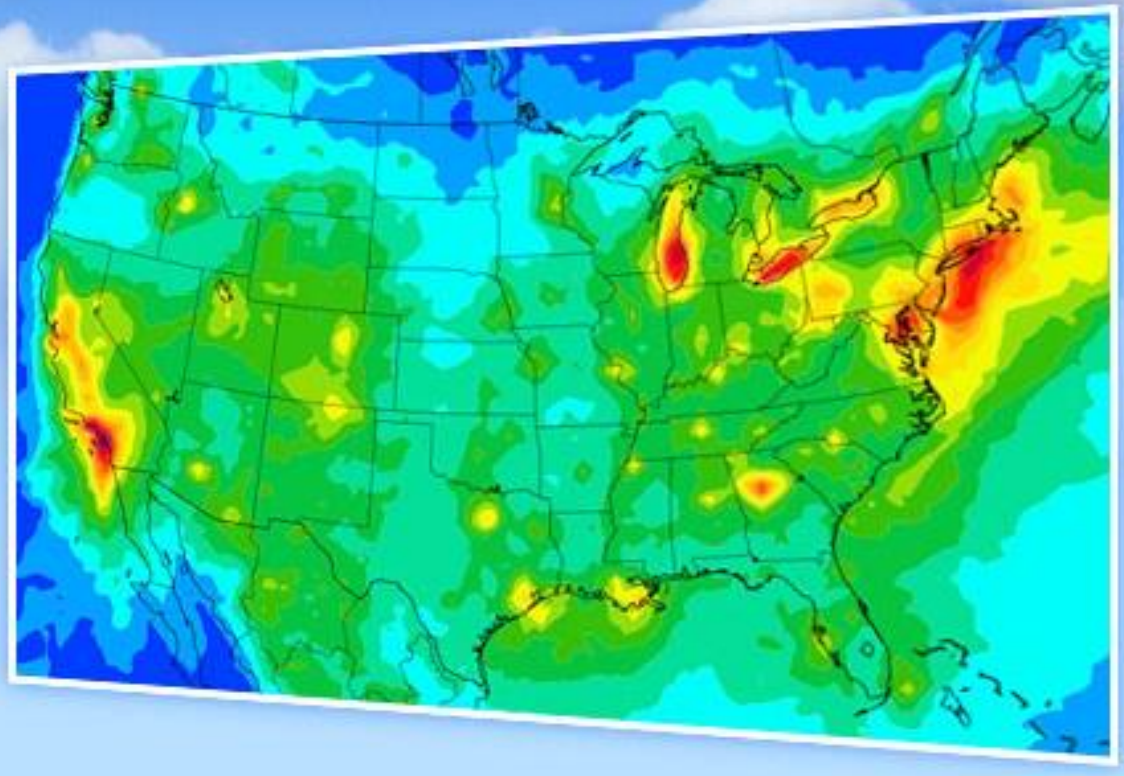
CAMx

Ozone
Particulates
Toxics



Modeling System Overview

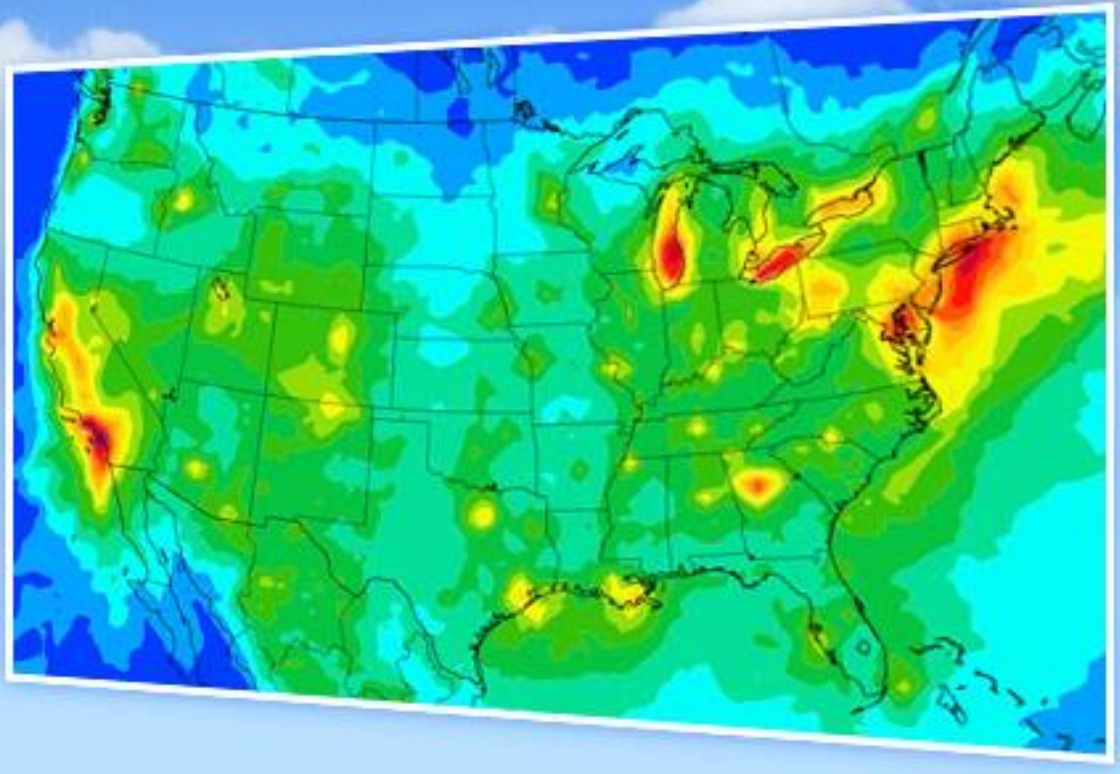
CAMX OVERVIEW
JULY 2020

TOPICS

- Atmospheric Dispersion Models
- CAMx v7 Overview
  - Features
  - Input/Output
  - Technical Formulation
  - Probing Tools
  - Computer Resources

CAMx

Ozone
Particulates
Toxics



Atmospheric Dispersion Models

RAMBOLL

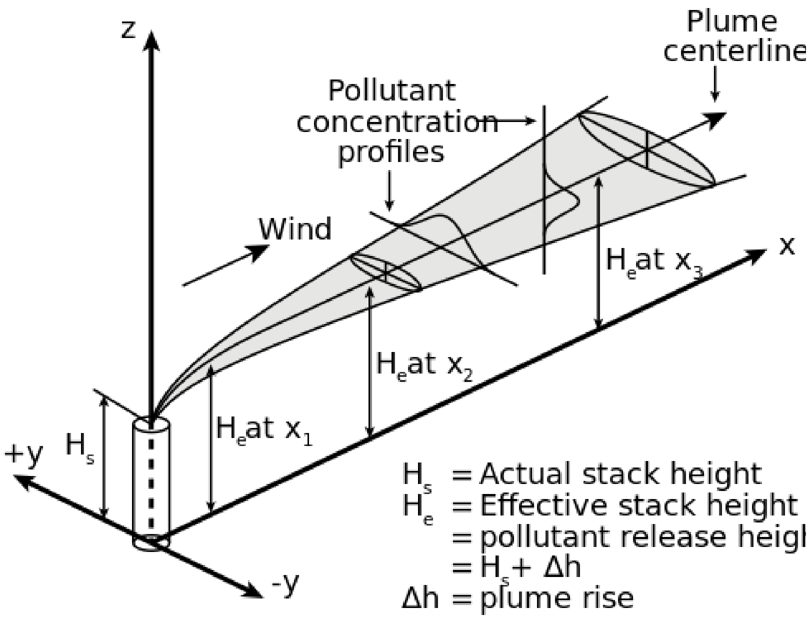
CAMX OVERVIEW
JULY 2020

DISPERSION MODELS
Overview

- All dispersion models solve some form of the “continuity equation”
  - A source-oriented “deterministic” or predictive method
  - Contrast to receptor-oriented “statistical” or diagnostic models
- Simulate how pollutant concentrations evolve in time/space from:
  - Emissions (sources)
  - Dispersion
    - Advection (transport by mean/resolved wind)
    - Turbulent diffusion (mixing by unresolved motion)
  - Chemical reactions (production/destruction)
  - Deposition (removal)

DISPERSION MODELS
Defined by Frame of Reference

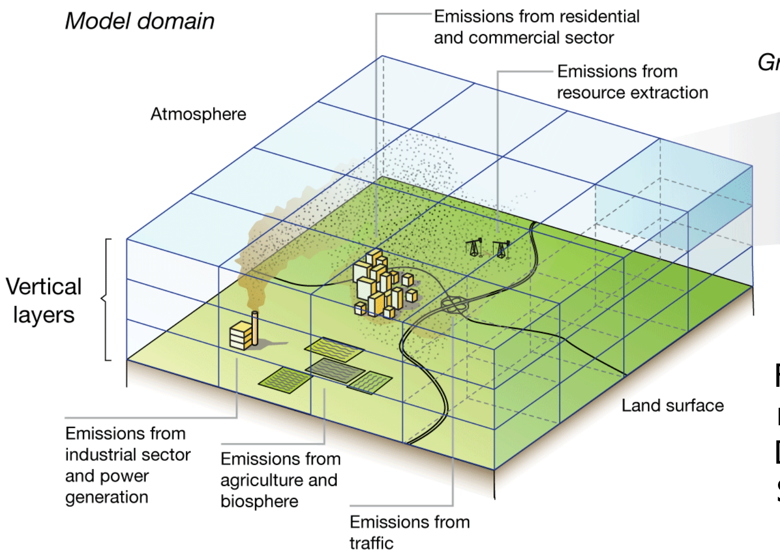
- Lagrangian: coordinate system follows air parcels
  - Plume and puff models: presume Gaussian concentration patterns
  - Plume coherency limits applicability, some non-physical consequences
  - Simple, less expensive
  - AERMOD, CALPUFF, SCIPUFF

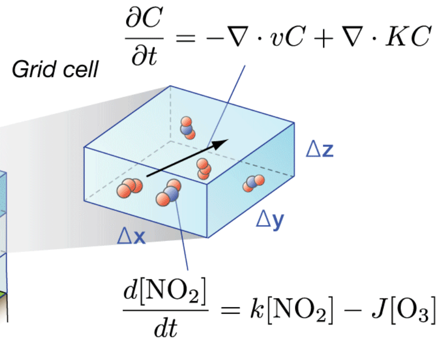


$$C(x,y,z,t) = \frac{Q}{2\pi . u . \sigma_y . \sigma_z} . \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left[\exp\left(-\frac{(z-H_{eff})^2}{2\sigma_z^2}\right)\right] + \exp\left(-\frac{(z+H_{eff})^2}{2\sigma_z^2}\right)$$

DISPERSION MODELS
Defined by Frame of Reference

- Eulerian: coordinate system is fixed in space
  - Grid models: no presumed concentration patterns, but pixelated results depend on grid resolution
  - Pollutants move consistently with resolved flow patterns
  - Complex, more expensive
  - CAMx, CMAQ, WRF-Chem



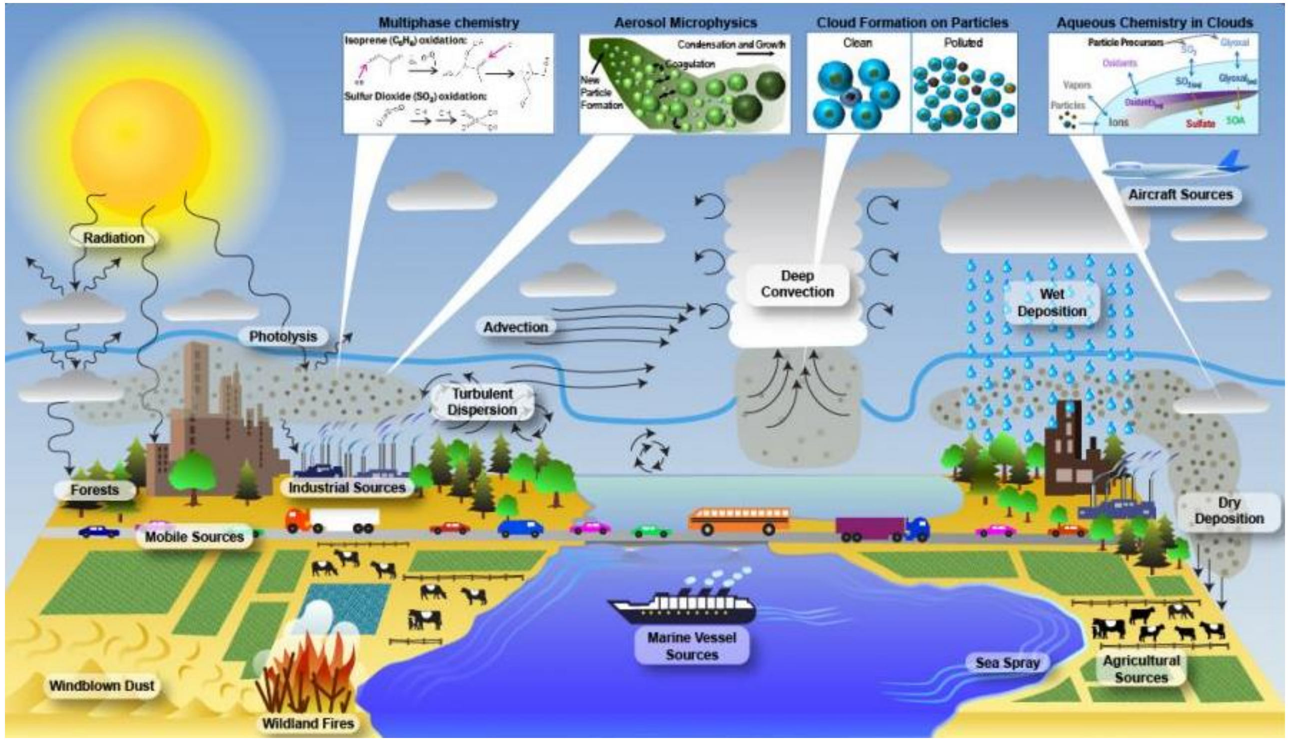


$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{V} c + \nabla \cdot K \nabla c + R_C + R_E + R_D$$

