

Applications of Source Contribution and Emissions Sensitivity Modeling to Assess Transport and Background Ozone Attribution

April 2014

Kirk Baker, Norm Possiel,
Brian Timin, Pat Dolwick

Source Sensitivity & Contribution Modeling Approaches

How will the modeled concentrations change based on changes to emissions?

Source sensitivity approaches

- Brute force zero out
- Decoupled Direct Method (DDM)

What are the various contributors to modeled concentrations?

Source contribution approaches

- Ozone and PM source apportionment (OSAT, APCA, PSAT)
- Adding additional inert PM_{2.5} tracers (carbon tracking)

**All techniques have strengths and limitations*

Brute Force Zero Out

Advantages

- Simple to execute and simple to interpret
- Efficient when examining the impact from a few sources or source groups

Disadvantages

- For larger problems, the approach becomes expensive due to iterative model runs
- When evaluating the impacts from many large emissions source groups, the impacts do not sum up to the original modeled concentrations due to nonlinearities in the system

Decoupled Direct Method (DDM)

Advantages

- Efficient when looking at a larger group of emissions sources or when a range of model response is desired
- Essentially provides a model response surface which can act as a stand alone reduced form model for future purposes

Disadvantages

- Most problems require additional pre-processing of emissions and staff expertise to interpret the results
- Technique most applicable to emissions perturbations <50%, less agreement with brute force for emissions changes >50%
- Summing sensitivities will not be equivalent to the original modeled concentration

Source Apportionment

Advantages

- Efficient when looking at a larger group of emissions sources
- Provides an estimate of the “resultant” air quality (does not perturb important atmospheric chemical processes)

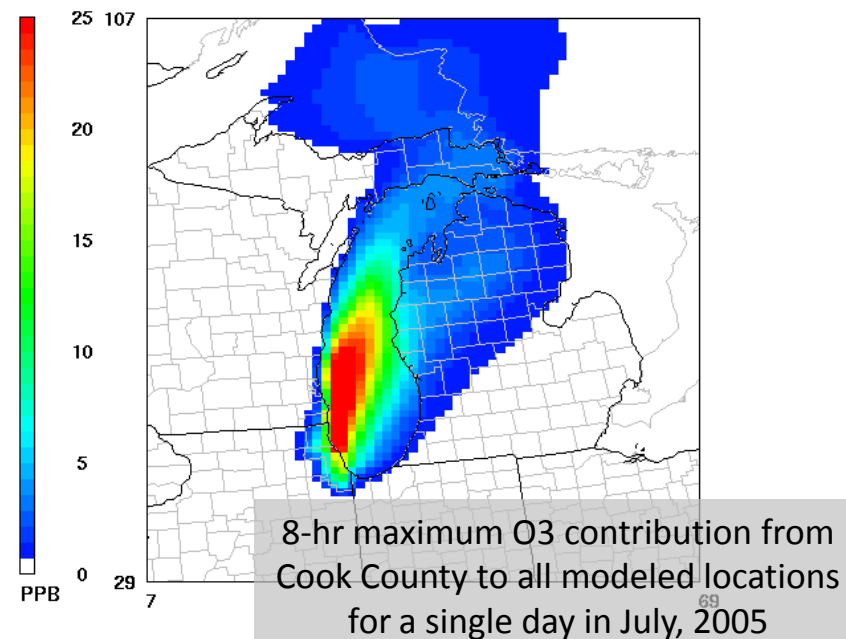
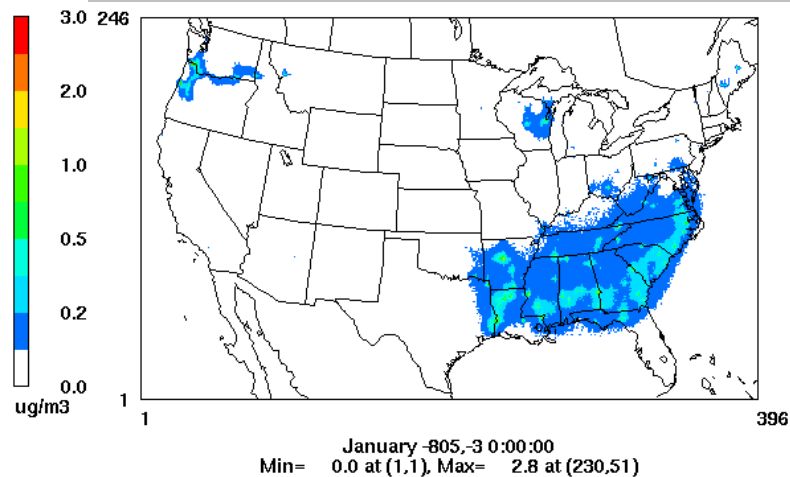
Disadvantages

- Most problems require additional pre-processing of emissions and staff expertise to interpret the results
- Technique does not provide information about how the model will respond to emissions changes

