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.

Recent AMD-sponsored enhancements:

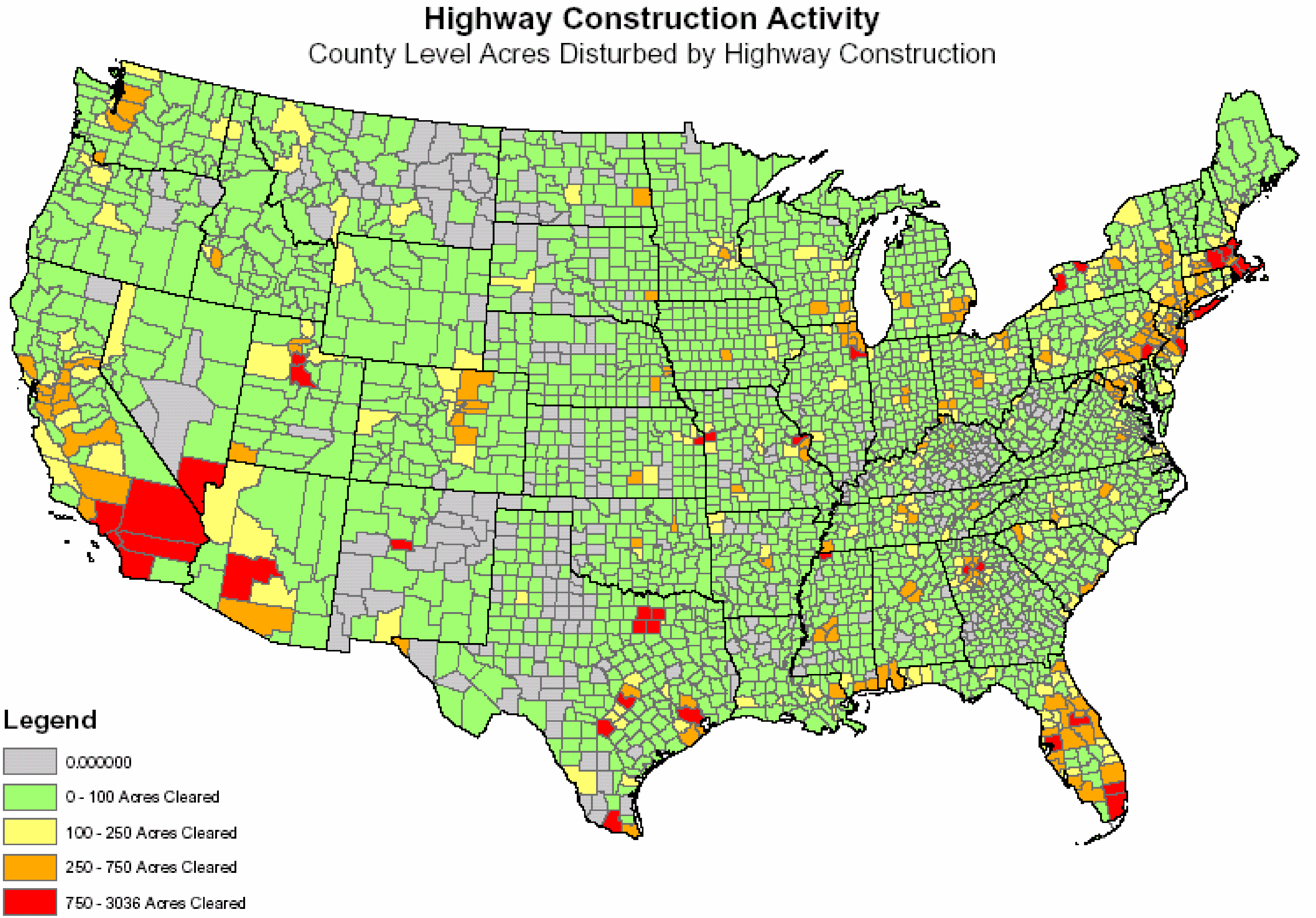
- Ability to ingest Continuous Emissions Monitoring (CEM) data
- Plume-in-grid (PinG) stack selection criteria
- Importation of projection packets (GROWIN module)
- Consulted on the integration of the criteria and toxic inventories
- Modified and corrected the plume rise algorithm
- Setup/modified GSPRO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

