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SCICHEM:
A Puff Model with Chemistry

Part 1: Description and SO_2/NO_2 Applications

Eladio Knipping, Naresh Kumar
Environment Sector
Electric Power Research Institute

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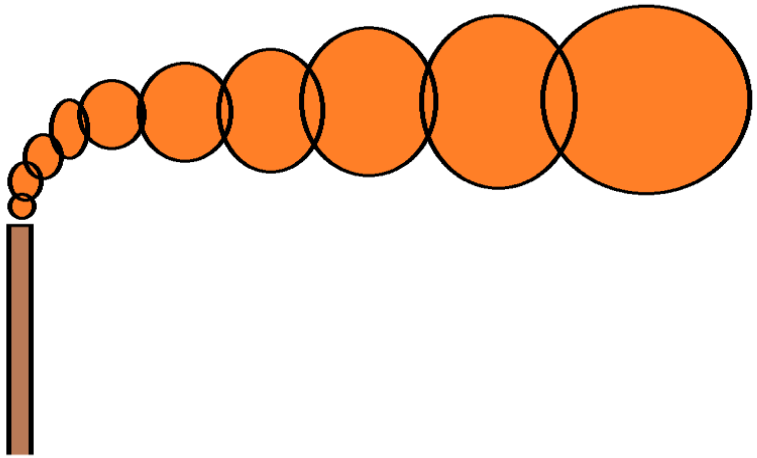
SCICHEM: SCIPUFF with Chemistry

Second Order Closure Integrated Puff Model (SCIPUFF) with Chemistry

- Plume represented as a succession of puffs
- Comprehensive puff chemistry treatment



SCICHEM Transport

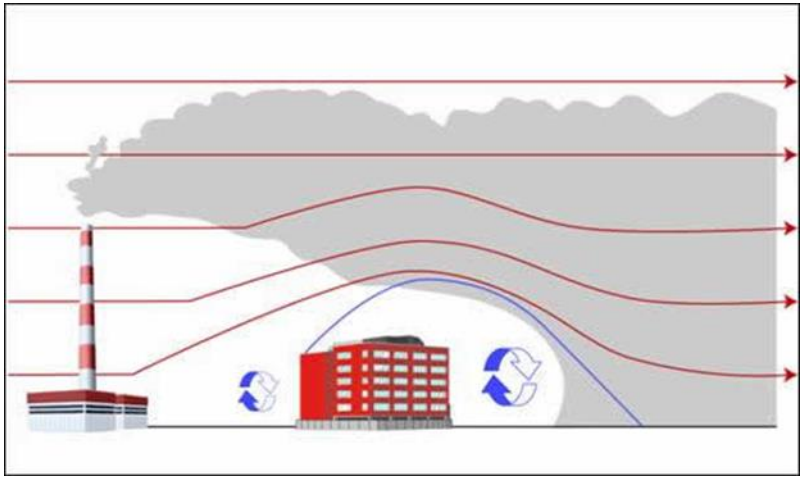
- Overlapping 3D puffs represent concentration field
- Solve ODE's for puff moments
- Wide range of scales
  - No fixed grid
  - No diffusion errors
- Inhomogeneous conditions
  - Spatial
  - Temporal

SCICHEM Chemistry

- No chemistry for tracer simulations and SO_2 simulations
- Optimized near-source NO-NO_2-O_3 chemistry for short-range 1-hour NO_2 assessments
- Full treatment of chemistry and dry and wet deposition, similar to treatments in photochemical grid models, such as CMAQ and CAMx

Other SCICHEM Features

- Nested meteorology grid
- Multiple source types: Point, area and volume
- Ability to read AERMOD-style input files for short-range applications
- Accounts for the effects of building downwash on point source plumes (PRIME algorithm)

