Overview of Emissions Modeling Support and Research for the CMAQ Modeling System

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Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.
Mission statement:

• Provide the best available emission estimate data to drive the CMAQ modeling system;

• Improve these estimates by building emission models that account for meteorological conditions; and,

• Develop innovative ways of evaluating these emissions.
Emissions Modeling Support and Research for the CMAQ Modeling System

- **AMD staff:** W. Benjey, T. Pierce, G. Pouliot (w/ contributions from J. Ching, D. Gillette, A. Gilliland, G. Gipson, P. Bhave, and J. Godowitch)

- **Outside collaborators:** OAQPS, ORD/NRMRL, CEP, CSC, EIIP, RPOs, IGAC/GEIA, Environment Canada, NCAR, and Washington State University

- **Selected R&D areas:** SMOKE, geographical data files, air quality forecasting, biogenic emissions, sea salt, fugitive dust, and NH3 inverse modeling
Sparse Matrix Operator Kernel Emissions System (SMOKE)

**Background:** SMOKE began under the sponsorship of AMD with the North Carolina Supercomputing Center (now CEP). As a community model, it is applicable to any pollutant, computationally efficient, and architecturally flexible. SMOKE may be downloaded at [www.cmascenter.org](http://www.cmascenter.org).

**Recent AMD-sponsored enhancements:**
- Ability to ingest Continuous Emissions Monitoring (CEM) data
- Plume-in-grid (PinG) stack selection criteria
- Importation of projection packets (GROWIN module)
- Consulted on the integration of the criteria and toxic inventories
- Modified and corrected the plume rise algorithm
- Setup/modified GSPRO speciation files for CB4, RADM, & SAPR99
- Incorporated various versions of BEIS3
Spatial Allocation of Emissions

**Spatial Allocator program:** Gridding spatial data poses a difficult challenge when processing raw emissions data. CEP (via funding from MIMS) has developed the Spatial Allocator program to replace SMOKE Tool, which was part of the old Models-3 modeling framework. Spatial Allocator does not require the use of expensive proprietary software. Downloads are available at [www.epa.gov/AMD/mims/software/spatial_allocator.html](http://www.epa.gov/AMD/mims/software/spatial_allocator.html).

**Spatial surrogates:** Used to distribute area source emissions. Working with CSC, we have used GIS to generate shape files for agriculture, airports, housing, population, major highways, ports, railroads, water, rural area, urban area, forest area, and roads. To support modeling of NH3 and fugitive dust emissions, we are creating shape files of paved roads, unpaved roads, vehicle miles traveled, construction activity, and agricultural tillage practices.
Sample of a spatial surrogate file created for SMOKE

Highway Construction Activity

County Level Acres Disturbed by Highway Construction

Legend

- 0.000000
- 0 - 100 Acres Cleared
- 100 - 250 Acres Cleared
- 250 - 750 Acres Cleared
- 750 - 3036 Acres Cleared
Increasing the speed of mobile source emission estimates by using polynomial functions to account for temperature
Atlanta, GA (PAR emissions, 32 km grid, June 12-30, 1999)
Estimating Biogenic Emissions for CMAQ

- **Biogenic Emissions Inventory System (BEIS):**
  - introduced by AMD in 1988 to estimate VOC emissions from vegetation and NO emissions from soils

- **BEIS3.09:**
  - default version in SMOKE 2.0
  - 1-km vegetation database (BELD3)
  - emission factors for isoprene, monoterpenes, OVOCs, and nitric oxide (NO)
  - environmental corrections for temperature and solar radiation (isoprene only)
  - speciation factors for the CBIV, RADM2, and SAPRC99 mechanisms
Estimating Biogenic Emissions for CMAQ

- **BEIS3.12:**
  - used in the current research version of CMAQ
  - emission factors for 34 chemicals, including 14 monoterpenes and methanol
  - MBO, methanol, isoprene modulated by solar radiation
  - soil NO dependent on soil moisture, crop canopy coverage, and fertilizer application
  - to be a module to SMOKE and released at www.epa.gov/asmdnerl/biogen.html
Flowchart of the Biogenic Emissions Inventory System (BEIS3)

Several areas of uncertainty exist
USGS North American Land Characteristics Data
(1 km, 21 broad classes, satellite-derived)

Assign crop areas to 1-km grid cells in a county, using USGS class and urban/rural IDs

Derive crop species distribution and total crop area (county-level)

Assign forest areas to 1-km grid cells

US Forest Inventory and Analysis (FIA) data
(county-level, 300,000 survey plots)