From AWMA Environmental Manager magazine, July 2012 issue on AQMEII: Douw Steyn, Peter Builtjes, Martijn Schaap, Greg Yarwood

DISPERSION MODELS
Eulerian Models – Advantages

- More realistic, comprehensive, explicit treatment of many processes:
  - Numerous emission types/sources
  - Complex meteorology
  - Complex non-linear chemistry
  - Multi-pathway pollutant removal
- Wide range of scales and applicability
  - Urban to global



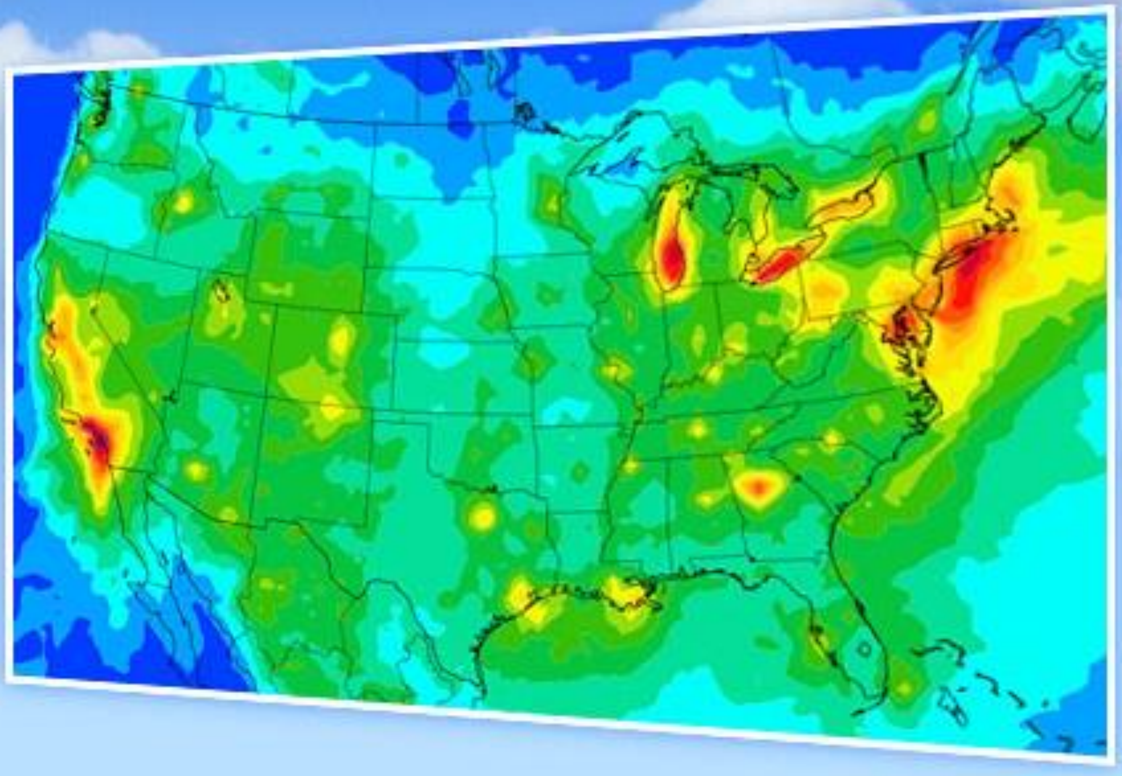
DISPERSION MODELS
Eulerian Models – Limitations

- Data intensive
  - Meteorology, emissions, initial/boundary conditions
  - Output can be complicated, non-intuitive to interpret
- Grid resolution
  - Affects accuracy, speed, data volume
  - Parameterized sub-grid processes
- Sophisticated numerical treatments
  - Operator splitting
  - Complex solvers affect model speed

- Applications require
  - ➢ Ample computing resources
  - ➢ Ample time investment
  - ➢ Ample knowledge/understanding
- Remedies
  - ➢ Parallelization over multiple CPUs
  - ➢ “Smart” solver technologies
  - ➢ Grid nesting/Plume-in-Grid
  - ➢ Probing Tools

CAMx

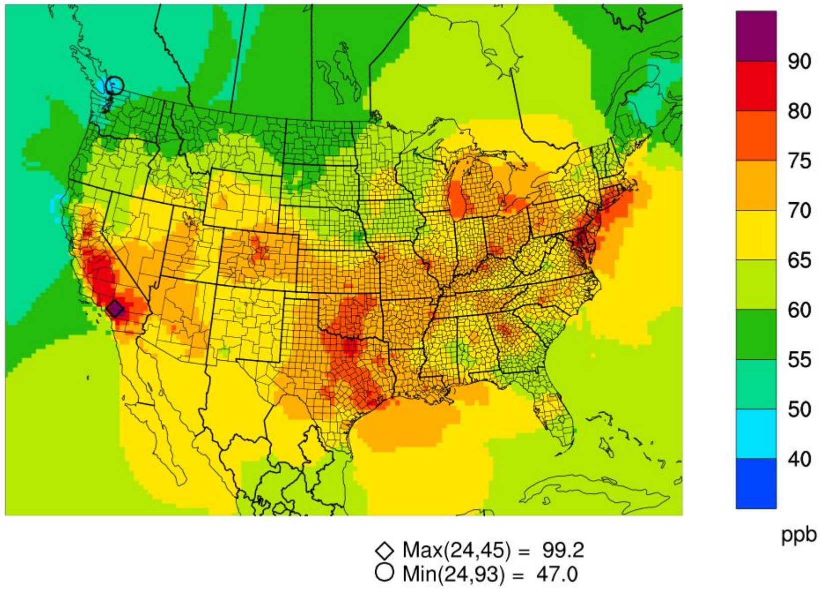
Ozone
Particulates
Toxics



Features

CAMx v7 FEATURES

- Regional tropospheric photochemical grid model
  - Multiple gas-phase chemical mechanisms
  - Comprehensive aerosol treatment
  - Mercury and toxics
- Large range of applicable scales:
  - Nested grids extend scales from ~1 to 1000's km
  - Individual point sources plumes (<< 1 km) via Plume-in-Grid
- Flexible "off-line" model
  - Meteorological and emission inputs derived from other models



CAMx v7 FEATURES

- Contemporary peer-reviewed algorithms
- Computationally and memory efficient
  - Parallelization: shared (OMP) and distributed (MPI) memory
  - Either or both can be used
- Flexible, but for experienced Linux users
- Well-vetted history
  - US EPA, States/municipalities, stakeholders, global user base
  - Extensive scientific publications on CAMx applications
- Freely available to the public (www.camx.com)

RAMBOLL

CAMx v7 FEATURES

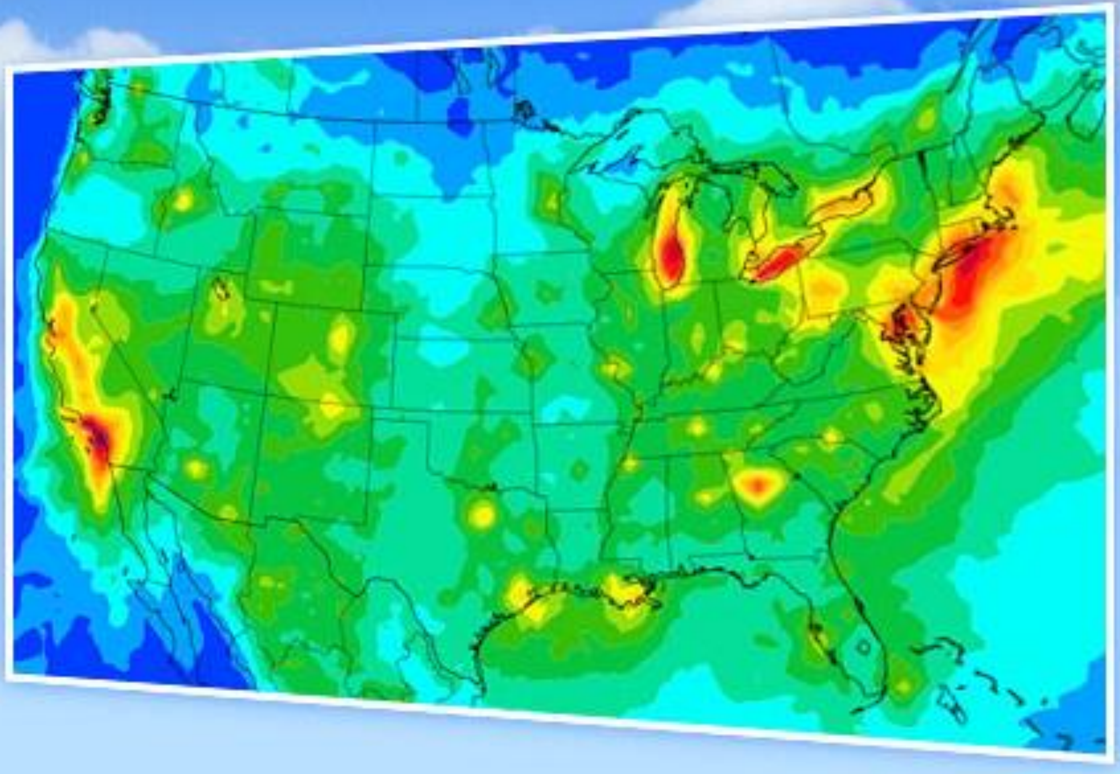
- 2-way or 1-way grid nesting
  - "Flexi-nesting": introduce/remove nested grids anywhere, any time
- Multiple map projections
  - Lambert, Polar, Mercator, UTM, Geodetic (latitude/longitude)
- Two advection options (PPM, Bott)
- Two dry deposition options (Wesely, Zhang)
- Plume-in-Grid (PiG) sub-model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

