Much ado about emission modeling …

Sigh no more, [colleagues], sigh no more,
[Emissions] were deceivers ever,
One foot in sea and one on shore,
*To one thing constant never.**

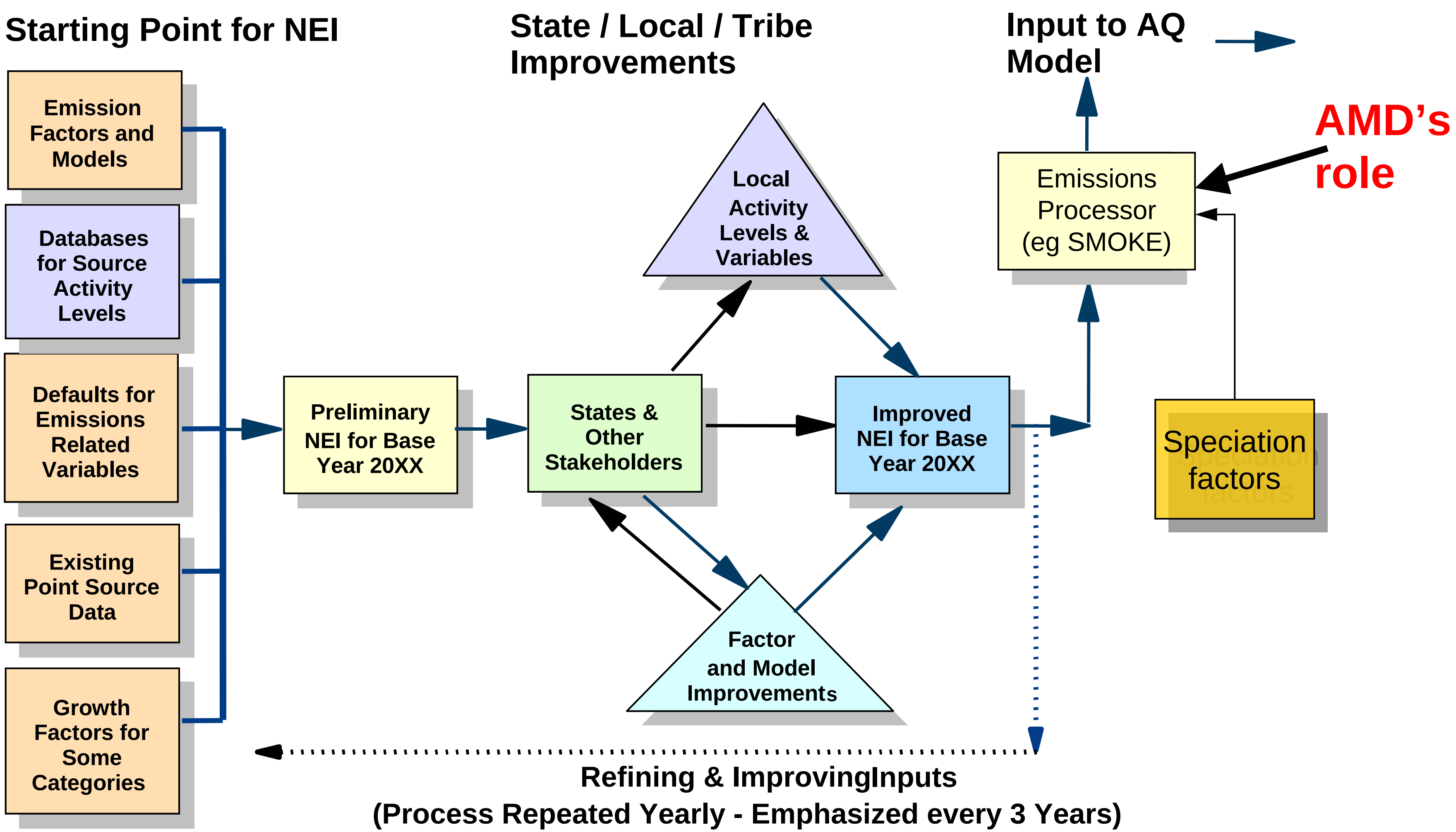
**w/ apologies to Wm. Shakespeare, from Much Ado About Nothing.*

T. Pierce
Atmospheric Modeling Division/NOAA
U.S. EPA/Office of Research and Development
Research Triangle Park, North Carolina

Much ado about emission modeling support and research …

- **AMD's role:** To obtain the best available emission estimate data for regional air quality modeling; to improve these estimates by building emission models that account for meteorological conditions; and, to develop innovative ways of evaluating emissions.
- **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**: EPA/OAQPS, EPA/ORD, RPOs, States/EIIP, CSC, USFS, IGAC/GEIA, Environment Canada, NCAR, and university researchers.
- **Selected R&D areas:** SMOKE, geographical data files, air quality forecasting, biogenic emissions, sea salt, fugitive dust, and NH3 inverse modeling

EPA's National Emissions Inventory



Courtesy T. Pace (EPA/OAQPS)

Much ado about emission modeling …

Purpose:

- to report on emission focus areas w/in AMD
- to suggest topics for future research
- to encourage collaboration

Outline:

- Ammonia
- Biogenic emissions
- Fugitive dust
- Air quality forecasting
- Wildfires

Much ado about ammonia emissions …

- 1994 – Battye et al., Development and selection of ammonia factors (EPA work assignment, W. Benjey)
- 1999 – Pierce and Bender, Examining the temporal variability of ammonia and nitric oxide emissions from agricultural processes (www.epa.gov/asmdnerl/awma_ei99.pdf)
- 2000 – CMU NH3 emissions model (www.cmu.edu/ammonia)
- 2003 – Gilliland et al., Seasonal NH3 emission estimates for the eastern United States based on ammonium wet concentrations and an inverse modeling method, J. Geophys. Res., 108 (D15), 4477, doi:10.1029/2002JD003063.
- 2004 – National Emission Inventory - Ammonia Emissions from Animal Husbandry Operations, Draft Report (www.epa.gov/ttn/chief/net/2002inventory.html)
- 2004 – Battye and Barrows, Review of ammonia emission modeling techniques for natural landscapes and fertilized soils, Draft Report (avbl for review at www.epa.gov/ttn/chief)

Much ado about ammonia emissions …

1998 National Emission Inventory for the U.S.

Source	NH3 emissions (x1000 tons)
Animal husbandry	3,520
Fertilizer	724
Industrial	691
Natural	0
Total	4,935

National Emission Inventory - Ammonia Emissions from Animal Husbandry Operations, Draft Report (2004)

Table 4-3. Comparison of 1999 and 2002 Ammonia NEIs

Animal Group	1999 NEI			2002 NEI		
	Population	Emission Factor (lb/head/yr)	Emissions (tons/yr)	Population	Emission Factor (lb/head/yr)	Emissions (tons/yr)
Cattle and Calves Composite	100,126,106	50.5	2,528,184	100,939,728	24.1	1,214,742
Hogs and Pigs Composite	63,095,955	20.3	640,424	59,978,850	14.32	429,468
Poultry and Chickens Composite	1,754,482,225	0.394	345,633	2,201,945,253	0.60	664,238
Sheep	6,768,448	7.43	25,144	6,685,000	7.43	24,835
Goats	1,820,268	14.1	12,833	1,989,799	14.1	14,028
Horses	2,578,238	26.9	34,677	5,300,000	26.9	71,285
Total	**1,928,871,240**	NA	**3,586,896**	**2,376,838,630**	NA	**2,418,595**

NA = Not applicable

33% reduction in NH3 emissions

Recommended Default Emission Factors for Natural Landscapes

Vegetation	Emission factors (ng m^{-2} s^{-1})	Estimated emissions in continental US (Gg/yr)
Forests	1.2	58
Grasslands	0.9	32
Shrublands	1.3	46
Deserts	0.3	<1
Total		137

=> ~5% of total U.S. inventory

Review of Ammonia Emission Modeling Techniques for Natural Landscapes and Fertilized Soils, Draft Report