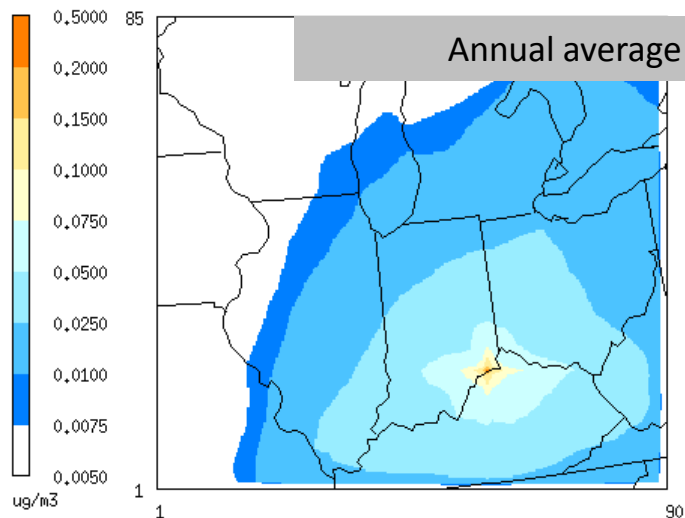
Source Sensitivity & Contribution

- Photochemical model source sensitivity approach (DDM) estimates sensitivity coefficients that relate emissions changes from specific emissions sources to model outcomes at each hour and grid cell
- Photochemical model source apportionment tracks the formation and transport of ozone and PM_{2.5} from specific emissions sources and calculates contribution at each hour and grid cell
- Source groups may be single sources, groups of sources (sector, fires, biogenics, etc), entire States, or entire Counties
 - Must identify before model simulations
- Receptors are each individual grid cell--which may be matched to any monitor located in the model domain
 - Do not need to identify receptors before model simulations

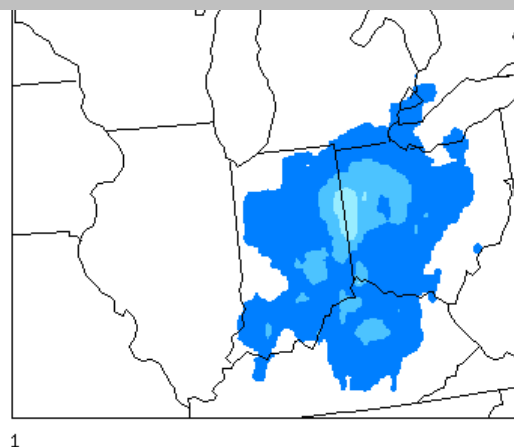
Annual average PM2.5 contribution from Pulp & Paper sector



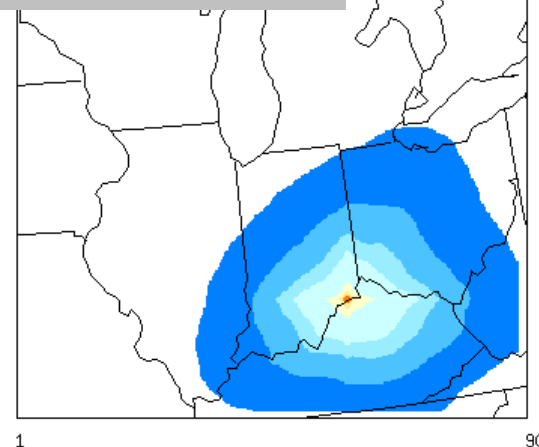
Annual Avg PM2.5 Sulfate



Annual Avg PM2.5 Nitrate



Annual Avg Primary PM2.5



Modeling to Assess Transport

Motivation for State-level Air Quality Attribution

- Section 110(a)(2)(D)(i)(I) (the “good neighbor” provision) of the Clean Air Act requires every state’s SIP to:
 - “...contain adequate provisions ... prohibiting, consistent with the provisions of this subchapter, any source or other type of emissions activity within the State from emitting any air pollutant in amounts which will ... contribute significantly to nonattainment in, or interfere with maintenance by, any other State with respect to any [NAAQS]”
- “Good neighbor” SIPs are required for each pollutant covered by a NAAQS (including each revision) and must also address identified precursors to those pollutants
- The “good neighbor” provision applies to all states regardless of whether they contain nonattainment areas
- Each state has an obligation to prohibit emissions that “significantly contribute to nonattainment” or “interfere with maintenance” of the NAAQS in another state

Regulatory History of Transport Rules

- NOx SIP call (1998) covered 1-hr ozone NAAQS
- CAIR (2005) covered the 1997 8-hr ozone and annual PM_{2.5} NAAQS
- CAIR court decision - 7/2008
- CAIR remand - 12/2008
- Transport Rule (proposal) - 7/6/2010
- Transport Rule/CSAPR (final) - 7/6/2011
- U.S. Court of Appeals D.C. Circuit issues stay 12/30/2011
- CSAPR vacated - 8/21/2012

Major Elements of Previous Interstate Transport Rules

- Identify air quality “need” – areas in the Eastern US projected to have nonattainment/maintenance problems in the future
- **Quantify State-specific contributions to model estimated future air quality**
- Use air quality thresholds to identify States to be covered by the rule
- **Define/quantify the amount of significant contribution (emissions) to be eliminated** (i.e. specify state emissions budgets)
- Structure of remedy & quantify the expected benefits of the rule