CAMx v7 FEATURES
Probing Tools

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

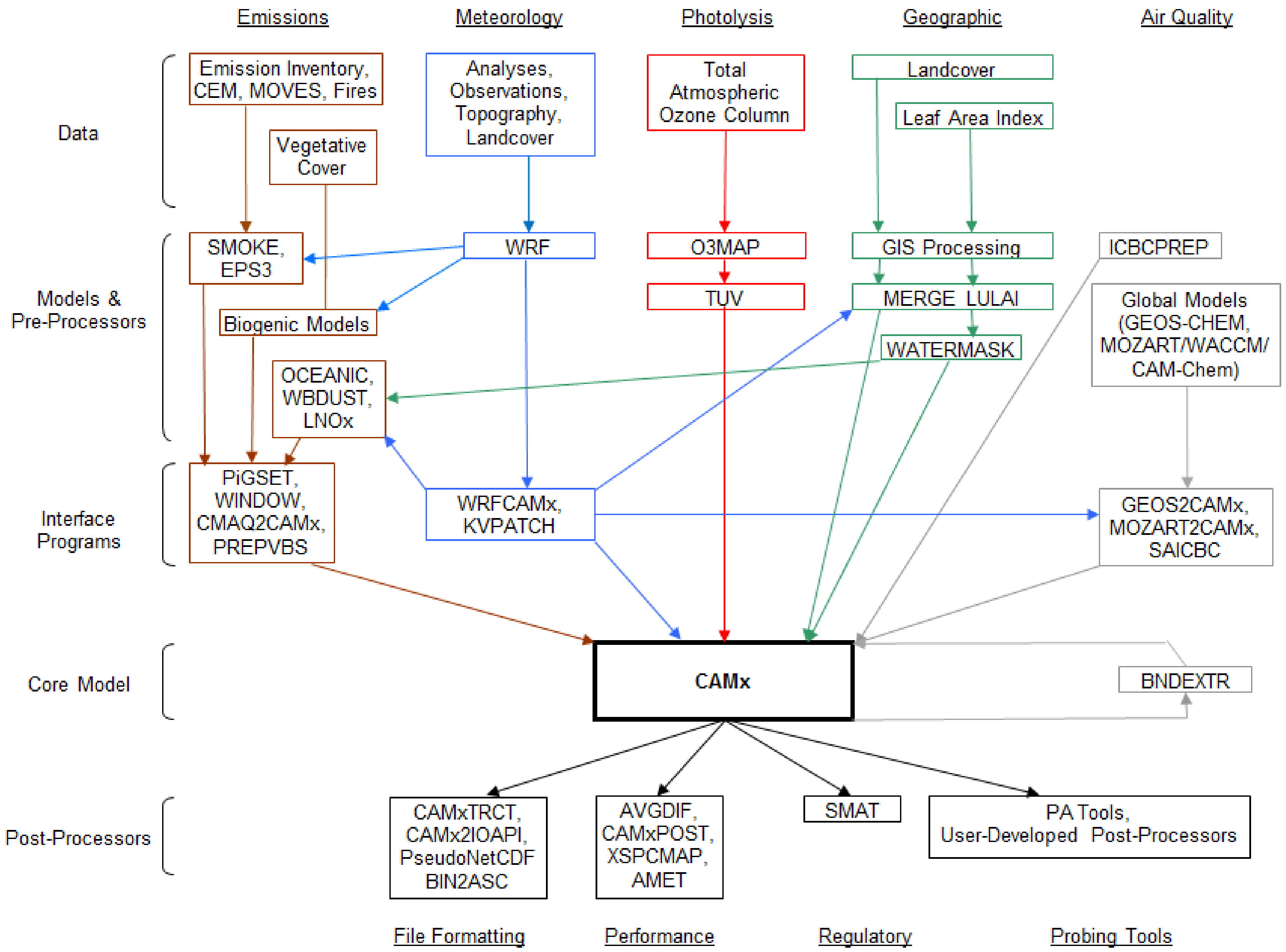
CAMx

Ozone
Particulates
Toxics



Input/Output

CAMx v7 MODELING SYSTEM



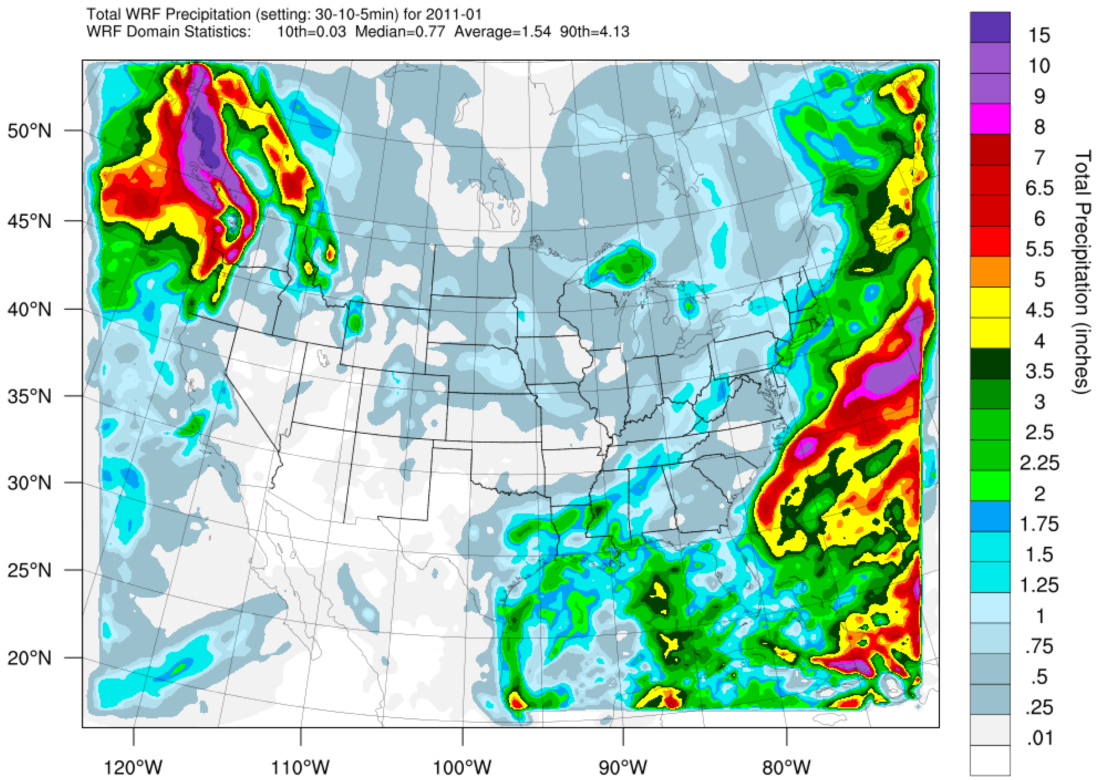
RAMBOLL

CAMx v7 INPUT/OUTPUT
Formats

- NetCDF formats for gridded model input and output files
  - NetCDF3 is traditional, uncompressible
  - NetCDF4 uses HDF5 data compression (conserves disk space)
    - Models/programs using NCF4 automatically read/write compressed files
    - No need to un-compress separately!
- Uncompressed CAMx netCDF I/O is compatible with EPA's Models-3 I/O-API convention
- CAMx allows mix of traditional Fortran binary and netCDF input files
- User can select traditional Fortran binary or netCDF output files

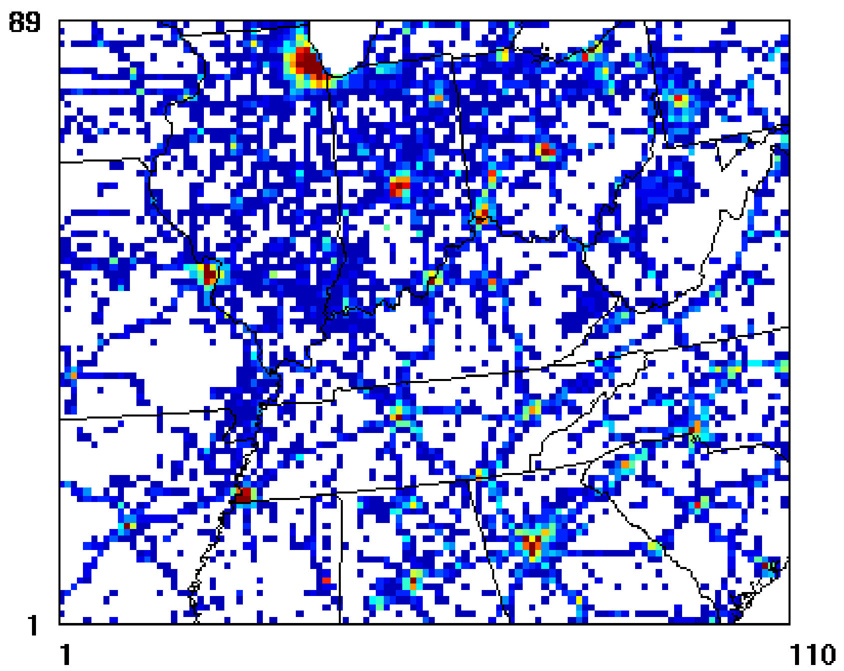
CAMx v7 INPUT/OUTPUT
Meteorology and Environmental Inputs

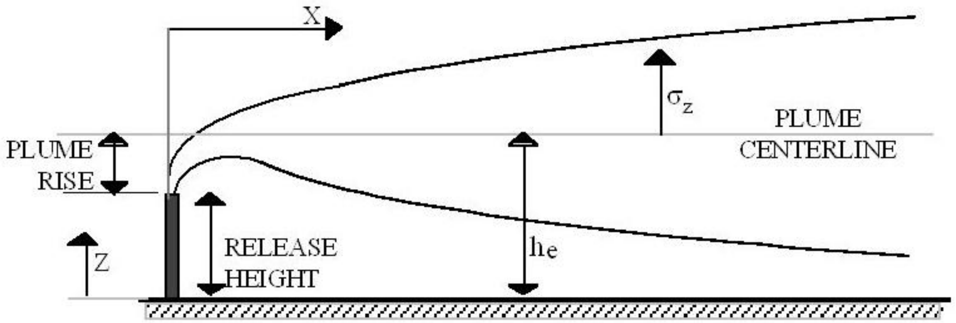
- Define state of the atmosphere and surface
  - 2D land cover, LAI, topography, snow cover
  - 3D wind, temperature, pressure, humidity, clouds, rain, turbulent diffusion rates
  - 3D vertical grid structure
- Pre-processor tool available to interface with the WRF meteorological model



CAMx v7 INPUT/OUTPUT
Emission Inputs

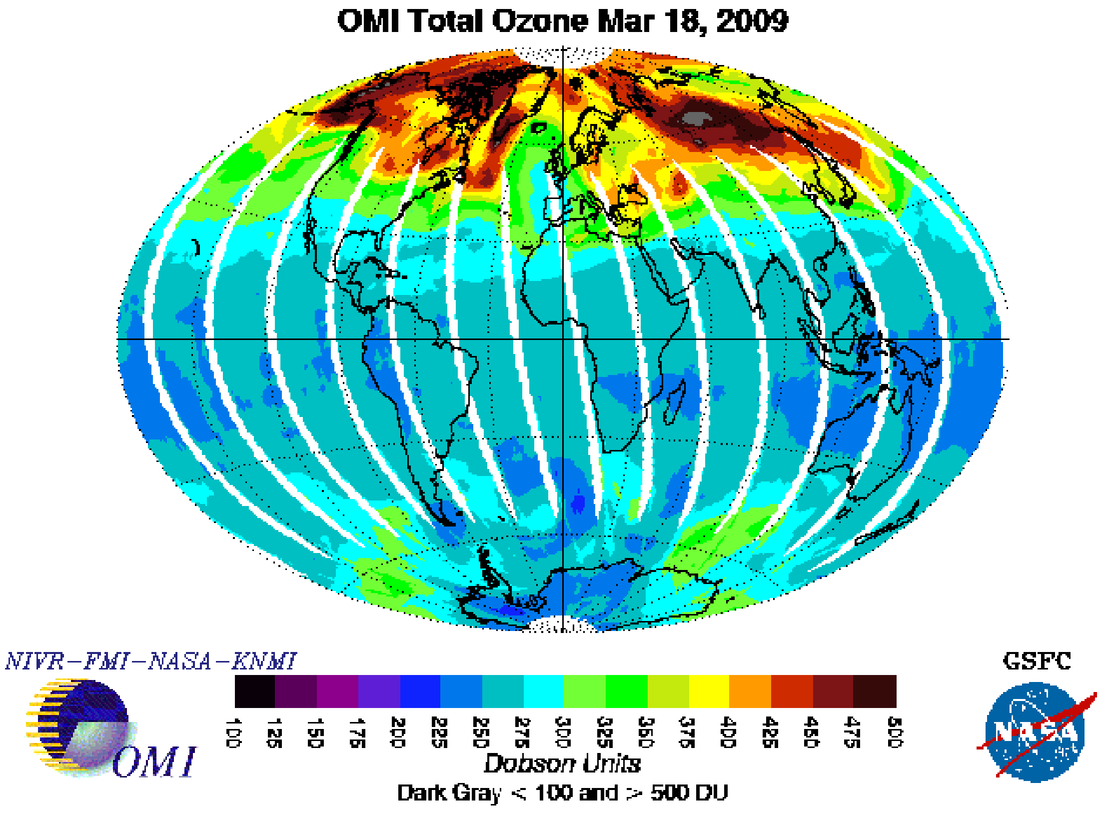
- Gridded surface emissions
  - Mobile, area, biogenic, etc.
  - Multiple input files by sector
- Gridded 3-D emissions
  - Aircraft, wildfire, lightning, etc.
  - Multiple input files by sector
- Elevated point emissions
  - Large industrial stacks or sources with plume rise
  - Model-calculated or user-specified plume rise by source
  - Multiple inputs file by sector





