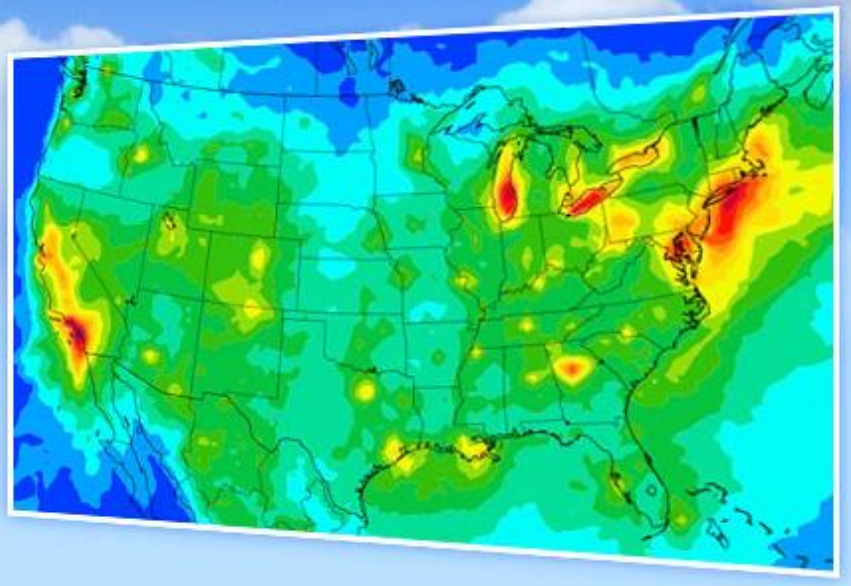
CAMx

Ozone
Particulates
Toxics



MODELING SYSTEM OVERVIEW
And Recent Updates

Chris Emery

RAMBOLL ENVIRON

CAMx OVERVIEW

- Regional/tropospheric photochemical grid model
- Large range of applicable scales:
  - Individual point sources plumes (<< 1 km) via Plume-in-Grid
  - Nested grids extend scales from ~1 to 1000's km
- Chemical species:
  - Photochemical gases (NOx, VOC, CO, ozone, halogens)
  - Inorganic and organic aerosols
    - Primary (emitted) and secondary (chemically formed)
    - Multiple size treatment options
  - Mercury and toxics

CAMx OVERVIEW

- Contemporary peer-reviewed algorithms
  - Multiple "Probing Tools"
  - Mass conservative and mass consistent numeric treatments
- Computationally and memory efficient
  - Parallelization: shared- (OMP) and distributed-memory (MPI)
  - Either or both can be used
- Flexible and relatively easy to use
  - For experienced Unix/Linux users
- Well-vetted history (EPA, States/municipalities, stakeholders)
- Freely available to the public (www.camx.com)

CAMx OVERVIEW
Model I/O

- Model input
  - Gridded and point emissions (direct from SMOKE, EPS3)
  - Meteorology (WRF, MM5, RAMS)
  - Geography (topography, land cover/LAI)
  - Initial/boundary conditions (MOZART/CAM-Chem, GEOS-Chem)
  - Chemistry (mechanism definition, photolysis information)
- Model output
  - N-hour average concentrations (2-D or 3-D)
  - N-hour dry/wet deposition accumulations
  - Others: PiG, Probing Tool, surface model, diagnostics

CAMx OVERVIEW
Chemistry

- Multiple gas-phase chemical mechanisms
  - Carbon Bond (CB05 and CB6 variants) and SAPRC07TC
  - Fast and accurate numerical solver (EBI)
- Comprehensive aerosol treatment
  - Aqueous sulfate and nitrate oxidation (RADM-AQ)
  - Partitioning among organic gases and aerosols (SOAP, VBS)
  - Partitioning among inorganic salts and acids (ISORROPIA)
  - Modal (CF) and sectional (CMU) size treatments
- Chemistry mechanisms optionally support mercury chemistry