Approach Used in CSAPR to Identify Future Nonattainment/Maintenance Receptors

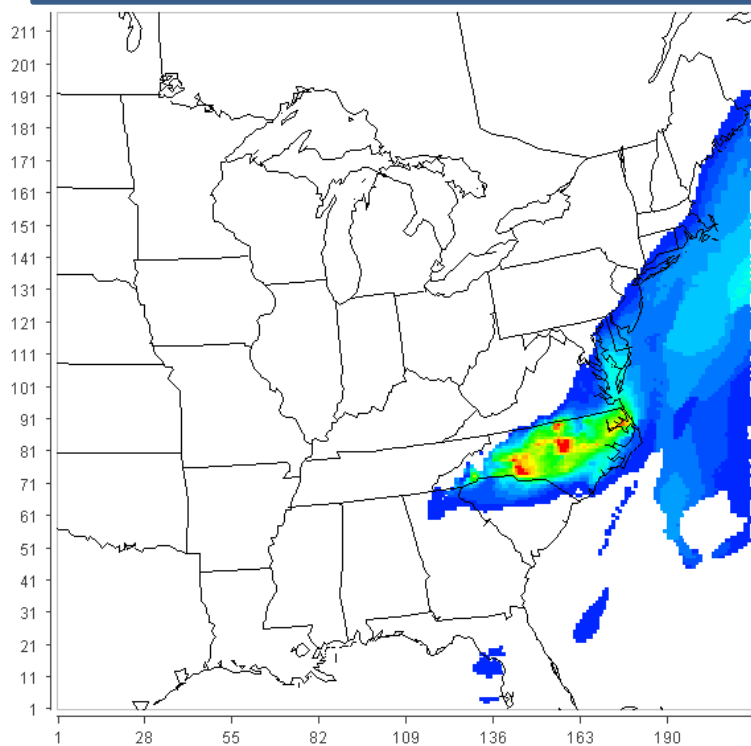
- Base year design values were projected to 2012 and 2014
 - Followed Modeled Attainment Demonstration guidance methodology
 - Modeling used to calculate % change in ozone between 2005 and 2012 or 2014 (relative response factor or RRF)
 - % change in ozone multiplied by base year ambient data
- Base year ambient design values taken from the period 2003-2007
 - Base model year is 2005; projected design value periods span 2005 (2003-2005, 2004-2006, 2005-2007)
 - Projected each of these periods and the 5-year weighted average
- Definition of Nonattainment and Maintenance (*could change in future Rules)
 - Future year projection of **average** design values used to determine nonattainment receptors
 - Future year projection of **maximum** design values used to determine maintenance receptors (maintenance considers variability due to meteorology and emissions)

Approach Used in CSAPR for Quantifying Contributions

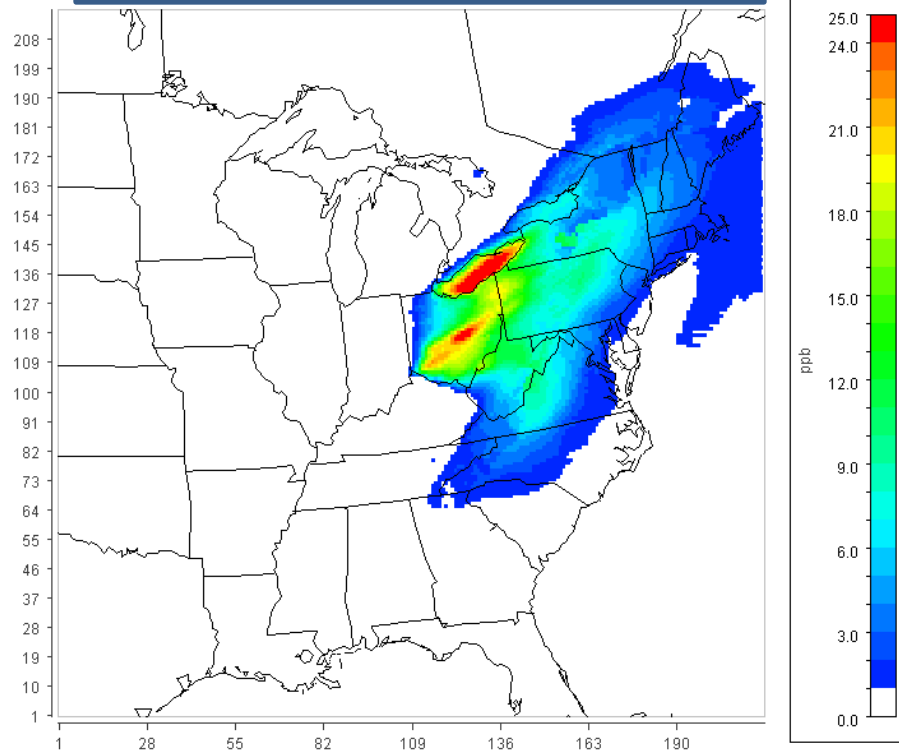
- Source apportionment: CAMx model; APCA method for ozone
 - Where ozone formation is VOC limited and source combination is biogenic VOC + anthropogenic NOX, the contribution is given to the anthropogenic NOX source
- Interstate contributions based on State total anthropogenic emissions: NOx emissions -> ozone
- The SMOKE emissions model enhanced to track emissions to specific States
- CAMx source apportionment outputs applied in a “relative sense” to calculate contributions to future year design values
 - Contributions *from* each state *to* each receptor site
 - Receptor sites are nonattainment and maintenance monitors

Single-Day Contribution to 8-Hr Daily Max Ozone (July 21, 2011)

