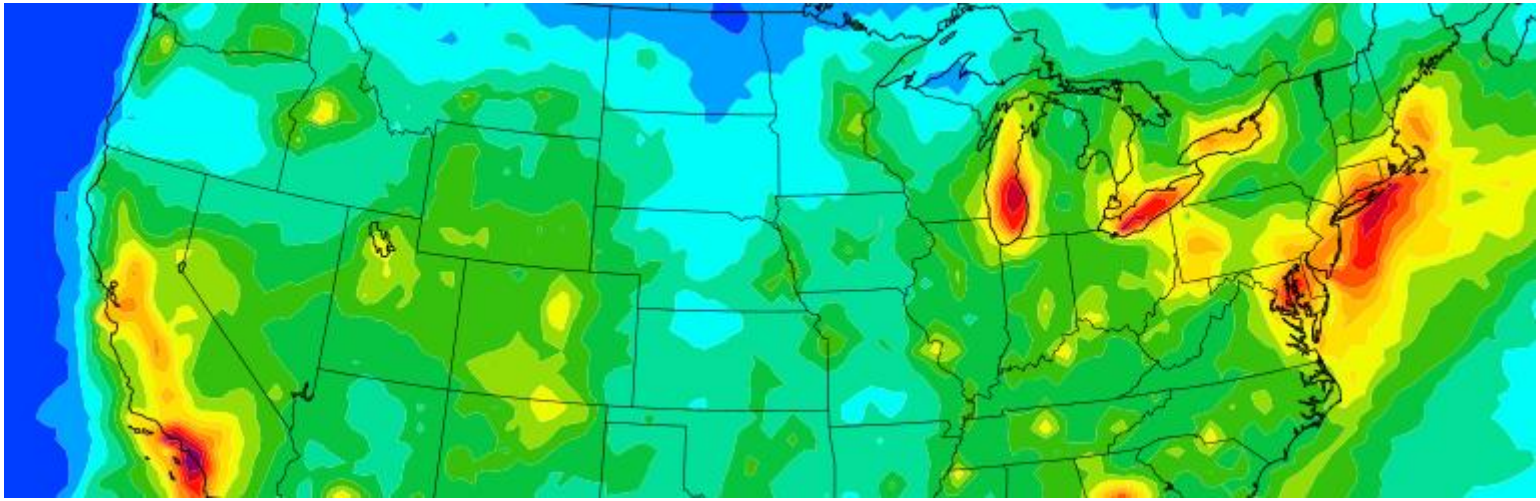
CMAQ and CAMx Overview and Recent Updates



2014 Midwest and Central States Air Quality Workshop

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ENVIRON

CMAQ Overview

- Community Multi-scale Air Quality modeling system, v5.0.1
  - Developed and maintained by EPA/ORD/NERL/AMAD
  - Distributed and supported by the Community Modeling and Analysis System (CMAS)
    - Center for Environmental Modeling for Policy Development (CEMPD), University of North Carolina at Chapel Hill (UNC) Institute for the Environment (IE)
    - www.cmas.org: source code, on-line documentation, links to other data, information, and papers
  - Open source, community-based contributions

CMAQ Overview

- Computer platforms
  - Linux multi-core work stations and cluster systems
- Source code
  - CVS version-controlled Fortran tar files
    - CVS must be installed prior
  - **Bldmake** extracts and builds a CMAQ executable
    - C and Fortran90 compilers must be installed prior
- Required 3rd-party libraries
  - MPICH for MPI distributed-memory parallelization
  - netCDF and I/O API (v3.1) file management routines
  - LAPCAK for bi-directional mercury module

CMAQ Overview

- Major system components
  - ICON/BCON: initial/boundary conditions
  - JPROC: clear-sky photolysis rates (now optional)
  - MCIP: meteorological interface with WRF, MM5
  - CCTM: chemistry-transport model
  - PROCAN: code for process analysis (optional)
  - CHEMMECH: chemical mechanism inputs (optional)
  - LTNG_2D_DATA: lightning NOx generator (optional)

