

RELEASE NOTES for CAMx v5.40, 10/10/11

The Comprehensive Air Quality Model with extensions (CAMx) is available at <http://www.camx.com>.

Join the CAMx User's Group by sending an e-mail message to:

majordomo "at" environ "dot" org

Put the words "subscribe CAMxusers" in the body of the message. When you subscribe, Majordomo will send you a reply that provides details on how to use this list server.

The "camxusers" group is meant for broadcasting useful information about CAMx and its pre- and post-processors to all users that subscribe to this group, or to ask about available datasets or issues that other users may have come across. It is not meant for asking how to run CAMx, how to prepare inputs, or why CAMx arrived at a particular prediction.

Please direct specific comments or questions about problems or bugs with CAMx or its support software to:

ask-camx "at" environ "dot" org

which comes directly to the developers.

Overview of Version 5.40

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V5.40 includes several updates, modifications and bug fixes from the previous release (v5.30). The new capabilities in CAMx include the next version of the Carbon Bond gas-phase photochemical mechanism (CB6) and an option to treat PM attenuation of clear-sky photolysis rates.

- \* New chemistry parameters files are provided to support CB6.
- \* Use the chemistry parameters files specifically labeled for v5.40. Default light extinction parameters are now set for all aerosol species and deposition parameters for many gas species have been updated.
- \* There are no changes to other input file formats from versions 4.3 through 5.3.
- \* There are no changes to core model output file formats from versions 4.4 through 5.3.
- \* There are no changes to Probing Tool outputs since version 5.1.

Since v5.0, CAMx is capable of distributed multi-processing using MPI. To use MPI you must have the MPICH or MPICH2 utility installed on your system. We strongly recommend using MPICH2. Guidance for running MPI and OMP parallelization is provided in the README file located in the source code directory, and in the CAMx User's Guide.

v5.40 Updates

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1. Version 6 of the Carbon Bond photochemical mechanism (CB6) is now available. All CB4 variants have been removed. The current gas-phase mechanisms include CB05, CB6, and SAPRC99, and all support CF and CMU PM chemistry and Process Analysis.

Implications: CB6 extensively revises CB05 with the core inorganic chemistry updated to 2010 and major revisions to the chemistry for aromatics, isoprene, alkenes, alkanes and oxygenates. Several long-lived and abundant VOCs are added explicitly and could be added to emission inventories. Several alpha-dicarbonyls are included because they are SOA precursors. Compared to CB05, more rapid ozone formation is expected for VOC sensitive conditions with less change in ozone for NOx-limited conditions. CB6 has greater computational requirements than CB05. CB6 can be used with CB05 format emission inventories.

2. The in-line TUV adjustment of clear-sky photolysis rates was expanded to account for the effects of simulated PM concentrations as the model runs. This update includes an improved way to define the PM model to use in concert with gas-phase chemistry: aerosol options are NONE, INERT, CF, and CMU.

Implications: Aerosol optical properties are defined in the chemistry parameters file and passed to the in-line TUV algorithm. The albedo/haze/ozone and clear-sky photolysis input files must be generated with the first haze bin set to zero opacity to avoid double-counting of haze effects. Arbitrarily named inert PM species with user-defined size bins can be specified in the chemistry parameters file. See the CAMx User's Guide for more details.

#### v5.40 Modifications

1. Improved MPI efficiency by reducing the amount of data passed back to the master node each hour.

Implications: MPI applications are faster with improved scalability to higher numbers of CPUs, especially for large applications (large/many grids, Probing Tools).

2. Two internal and transparent structural modifications:
  - a) Dimensions and MPI passing of "height" and "depth" arrays are handled similarly as all other met variables;
  - b) Radicals and 'state' species concentrations are combined into a single vector.

Implications: No changes in model speed or to output concentrations relative to v5.30.

3. PiG puff growth rates were modified to ignore growth contributions from horizontal and vertical shear during

stable/nighttime conditions. Shear effects remain during neutral/unstable/daytime conditions. Reduced minimum limits on vertical diffusivity, turbulent flux moment, and nighttime PBL depth.

Implications: These changes stem from comparing observed nocturnal plume dimensions against PiG. PiG puff behavior will change potentially significantly at night and above the boundary layer, usually leading to longer lifetimes before dumping to the grid.

#### v5.30 Bug Fixes

1. Improved the vertical advection of source apportionment tracers.

Implications: The source apportionment vertical advection routine was found to cause small spurious tracer concentration increments that could grow in time. Negligible to minor impacts in source apportionment results (OSAT and PSAT) should be expected.

2. The internal dimensioning of landuse arrays was improved to be more robust.

Implications: This fix alleviates a model crash when dry deposition is turned off. In such cases the number of landuse categories was not set and prohibited dynamic allocation of certain variables.

3. Fixed a bug in domain decomposition for MPI with 2 or more nests of the same generation.

Implications: Domain decomposition is now performed correctly and alleviates possible model crashes. The nested boundary conditions are now inherited from the correct grid.

4. Fixed a bug that prohibited nested grids from inheriting the source area map from the parent when running DDM.

Implications: If a DDM run included a nest but only a source area map for the parent was provided, all of the cells in the nest would be assigned to region 0. This would effectively eliminate them from the DDM calculations. This has been fixed.

5. Changed the meteorological update of boundary conditions for OSAT/DDM (used to convert from mixing ratio to density) to only apply at true grid boundaries, not MPI slice boundaries.

Implications: Insignificant impact on output tracer/DDM fields at the seam of the MPI slices.

6. Code that handles seasonal LAI adjustments in routine SRFRUF was simplified to be consistent with routine DRYDEP.

Implications: No impact on output concentrations or deposition.

7. A flag was added to explicitly turn off chemistry in PiG when the user-defined Mechanism 10 is run.

Implications: This change ensures that no chemistry is run in PiG with Mech 10 invoked.

8. Fixed a bug that caused an error when reading the boundary condition file for source apportionment when timestamp crossed over the new year.

Implications: Now adjusts date/time properly for crossing over a new year.

9. Fixed a bug in several file-writing routines that caused an improper date stamp on concentration and deposition output files at midnight of a new year.

Implications: No impact for most users, except now post-processors and boundary extraction programs will work more correctly when crossing over a new year.