Contribution from North Carolina



Contribution from Ohio

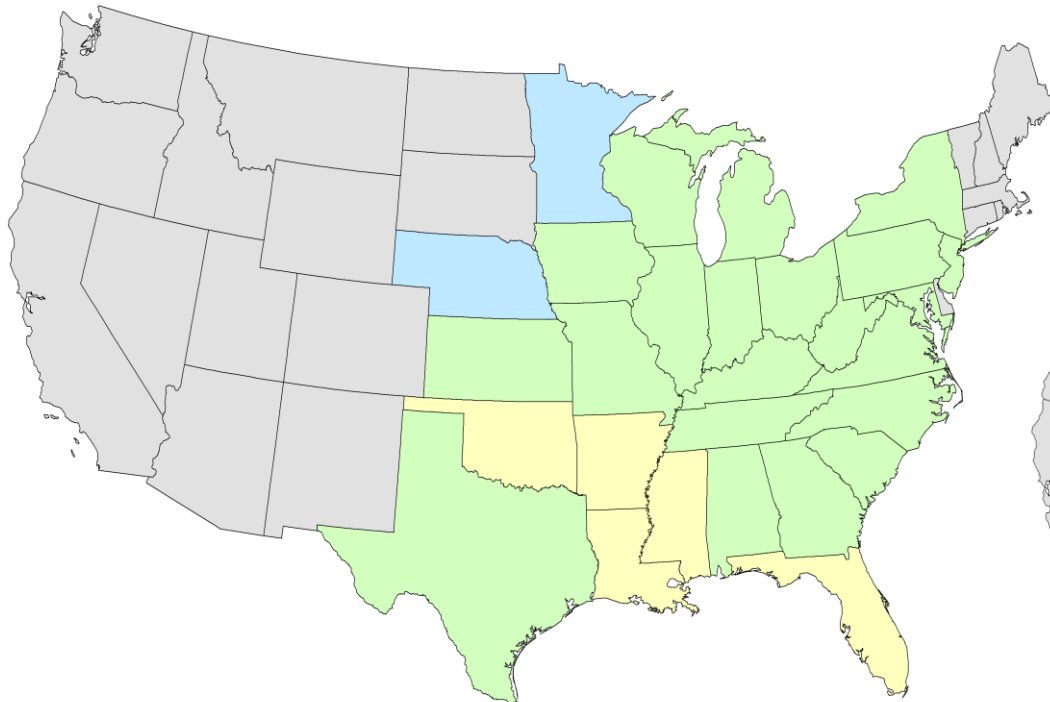


CSAPR Air Quality Contribution Thresholds

- In CSAPR, air quality contributions were evaluated against thresholds defined as 1 percent of the NAAQS
 - 8-hr Ozone (0.8 ppm 1997 NAAQS)
 - 0.08 ppm
 - Annual avg PM_{2.5} (15.0 µg/m³ 1997 NAAQS)
 - 0.15 µg/m³
 - Daily average PM_{2.5} (35 µg/m³ 2006 NAAQS)
 - 0.35 µg/m³
- States which contributed ozone at or above the thresholds to future year nonattainment of maintenance sites in other (i.e., downwind) states were included in the rule

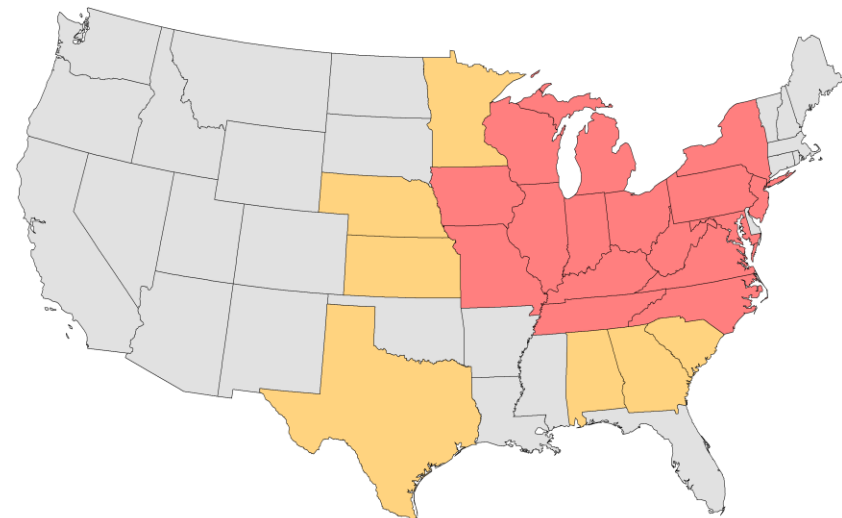
States Included in CSAPR

Total Program Coverage



- States controlled for both fine particles (annual SO₂ and NO_x) and ozone (ozone season NO_x) (21 States)
- States controlled for fine particles only (annual SO₂ and NO_x) (2 States)
- States controlled for ozone only (ozone season NO_x) (5 States)
- States not covered by the Transport Rule

Group 1 versus Group 2 SO₂ States



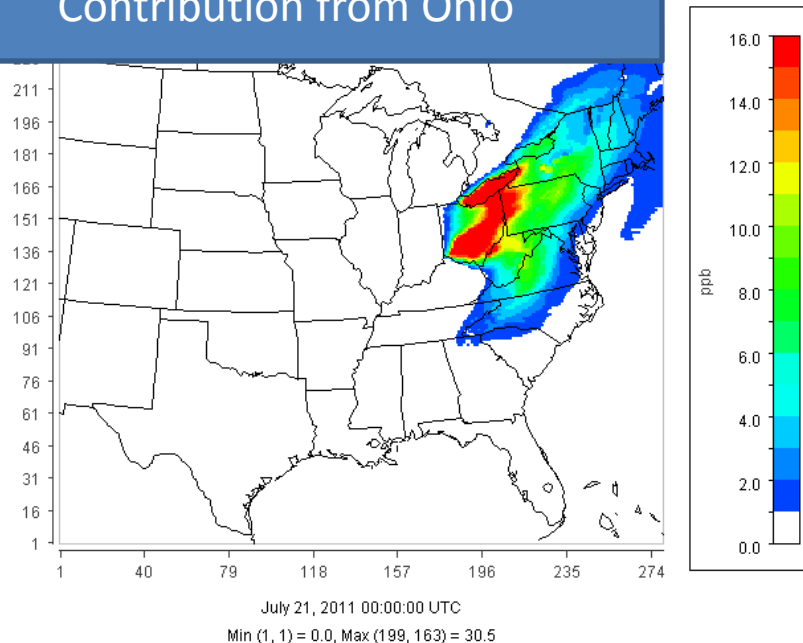
- Group 1 States (16 States)
- Group 2 States (7 States)
- States not covered by the annual Transport Rule

- 23 states are required to reduce both annual SO₂ and NO_x emissions
- 26 states are required to reduce NO_x emissions during the ozone season (May-Sept.)

