SCICHEM for Regulatory Modeling

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General Overview of SCICHEM

- SCICHEM is a Lagrangian photochemical puff model with different options for gas and aerosol chemistry schemes, the most detailed of which are consistent with the mechanisms found in photochemical grid models.

- SCICHEM is able to model the dispersion of primary pollutants and the formation of secondary pollutants
  - SCICHEM can explicitly model the conversion of NO to NO_2
  - SCICHEM can be used to model ozone and secondary $PM_{2.5}$
  - SCICHEM can be used for near-source applications as well as long-range transport applications
    - Option to use simple chemistry for near-source applications

SCICHEM 3.0 Features

- Chemistry
  - CB05 gas-phase chemistry mechanism
  - Aerosol and aqueous chemistry modules based on CMAQ 4.7.1
- Dispersion
  - Incorporates last 10 years of improvements in SCIPUFF (developed independently of SCICHEM)
- Source Treatment
  - Point, area, and volume sources
  - Building downwash algorithm
- Option to read input files in keyword format (similar to AERMOD inputs)
- Detailed specification of background concentrations based on photochemical grid modeling simulation

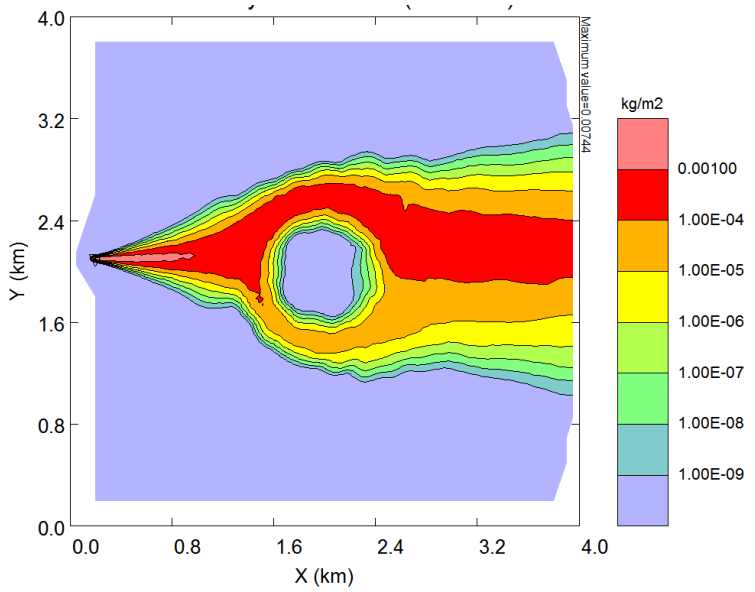
SCICHEM History

- First version developed in late 1990s
  - SCIPUFF (dispersion component) evaluated with tracer experiments and AERMOD databases
  - SCICHEM evaluated with power plant plume measurements
  - Sporadic incremental upgrades through 2010

- Major upgrade effort initiated in 2011
  - Beta 1 (for 1-hour NO_2 and SO_2) released in 2013
  - Beta 2 (for both primary and secondary impacts) released in 2014
  - Model updated to respond to beta-tester feedback and comments and include new features
  - Final version, SCICHEM 3.0, released on August 10, 2015
  - **http://sourceforge.net/projects/epri-dispersion/**

SCICHEM Evaluations

- **Theoretical Studies**
  - Buoyant plumes in shear flow
  - Laboratory diffusion measurements
  - Flow around a hill

