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EQUATES

EPA's Air QUAlity TimE Series Project

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**Retired*

19th Annual CMAS Conference
October 28, 2020

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Background

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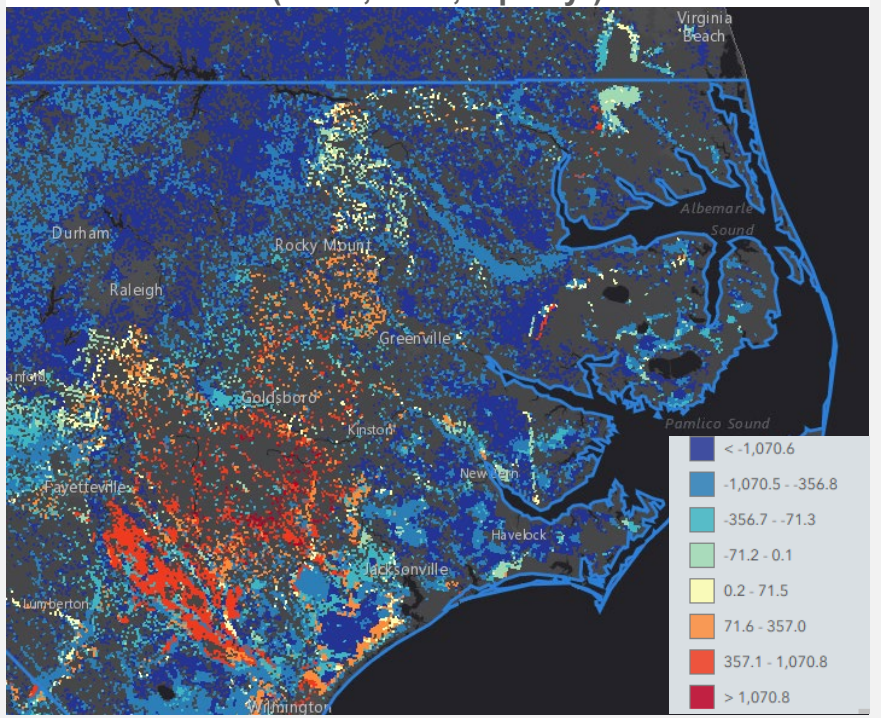
Applications of Multiyear CMAQ Simulations

- Decadal and multidecadal CMAQ simulations have been used for a wide variety of applications
- CMAQv5.0.2 annual deposition estimates for 2002-2012 are currently being used by **TDEP, CASTNET, EnviroAtlas, Critical Loads Mapper,** and to support **nutrient assessments**
  - These EPA tools and data products are missing deposition trends in more recent years
- 2002 - 2017 **model/observation "fused" ozone and $PM_{2.5}$ surfaces** have been used for numerous epidemiological studies
  - Different years use different CMAQ versions (v4.6-v5.3), leading to discontinuities in bias of fused surfaces

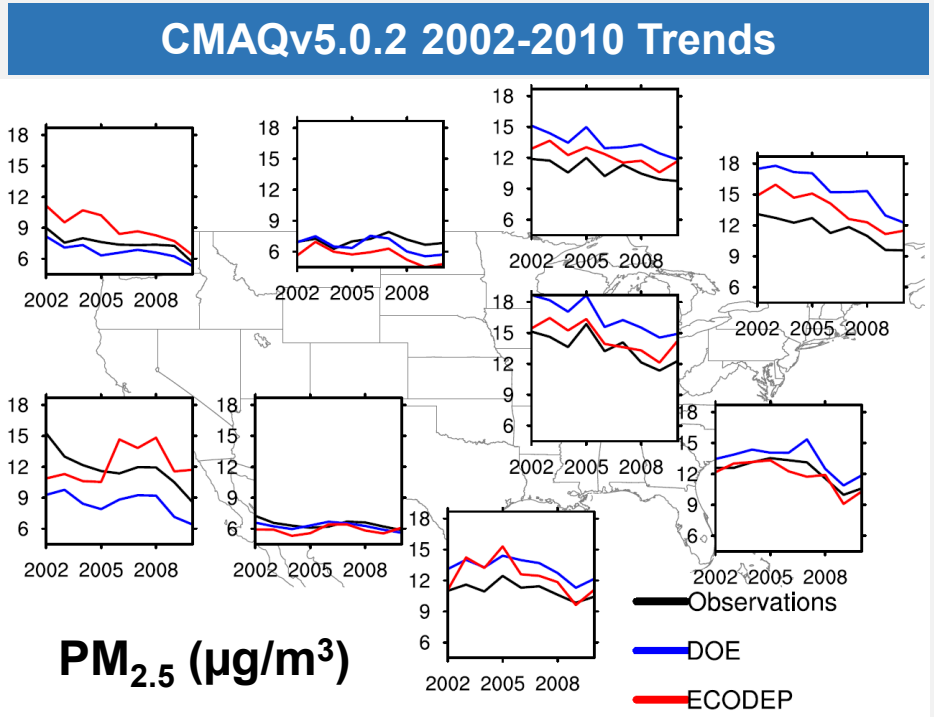
Screen shot from Critical Loads Mapper

Exceedance of Forest Acidification by Total N (TDEP, 2015, eq/ha-yr)



EQUATES: EPA's Air QUAlity TimE Series Project

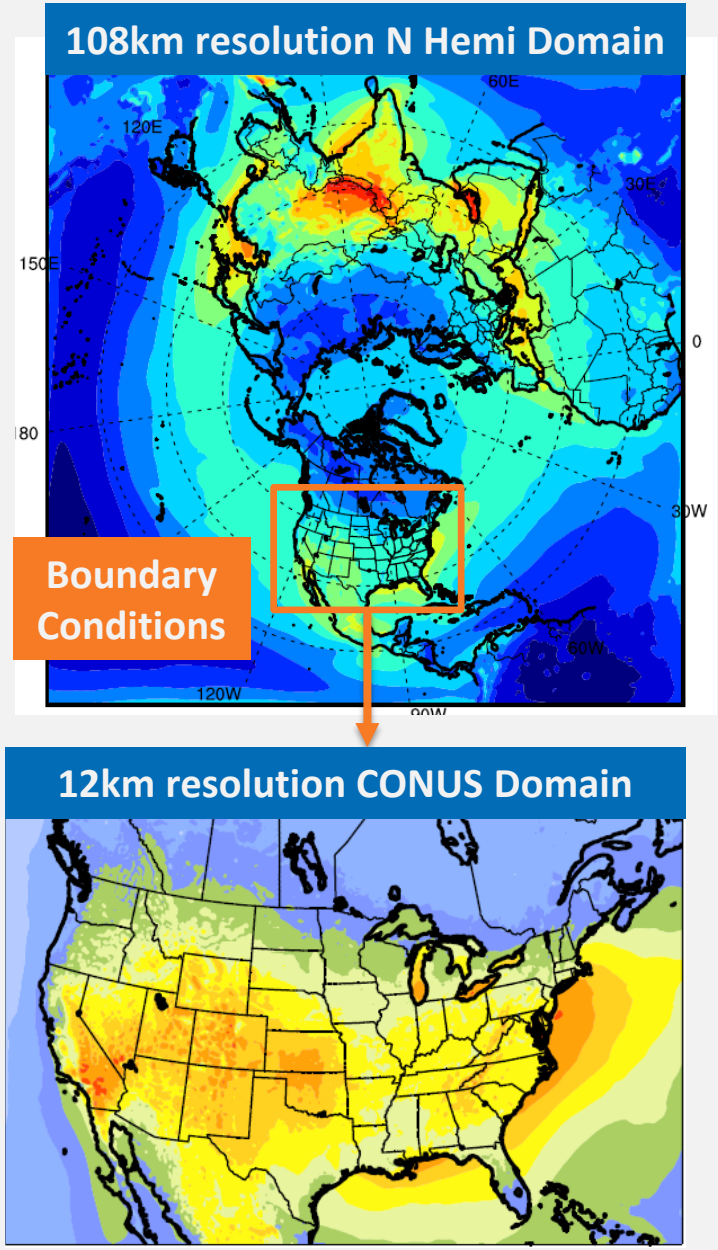
- New CMAQv5.3.2 time series will:
  - Include more recent years (2002-2017)
  - Address known biases in older versions of the air quality, meteorology, and emission models
  - Provide a consistent set of emissions, meteorology, and air quality estimates appropriate for a range of applications
- EQUATES will supersede previous CMAQ time series and provide a unified set of modeling data across applications