CAMx OVERVIEW
Model Options

- 2-way or 1-way grid nesting
  - "Flexi-nesting": introduce/remove nested grids anywhere, any time
- Multiple map projections
  - Lambert, Polar, Mercator, Geodetic (latitude/longitude), UTM
- Two advection options (PPM, Bott)
- Two dry deposition options (Wesely89 or Zhang03)
- Plume-in-Grid (PiG) sub-model
  - Two chemistry options (NOx-O_3 with PM, full gas-phase)
- Surface chemistry/re-emission model
  - User-defined heterogeneous chemistry on soil, vegetation, snow

CAMx OVERVIEW
Probing Tools

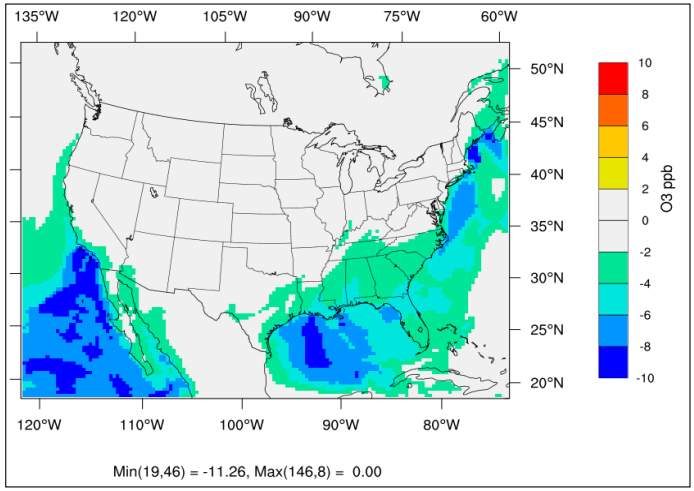
- Source Apportionment Technology (O/PSAT)
  - Track attribution to emissions by category and region
- Decoupled Direct Method (DDM, HDDM)
  - Track sensitivity to emissions by category and region
- Process Analysis tools (IPR, IRR, CPA)
  - Additional information helps explain model predictions
- Reactive Tracer sub-model (RTRAC, RTCMC)
  - Run additional gas and PM species (toxics) with separate chemistry

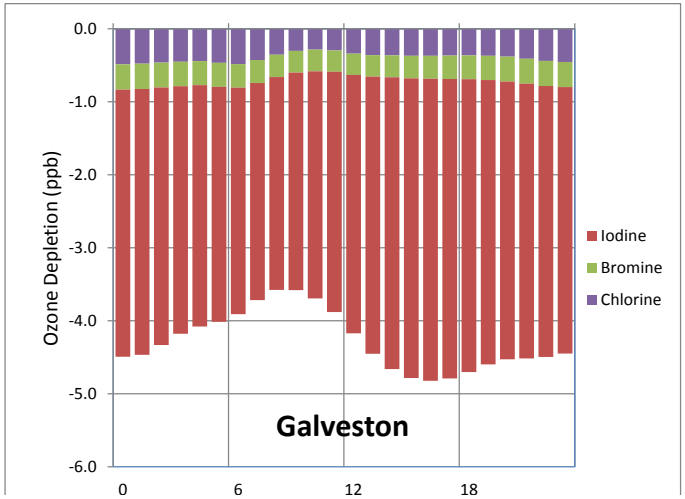
UPDATES IN CAMx v6.2 (2015)
Volatility Basis Set (VBS) for Organic Aerosols

- A unified framework for gas-aerosol partitioning and chemical aging of primary and secondary OA
  - An option to the original/simpler "SOAP" treatment
  - Implements current knowledge with upgrade path
- Condensed 2-D approach: "1.5-D"
  - Evolves CG/OA from VOC/IVOC by oxidation state and volatility
    - 5 volatility "bins" for each of 4 VOC/IVOC/POA source types
    - Anthropogenic, Biogenic, Fires, Meat Cooking
  - Works with CB05/CB6r2 and 2-mode CF size model
    - Not currently linked into Probing Tools or CMU section size model
- Requires emissions speciation of POA/IVOC by source sector (in progress)