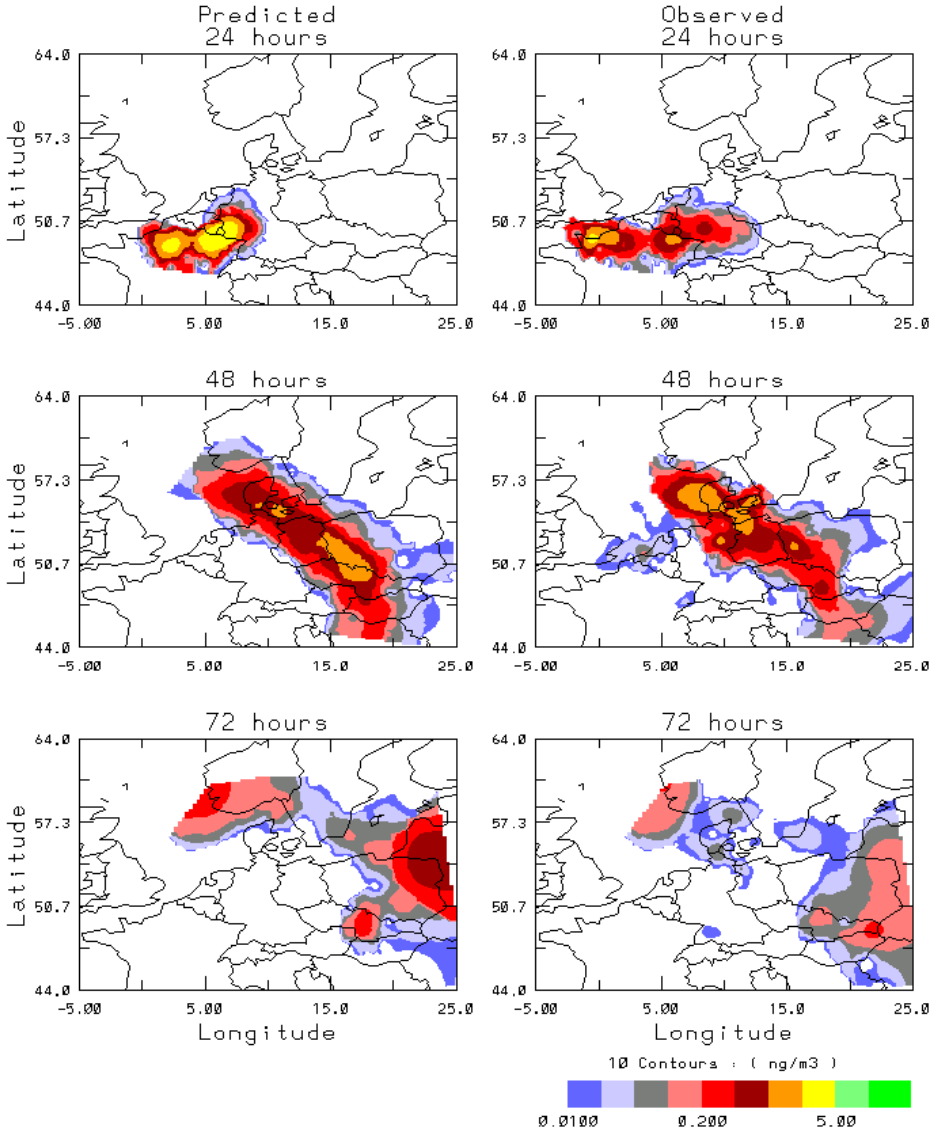


Flow around a hill

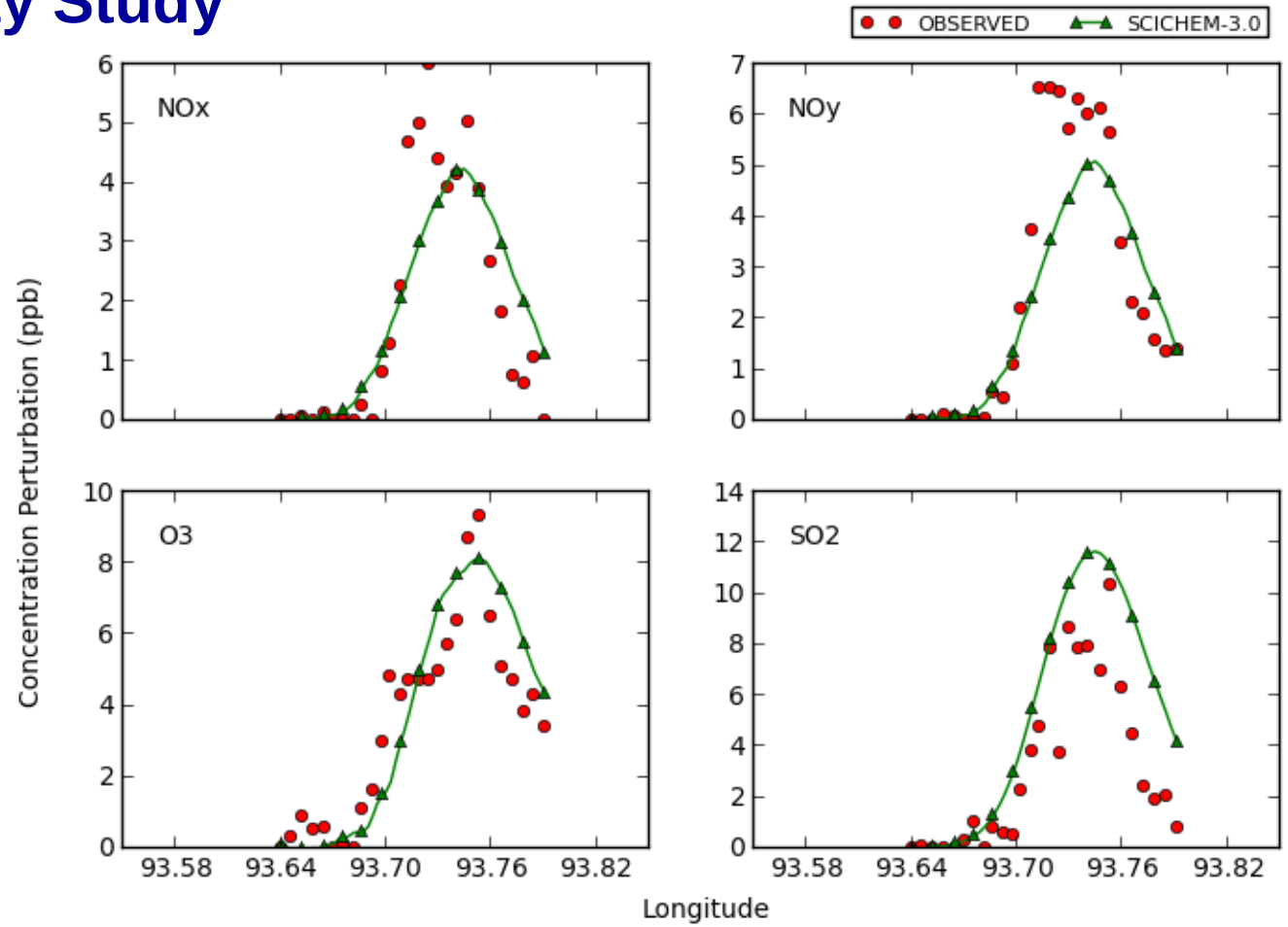
- **Evaluation with tracer studies**
  - European Tracer Experiment
  - AERMOD evaluation databases

- **Evaluation with aircraft measurements**
  - TVA Cumberland power plant plume
  - Dolet Hills power plant plume
  - Evaluation with 2013 SENEX measurements (ongoing)
  - Evaluation with SEARCH measurements (exploratory research study)

Long-Range Transport Evaluation with Tracer Studies
European Tracer Experiment (ETEX) 1994



