CAMx Modeling System Overview
TOPICS

• Atmospheric Dispersion Models

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

\[ C(x, y, z, t) = \frac{C}{2\pi H_0 \sigma_x \sigma_y} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{(z - H_0)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + H_0)^2}{2\sigma_z^2}\right) \]

- \( H_0 = \) Actual stack height
- \( H_e = \) Effective stack height
- \( \Delta h = \) pollutant release height
- \( \Delta h = H_0 + \Delta h \)
**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

\[
\frac{\partial C}{\partial t} = -\nabla \cdot \vec{v} C + \nabla \cdot \vec{K} C
\]

\[
\frac{\partial c}{\partial t} = -\nabla \cdot \vec{V} c + \nabla \cdot K \nabla c + R_c + R_E + R_D
\]

\[
\frac{d[NO_2]}{dt} = k[NO_2] - J[O_3]
\]

From AWMA Environmental Manager magazine, July 2012 issue on AQMEII:
Douw Steyn, Peter Builjes, 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 Features

- Ozone
- Particulates
- Toxics
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)
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
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
• “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
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
• 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
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
TECHNICAL FORMULATION
Gas-Phase Photochemistry

- Ozone, NOx, VOC, CO, halogens, CH₄, 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
    - 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 NH₃ “emission potentials” by land cover type (Whaley et al., 2018)
  - Define temperature-dependent compensation points along circuit
  - Determine direction and magnitude of the net NH₃ flux
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

Probing Tools

Ozone
Particulates
Toxics
**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, SO₂, NH₃, VOC, primary PM)
- Tracks secondary products (O₃, SO₄, NO₃, NH₄, 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
- Distinguishes ozone production under NOx and VOC sensitive conditions – accounts for non-linear photochemistry
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\textsuperscript{st}-order (DDM) and 2\textsuperscript{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

Ozone production rate
Ozone from VOC-sensitive chemistry
Ozone from NOx-sensitive chemistry
**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
PROBING TOOLS
Reactive Tracers (RTCMMC)

- 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
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
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

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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
CAMx WEBSITE
http://www.camx.com

A multi-scale photochemical modeling system for gas and particulate air pollution
Version 7.00 posted May 31, 2020

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