Spatial Allocation of Emissions

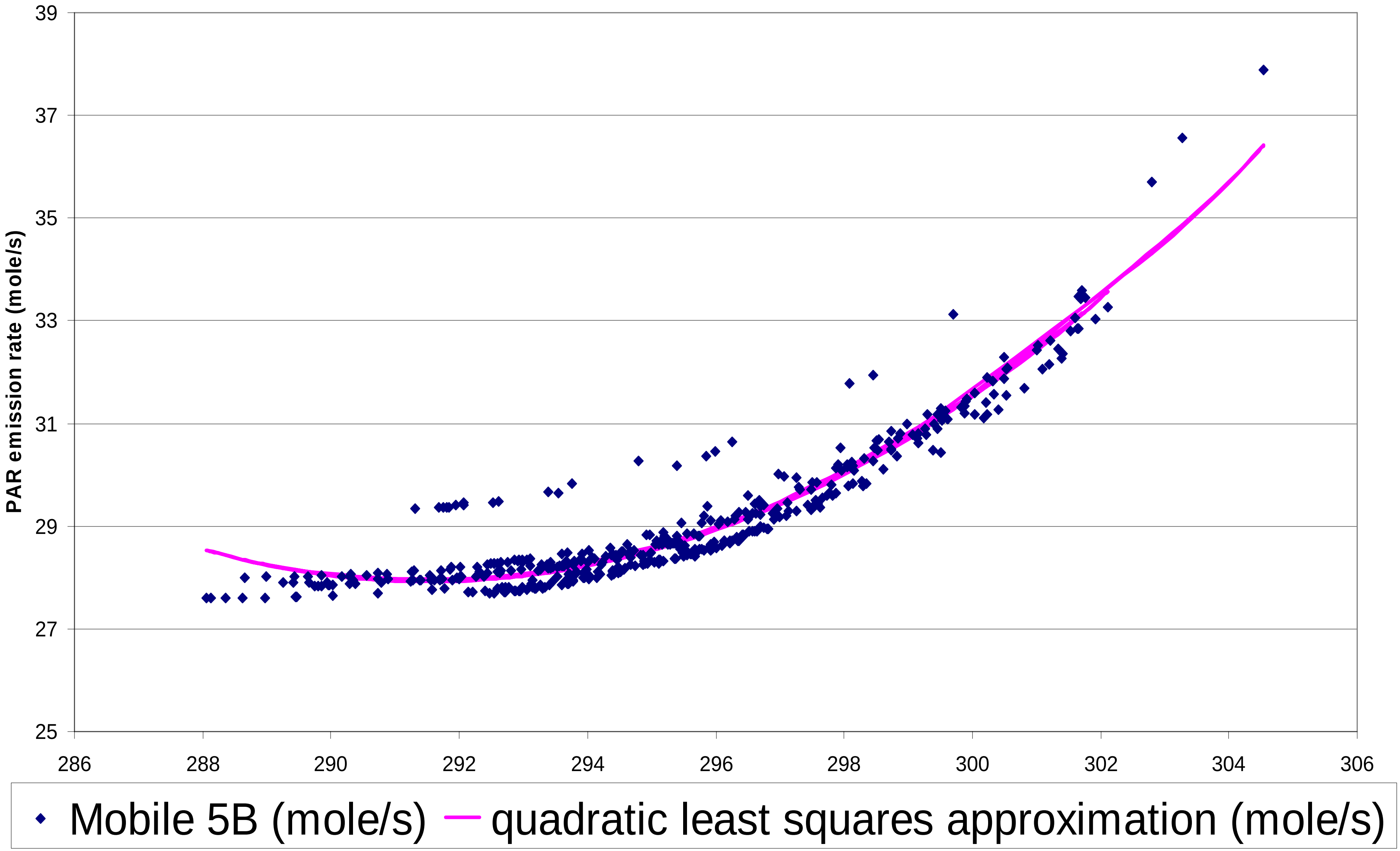
Spatial Allocator program: Gridding spatial data poses a difficult challenge when processing raw emissions data. CEP (via funding from MIMS) has developed the Spatial Allocator program to replace SMOKE Tool, which was part of the old Models-3 modeling framework. Spatial Allocator does not require the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

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



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)



