Bidirectional Ammonia Flux Modeling in the CMAQ-EPIC System

Jonathan Pleim[1] and Limei Ran[2]

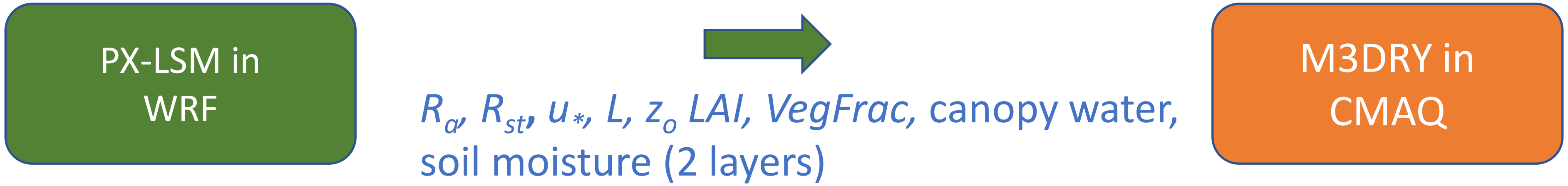
1 EPA/ORD/CEMM

2 USDA/NRCS

Outline

- Dry deposition in the Community Multiscale Air Quality (CMAQ) model
    - CMAQ dry deposition is linked with Pleim-Xiu land surface model (PX-LSM) in WRF
- Ammonia bidirectional flux modeling
    - Soil ammonia from the Environmental Policy Integrated Climate (EPIC) model is used to compute bidirectional NH_3 fluxes in CMAQ
- New aerosol dry deposition modeling in CMAQ
    - The addition of new microscale impaction term greatly improves model compared to size resolved measurements

Dry deposition and bidirectional flux



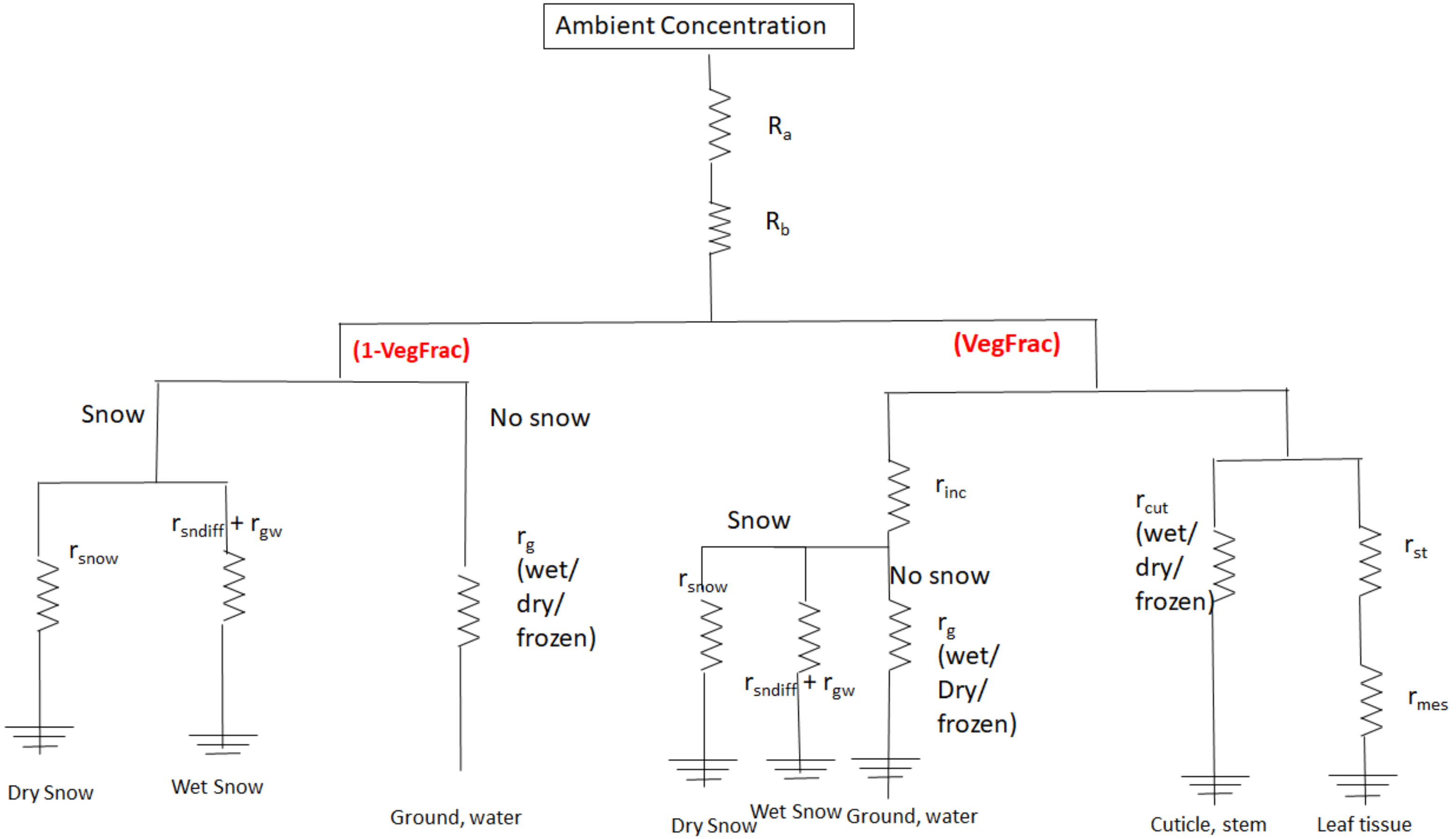
PX-LSM in WRF

R_a, R_{st}, u_*, L, z_o *LAI*, *VegFrac*, canopy water, soil moisture (2 layers)

M3DRY in CMAQ

- PX-LSM (*Pleim & Xiu, 1995; Xiu & Pleim, 2001*) is a land surface model with Jarvis-type stomatal conductance available in the WRF model (Gilliam & Pleim, 2010)
  - Three pathways for WV flux: stomatal transpiration, evaporation from wet cuticle and other surfaces, and flux from soil
  - Key feature is the soil moisture and temperature nudging system (Pleim & Xiu, 2003, Pleim & Gilliam, 2009)
- M3dry (*Pleim et al., 2001; Pleim & Ran, 2011*) was designed as adjunct to the PX-LSM in the WRF model so that chemical fluxes are consistent with heat and moisture fluxes.
  - WV stomatal resistance from LSM scaled by gas diffusivity used for stomatal dry deposition pathway R_{st}
  - Surface resistances (R_g, R_{cut}) scaled by reactivity and solubility

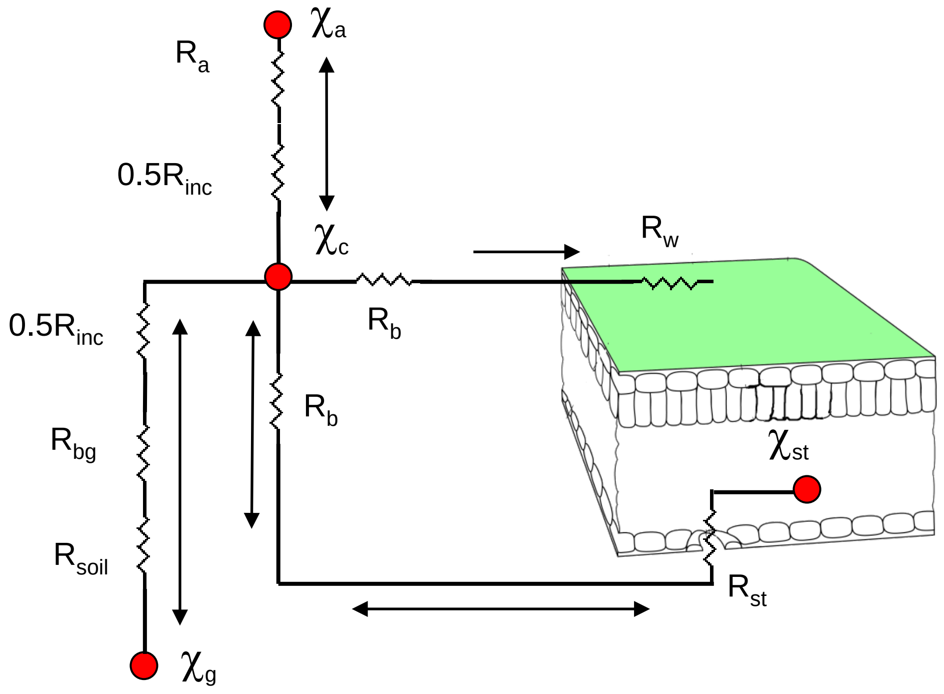
M3Dry Resistance Schematic



- The basic concept is that surface resistances (cuticle, ground, snow) for each chemical species are scaled by relative reactivity for dry surfaces and solubility for wet surfaces.
- In recent years dependencies on soil moisture and RH have been added for ozone and ammonia

CMAQ – EPIC NH3 bidirectional flux

- Bidirectional NH_3 flux modeling in CMAQ :
  - Based on simple resistance algorithm developed from field measurements in NC
  - Bidirectional flux from compensation concentrations in soil and plant stomata
  - Directly linked with daily output from the Environmental Policy Integrated Climate (EPIC) model