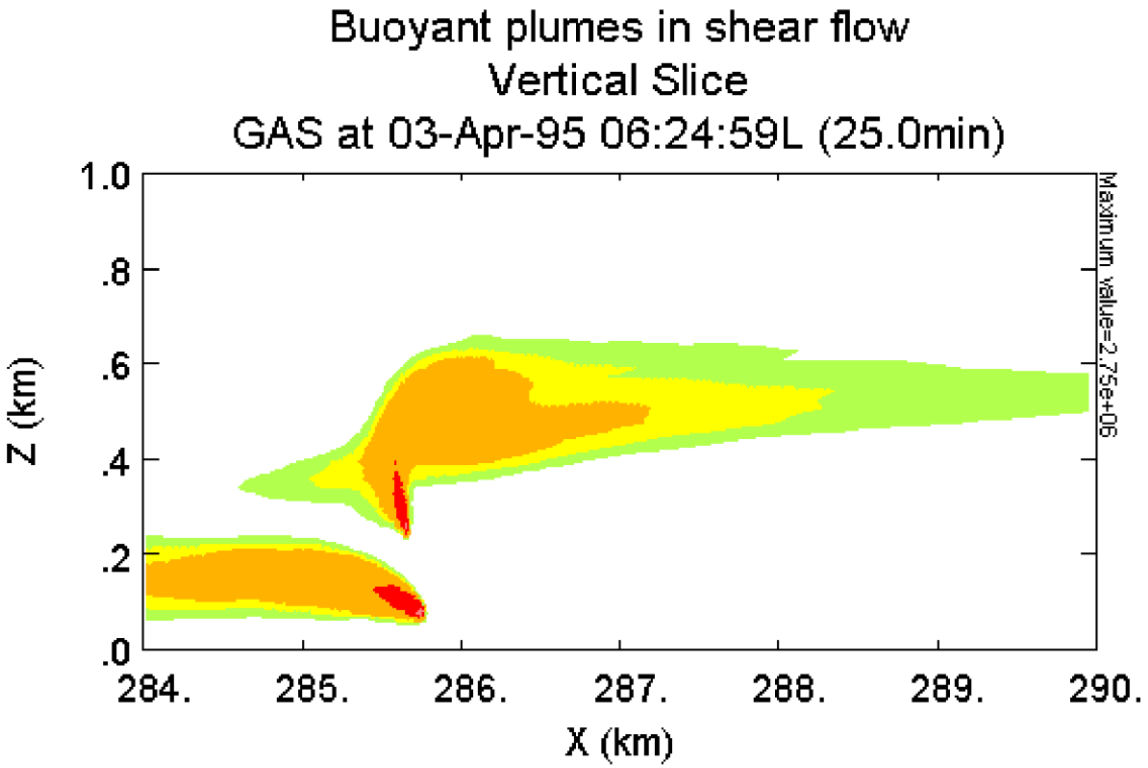


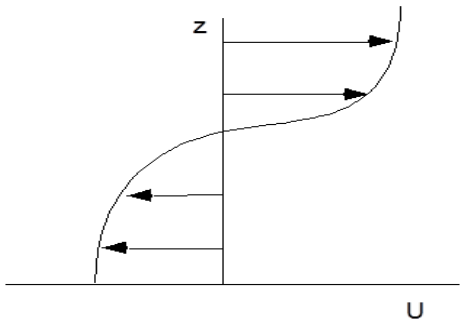
SCICHEM Applications

- **Theoretical Studies**
  - Bouyant plumes in shear flow
  - Laboratory diffusion measurements (Deardorff and Willis, 1974) *
  - Flow around a hill
- **Tracer studies**
  - European Tracer Experiment *
  - AERMOD evaluation databases
- **Short-range applications**
  - 1-hour NO_2 application
- **Long-range applications (O_3 and $PM_{2.5}$)**
  - TVA Cumberland power plant plume
  - Four Corners single-source impacts

