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Ammonia Emissions Enhancements with Deep Learning CTM (Forward-Backward) and Remote-sensing Observations

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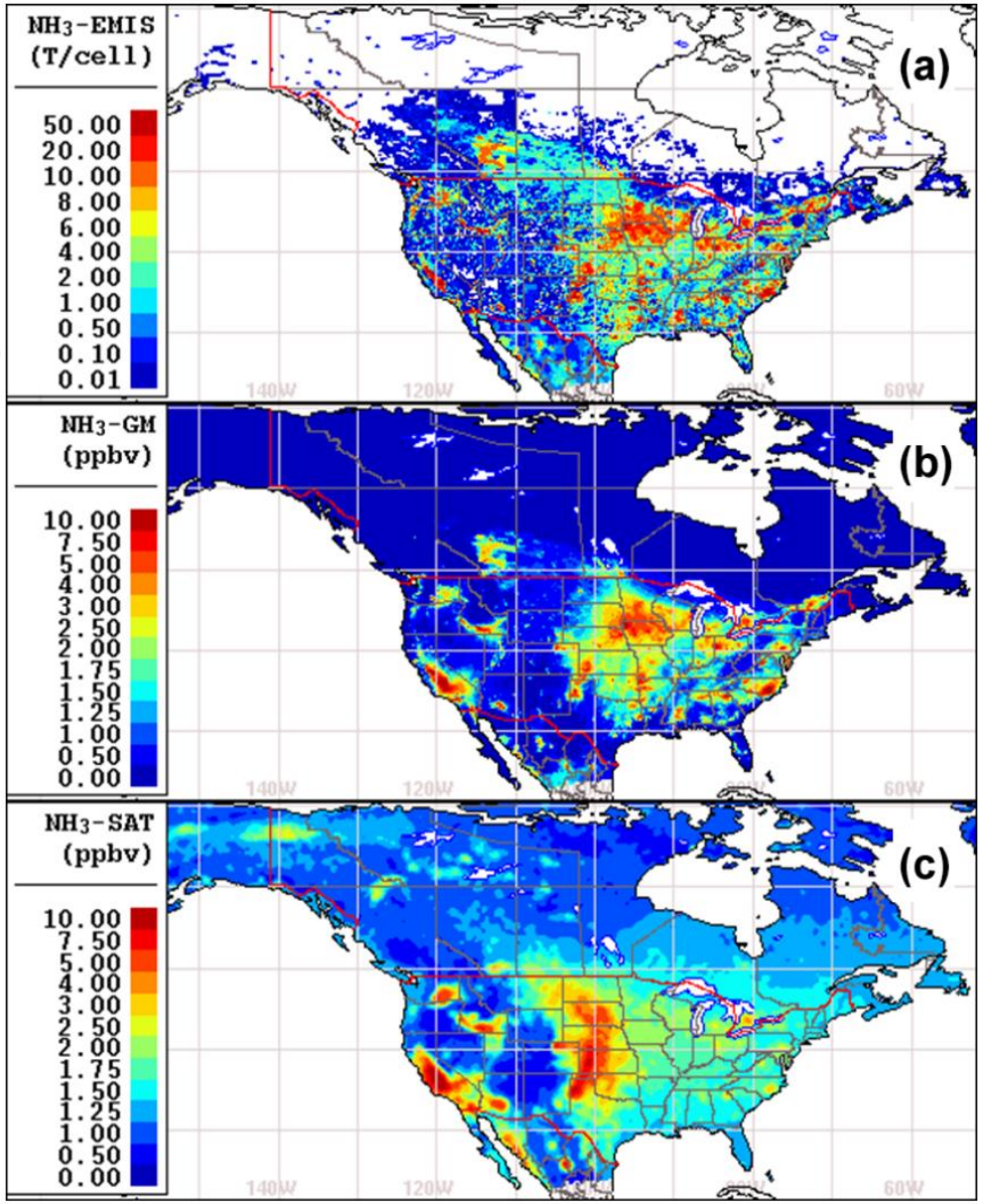
Motivation