CMAQ Overview

- CCTM major features
  - Single-grid, 1-way nesting supported
  - CB05, SAPRC07, SAPRC99 photochemistry
    - ROS3, EBI, SMVGEAR solvers
    - Chlorine, mercury, toxics can be included in CB05
    - External clear-sky photolysis rates OR in-line photolysis rates
      - Account for modeled O_3, PM, clouds, temperature
  - PM chemistry; 3-mode size treatment
    - AERO5: primary, inorganic, organic components
    - AERO6: splits primary PM into many elemental species
    - ISORROPIA (v2.1) for inorganic chemistry
    - RADM-AQ for aqueous chemistry
    - SOA chemistry: 10 anthro, 7 bio semi/non-volatile species

CMAQ Overview

- CCTM major features (continued)
  - Horizontal & vertical advection
    - Mass conservative and consistent
    - Piecewise Parabolic Method
    - In-line vertical velocity from input density, horizontal winds
  - Vertical diffusion
    - Asymmetric Convective Model (ACM2)
  - Multiple cloud treatments (chemistry, wet removal)
    - Grid-resolved clouds (from met model)
    - Precipitating sub-grid clouds (diagnosed)
    - Non-precipitating sub-grid clouds (diagnosed)
    - Sub-grid cloud convective mixing using ACM2

CMAQ Overview

- CCTM major features (continued)
  - Dry deposition
    - M3DRY tied to WRF/MM5 Pleim-Xu surface model
    - Bi-directional ammonia and mercury
    - MOSAIC configuration outputs landuse-specific fluxes
  - Emissions
    - Gridded, speciated, temporalized (SMOKE, CONCEPT)
    - In-line BIES3 option for biogenics
    - In-line point source plume rise option
    - In-line windblown dust option
    - In-line sea salt option
  - Process Analysis – informs on physical/chemical processes

New in CMAQ v5.0

- v5.0 released February 2012
  - v5.0.1 released July 2012
    - Bug fixes and minor code enhancements
- PM updates
  - AERO6 treatment
  - ISORROPIA v2.1
  - Updates to SOA yield parameterization
  - Other code/efficiency improvements
  - In-line windblown dust module
  - Sulfur chemistry updates

New in CMAQ v5.0

- Gas chemistry updates
  - CBO5
    - Updated toluene/xylene reactions
    - Revised rate constants for N_2O_5 hydrolysis
  - SAPRC07
    - Updated organic and inorganic reactions
    - Updated photolysis rates
    - Better representation of reactions in low-NOx conditions
    - Additional explicit species with high emissions, high toxicity, or high SOA formation
  - Enhanced in-line photolysis model
  - Expanded surface albedo calculation
    - Land use, zenith angle, seasonal vegetation, snow/sea ice

New in CMAQ v5.0

- Updated sub-grid cloud module
  - Coordinated with MCIP v4.0
  - Minimum grid resolution was removed
- Updated ACM2 vertical diffusion
  - Modified diffusivity for stable conditions
  - Reduced minimum diffusivity
  - Coordinated with WRF v3.4
- Updated vertical advection
  - Based on WRF method
  - Zero flux top boundary condition