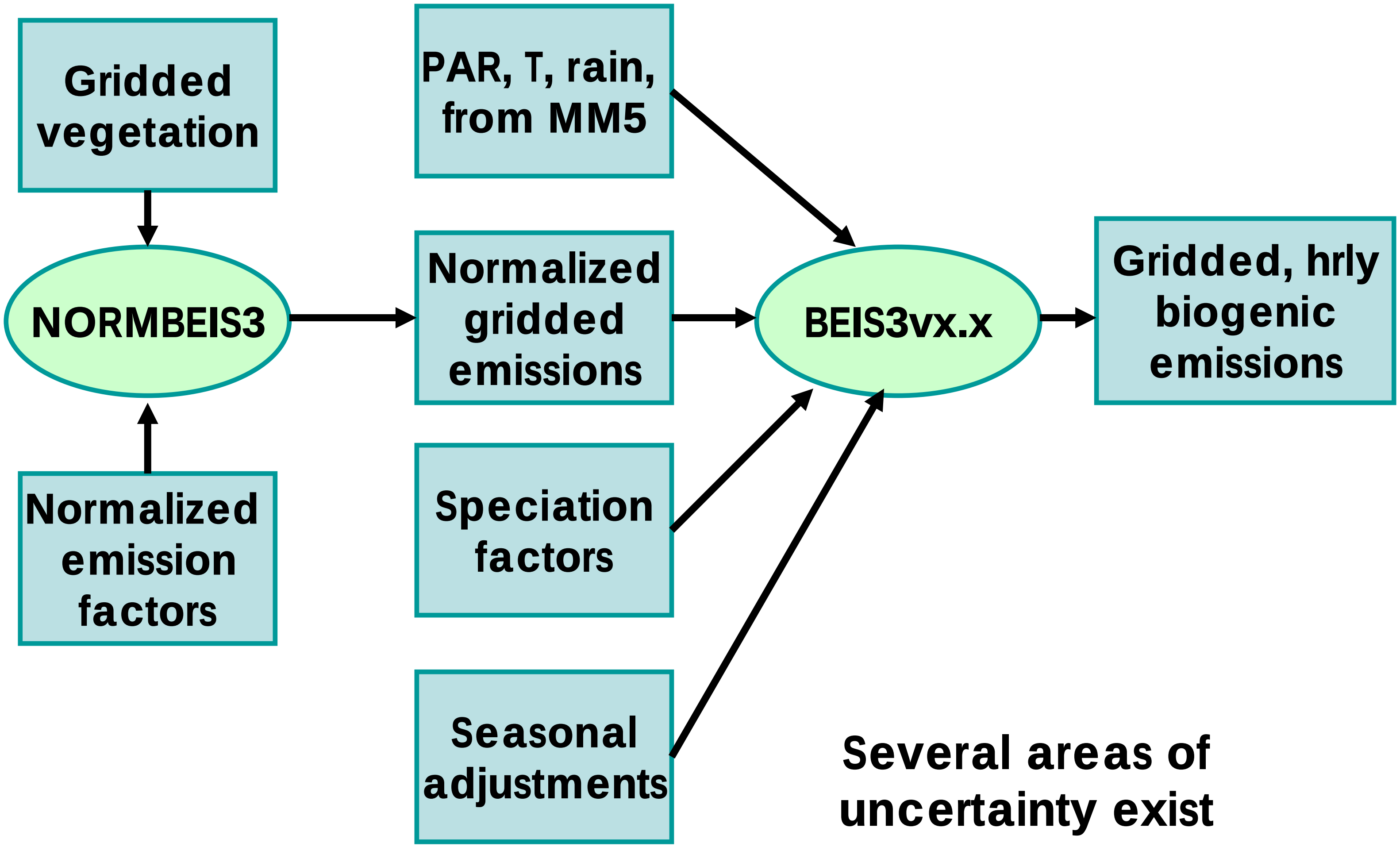
Estimating Biogenic Emissions for CMAQ

- **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

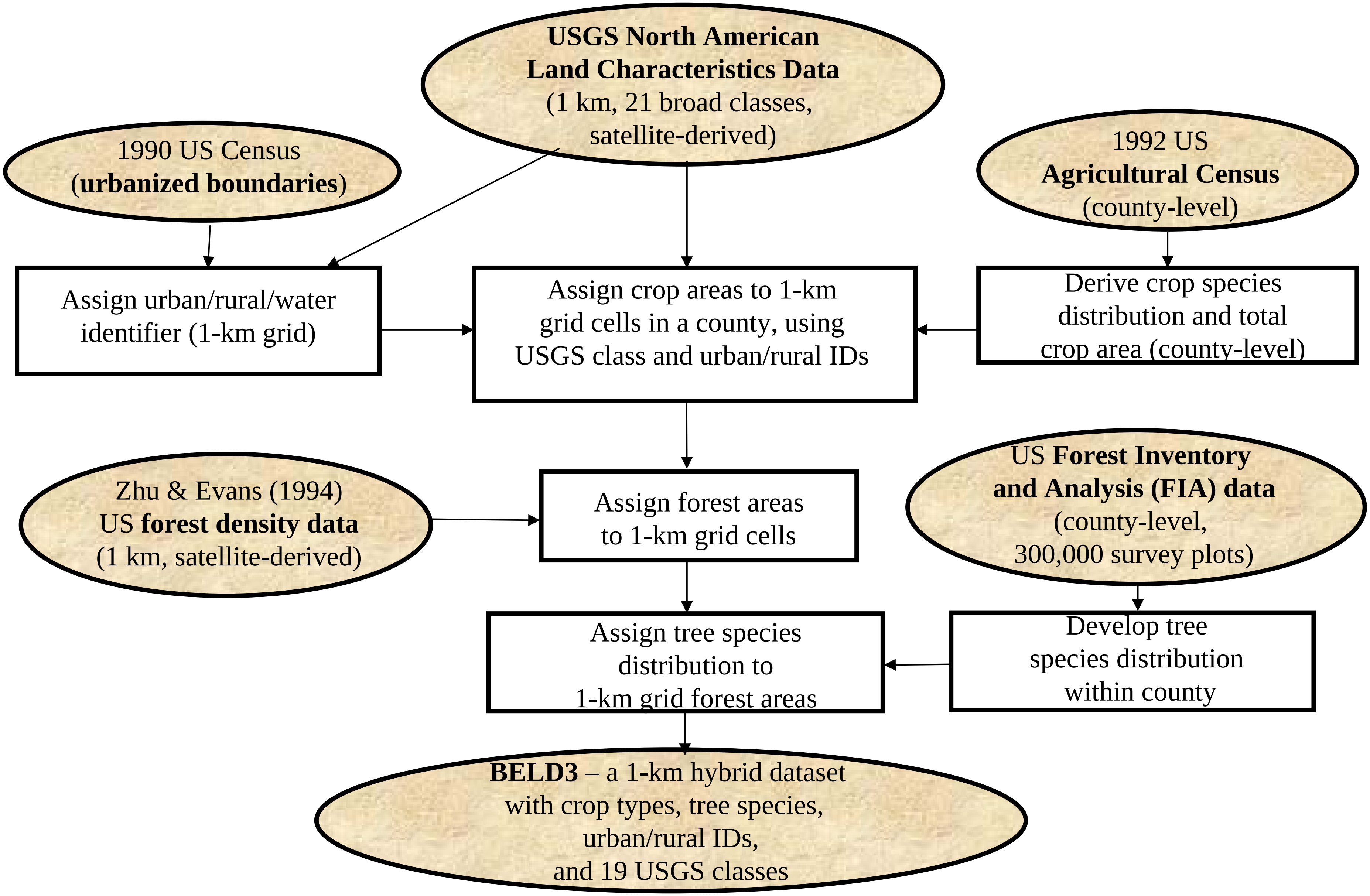
- **BEIS3.12:**
  - used in the current research version of CMAQ
  - emission factors for 34 chemicals, including 14 monoterpenes and methanol
  - MBO, methanol, isoprene modulated by solar radiation
  - soil NO dependent on soil moisture, crop canopy coverage, and fertilizer application
  - to be a 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

Creating Gridded Vegetation Data for the Biogenic Emissions Landuse Database (BELD3)



BELD3 – 229 vegetation classes

USGS classes

USGS_drycrop
USGS_irrcrop
USGS_cropgrass
USGS_cropwdlnd
USGS_grassland
USGS_shrubland
USGS_shrubgrass
USGS_savanna
USGS_decidfores
USGS_evbrdleaf
USGS_coniferfor
USGS_mxforest
USGS_water
USGS_wetwoods
USGS_sprsbarren
USGS_woodtundr
USGS_mxtundra
USGS_snowice
USGS_urban

