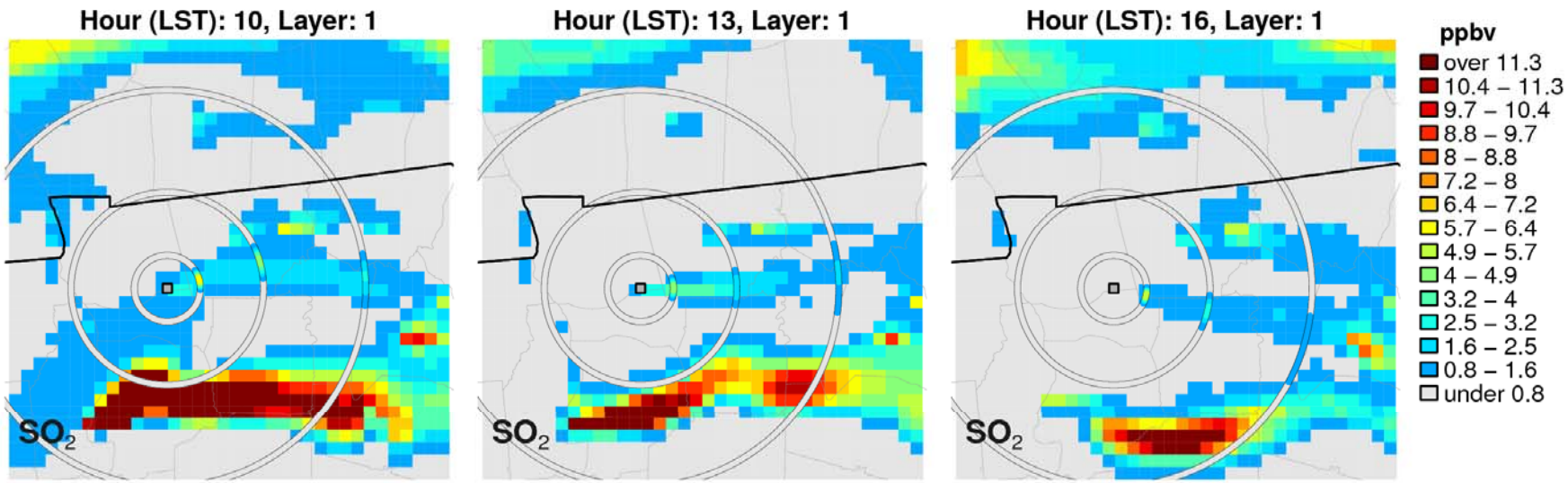




Comparison of Absolute Concentrations: CMAQ and SCICHEM-WRF

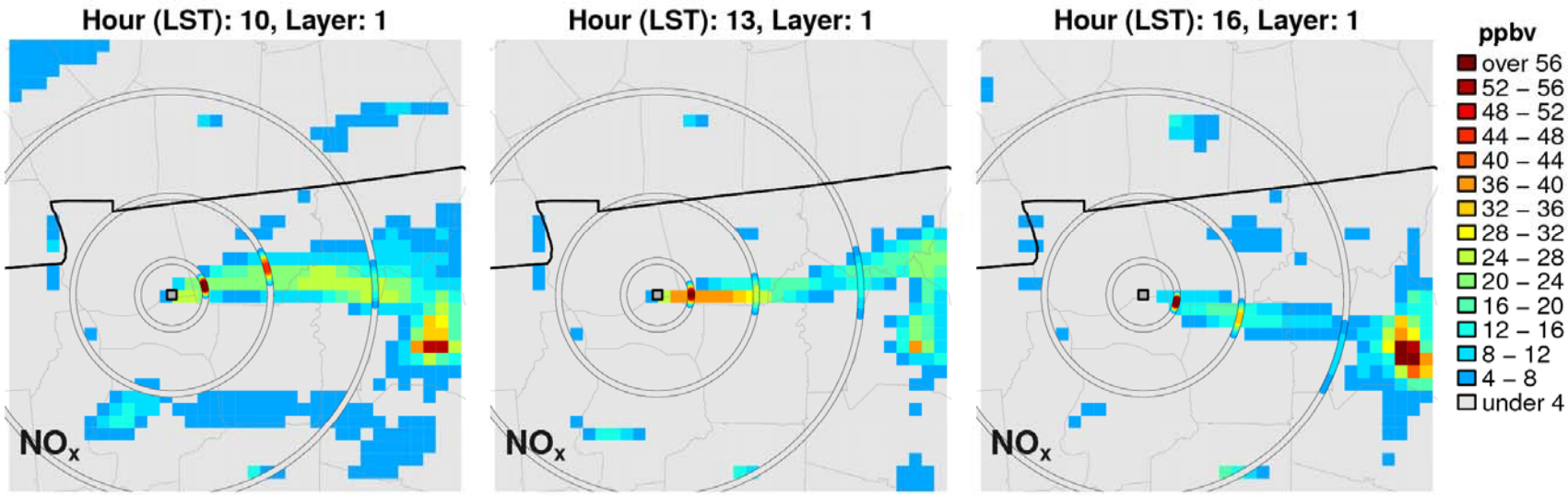
- *Overlay SCICHEM-WRF predictions at receptor rings onto CMAQ spatial concentration fields*