- **NH_3 :** Animal manure, production, and Application of fertilizers
  - Short lifetime of NH_3 (τ = 0.5-5 days or less)
  - Deposited to the surfaces near its source with relatively high dry deposition.
  - Ecosystem eutrophication
- **NH_4^+** : Neutralization process of acid gases (H_2SO_4, HNO_3 and HCl) by NH_3 at the surface on $PM_{fine} \leq 2.5\mu m$
  - NH_4HSO_4, $[NH_4]_2SO_4$, $[NH_4]_3H[SO_4]_2$, NH_4NO_3, NH_4Cl,,,,
  - Role of degradation of visibility in the local area
  - Longer lifetime of NH_4^+ approximately 5~10 days
  - Ecosystem acidification from ammonium oxidation in the atmosphere
  - Sensitive spatiotemporal patterns by meteorology, events, and acid gases.
- **Top-down vs. Bottom-up NH_3 emissions are quite different**
  - Swine NH_3 emissions from Iowa and NC relatively overestimated?
  - Beef NH_3 emissions from Texas, Kentucky, and Nebraska are the main NH_3 in Central US

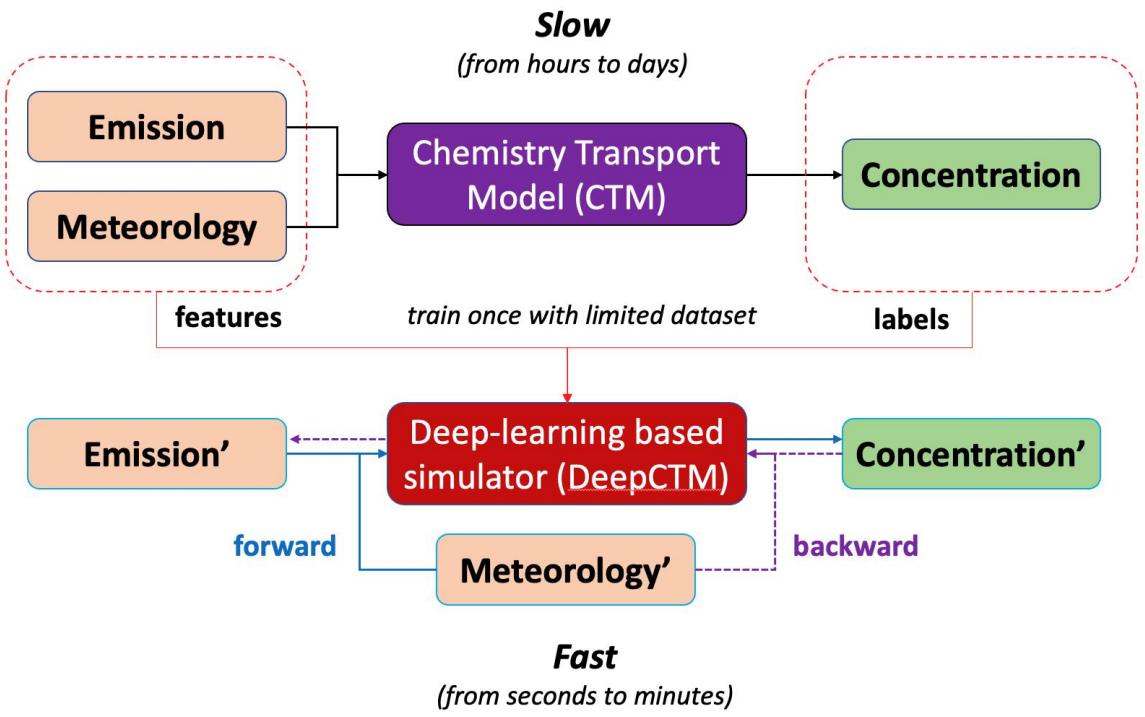


(Shepard et al., 2020)