Crop types (USDA)

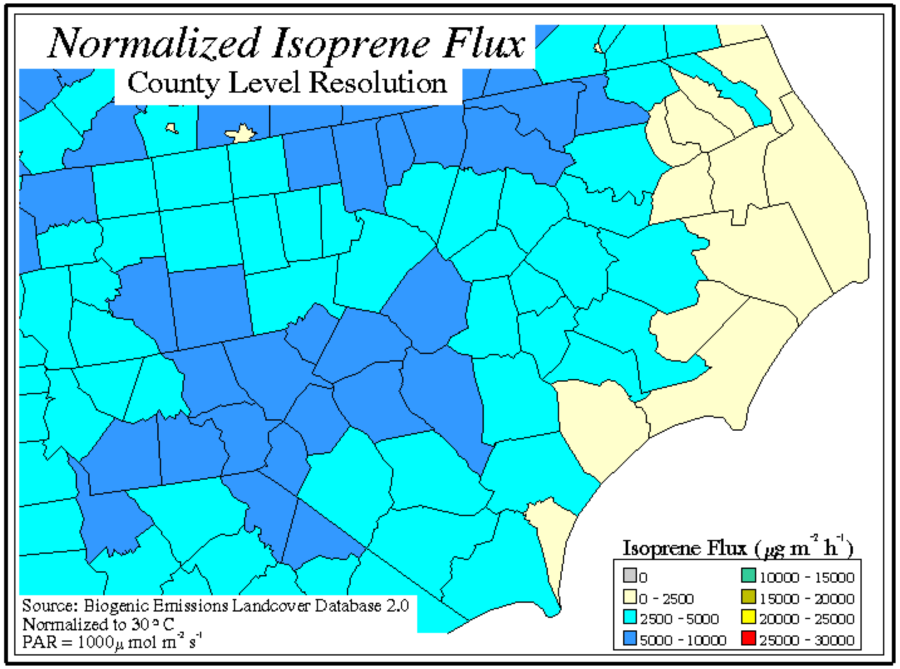
Alfalfa
Barley
Corn
Cotton
Grass
Hay
Misc_crop
Oats
Pasture
Peanuts
Potatoes
Rice
Rye
Sorghum
Soybeans
Tobacco
Wheat

tree species/genera (FIA)

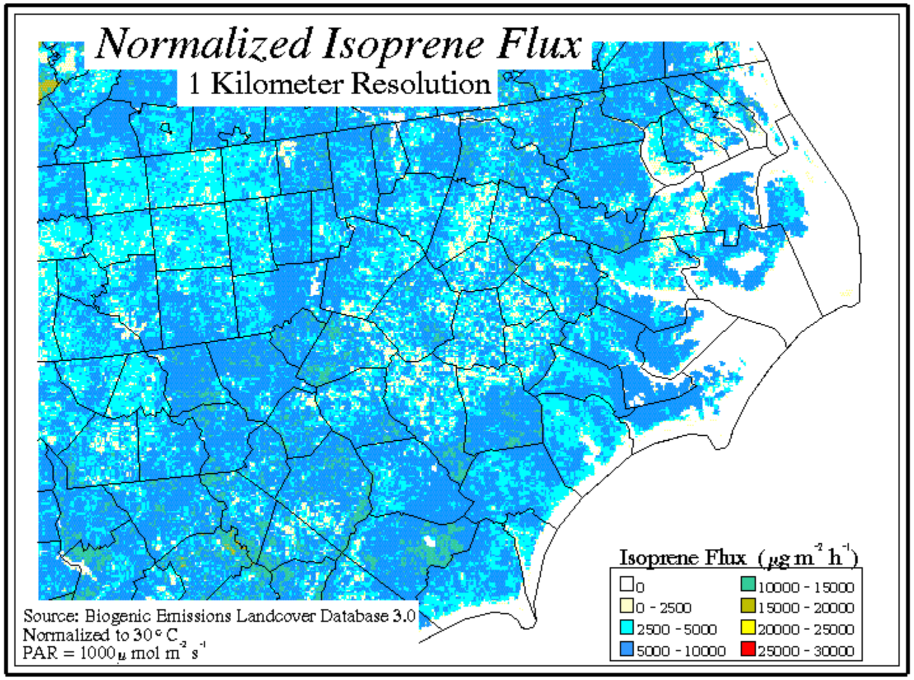
Acacia
Ailanthus
Alder
Apple
Ash
Basswood
Beech
Birch
Bumelia_gum
Cajeput
Califor-laurel
Cascara-buckthor
Castanea
Catalpa
Cedar_chamaecyp
Cedar_thuja
Chestnut_buckey
Chinaberry
Cypress_cupress
Cypress_taxodiu
Dogwood
Douglas_fir
East_hophornbea
Elder
Elm
Eucalyptus
Fir_balsam
Fir_CA_red
Fir_corkbark
Fir_fraser
Fir_grand
Fir_noble
Fir_Pacf_silver
Fir_SantaLucia
Fir_Shasta_red
Fir_spp
Fir_subalpine
Fir_white
Gleditsia_locus
Hackberry
Hawthorn
Hemlock
Hickory
Holly_American
Hornbeam
Incense_cedar
Juniper
KY_coffeetree
Larch
Loblolly_bay
Madrone
Magnolia
Mahogany
Maple_bigleaf
Maple_bigtooth
Maple_black
Maple_boxelder
Maple_FL
Maple_mtn
Maple_Norway
Maple_red
Maple_RkyMtn
Maple_silver
Maple_spp
Maple_striped
Maple_sugar
Mesquite
Misc-hardwoods
Mixed_conifer
Mountain_ash
Mulberry
Nyssa
Oak_AZ_white
Oak_bear
Oak_black
Oak_blackjack
Oak_blue
Oak_bluejack
Oak_bur
Oak_CA_black
Oak_CA_live
Oak_CA_white
Oak_canyon_live
Oak_chestnut
Oak_chinkapin
Oak_delta_post
Oak_Durand
Oak_Emery
Oak_Engelmann
Oak_evergreen
Oak_Gambel
Oak_interio_liv
Oak_laurel
Oak_live
Oak_Mexicanblue
Oak_Northrn_pin
Oak_Northrn_red
Oak_nuttall
Oak_OR_white
Oak_overcup
Oak_pin
Oak_post
Oak_scarlet
Oak_scrub
Oak_shingle
Oak_Shumrd_red
Oak_silverleaf
Oak_Southrn_red
Oak_spp
Oak_swamp_cnut
Oak_swamp_red
Oak_swamp_white
Oak_turkey
Oak_water
Oak_white
Oak_willow
Osage-orange
Paulownia
Pawpaw
Persimmon
Pine_Apache
Pine_Austrian
Pine_AZ
Pine_Bishop
Pine_blackjack
Pine_brstlcone
Pine_chihuahua
Pine_Coulter
Pine_digger
Pine_Ewhite
Pine_foxtail
Pine_jack
Pine_Jeffrey
Pine_knobcone
Pine_limber
Pine_loblolly
Pine_lodgepole
Pine_longleaf
Pine_Monterey
Pine_pinyon
Pine_pinyon_brd
Pine_pinyon_cmn
Pine_pitch
Pine_pond
Pine_ponderosa
Pine_red
Pine_sand
Pine_scotch
Pine_shortleaf
Pine_slash
Pine_spruce
Pine_sugar
Pine_Swwhite
Pine_tablemtn
Pine_VA
Pine_Washoe
Pine_whitebark
Pine_Wwhite
Pine_yellow
Populus
Prunus
Redbay
Robinia_locust
Sassafras
Sequoia
Serviceberry
Silverbell
Smoketree
Soapberry_westr
Sourwood
Sparkleberry
Spruce_black
Spruce_blue
Spruce_Brewer
Spruce_Engleman
Spruce_Norway
Spruce_red
Spruce_Sitka
Spruce_spp
Spruce_white
Sweetgum
Sycamore
Tallowtree-chins
Tamarix
Tanoak
Torreya
Tung-oil-tree
Unknown_tree
Walnut
Water-elm
Willow
Yellow_poplar
Yellowwood
Yucca_Mojave