Hogrefe et al. 2018 CMAS presentation:
https://www.cmascenter.org/conference/2018/agenda.cfm

Overview of EQUATES Modeling Effort

- 2002-2017 CMAQv5.3.2 simulation over the Northern Hemisphere (**N Hemi**) and the contiguous US (**CONUS**)
- N Hemi simulation will provide the boundary conditions for the CONUS simulations
- New meteorological and emissions inputs are being developed for N Hemi and CONUS simulations



Improvements Over Existing CMAQ Simulations

	CMAQv5.0.2 "DOE" Xing et al. (2013)	CMAQv5.0.2 "ECODEP" Zhang et al. (2019)	CMAQv5.3.2
Model	CMAQv5.0.2 (CB05_AERO6; w/o bidirectional NH_3)	CMAQv5.0.2 (CB05TUCL-AERO6; w/ bidi NH_3)	**CMAQv5.3.2 (CB6R3-AERO7; w/bidi NH_3)**
Date range	1990 - 2010	2002 – 2012	**2002 – 2017**
Domain/ Resolution	108km N Hemi + 36km CONUS	12km CONUS	**108km N Hemi + 12km CONUS**
Meteorology	WRF3.4	WRF3.4	**WRFv4.1.1**
Emissions	NEI data (2002 or 2005 base year + scaling factors and emissions constraints; climatological fires, no CMV)	Various NEIs / Modeling Platforms	**2017 NEI as primary base year; consistent methods used for each sector (when feasible) to avoid artificial step changes**
Boundary Conditions	N Hemi CMAQv5.0.2	GEOS-Chem	**N Hemi CMAQv5.3.2**

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Meteorology

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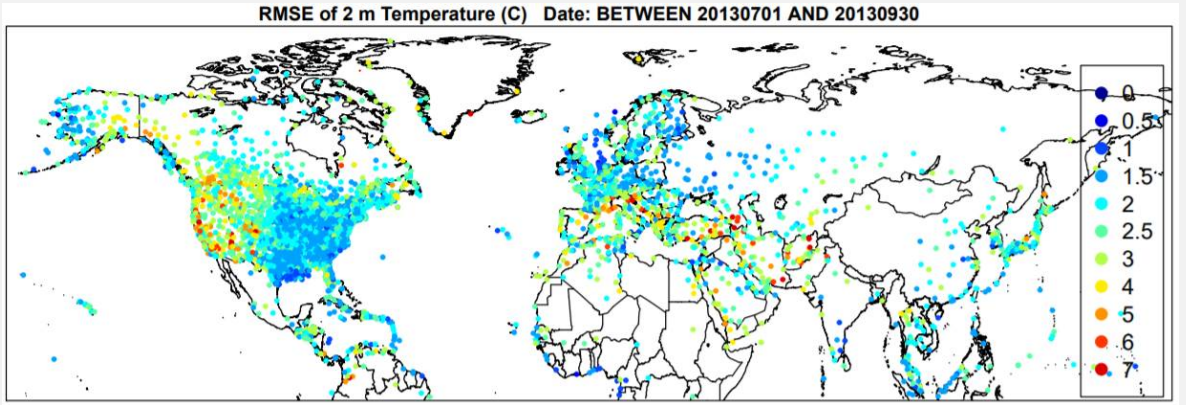
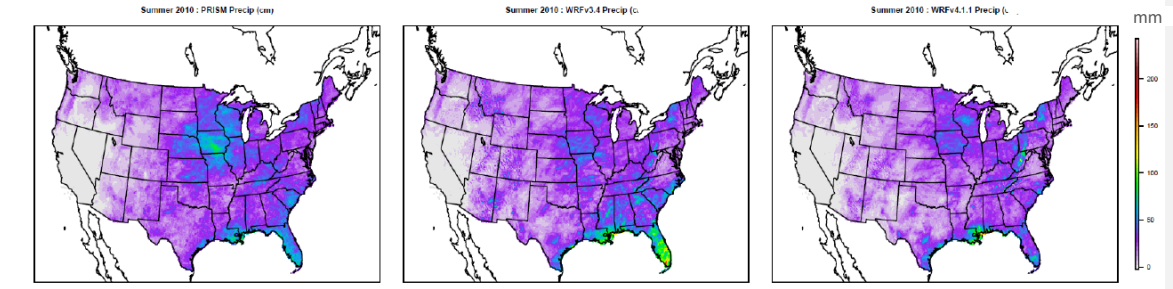
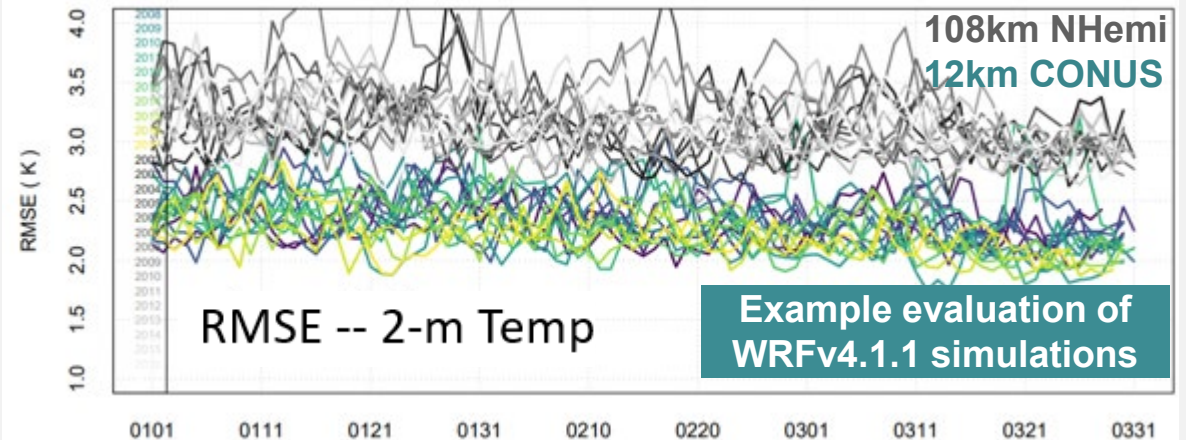
WRFv4.1.1 Meteorology

- 2002-2017 CONUS and N. Hemi WRFv4.1.1 estimates were evaluated against weather stations, radiosonde data, and PRISM precipitation fields.
- Bias and error in WRFv4.1.1 temperature, wind speed, and mixing ratio are comparable to WRFv3.4 and other more recent model versions.
- WRFv3.4 high bias in precipitation across multiple seasons/regions is reduced or eliminated in v4.1.1 simulations. WRFv4.1.1 simulations show a low precipitation bias in eastern US (next 2 slides).
- New hybrid vertical coordinate system in WRF (Beck et al. 2020) reduces high precipitation bias at high elevation locations in western states (see slide 10).