New in CMAQ v5.0

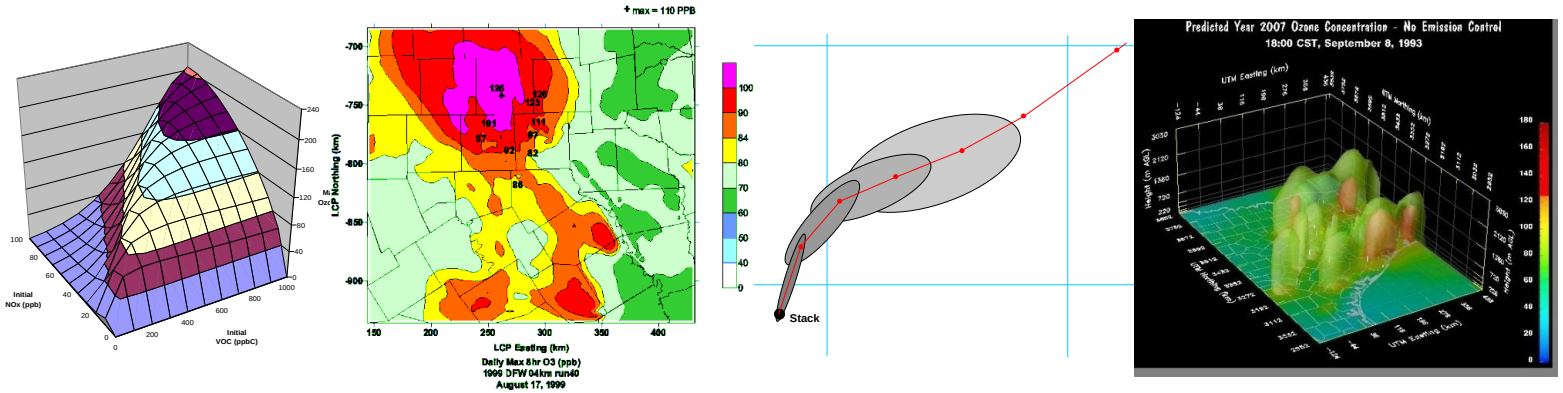
- Optional lightning NOx treatments
  - Off-line, from a 4-D file
  - In-line, informed by lightning detection data
  - Fully in-line (automated from input met)
- Updated dry deposition
  - Bi-directional ammonia and mercury
  - New mesophyll resistance
  - Option to output land use specific deposition velocity and flux

Coming in CMAQ v5.0.2

- Expected release in April 2014
  - EPA “base” model
  - Separate “instrumented community” versions
  - WRF-CMAQ coupled system
- Instrumented Models
  - Integrated Source Apportionment Method (ISAM)
  - Direct Decoupled Method (DDM) for ozone and PM
  - Sulfur Tracking by chemical/physical process (like PA)
- Chemistry updates
  - Volatility Basis Set (VBS) for SOA
  - SOA yield updates
  - Photolysis updates (CB05 quantum yields, snow, LU)
- Advanced Plume Treatment (APT)
  - Plume-in-Grid based on SCICHEM puff model

CAMx Overview

- Comprehensive Air quality Model with extensions, v6.10
  - Developed, maintained, distributed, and supported by ENVIRON Corporation
    - www.camx.com: source code, documentation, links to other data, information, and papers
  - Open source, community-sponsored developments



CAMx Overview

- Computer platforms
  - Linux multi-core work stations and cluster systems
- Source code
  - Fortran/C tar files
  - **Makefile** builds a CAMx executable
    - C and Fortran90 compilers must be installed prior
    - OMP-compatible compilers needed for shared-memory parallelization
- Required 3rd-party libraries
  - MPICH, MVAPICH or OpenMPI for MPI distributed-memory parallelization
- OMP and/or MPI parallelization can be used

CAMx Overview

- Supporting tools
  - GEOS2CAMx, MOZART2CAMx: initial/boundary conditions
  - TUV/O3MAP: clear-sky photolysis rates
  - WRFCAMx, MM5CAMx, RAMSCAMx: meteorological interface with WRF, MM5, RAMS
  - KVPATCH: adjusts diffusivity for LU, clouds (optional)
  - PIGSET: sets point sources for PiG treatment (optional)
  - SEASALT: calculates sea salt emissions (optional)
  - CAMx2IOAPI: translates CAMx output to Models-3 netCDF/IO-API formats (optional)
  - CMAQ2CAMx: translates CMAQ emissions, IC/BC to CAMx formats (optional)

CAMx Overview

- CAMx major features
  - 2-way nesting, 1-way nesting supported
    - Flexi-nesting
  - CB6, CB05, SAPRC99 photochemistry
    - EBI, IEH, LSODE solvers
    - Halogens, mercury can be included in CB6/CB05
    - Toxics treated by RTRAC add-on
    - External clear-sky photolysis rates
      - In-line adjustment for modeled PM, clouds, temperature, pressure
  - PM chemistry; 2-mode or sectional size treatments
    - primary, inorganic, organic components
    - ISORROPIA (v1.7) for inorganic chemistry
    - RADM-AQ for aqueous chemistry
    - SOAP for organic aerosols: 9 semi/non-volatile species