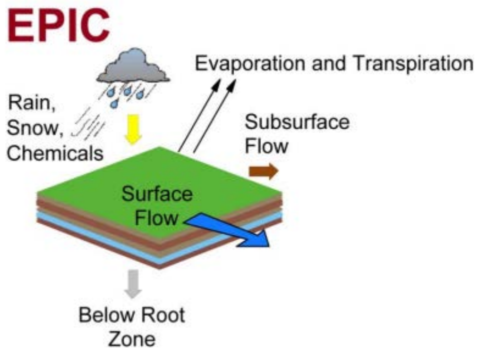


Pleim et al 2013, JGR

	Resistance to deposition
R_a	Aerodynamic resistance
R_b	Laminar boundary layer resistance
R_{inc}	In-canopy aerodynamic resistance
R_{bg}	Ground laminar boundary layer resistance
R_w	Cuticular resistance
R_{st}	Stomatal resistance
χ_a	Atmospheric concentration
χ_c	Canopy compensation point
χ_g	Soil compensation point concentration
χ_{st}	Stomatal compensation point concentration
R_{soil}	Soil resistance

Environmental Policy Integrated Climate - EPIC

- **EPIC - field scale terrestrial ecosystem model at daily time step:**
  - Initially constructed and named as the Erosion Productivity Impact Calculator in the early 1980s based on the daily runoff hydrology submodel of the CREAMS (Chemicals, Runoff, and Erosion from Agricultural Management Systems) model (Knisel, 1980)
  - Growth of ~ 120 plant species including food crops, native, grasses, and trees
  - Used to assess climate change effects on crop yields, soil carbon sequestration and GHG emissions
  - Nutrient (N-P-K) cycling and nutrient loss in water and sediment
  - Wind and water erosion
  - Draining and Irrigation
  - Pesticide and salt fate and transport
  - Integrated modeling with water and air quality
  - Economic-environmental accounting with alternative practices

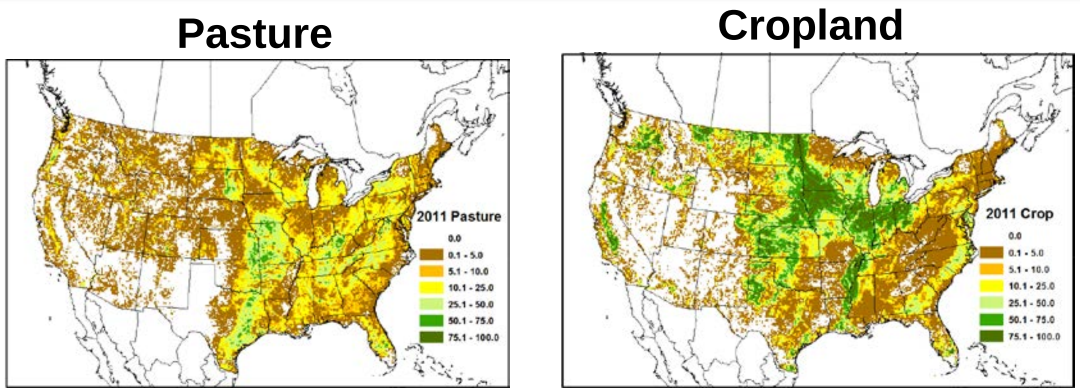


Williams et al. (1984, 1989, 1990, 1995, 2008), Sabbagh et al. (1991), Stockle et al. (1992a), Kiniry et al. (1992, 1995), Potter et al. (1998), Izaurralde et al. (2004, 2006, 2012, 2017), de Barros et al. (2004), Gassman (2005, 2011), Wang et al. (2012), Ellen et al. (2012), Ran et al. (2019), …

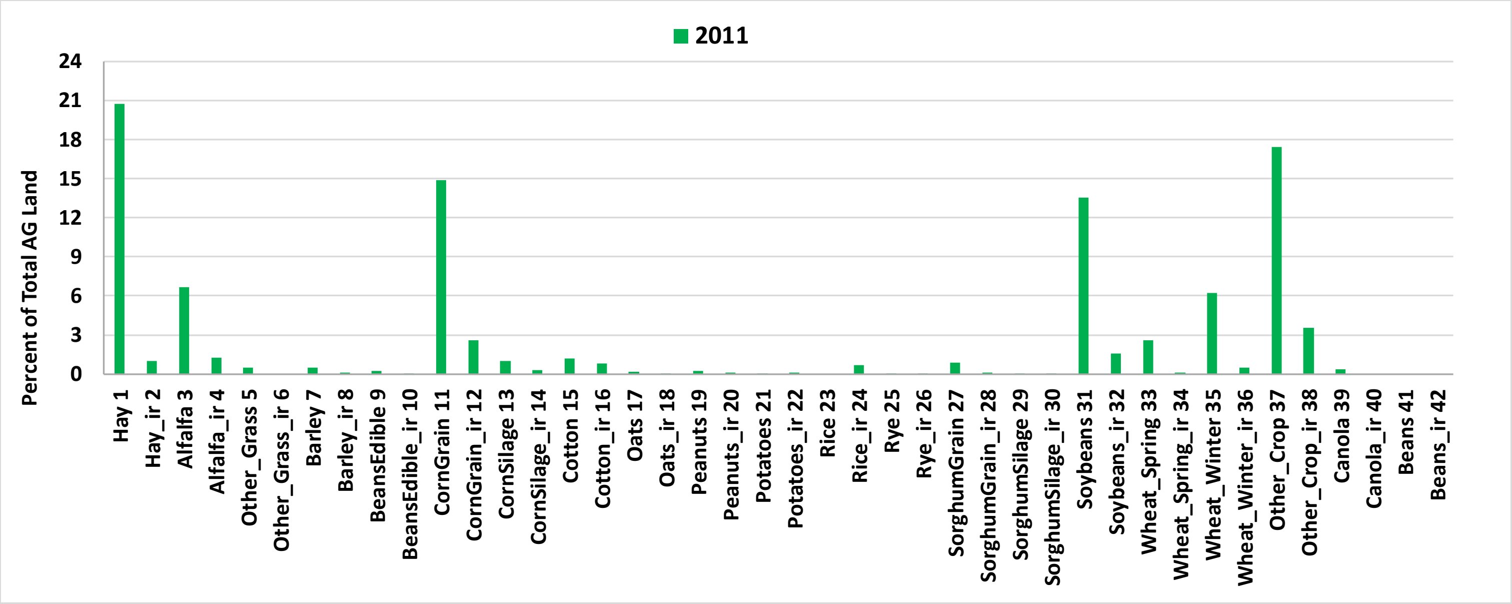
https://epicapex.tamu.edu/about/epic/

EPIC application to 12 km CONUS grid

- 21 grassland and cropland types with rainfed and irrigated information
- Crop fractions at each modeling grid cell are estimated based on 2011 NLCD data and 2012 USDA agricultural census



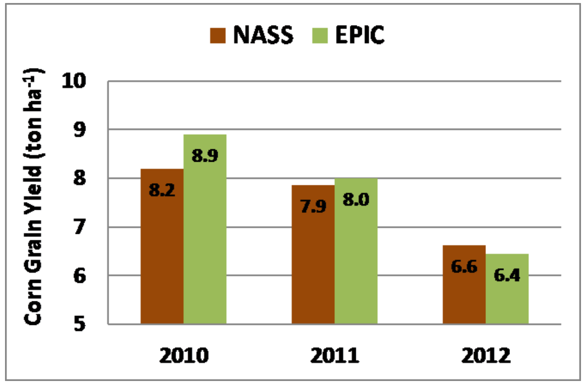
Agriculture land (%) in CMAQ 12 km domain grid cells

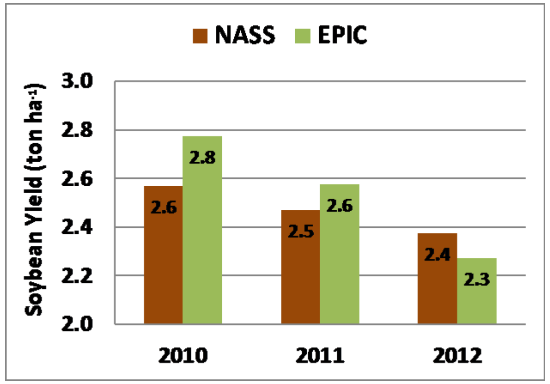


- Pasture (1 to 6): ~30% of total FEST-C EPIC agricultural land
- Dominant crops: hay, corn grain, soybean, and other crops