SO_2 Concentration:
CMAQ and SCICHEM-WRF



Preliminary results; subject to change

NO_x Concentration:
CMAQ and SCICHEM-WRF

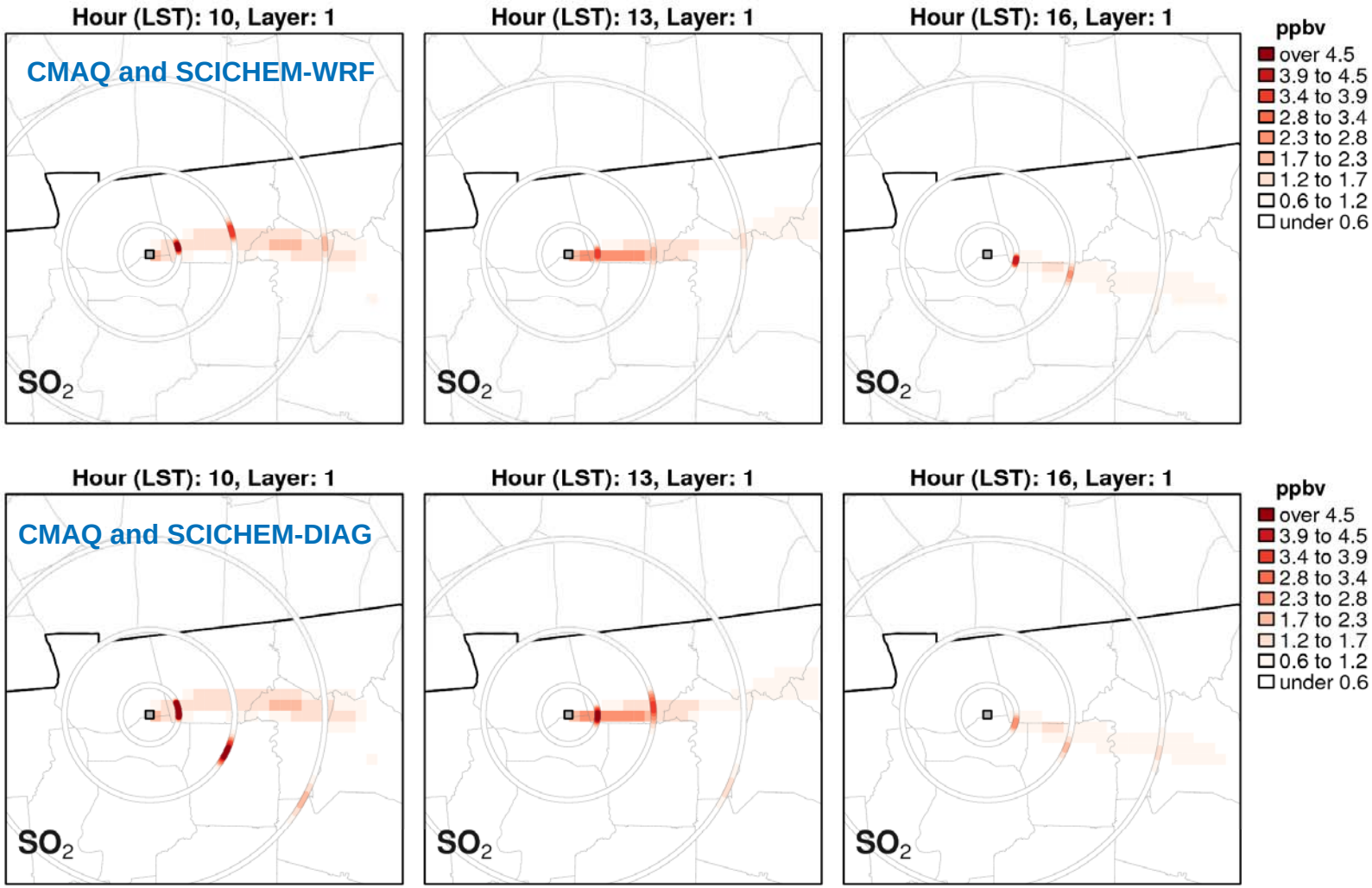


Preliminary results; subject to change

Comparison of Plume Concentrations: CMAQ, SCICHEM-WRF, SCICHEM-DIAG

- *Estimate plume concentrations for CMAQ and SCICHEM by subtracting zero-out predictions from base-case predictions*
- *Overlay SCICHEM plume concentrations at receptor rings onto CMAQ plume-concentration fields*