BEIS3 - Improved spatial resolution

BEIS2/BELD2



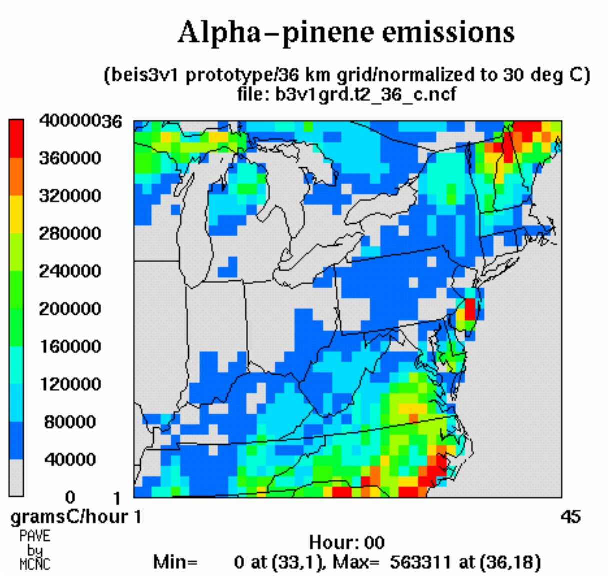
BEIS3/BELD3

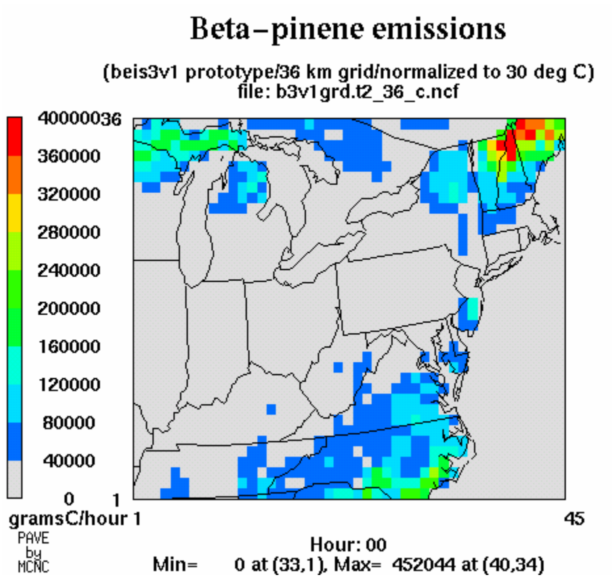


BEIS3 – Chemical species

34 chemical species

- isoprene
- methyl-butenol
- a-pinene
- b-pinene
- d3-carene
- d-limonene
- camphene
- myrcene
- a-terpinene
- b-phellandrene
- sabinene
- p-cymene
- ocimene
- a-thujene
- terpinolene
- g-terpinene
- methanol
- ethene
- propene
- ethanol
- acetone
- hexanal
- hexenol
- hexenylacetate
- formaldehyde
- acetaldehyde
- butene
- ethane
- formic acid
- acetic acid
- butenone
- carbon monoxide
- ORVOCs
- nitric oxide