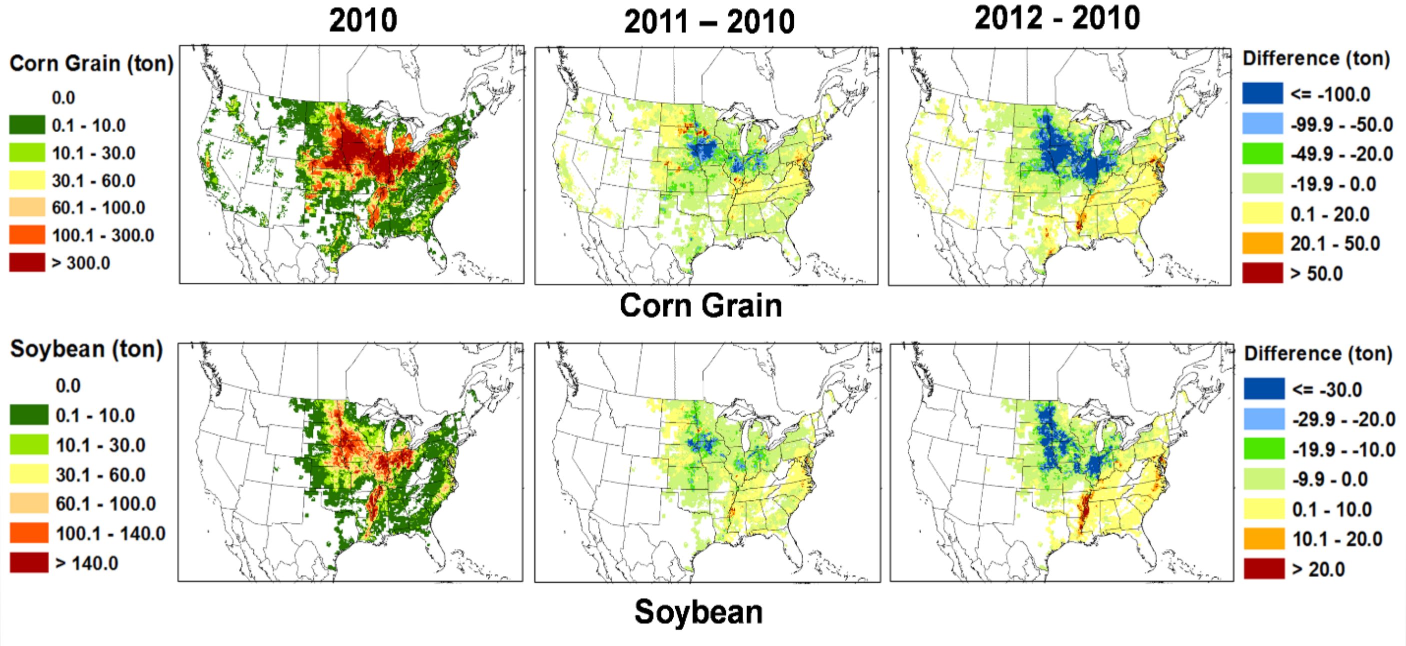
Percent of the domain agriculture land by crop types for 2011 NLCD and 2012 census

Integrated Agriculture - yield





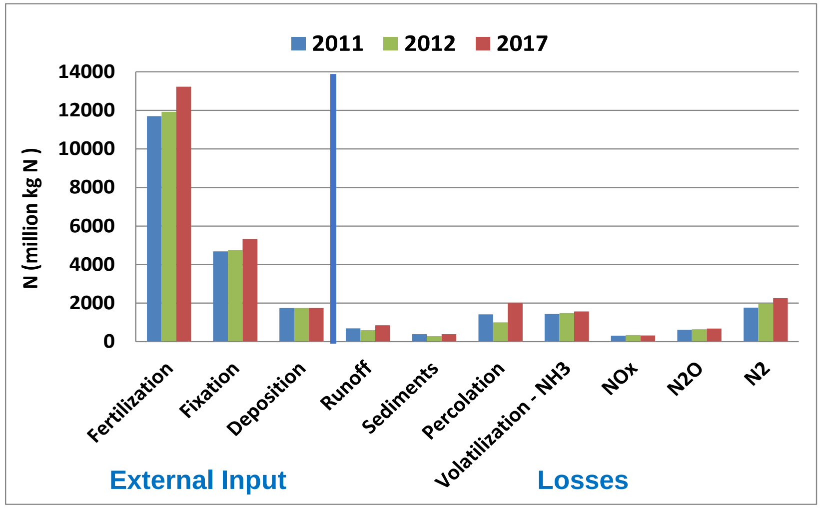
- EPIC does well in simulating yields for corn grain and soybeans
  - Decreasing trend consistent with USDA National Agriculture Statistic Service (NASS) reports (due to drought)
  - EPIC has high yields in normal precipitation year 2010 (no insect and storm loss in EPIC)

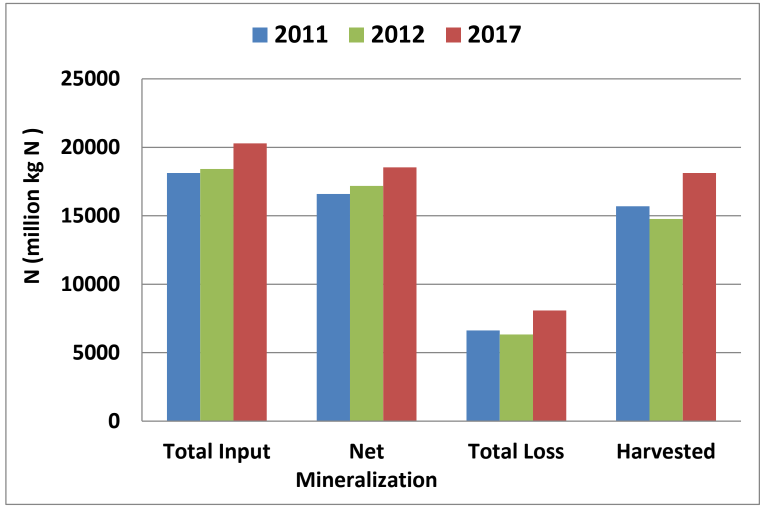


- 2010 most productive year
- Reduced production is most obvious in the Corn Belt region for 2012
- Production increase in the southeast and lower Mississippi Valley for 2012

Recent EPIC enhancements – N_2O and NO_x

N_2O emissions with other N pathway budgeting over CONUS





Data source: Luo et al., 2022. Integrated Modeling of US Agricultural Soil Emissions of Reactive Nitrogen and Associated Impacts on Air Pollution, Health, and Climate. Environmental Science & Technology, 56(13), pp.9265-9276.

Simulated N in different pathways reflects the weather conditions over the 3 years

- 2011 – severe drought in SW-Texas
- 2012 – severe drought in west and Plains states - Corn Belt regions (lowest N loss and in harvested)
- 2017 – normal and moist, associated with high N input-output

- **N_2O is simulated in EPIC from both nitrification and denitrification**
- **NO + HONO from nitrification**

CMAQ - EPIC Bidirectional flux

- Every day compute Γ in 2 soil layers (1 cm and 5 cm) from NH_3 in soil, soil moisture, soil characteristics, soil pH, and CEC, all from EPIC for each of 42 crop types:

$$NH_4^+{}_{aq} = \frac{L1\_NH_3}{d_1 w_1}$$

$L1\_NH_3$ is NH_3 in soil, d_1 is soil layer thickness, w_1 is soil moisture

$$\Gamma = \frac{NH_4^+{}_{aq}}{H^+}$$

Aggregated from 42 crops to total ag fraction of grid cell

$$\chi_g = F_{avail} \frac{A}{T_L} 10^{-B/T_L} \Gamma_g$$

F_{avail} = Max (1. – 0.038 CEC, 0.3)   CEC = cation exchange capacity (Williams 1995)

- Use the larger of the 2 layers: $\Gamma = \max(\Gamma_1, \Gamma_2)$ (almost always layer 1)
- FEST-C/EPIC is described and evaluated by Ran et al 2019
- Bidi-EPIC is described and evaluated by Pleim et al 2019