SO_2 Difference (Base - Zero out):
CMAQ, SCICHEM-WRF, SCICHEM-DIAG



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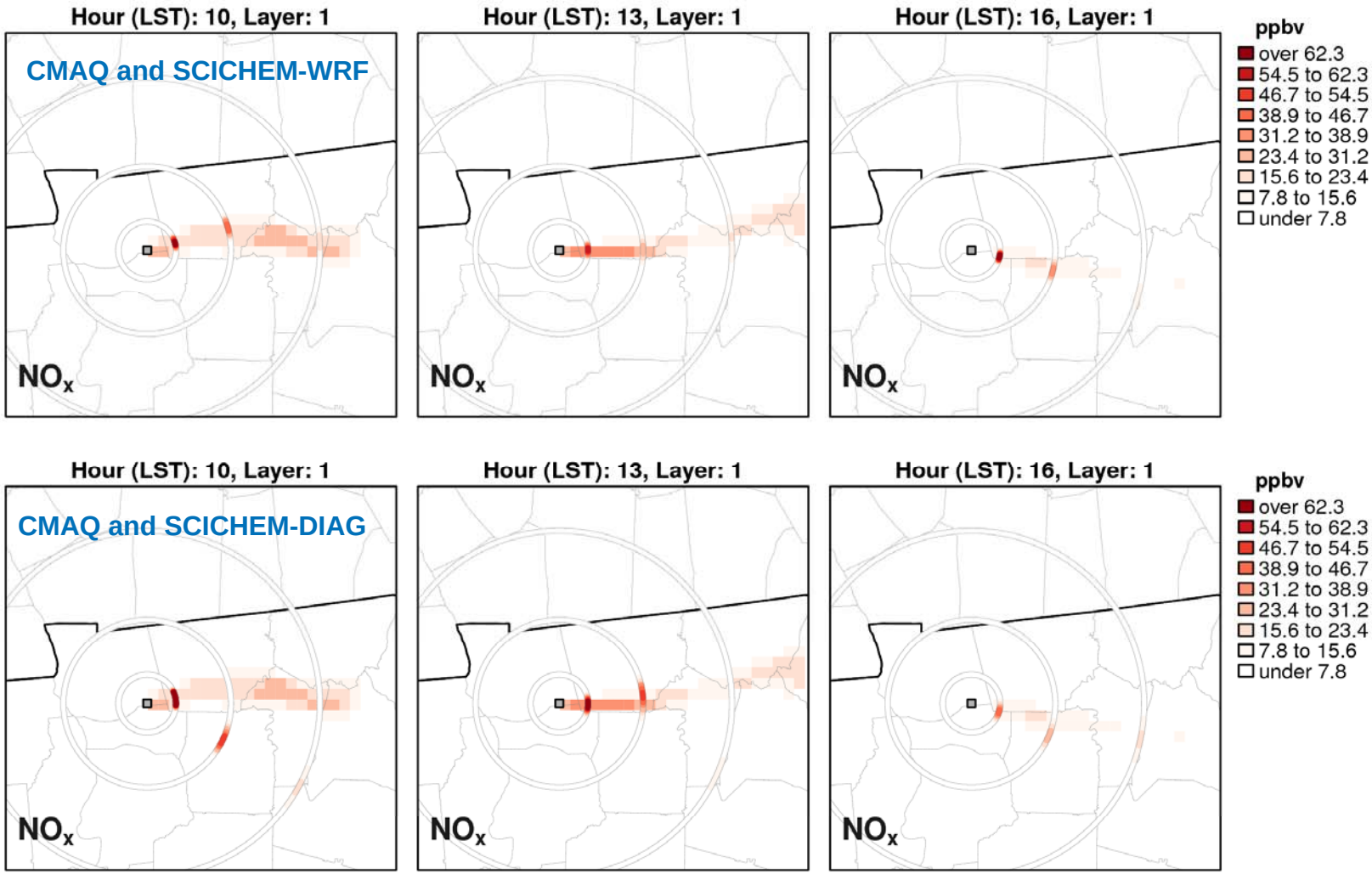
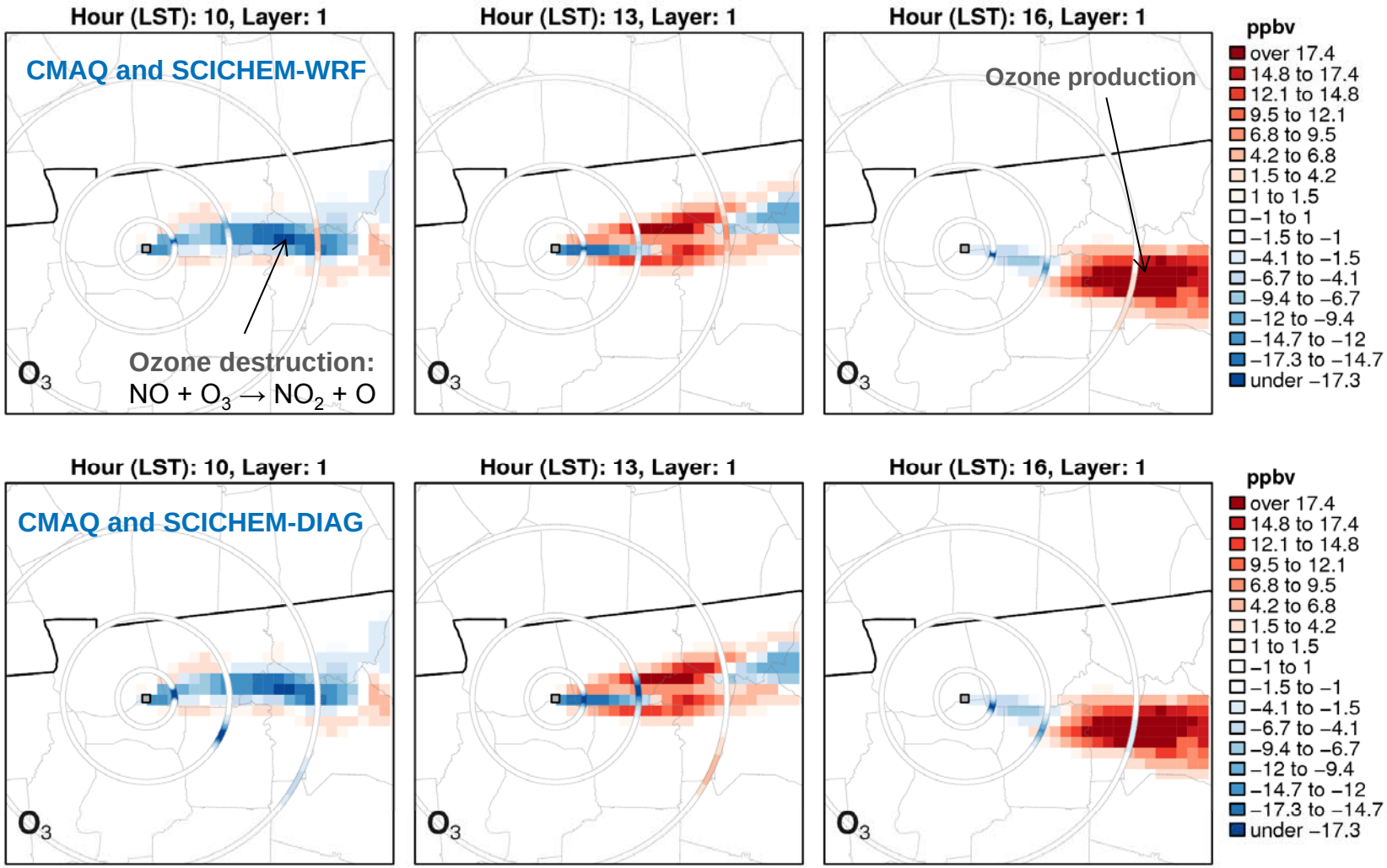
NO_x Difference (Base - Zero out):
CMAQ, SCICHEM-WRF, SCICHEM-DIAG