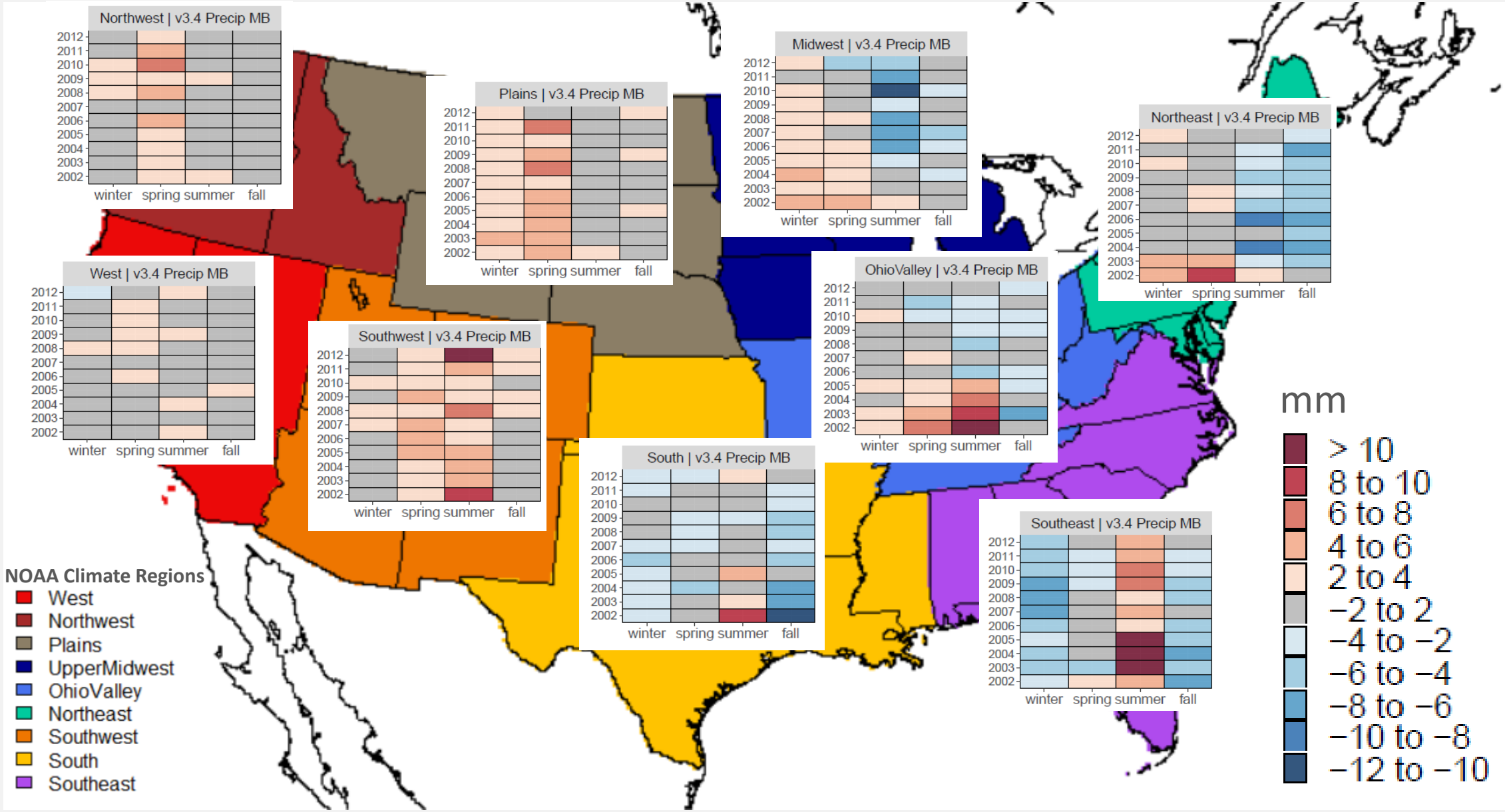


Summer 2010: PRISM, WRFv3.4, WRFv4.1.1 Precipitation

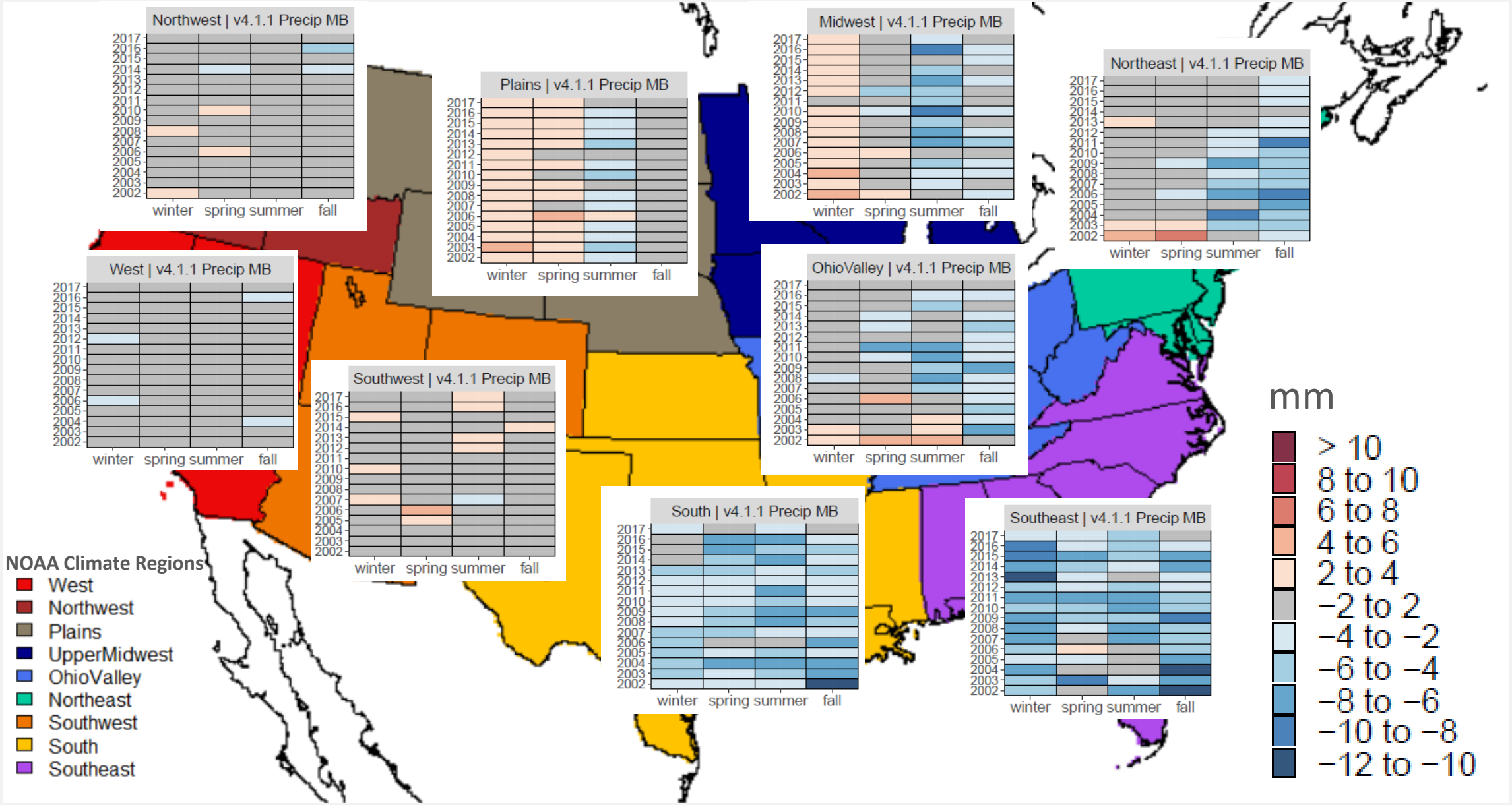




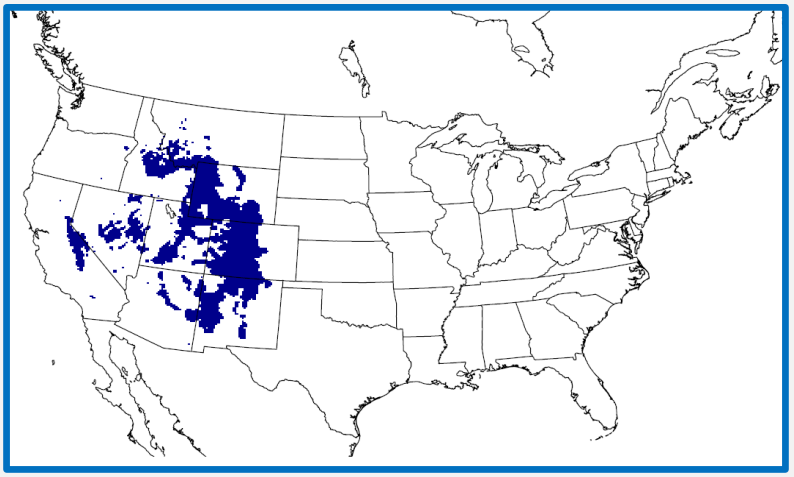
WRFv3.4 - PRISM Mean Bias in Seasonal Total Precipitation (2002-2012)