CMAQ NH_3 concentration vs CrIS

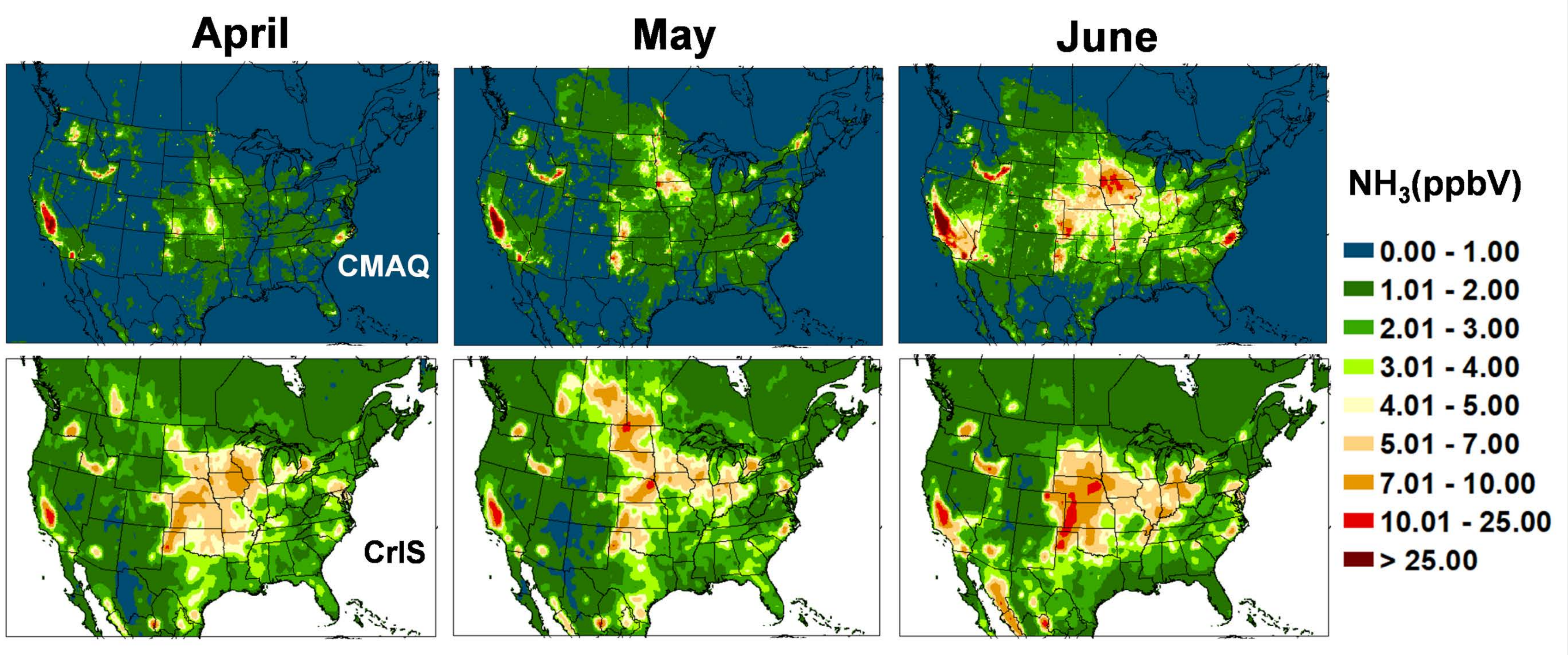
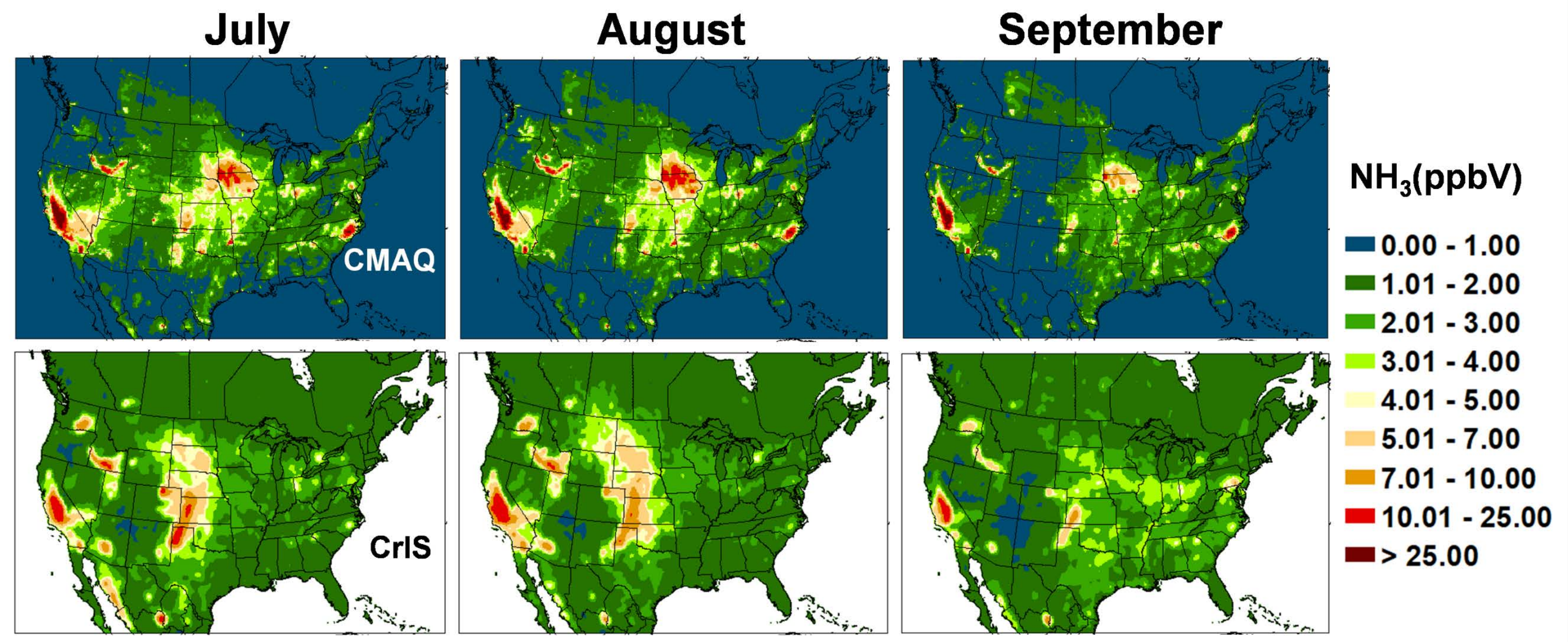


Figure from *Pleim et al., 2019, JAMES*

- CrIS satellite retrievals provided by Mark Shephard (Shephard and Cady-Pereira, 2015)
- Model NH_3 is low compared to CrIS in Spring but similar during growing season