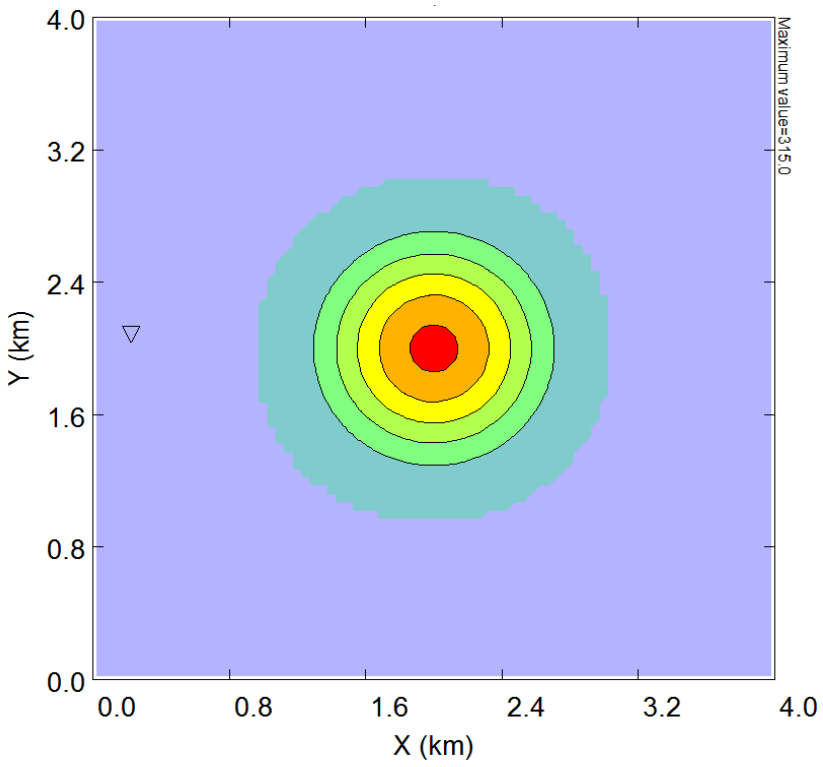
* Not shown

Buoyant Plumes in Shear Flow

