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
SCICHEM Evaluations

- **Theoretical Studies**
  - Buoyant plumes in shear flow
  - Laboratory diffusion measurements
  - 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

Peaks for NO$_y$, SO$_2$ and O$_3$ are within 20% of observed values

Traverse 3, 18 km downwind
Dolet Hills, Northeast Texas Air Care (NETAC) 2005 Air Quality Study

- 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
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):

  - Open Access Article