Proposed temporal adjustment factors for NH3 emissions from natural landscapes

Proposed seasonal allocation:
Spring = 0.143
Summer = 0.714
Autumn = 0.143
Winter = 0.000

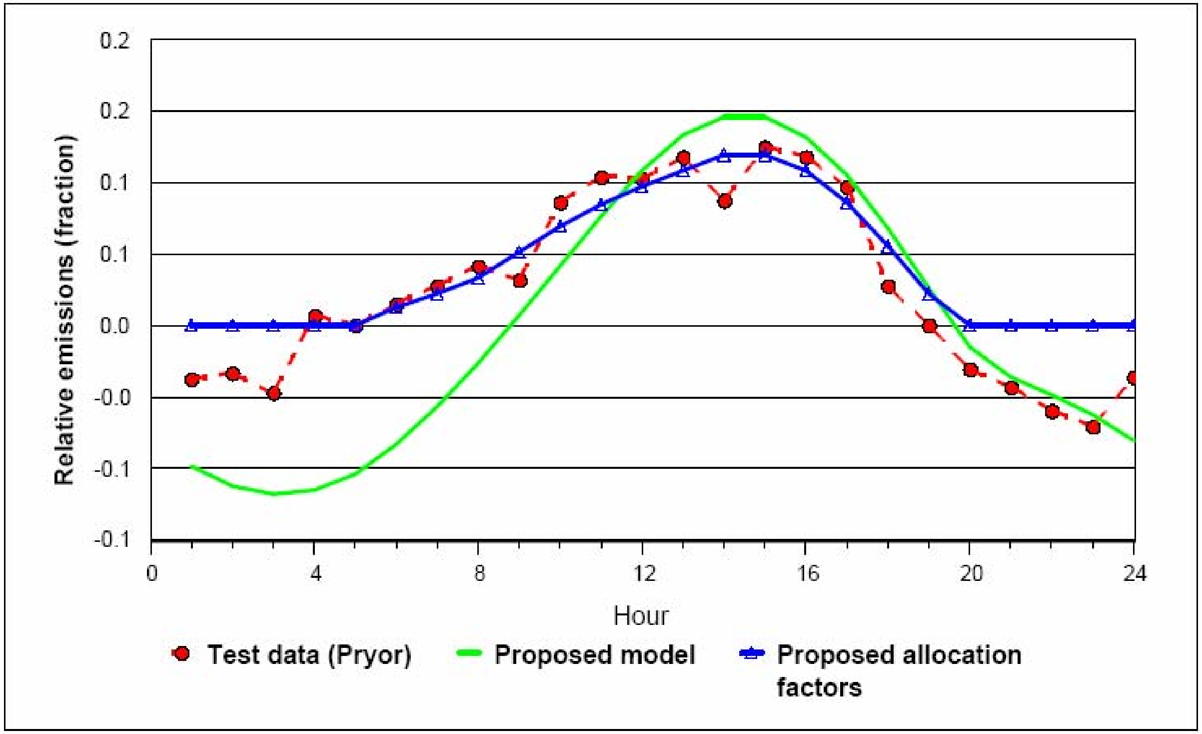


Figure 8. Comparison of proposed diurnal allocation factors with measured and modeled diurnal values.

Review of Ammonia Emission Modeling Techniques for Natural Landscapes and Fertilized Soils, Draft Report

Proposed temporal adjustment factors for NH3 emissions from fertilized soils

Proposed seasonal allocation:
Use CMU's county-wide, monthly values

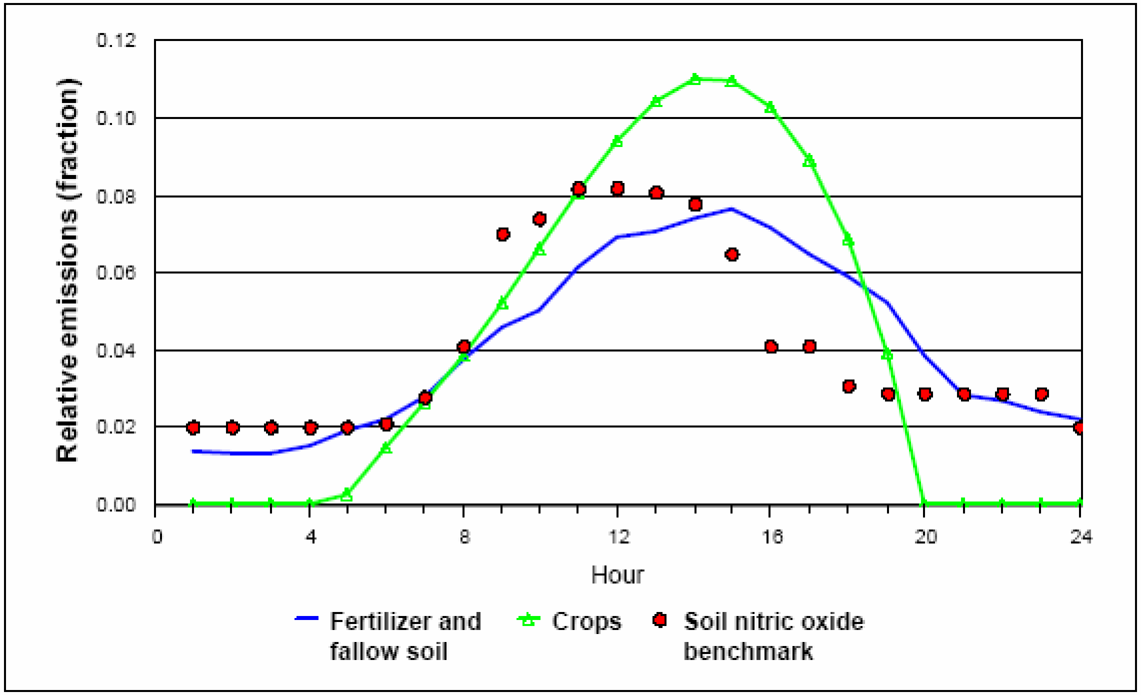


Figure 12. Diurnal allocation factors for NH_3 from fertilizer, crops, and fallow soil, compared with the profile for nitric oxide from soil.