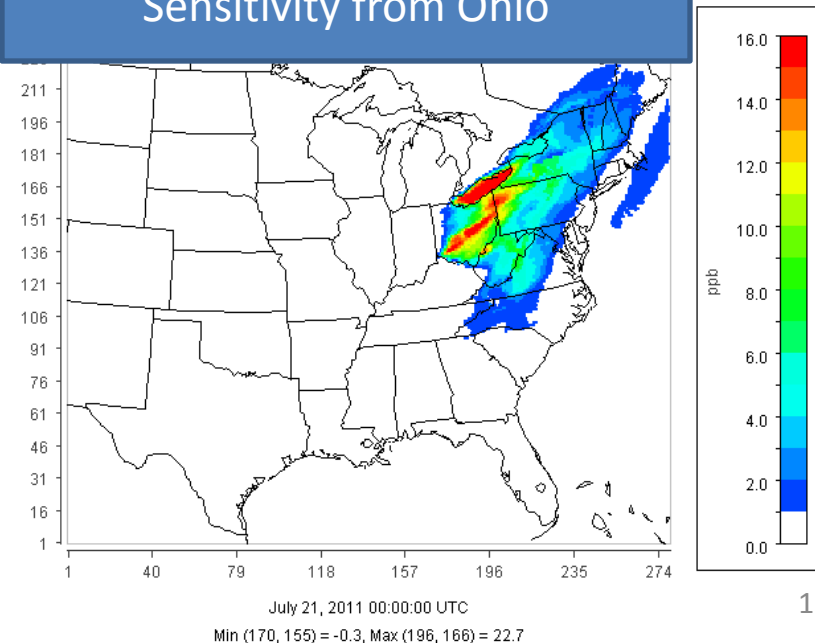
Source Sensitivity Modeling (HDDM)

- In addition to knowing a State's contribution, we may need an estimate of how ozone will change at a specific receptor when the State's emissions change (estimate of response)
- One option is the Higher Order Decoupled Direct Method (HDDM); provides an estimate of how ozone will change based on changes in "tagged" States
- The HDDM approach was used to support the Ozone NAAQS REA

Contribution from Ohio



Sensitivity from Ohio



AQ Modeling Platform for New Transport Rule

- Base year for meteorology: annual 12 km simulation of 2011
- Current year emissions based on 2011 NEI; projected to 2018
 - EPA made the 2011 and 2018 inventories available for comment prior to proposal; “comment period” over but we are still open to suggestions
- Updated emissions modeling & processing for source apportionment
- Updated photochemical model (CAMxv6.1) & gas phase chemistry (CB6r2)
 - Includes more explicit treatment of organic nitrate NO_x recycling
- Source apportionment for 2018
 - Contributions tracked anthropogenic emissions from 48 States individually, all Tribal lands in aggregate, biogenic emissions, and “everything else” which includes fires, offshore emissions, other countries, etc.
- Review/update for each post processing step
 - Programs were simplified and steps were consolidated where possible
 - The process for estimating contributions no longer requires the use of the MATS attainment test software or the SAS statistical software package

Updated Emissions Modeling and Post-Processing Source Apportionment Outputs

- SMOKE tracks State FIPS codes throughout emissions modeling process to maintain each source's State identity
 - This is fairly simple for point sources
 - Previously SMOKE generated separate emissions for each State (i.e. 25 different NO species for 25 different States)
 - Now SMOKE optionally processes and outputs gridded 2D emissions as point source format files to minimize excessively large emissions files
- The WRF2CAMX processor was modified to generate sub-grid scale non-precipitating clouds based on vertical RH profile
- Post-processing streamlined into fewer programs/scripts
 - Convert regular model and source apportionment ozone to local time 8-hr daily maximums (source contribution 8-hr max paired with regular model output in time and space)
 - Percent contribution estimated for each State
 - Percent contribution multiplied by future year design value to estimate a contribution in ppb

“Background Ozone”

OTHER USES FOR SOURCE ATTRIBUTION TOOLS

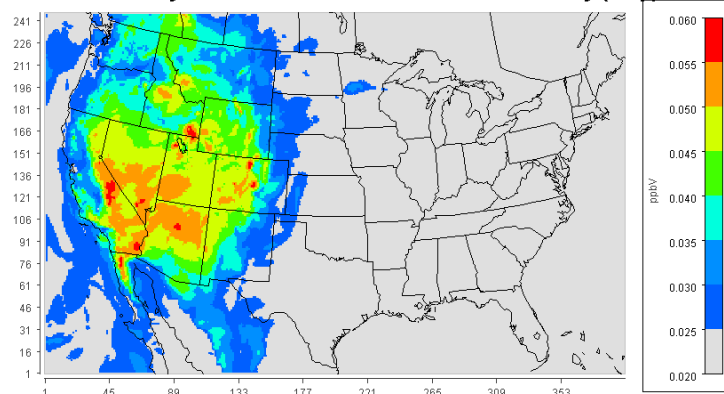
Methods for Estimating “Background” Ozone

- As noted in the recent ozone ISA, there are limitations associated with the existing definitions of USB, NAB, and NB:
 - Unrealizable, hypothetical, counterfactual scenarios have limited application in an implementation context.
 - Non-linearities in ozone chemistry, especially in urban areas, can hinder interpretation of space/time-specific background contributions.
 - Individual impacts may not sum up to aggregate impacts in brute force modeling (due to non-linearities) making it harder to parse out the proportions of various background sources.
- EPA is investigating several potential companion assessments of boundary contributions to compliment the zero-out analyses.
 - OSAT source apportionment
 - Reactive tracer probing tools
 - Higher-order direct decoupled method (HDDM)
- It is expected that the output from each of these methodologies could potentially be combined to build a more complete characterization of background ozone.