CAMx Overview

- CAMx major features (continued)
  - Horizontal & vertical advection
    - Mass conservative and consistent
    - Horizontal: Piecewise Parabolic Method or Bott
    - In-line vertical velocity from input density, horizontal winds
    - Vertical: Implicit hybrid centered/upstream scheme
  - Vertical diffusion
    - K-theory – implicit solver
    - Asymmetric Convective Model (ACM2) – explicit solver
  - Multiple cloud treatments (chemistry, wet removal)
    - Grid-resolved clouds (from met model)
    - Precipitating sub-grid clouds (diagnosed)
    - Non-precipitating sub-grid clouds (diagnosed)
    - No sub-grid cloud convective mixing

CAMx Overview

- CAMx major features (continued)
  - Dry deposition
    - Zhang gas/PM treatment (26 LU categories), OR
    - Wesely gas, Slinn&Slinn PM treatments (11 LU categories)
  - Surface model
    - Deposition, surface chemistry, re-emission
  - Plume-in-Grid (PiG)
    - Fast inorganic (NOy) chemistry and PM (GREASD)
    - CB6/CB05/SAPRC99 organic (NOx+VOC) chemistry (IRON)
  - Emissions
    - Gridded, speciated, temporalized (SMOKE, CONCEPT, EPS3)
    - All emissions are supplied via external files
    - In-line point source plume rise or set externally

CAMx Overview

- CAMx major features (continued)
  - Probing Tool extensions
    - Ozone/PM source apportionment technology (O/PSAT)
    - Direct Decoupled Method (DDM)
      - High order (HDDM) for gases
      - First order for PM
    - Process Analysis – informs on physical/chemical processes
      - Integrated Process Rates (IPR)
      - Integrated Reaction Rates (IRR)
      - Chemical Process Analysis (CPA)
    - Reactive Tracers – toxics and other compounds
      - Linear chemistry (RTRAC), complex mechanisms (RTCMC)

New in CAMx v6.0

- v6.0 released May 2013
- I/O unification
  - Consistent UAM fortran binary formats for all 2/3-D data
  - Header record expanded to be more fully self-documenting
- Photolysis updates
  - Simplification of photolysis-related input processing
  - More in-line automation within CAMx
  - Expanded “lookup” dimensions for photolysis rates
- Updates to CB6 mechanism
  - Addition of iodine chemistry
  - CB6r1: isoprene and aromatic revisions, more NOx recycling from organic nitrates (ONs)
- Updates to mercury chemistry (Cl $\rightarrow$ Br)

New in CAMx v6.1

- v6.1 released April 2014
- More updates to CB6 mechanism (CB6r2)
  - ONs split between simple gas-phase alkyl nitrates (reservoir of NO_2) and multi-functional ONs that partition into OA (subsequent hydrolysis to nitric acid)
  - Adds emitted (or excess, or local) methane (ECH4)
- Updates to PiG
  - Condensed gas-phase chemical mechanism for GREASD PiG
  - Reduced nocturnal puff growth rates
  - Other minor updates to improve performance
- Added PM-DDM (first order sensitivity)

New in CAMx v6.1

- Added a surface sub-model
  - Deposition/chemistry/re-emission
  - Irreversible loss to soil leaching and vegetation penetration, and removal by precipitation
  - Wesely deposition option only
- Expanded RTRAC coupling to core model mechanisms/species

Coming in CAMx v6.2

- Expected release late 2014
  - Volatility Basis Set (VBS) for SOA
  - Explicit SOA formation from benzene
  - Top boundary condition from global models
    - Explicit source of stratospheric constituents
  - Link surface model to Zhang deposition option
- Other/later updates
  - Sub-grid convective cloud model
    - Vertical mixing/entrainment, chemistry, wet removal
  - Ozone deposition interaction with oceanic halogen release