Preliminary results; subject to change

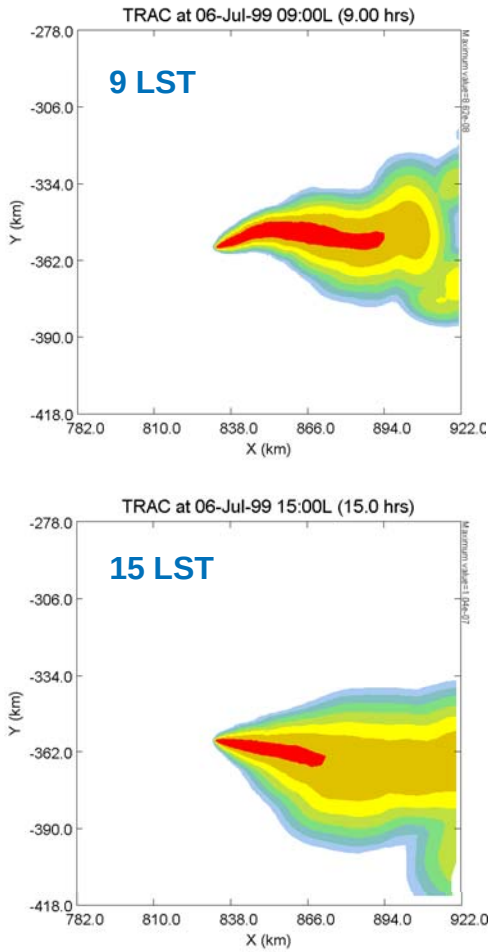
O_3 Difference (Base - Zero Out):
CMAQ, SCICHEM-WRF, SCICHEM-DIAG