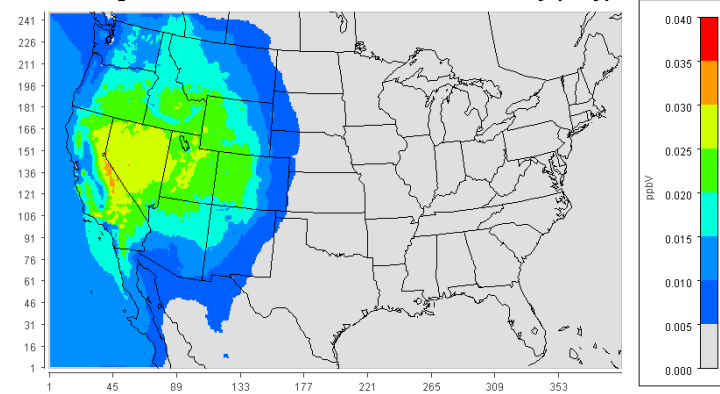
Source Apportionment Approach

- Source apportionment modeling is especially useful when boundary contributions are desired without perturbing chemistry.
- Five individual boundary contributions can be tracked separately or aggregate together.
- EPA is doing CAMx (APCA) source apportionment modeling for a 2007 base.
- Boundary condition files from GEOS-Chem

Maximum hourly ozone contribution from West boundary (July)



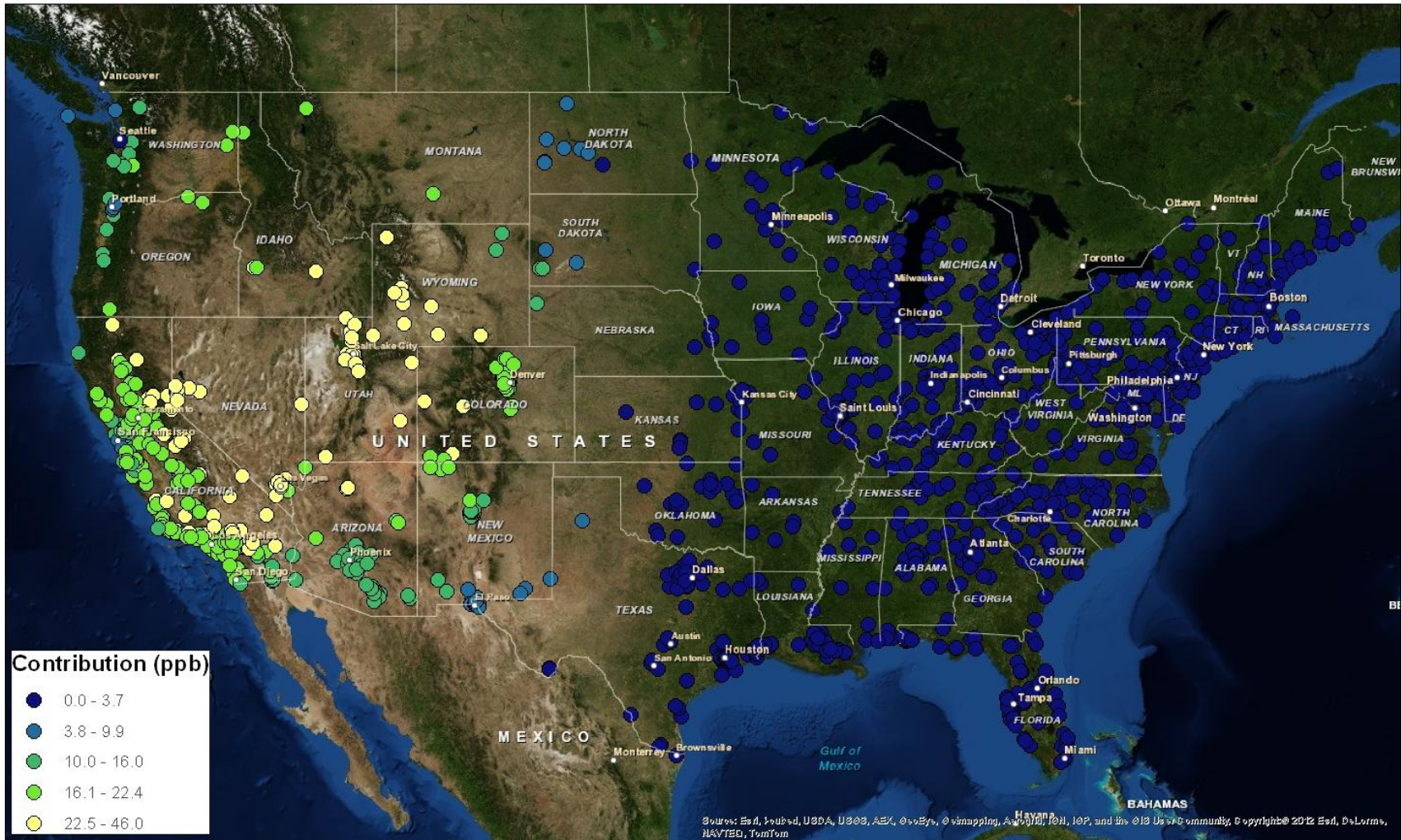
Average ozone contribution from West boundary (July)