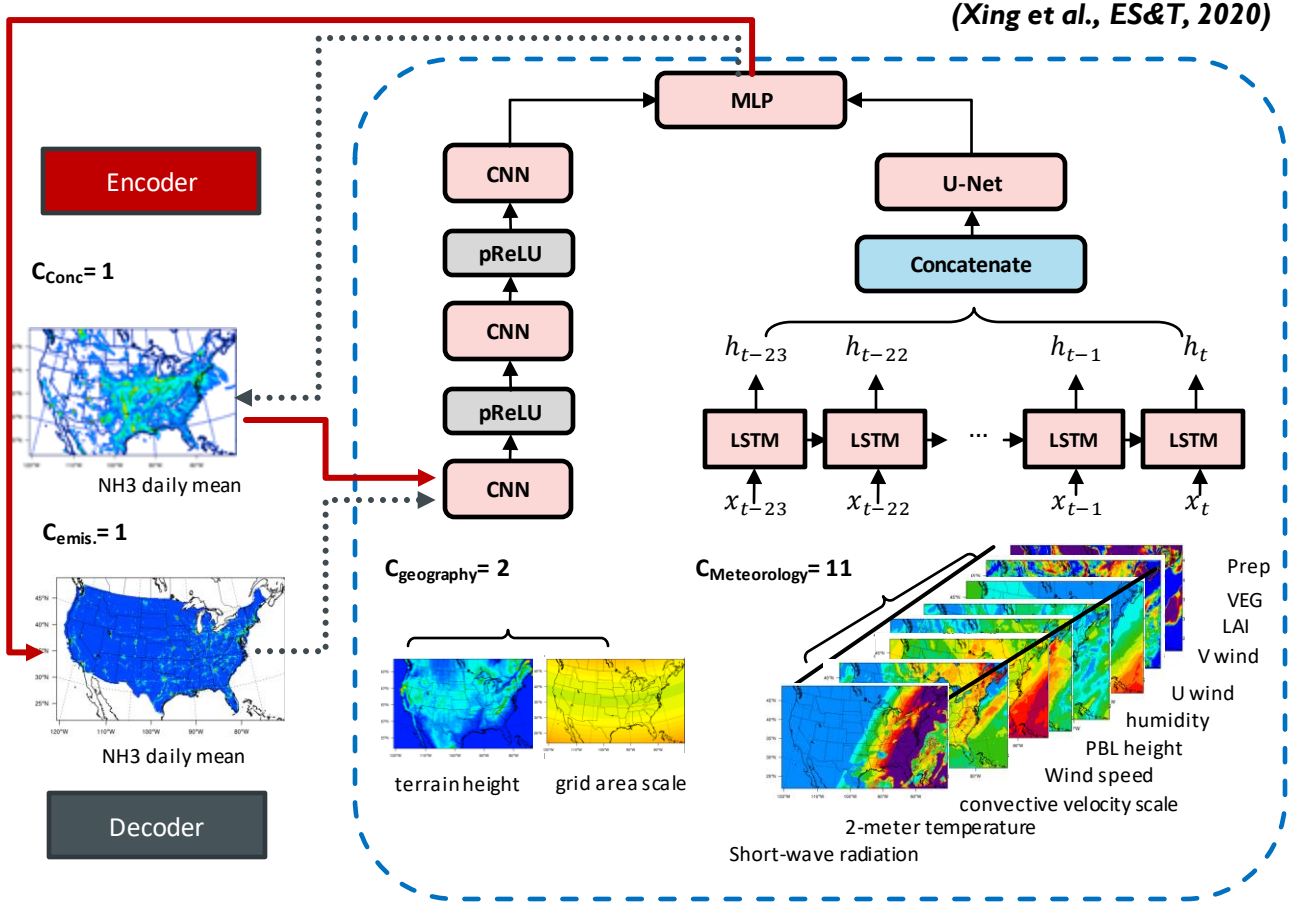
DeepCTM-VAE Applications with Observations

- **Objectives**
  - Bottom-up NH_3 Emissions Comparison against Top-down NH_3 Emissions
  - Understand the differences and identify the solution to enhance the bottom-up Inventory
- **Deep-Learning Chemical Transport Model (Decorder)**
  - Development of DeepCTM (forward) based on the CMAQ CONUS12 simulation to understand the non-linear relationship between emissions and air quality
- **Variational AutoEncoder (VAE) Applications with CrIS Remote-sensing Observations**
  - Development of VAE (Backward) over the U.S.
  - Data Assimilation: Surface NH_3 concentrations based on the CrIs remote-sensing and monitoring observations.
  - Development of top-down NH_3 emissions inventory over the U.S. and compare them against the bottom-up emissions (USEPA NEI)

