DEASCO3 – Revised 2002 Base B Simulation Specifications

Scenario Name: CAMx OSAT/PSAT 2002 Base Simulation version B

DEASCO3 Code: "SA_Base02b"

Date Specifications Prepared: May 1, 2012

Time Window for Modeling/Analysis: Emissions modeling start date – use existing Base02b emissions & lightning NOx emissions; Start simulation on April 25, 2012; Complete results analysis by May 31, 2012.

Description: 2002 Annual 36 km CAMx ozone and particulate source apportionment technology (OSAT/PSAT) model simulation using actual 2002 emissions

Purpose/Objective: Identify contributions of fire emissions to modeled 8-hour ozone concentrations for actual 2002 year conditions.

Expected Analysis Methods: Specific analysis methods will generally be determined based on the nature of the simulation and the stated purpose and objectives. These typically involve a number of standard post-processing products used to elucidate relevant modeling results and analyses and aid in summarizing and interpreting the simulation results. For the present simulation these would include:

- Source Apportionment Tracers - run ozone, NO_X, VOC, primary PM, SO_4 and NO_3 tracers, state-specific source regions in western U.S. and 3 source categories
    - Ozone Source Apportionment Technology (OSAT)
    - Particulate Source Apportionment Technology (PSAT)
- Spatial plots and/or animations of modeled contributions of fire emissions to 8-hour ozone concentrations, overlaid with observed daily maximum 8-hour ozone concentrations
- Other displays TBD based on discussions with DEASCO3 team and FLM "inner circle" collaborators

Input Data:

Emissions – Emission data are based on Base02b emission inventory (see WRAP RMC SpecSheet[1] for reference). The three OSAT emission source groups include:

- Biogenic
    - BEIS3 biogenic emissions

[1] http://pah.cert.ucr.edu/aqm/308/spec_sheets/RMC_Model_run_specification_base02b_05_10_2006.doc

- All Fires
  - CENRAP area source fires
  - WRAP wild/prescribed/agricultural point source fires
  - CENRAP and VISTAS point source fires
  - Canadian point source fires
- Everything else
  - Area sources except dust
  - Wind-blown/road dust emissions
  - On-/off-road mobile sources
  - Eastern pacific commercial shipping lane
  - Off-shore area/point sources
  - Ammonia emissions
  - WRAP Oil & gas emissions
  - Point sources
- New Emissions
  - Add lightning NOx emissions from CRC Background Study[2]

Emissions Processing Approach

- Start with CMAQ pre-merged emission files from WRAP RMC archives
- Merge CMAQ emissions files for each OSAT source group
- Convert the merged CMAQ emissions files into CAMx emissions file format using CMAQ2CAMx

<u>Other Ancillary Inputs and Model Settings</u>

- See "Summary of Key Findings" in the below section.
- Time period simulated – annual, actual year, meteorology for 2002 used
- Source apportionment (OSAT/PSAT):
  - 24 Source Regions (see Figure 1 and Table 1 below)
  - 3 Source Categories: (1) Biogenic+Lightning; (2) All Fires (WF, Rx, Ag); and (3) Remainder
  - Initial Concentration (IC) and stratified Boundary Condition (BC) adds 6 Source Groups
  - 78 Source Groups (78=24×3+6) with OSAT (4 Tracers), PSAT SO4 (2 Tracers), PSAT NO3 (7 Tracers) and PSAT Primary PM (6 Tracers) means we are adding 1482 new species to simulation
  - Running all the tracers in a single simulation is not practical (memory and run time issues) → Two separate runs: (1) OSAT; and (2) PSAT
    - For OSAT, run with 24 Source Regions as in Table 1 (results in 312 new tracer species)
    - For PSAT, run with just one source region and no stratified BC (results in 75 new tracer species)

[2] Koo et al., Natural emissions for regional modeling of background ozone and particulate matter and impacts on emissions control strategies, Atmos. Environ., 44, 2372-2382, 2010.

Table 1. Definitions of the 24 Source Regions to be used in the DEASCO3 2002 OSAT source apportionment run.