UPDATES IN CAMx v6.2 (2015)
Oceanic Halogen Chemistry

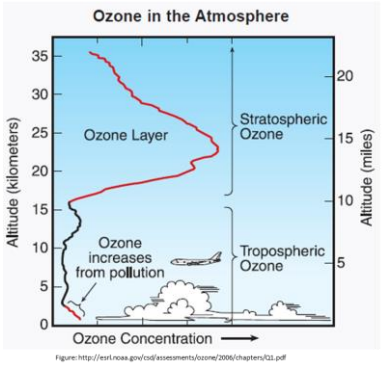
- Issue
  - O_3 over Gulf of Mexico is too high
  - Oceanic halogens deplete O_3
- Approach
  - Add gas-phase reactions involving I, Br, Cl
  - CB6r2h: adds 41 species, 89 reactions
- Evaluation
  - Test on June 2006 Texas modeling database
  - O_3 reductions of >6 ppb along Texas coastline

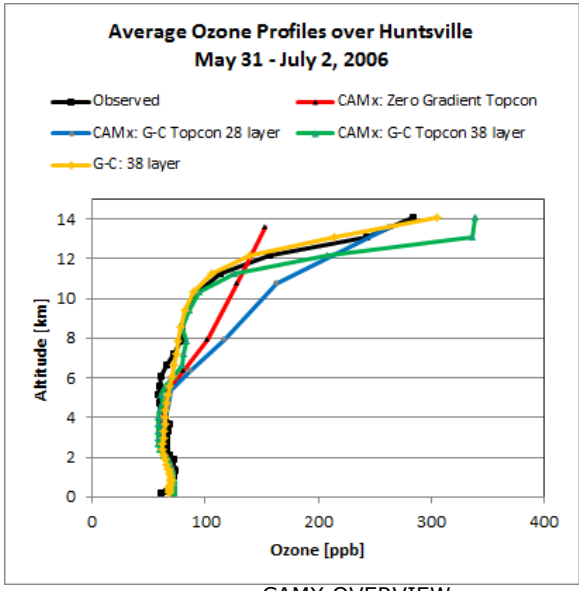




UPDATES IN CAMx v6.2 (2015)
Top Boundary Conditions from Global Models

- Issues
  - Poor UT/LS O_3 and NOy
  - Stratospheric O_3 impact at surface
  - Long-lived NOx reservoir (PAN)
  - Original implicit top BC is inadequate
- Approach
  - Explicit top BC from global models (GEOS-Chem and MOZART)
  - Improved UT/LS NO_2 and O_3
    - Allow comparison to column satellite data
  - Good vertical resolution aloft is important
    - Vertical transport over mountain areas





UPDATES IN CAMx v6.3 (2016)
Ozone Source Apportionment Update (OSAT3)

- Issue
  - O_3 can "hide from view" as NO_2

    $O_3 + NO \rightarrow NO_2$

    $NO_2 + hv \rightarrow \rightarrow O_3$
  - OSAT2 attributes "hidden O_3" to local sources rather than transport
- Approach
  - Track odd oxygen and nitrogen through NOy cycle
    - Accounts for NOx recycling of ozone
    - Harmonizes the N-tracers in OSAT and PSAT to a single method
    - Extends 4 N/V precursor tracers to 10
  - Reduces local O_3 production from NOx, increases transported O_3 production

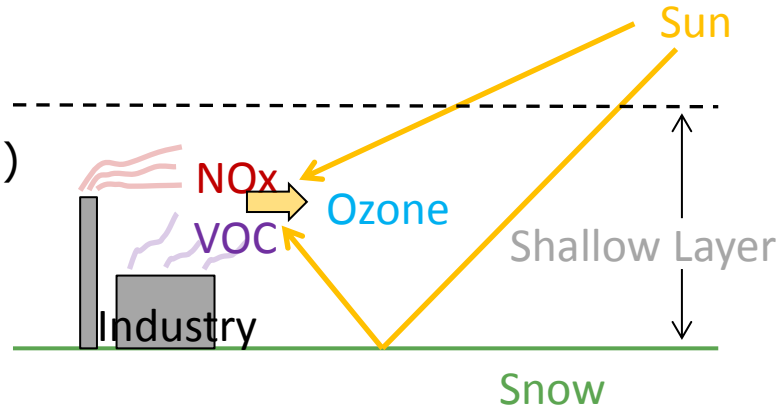
UPDATES IN CAMx v6.3 (2016)
SA Source Regions Over Fractional Cells