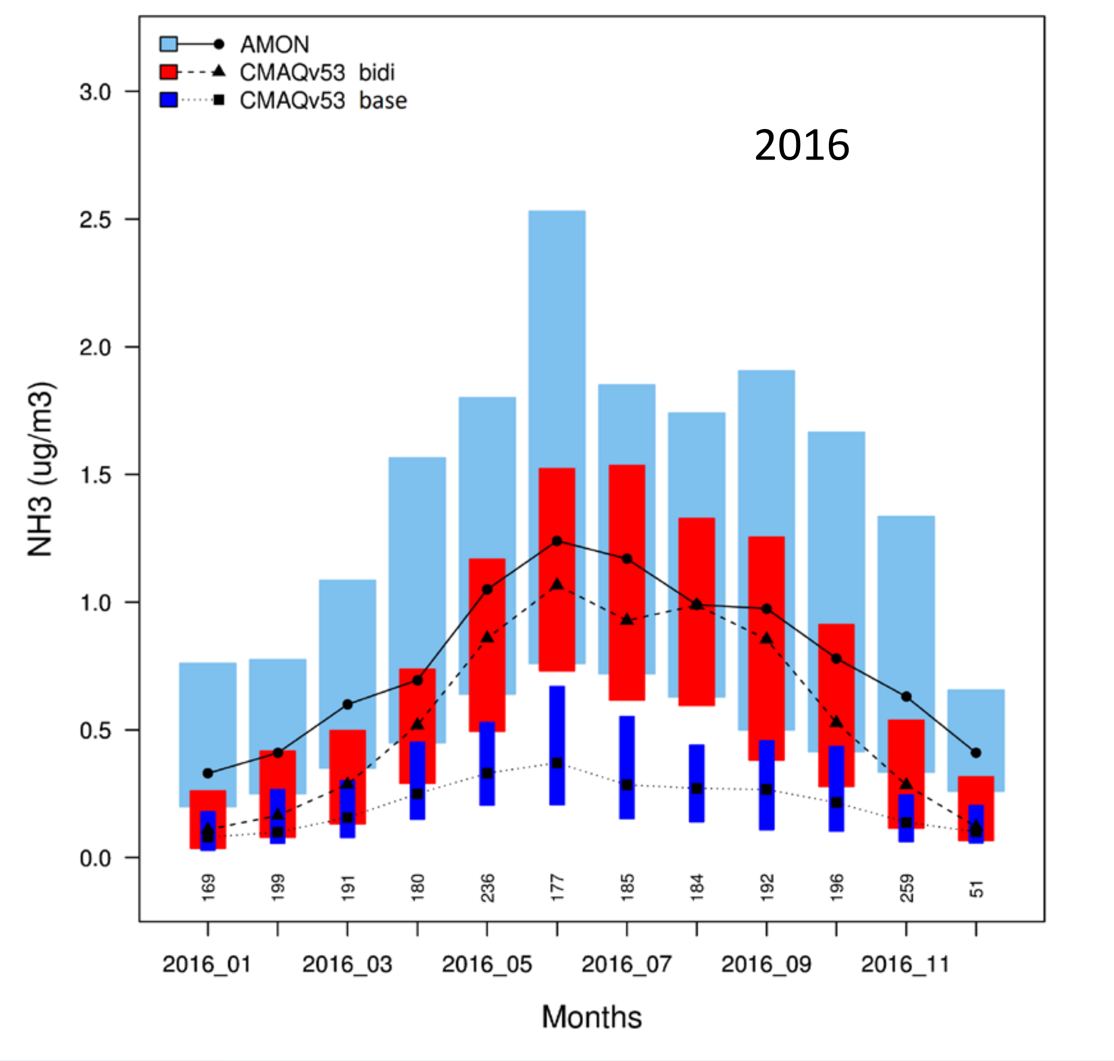
CMAQ NH4 concentration vs CrIS

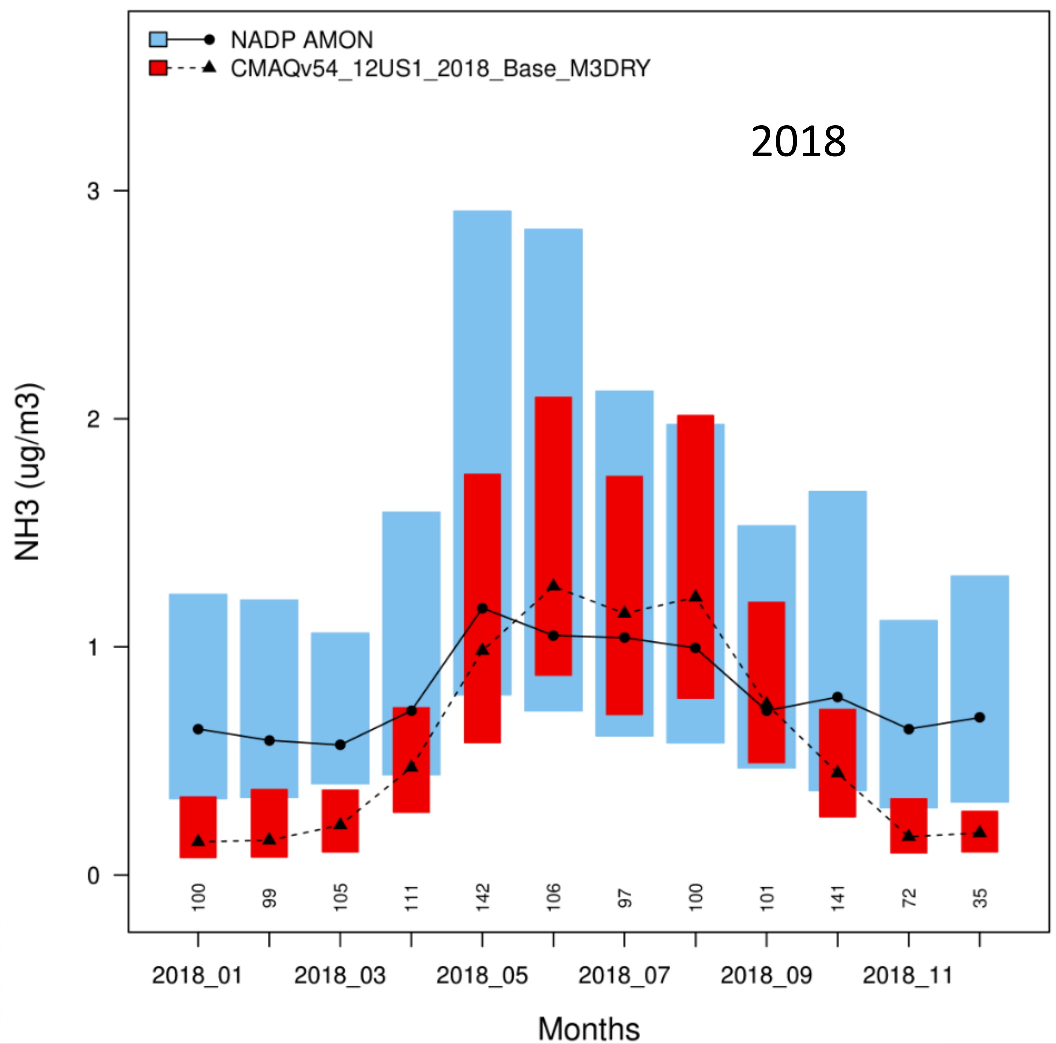


Figures from *Pleim et al., 2019, JAMES*

- High concentration areas are similar
- Model NH_3 is much greater than CrIS in Iowa and southeastern NC which are intensive hog production spots

NH_3 concentration Model vs AMON





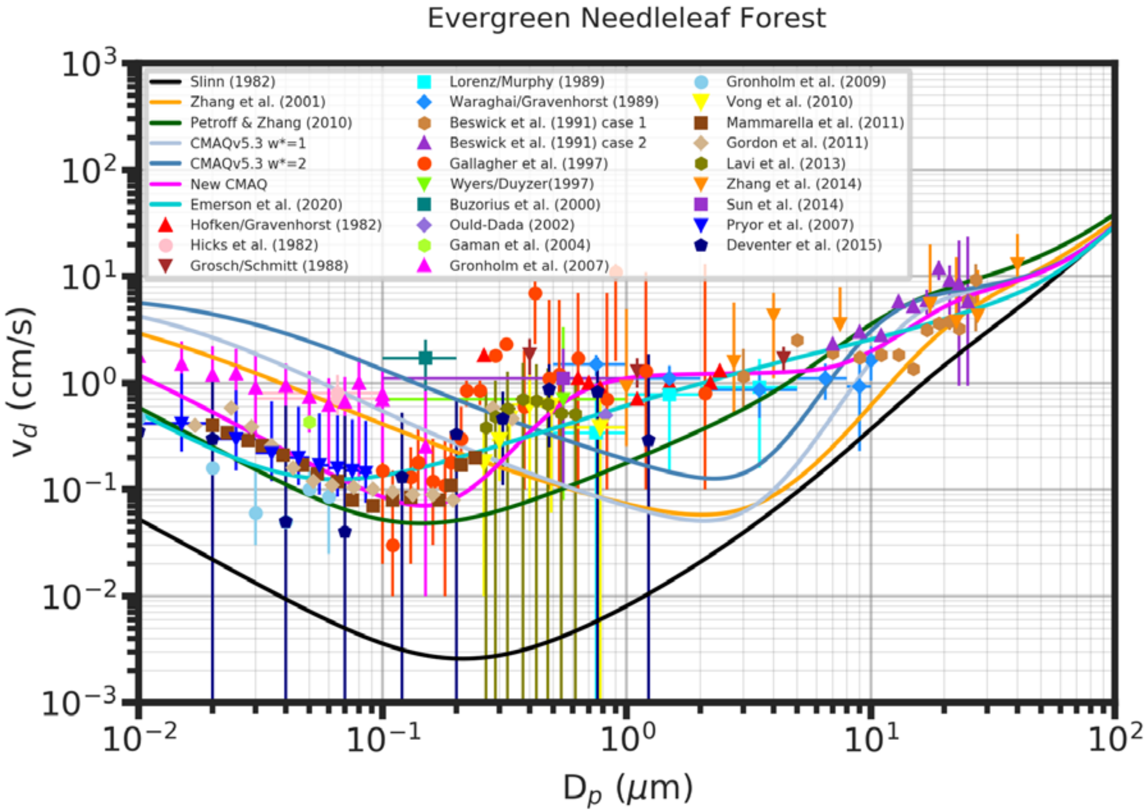
Next steps for EPIC-CMAQ

- Evaluate and improve agriculture model – EPIC
  - Update soil properties such as soil texture, CEC, pH, C-N-P content
  - Update cropland management including fertilizer type, timing, method, and manure application
  - Crop information – crop type, area, irrigation
  - N-cycling with N_2O and NO_X emissions using USDA N_2O monitoring network data
  - Harmonize volatilization in EPIC and CMAQ

    two-way flux should balance in both models
- CMAQ bidi improvement
  - Apply EPIC with realistic fertilization – current model uses crop N demand (less than actual)

New model for aerosol dry deposition

- Current models do not compare well with measurements especially for forests
- Hypothesis: Missing process involves effects of microscale features such as leaf hairs, ridges, or thick epicuticular wax layers for broadleaf and edge effects for long narrow needleleaf
- New model includes new microscale impaction process
- Follows observations across size spectra much better, especially in accumulation mode