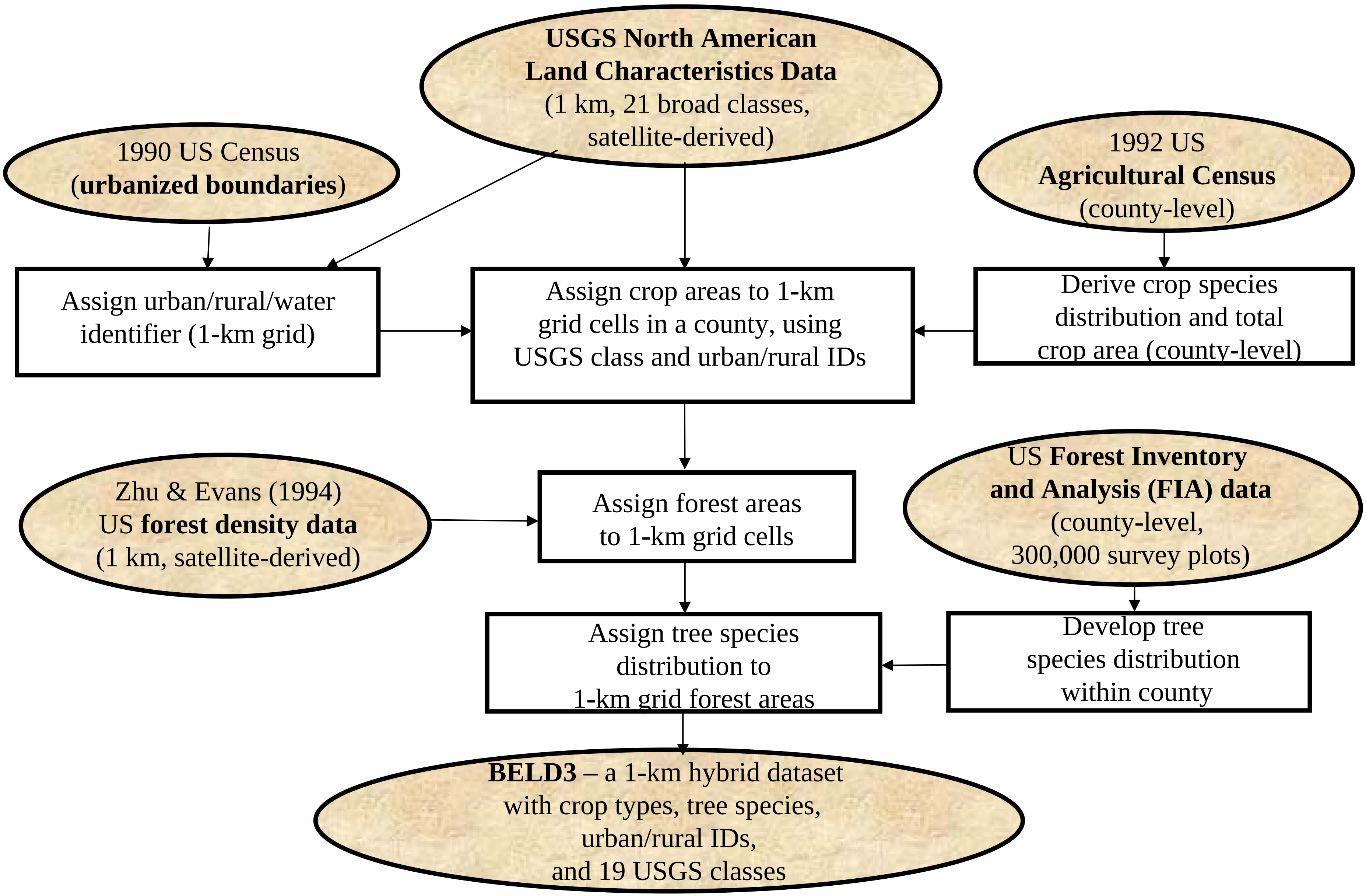
Much ado about biogenic emissions …

- **Biogenic Emissions Inventory System (BEIS):**
  - introduced by AMD in 1988 to estimate VOC emissions from vegetation and NO emissions from soils
- **BEIS3.09:**
  - current default version used for regulatory modeling
  - 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

Much ado about biogenic emissions …

- **BEIS3.12:**
  - current research version of CMAQ and in 2001 NEI
  - 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
  - avbl as a module to SMOKE and can be downloaded from www.epa.gov/asmdnerl/biogen.html

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)

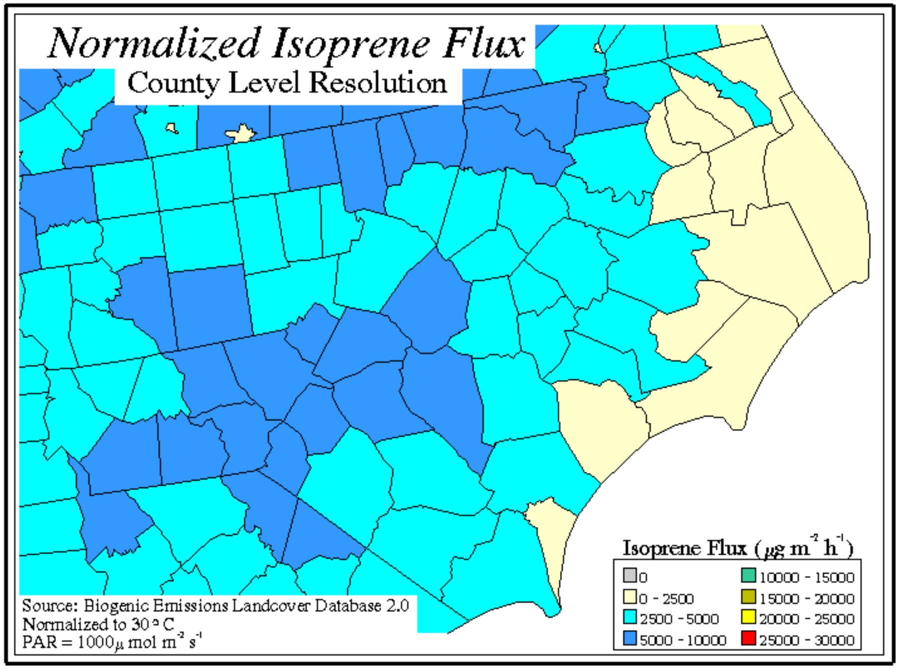
Alfalfa
Barley
Corn
Cotton
Grass
Hay
Misc_crop
Oats
Pasture
Peanuts
Potatoes
Rice
Rye
Sorghum
Soybeans
Tobacco
Wheat

tree species/genera (FIA)

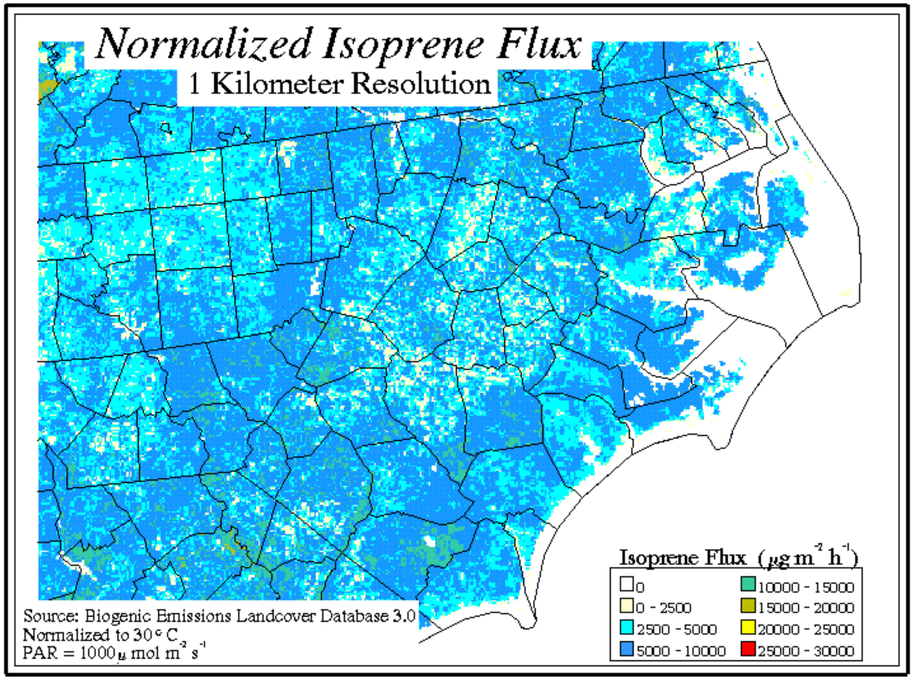
Acacia
Ailanthus
Alder
Apple
Ash
Basswood
Beech
Birch
Bumelia_gum
Cajeput
Califor-laurel
Cascara-buckthor
Castanea
Catalpa
Cedar_chamaecyp
Cedar_thuja
Chestnut_buckey
Chinaberry
Cypress_cupress
Cypress_taxodiu
Dogwood
Douglas_fir
East_hophornbea
Elder
Elm
Eucalyptus
Fir_balsam
Fir_CA_red
Fir_corkbark
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
Yellowood
Yucca_Mojave

