ATTACHMENT T

NYSDEC Technical Support Document TSD-1d

TSD-1d

8hr Ozone Modeling using the SMOKE/CMAQ system

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Air Quality Modeling Domain

The modeling domain utilized in this application represented a sub-set of the inter-RPO's continental modeling domain that covered the entire 48-state region with emphasis on the Ozone Transport Region. The OTC modeling domain at 12km horizontal mesh is displayed in Figure 1 is part of the 36km continental domain that is designed to provide boundary conditions (BCs). The particulars of the two modeling domains are:

The 36km domain covered the continental US by a 149 by 129 mesh in the east-west and north-south directions, respectively. The domain is based on Lambert Conformal Projection with the center at (97ºW 40ºN) and parallels at 33ºN and 45ºN. As evident from Figure 1, the 12km domain utilized in this analysis covers most areas of the eastern US and has 172 by 172 mesh in the horizontal. Both domains utilize 22 layers in the vertical extending to about 16km with 16 layers placed within the lower 3km.

Photochemical Modeling -- CMAQ

The CMAQ (version 4.5.1) with CB4 chemistry, aerosol module for $PM_{2.5}$ and RADM cloud scheme was utilized in this study. Photochemical modeling was performed with the CCTM software that is part of the CMAQ modeling package. Version 4.5.1 of this modeling software was obtained from the CMAS modeling center at http://www.cmascenter.org. The following module options were used in compiling the CCTM executable:

- Horizontal advection: yamo
- Vertical advection: yamo
- Horizontal diffusion: multiscale
- Vertical diffusion: eddy
- Plume-in-Grid: non operational
- Gas phase chemical mechanism: CB-4
- Chemical solver: EBI
- Aerosol module: aero3
- Process analysis: non operational

The following computational choices were made during compilation:

- Compiler version: PGI 6.0
- Fortran compiler flags:-Mfixed -Mextend -Bstatic -O2 -module ${MODLOC} -I.
- C compiler flags： -v -O2 -I${MPICH}/include
- IOAPI library: version 3.0
- NETCDF library: version 3.6.0
- Parallel processing library version: mpich 1.2.6
- Static compilation on 32-bit system

The following choices were made for running the executable:

- Number of processors: 8
- Domain decomposition for parallel processing: 4 columns, 2 rows
- Number of species written to the layer-1 hourly-average concentration output (ACONC) file: 39 (O3, NO, CO, NO2, HNO3, N2O5, HONO, PNA, PAN, NTR, NH3, SO2, FORM, ALD2, PAR, OLE, ETH, TOL, XYL, ISOP, ASO4I, ASO4J, ANO3I, ANO3J, ANH4I, ANH4J, AORGAI, AORGAJ, AORGPAI, AORGPAJ, AORGBI, AORGBJ, AECI, AECJ, A25I, A25J, ACORS, ASEAS, ASOIL)
- Each daily simulation was performed for 24 hours starting at 05:00 GMT (00:00 EST)

The following postprocessing steps were performed using utility tools from the "ioapi" software package obtained from http://www.baronams.com/products/ioapi/AA.html#tools:

- Extract and combine the following species for each hour for the first 16 model layers from the full 3-D instantaneous concentration output file: O3, CO, NO, NO2, NOY_1 (=*NO* + *NO2* + *PAN* + *HNO3*), NOY_2 (=*NO* + *NO2* + *PAN* + *HNO3* + *HONO* + *N2O5* + *NO3* + *PNA* + *NTR*), HOX (=*OH* + *HO2*), VOC (=*2*ALD2* + *2*ETH* + *FORM* + *5*ISOP* + *2*OLE* + *PAR* + *7*TOL* + *8*XYL*), ISOP, PM2.5 (=*ASO4I* + *ASO4J* + *ANO3I* + *ANO3J* + *ANH4I* + *ANH4J* + *AORGAI* + *AORGAJ* + *1.167*AORGPAI* + *1.167*AORGPAJ* + *AORGBI* + *AORGBJ* + *AECI* + *AECJ* + *A25I* + *A25J*), PM_SULF (=*ASO4I* + *ASO4J*), PM_NITR (=*ANO3I* + *ANO3J*), PM_AMM (=*ANH4I* + *ANH4J*), PM_ORG_SA (=*AORGAI* + *AORGAJ*), PM_ORG_PA (=*1.167*AORGPAI* + *1.167*AORGPAJ*), PM_ORG_SB(=*AORGBI* + *AORGBJ*), PM_ORG_TOT (=*AORGAI* + *AORGAJ* + *1.167*AORGPAI* + *1.167*AORGPAJ* + *AORGBI* + *AORGBJ*), PM_EC (=*AECI* + *AECJ*), PM_OTH (=*A25I* + *A25J*), PM_COARS (=*ACORS* + *ASEAS* + *ASOIL*), SO2, HNO3, NH3, H2O2
- Extract all species for all model layers for the last hour of each daily instantaneous concentration output file to enable "hot" restarts of modeling simulations
- Create daily files of hourly running-average 8-hr ozone concentrations with time stamps assigned to the first hour of the averaging interval