24 Source Regions corresponding to 16 individual western states and separate groups for Texas+New Mexico, Great Basin, North Great Plains, Northeastern Quarter, Southeastern Central, Canada, Mexico, and offshore								
16 individual states	**Tex-Mex**	**Great Basin**	**North Great Plains**	**NE Quarter**	**SE Central**	**Canada**	**Mexico**	**Offshore**
Alabama	Texas	Nevada	South Dakota	West Virginia	North Carolina	Canada	Mexico	Offshore
Arizona	New Mexico	Utah	Minnesota	Delaware	Tennessee			
California			Iowa	Maryland	Mississippi			
Colorado			North Dakota	Virginia				
Florida			Nebraska	New Jersey				
Georgia			Missouri	Pennsylvania				
Kansas				New York				
Idaho				Vermont				
Montana				New Hampshire				
Oklahoma				Maine				
Oregon				Massachusetts				
South Carolina				Connecticut				
Washington				Rhode Island				
Wyoming				Wisconsin				
Louisiana				Michigan				
Arkansas				Illinois				
				Ohio				
				Indiana				
				Kentucky				

Results

Relevant Output Products

- Spatial plots or animations of modeled contributions of fire emissions to 8-hour ozone concentrations, overlaid with observed daily maximum 8-hour ozone concentrations.
- Spreadsheets of observed and modeled total and modeled fire contributions for ozone, NO_X, EC, OC, SO_4, NO_3 and other $PM_{2.5}$ at monitoring sites (AQS, IMPROVE, CASTNet and STN).
- Animation of gridded fire emissions and fire ozone contributions.
- Other TBD.

Summary of Key Findings

Source apportionment (OSAT/PSAT) simulations for 2002 are being performed with modified CAMx v5.40 that can get separate contributions of stratospheric and tropospheric ozone boundary conditions. Table 2 tabulates the overall information for the simulations. The domain setup is tabulated in Table 3. The CAMx runtime options are shown in Table 4. Figure 1 shows

the modeling domain used in the simulation with the Source Regions defined. The three emission source groups are described in Table 5. The initial and boundary conditions for the simulation came from a 2002 GEOS-CHEM simulation. We allowed 2 weeks of spin-up days prior to the beginning of simulation.

Table 2. DEASCO3 2002 CAMx run specs.

Simulation specs	Description
Model	Modified CAMx v5.40 (www.camx.com)
OS / Compiler	Linux / pgf90 8.0-2 64-bit
Compute node	Dual hexa-core Intel Xeon CPUs w/ 48 GB of RAM
Domain setup	see Table 3
Runtime options	see Table 4
Source region	24 source regions, see Figure 1
Emission source groups	Base02b, 3 source categories, see Table 5
Initial Condition	IC from a 2002 GEOS-CHEM simulation
Boundary Conditions	3-hourly BC from a 2002 GEOS-CHEM simulation

Table 3. 2002 CAMx Domain setup.

WRAP PSAT specs	Description
Map projection	Lambert projection (RPO unified grid)
Center meridian	-97
Center longitude	-97
Center latitude	40
True latitude 1	45
True latitude 2	33
Number of columns	148
Number of rows	112
Number of layers	19
Grid resolution	36 km
Time zone	UTC

Table 4. CAMx runtime options.

WRAP PSAT specs	Description
Advection solver	PPM
Chemistry parameters	CAMx5.4.chemparam.6_CF (CB05 chemistry mechanism)
Chemistry solver	EBI
Plume-in-grid	not used
Probing tool	OSAT source apportionment for ozone, NO_X and VOC (w/ 24 Source Regions) PSAT source apportionment for SO_4, NO_3 and primary PM (w/ 1 Source Region)
Dry/wet deposition	TRUE (turned on)
Staggered winds	TRUE (turned on)