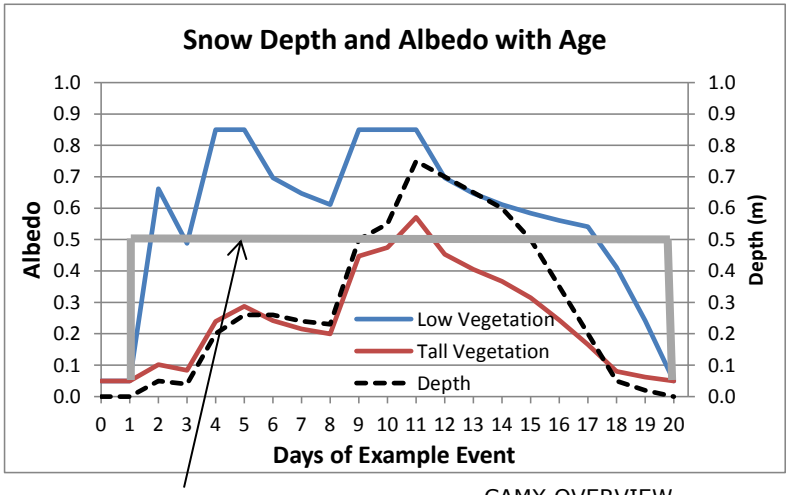
- Issue
  - SA source regions are defined by digital maps of whole grid cells
  - Region maps can be defined for each grid to maximize resolution
- Approach
  - Allocate fractional portions of each grid cell to multiple source regions
    - E.g., multiple counties or states intersecting within a single cell
  - Maintain the original integer region map file as default
  - Utilize information from SMOKE report files on the spatial allocation factors
  - Allow user to weight fractional areas by criteria pollutant (NOx, VOC, SO_2, PM or all)

UPDATES IN CAMx v6.3 (2016)
Improved Snow Cover Treatment

- Issue
  - Rural winter ozone events in O&G basins in the western US (cold, stagnant, stable)
  - NOx + fugitive VOC (alkanes) + shallow mixing + high albedo

    → O_3 > 100 ppb
  - Surface albedo is critical
- Approach
  - Adapt WRF snow albedo technique
  - Depends on landuse, snow depth/age
- Tested in Uinta Basin of Utah
  - Results in much higher ozone