Results are preliminary and subject to change

Source apportionment ozone impacts: Western boundary

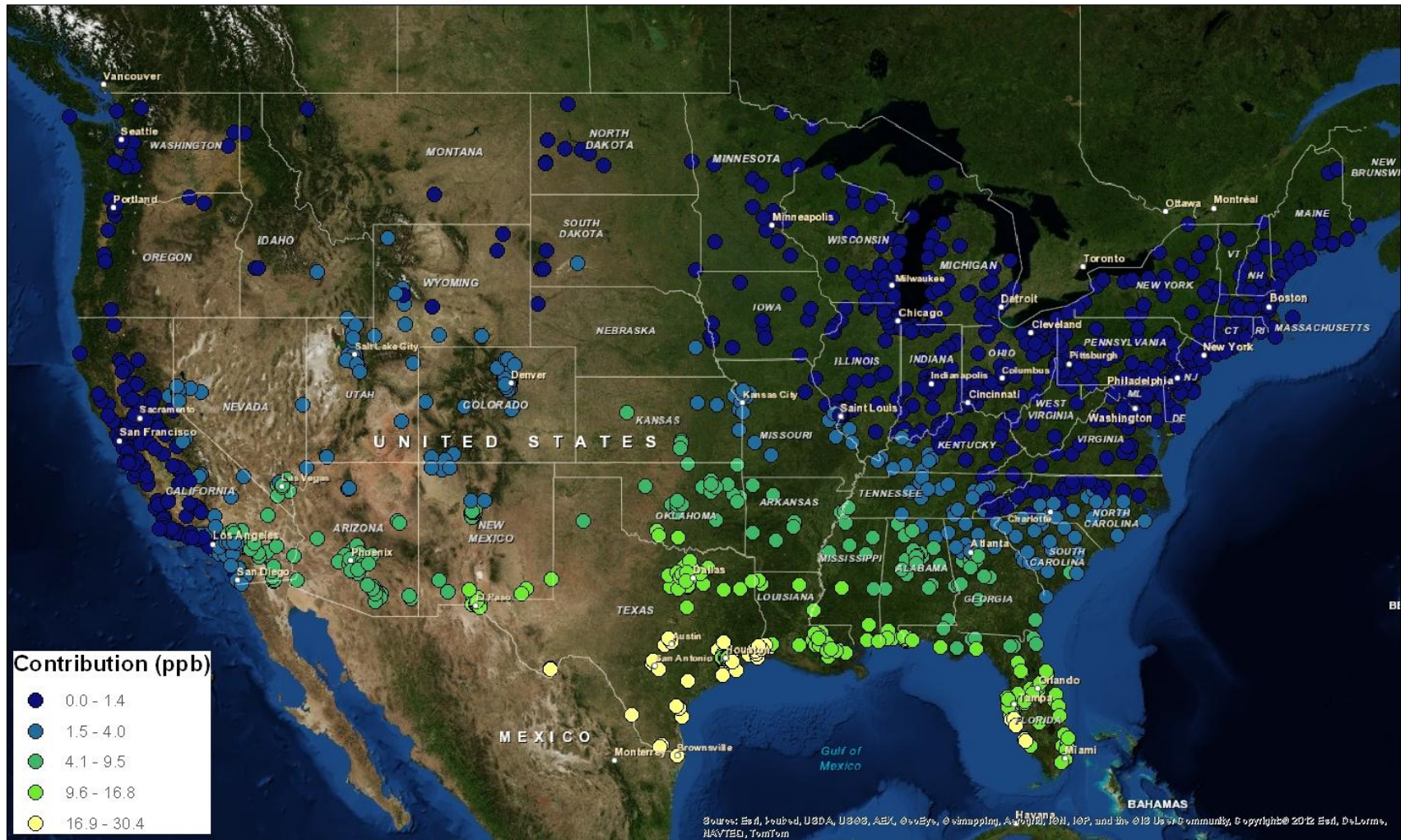
July average contribution to MDA8 from Western boundary



**note difference scales on each plot*

Source apportionment ozone impacts: Southern boundary

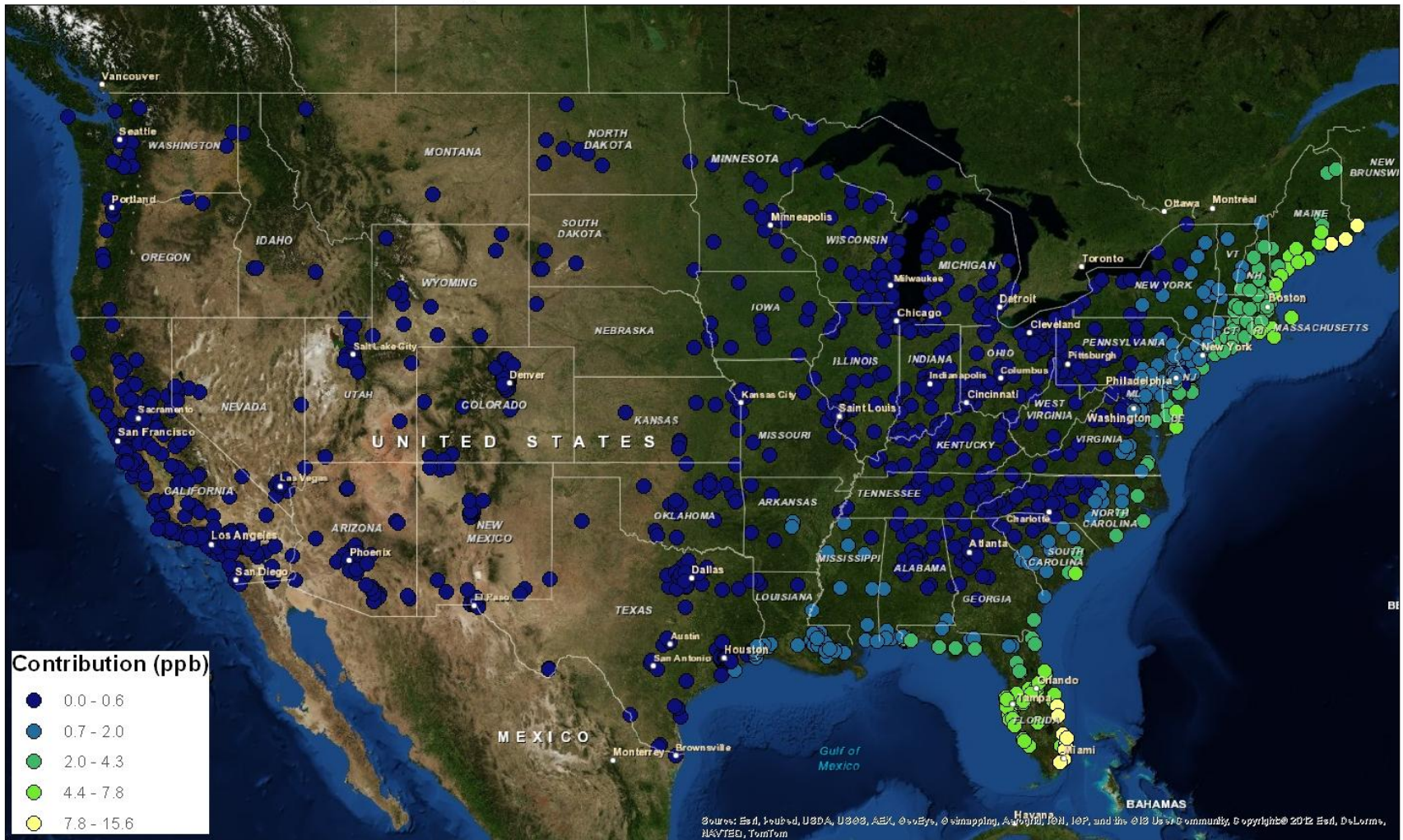
July average contribution to MDA8 from Southern boundary