WRFv4.1.1 - PRISM Mean Bias in Seasonal Total Precipitation (2002-2017)

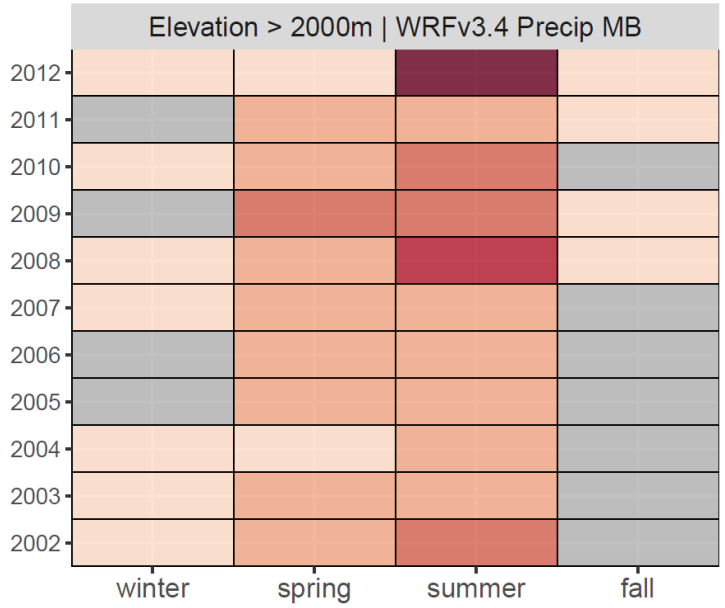


WRFv3.4 vs WRFv4.1.1 Precipitation Mean Bias at High Elevation Grid Cells

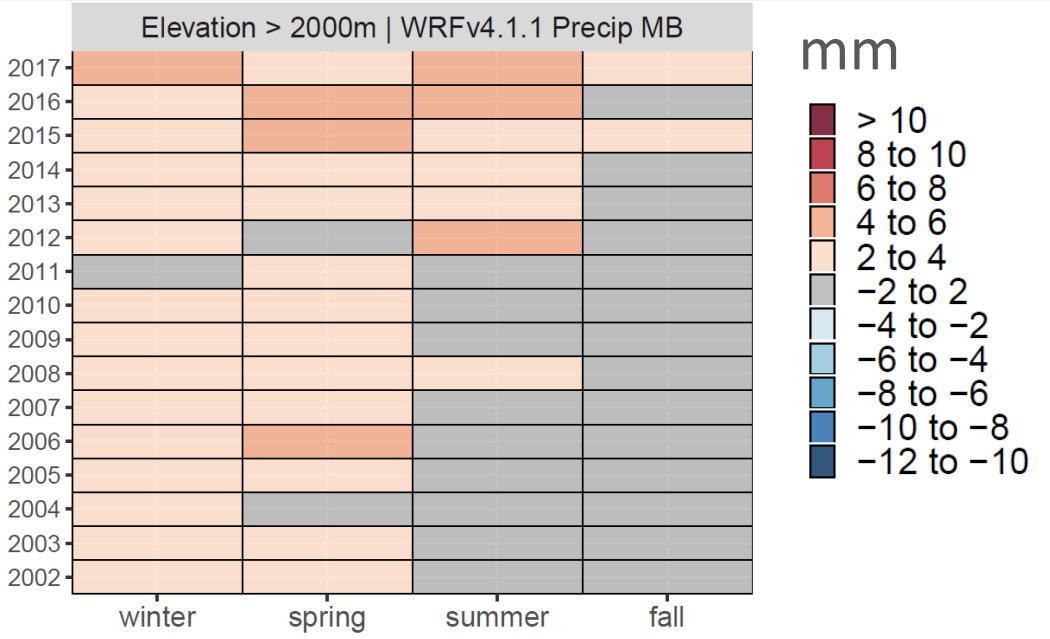


CMAQ Grid Cell Mask for High Elevation (>2000m)

WRFv3.4 – PRISM MB



WRFv4.1.1 – PRISM MB



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Northern Hemisphere Emissions

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Development of Northern Hemisphere Emissions

- Started with 2010 **HTAPv2.2** emissions (Janssens-Maenhout et al.). This allowed us to leverage previous EPA efforts to speciate, temporally and vertically allocate HTAP emissions
- To estimate interannual variability, we used the long-term record from Community Emissions Data System (**CEDS**; Hoesly et al.)
  - Scaled 2010 forward/backward using year/country/sector scaling factors based on CEDS 2002-2014 trends
  - Used a flat trend for 2014-2017
- Biogenic VOC emissions and Soil NO emissions (important precursors to ozone and particulate) were developed from Copernicus Atmospheric Modeling System (**CAMS**) emissions
- Supplemented emissions with data from additional sources (see next 2 slides)

Atmos. Chem. Phys., 15, 11411–11432, 2015
www.atmos-chem-phys.net/15/11411/2015/
doi:10.5194/acp-15-11411-2015
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Atmospheric Chemistry and Physics

HTAP_v2.2: a mosaic of regional and global emission grid maps for 2008 and 2010 to study hemispheric transport of air pollution

G. Janssens-Maenhout[1,12], M. Crippa[1], D. Guizzardi[1], F. Dentener[1], M. Muntean[1], G. Pouliot[2], T. Keating[3], Q. Zhang[4], J. Kurokawa[5], R. Wankmüller[6], H. Denier van der Gon[7], J. J. P. Kuenen[7], Z. Klimont[8], G. Frost[9], S. Darras[10], B. Koffi[1], and M. Li[4,11]

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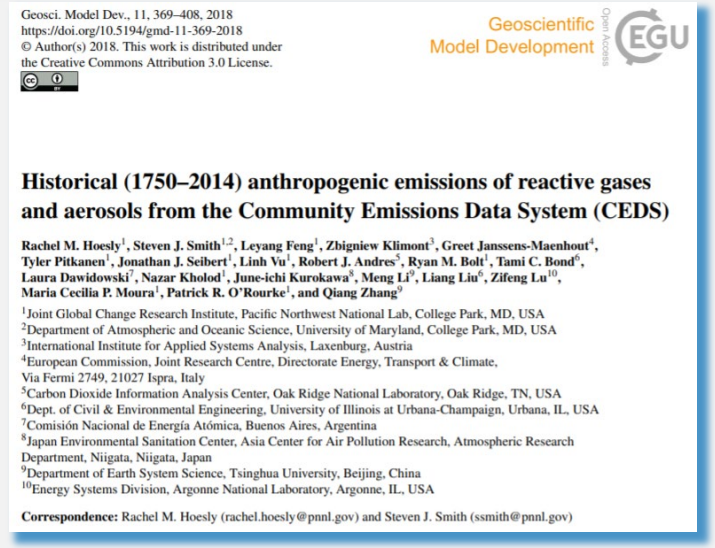

Geosci. Model Dev., 11, 369–408, 2018
https://doi.org/10.5194/gmd-11-369-2018
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Geoscientific Model Development

Historical (1750–2014) anthropogenic emissions of reactive gases and aerosols from the Community Emissions Data System (CEDS)