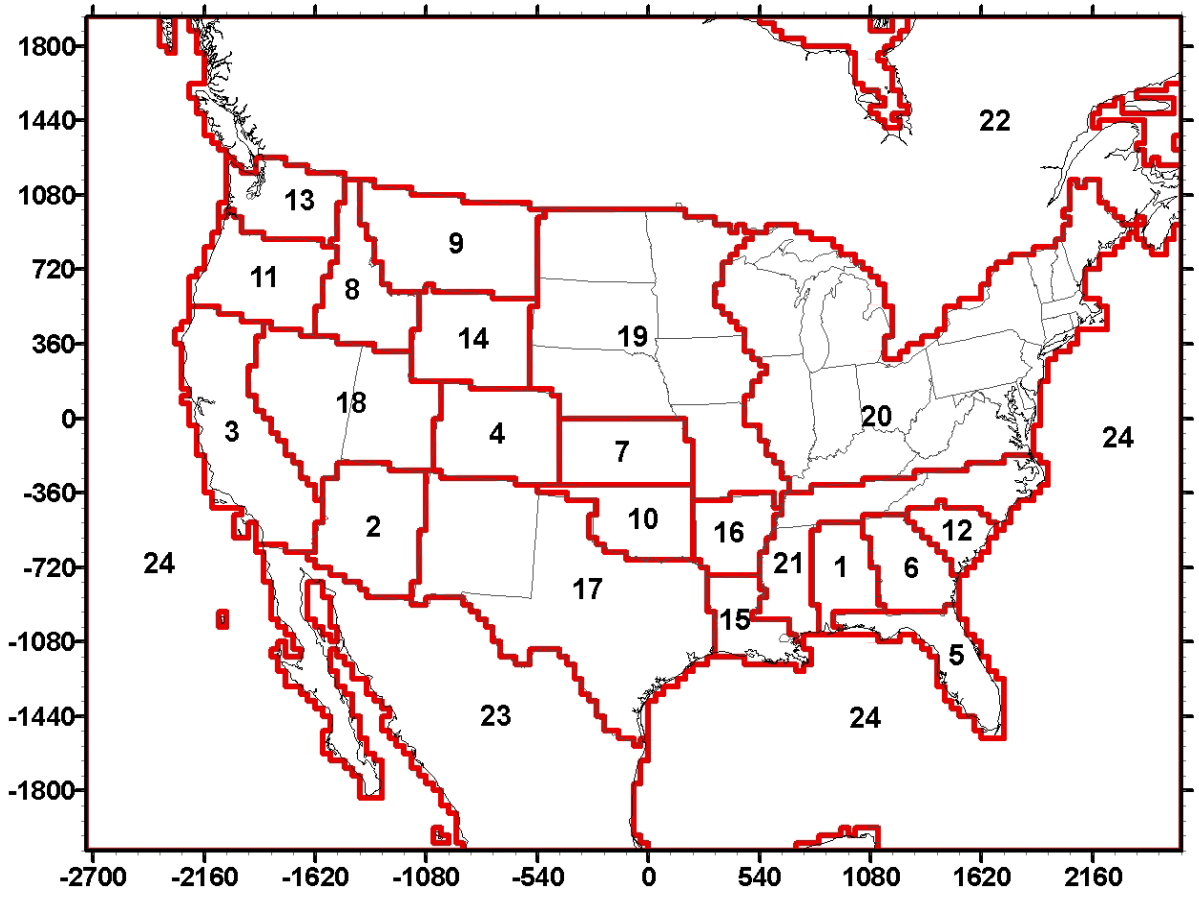

Figure 1. Modeling domain for the DEASCO3 2002 OSAT/PSAT simulation (24 source regions shown in red).

Table 5. DEASCO3 OSAT/PSAT emission source groups

Emissions Source Groups	Low-level Sources	Elevated Sources
1	Biogenic sources	Lightning
2	All fires (low-level)	All fires (elevated)
3	Everything else (low-level)	Everything else (elevated)

Interpretation/Recommendations

Will obtain separate contribution of fire emissions, as well as natural (biogenic+lightning) and anthropogenic emissions, from 24 Source Regions to ozone through CONUS domain. Also will have separate contributions due to stratospheric ozone and international transport (i.e., tropospheric ozone boundary conditions).

Analysis approach: Animations of modeled total ozone, modeled ozone due to all fires, fire emissions and observed ozone concentrations focusing on daily maximum ozone concentrations and 36 km CONUS domain. Subregional animations for Case Studies. Extract modeling results at monitoring sites for use in Empirical Tool.