**note difference scales on each plot*

Source apportionment ozone impacts: Eastern boundary

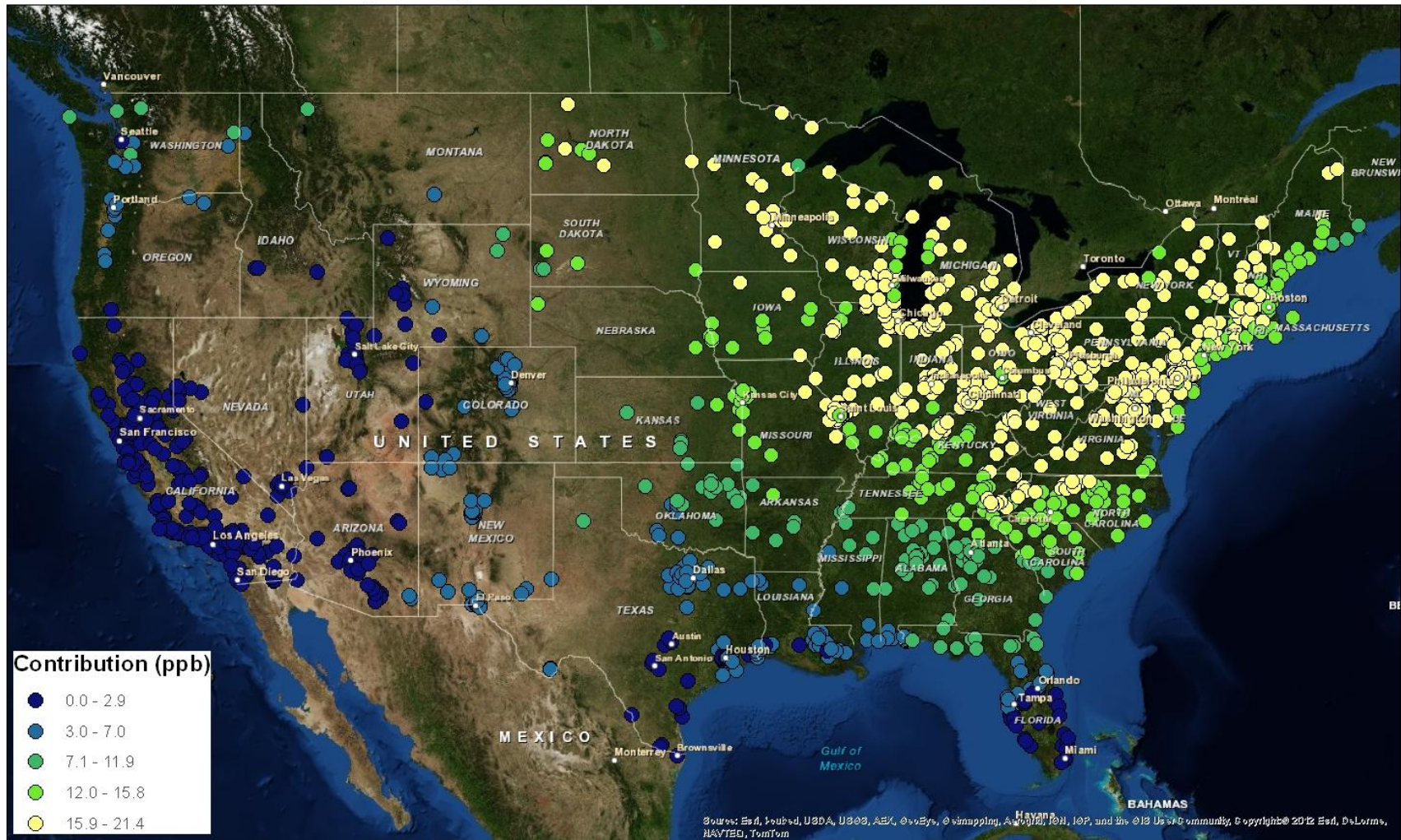
July average contribution to MDA8 from Eastern boundary



**note difference scales on each plot*

Source apportionment ozone impacts: Northern boundary

July average contribution to MDA8 from Northern boundary



**note difference scales on each plot*

More Information

CSAPR Web Site

- www.epa.gov/crossstaterule/
 - Regulatory Actions
 - Link to the TR/CSAPR docket
 - Air Quality Modeling TSD
 - Emissions Inventory TSD
 - Significant Contribution TSD
 - IPM-predicted EGU emissions
 - Ozone and annual and daily PM2.5 contributions from each state to each receptor site
 - Costs and Benefits of the rule

Ozone NAAQS Policy Assessment document (Feb 2014)

- http://www.epa.gov/ttn/naaqs/standards/ozone/s_o3_2008_pa.html