Assign tree species distribution to 1-km grid forest areas

Develop tree species distribution within county

BELD3 – a 1-km hybrid dataset with crop types, tree species, urban/rural IDs, and 19 USGS classes

1990 US Census (urbanized boundaries)
Assign urban/rural/water identifier (1-km grid)

1992 US Agricultural Census (county-level)

Zhu & Evans (1994) US Forest density data
(1 km, satellite-derived)
Beld3 - 229 vegetation classes

Tree species/genera (FIA)

USGS classes
- Alfalfa
- Barley
- Corn
- Cotton
- Grass
- Hay
- Misc_cropland
- Oats
- Pasture
- Peanuts
- Potatoes
- Rice
- Rye
- Sorghum
- Soybeans
- Tobacco
- Wheat

Crop types (USDA)
- Ash
- Basswood
- Beech
- Birch
- Bumelia_gum
- Cajeput
- Califor-laurel
- Cascara-buckthorn
- Castanea
- Catalpa
- Cedar_chamaecyp
- Cedar_thuja
- Chestnut_bucky
- Chinaberry
- Cypress_cupress
- Cypress_taxodi
- Dogwood
- Douglas_fir
- East_hophornbea
- Elder
- Elm
- Eucalyptus
- Fir_balsam
- Fir_CA_red
- Fir_corkbark
- Fir_frazer
- Fir_grand
- Fir_noble
- Fir_Pacif_silver
- Fir_SantaLucia
- Fir_Shasta_red
- Fir_spp
- Fir_subalp
- Fir_white
- Gleditsia_locus
- Hackberry
- Hawthorn
- Oak_CA_black
- Oak_CA_canyon
- Oak_CA_light
- Oak_CA_white
- Oak_chinkapin
- Oak_cheesn
- Oak_chinkapin
- Oak_delta_post
- Oak_durand
- Oak_envergreen
- Oak_gambel
- Oak_actino
- Oak_laurel
- Oak_live
- Oak_Mexicanblue
- Oak_north
- Oak_north
- Oak_north
- Oak_nuttall
- Oak_OH_white
- Oak_overcup
- Oak_pin
- Oak_post
- Oak_scarlet
- Oak_scrub
- Oak_shingle
- Oak_shump
- Oak_silverleaf
- Oak_southern
- Oak_spp
- Oak_spruce
- Oak_swamp_cnut
- Oak_swamp_red
- Oak_swamp_white
- Oak_turkey
- Oak_water
- Oak_white
- Oak_willow
- Osage-orange
- Pawpaw
- Persimmon
- Pine_Apache
- Pine_Austri
- Pine_AZ
- Pine_Bishop
- Pine_blackjack
- Pine_bristlecone
- Pine_chihuahua
- Pine_Coulter
- Pine_digger
- Pine_Ewhite
- Pine_foxtail
- Pine_jack
- Pine_Jeffrey
- Pine_knobcone
- Pine_limb
- Pine_lobo
- Pine_lodgepole
- Pine_monterey
- Pine_pinyon
- Pine_pinyon_brd
- Pine_pinyon_cm
- Pine_pitch
- Pine_pond
- Pine_ponderosa
- Pine_red
- Pine_sand
- Pine_scotch
- Pine_shortleaf
- Pine_spruce
- Pine_sugar
- Pine_swhite
- Pine_tablemtn
- Pine_VA
- Pine_Washoe
- Pine_whitebark
- Pine_Wwhite
- Pine_yellow
- Populus
- Prunus
- Redbay
- Robinia_locust
- Sassafras
- Sequoia
- Serviceberry
- Silverbell
- Smoketree
- Soapberry_west
- Sourwood
- Sparkleberry
- Spruce_black
- Spruce_blue
- Spruce_brewer
- Spruce_engleman
- Spruce_norway
- Spruce_red
- Spruce_Sitka
- Spruce_spp
- Spruce_white
- Sweetgum
- Sycamore
- Tallowtree-china
- Tamarix
- Tanoak
- Torrey
- Tung_oil-tree
- Unknown_tree
- Walnut
- Water_elm
- Willow
- Yellow_poplar
- Yellowwood
- Yucca_Mojave
BEIS3 - Improved spatial resolution

BEIS2/BELD2

BEIS3/BELD3
BEIS3 – Chemical species

34 chemical species

isoprene ethene
methyl-butenol propene
a-pinene ethanol
b-pinene acetone
d3-carene hexanal
d-limonene hexenol
camphene hexenylacetate
myrcene formaldehyde
a-terpinene acetaldehyde
b-phellandrene butene
sabinene ethane
p-cymene formic acid
ocimene acetic acid
a-thujene butenone
terpinolene carbon monoxide
g-terpinene ORVOCs
methanol nitric oxide
Comparison of BEIS3.09 v BEIS3.12 for 2001 – Domain total emissions