BEIS3 - Improved spatial resolution

BEIS2/BELD2



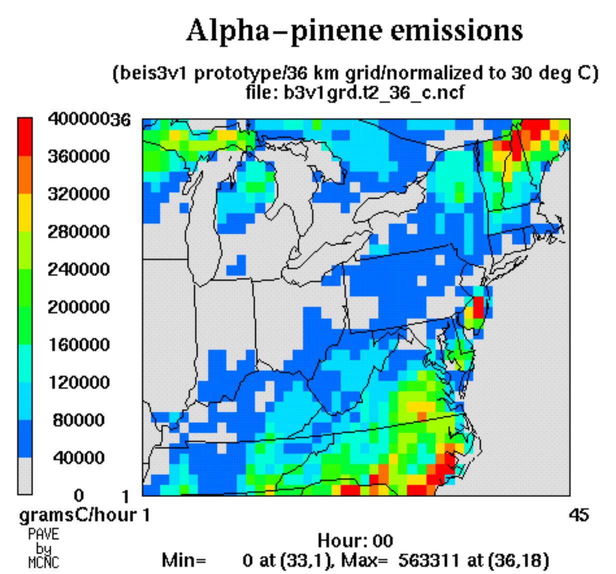
BEIS3/BELD3

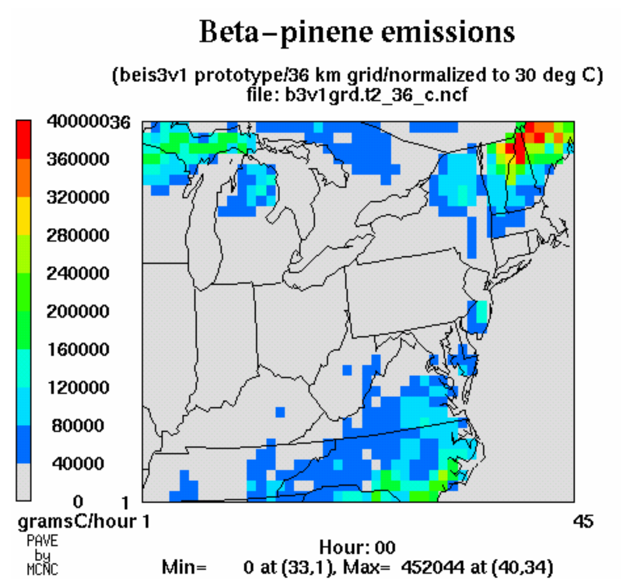


BEIS3 – Chemical species

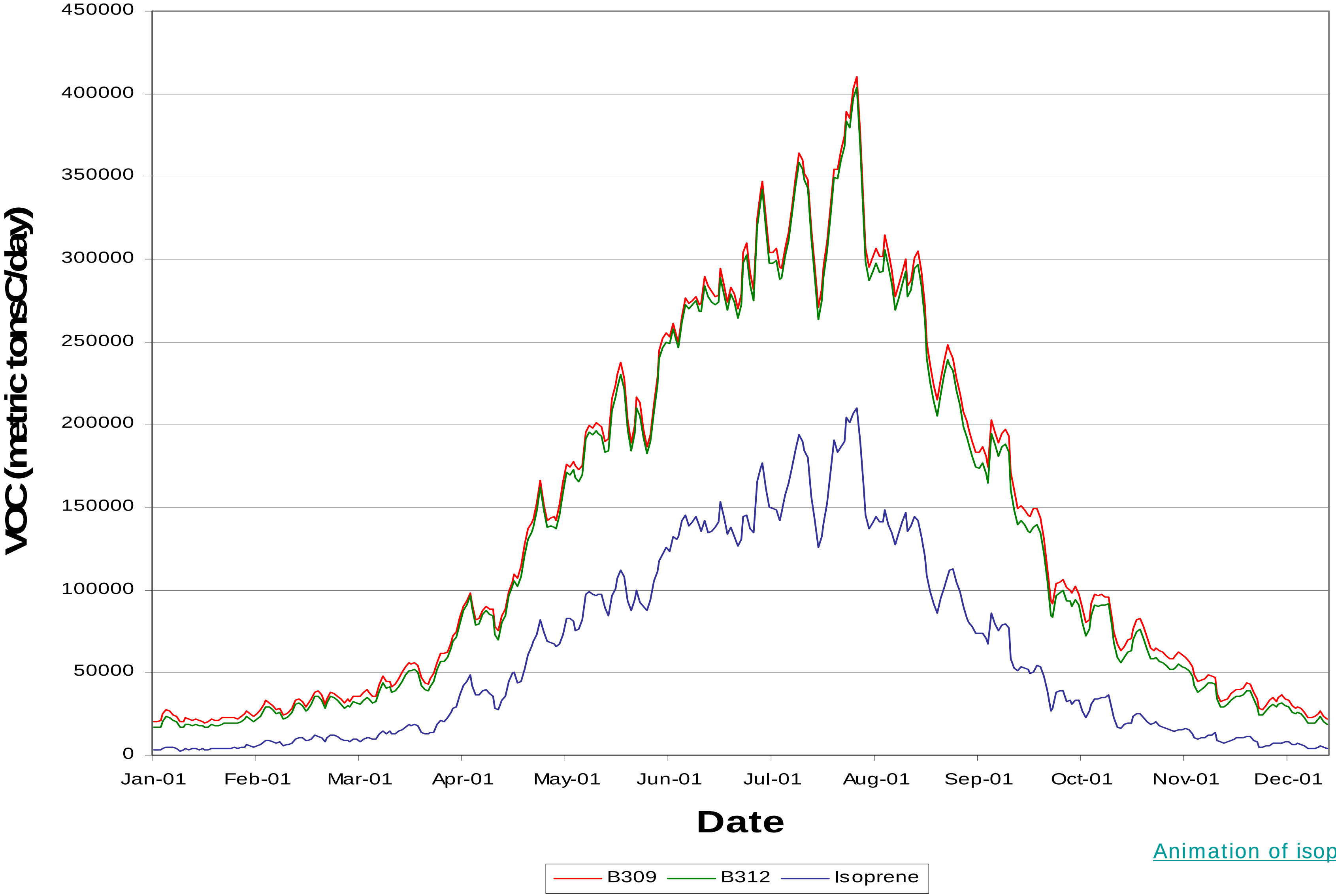
<u>34 chemical species</u>

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



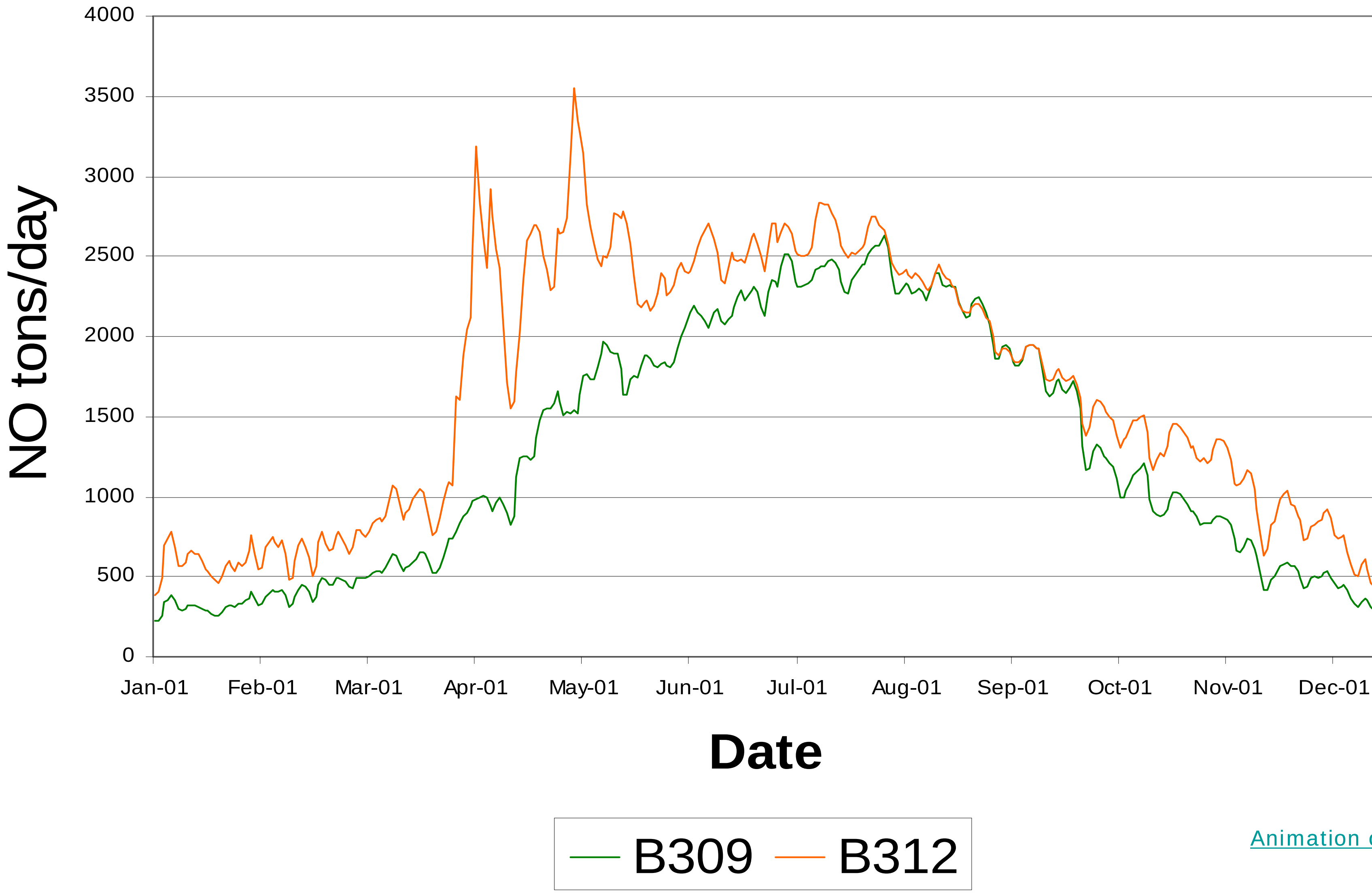


Comparison of BEIS3.09 v BEIS3.12 for 2001 Domain total emissions



Animation of isoprene

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