New model ▬

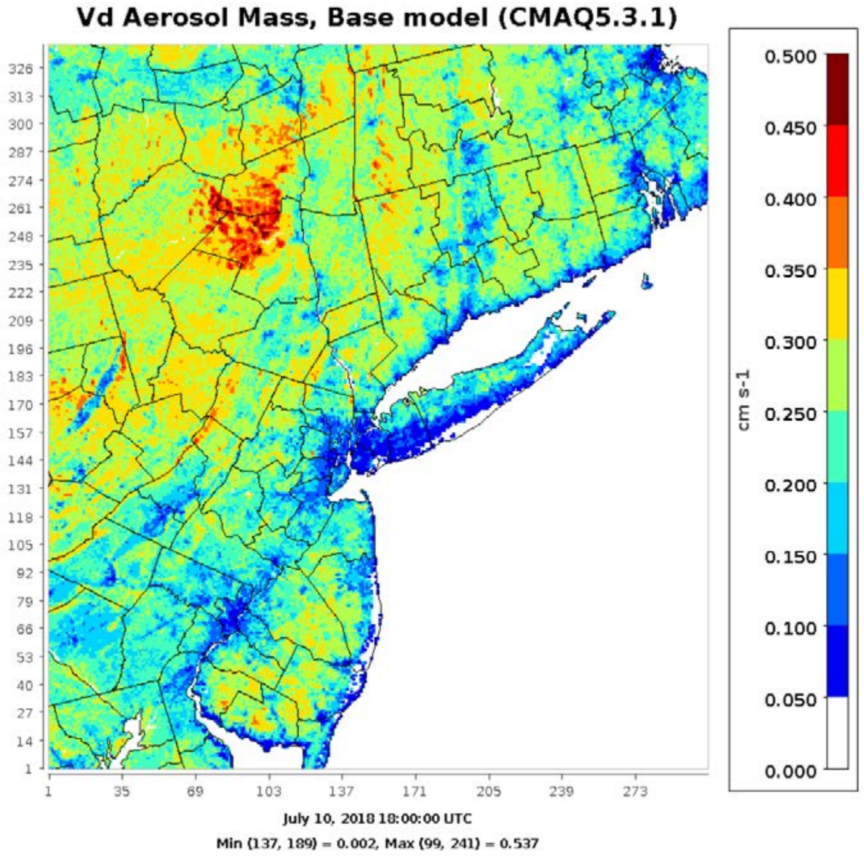
CMAQv5.3 w*=1 ▬

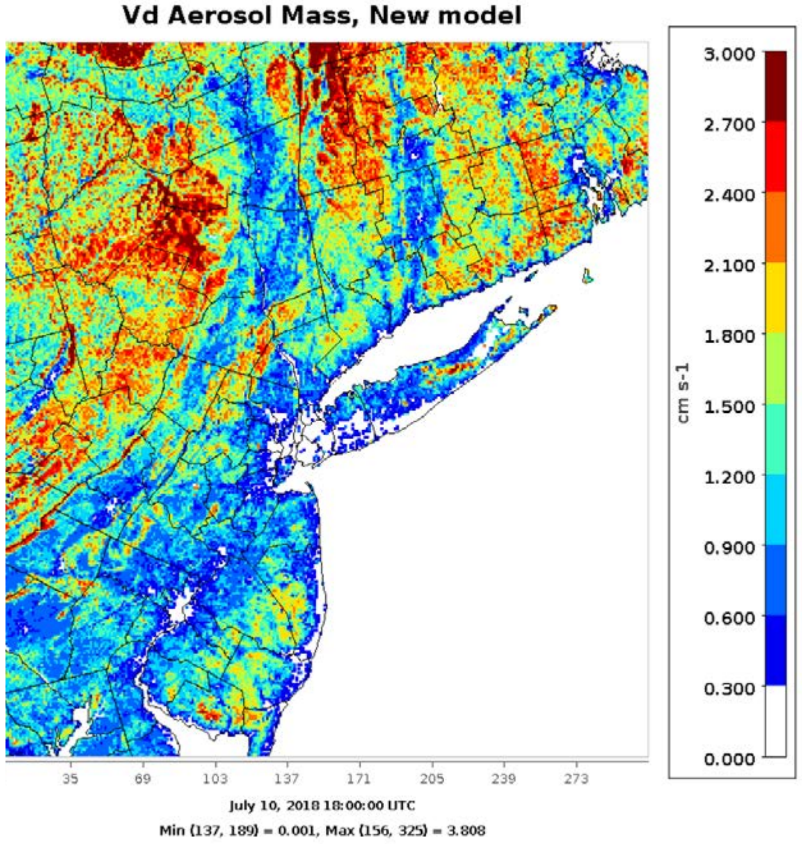
CMAQv5.3 w*=2 ▬

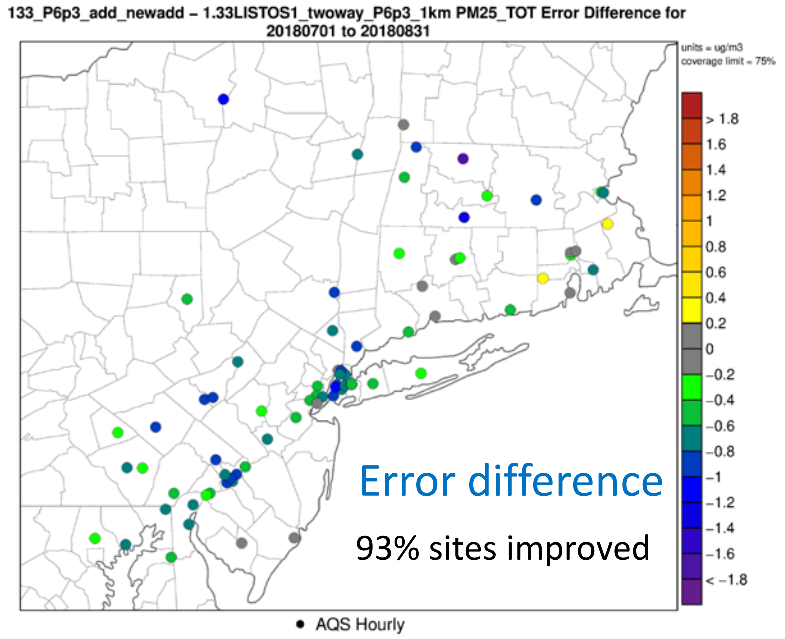
Zhang et al 2001 ▬

Pleim et al., 2022

V_d for accumulation mode mass – July 10, 2018 (18Z)







Error difference

93% sites improved

WRF-CMAQ model at 1.33 km grid resolution for LISTOS 2018
New model much higher V_d especially for forested areas

Reduces error in simulated $PM_{2.5}$ averaged over July - August 2018

Conclusions

- Dry deposition model in CMAQ (M3Dry) is linked to PX-LSM in WRF
  - Stomatal pathway constrained by soil assimilation scheme
- The ammonia bidirectional flux model is linked to the EPIC agriculture-ecosystem model
  - Development of EPIC is being advanced at the USDA
- New aerosol dry deposition model compares well with size resolved dry deposition velocity measurements.
  - Modeled dry deposition of PM2.5 greatly increased

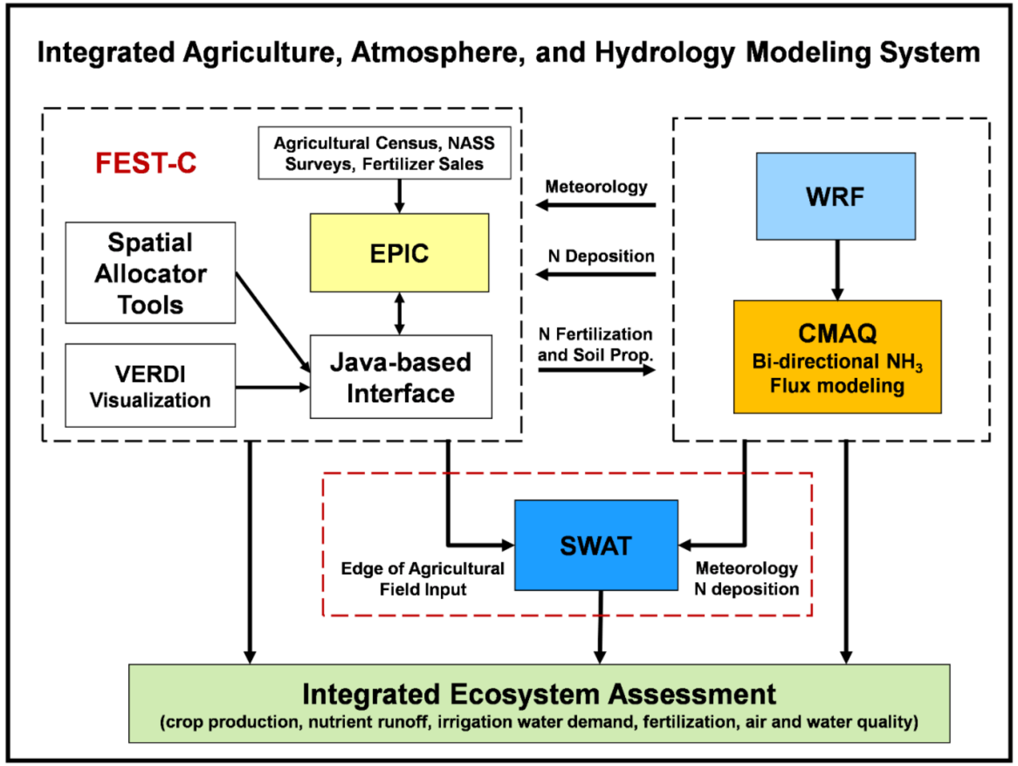
References

- Gilliam, R.C., and Pleim, J.E., 2010, An evaluation of the Pleim-Xiu land surface model, surface-layer and asymmetric convective model in version 3.0 of WRF ARW, J. Appl. Meteor. Climatol, 49, 760-774.
- Pleim, J.E., Ran, L., Saylor, R.D., Willison, J. and Binkowski, F.S., 2022. A New Aerosol Dry Deposition Model for Air Quality and Climate Modeling. *Journal of Advances in Modeling Earth Systems*, *14*(11).
- Pleim, J. E., Ran, L., Appel, W., Shephard, M. W., & Cady-Pereira, K. (2019). New bidirectional ammonia flux model in an air quality model coupled with an agricultural model. *Journal of Advances in Modeling Earth Systems*, *11*(9), 2934-2957.
- Pleim, J. E., Bash, J. O., Walker, J. T., & Cooter, E. J. (2013). Development and evaluation of an ammonia bidirectional flux parameterization for air quality models. *Journal of Geophysical Research: Atmospheres*, *118*(9), 3794-3806.
- Pleim, J., & Ran, L. (2011). Surface flux modeling for air quality applications. *Atmosphere*, *2*(3), 271-302.
- Pleim, J.E., and Gilliam, R., 2009, An indirect data assimilation scheme for deep soil temperature in the Pleim-Xiu land surface model. J. Appl. Meteor. Climatol., 48, 1362–1376.
- Pleim, J. E., and A. Xiu, 2003, Development of a land surface model. Part II: Data Assimilation. J. Appl. Meteor., 42, 1811-1822.
- Pleim, J. E., Xiu, A., Finkelstein, P. L., & Otte, T. L. (2001). A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. *Water, Air and Soil Pollution: Focus*, *1*(5-6), 243-252.
- Pleim, J. E. and A. Xiu, 1995. Development and testing of a surface flux and planetary boundary layer model for application in mesoscale models. J. Applied Meteorology, 34, 16-32.
- Pye, H. O. T., Zuend, A., Fry, J. L., Isaacman-VanWertz, G., Capps, S. L., Appel, K. W., et al. (2018). Coupling of organic and inorganic aerosol systems and the effect on gas–particle partitioning in the southeastern US. Atmospheric Chemistry and Physics, 18(1), 357–370. https://doi.org/10.5194/acp-18-357-2018
- Ran, L., Yuan, Y., Cooter, E., Benson, V., Yang, D., Pleim, J., ... & Williams, J. (2019). An integrated agriculture, atmosphere, and hydrology modeling system for ecosystem assessments. *Journal of Advances in Modeling Earth Systems*.
- Xiu, A. and J. E. Pleim, 2001, Development of a land surface model part I: Application in a mesoscale meteorology model. J. Appl. Meteor., 40, 192-209

Extras

Fertilizer Emission Scenario Tool for CMAQ
(FEST-C)

- FEST-C: https://www.cmascenter.org/fest-c/
  - First release of FEST-C v1.0 in October 2013
  - Current release FEST-C V1.4 in September 2018
- Contains Java-based interface, adapted EPIC (Environmental Policy Integrated Climate), tools
- Conducts EPIC simulations integrated with WRF and CMAQ
- Generates EPIC output for CMAQ modeling with the bi-directional NH_3 options
- Generates EPIC and WRF/CMAQ files for integrated watershed hydrology and water quality SWAT (Soil & Water Assessment Tool) simulations



Integrated Agriculture, Atmosphere, and Hydrology Modeling System

FEST-C

Agricultural Census, NASS Surveys, Fertilizer Sales

EPIC

Spatial Allocator Tools

VERDI Visualization

Java-based Interface

Meteorology

N Deposition

N Fertilization and Soil Prop.

