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SCICHEM:
A Puff Model with Chemistry

Part 2: Ozone and Particulate Matter

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SCICHEM Full Chemistry Description

- Full treatment of chemistry and dry and wet deposition, similar to treatments in photochemical grid models, such as CMAQ and CAMx
- CB05 gas-phase chemistry
- CMAQ AERO5 aerosol module, including ISORROPIA and SOA modules
- RADM aqueous-phase chemistry

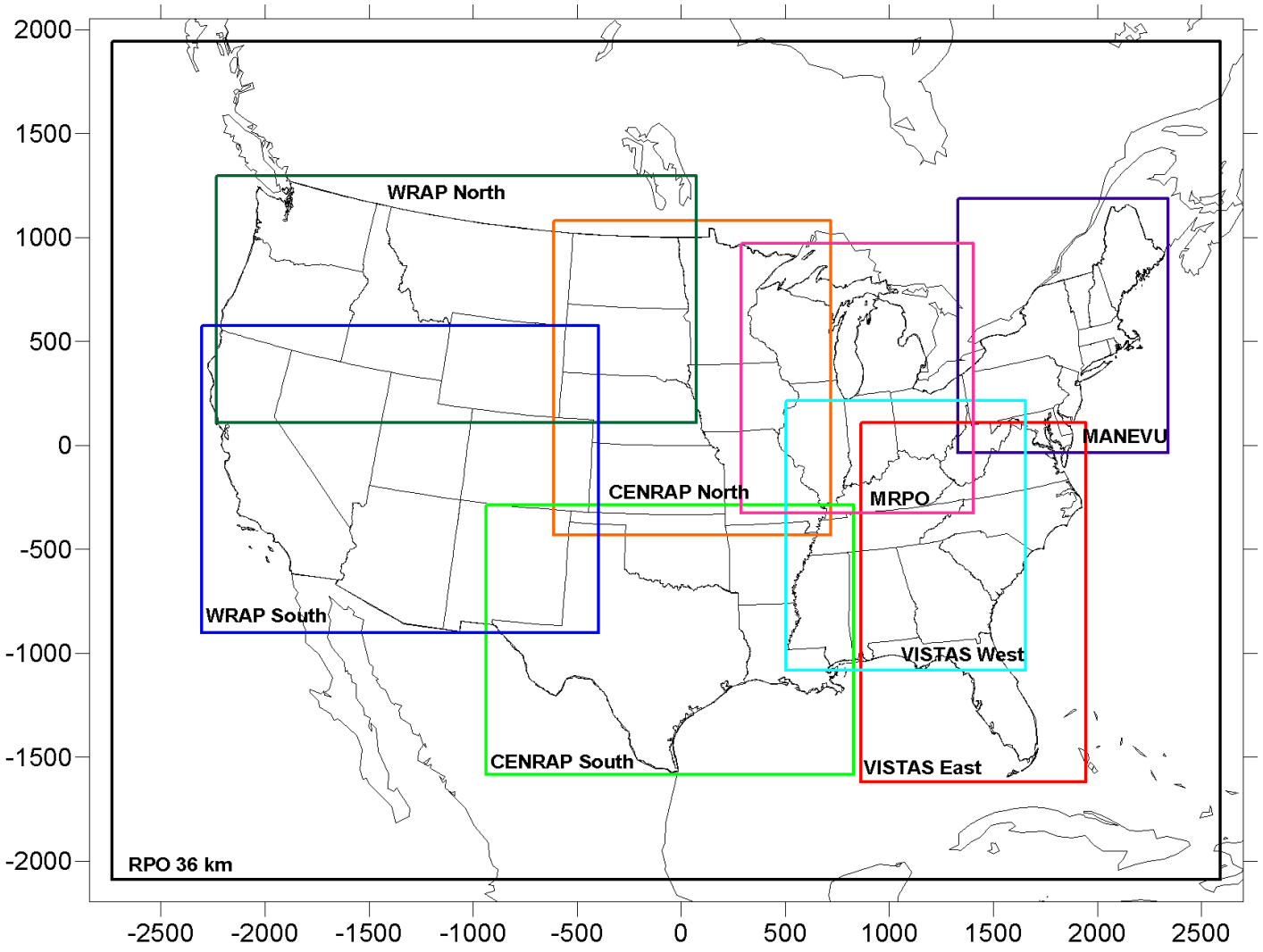
SCICHEM for Secondary Pollutants (Long-Range Applications)