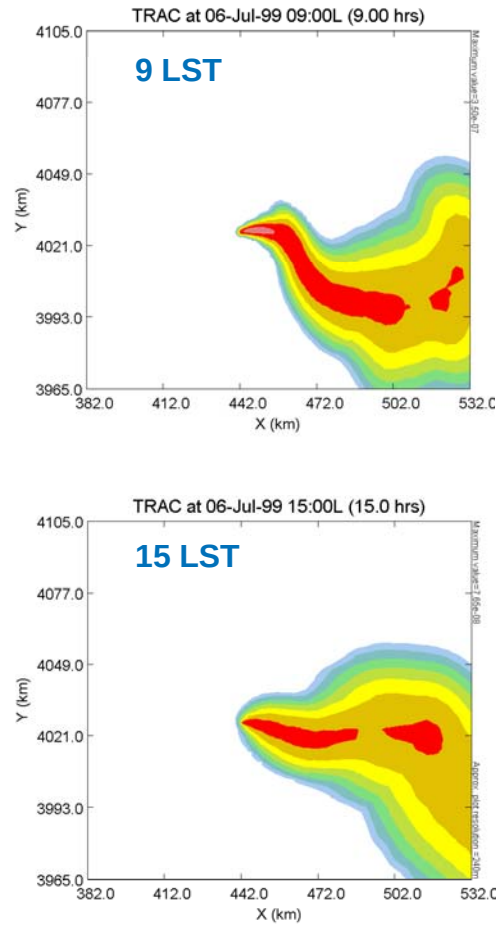
Preliminary results; subject to change

Surface Tracer Concentration:
SCICHEM-WRF and SCICHEM-DIAG

SCICHEM-WRF



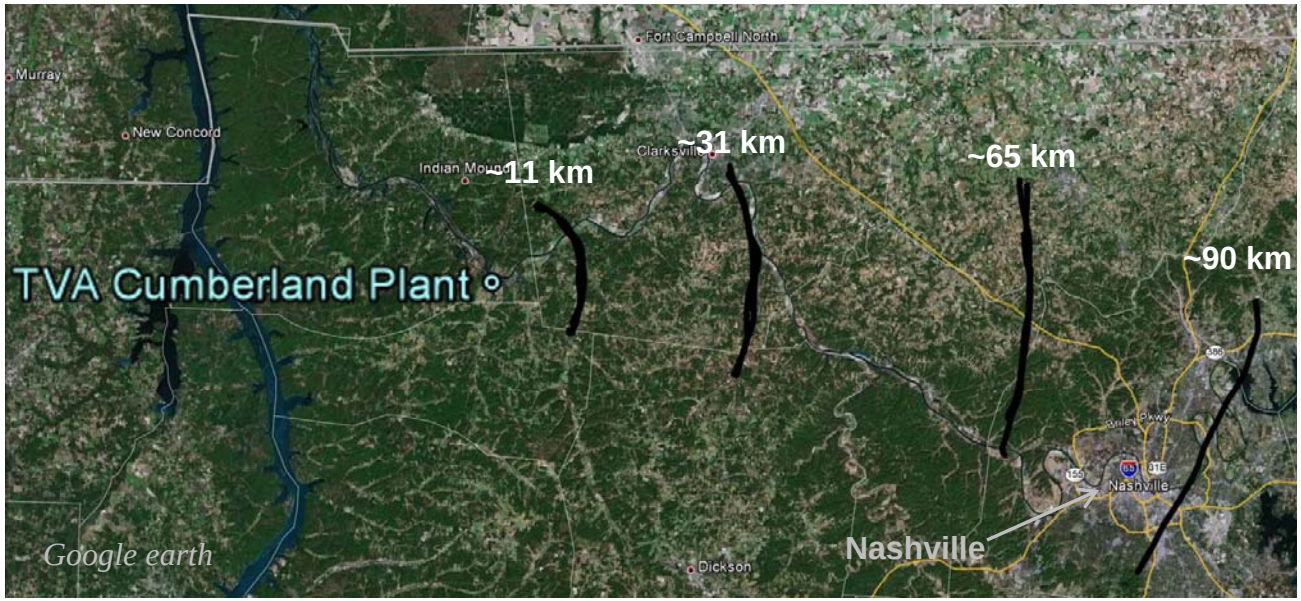
SCICHEM-DIAG



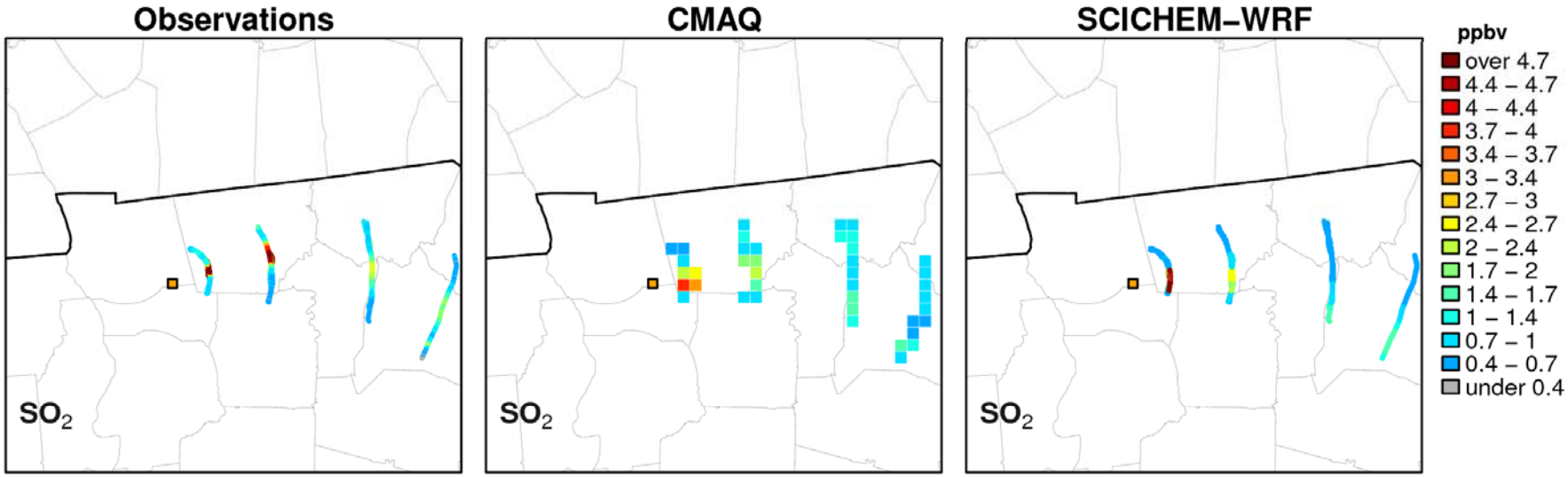
Preliminary results; subject to change

TVA Bell 205 Helicopter Observations

- 12 traverses of plume downwind of the TVA power plant on 6 July 1999 at an average altitude of 500 m
  - Clear day with light winds from west/northwest
- Observed species in include O_3, NO, NO_2, and SO_2