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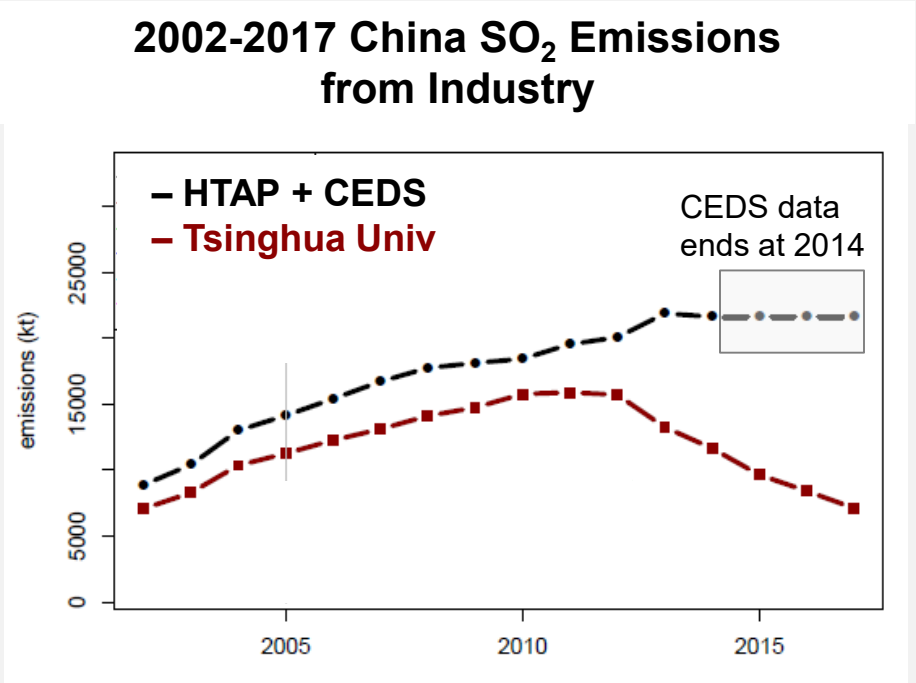
EQUATES

Development of Northern Hemisphere Emissions

- **China emissions** are based on trends from Zhao et al. (2018) (Tsinghua University)
  - Zhao et al. inventory includes decreasing SO_2 emissions from industry starting in 2013
  - This decreasing trend is qualitatively consistent with satellite trends in SO_2 columns, e.g., Krotkov et al. (2016); van der A et al. (2017)

- **Canada emissions** are provided by Environment and Climate Change Canada, based on their new long-term (1990-2018) Air Pollutant Emissions Inventory (APEI) Trends database



Trends from Zhao et al. (Tsinghua University) capture decreases in China SO_2 emissions driven by controls in the industry sector (iron, steel, cement)

Northern Hemisphere Emissions Methods Table

Sector	Data Source
Fires	N. America: SMARTFIRE2 + Bluesky Outside N. America: FINNv1.5
N. America; non-fire sectors	See slides 13-19
Soil NO	Hourly CAMS soil NO v2.1 data (CAMS_D81.3.6.1, CAMS_D81.3.8.2; extension of Yienger and Levy (1995)) for 2002-2017 based on monthly mean values + diurnal scaling factors.
Biogenic VOCs	Hourly CAMS biogenic VOCs v2.2 data (Sindelarova et al.; extension of Megan2.1) for 2002-2017 based on monthly mean values + diurnal scaling factors.
NO from lightning	GEIA based monthly climatology using vertical profiles applied by season and latitude
Canada emissions	2002-2017 Air Pollutant Emission Inventory (APEI) time series developed by Environment and Climate Change Canada
China emissions	China Inventory documented in Zhao et al. (2018) for 2005-2015. 2002-2004 created using CEDS scaling factors. 2016-2017 trends provided by Haotian Zheng (personal communication)
Mexico emissions	New 2016 inventory from Mexico's Secretariat of Environment and Natural Resources (SEMARNAT) scaled backward with CEDS scaling factors
All other sectors/regions	2010 HTAPv2.2 emissions + year specific scaling factors by country/sector using CEDS emissions for 2002-2014. 2015-2017 created using 2014 CEDS scaling factors.

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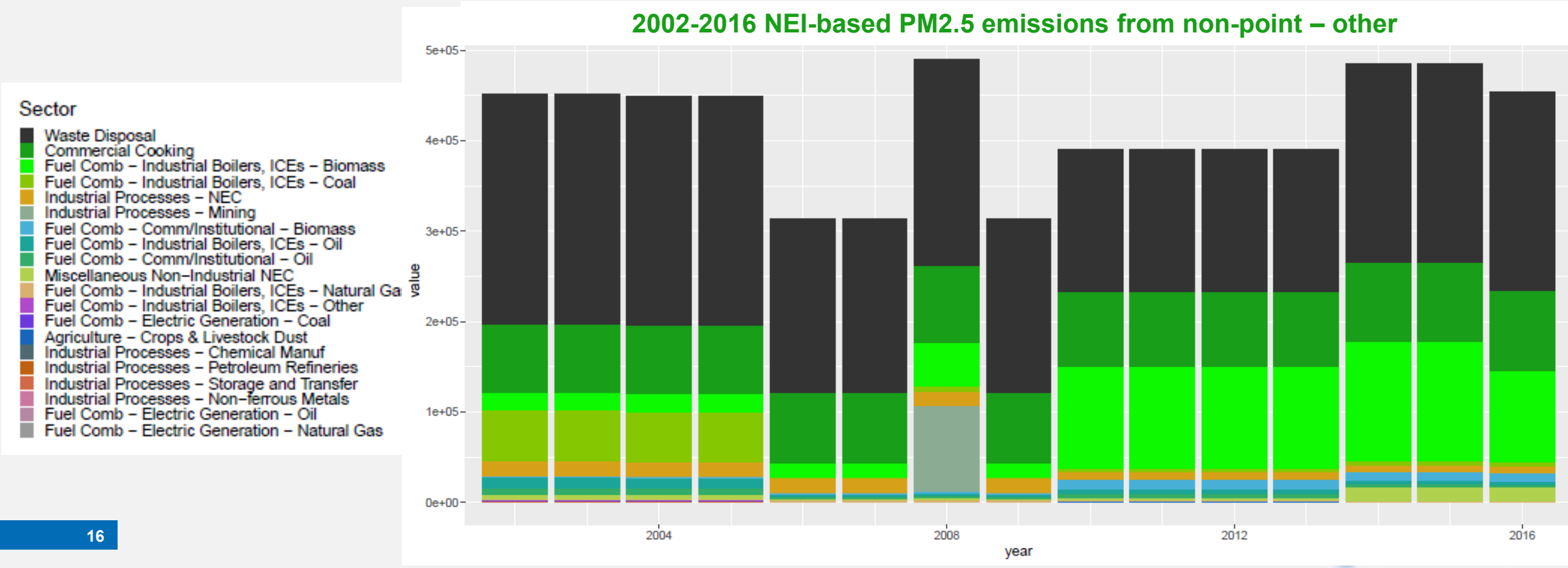
US Emissions

EQUATES

US Emissions

- EQUATES team examined trends in existing NEI/modeling platform emissions datasets and identified issues with changing methodologies.



Development of 2002-2017 US Emissions

Sector Categories in Collaborative 2016v1 Emissions Modeling Platform

Mobile
- On-road Vehicles
- Non-road Equipment
- C1/C2 Commercial Marine Vessels
- C3 Commercial Marine Vessels
- Rail

Point
- EGU
- Oil & Gas
- Non IPM (not EGU or oil & gas)
- Agricultural Field Burning
- Wild/Prescribed Fire
- Airports

Nonpoint
- Agriculture
- Area Fugitive Dust
- Oil & Gas
- Residential Wood Combustion
- Other

Biogenic (BEIS)

For each sector we are applying one of four approaches:

1. Develop new methods for creating consistent emissions for all years
2. Use 2016 or 2017 model platform emissions scaled with backcasting factors based on activity data and/or control information
3. Use existing modeling platform data
4. Leave flat at 2017 NEI levels

Highlights of New Emissions Modeling

- New fire emission inventory (wild, prescribed, and agriculture)
  See presentation by George Pouliot in this session

- New method for estimating organic emissions from volatile chemical products (VCP)
  See presentation by Karl Seltzer in this session

- New 2002-2017 EPIC simulations to support CMAQv5.3.2 modeling of bidirectional exchange of ammonia

- New MOVES nonroad and onroad mobile emissions modeling of NEI years; new onroad mobile inventories from CARB (EMFAC2017 model); new nonroad inventories from TCEQ (TexN2 model)