- **Evaluation Study**
  - Model evaluation for reactive gases using aircraft plume measurements, e.g., Cumberland plume
- **Regulatory Applications**
  - Single-source Class I area impact studies, e.g., Four Corners
- Background chemistry based on grid model (CMAQ) simulation results

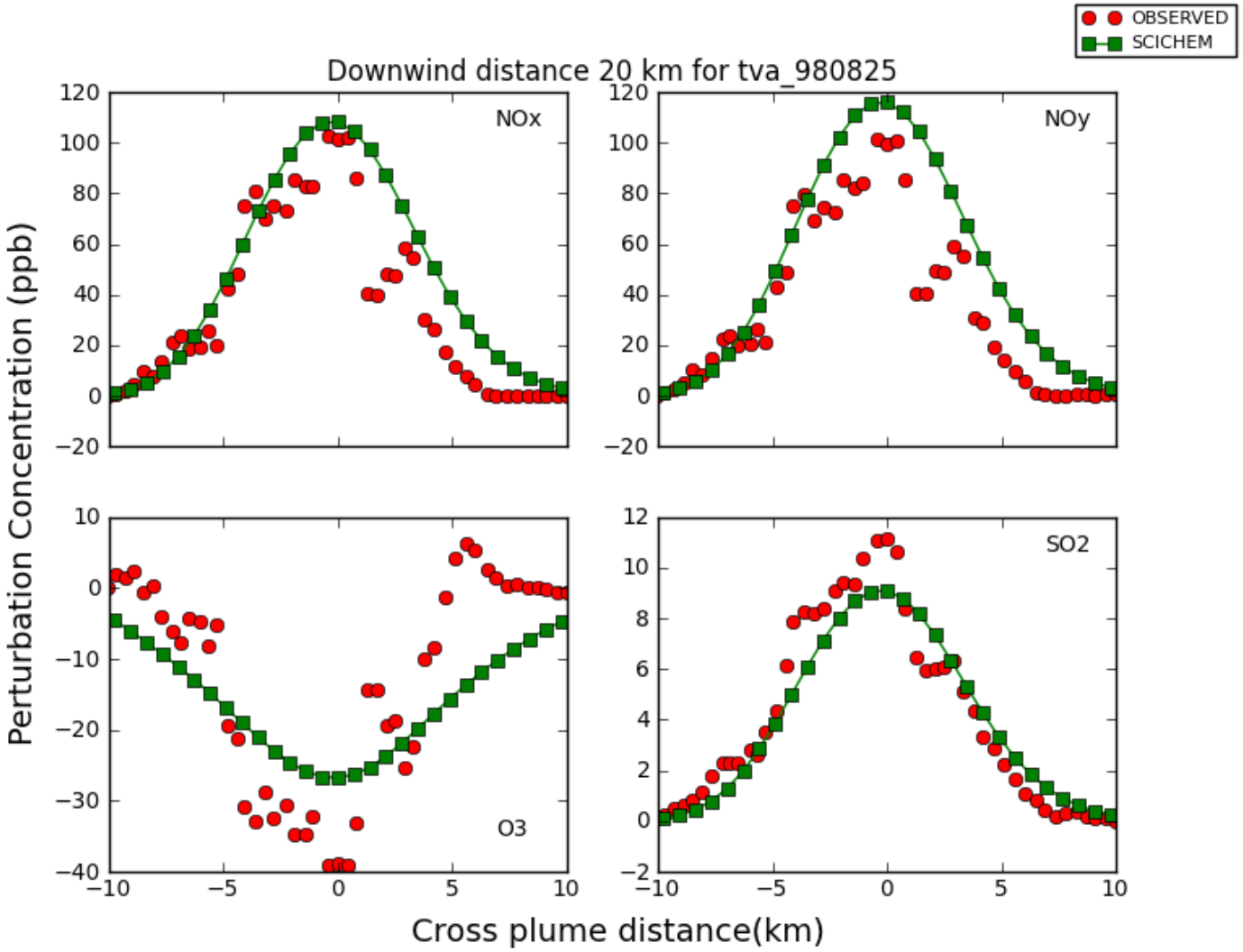
Background Chemistry Specification

- Monthly average, diurnally varying ambient concentration files generated for a representative year for eight regions of the contiguous US (CONUS)
  - Regions based on the Regional Planning Organizations (RPOs) modeling domains
- Calculated from a 36 km CONUS simulation with CMAQ, using the 2005 inputs for the Cross-State Air Pollution Rule (CSAPR)
  - The CMAQ results are horizontally averaged over a given region and hourly varying concentrations are provided for three vertical layers (0 to 300 m, 300 to 1000 m, and 1000 to 3000 m) for each month
- Two other options:
  - Constant values for all background species
  - Prescribe full 4-D background derived from a photochemical model simulation