WRF

CMAQ
Bi-directional NH_3 Flux modeling

SWAT

Edge of Agricultural Field Input

Meteorology
N deposition

Integrated Ecosystem Assessment
(crop production, nutrient runoff, irrigation water demand, fertilization, air and water quality)

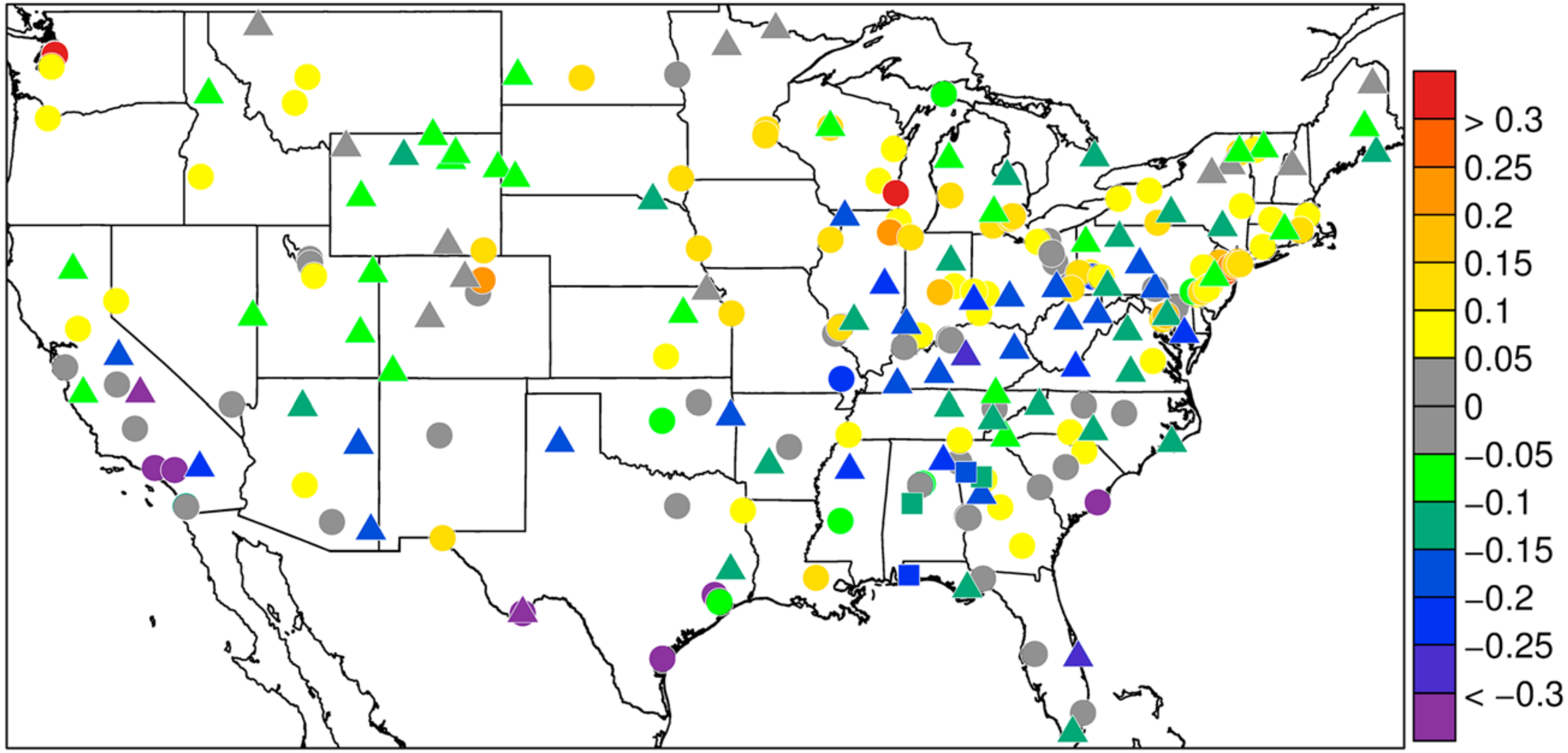
FEST-C with EPIC and integration tools is the centerpiece of this Integrated modeling system

FEST-C V1.4 and integrated modeling are described in details by Ran et al. 2019 (JAMES)

Key resistances

- Resistances passed from WRF/PX-LSM
  - Aerodynamic resistance: $$R_a = \frac{\phi_{hn}}{u_* k}\left[ln\left(\frac{z}{z_o}\right) - \psi_h\left(\frac{z}{L},\frac{z_o}{L}\right)\right]$$
  - Bulk stomatal resistance: $$R_{st} = \left[\frac{F_1(PAR)F_2(w_2)F_3(RH_s)F_4(T_a)}{LAI}\right]^{-1}$$
  - Additional parameters passed from WRF: u_*, L, z_o *LAI, VegFrac,* canopy water, soil moisture (2 layers)
- Resistances computed in CMAQ
  - Quasi-laminar boundary layer resistance: $R_b = \frac{B^{-1}}{u_*}\left(\frac{Sc}{Pr}\right)^{2/3}$
  - R_{cut}, R_{ground} scaled by relative reactivity and solubility of wet
  - Special functions
    - $R_g(O_3) = 200 + 300\ W_g/W_{fc}$
    - $R_{cut}(O_3) = 2000$ * (1.0 -rh_func) + $r_{wet}(O_3)$ * rh_func
      - rh_func = max(0.0,(RH- 70.0)/30.0)
    - $R_{cut}(NH_3) = r_{wet}(NH_3)$ + 100.0-max(RH,60.0)

