

PMDETAIL – 2011 PSAT Simulation Specifications

Scenario Name: CAMx 2011 PSAT Simulation (preliminary and full scenarios)

PMDETAIL Code: “PSAT11pre” and “PSAT11full”

Date Last Updated: June 5, 2014

Time Window for Modeling/Analysis: Modeling start date – late June 2014 for PSAT11pre.

Description: 36/12 km CAMx particulate source apportionment technology (PSAT) simulation of 2011 annual period using the 3SAQS 2011 base case modeling platform with revised 2011 fire emissions from Air Sciences that includes levoglucosan emissions from fires.

Purpose/Objective

- PSAT11pre – (1) Identify the filter samples for detailed re-analysis by CSU; (2) select 10-20 case studies for the CAMx VBS modeling by ENVIRON and PMCAMx-SR VBS modeling by CMU; and (3) identify periods in PSAT11full to turn on PSAT SOA tracers.
- PSAT11full – Obtain separate contributions of fine particulate matter (PM_{2.5}) concentrations due to emissions from wildfires (WF), prescribed burns (Rx), agricultural burning (Ag), and other biomass burning (BB) to modeled PM concentrations for the 2011 annual period

Input Data

Emissions – Emission data are based on the 3SAQS 2011 base case modeling database which includes the revised 2011 fire emissions with levoglucosan from Air Sciences. The five types of PSAT emission source groups for PSAT11full are:

- Wildfires (WF)
- Prescribed burns (Rx)
- Agricultural burning (Ag)
- Other biomass burning (BB)
- Everything else

PSAT11pre will use a combined fire (WF+Rx+Ag) source category.

Emissions Processing Approach

- Re-process 2011 NEI point and non-point emissions to separate out emissions associated with biomass burning (e.g., fireplaces, woodstoves, biomass generation, open pit burning, etc.).
- Add levoglucosan emissions to 2011 NEI biomass burning sources (e.g., ratio off of PM_{2.5}).
- Prepare the source apportionment emission inputs for four fire types (WF, Rx, Ag & BB) using the CAMx compact point source feature.

Other Ancillary Inputs and Model Settings

- CAMx v6.10 (www.camx.com; released on April 4, 2014).
- The Carbon Bond 6 Revision 2 (CB6r2) mechanism.
- The met/ozone column/photolysis rate inputs from the 2011 3SAQS base case modeling database.
- Time period simulated: Annual period of 2011.
- Domains: 36 km CONUS and 12 km WESTUS (PSAT11full only) domains using two-way grid nesting (Figure 1).
- Source apportionment (PSAT11full):
 - 1 Source Region.
 - 5 Source Categories: (1) WF; (2) Rx; (3) Ag; (4) BB; and (5) Remainder.
 - Initial Concentration (IC) and Boundary Condition (BC).
 - PSAT tracers.
 - 2 tracers for sulfur
 - 7 tracers for nitrogen
 - 20 tracers for SOA (only for selected sub-periods)
 - 6 tracers for primary PM
 - Total 105 (or 245 w/ SOA tracers) source group tracers.
- Spin-up:
 - December 22-31, 2010 (10 days).
- Multi-Processing Strategy
 - Each run will use 24 CPUs using 12 CPUs with MPI (domain decomposition) and 2 CPUs with OpenMP (compiler directives) multiprocessing approaches.

Modeling Scenarios

	PSAT11pre	PSAT11full
Modeling Grid	36 km only	36/12 km 2-way nesting
PSAT Source Category	<ul style="list-style-type: none">• Combined fires (WF+Rx+Ag; BB not separated from point/non-point emissions)• Everything else	<ul style="list-style-type: none">• WF• Rx• Ag• BB• Everything else
PSAT Tracer	<ul style="list-style-type: none">• Primary PM	<ul style="list-style-type: none">• Sulfur• Nitrogen• SOA (for selected sub-periods)• Primary PM