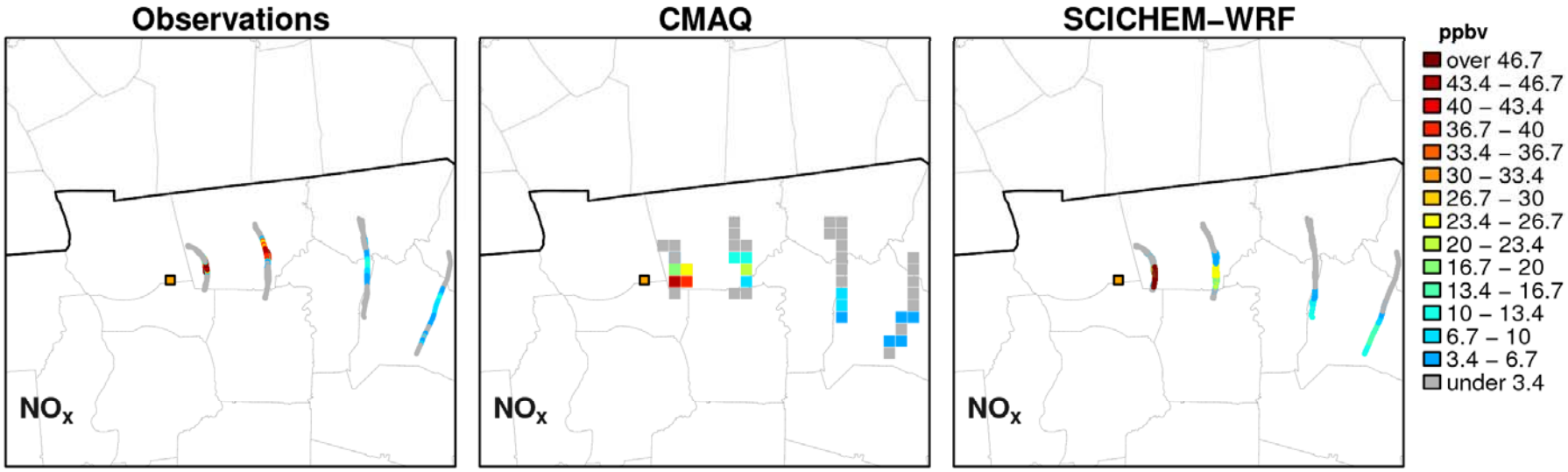


SO_2 for Plume Transects on July 6th



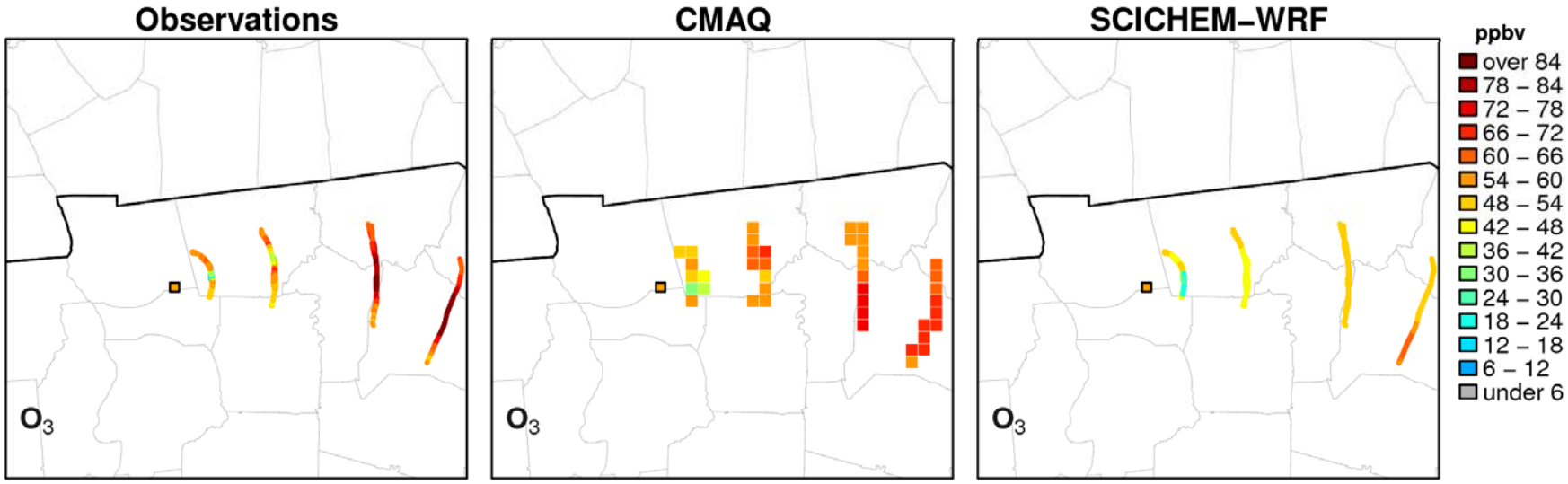
Preliminary results; subject to change

NO_x for Plume Transects on July 6th



Preliminary results; subject to change

O_3 for Plume Transects on July 6th