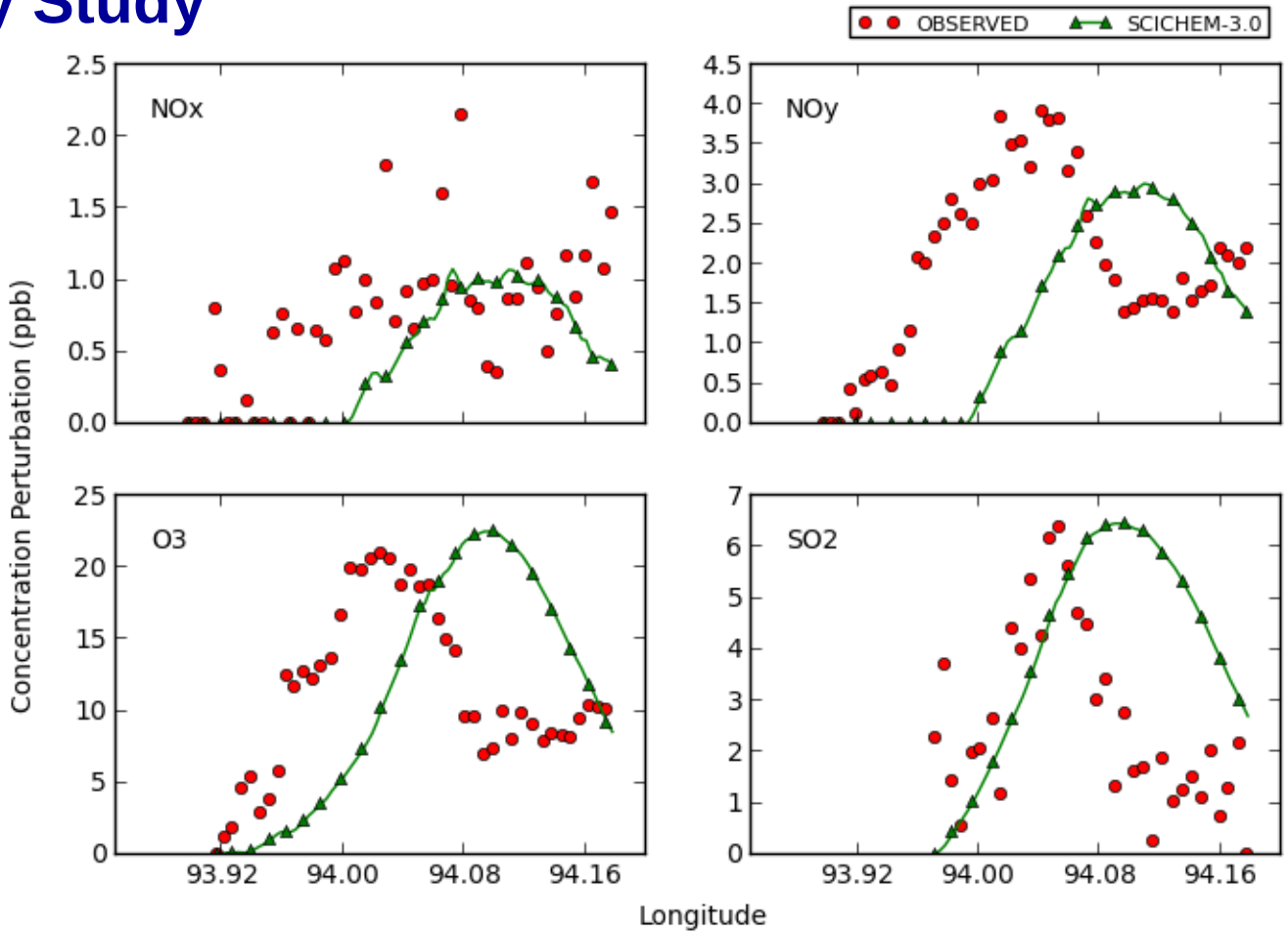
Dolet Hills, Northeast Texas Air Care (NETAC) 2005 Air Quality Study