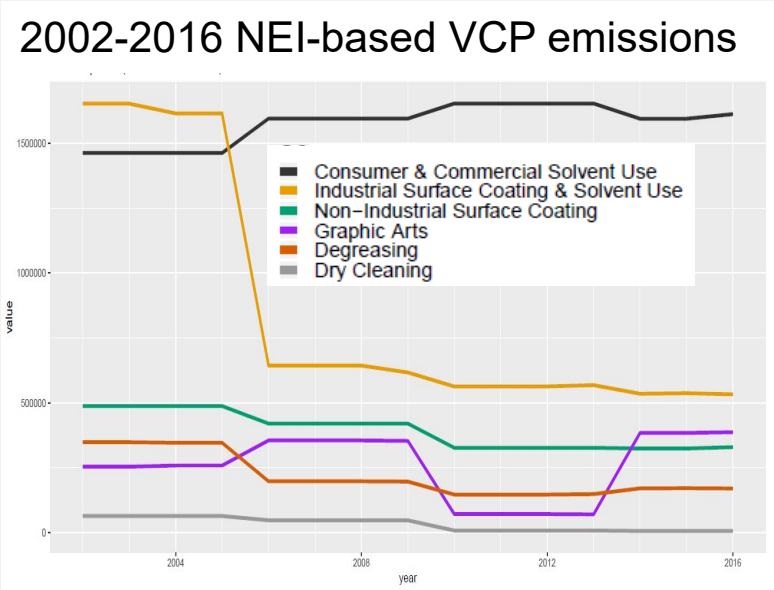
- New consistent time series of rail and commercial marine vehicle emissions developed by scaling 2016 model platform emissions with activity and control information

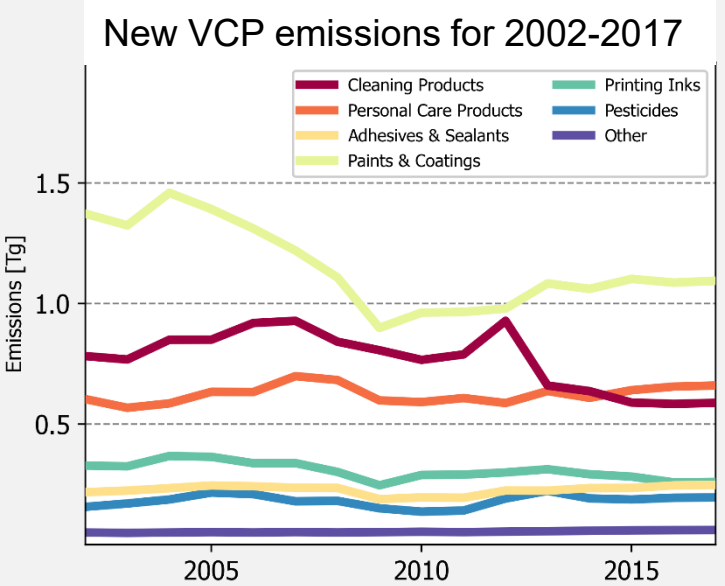
- See slides 25-29 for summary methods tables for all sectors

Examples of Emissions Updates: Solvents and Agriculture

VOC Emissions from VCPs

- NEI-based emissions trend has step-changes driven by methods changes between NEIs
- Time series simulations will leverage new VCPy inventory (see presentation by Karl Seltzer)

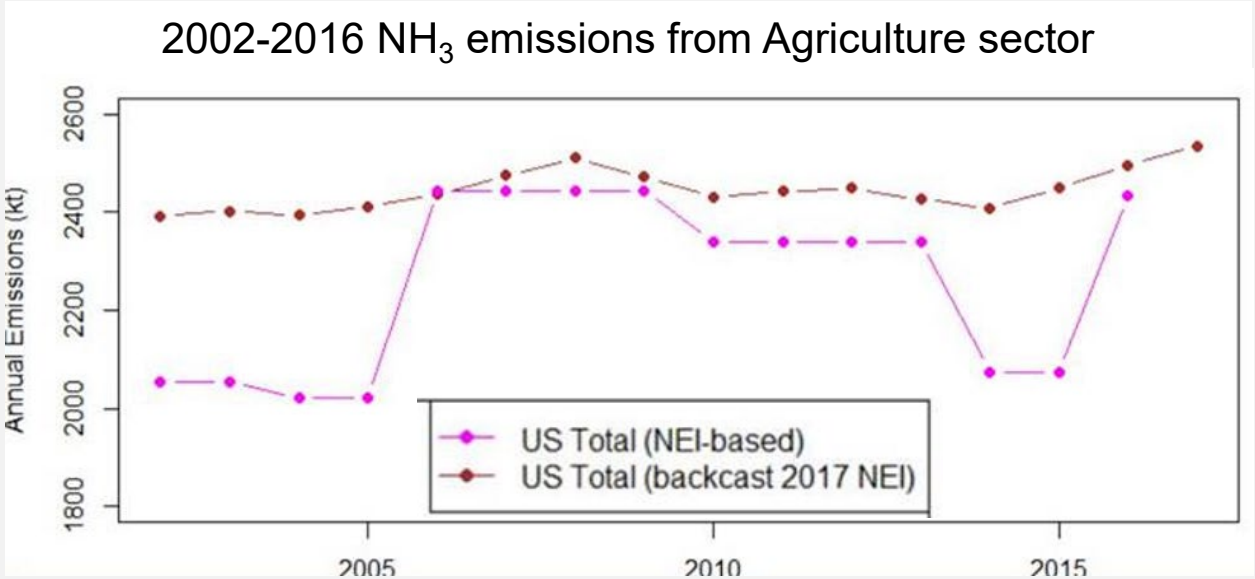




NH_3 Emissions from Agriculture (excluding fertilizer emissions*)

- NEI-based emissions trend has step-changes driven by methods changes between NEIs
- New emissions are based on 2017 NEI and backcasting factors based on USDA animal head counts

*fertilizer emissions are estimated with EPIC+CMAQ w/ bidirectional exchange of ammonia



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CMAQ Simulations

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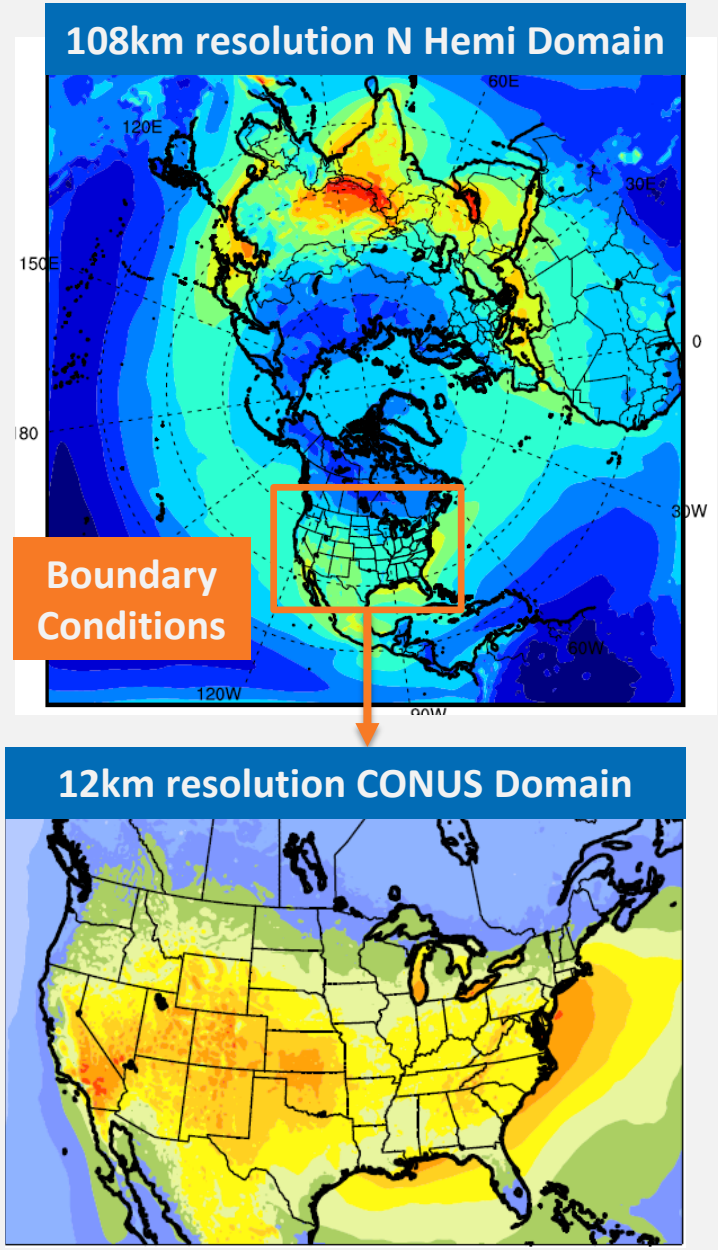
CMAQv5.3.2