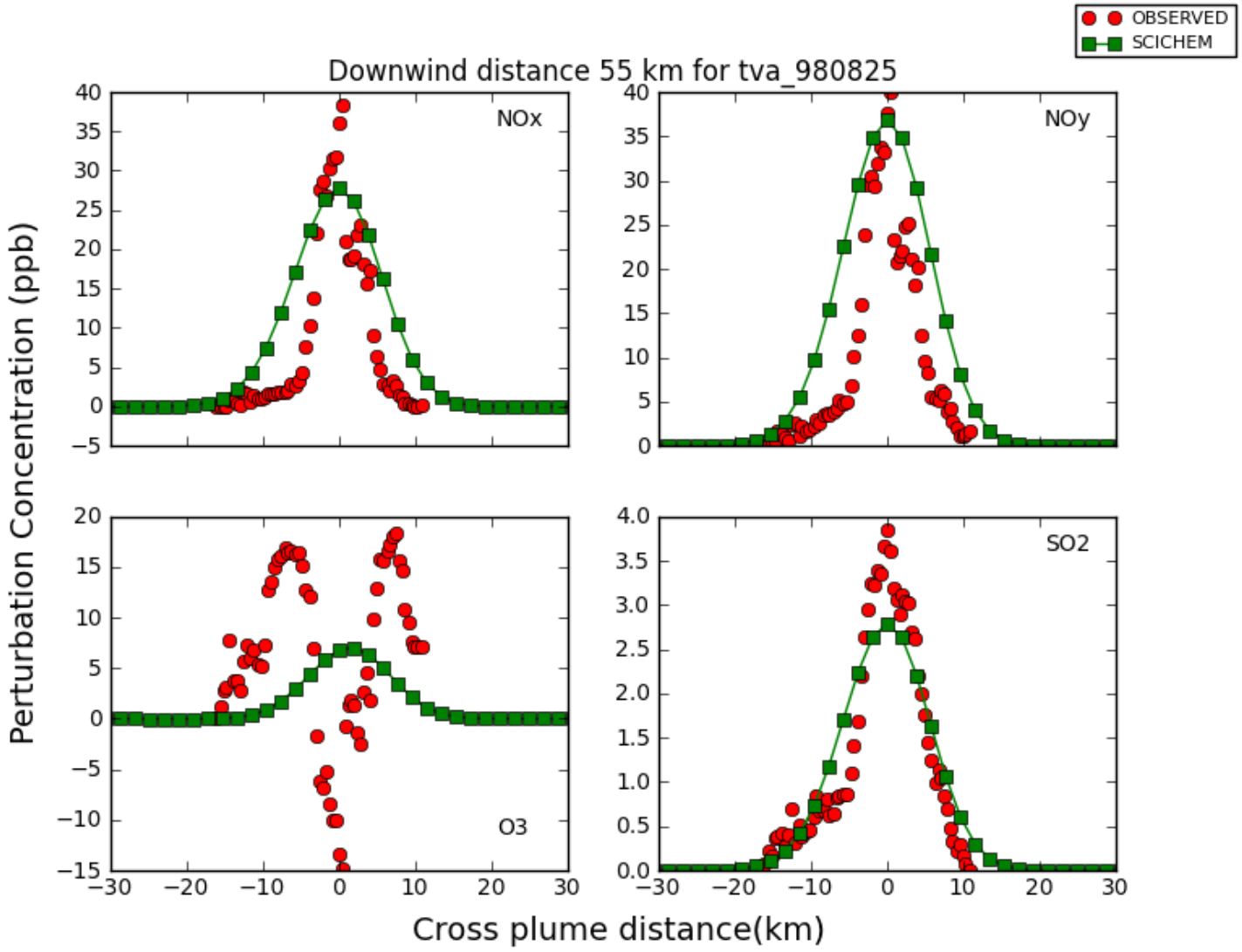
Background Chemistry Regions



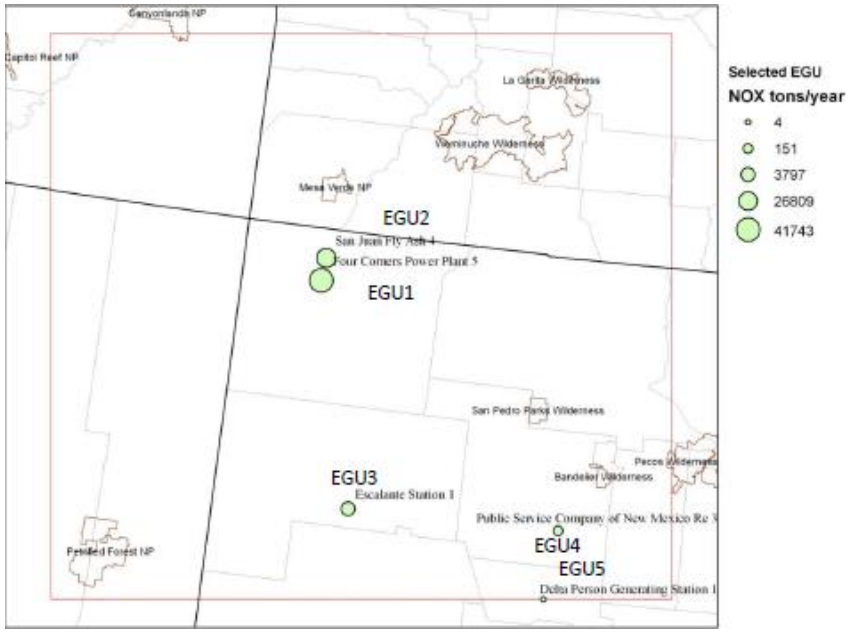
Cumberland Plume Comparisons at 20 km Downwind