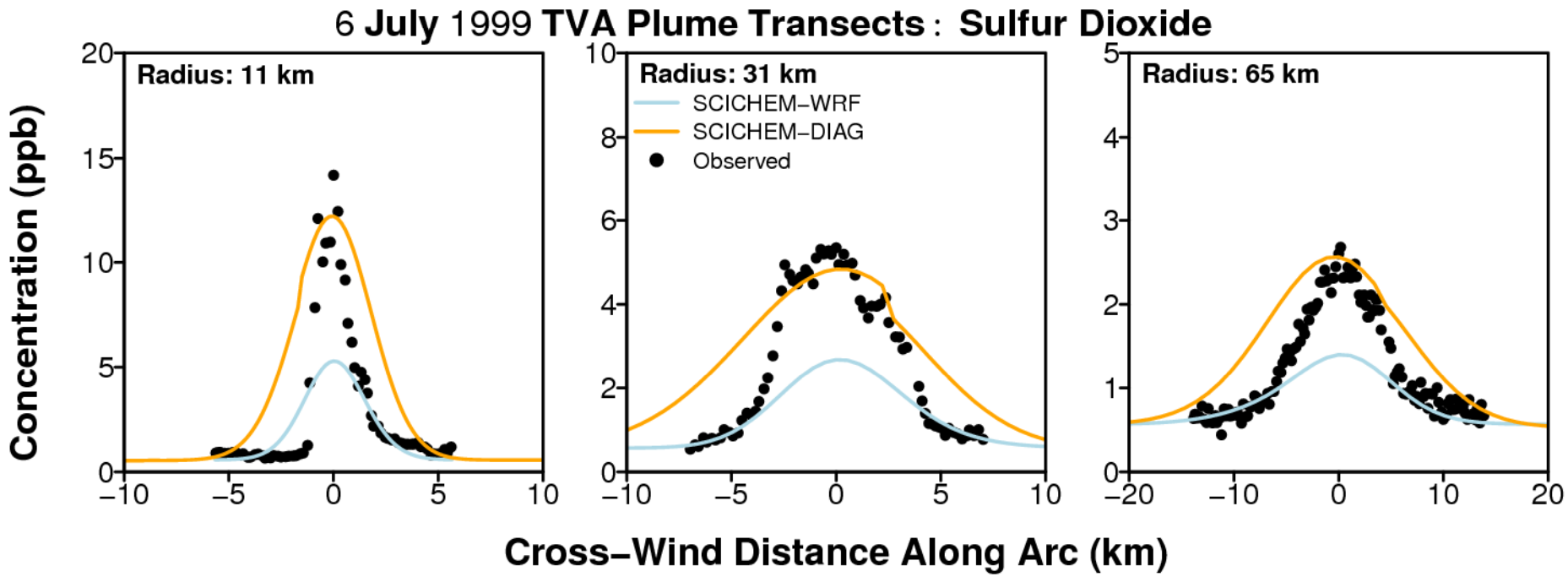
Preliminary results; subject to change

Comparison of Centered Profiles: Observed, SCICHEM-WRF, SCICHEM-DIAG

- *Find max/min in concentration along plume transect or receptor arc*
- *Center concentrations to max/min value*
- *Compare centered profiles for model and observations*