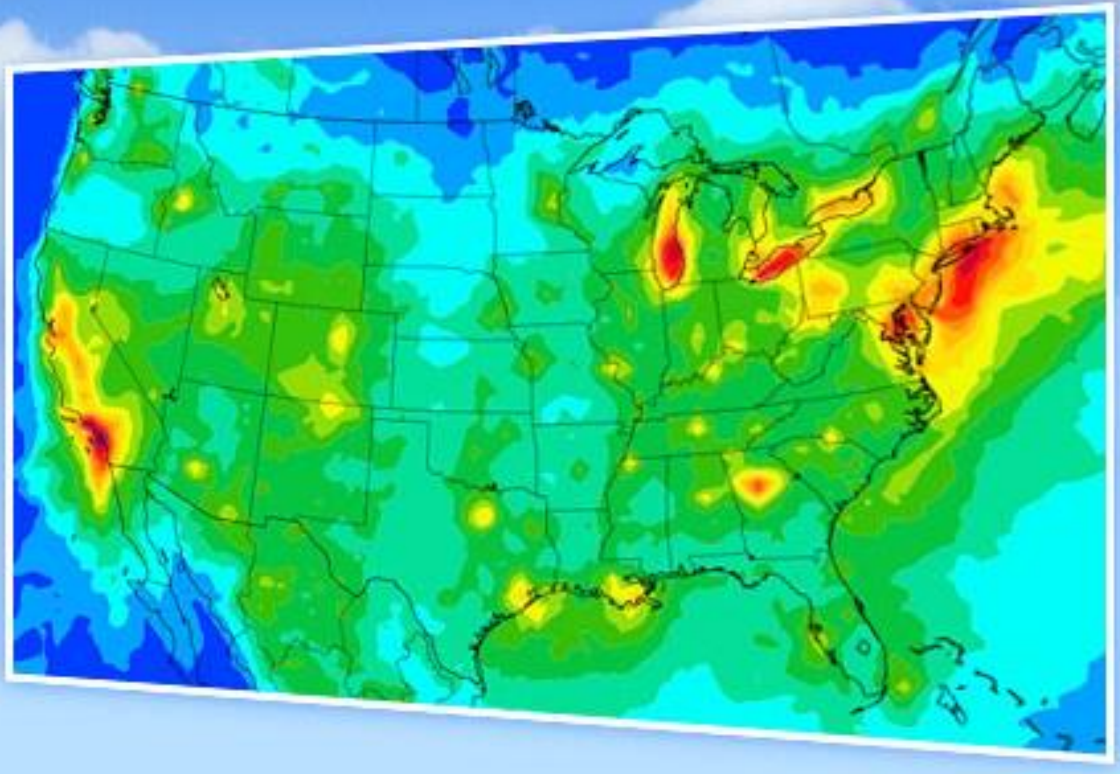
CAMx v7 INPUT/OUTPUT
Other Inputs

- Initial conditions define initial state of the atmosphere at the start of a simulation
- Boundary conditions define pollutant fluxes into the domain from the lateral and top boundaries
  - Pre-processors available for global model downscaling
    - GEOS-Chem, MOZART/WACCM/CAM-Chem
    - Hemispheric CAMx (H-CAMx)
- Clear-sky photolysis rates and total atmospheric ozone column
- Chemistry parameters file defines species and reaction mechanisms



CAMx

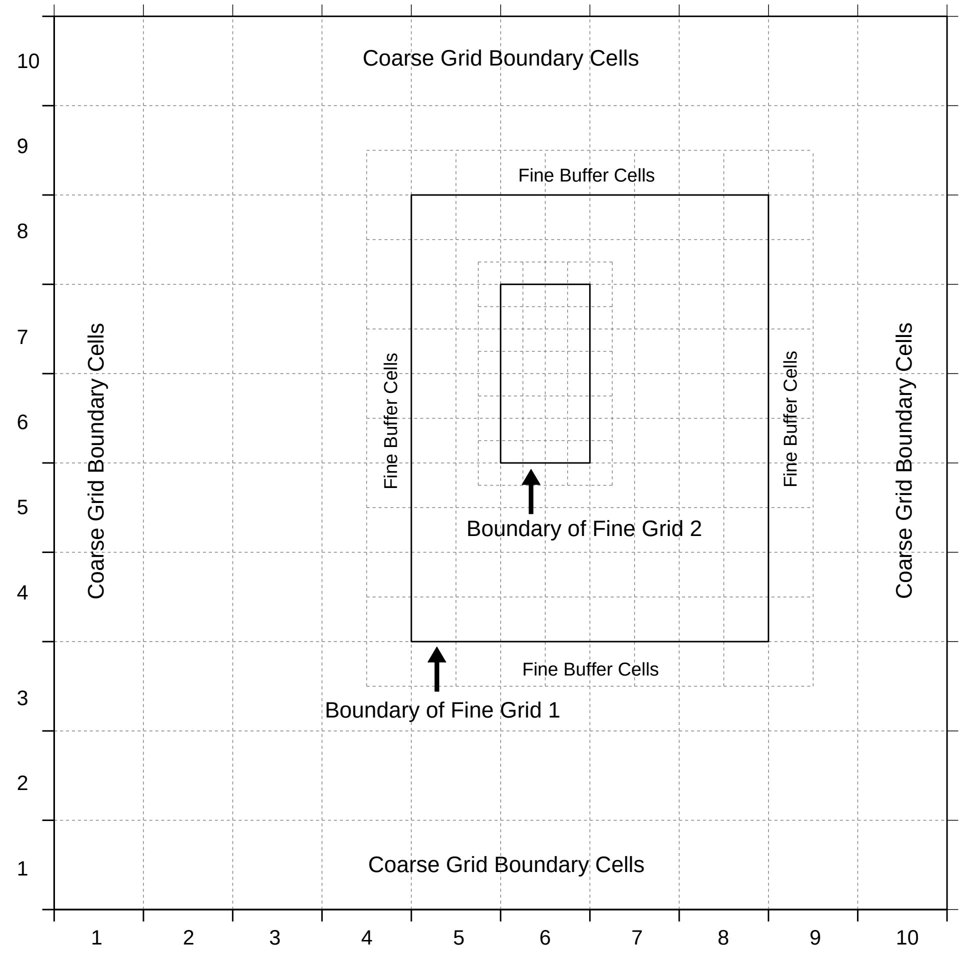
Ozone
Particulates
Toxics



Technical Formulation

TECHNICAL FORMULATION
Computational Grids

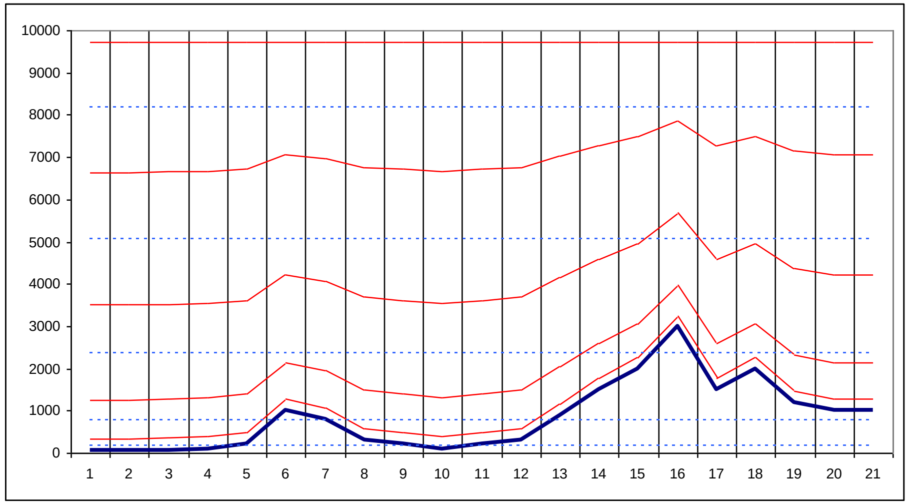
- “Master” and “nested” grids
  - All nests defined relative to master
  - Arbitrary mesh factors allowed (2, 3, 5, etc.)
  - **BUT** telescoping grids must have lowest common denominator
  - Nests need internal “buffer” cells to hold boundary conditions



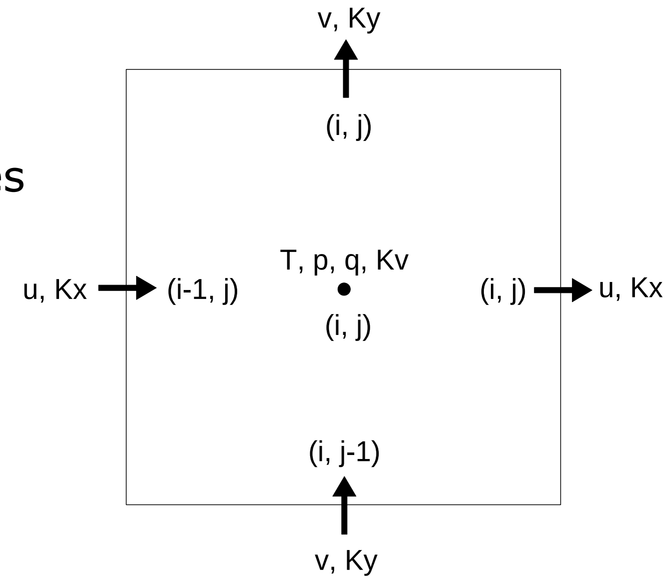
RAMBØLL

TECHNICAL FORMULATION
Computational Grids

- Terrain-following vertical height coordinate
  - Usually based on met model structure (WRF)
  - Time-varying structure allowed
  - No vertical nesting

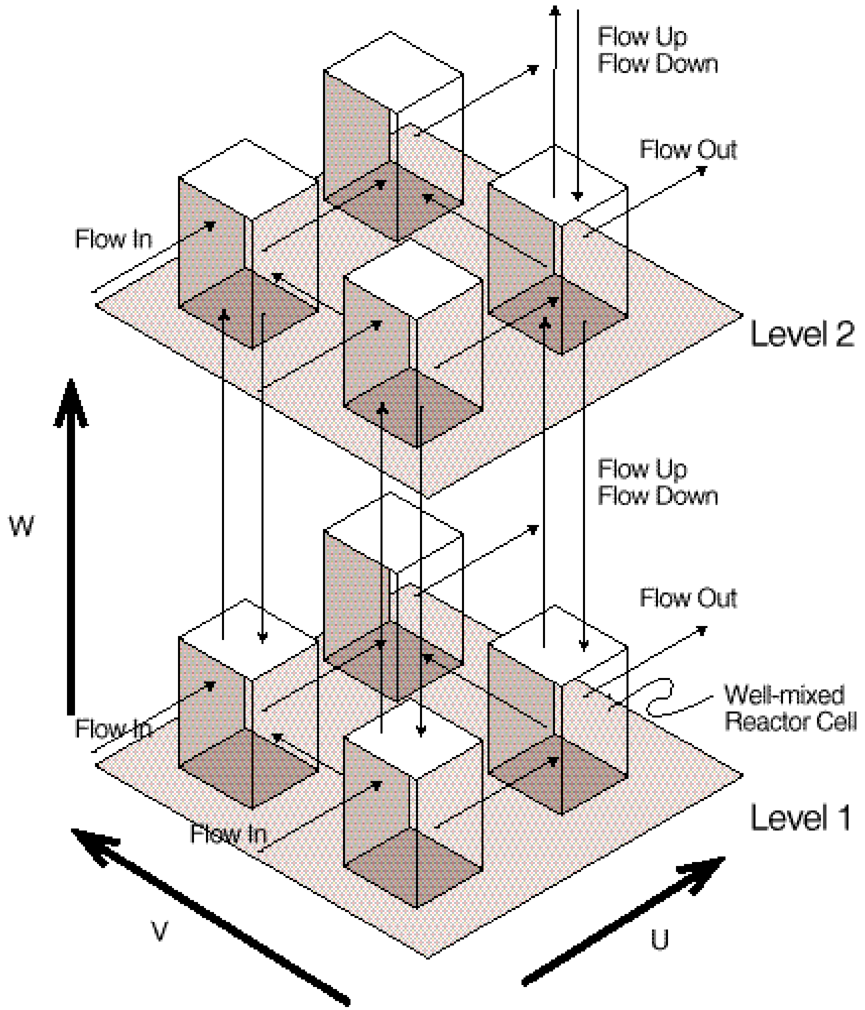


- Grid cell arrangement
  - Variables are "staggered"
  - Most are carried at cell center and represent cell averages
  - Transport fluxes are carried at cell edges



TECHNICAL FORMULATION
Transport

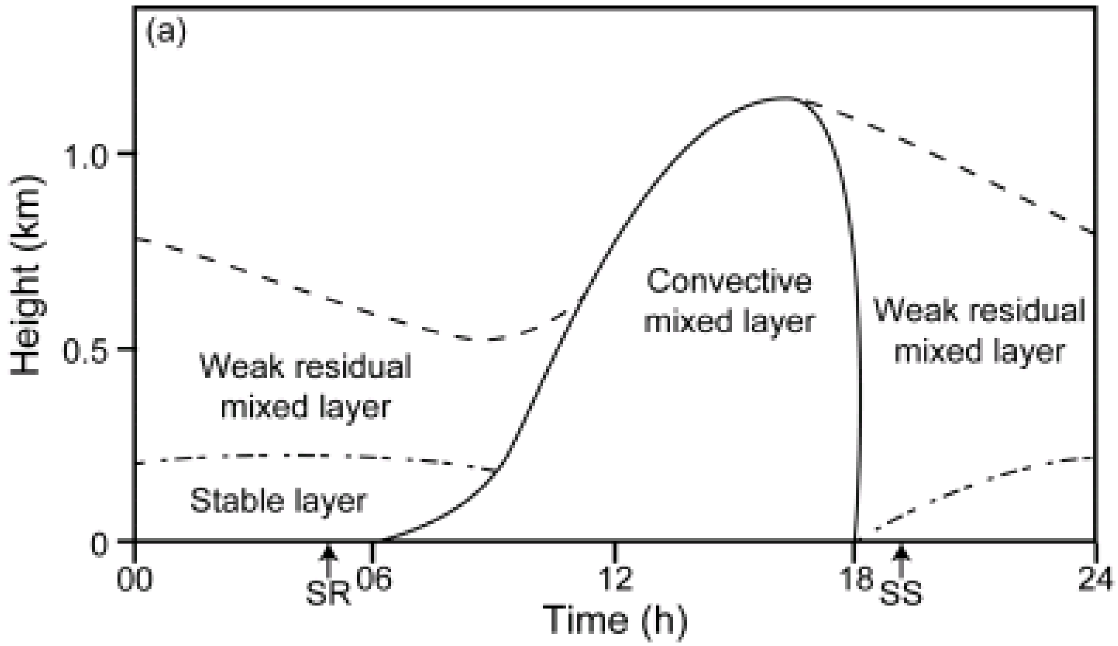
- Horizontal advection solver options:
    - Bott (1989): area-preserving flux-form solver
    - Colella and Woodward (1984): piecewise-parabolic method
- Vertical advection solved with centered hybrid implicit scheme (Emery et al., 2011)
    - Accounts for time-varying layer structure
    - Maintains mass conservation/consistency
    - Reduces numerical diffusion