Traverse 3, 18 km downwind

- Peaks for NO_y, SO_2 and O_3 are within 20% of observed values

Dolet Hills, Northeast Texas Air Care (NETAC) 2005 Air Quality Study



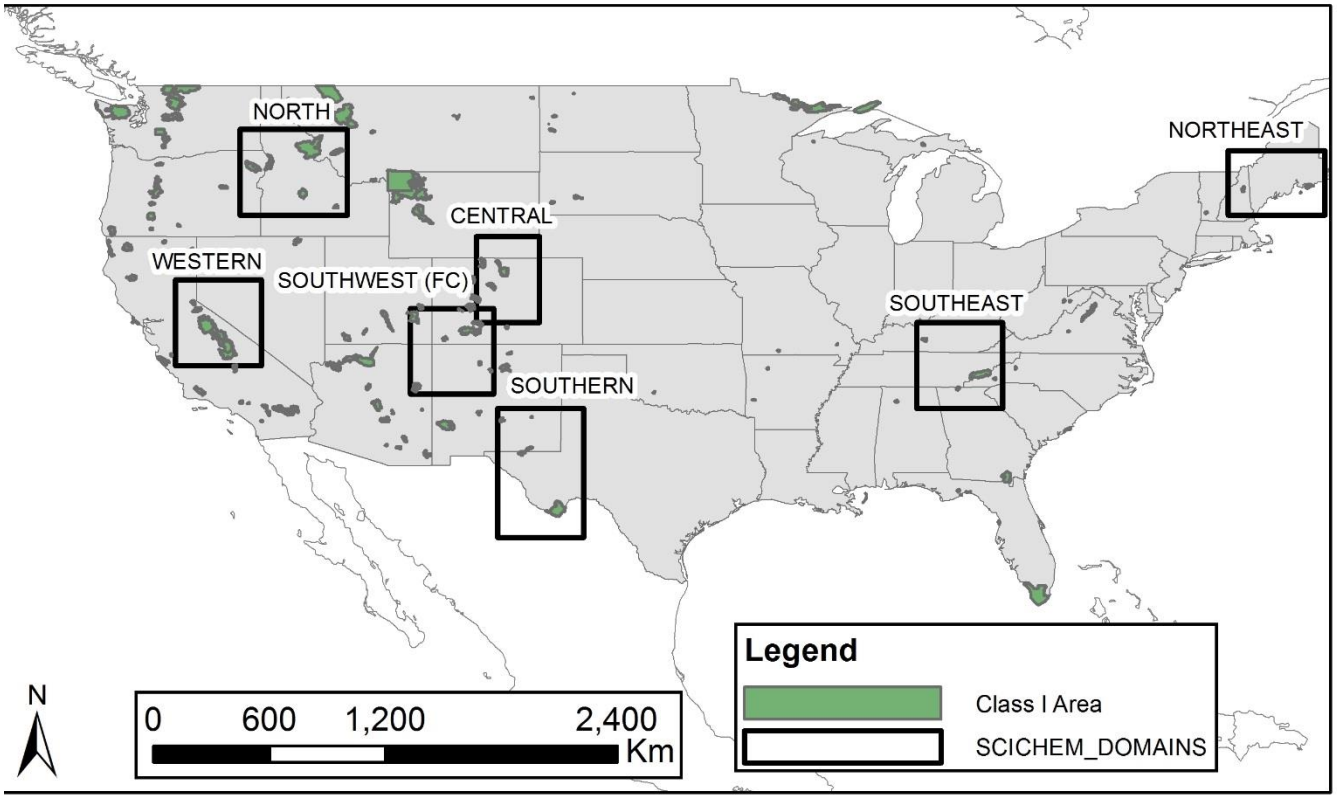
Traverse 6, 54 km downwind

- 20 ppb peak ozone production in measurements and modeling

SCICHEM Model Testing (Stress Testing)

