

Overview of Regional Air Quality Modeling at Ozone Research Center

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Regional Photochemical Air Quality Modeling Resources at ORC

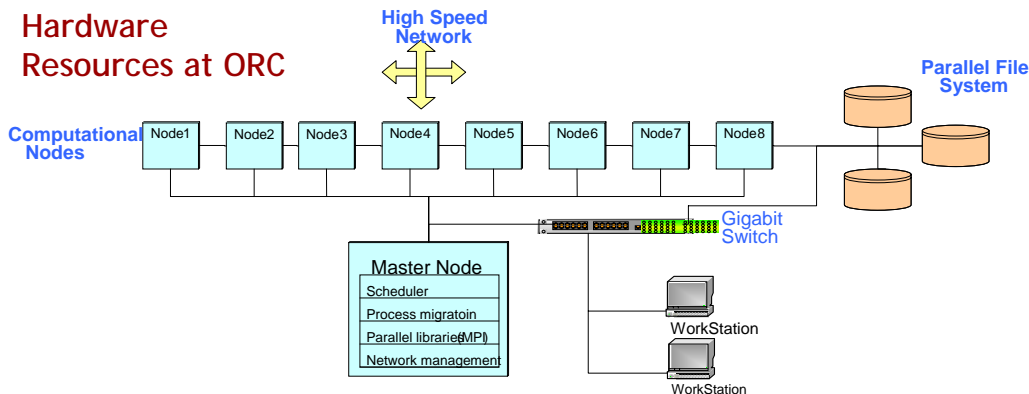
ORC maintains operational installations of multiple regional photochemical models:

- Community Multiscale Air Quality (CMAQ version 4.4 and version 4.5), Comprehensive Air-quality Model (CAMx version 4.20), Regional Modeling System for Aerosols and Deposition (REMSAD version 8.0)

The following MODELS3/CMAQ implementation is used for the regional modeling presented here:

- Air Quality Models: Community Multiscale Air Quality (CMAQ version 4.4 and version 4.5)
- Emissions Processor: Sparse Matrix Operator Kernel Emissions (SMOKE version 2.1 and version 2.2)
- Meteorology Processor: Meteorology-Chemistry Interface Processor (MCIP version 2.2.2 and version 3)
- Scientific Libraries: NETCDF, IOAP, MPI
- Compiler: Portland Group Fortran, pgcc, gcc
- Statistical/Numerical Modeling and Visualization Tools: MATLAB, SAS, ArcGIS/ArcIMS, PERL, Shell Scripting and Fortran

Hardware Resources at ORC



- Cluster I (Chrysothemis)**
 - Processor: AMD Athlon XP 1800+ 1.6GHz
 - Number of Processors : 16
 - Memory: 512 MB x 16
 - Storage: 40 GB x 16
 - Network: Gigabit Ethernet
- Cluster II (Purchase in Progress)**
 - Processor: AMD Dual Core Opteron with 64 bit + 2.2GHz
 - Number of Processors : 4
 - Memory: 2 GB x 4
 - Storage: 40 GB x 16
 - Network: Gigabit Ethernet
- Storage (Promise RAID 1, II)**
 - Supported with 6 TeraBytes of disk space; expansion is in progress
 - Regular backups using USB disk (5 x 300 GB) and SDLT tape drive (10 x 160 GB)
- Uninterrupted Power Supply (UPS)**
 - All Server and Disk Arrays are supported with multiple UPS
- Workstations**
 - Multiple PCs running Windows XP/ Linux with NFS and SMBFS file system support

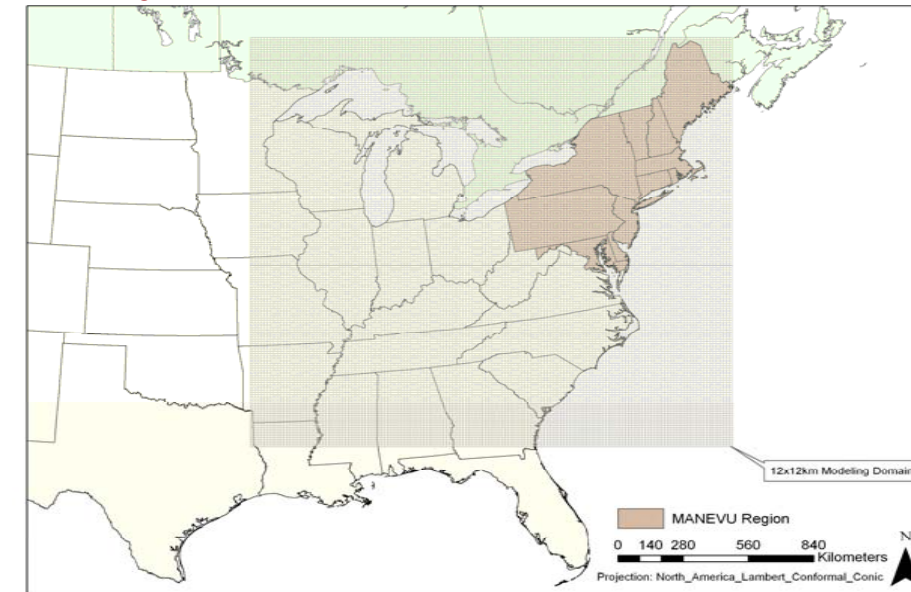
Ongoing Regional Air Quality Modeling work at ORC for SIP Support