DeepCTM: Deep-Learning CTM



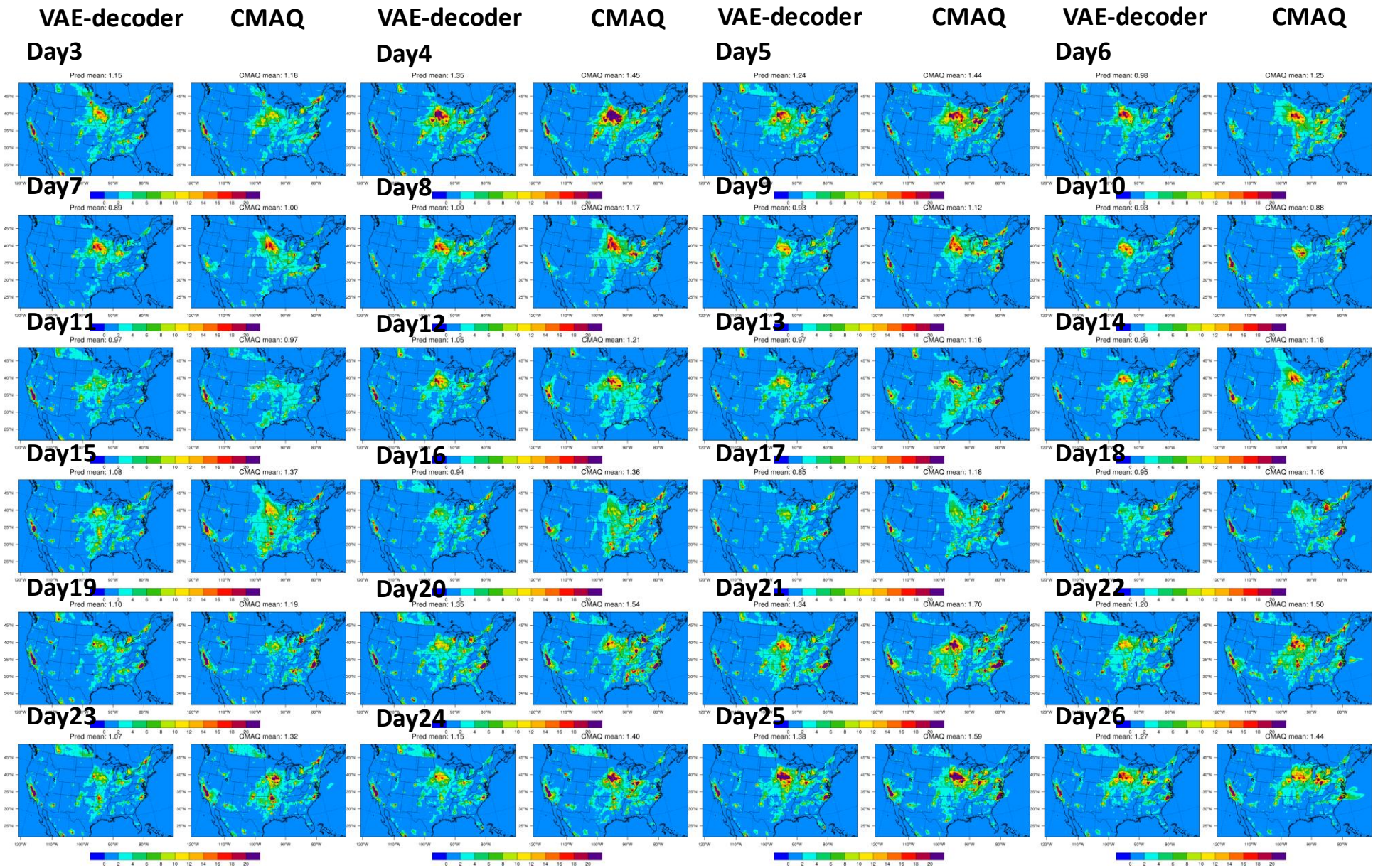
(Xing et al., ES&T, 2020)



- Study the impacts from the inputs (Emissions, Meteorology, Concentrations, and Time)
- Computationally highly efficient (<2 minutes) to execute DeepCTM once the training of DeepCTM is complete

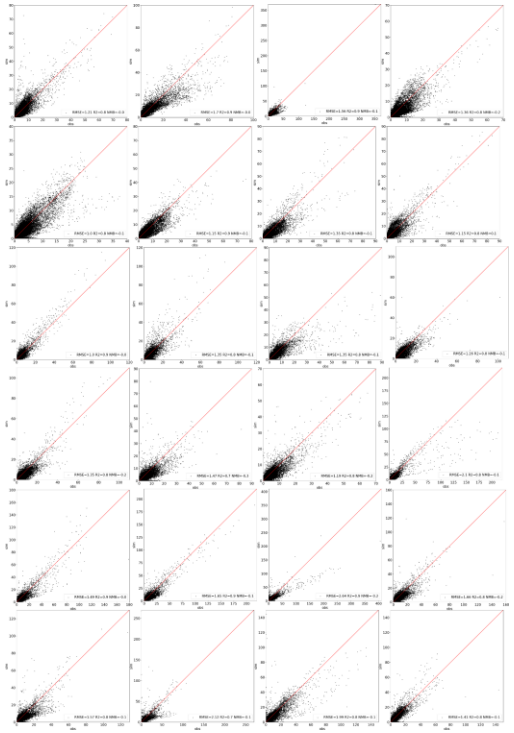
UNet: capture the cross-space interaction
LSTM: capture the temporal variation

Performance of VAE-decoder (forward: emis->conc)