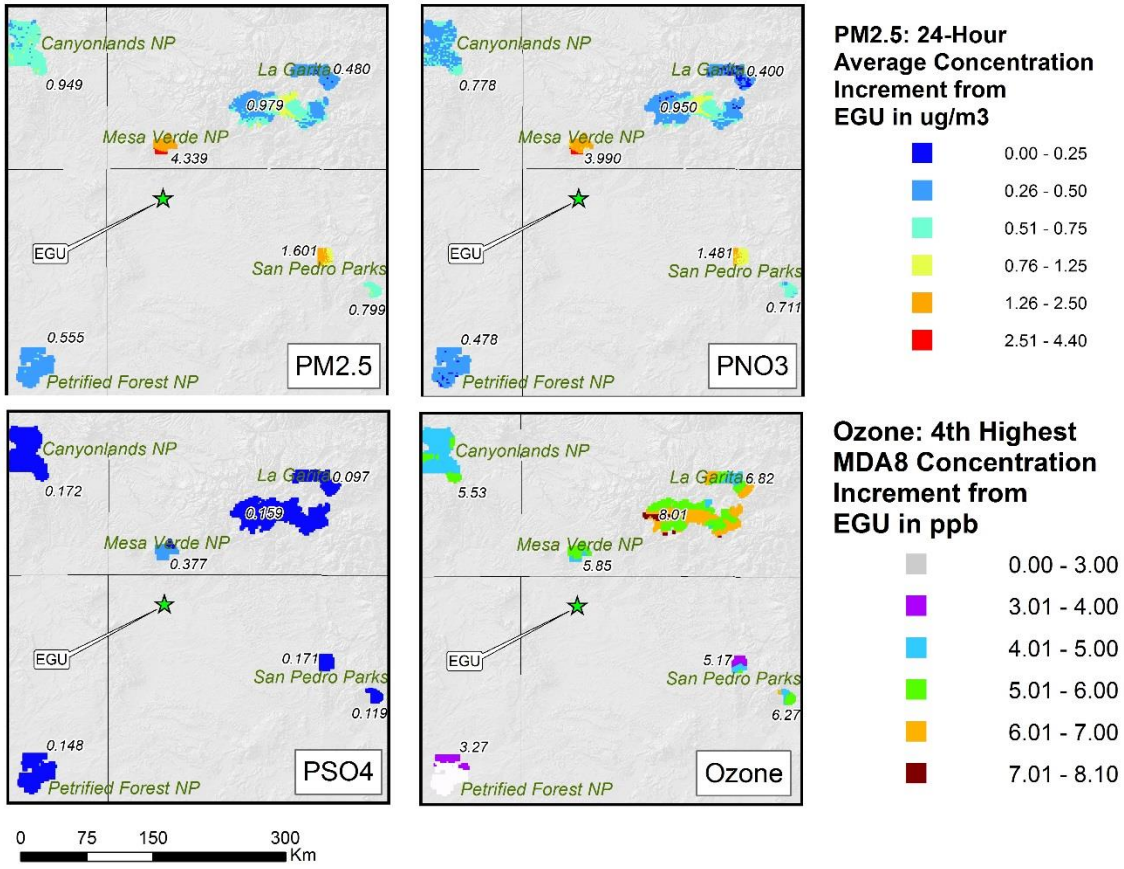
- During the beta period, comments were received that SCICHEM had not been “stress tested”
  - Questions arose whether the model could simulate a variety of conditions and sources for annual simulations
- Objectives
  - Test robustness of model for long-term (annual) applications for a range of meteorological conditions and source types
  - Demonstrate calculation of secondary impacts in Class I areas
- Hypothetical sources
  - Power plant
  - Flare with highly reactive VOC (HRVOC) emissions
  - Petrochemical complex plume
- Modeling domains
  - Several domains across the US with multiple Class I areas in the domain

Domains for Model Testing



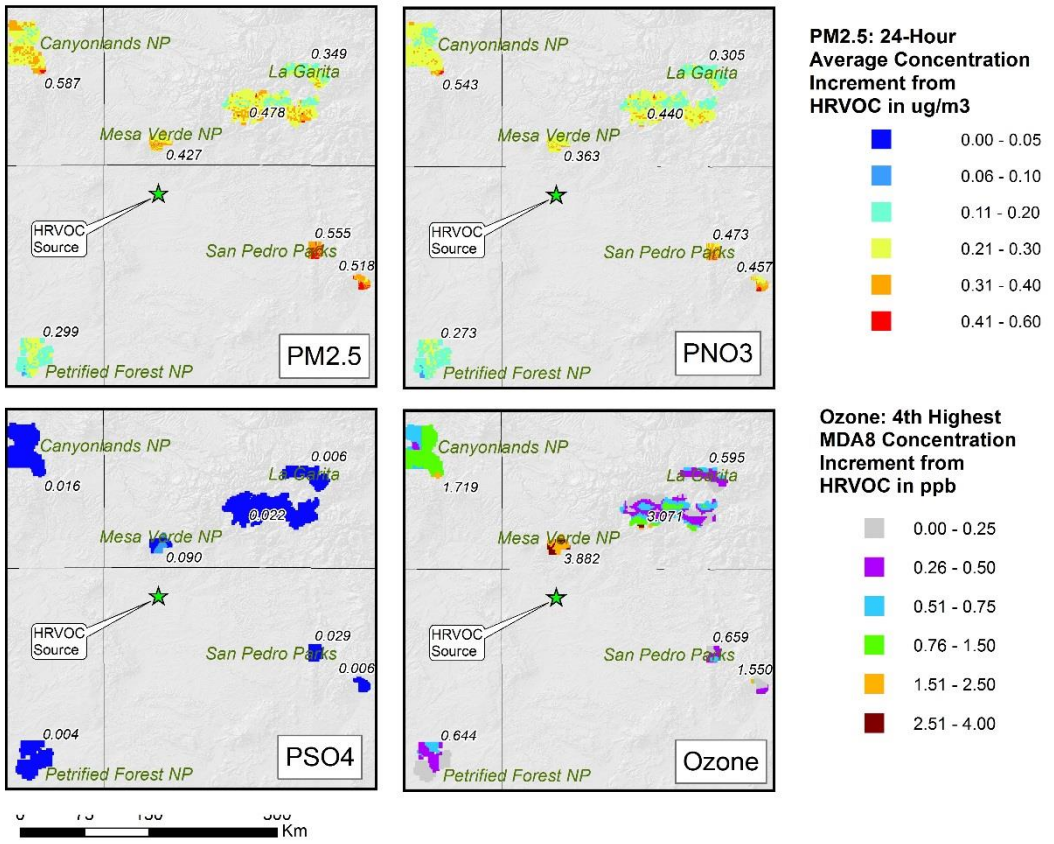
Annual Power Plant Impacts: Four Corners Domain