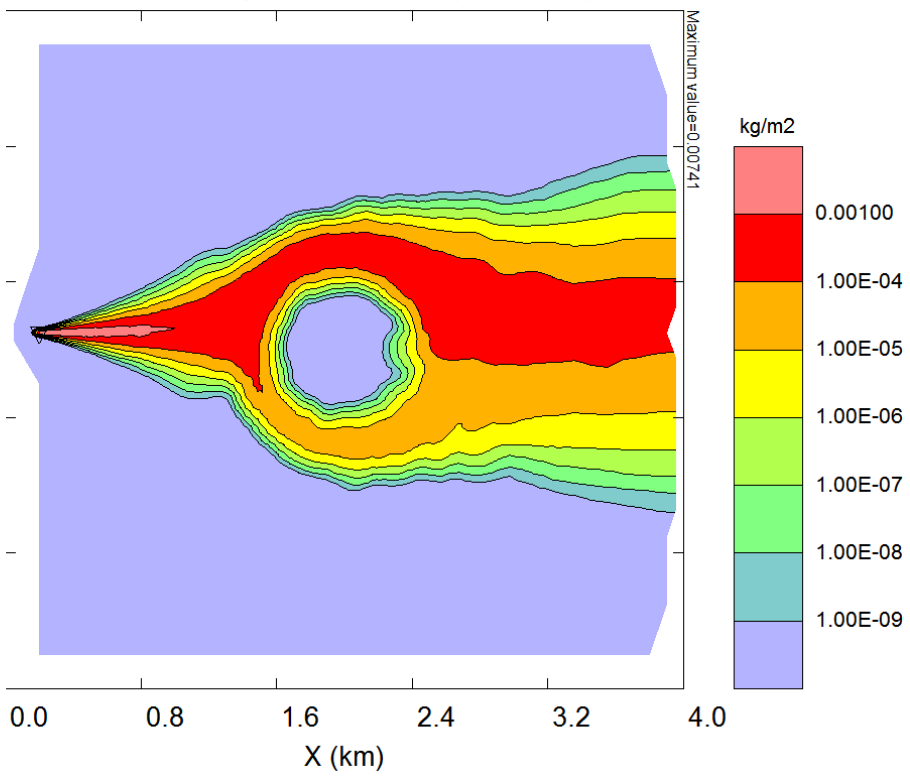




Flow Around a Hill

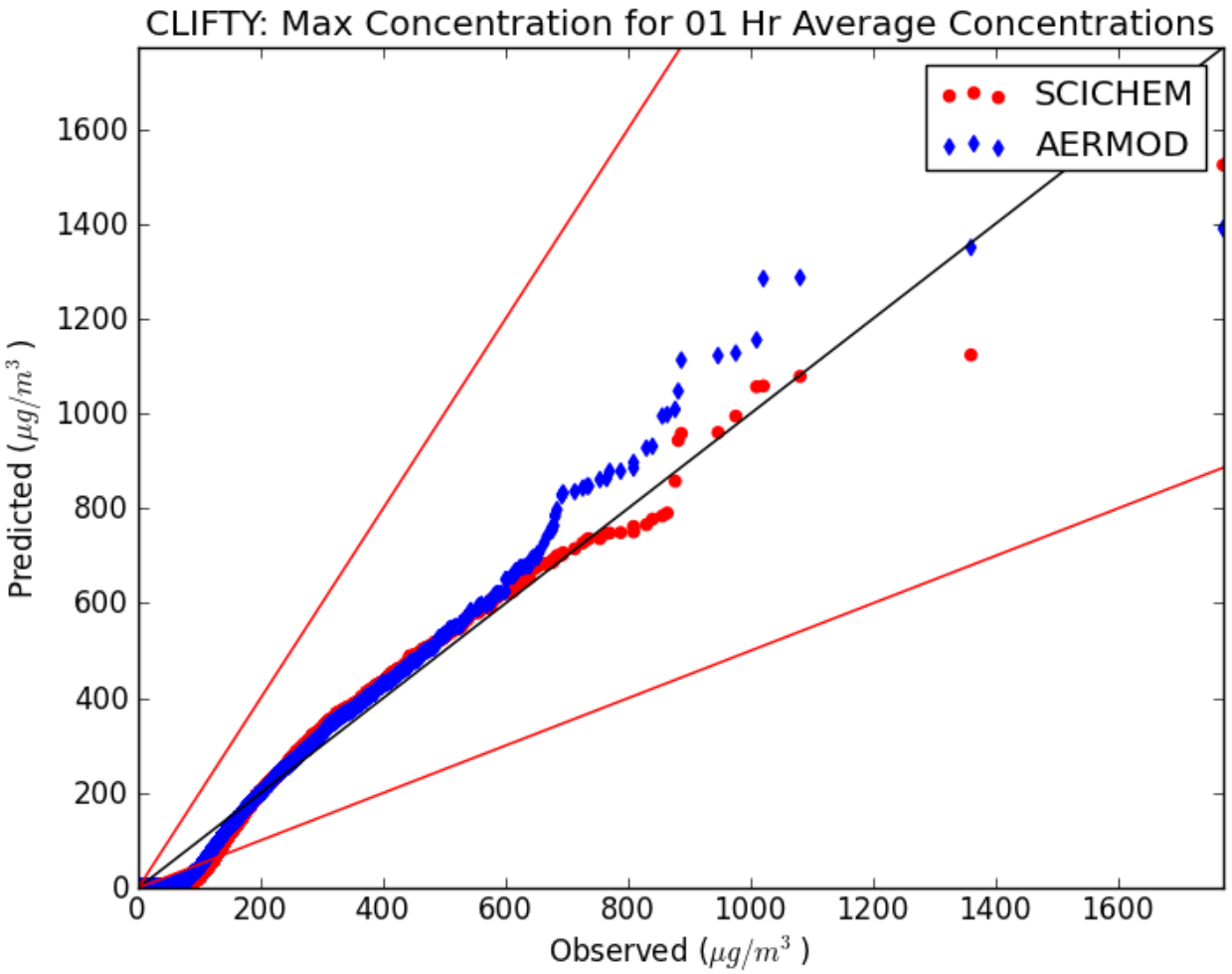