RAMBOLL

TECHNICAL FORMULATION
Transport

- Horizontal diffusion solved with explicit scheme
  - 2-D simultaneous (Smagorinsky, 1963)
- Vertical diffusion (2 options):
  - Standard K-theory solved with implicit scheme
  - ACM2 (Pleim, 2007) non-local convection solved semi-implicitly
  - Dry deposition flux used as surface boundary condition



RAMBOLL

TECHNICAL FORMULATION
Gas-Phase Photochemistry

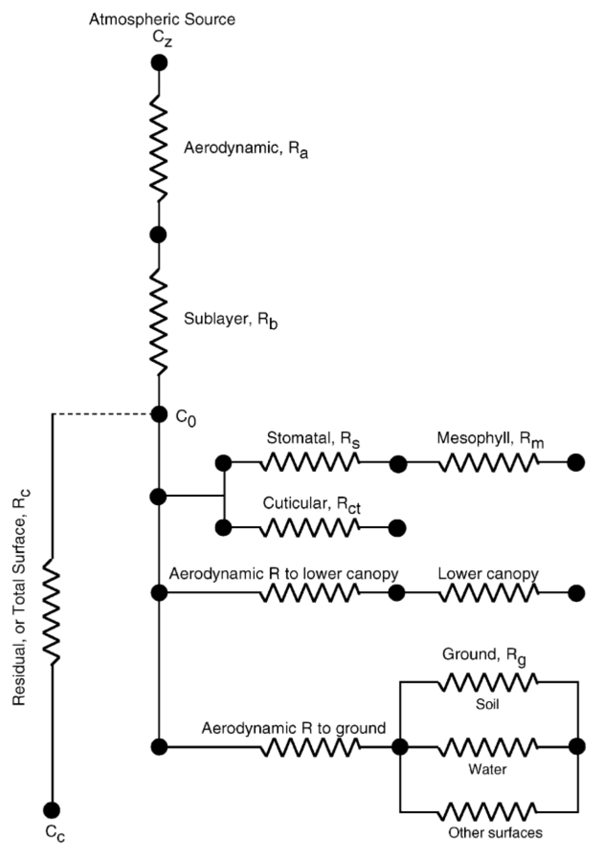
- Ozone, NOx, VOC, CO, halogens, CH_4, inorganic and organic radicals and products
- Gas-phase mechanisms currently supported:
  - CB05 (Yarwood et al., 2005)
  - CB6r2h (Yarwood et al., 2014)
  - CB6r4 (Emery et al., 2015, 2016, 2019)
  - SAPRC07TC (Carter, 2010, Hutzell et al., 2012)
- TUV pre-processor generates lookup table of clear-sky photolysis rates
  - Dimensions include zenith angle, altitude, ozone column, surface albedo
  - Cloud/aerosol adjustments applied within CAMx

TECHNICAL FORMULATION
Aerosol Chemistry

- Primary elemental/organic carbon, dust, sea salt, elemental metals and cations
- Secondary sulfate, nitrate, ammonium, chloride, organic aerosols
- Chemical treatments:
  - Aqueous sulfate, nitrate, SOA chemistry (Chang et al., 1987; Ibusuki and Takeuchi, 1987; Martin and Good, 1991; Jacobson, 1997; Ortiz-Montalvo et al., 2012; Lim et al., 2013)
  - Chemistry and partitioning among organic gases and aerosols: SOAP (Strader et al., 1999) or the Volatility Basis Set (Koo et al., 2014)
  - Partitioning among inorganic acids, cations and aerosols: ISORROPIA (Nenes et al., 1998, 1999) or EQSAM (Metzger et al., 2016)
  - Modal (CF) and sectional (CMU) size treatments

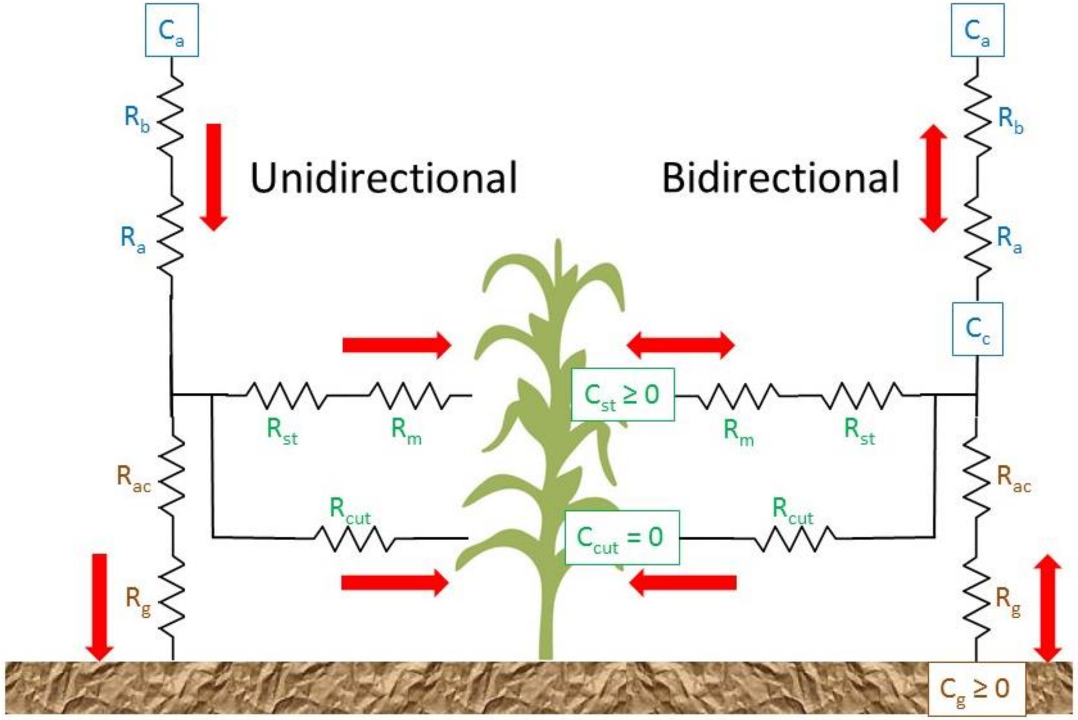
TECHNICAL FORMULATION
Pollutant Removal

- Dry deposition
  - Deposition velocity depends on surface type and seasonal characteristics
    - Resistance model analogous to an electric circuit
  - Wesely (1989), Slinn and Slinn (1980)
    - Dependencies include: season, land cover, solar flux, surface stability, surface wetness, gas solubility and diffusivity, aerosol size
  - Zhang (2001, 2003)
    - Resistances include dependence on Leaf Area Index (LAI) and snow cover
    - Default LAI set according to landuse; can be adjusted according to satellite-derived LAI



TECHNICAL FORMULATION
Bidirectional Ammonia Deposition/Emission

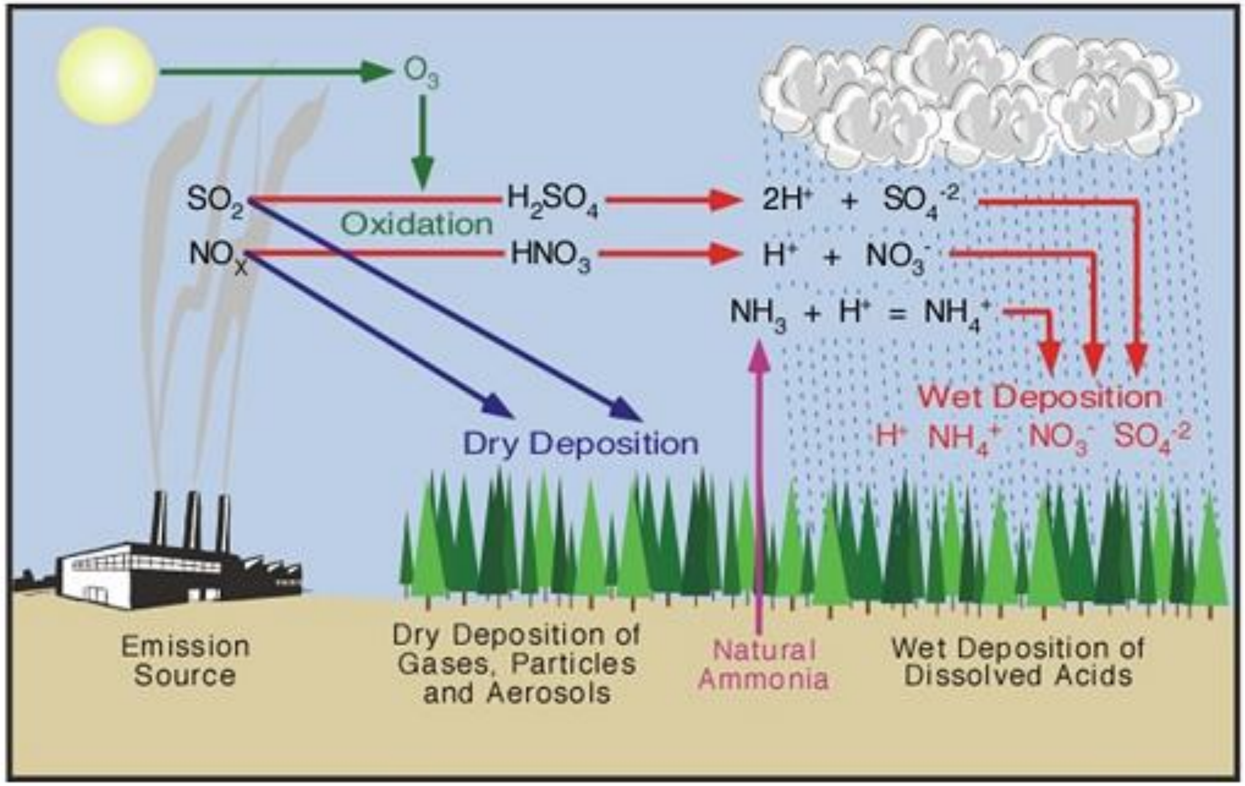
- "BiDi" algorithm of Zhang et al. (2010)
  - Implemented within CAMx Zhang dry deposition function
- Assigns NH_3 "emission potentials" by land cover type (Whaley et al., 2018)
  - Define temperature-dependent compensation points along circuit
  - Determine direction and magnitude of the net NH_3 flux



RAMBOLL

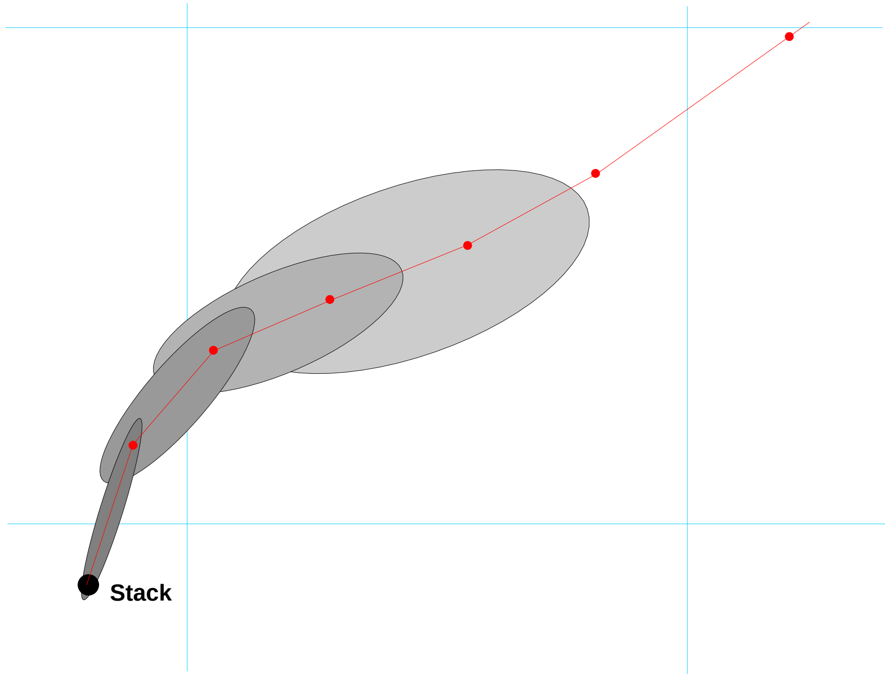
TECHNICAL FORMULATION
Pollutant Removal

- Wet scavenging
  - First order removal rate based on scavenging coefficient (Seinfeld and Pandis, 1998)
  - Gas rates depend upon solubility and diffusivity
  - Aerosol rates depend upon size and density
  - Separate rates determined for in-cloud and below-cloud processes, rain vs snow