Ammonium PM2.5 for May – September 2016

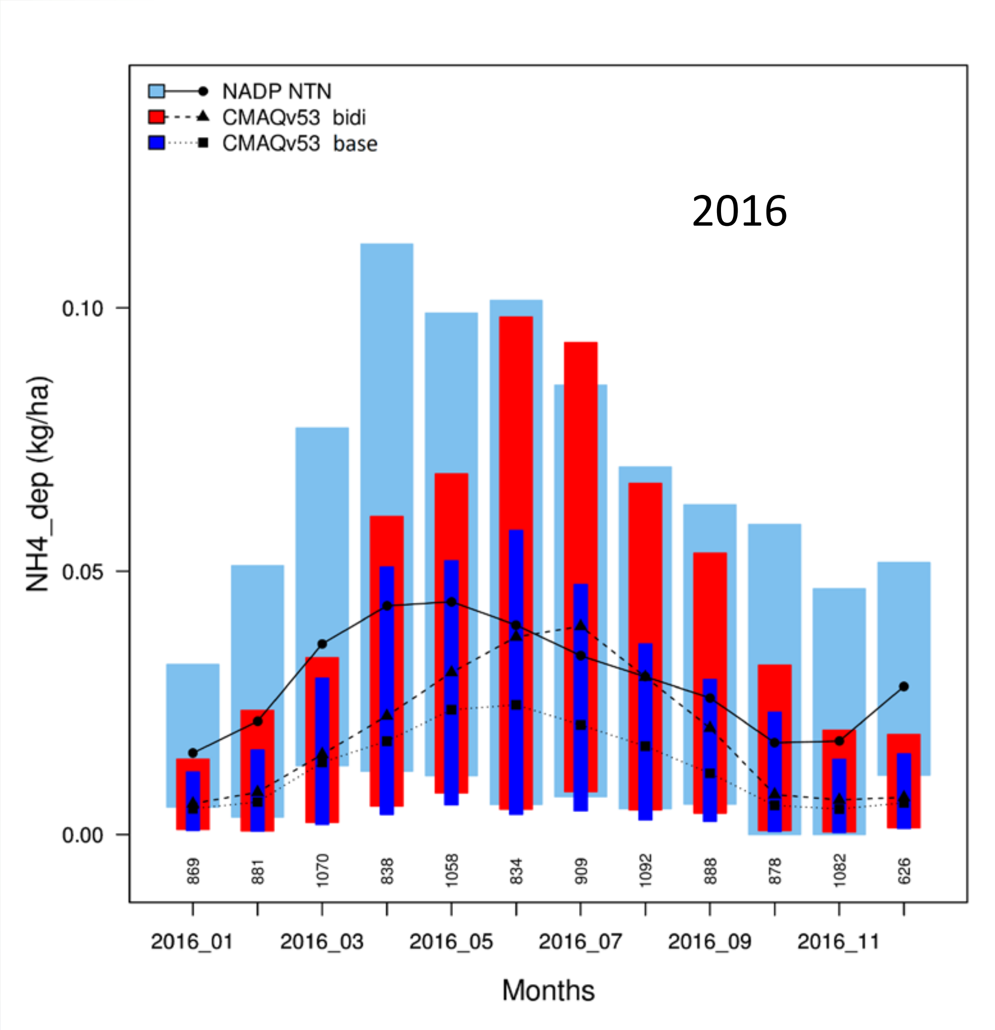


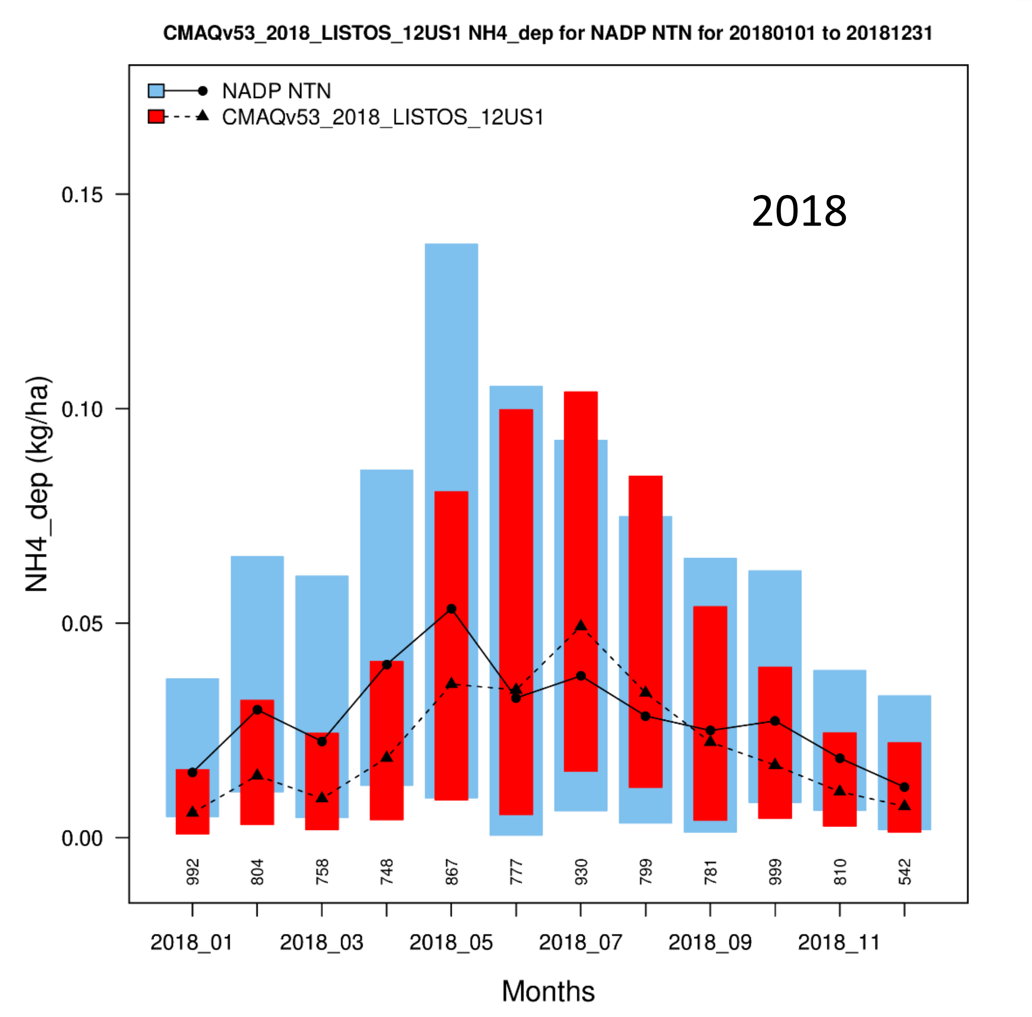
CIRCLE=CSN; TRIANGLE=CASTNET; SQUARE=SEARCH_Daily;

- The model is often low compared to CASTNet and SEARCH but high compared to CSN
- Analysis by Pye et al. (2018) concluded that CSN tends to underestimate NH_4^+ concentrations

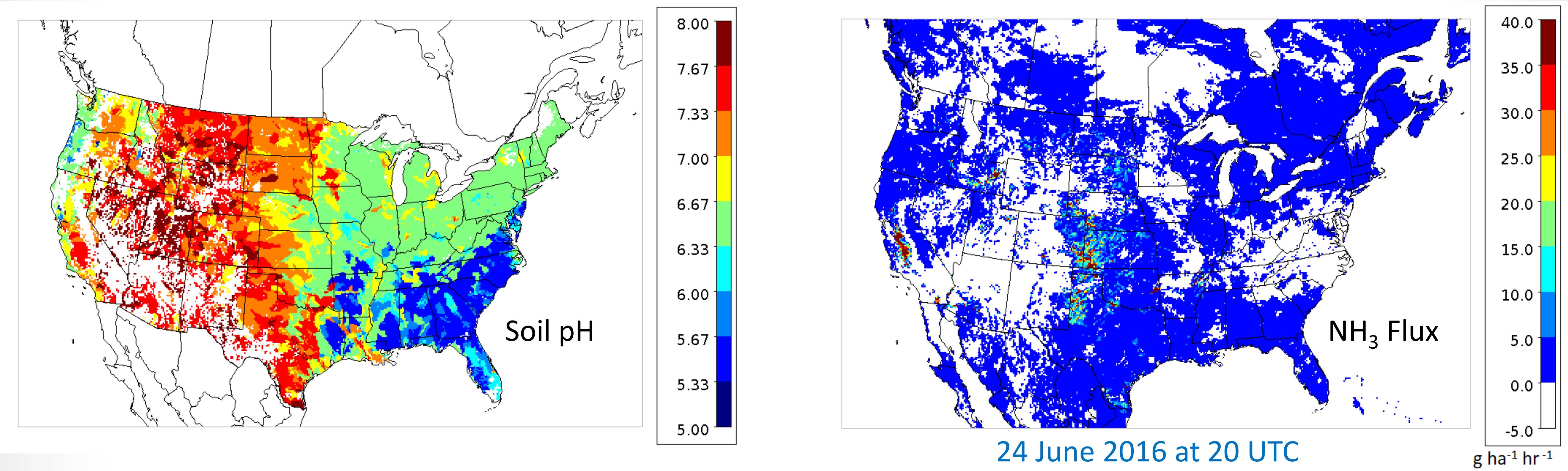
EPA

NH4 Wet Deposition from NADP NTN




CMAQv53_2018_LISTOS_12US1 NH4_dep for NADP NTN for 20180101 to 20181231

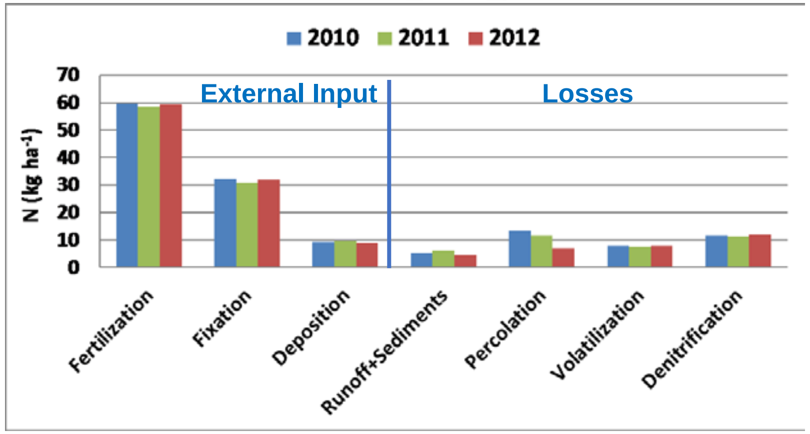
High Concentrations in Central Valley

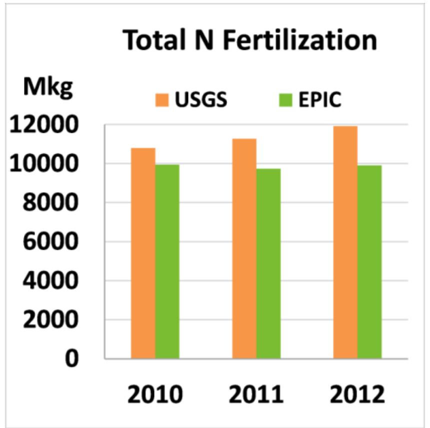


24 June 2016 at 20 UTC

- High concentrations in Central Valley of CA result from sporadic extreme fluxes
- Extreme Γ values occur in grid cells where individual crops occasionally have extremely high soil NH_4 concentrations in areas with high soil pH.
- E.g.: The flux in a cell in CA on June 1 is dominated by irrigated cotton which is only 8.8% area of the cell but with high NH4 soil mass, low soil water, and high pH results in Γ = 15, 000,000 leading to a grid cell $\Gamma = 1{,}900{,}000$

Integrated Agriculture: N budget

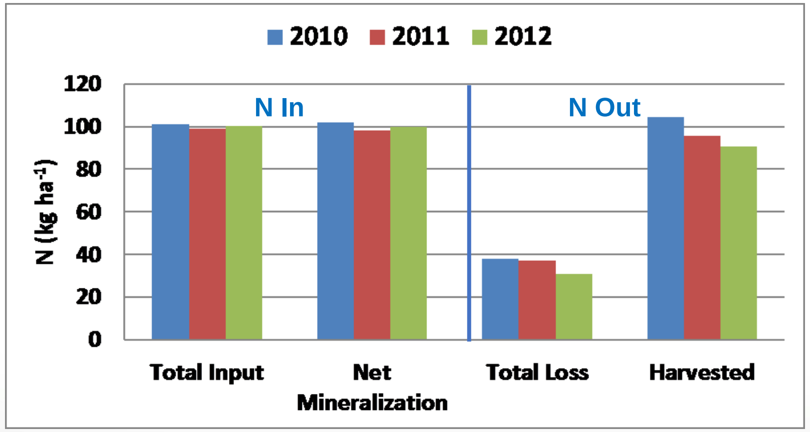




- Total input is similar among the 3 years
- N total loss and N in harvested plants are much more sensitive to year-specific weather conditions with a decreasing trend
- Reasonably lower than USGS sale-based fertilization as EPIC is a need-based model

Total Input = Fertilization + Fixation + Deposition

Total N Loss = Runoff + Sediments + Percolation + Volatilization + Denitrification



N In = Total Input + Net Mineralization

N Out = Total Loss + Harvested

- Specific-year weather plays a dominant role in dictating how much N leaves the field through either the loss pathways or harvesting
- But, weather has much less impact on overall N input

Detailed analysis in a paper by Ran et al. 2019 JAMES