The following files are archived on LTO2 computer tapes (each tape holds approximately 200 Gb of data) for each day:

- Aerosol/visibility file
- Layer-1 hourly-average concentration output file (contains 39 species)
- Dry deposition file
- Wet deposition file
- Extracted 16-layer species file
- Restart file (last hour of full 3-D instantaneous concentration file)
- Hourly 8-hr concentration file

Photolysis Rates

One of the inputs to CMAQ is the photolysis rates. In this study, photolysis rate lookup tables were generated for each day of 2002 with the JPROC software that is part of the CMAQ modeling package. This software was obtained from the CMAS modeling center at http://www.cmascenter.org. Rather than using climatological ozone column data, daily ozone column measurements from the NASA Earthprobe TOMS instrument were downloaded from ftp://toms.gsfc.nasa.gov/pub/eptoms/data/ozone/Y2002/ and used as input to the JPROC processor. It should be noted that TOMS data were missing for the time period from August 3 – 11, 2002. The missing period was filled as follows-- TOMS data file for August 2 was used as JPROC input for August 3rd through August 7th, and the TOMS data file for August 12th was used as JPROC input for August 8th through August 11th.

Boundary Conditions (BCs)

The boundary conditions for the 12km grid were extracted from the 36km CMAQ simulation. The 36km simulation utilized boundary conditions that were based on a one-way nest approach to GEOS-CHEM global model outputs (Moon and Byun 2004, Baker 2005). As stated above, the intent of the 36km CMAQ simulation was to provide the BCs for the 12km model that would be more reflective of the emissions and meteorology rather than to use either clean or arbitrary pollutant fields. Also, in this study the CMAQ simulations utilized a 15-day ramp-up period, thereby minimizing the propagation of the boundary fields into the areas of concern. A report on the setup and application of the 36km CMAQ and the extraction of the BCs is available from NYSDEC.

Meteorological data

The meteorological data for this study was based on MM5 modeling (see Meteorological Modeling, 2007). The MM5 fields are then processed by MCIP version 3.0, a utility available as part of the CCTM software from CMAS Modeling Center (see http://www.cmascenter.org) to provide CMAQ model-ready inputs.

Emissions

The emissions data for 2002 were generated by individual states within the OTR and were assembled and processed through the Mid Atlantic Northeast Visibility Union (MANE-VU), a Regional Planning Organization (RPO). These emissions were then processed by NYSDEC using SMOKE processor to provide CMAQ compatible inputs (Anthro-Emissions 2006). The 2002 emissions for the non-OTR areas within the modeling domain were obtained from the corresponding RPOs and were processed using SMOKE, in a manner similar to that of the OTR.emissions. Details of this processing are outlined in the report (Pechan 2007), and the hourly biogenic emissions (Bio-Emissions, 2006)

CMAQ simulations

CMAQ simulations were performed using the one-way nesting approach in which we perform the continental CMAQ simulation at 36km grid spacing. For this simulation we utilized clean initial conditions with boundary conditions extracted from the simulation of GEOS-CHEM global chemical model. The interface program used in this application was developed by University of Huston (Moon and Byun 2004), which was applied to obtain hourly 36km boundary concentrations from GEOS-CHEM outputs. The CMAQ 36km simulation was initiated from December 15, 2001 with the first 15 days as spin up period and terminated on December 31, 2002. The simulation utilized the 2002 emissions data available from the RPOs and 2002 MM5 meteorological fields developed by the University of Maryland (TSD-1a). The hourly boundary fields for the 12km CMAQ domain were obtained by application of BCON program to the 3-D concentration fields generated by the 36km CMAQ simulation.

The 12km simulations for both base and future year were assigned the boundary conditions based on the 36km CMAQ simulation and clean initial conditions. The simulation period covered was from April 15 through September 30, with the first 15 days of April set as ramp-up or spin-up period and that only data from May 1 through September 30 were used in the analysis. Details on CMAQ setup and run scripts are available from NYSDEC.

References

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