Cumberland Plume Comparisons at 55 km Downwind

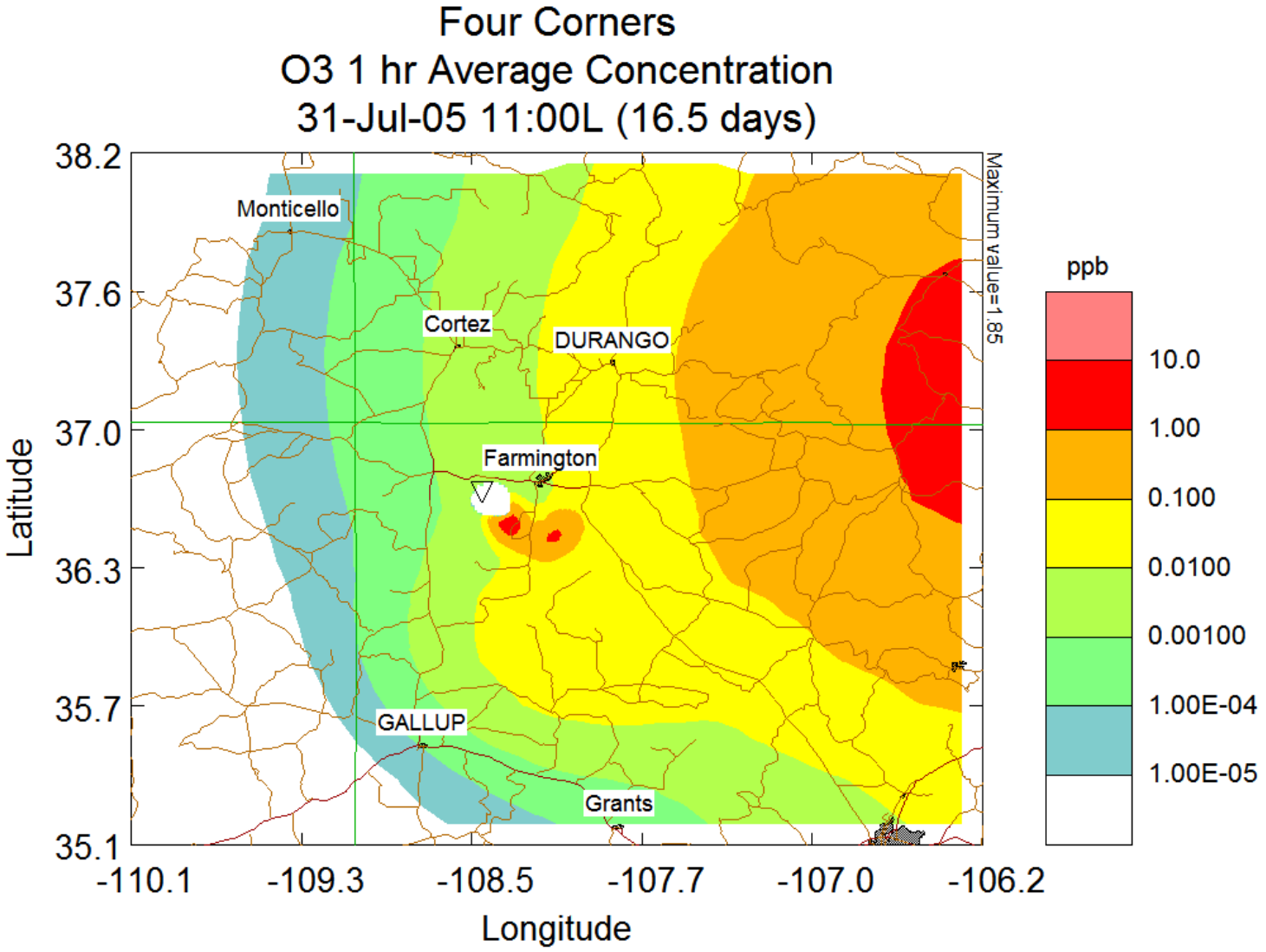


Four Corners (FC) Single-Source Application

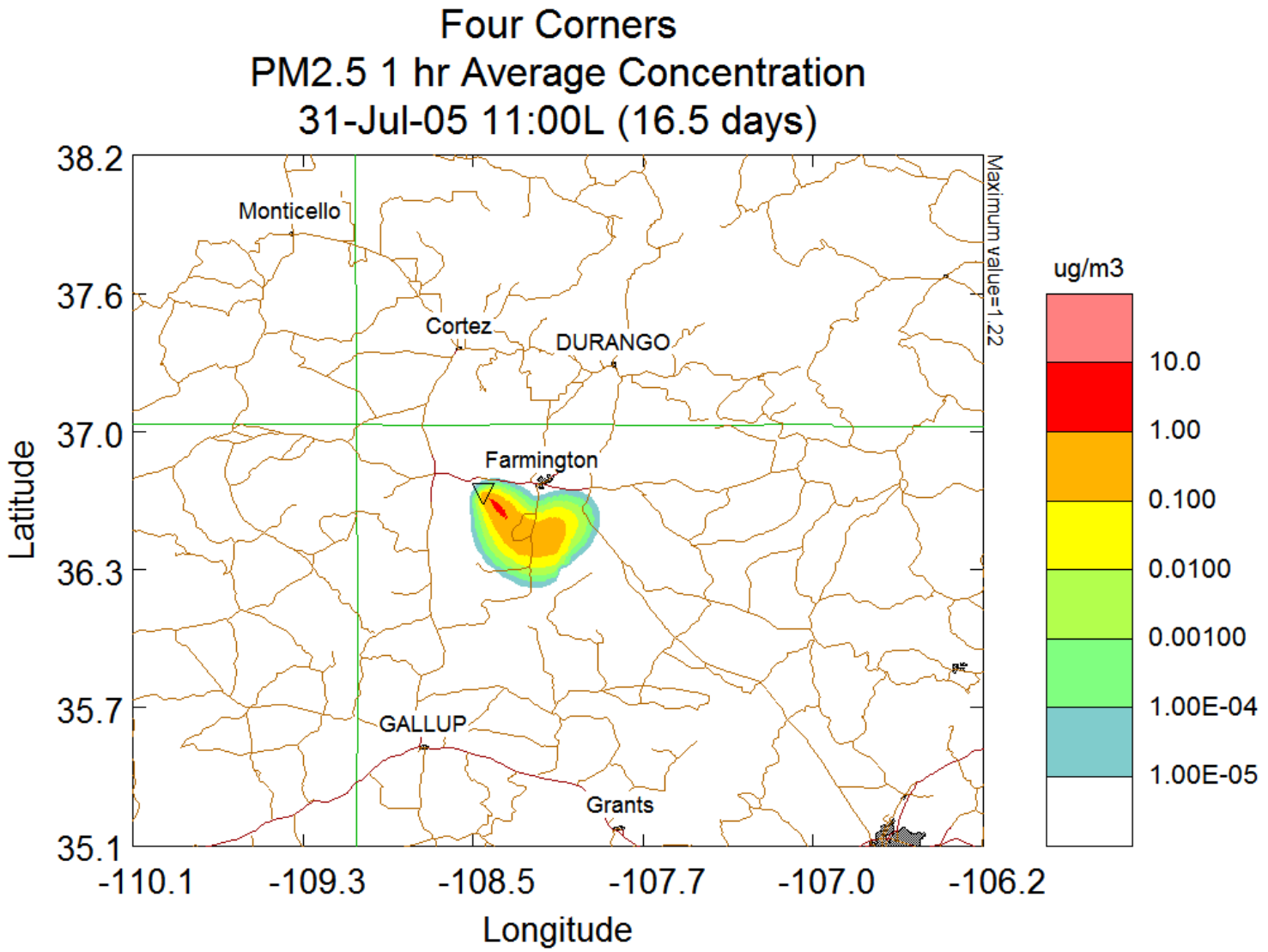


- 4-km domain
- Annual WRF meteorology converted to SCICHEM MEDOC format files using MMIF 3.1
- Background chemistry for "WRAP South" region
- Annual simulation for EGU1 impacts
- Representative results shown for 17-day simulation (July 15-31) included with SCICHEM 3.0b2

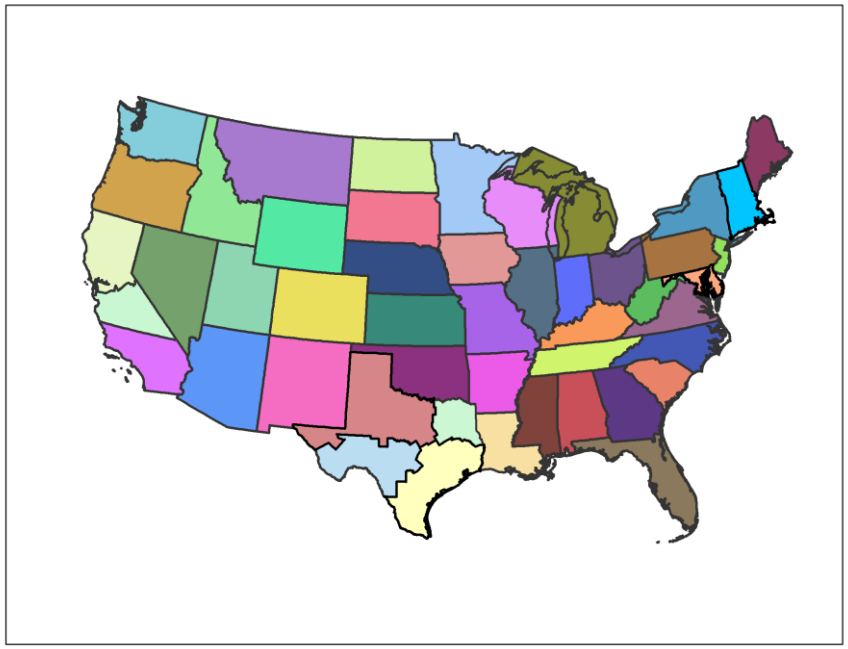
Ozone: Noon, July 31, 2005



$PM_{2.5}$: Noon, July 31, 2005



Potential Modified Regions



- Different regions for background chemistry could be defined based on states, groups of states or partial states, as shown to the left
- Plumes are bound to transport across regions, so modeling could be performed with different backgrounds to test the sensitivity of results to those assumptions

SCICHEM Runtimes

- System:
  - Linux workstation (4 Processor Intel Core2 Quad CPU Q9650 @3.00GHz)
- 15-hour TVA plume study (full chemistry): 5 minutes
  - Extrapolates to ~50 hours for full year
- Annual Four Corners simulation (full chemistry): 80 hours

SCICHEM Summary

- The full chemistry version of SCICHEM incorporates chemistry from highly tested Eulerian models
- SCICHEM has been tested against aircraft data with favorable performance
- SCICHEM 3.0 can be an appropriate model for single-source O_3 and $PM_{2.5}$ applications
- Release of SCICHEM 3.0 Beta 2 will occur in first half of 2014
  - http://sourceforge.net/projects/epri-dispersion/
- Await feedback from users and then formally release final version