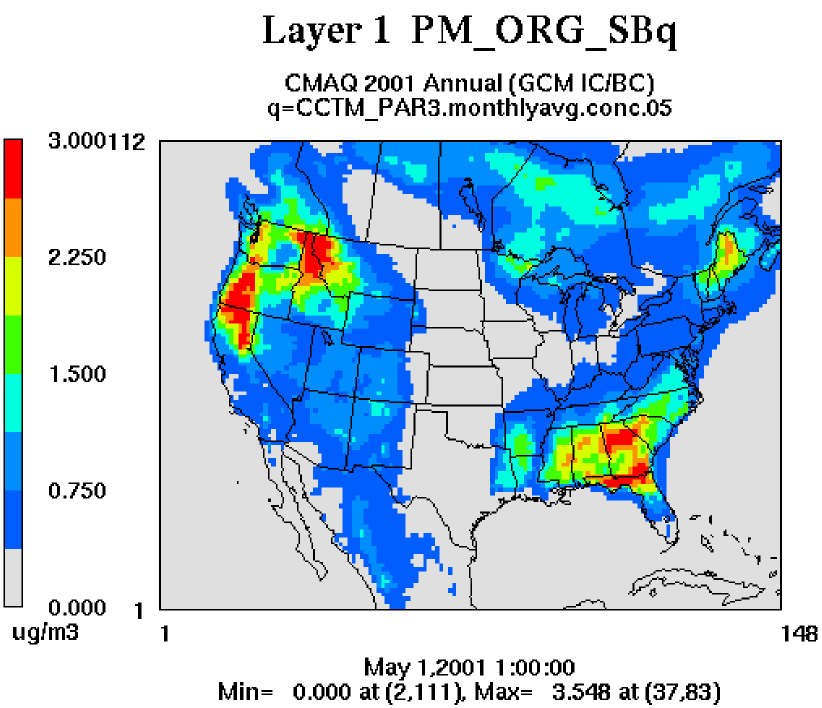
Animation of NO

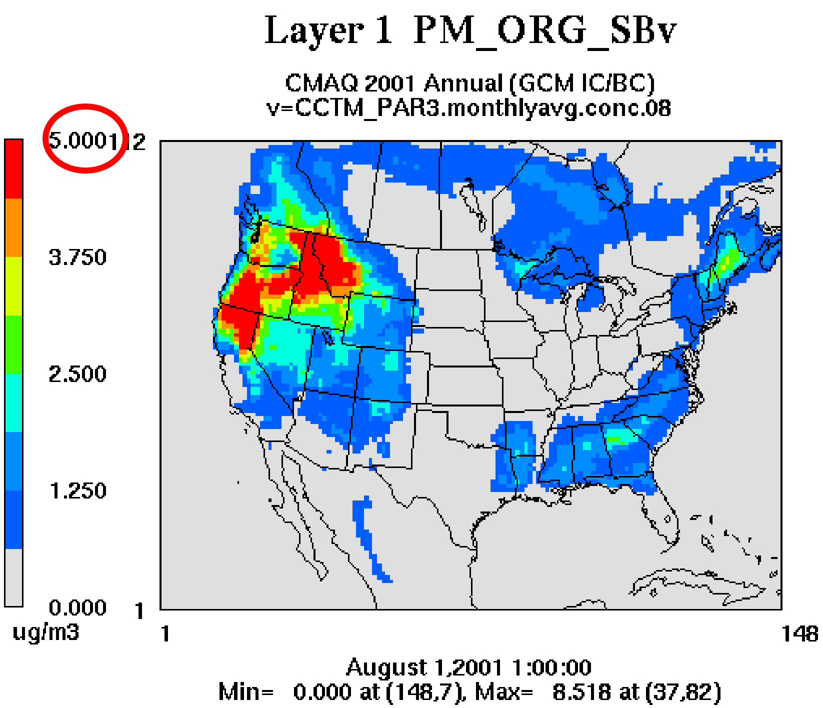
Comparison of BEIS3.09 v BEIS3.12 for 2001 Domain total emissions (10^3 metric tons)

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

The latest modeling "crisis" – high biogenic organic aerosol concentrations in the northwestern U.S. …

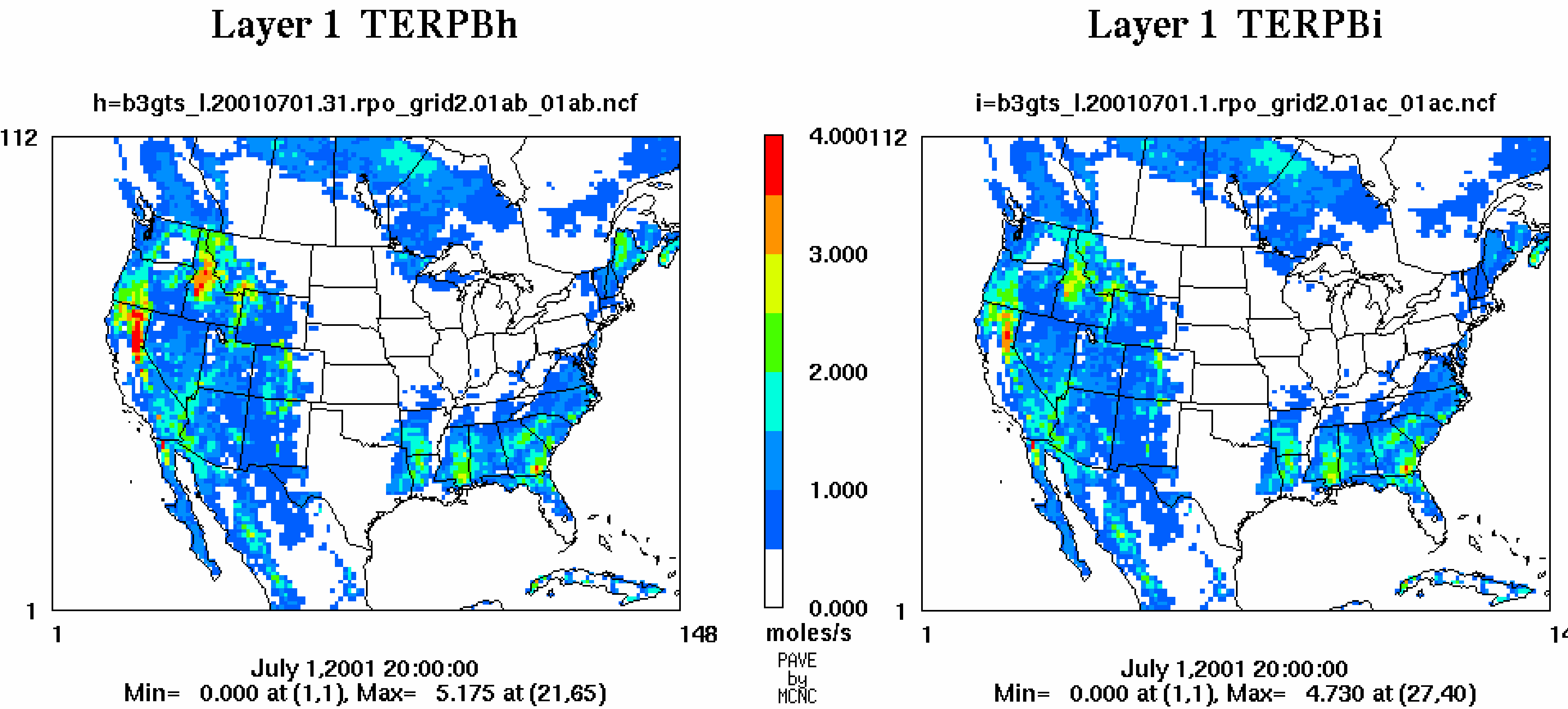
Are the monoterpene emission factors too high?