Levoglucosan Modeling

CAMx is modified to model total (gas + aerosol) levoglucosan. Two levoglucosan tracers are added: One as an inert species (LEVO) and the other with chemical decay (LVGC). Chemical

decay of levoglucosan is modeled by a second-order oxidation reaction with hydroxyl (OH) radicals:

$$[\text{LVGC}] = [\text{LVGC}]_0 \exp(-k [\text{OH}] t)$$

We employ the effective rate constant (k) of $3 \times 10^{-11} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ estimated by Hennigan et al. (2011) which is based on the smog chamber studies during the third Fire Lab at Missoula Experiment (FLAME III) using various fuels commonly burned in North American wildfires. Both LEVO and LVGC will be removed by wet and dry deposition as a component of internally-mixed fine particle ($\text{PM}_{2.5}$).

Results

Relevant Output Products

- List of filter samples identified for re-analysis by CSU (PSAT11pre).
- 10-20 case studies selected for the subsequent VBS modeling by ENVIRON and CMU (PSAT11pre).
- Spatial plots and/or animations of modeled contributions of 2011 fire emissions to $\text{PM}_{2.5}$ concentrations, overlaid with observed $\text{PM}_{2.5}$ concentrations (PSAT11full).
- Database of observed and modeled total and modeled fire contributions for SO_4 , NO_3 , EC, OC, and other $\text{PM}_{2.5}$ at monitoring sites (IMPROVE, CSN and FRM): For use with the Empirical Assessment Tool (PSAT11full).
- Other TBD.

Interpretation/Recommendations

Will obtain separate contribution of 2011 fire emissions to $\text{PM}_{2.5}$ throughout the CONUS and WESTUS domains for use with the Empirical Assessment Tool. Generate spatial plots of modeled $\text{PM}_{2.5}$, fire contributions, fire emissions and observed $\text{PM}_{2.5}$. Additional displays will be generated as needed.

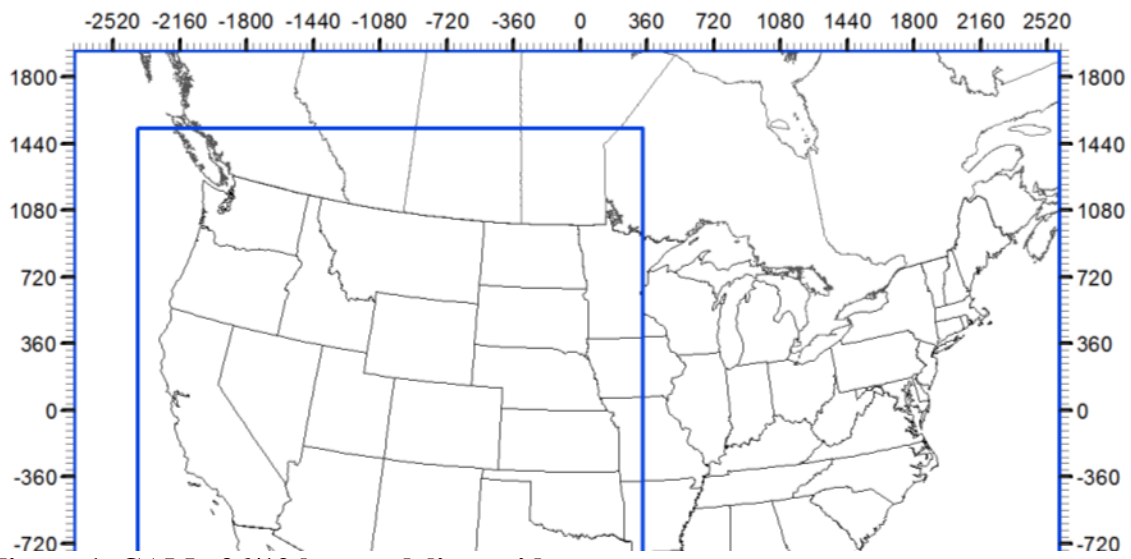


Figure 1. CAMx 36/12 km modeling grids.