Simulation	Time period	Groups Involved	Regional Collaborators in Joint Modeling work
2002 Base Year	Annual	Regional Collaboration	Mid-Atlantic Regional Air Management Association (MARAMA)
2009 Base Year	Annual	Regional Collaboration	New York State Department of Environmental Conservation (NYDEC)
2009 Regional Control Strategy	Annual	Regional Collaboration	New Jersey Department of Environmental Protection (NJDEP)
2009 Local Control Strategy	Episode (August 1 st to August 15 th , 2002)	ORC - NJDEP	Northeast States for Coordinated Air Use Management (NESCAUM)
Sensitivity Analysis	Episode (August 1 st to August 15 th , 2002)	ORC - NJDEP	University of Maryland (UMD)
			Ozone Research Center (ORC)

Sensitivity Analysis to Determine the Impact on Ozone and PM2.5 Levels of:

- Improved Temporal Profiles for Point Sources on Ozone and PM2.5
- Domain-wide SO₂ reductions
- Improved Temporal Profiles for Mobile Sources
- Different numerical modules in CMAQ 4.4 and CMAQ 4.5

Modeling Domain

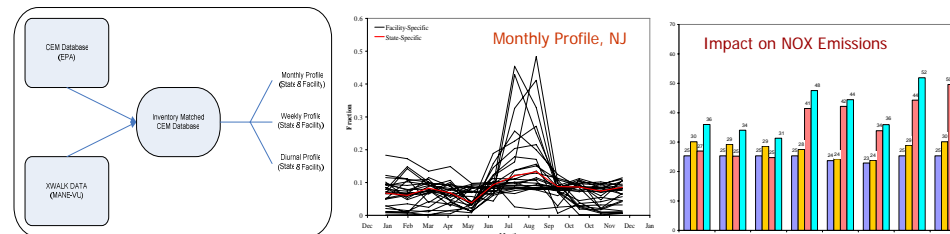
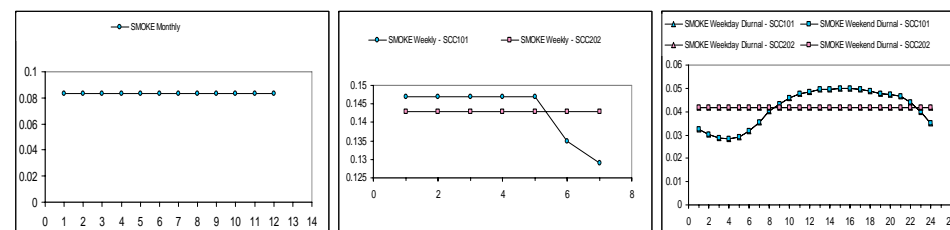


Sensitivity Analysis and Control Strategy Runs

Impact of Improved Temporal Profiles for Point Sources on Ozone / PM2.5

Motivation:

- Electric Generating Units (EGUs) emit 70% SO₂ and 20% NO_x in Mid-Atlantic/Northeast Visibility Union (MANE-VU) region
- SMOKE underestimates temporal distribution of emissions from EGUs
- Continuous Emissions Monitoring (CEM) data are used to improve temporal profiles of emissions



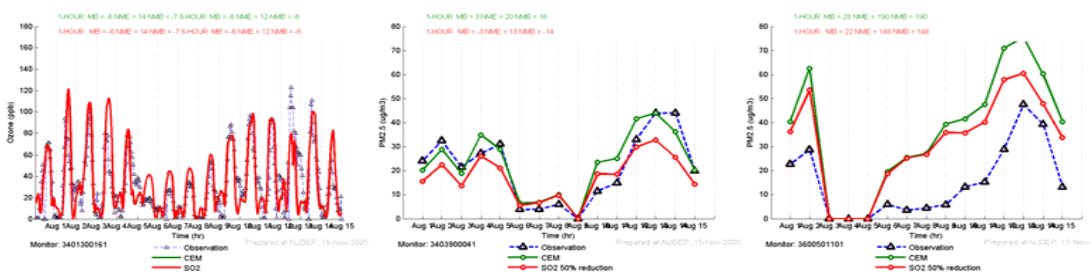
Findings:

- CEM-based state and facility-specific temporal profiles changed substantially hourly emissions
- Ozone prediction performance improved

Impact of SO₂ Reduction

Motivation

- Quantify the impact of 50% domain-wide SO₂ reduction



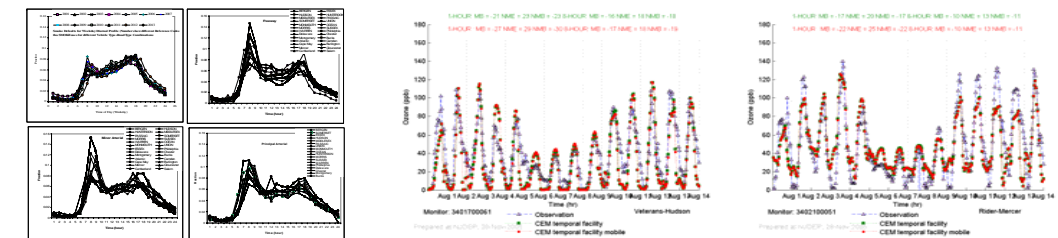
Findings

- No significant change in ozone is observed
- PM2.5 over-estimation is reduced (problem with CMAQ version 4.4)

Impact of Improved Temporal Profiles for Mobile Sources on Ozone

Motivation

- Quantify the impact of improved VMT profiles on Ozone



Findings

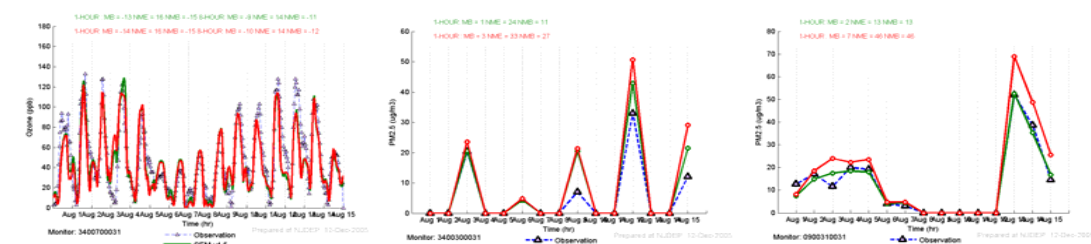
- Slight but quantifiable improvements in ozone predictions
- Weekend performance worse than SMOKE defaults (probably due to lack of actual weekend VMT data)

Comparison of CMAQ 4.4 and CMAQ 4.5 Performance

Motivation

- Differences in the 2 CMAQ versions are significant

- Aerosols**
 - Added sea salt (fine equilibrium; non-interactive coarse mode) - aeor4
 - Updated aerosol dry deposition algorithm
 - Updated mechanism include files to remove any aerosol species with zero concentrations for aeor4
 - Updated ISORROPIA to v1.5 (25 Oct 2003) and fixed some discontinuities
 - Added diagnostic variables to calculate PM2.5 concentrations
 - Corrected bug in mode merging to reduce mode crossover
 - Modified SO4 used in ISORROPIA call
 - Corrected inconsistency in MINLZSG (aerodepr)
 - Corrected the EMSULF (H2SO4 emissions) unit conversion bug
- Chemistry**
 - Added CBA/chlorine chemistry and associated EBI solver
 - Added CBA/air toxics and SAPRC99/air toxics chemistry and associated EBI solvers
 - Added degradation algorithm to the generalized solvers
 - Corrected treatment of convergence failures in EBI solvers
 - No longer support the RAD2 mechanism
 - P-In-G & PBL modeling
 - Improved calculation of plume centerline
 - Fixed bug in the aerosol species array subscripting
 - Corrected error in non-reactive species NH3 fluxes and dry deposition
 - Updated to use PURB (% urban) for setting minimum Kz
- Clouds**
 - Added new sub-grid cloud mixing algorithm/module (based on ACM)
 - Added new cloud diagnostic variables
 - Corrected the interpolation times for resolved clouds (to time-step midpoint) and for subgrid clouds (to half hour)
- Advection**
 - Added new mass continuity scheme
- Other**
 - Added dynamic vertical layer allocation
 - Added primary carbon source apportionment capability
 - Added sulfate tracking capability



Findings

- Few ppb improvements on ozone
- PM_{2.5} improves significantly (due to improvements in CMAQ 4.5 aerosol module)

Acknowledgements

Base Funding for the Ozone Research Center is Provided by the State of New Jersey Department of Environmental Protection (NJDEP - Contract AQ05-011).