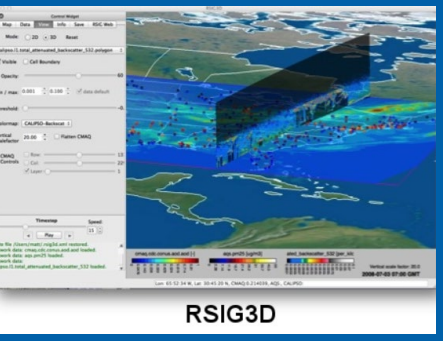
- **CMAQv5.3 improvements over v5.0.2**
  - Improved treatment of organic aerosols in aero7 module, leading to improved seasonal and diurnal patterns for $PM_{2.5}$
  - Improvements in vertical mixing introduced in v5.1 significantly reduces bias in morning and evening transition hours
  - Improvements in deposition algorithms introduced in v5.3 including land use specific deposition estimates and improved ozone dry deposition
  - Numerous additional updates! (See slides 30-32)

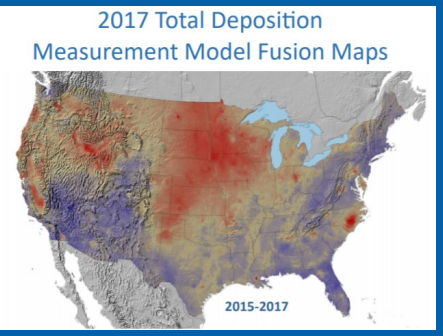
- Chemical mechanism
  - 108km NHemi: cb6r3m_ae7_kmtbr
  - 12km CONUS: cb6r3_ae7_aq

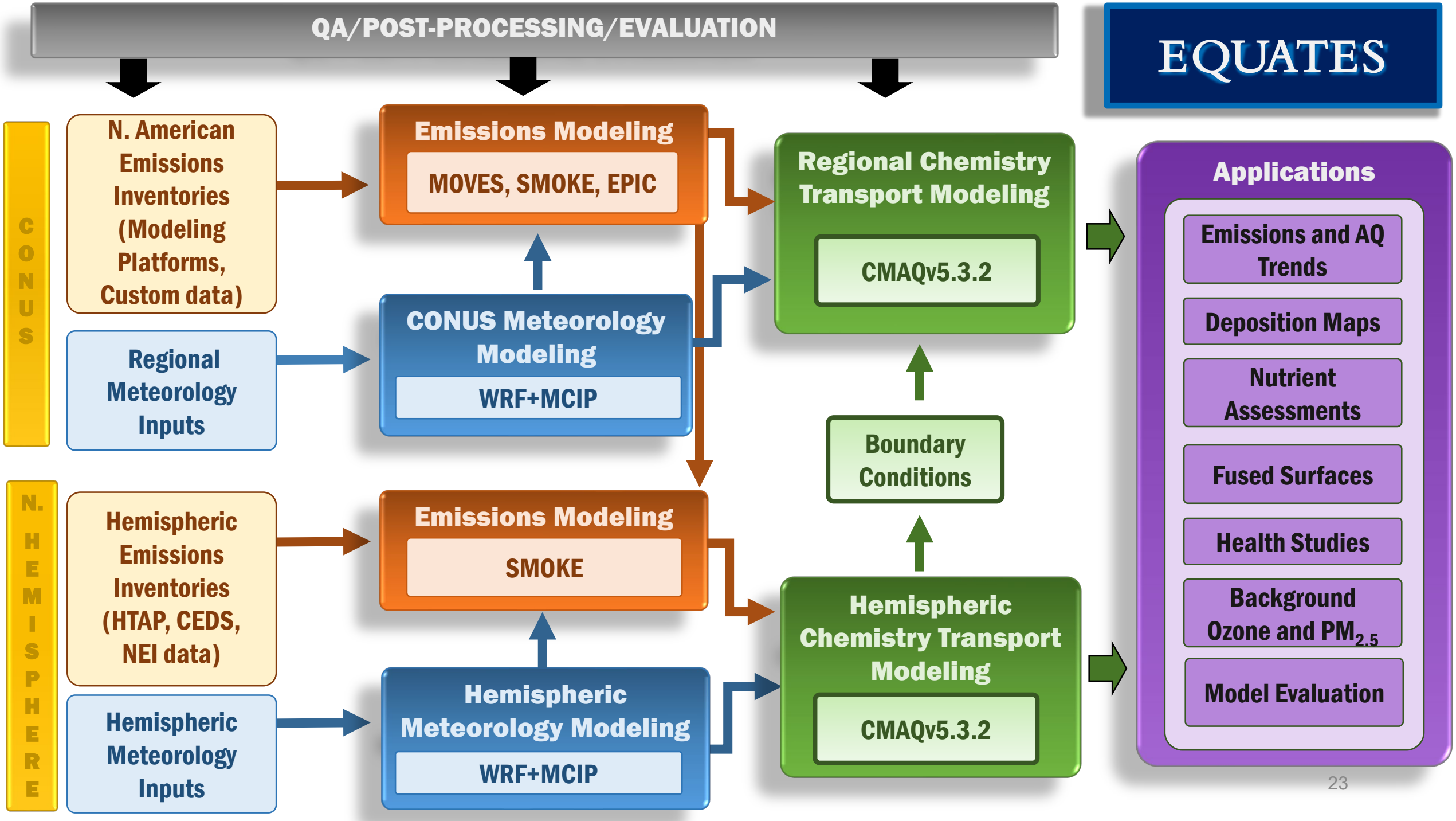


EQUATES Progress and Next Steps

- WRF simulations are complete (NHemi and CONUS)
- Northern Hemisphere (except US) emissions are complete
- 2020: US emissions will be completed this fall and then CMAQ simulations will begin
- 2021: Data will be post-processed to meet various collaborator needs and shared across multiple platforms
  - New TDEP maps added to other EPA tools and data products (e.g., EnviroAtlas, Critical Loads Mapper)
  - Subset of model inputs/outputs publicly posted (e.g., CMAS data warehouse, RSIG)






QA/POST-PROCESSING/EVALUATION
EQUATES
CONUS
N. HEMISPHERE
N. American Emissions Inventories (Modeling Platforms, Custom data)
Regional Meteorology Inputs
Hemispheric Emissions Inventories (HTAP, CEDS, NEI data)
Hemispheric Meteorology Inputs
Emissions Modeling
MOVES, SMOKE, EPIC
CONUS Meteorology Modeling
WRF+MCIP
Emissions Modeling
SMOKE
Hemispheric Meteorology Modeling
WRF+MCIP
Regional Chemistry Transport Modeling
CMAQv5.3.2
Boundary Conditions
Hemispheric Chemistry Transport Modeling
CMAQv5.3.2
Applications
Emissions and AQ Trends
Deposition Maps
Nutrient Assessments
Fused Surfaces
Health Studies
Background Ozone and PM2.5
Model Evaluation

For more information on the slides in this presentation, please contact:

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Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA.