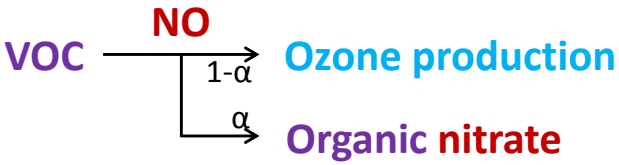




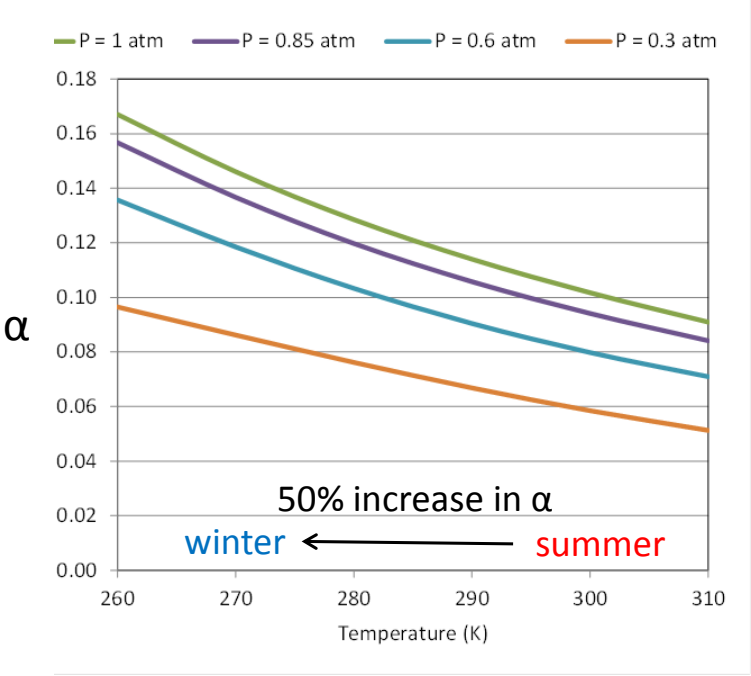
Original albedo assumption

UPDATES IN CAMx v6.3 (2016)
CB6 Cold Temperature Chemistry (CB6r3)

- Issue
  - Models set constant branching ratio (α) for organic nitrate formation



  - Addresses summer conditions
  - But α depends on temperature and pressure (altitude)
- Approach
  - Include T/P dependency in CB6r3
- Tested in Uinta Basin of Utah
  - Results in slightly lower ozone



UPDATES IN CAMx v6.3 (2016)
Model Speedup

- Objective
  - Improve algorithm efficiency, expand parallelization, increase model speed
- Method
  - Use a code profiler to track timing in each routine/process and CPU (parallelization)
  - Identify and prioritize areas of the code for improvements
  - Test compiler options, identify fast configuration w/o accuracy impacts
  - Revise code, implement new optimized routines in order of priority
- Results
  - Runtimes reduced ~15-50% (depends on chipset, compiler, model configuration)

UPDATES IN CAMx v6.3 (2016)
SAPRC and Map Projections

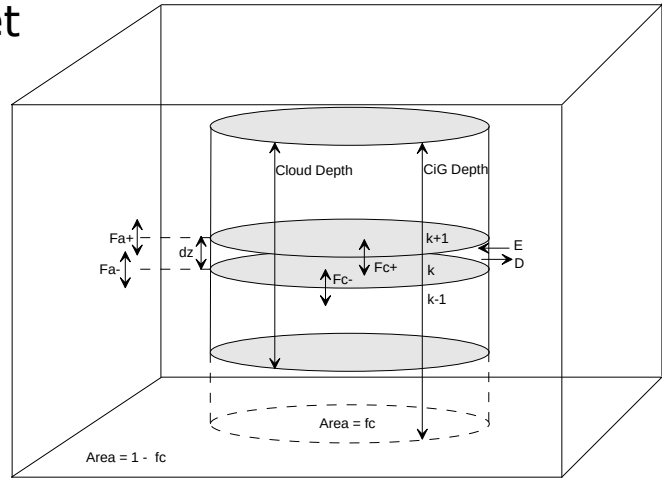
- SAPRC07TC
  - Replaces outdated SAPRC99
  - Consistent with CMAQ so that emissions work in either model
  - Does not include EPA's isoprene chemistry update
  - 117 species, 565 reactions, supports toxics (a BIG mechanism)
- Map projections
  - Added WRF's definitions for polar stereographic and Mercator
  - Supports high- and low-latitude applications globally
- Updates to several CAMx pre-processors
  - Notably WRFCAMx meteorological interface

SHORT-TERM UPDATES (LATE 2016)

- TCEQ-sponsored condensed halogen chemistry (Spring 2016)
  - CB6r2h is disproportionately slow, Ix reactions most important
  - FASTER: CB6r2 + 16-reaction inorganic Ix mechanism (I-16b)
  - Add In-line Ix emissions = function of O_3, SST, wind speed
- EPA-sponsored Chemistry Improvements (Summer 2016)
  - I-16b + CB6r3 = CB6r4
  - SOAP and RADM-AQ updates
  - Wet deposition update
- Other
  - ACM2 speedup to parallel updates in CMAQ v5.1
  - CPA extensions to new mechanisms