Preliminary CMAQ modeling plots

BEIS3.12 -- Change in the monoterpene emission factor for spruce and fir from 2.6 ug/g-hr to 1.5 ug/g-hr



Example for Lassen County, California – Effect of changing the monoterpene emission factor for spruce and fir from 2.6 ug/g-hr to 1.5 ug/g-hr

Tree type	Fraction	B3.12 efac (ug/m2-hr)	B3.13 efac (ug/m2-hr)
Jeffrey pine	0.29	1820	1820
Ponderosa pine	0.28	1820	1820
White fir	0.22	3900	2250
Lodgepole pine	0.05	1820	1820
Incense cedar	0.04	132	132
Calif. red fir	0.04	3900	2250
Calif. blk oak	0.01	86	86
Juniper	0.01	371	371
Oreg. wht oak	0.01	86	86
Douglas fir	0.01	3900	2250
Total/Wtd avg	0.97	**2265**	**1800**

=> Changing efac for spruce & fir lowered monoterpene emissions by ~20%

Much ado about biogenic emissions …

- Proposed future priorities:
  - Examine climatic adjustments of monoterpene emissions and evaluate flux estimates w/ field data
  - Incorporate isoprene seasonality
  - Combine the BEIS3 and the WRF-Chem/MEGAN platforms

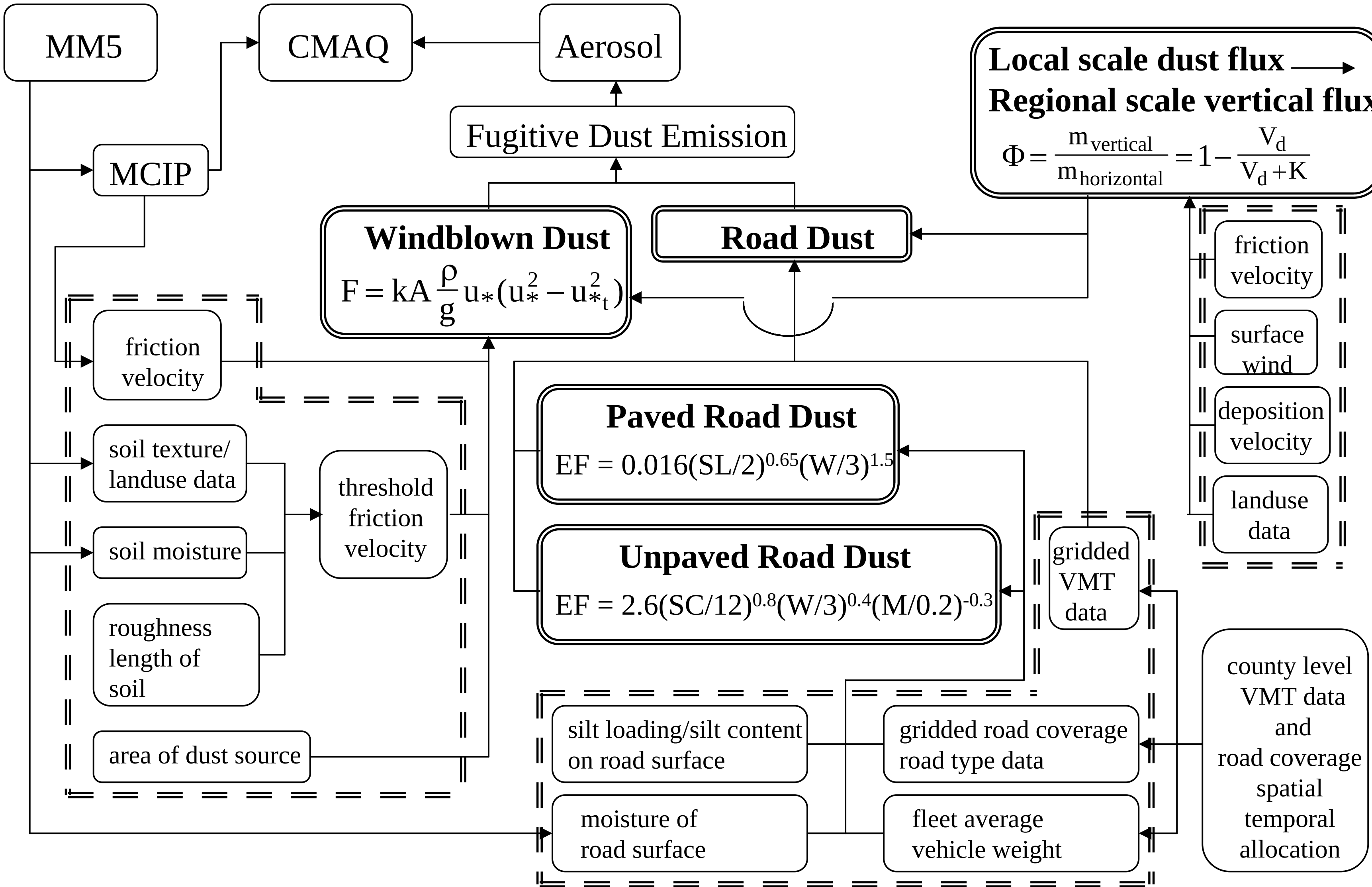
Much ado about fugitive dust emissions…

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

- Dr. Shan He has developed an wind blown dust algorithm for CMAQ based on the work of Gillette. The algorithm uses threshold friction velocity parameterizations and incorporates gridded databases of soil type, surface soil moisture content, meteorology, and vegetation. It also estimates the interception of dust particles by vegetation. Unfortunately w/ Shan's departure, this effort is "collecting dust".