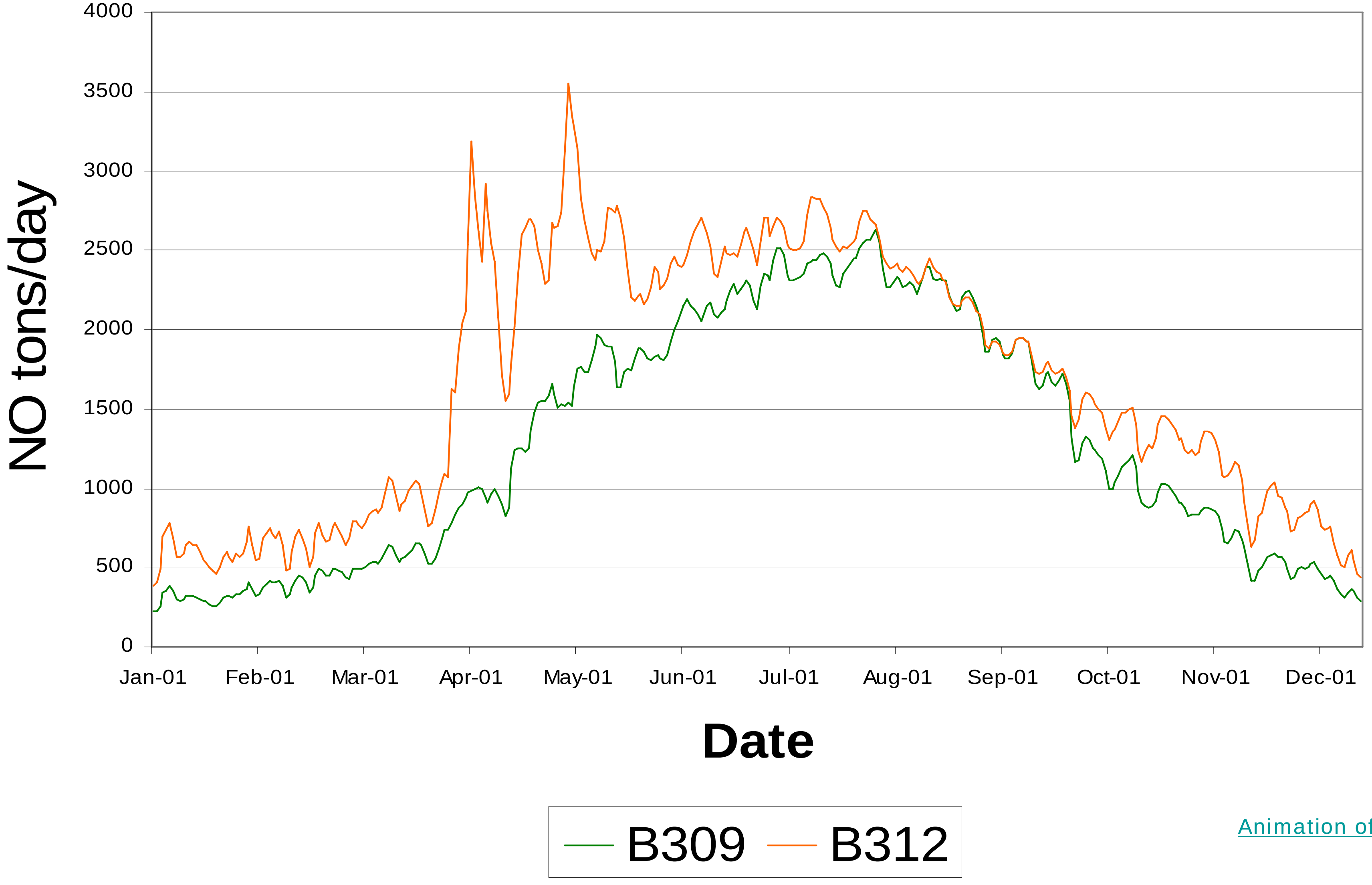




Comparison of BEIS3.09 v BEIS3.12 for 2001 – Domain total emissions

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)

Compound	BEIS3.09	BEIS3.12	% change
Soil NO	467	609	+30%
Total VOC	50,320	48,365	-4%
Isoprene	22,141	22,141	0%