TERRAIN

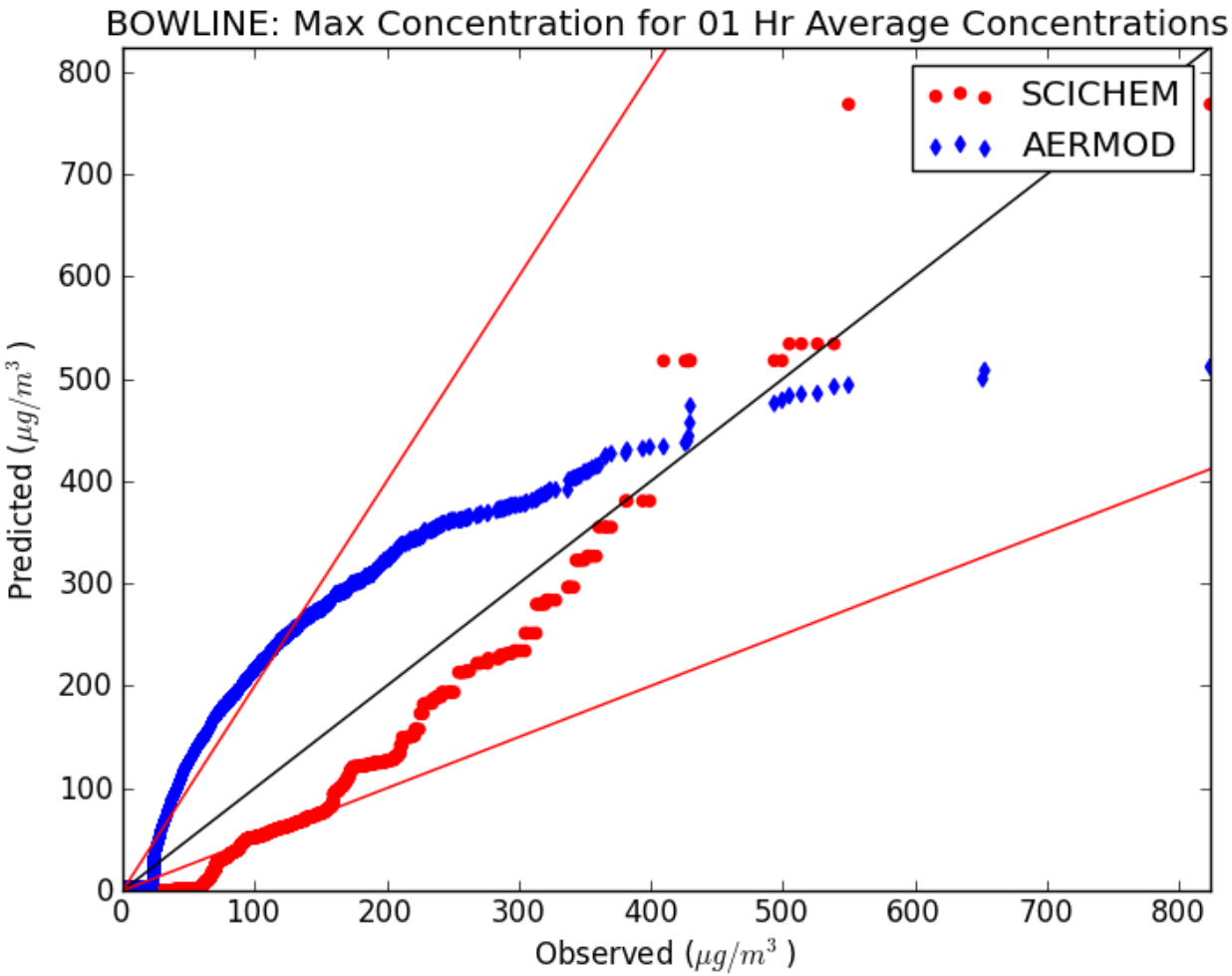


Integrated Concentration