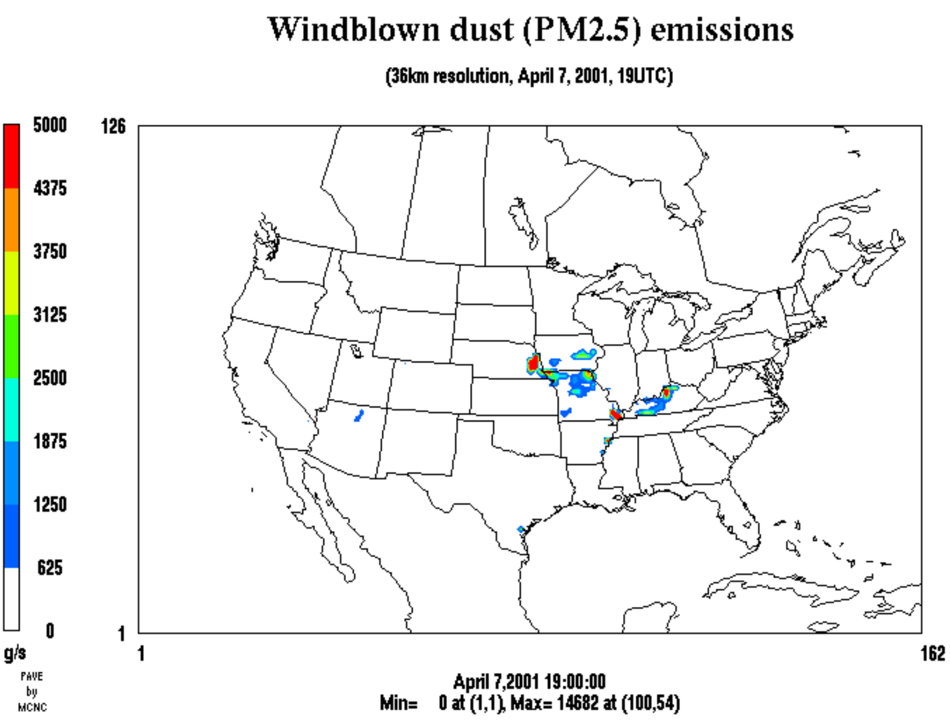
- G. Pouliot has been working on an improved algorithm for other fugitive dust sources.

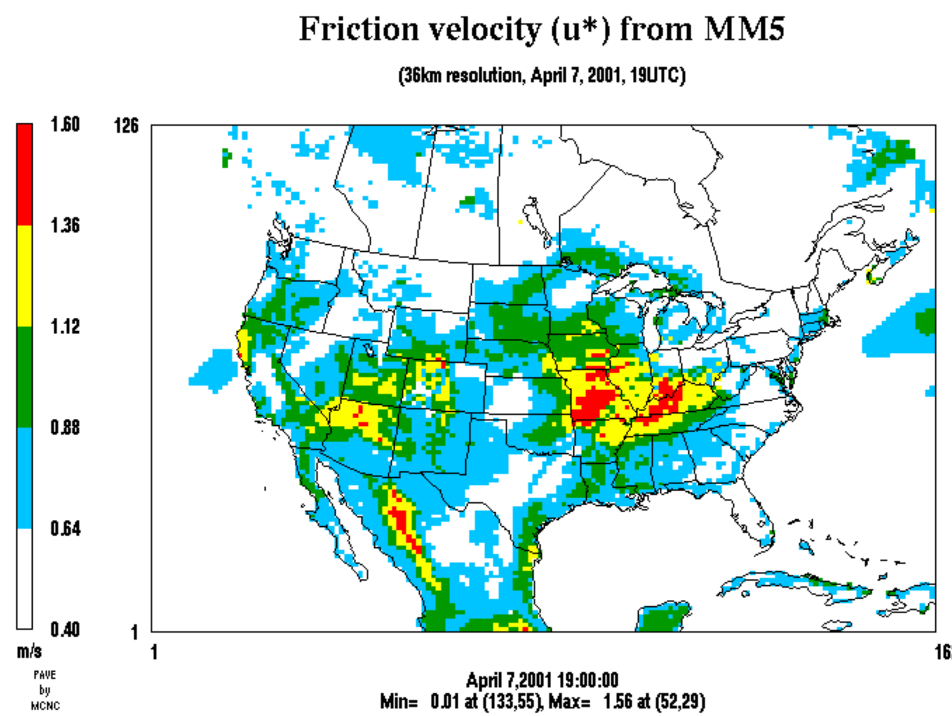
Proposed Fugitive Dust Emission Model



Courtesy of Dr. Shan He

Windblown Fugitive Dust Emissions Estimated with the "He" Algorithm





Fugitive Dust Emissions from Unpaved Roads

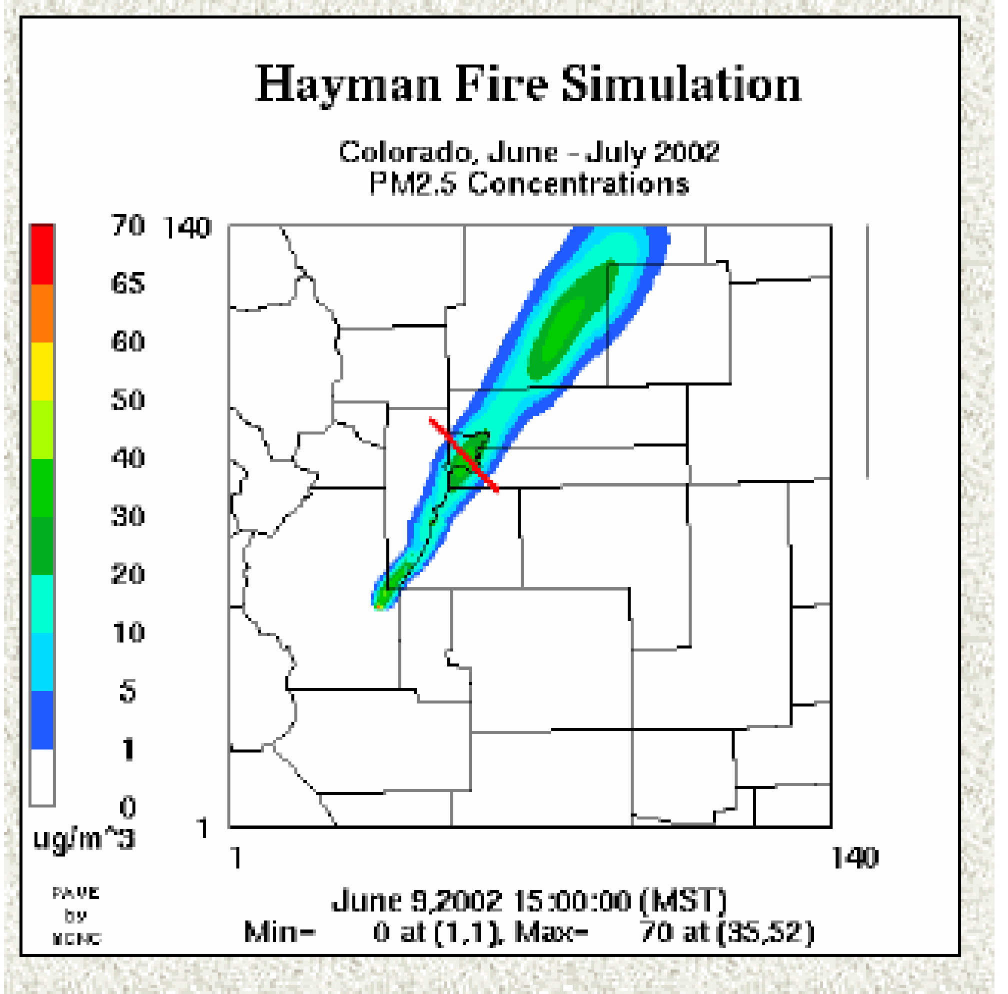
Current method	Proposed method
Does not account for removal by vegetation	Incorporate transport fraction developed by Dr. Shan He
FHWA road mileage	TIGER data to grid unpaved roads from county data
Uses monthly rainfall from a single station in a state	Simulate the moisture content of the road surface 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 later in 2004.