Sea Salt Emissions

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

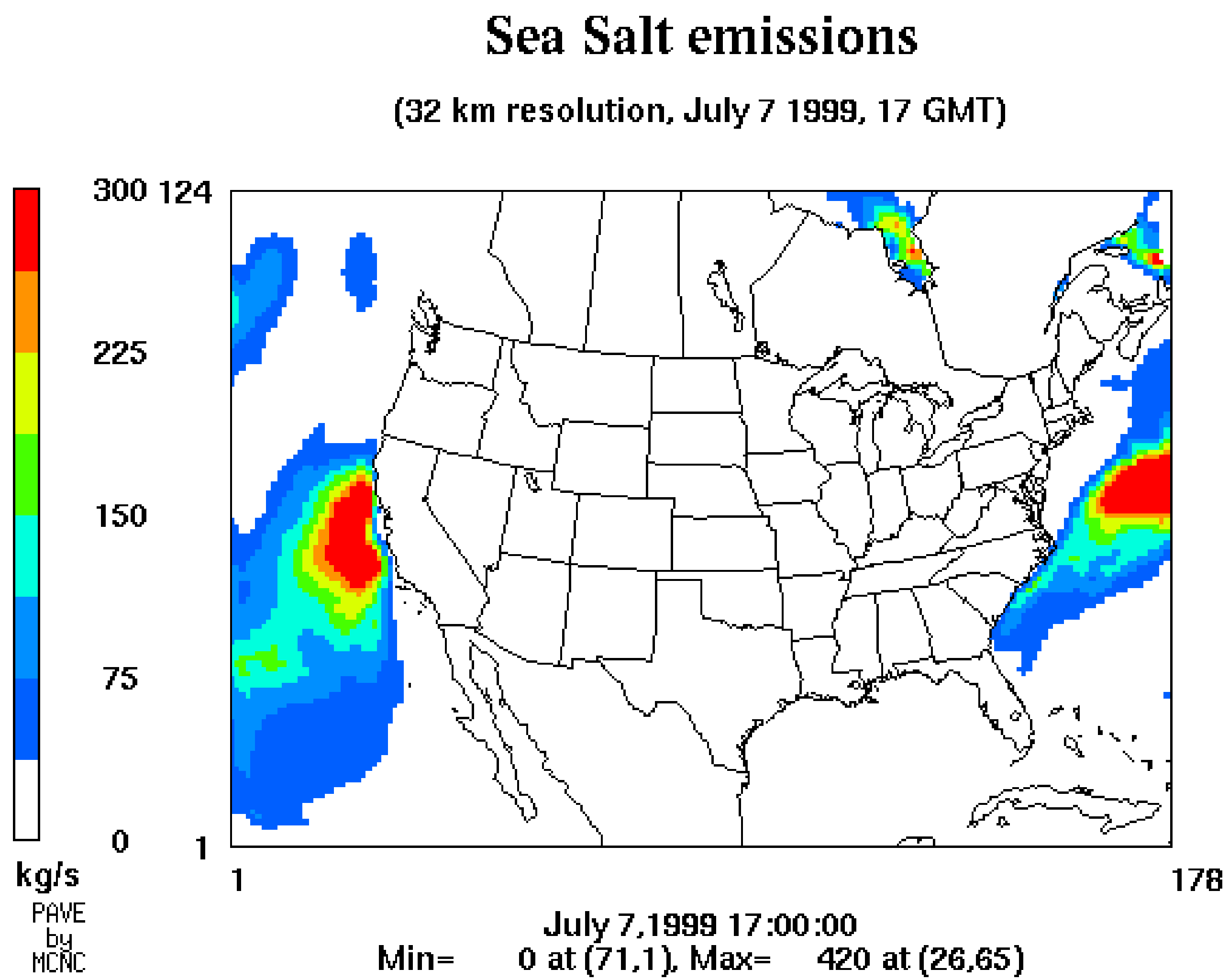
- Among available sea spray generation functions, Smith and Harrison (*Journal of Aerosol Science* **29**:S189-S190, 1998) appear best-suited for CMAQ.

- 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



Fugitive Dust Emissions

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

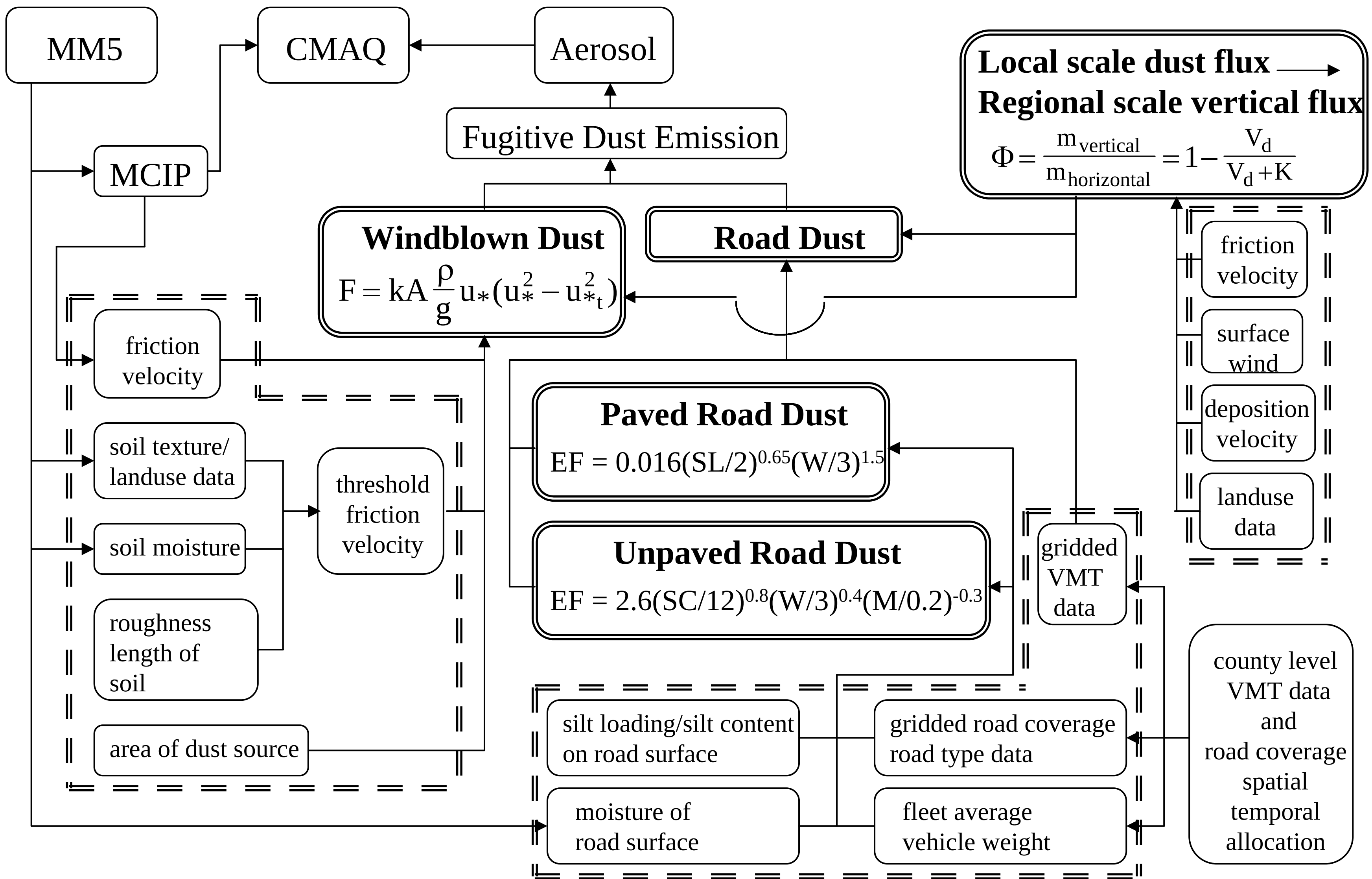
• To account for this discrepancy, He et al. (2002, Proceedings of the Annual Conference of the American Association for Aerosol Research, Charlotte, NC) developed an wind blown dust algorithm for CMAQ based on the work of Gillette.