- Maximum 24-hour average $PM_{2.5}$ impact ranges from 0.5 to 4.3 ug/m^3
  - Max PM NO_3: 0.4 to 4 ug/m^3
  - Max PM SO_4: 0.1 to 0.4 ug/m^3
- 4th highest 8-hour average ozone impact ranges from 3.3 to 8 ppb



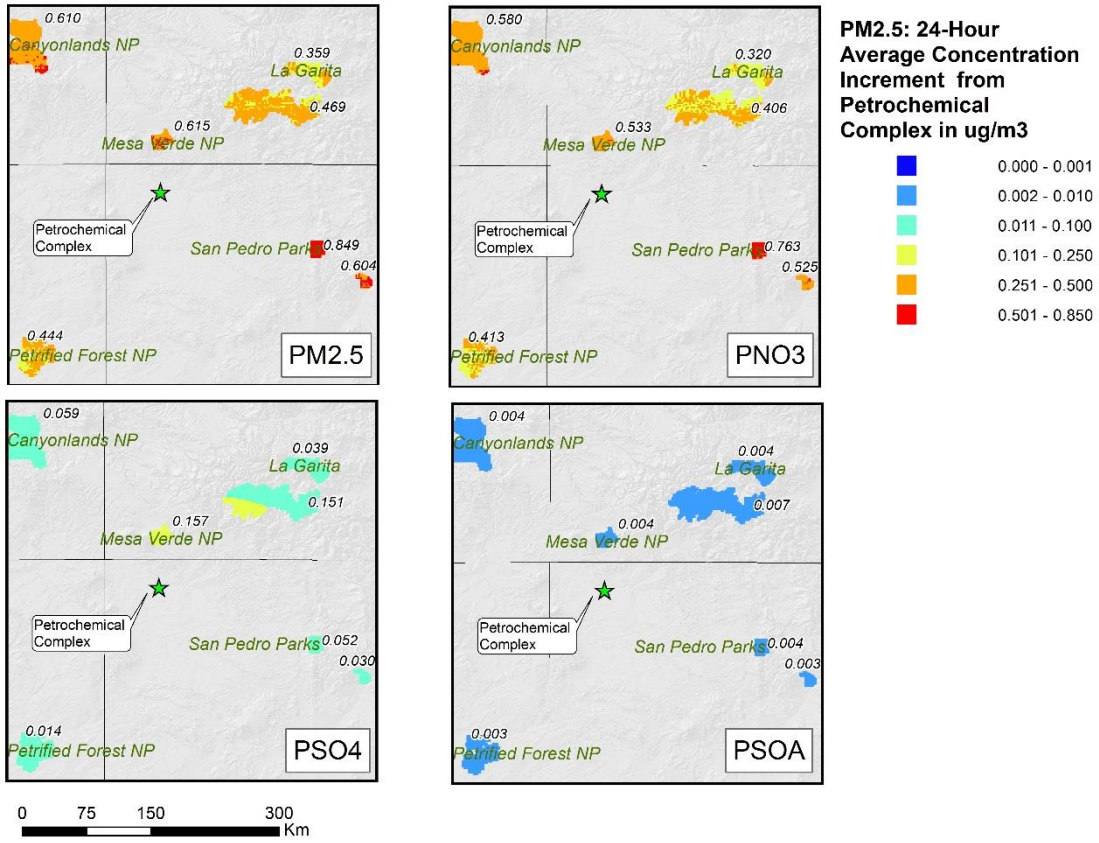
HRVOC Flare Impacts: Four Corners Domain