Much ado about wildland fire emissions …

- Current 2001 inventory includes monthly estimates by state
- For 2002, the RPOs are producing an event-based, location-specific inventory
- With support from OAQPS and EIIP, an IAG is being established w/ USFS to integrate BlueSky into SMOKE:
    - ➢ will provide framework for producing model-ready emissions from wildfires
    - ➢ will include updated fuel characteristics
    - ➢ will need support for plume rise and vertical allocation

BlueSky is a working system developed by the USFS for forecasting smoke from prescribed burns and wildfires. It has many of the components needed for an emissions module to CMAQ/SMOKE. (www.blueskyrains.org)

Actual simulation from the BlueSky system



Much ado about wildland fire emissions …

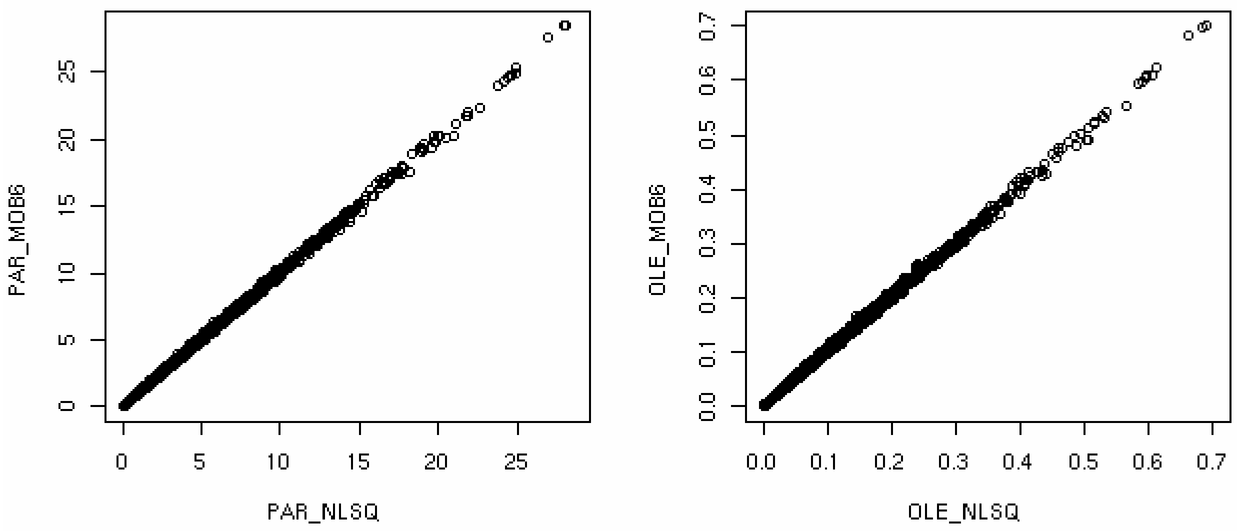
- Proposed future priorities:
  - ➢ Include RPO inventory as soon as practical for 2002 CMAQ simulations
  - ➢ Integrate BlueSky into SMOKE and evaluate CMAQ model performance

Much ado about AQ forecast emissions …

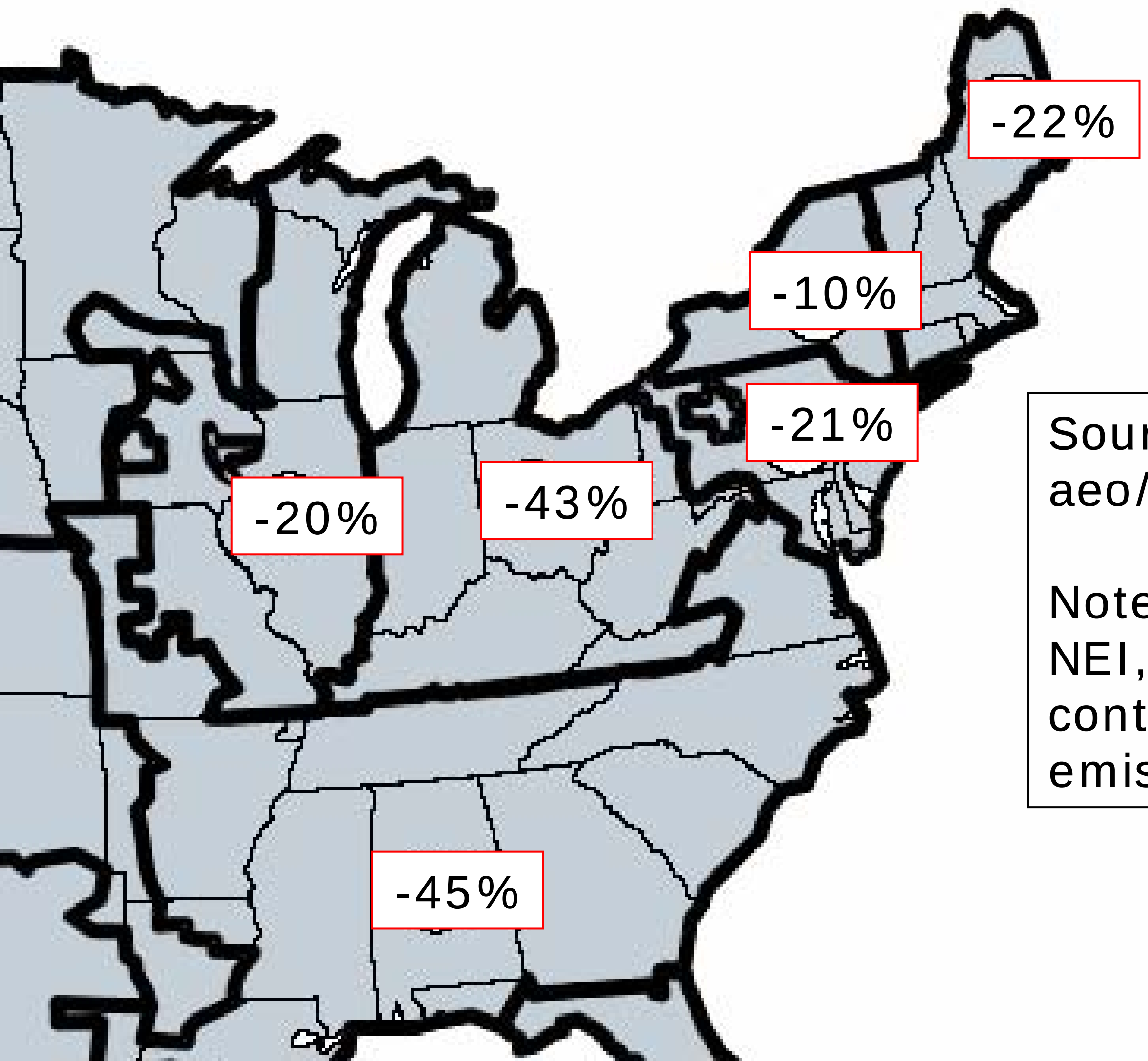
- Work performed by G. Pouliot
- Priorities for 2004:
  - ➢ Incorporate and streamline Mobile6 calculations
  - ➢ Account for significant reductions in electrical generating unit (EGU) NOx emissions

Emissions for air quality forecasting – using simple regression to account for hourly temperature effects in Mobile6

Comparison of VOC emissions from Mobile6 vs. NLSQ regression across the NE AQ forecast domain for August 4, 2003



Emissions for air quality forecasting – change in NOx EGU emissions from 2001 to 2004



Source:www.eia.doe.gov/oiaf/aeo/supplement/

Note: according to the 1998 NEI, electric utilities contributed ~25% of NOx emissions

Much ado about AQ forecast emissions …

- Proposed future priorities:
  - ➢ Adjust EGU emissions as a function of predicted temperature (based on analysis of existing CEM data)
  - ➢ Incorporate satellite-derived wildfire emissions
  - ➢ Perform sensitivity analysis of the effect of emission changes resulting from voluntary control measures

Much ado about emission modeling…

Then sigh not so, but let them [emissions] go,
And be you blithe and bonny,
Converting all your sounds of woe
*Into hey nonny, nonny.**

**w/ apologies once again to Wm. Shakespeare,*
from Much Ado About Nothing.