North America Emissions

Sector	Methodology
Point - EGU	Use existing data for all years but processed using most recent tools/methods. For non-CEM sources with partial year reporting (based on EIA information), update temporal profiles.
Point – Oil & Gas	Use existing modeling platform data
Nonpoint – Oil & Gas	Emissions for NEI years from 2017 Nonpoint Oil and Gas Production Emission Estimation Tool. Interpolation between NEI years.
Mobile – Onroad	New MOVES runs and new estimates of VMT (and other activity data) for NEI years. For the non-NEI years use national adjustments to the MOVES emission factors (+/- 1 yr) based on vehicle type. Run SMOKE-MOVES for all years using year-specific met. Process gasoline and diesel emissions separately. CA onroad emissions using EMFAC2017 were provided by CARB for all years.
Mobile – Nonroad	5 NEI years of nonroad runs using MOVES2014b + interpolate remaining years CA: CA provided 2011, 2014, 2017. Interpolate for 2012-2013, 2015-2016. Scale back from 2011 using MOVES data to create 2002-2010 TX: 2017, 2010, 2002 TexN2 runs from TCEQ + interpolate remaining years Gasoline and diesel emissions will be processed separately for nonroad

North America Emissions

Sector	Methodology
Mobile - Nonroad - C1/C2 Commercial Marine Vessels	2016, 2017 – use modeling platform data (2016 is based off of adjusted 2017 data) 2002 -2015: OTAQ developed regional (by PADD) backcasting factors (base year 2016 was based off of 2017 NEI data) using regional fuel consumption as an activity surrogate with additional pollutant-specific adjustments for fuel standards (ECA and non-ECA adjustments)
Mobile - Nonroad - C3 Commercial Marine Vessels	2016, 2017 – use modeling platform data (methods are consistent) 2002 -2015: OTAQ developed regional (by PADD) backcasting factors (base year = 2016) using regional fuel consumption as an activity surrogate with additional pollutant-specific adjustments for fuel standards (ECA and non-ECA adjustments)
Mobile – Nonroad – Rail	2016, 2017 – use modeling platform data (2016 is based off of adjusted 2017 data) 2002 -2016: OAQPS+OTAQ developed backcasting factors (base year = 2016) using fuel sales data as an activity surrogate with additional adjustment for specific pollutants to account for regulation and sulfur technology
Airports	Use 2017 platform and backcast based on FAA Terminal Area Forecast data for 2002-2017

North America Emissions

Sector		Methodology
Nonpoint – Residential Wood Combustion		Use 2017 inventory and backcast based on national-level EIA/SEDS residential wood consumption data
Point – non-IPM **Nonpoint – other**	**Fuel Combustion** (except for nonpt biomass) **Industrial Processes** **Commercial Cooking**	Use existing modeling platform data which includes large emissions reductions from control programs such as the NOx SIP Call
	Fuel Combustion – Commercial Biomass (nonpt only)	Use 2017 inventory and backcast based on national-level EIA/SEDS commercial wood consumption data
	Fuel Combustion – Industrial Biomass (nonpt only)	Use 2017 inventory and backcast based on national-level EIA/SEDS industrial wood consumption data
	Waste Disposal	Use 2017 inventory for all years, except composting. For composting use 2017 values and backcast using linear interpolation of values in Table 7-19 from EPA report EPA 430-R-16-002
	Gas Stations	Linear interpolation between 2002 and 2017 modeling platform data. Remove stage 2 gas station SCCs from 2002 to avoid double counting with MOVES refueling emission
	Solvents	**New VCPy inventory – see presentation by Karl Seltzer in this session**
	All others (including Bulk Gasoline Terminals, Misc Non-Industrial NEC, Mobile)	Use 2017 inventory for all years, using 2016/2017 temporal profiles.

North America Emissions

Sector	Methodology
Nonpoint – Agriculture	- NH3 fertilizer emissions from EPIC+CMAQ w/ bidirectional exchange of ammonia - Use 2017 values (developed from CMU model) and backcast using USDA animal head counts
Nonpoint – Area Fugitive Dust	- Unpaved road dust: use 2017 estimates and use a national scaling factor to scale back based on national VMT (same VMT created for onroad emissions) - Paved road dust: use 2017 estimates and use state-specific scaling factors to scale back based on VMT totals by state (same VMT created for onroad emissions) - Ag dust from livestock: use the 2017 values and backcast using USDA animal head counts - All other afdust sectors (including dust from crop tilling) - Use 2017 values for all years - In all cases, the year specific met adjustments are applied

North America Emissions

Sector	Methodology
Point – Wild and Prescribed Fires	Year-specific fires from SMARTFIREv2 + BlueSky pipeline. Updated approach for Flint Hills (using year specific county level acres for Spring Burning) and grassland fires **See presentation by George Pouliot in this session**
Point – Agricultural Fires	New approach for sugarcane. **See presentation by George Pouliot in this session**
Biogenics	BEIS model run online in CMAQ, with new BELD5 land use database

CMAQv5.3

CMAQv5.3 System Updates

- Incorporated updated instrumented models: Sulfur Tacking, Integrated Source Apportionment (ISAM) consistent with science process updates. Improvements in computational efficiency of these instrumented techniques have led to substantially faster run times to support their practical applications.
- A new emissions interface allows for substantial flexibility in the way emissions are mapped, scaled, and checked for quality and can greatly simplify the task of assessing air quality improvements resulting from emission changes.
- Incorporated updates (new data sources, updated vertical coordinate system) to CMAQ and the Meteorology-Chemistry Interface Processor (MCIPv5.0) to increase scientific consistency between the atmospheric dynamics and chemistry calculations.

New Features and Processes in v5.3

- Updated marine chemistry to represent impacts of (1) halogen chemistry on ozone depletion and sulfate formation and (2) dimethyl sulfide on aerosol sulfate.
- Expanded the representation of secondary pollutant formation in clouds (AQCHEM-KMT2).
- Updated aerosol module (AERO7) that explicitly tracks 84 particulate species .
- Updated pathways for secondary organic aerosol formation from biogenic VOCs .
- Harmonized treatment of water uptake to aerosol organic phase to improve representation of aerosol chemistry, mixing, state and optical properties.
- Improved the representation of bi-directional exchange of ammonia at the surface. Improved representation of O_3 dry deposition to snow.
- Incorporated a new deposition module – the Surface Tiled Aerosol and Gaseous Exchange (STAGE) model to estimate land-use specific deposition.

CMAQv5.2

CMAQv5.2 System Updates

- Incorporated updates to representation of organic nitrate lifetimes and halogen chemistry for better representation of tropospheric chemistry on hemispheric scales.
- Added new sources of secondary organic aerosols (heterogeneous uptake of glyoxal and methylglyoxal in CB6) and updated properties of traditional secondary organic aerosol. The volatility of both secondary and primary organic compounds are now treated consistently with each other.
- Incorporated updated instrumented models: DDM-3D, Sulfur Tacking, Integrated Source Apportionment (ISAM) consistent with science process updates.

New Features and Processes in v5.2

- Incorporated the CB6 chemical mechanism to incorporate new information on gas-phase kinetics.
- Incorporated representation of stratosphere-troposphere exchange process on three-dimensional O_3 distributions, using a space and time varying potential vorticity scaling approach.
- Incorporated a new physics based windblown dust emission model that yields better agreement with observations of fine and coarse PM and constituents.
- Added a new model species to account for the organic aerosol compounds resulting from combustion processes.

CMAQv5.1

CMAQv5.1 System Updates

- Improved consistency in representation of radiation attenuation by clouds between WRF and photolysis module in CMAQ.
- Included the Rodas3 Rosenbrock solver to solve cloud chemistry, kinetic mass transfer, ionic dissociation, and wet deposition.
- Improvements to the land-surface model and ACM mixing scheme to enable finer-scale applications.
- Improvements in representation of aerosol mixing state and optical properties for 2-way coupled WRF-CMAQ configurations.

New Features and Processes in v5.1

- Incorporated the RACM2 chemical mechanism.
- Included detailed representation of impacts of halogen chemistry on O_3 in marine environments. Improved representation of O_3 in coastal regions as well as representation of O_3 loss in air masses transported intercontinentally across vast oceans.
- New secondary organic aerosol (SOA) sources from isoprene, alkanes, and polyaromatic hydrocarbons (PAHs).
- Incorporation of new binary nucleation and updates to $PM_{2.5}$ emission size distribution to improve aerosol size distribution simulation.
- Included gravitational settling for coarse aerosols.