LONG-TERM UPDATES (2017)
Sub-grid convection

- "Cloud-in-Grid" (CiG)
  - Shallow/deep convective transport, en/detrainment
  - Explicit cloud-scale aqueous chemistry and wet deposition
  - Leverages recent advances in WRF Kain-Fritsch (KF) convection algorithm
    - KF cloud properties and convective fluxes define CiG transport, chemistry, scavenging
- Implemented for core model
  - Analyzed O_3, NOx, CO against 3-D aircraft data from 2013 Houston DISCOVER-AQ
- Needs extension to Probing Tools



Thank you

www.camx.com

TECHNICAL FORMULATION
Source Apportionment (SA)

- Apportions simulated ozone and PM to emissions and initial/boundary conditions
  - Emissions can be split by source region and/or source category
  - Apportionment provided throughout the modeling domain
- Tracks precursor emissions (NOx, SO_2, NH_3, VOC, primary PM)
- Tracks secondary products (O_3, SO_4, NO_3, NH_4, SOA)
  - Can choose which species groups to track: ozone, sulfur, nitrogen, organics, primary PM, Hg
- Associates ozone/PM production with precursors present when formed– SA is tied into the model's chemical mechanism
- Distinguish ozone production under NOx and VOC sensitive conditions – accounts for non-linear photochemistry

TECHNICAL FORMULATION
Decoupled Direct Method (DDM)

- Calculate 1st-order (DDM) and 2nd-order (HDDM) derivatives, or sensitivities
  - Sensitivity of a concentration output to an emissions or IC/BC input
    - PM: DDM only
    - Ozone: DDM or HDDM
  - Calculate many sensitivities at once
  - Emissions may be specified by region and/or category
- Applications
  - Estimate effects of emission changes
  - Rank relative importance of source region/categories to ozone reduction potential, or other species

TECHNICAL FORMULATION
Process Analysis (PA)

- Gather and report additional information on model processes
  - Chemistry, deposition, emissions, etc.
  - Over entire modeling grid or user-defined analysis domains
- Explain "how the model got the answer it got"
  - Requires post-processing to be useful
- Integrated Process Rate (IPR) – mass budgets
- Integrated Reaction Rate (IRR) – detailed chemical rates
- Chemical Process Analysis (CPA) – key chemical rates

TECHNICAL FORMULATION
Reactive Tracers (RTRAC)

- Independent reactive gas and/or inert particle tracers (e.g., air toxics)
  - Assumes reactive species have minimal impact on photochemistry
  - Each tracer can be "tagged" for source apportionment
- Tracers operate in parallel to the CAMx host model
  - Tracer decay/production driven by modeled oxidant levels and photolysis rates
  - "Recursive tracers" allows for several generations of products: secondary toxics
- Can use IRON PiG and sampling grid for "fenceline" dispersion calculations

COMPUTER RESOURCES
Hardware and Software

- Modern Intel or AMD multi-core chipsets
  - Single/multiple servers or cluster environments, big memory (16+ Gb)
  - High volume RAID for data I/O, hard drives for backup (Tb)
- Linux OS (MS Windows not supported)
  - Any "flavor" (RedHat, Suse, Mandrake, etc.)
  - Apple/Mac OSX
- FORTRAN90 for Linux, supporting OMP
  - Recommend Intel or Portland Group Compilers (supports Gnu F90)
  - Absoft for Mac OSX
- 3rd party MPI libraries (MPICH3, OpenMPI, MVAPICH)

COMPUTER RESOURCES
Speed, Memory, Parallelization Scalability

- Depends on:
  - Number and sizes of grids
  - Chemistry mechanism/solver
  - Core model vs. PiG vs. Probing Tools
- CAMx v6.2 on the EPA 2011 Modeling Platform:
  - Single 12-km US grid (396x246, 25 layers), CB6r2 + CF PM, no PiG
  - 2.60 Ghz Intel Xeon chipsets, 24 hyper-threaded cores, PGF v15.7-0, MPICH v3.1.4

V6.3 looks to be ~20% faster

OMP	MPI	Total Cores	Duration (hr)
12	0	12	4:05:12
12	2	24	3:30:47
8	3	24	2:59:08
6	4	24	2:36:10
4	6	24	2:35:17
3	8	24	2:27:34
2	12	24	2:25:25
1	24	24	3:06:57