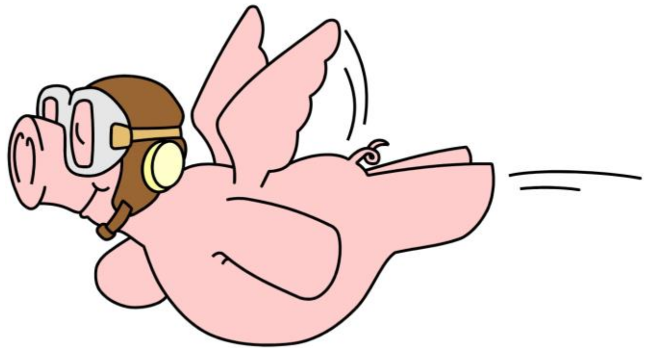
DISPERSION MODELS
Plume-in-Grid (PiG)

- Incorporates Lagrangian puff treatment into grid model framework
- Explicitly addresses point source plume-scale dispersion and chemistry
  - Overcomes grid scale limitations
- Provides practical advantages of Lagrangian methods
  - Removes shape limitations at large scales by transferring plume mass to grid when adequately resolved downwind
  - Allows cost effective application from plume to regional scales



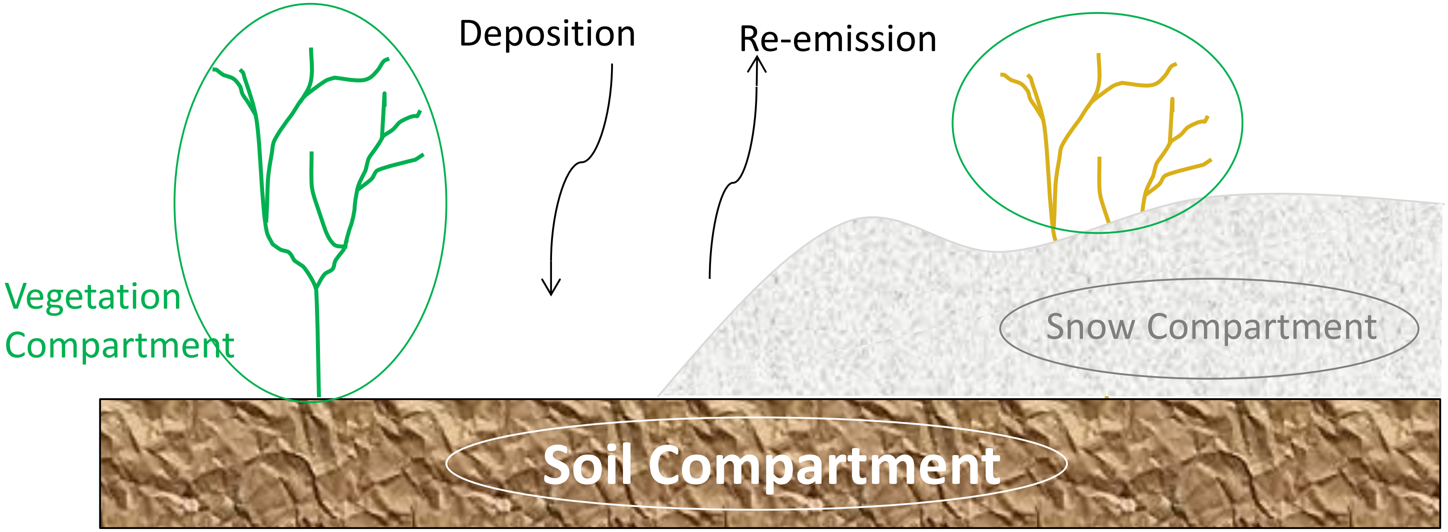
TECHNICAL FORMULATION
Plume-in-Grid (PiG)

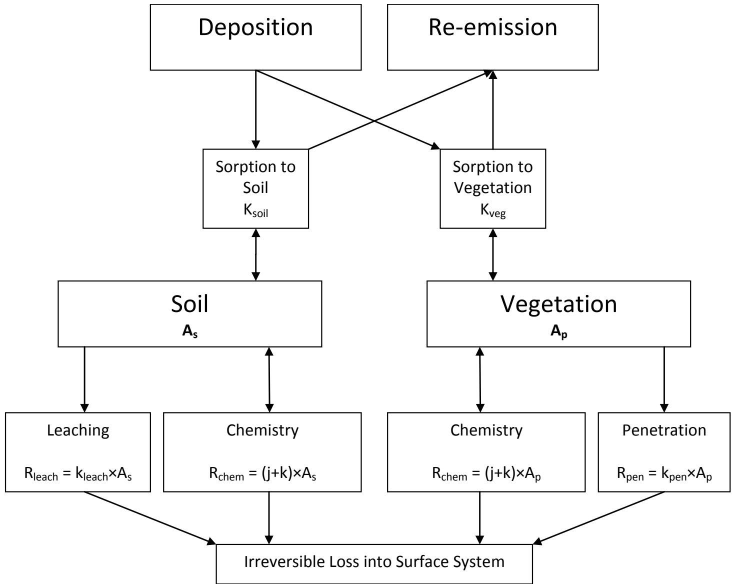
- GREASD PiG (fast chemistry):
  - Early inorganic NOx-O_3 chemistry from large NOx sources
  - Works with PM and SAT
  - Does not work with other Probing Tools
- IRON PiG (***slow*** chemistry):
  - Full gas-phase photochemistry
  - Incremental chemistry relative to grid concentrations
  - No PM
  - Works with RTRAC
  - Does not work with other Probing Tools



TECHNICAL FORMULATION
Surface Model

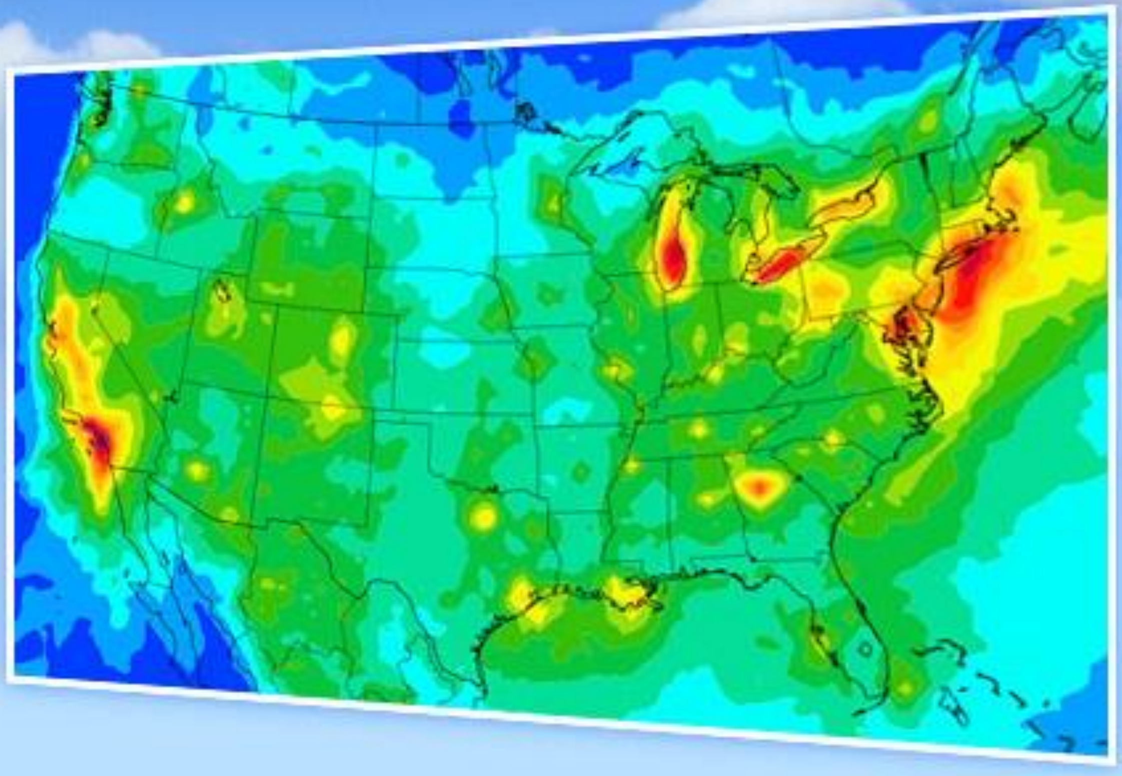
- Deposition/Chemistry/Re-emission
  - Uses deposited mass from dry deposition module
  - User-selected species and heterogeneous chemical reactions/rates
  - Re-emits volatile products back to atmosphere





CAMx

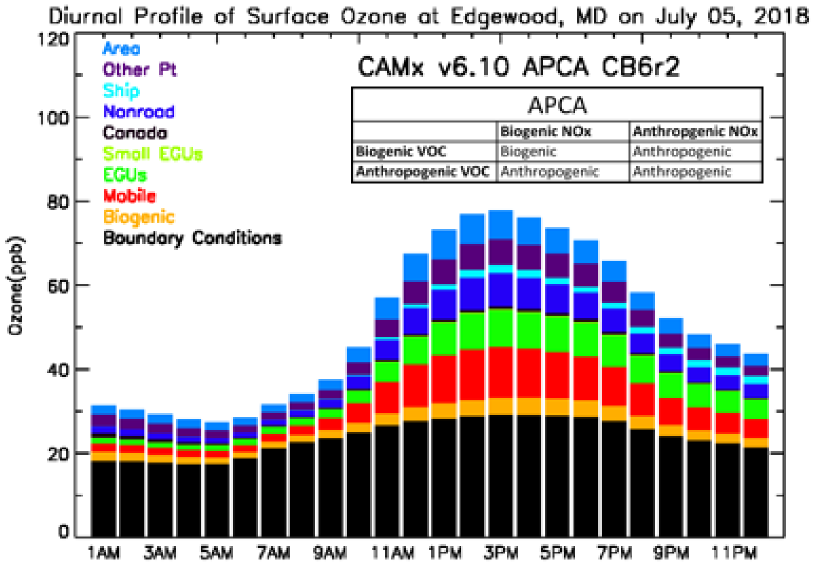
Ozone
Particulates
Toxics



Probing Tools

PROBING TOOLS
Source Apportionment Technology (SAT)

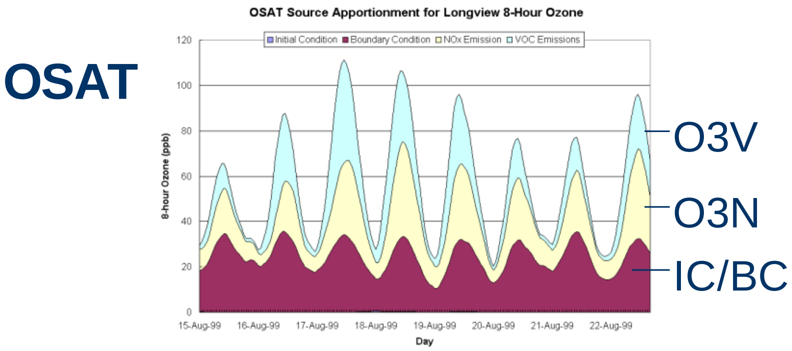
- Apportions simulated ozone and PM to emissions and initial/boundary conditions
  - Emissions can be split by source region and/or source category
  - Apportionment provided throughout the modeling domain
- Tracks precursor emissions (NOx, SO_2, NH_3, VOC, primary PM)
- Tracks secondary products (O_3, 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 – SAT is tied into the model's chemical mechanism
- Distinguish ozone production under NOx and VOC sensitive conditions – accounts for non-linear photochemistry

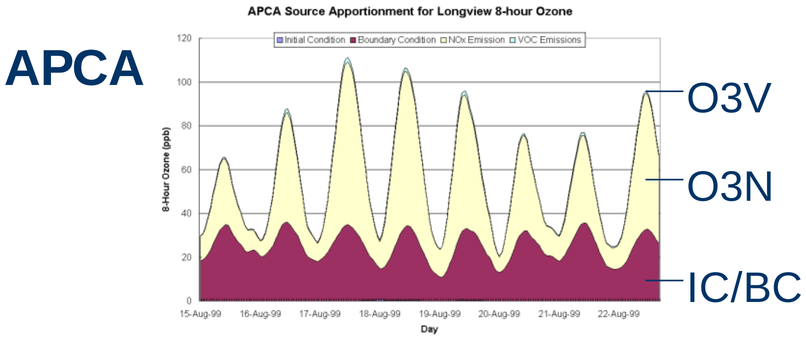


RAMBOLL

PROBING TOOLS
Source Apportionment (SA)