• 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.

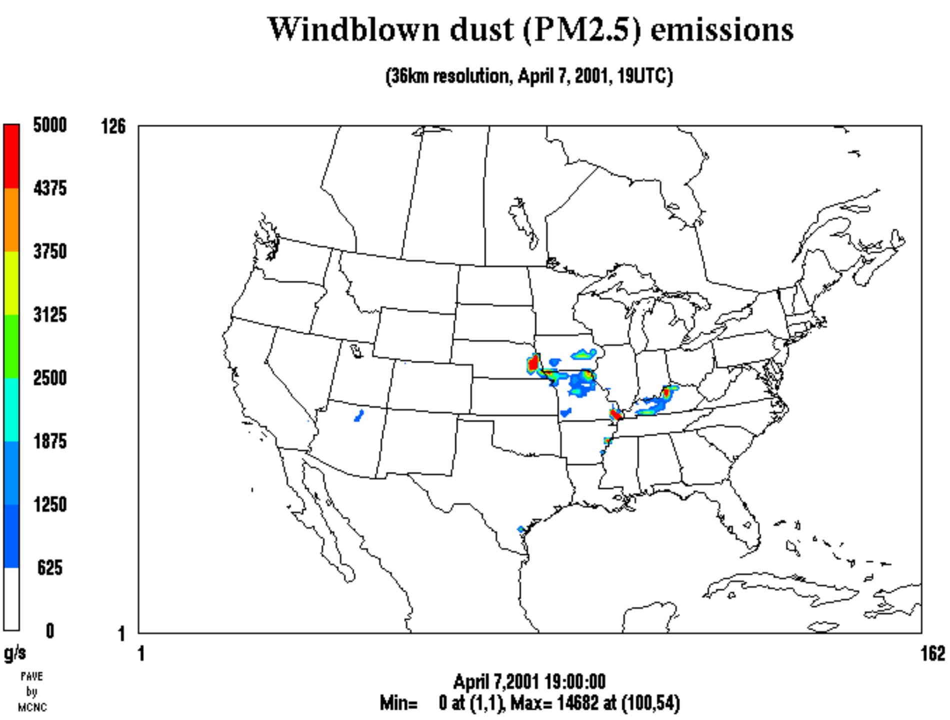
• CMAQ simulations have begun and are being evaluated for a multi-day windblown dust episode from April 2001.

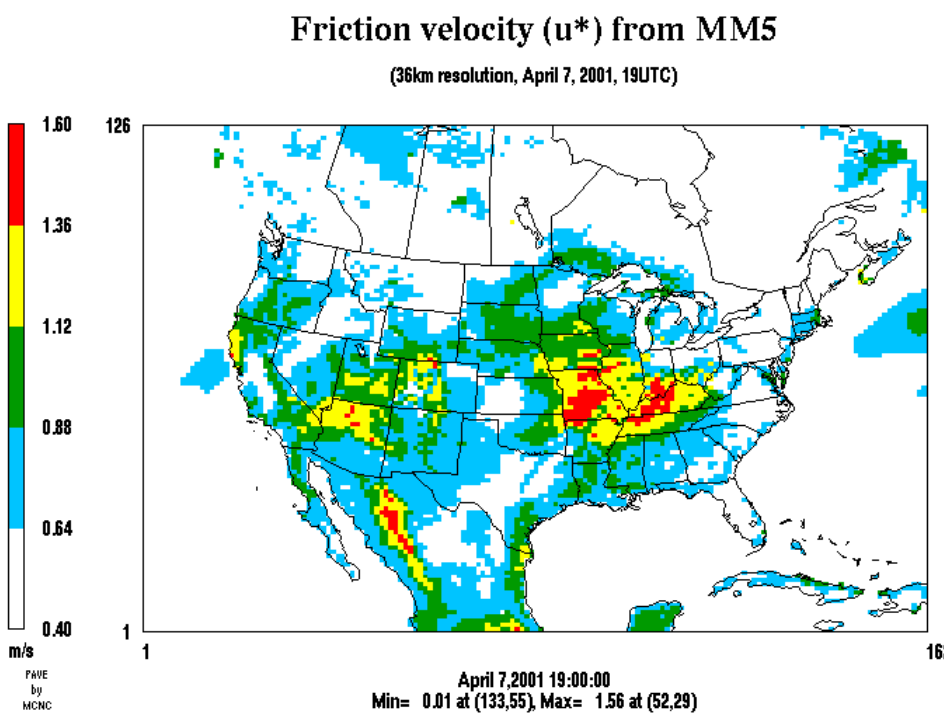
Proposed Fugitive Dust Emission Model for CMAQ



Courtesy of Dr. Shan He

Windblown Fugitive Dust Emissions Estimated with the "He" Algorithm





Fugitive Dust Emissions from Unpaved Roads

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

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.