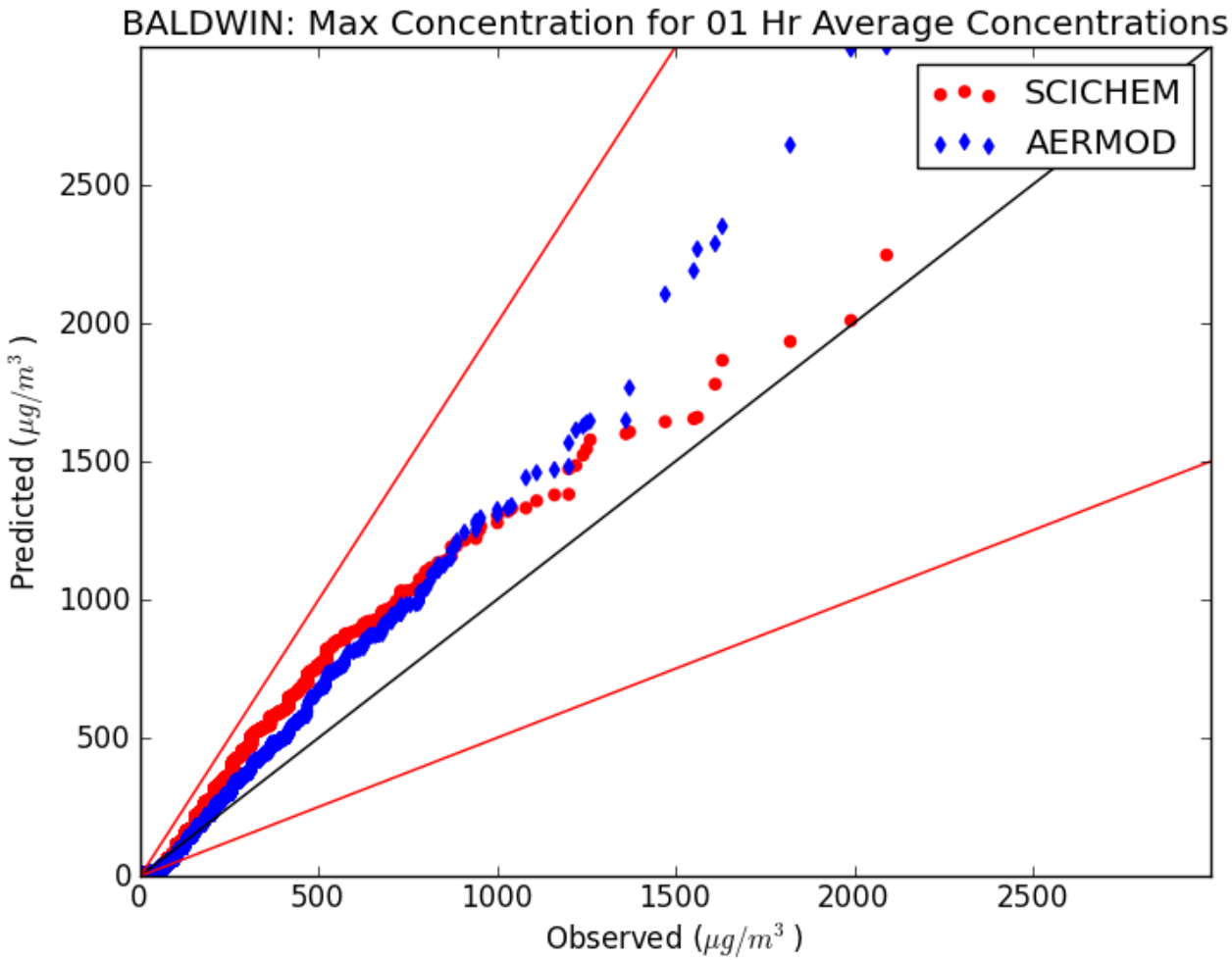
SCICHEM Performance: Clifty SO_2 Q-Q Plot