Animation of isoprene
Comparison of BEIS3.09 v BEIS3.12 for 2001 – Domain total emissions

Animation of NO
Comparison of BEIS3.09 v BEIS3.12 for 2001 – Domain total emissions (10^3 metric tons)

<table>
<thead>
<tr>
<th>Compound</th>
<th>BEIS3.09</th>
<th>BEIS3.12</th>
<th>% change</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil NO</td>
<td>467</td>
<td>609</td>
<td>+30%</td>
</tr>
<tr>
<td>Total VOC</td>
<td>50,320</td>
<td>48,365</td>
<td>-4%</td>
</tr>
<tr>
<td>Isoprene</td>
<td>22,141</td>
<td>22,141</td>
<td>0%</td>
</tr>
</tbody>
</table>
Sea Salt Emissions

• The aerosol module within the CMAQ modeling system needs to account for sea salt emissions over marine environments.


• Their equations have been adapted to compute sea salt emissions as a function of marine area, vertical wind profile, and roughness length.

• A test case using a version of CMAQ has been created with a 32-km gridded national domain for a 15-day period in July 1999.

Courtesy of Dr. Michelle Mebust
Estimate of Sea Salt Emissions for CMAQ

Sea Salt emissions

(32 km resolution, July 7 1999, 17 GMT)

Min= 0 at (71,1). Max= 420 at (26,65)
Fugitive Dust Emissions

• Fugitive dust emissions tend to be overestimated in atmospheric transport models (Gillette, 2001, www.wrapair.org/forums/dejf/documents/).

• To account for this discrepancy, He et al. (2002, Proceedings of the Annual Conference of the American Association for Aerosol Research, Charlotte, NC) developed an wind blown dust algorithm for CMAQ based on the work of Gillette.

• Algorithm uses threshold friction velocity parameterizations and incorporates gridded databases of soil type, surface soil moisture content, meteorology, and vegetation.

• Algorithm tries to account for the sub-grid scale variability of land use, and the interception of uplifted dust particles by vegetation.

• CMAQ simulations have begun and are being evaluated for a multi-day windblown dust episode from April 2001.
Proposed Fugitive Dust Emission Model for CMAQ

CMAQ

MM5

MCIP

Aerosol

Fugitive Dust Emission

Windblown Dust
\[ F = kA \frac{\rho}{g} u_*(u^2 - u_*^2) \]

Road Dust

Paved Road Dust
\[ EF = 0.016(SL/2)^{0.65}(W/3)^{1.5} \]

Unpaved Road Dust
\[ EF = 2.6(SC/12)^{0.8}(W/3)^{0.4}(M/0.2)^{-0.3} \]

Local scale dust flux
Regional scale vertical flux
\[ \Phi = \frac{m_{\text{vertical}}}{m_{\text{horizontal}}} = 1 - \frac{V_d}{V_d + K} \]

friction velocity
surface wind
deposition velocity
landuse data
gridded VMT data
county level VMT data and road coverage spatial temporal allocation

soil texture/landuse data
friction velocity
friction velocity
soil moisture
roughness length of soil
area of dust source

silt loading/silt content on road surface
moisture of road surface
gridded road coverage road type data
fleet average vehicle weight

Courtesy of Dr. Shan He
Windblown Fugitive Dust Emissions Estimated with the "He" Algorithm
# Fugitive Dust Emissions from Unpaved Roads

<table>
<thead>
<tr>
<th>Current method</th>
<th>Proposed method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Does not account for removal by vegetation</td>
<td>Incorporate transport fraction developed by Dr. Shan He</td>
</tr>
<tr>
<td>FHWA road mileage</td>
<td>TIGER data to grid unpaved roads from county data</td>
</tr>
<tr>
<td>Uses monthly rainfall from a single station in a state</td>
<td>Simulate the moisture content of the road surface using gridded solar radiation, dew point, wind speed and rainfall data.</td>
</tr>
<tr>
<td>Based on published AP-42 methodology and used in EPA’s NEI.</td>
<td>Status: Unpaved road data have been gridded and the emissions algorithm will be tested winter 2004.</td>
</tr>
</tbody>
</table>
Emissions Modeling for CMAQ – Work in progress

• Other emissions-related work includes the following:
  – support for the global climate change program
  – support for toxics and fine-scale modeling
  – ammonia
  – wildland fires
  – lightning NO
  – mobile sources

• The emissions work group is striving to interact more closely with the model evaluation team.

• QA of emission estimates for CMAQ will continue to be an important responsibility.