- Maximum 24-hour average $PM_{2.5}$ impact ranges from 0.3 to 0.6 ug/m^3
  - Max PM NO_3: 0.3 to 0.5 ug/m^3
  - Max PM SO_4: < 0.1 ug/m^3
- 4th highest 8-hour average ozone impact ranges from 0.6 to 3.9 ppb



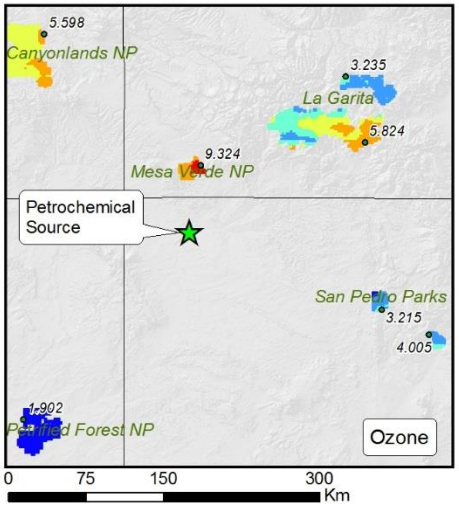
Petrochemical Complex PM Impacts: Four Corners Domain

- Includes small amount of SOA precursor (toluene, xylene) emissions
- Maximum 24-hour average $PM_{2.5}$ impact ranges from 0.36 to 0.85 ug/m^3
  - Max PM NO_3: 0.32 to 0.76 ug/m^3
  - Max PM SO_4: < 0.2 ug/m^3
  - Max PM SOA: 0.003 to 0.007 ug/m^3



Petrochemical Complex Ozone Impacts

- 4th highest 8-hour average ozone impacts
  - 1.9 to 9.3 ppb



Ozone: 4th Highest MDA8 Concentration Increment from Petrochemical Complex in ppb

0.00 - 2.00 | 2.01 - 3.00 | 3.01 - 4.00 | 4.01 - 5.00 | 5.01 - 7.00 | 7.01 - 9.40

Summary of Stress Testing

- Annual model testing successfully conducted for selected domains and source scenarios
  - Scenarios include a power plant with NOx and SO_2 emissions, a HRVOC flare, and a petrochemical complex with VOC, NOx and SO_2 emissions
  - Runtimes for annual simulation range from 20 to 80 hours depending on the domain and source scenario (for these simulations including secondary pollutants)
  - Model is robust

SCICHEM Conclusions

- SCICHEM has been thoroughly evaluated throughout its history of development and shown to be a robust model that can handle different sources under different chemical and meteorological regimes

- SCICHEM has been demonstrated that it can be used to simulate pollutant concentrations accurately for different applications
  - Short-range SO_2 simulations
  - Short-range NO_2 simulations
  - Long-range O_3 and secondary $PM_{2.5}$ simulations

- Representative runtimes
  - 15-30 minutes for annual SO_2 simulations
  - 20-40 minutes for annual NO_2 simulations
  - 20-80 hours for annual simulations with secondary pollutants

SCICHEM Reference

- Additional details on SCICHEM can be found in the following peer-reviewed journal publication (in addition to documentation included with the model):

- Chowdhury, B.; Karamchandani, P. K.; Sykes, R. I.; Henn, D. S.; Knipping. E., Reactive puff model SCICHEM: Model enhancements and performance studies. *Atmospheric Environment.* **2015,** *117,* 242-258.
  - Open Access Article
  - http://www.sciencedirect.com/science/article/pii/S1352231015302119