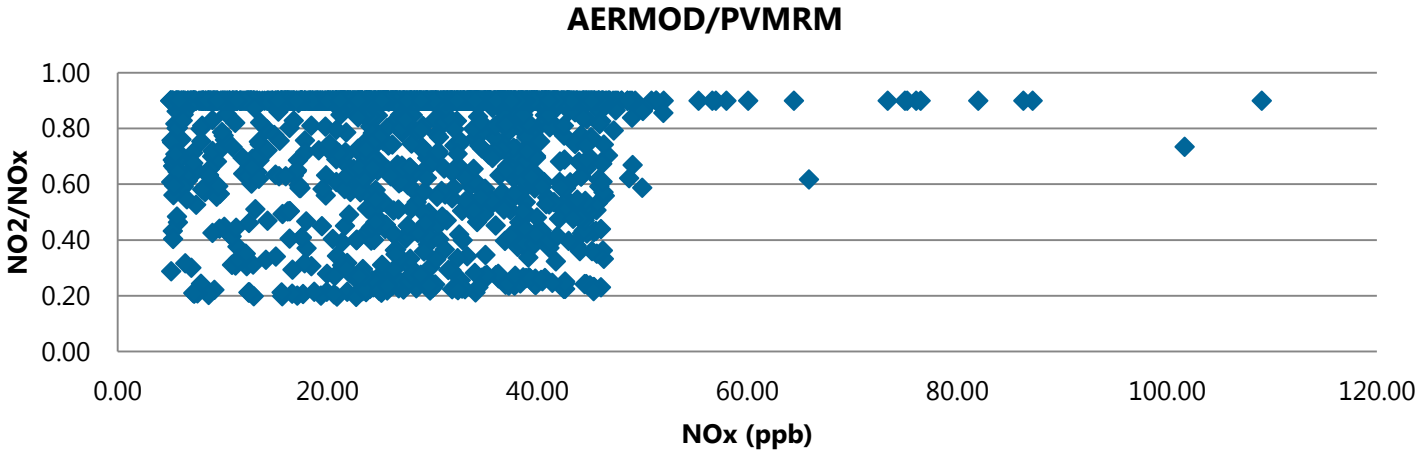
SCICHEM Performance: Bowline Q-Q Plot

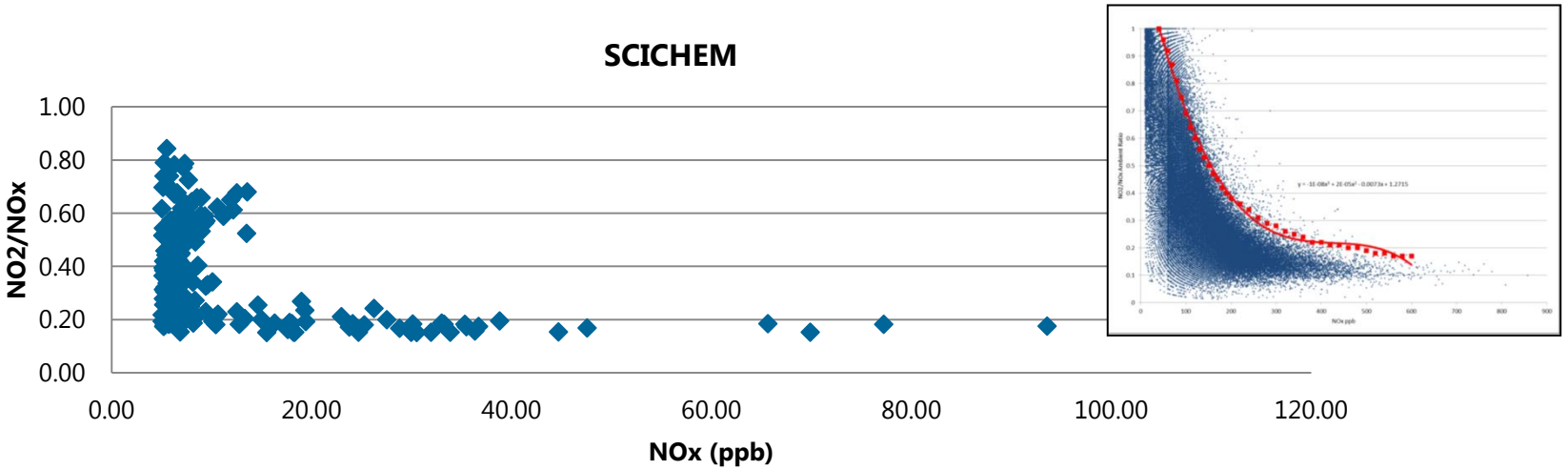


SCICHEM Performance: Baldwin SO_2 Q-Q Plot



SCICHEM Application for NO_2





SCICHEM NO_2/NOx ratios more consistent with observations

SCICHEM Runtimes

- System:
  - Linux workstation (4 Processor Intel Core2 Quad CPU Q9650 @3.00GHz)

- Annual 1-hour SO_2 (no chemistry): 7 minutes
- Annual 1-hour NO_2 (near-source chemistry): 1 hour

SCICHEM Summary

- SCICHEM can simulate conditions that steady-state models cannot replicate
- SCICHEM performance for is similar or better than AERMOD for SO2 evaluation databases
- SCICHEM can explicitly simulate the conversion of NO to NO2 in the atmosphere
- SCICHEM 3.0 Beta 1 released in June 28, 2013
- 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