- Source Apportionment is ***NOT*** Sensitivity
  - SA ***can*** identify what precursors participated in ozone/PM production in a specific chemical environment or scenario (culpability)
  - SA is ***limited*** for predicting responses to precursors controls when chemical responses are non-linear
- Alternate ozone apportionment methodologies:
  - OSAT: standard approach
  - APCA: attributes ozone production preferentially to anthropogenic (controllable) sources, such as when urban NOx and biogenic VOC combine to form ozone



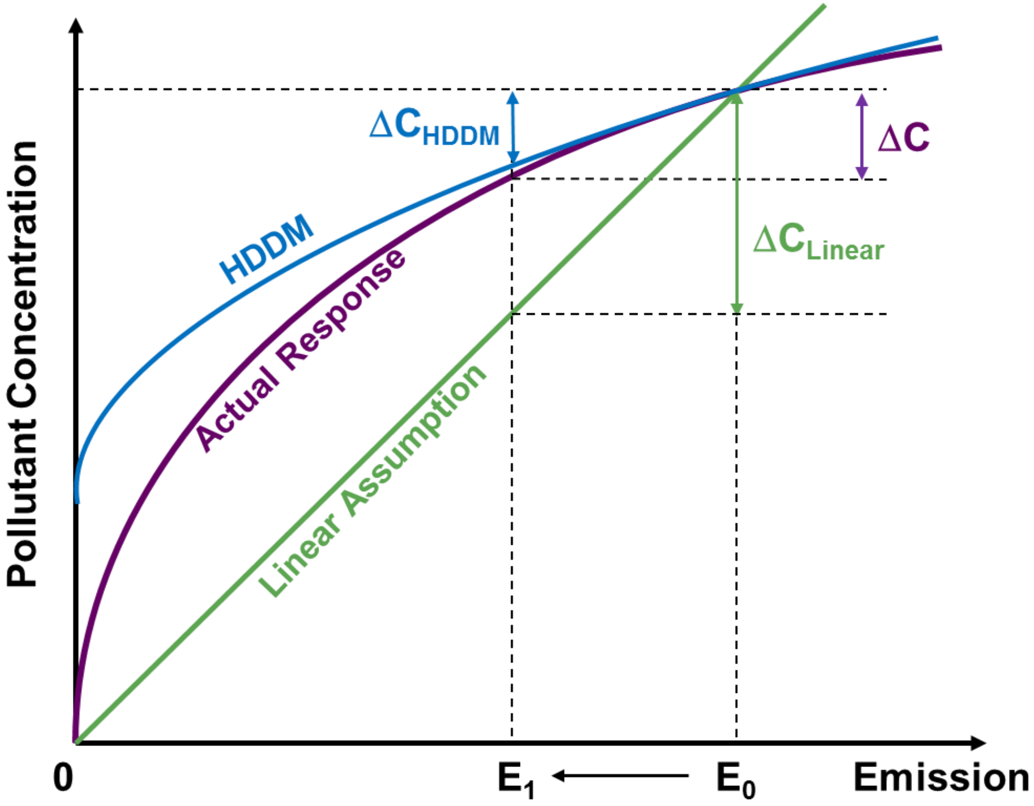


PROBING TOOLS
Decoupled Direct Method (DDM)

- Calculate 1^{st}-order (DDM) and 2^{nd}-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 in a single model run
  - Rank relative importance of source region/categories to ozone reduction potential, or other species

PROBING TOOLS
Decoupled Direct Method (DDM)

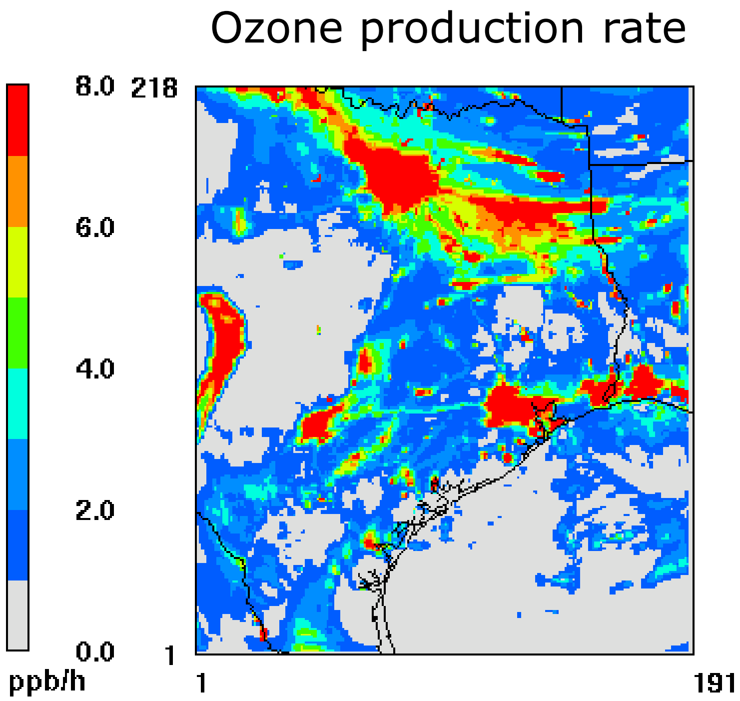
- Sensitivity is ***NOT*** Source Apportionment
  - It ***can*** predict ozone response to precursor controls:
    - DDM: small-moderate (near-linear) changes
    - HDDM: larger (non-linear) changes
  - It is ***limited*** for source attribution (culpability) because sensitivities can be negative
- DDM is slower than SA, but:
  - Provides information for every species (not just ozone or PM components)
  - More flexibility in selecting which parameters to track

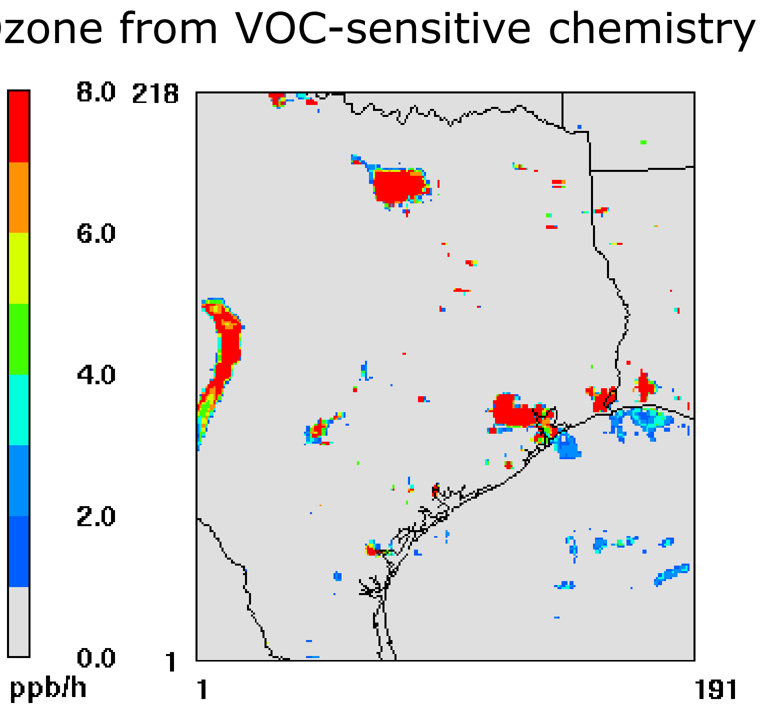


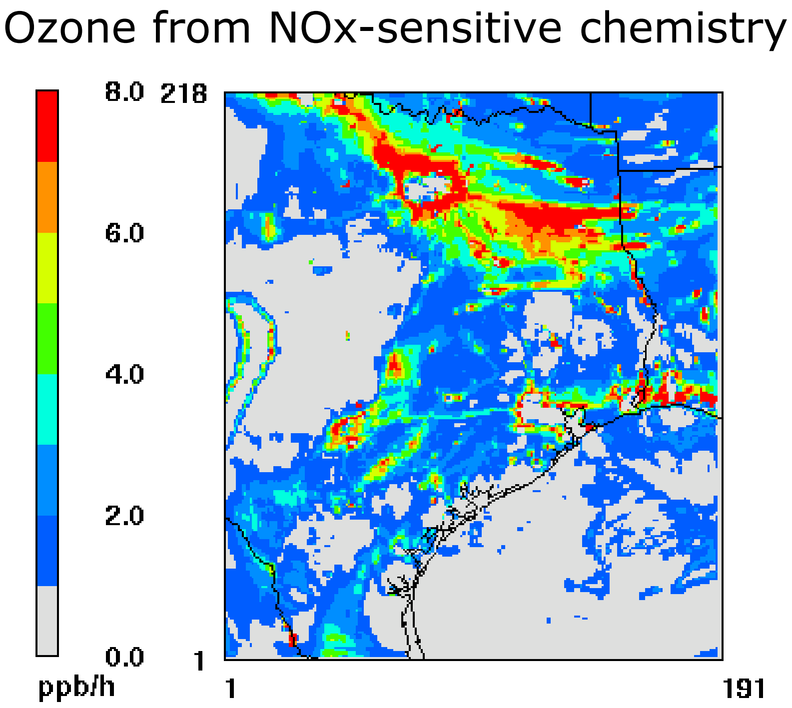
PROBING TOOLS
Process Analysis (PA)

- 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 by each physical and chemical process
- Integrated Reaction Rate (IRR) – detailed chemical rates reported by the mechanism
- Chemical Process Analysis (CPA) – key chemical rates most important for diagnosing and evaluating chemical processing

PROBING TOOLS
Process Analysis (PA) – Example from CPA

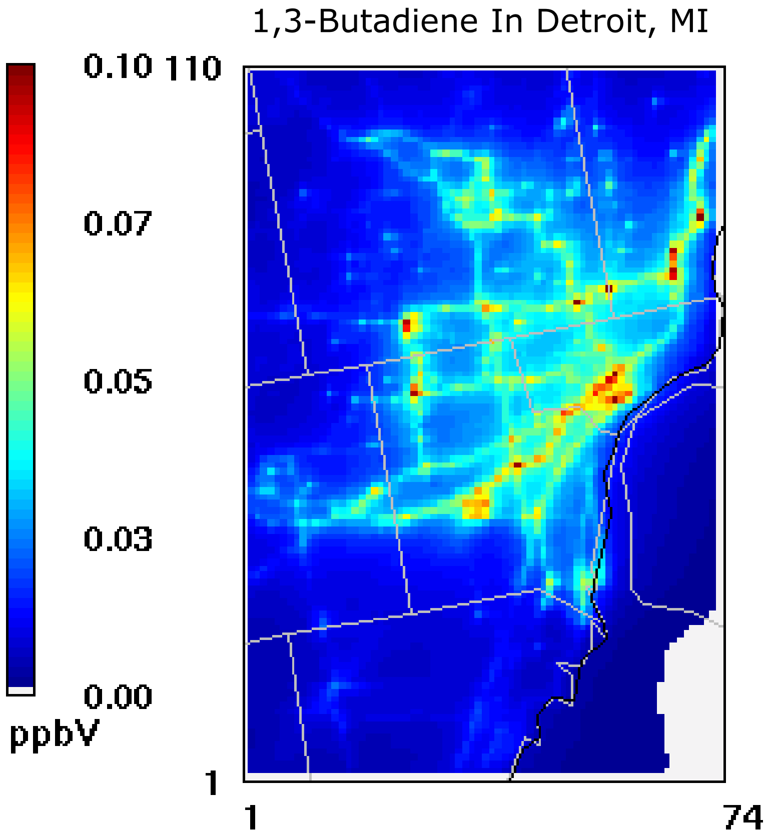






PROBING TOOLS
Reactive Tracers (RTRAC)

- Add sets of 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" allow for several generations of products: secondary toxics
- Can use IRON PiG and sampling grid for "fenceline" dispersion calculations