SO_2 Centered Profiles

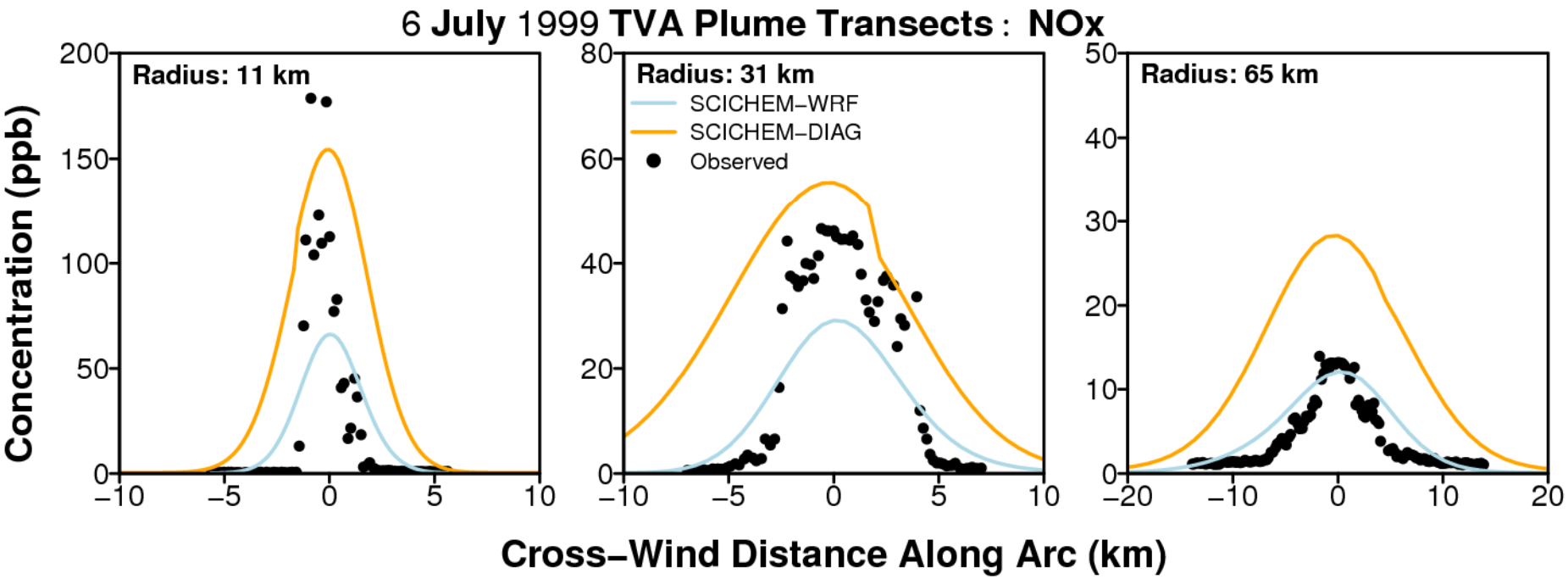
Observations, SCICHEM-WRF, SCICHEM-DIAG



Preliminary results; subject to change

NO_x Centered Profiles

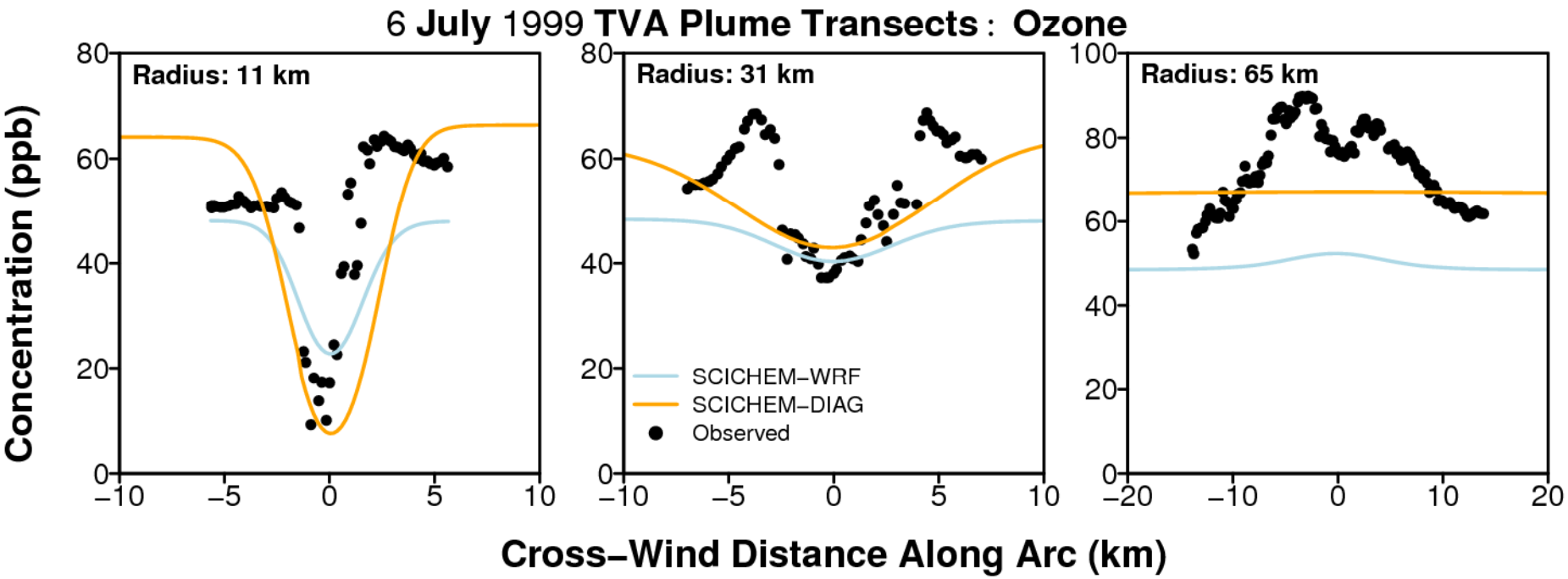
Observations, SCICHEM-WRF, SCICHEM-DIAG



Preliminary results; subject to change

O_3 Centered Profiles

Observations, SCICHEM-WRF, SCICHEM-DIAG



Preliminary results; subject to change

Summary of Preliminary Work

- Preliminary tools were developed for using SCICHEM
  - Process model inputs/outputs
  - Compare SCICHEM results with CMAQ results and observations
- SCICHEMv2.1 and CMAQv4.7.1 simulations were conducted for 6 July 1999 TVA Cumberland Plant case
- Reasonable model behavior was observed, e.g.,
  - Elevated SO_2 and NO_x concentration in plume
  - SO_2 and NO_x concentration profiles broaden and have lower peaks in afternoon and further from source due to dilution
  - O_3 titration in NO_x-rich, VOC-poor plume; O_3 production far from source
  - SCICHEM and CMAQ predictions are qualitatively similar

Preliminary results; subject to change

Next Steps

- Explore the impact of different treatments of ambient background concentrations in SCICHEM
- Extend the study to consider NO_x oxidation products (i.e., NO_z), $PM_{2.5}$, and vertical profiles
- Consider additional plume observation studies
- Compare with CMAQ-APT (Advanced Plume Treatment) when available
- Simulate longer periods and larger domains

Preliminary; subject to change

Acknowledgments

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