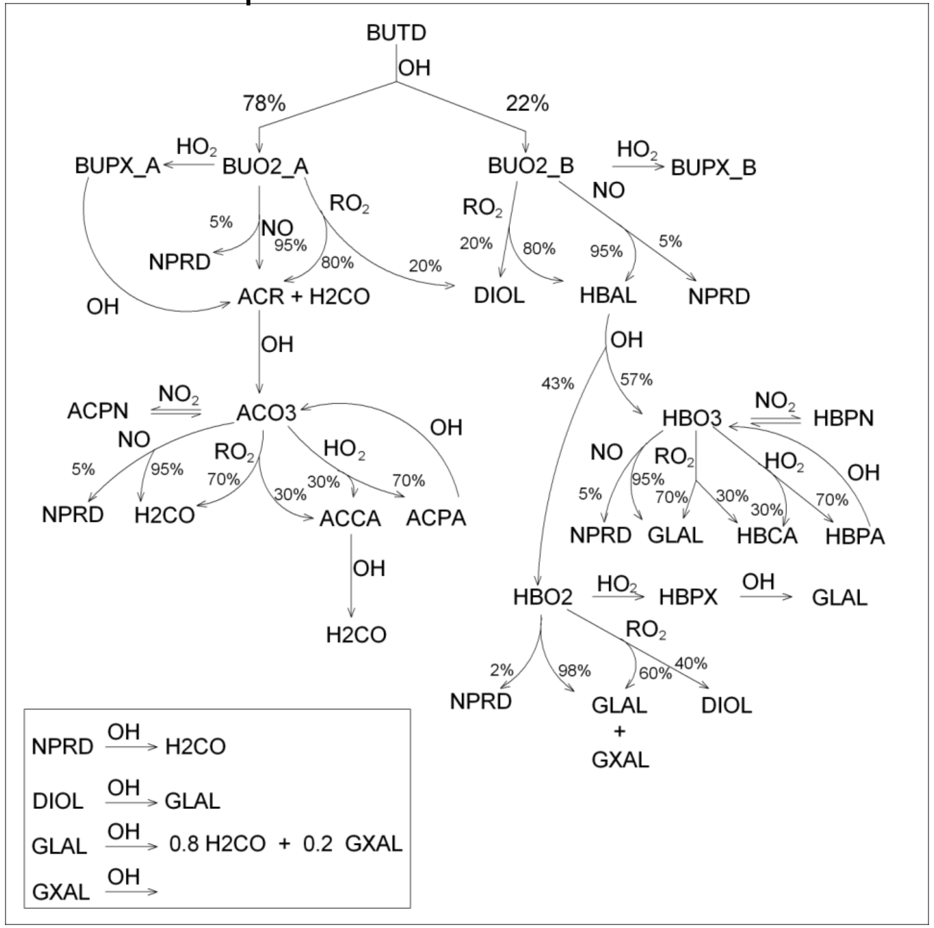


RAMBOLL

PROBING TOOLS
Reactive Tracers (RTCMC)

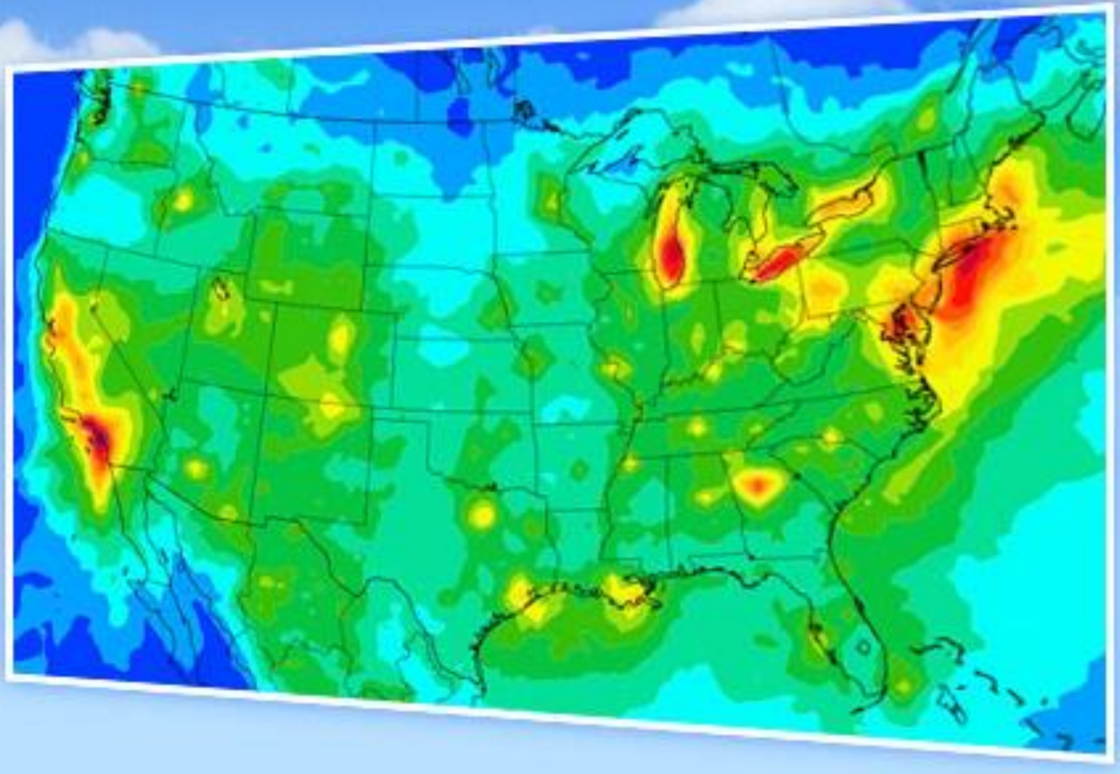
- RTCMC allows RTRAC to treat more complex chemistry
    - Reads external mechanism from text file
    - Automatically builds mechanism for LSODE solver at model startup
    - Performs independent chemical integration
        - Complex non-linear interactions among tracers and CAMx "core" species
- Adds mechanism flexibility
- Removes need to code separate mechanisms by hand
- Tracer apportionment possible, depends on chemical complexity

Example Butadiene Mechanism



CAMx

Ozone
Particulates
Toxics



Computer Resources

COMPUTER RESOURCES
Hardware and Software

- Modern Intel or AMD multi-core chipsets
  - Single servers or cluster environments
  - Fast networking among servers/nodes
  - High volume RAID for data I/O, hard drives for backup (TBs)
- Linux OS – any distribution/version (MS Windows not supported)
- Fortran90 for Linux, supporting OMP:
  - Commercial: Intel, Absoft/OSX
  - Free: Portland Group, Sun/Oracle, Gnu Fortran
- 3rd party libraries
  - MPI: MPICH, OpenMPI, MVAPICH
  - NetCDF: v3 or v4/HDF5

COMPUTER RESOURCES
Speed, Memory, Parallelization Scalability

- Depends on:
  - Number, sizes and resolution of grids
  - Chemistry mechanism/solver
  - Use of PiG and Probing Tools
  - Parallelization:
    - Larger/complex CAMx applications scale better because un-parallelized overhead processes (e.g., model setup, I/O, etc.) are small fractions of run time
  - Fast network (InfiniBand) and I/O (solid state drives) become important with many compute cores spread over many nodes such as in a cluster environment
  - We recommend using OMP and MPI in combination
  - Conduct tests to determine which OMP/MPI combinations work best for your application

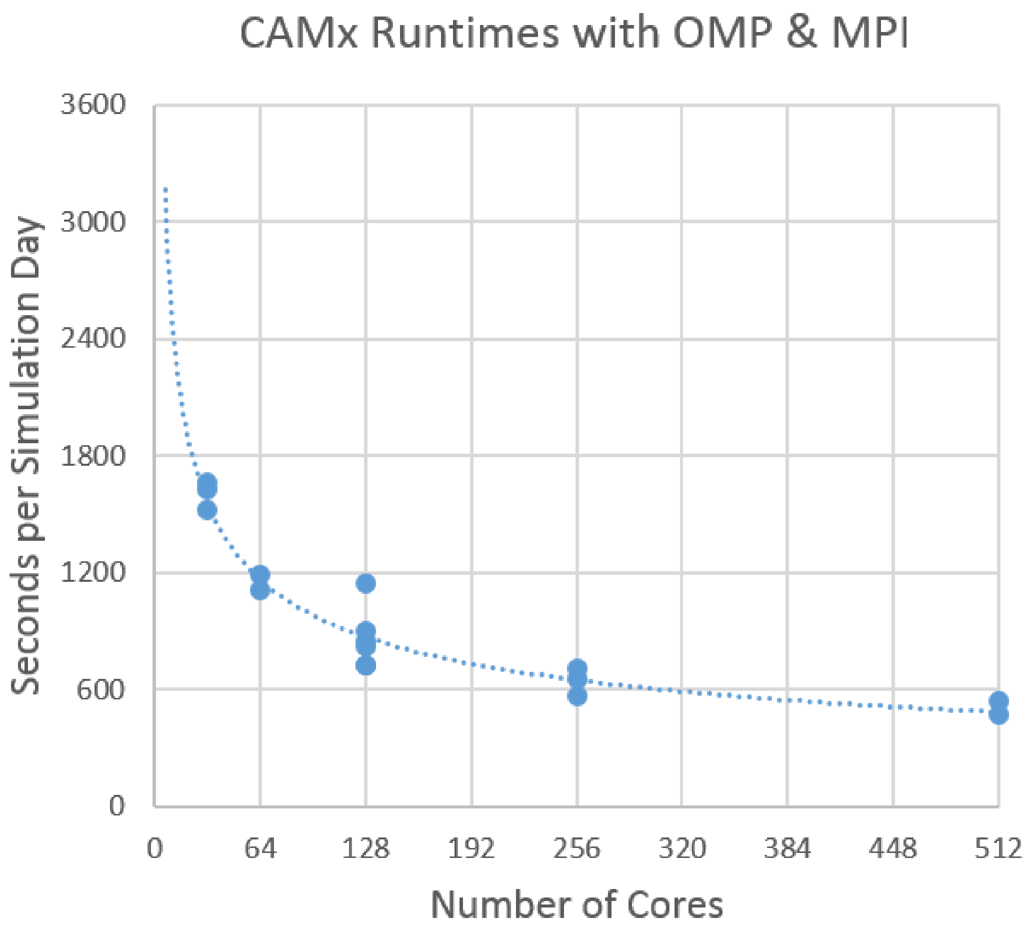
COMPUTER RESOURCES
Run Time Scaling, Example 1

- 24-hour simulation
- CAMx v6.4 with 3 nested grids:
  - 36-km (148x112), 12-km (149x110), 4-km (191x218), 28 layers
- CB6r4, no PM, no PiG, no Probing Tools
- Portland PGF90 v13.4, Intel IFORT v15.0 with OMP and MPICH v3.1.4
- 2.60 Ghz Intel Xeon chipset, 48 hyper-threaded cores

v6.4	PGF13.4			IFORT15.0		
MPIxOMP	Total	Factor	Scaling	Total	Factor	Scaling
1x1	7:16:41			6:29:43		
1x3	2:53:32	2.5	84%	2:34:35	2.5	84%
1x6	1:36:30	4.5	75%	1:27:38	4.4	74%
1x12	0:59:43	7.3	61%	0:54:52	7.1	59%
1x24	0:44:31	9.8	41%	0:44:40	8.7	36%
3x1	2:44:33	2.7	88%	2:22:18	2.7	91%
6x1	1:32:55	4.7	78%	1:22:48	4.7	78%
12x1	0:52:18	8.3	70%	0:47:25	8.2	68%
24x1	0:42:57	10.2	42%	0:40:10	9.7	40%
47x1	0:35:17	12.4	26%	0:34:09	11.4	24%
3x8	0:42:32	10.3	43%	0:35:01	11.1	46%
4x6	0:35:30	12.3	51%	0:33:40	11.6	48%
6x4	0:45:54	9.5	40%	0:33:13	11.7	49%
8x3	0:47:09	9.3	39%	0:33:58	11.5	48%
12x2	0:36:29	12.0	50%	0:33:27	11.7	49%

COMPUTER RESOURCES
Run Time Scaling, Example 2

- 24-hour simulation
- CAMx v6.4, US EPA national modeling grid:
  - 12-km (225x225), 25 layers
- CB6r2 + CF aerosols, PiG for major point sources
- SAT (9 regions x 1 sector, Ozone, Sulfur, Nitrogen groups, 220 total tracers)
- EPA's HPC system (Atmos); combinations of OMP and MPI, and combinations of standard disk and solid state (RAM) I/O



RAMBOLL

CAMx WEBSITE
http://www.camx.com

HOME ABOUT DOWNLOAD PUBLICATIONS CONTACT US

RAMBOLL ENVIRON

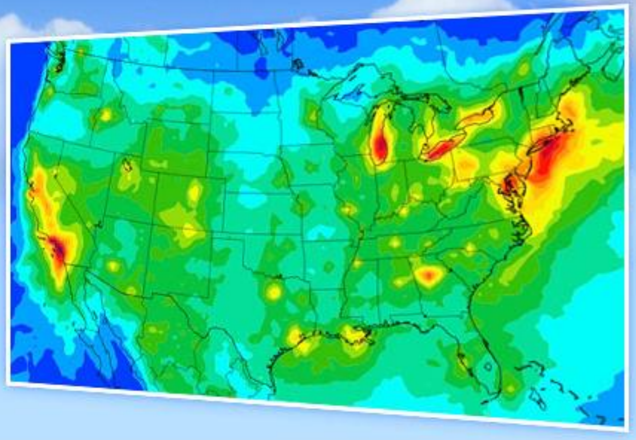
CAMx Ozone Particulates Toxics

Comprehensive Air Quality Model with Extensions

A multi-scale photochemical modeling system for gas and particulate air pollution

Version 7.00 posted May 31, 2020

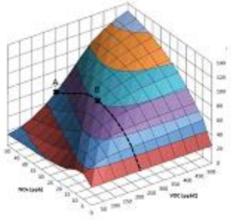
Go to CAMx Download



Why CAMx

- Simulate air quality over many geographic scales
- Treat a variety of inert and chemically active pollutants
  - photochemical gases, particulates, mercury and toxics
- Conduct source attribution, sensitivity, and process analyses
- Apply distributed- and shared-memory parallelization

CAMx In Action...



Overview presentation of features and formulation

Visit our on-line library of papers and reports

END