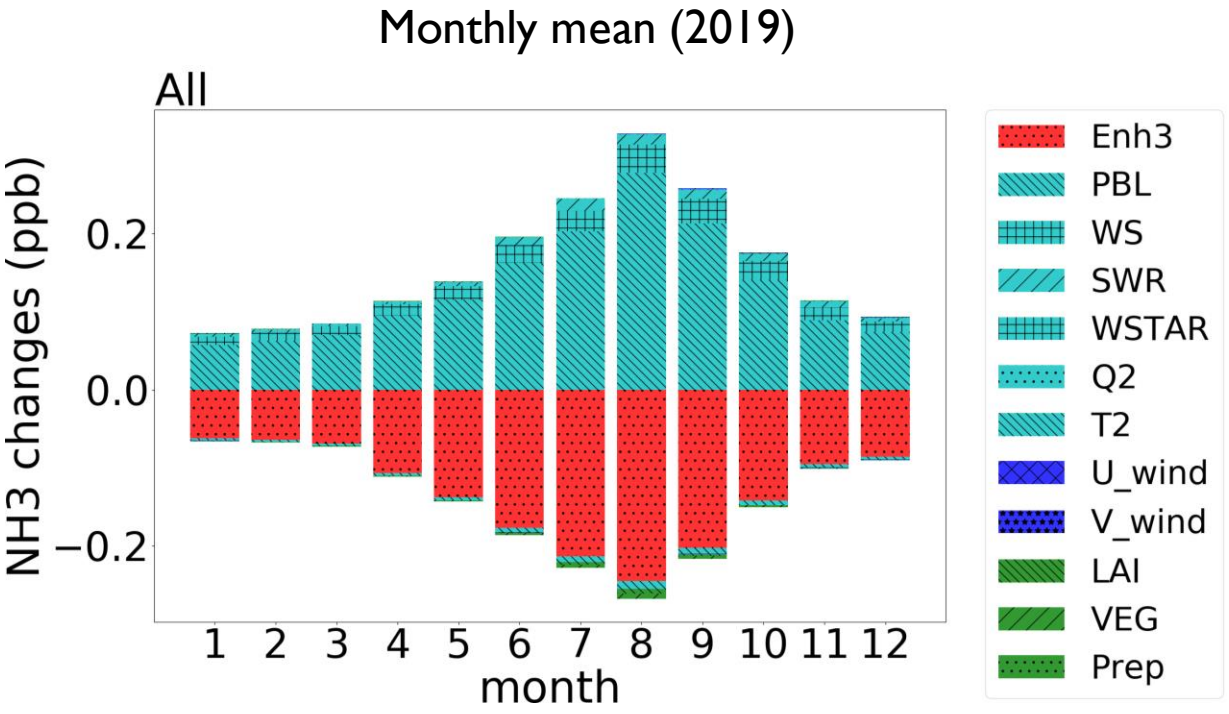
Daily NH_3 (ppb)

June 2020: Day 3-27



RMSE<3.0; R2>0.8

The Feature Impacts on NH_3 Concentrations

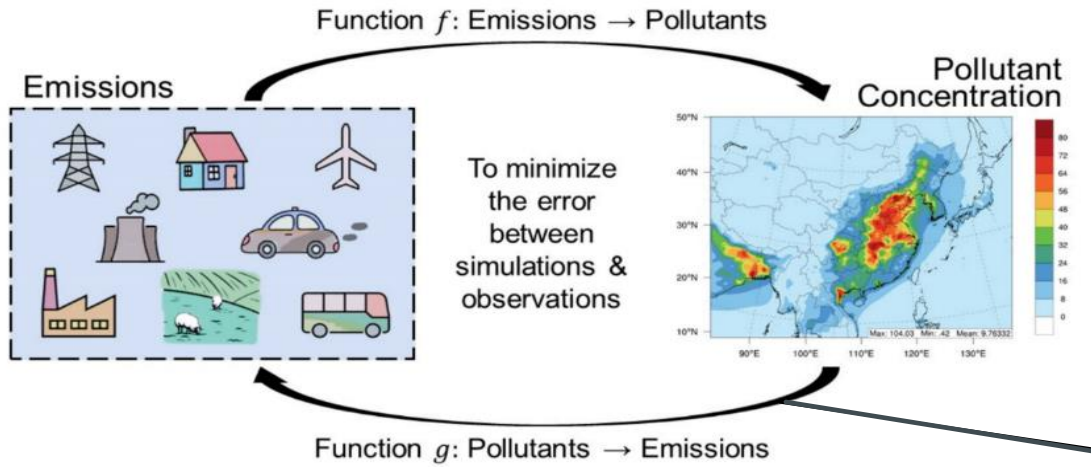


modulating each feature one-by-one

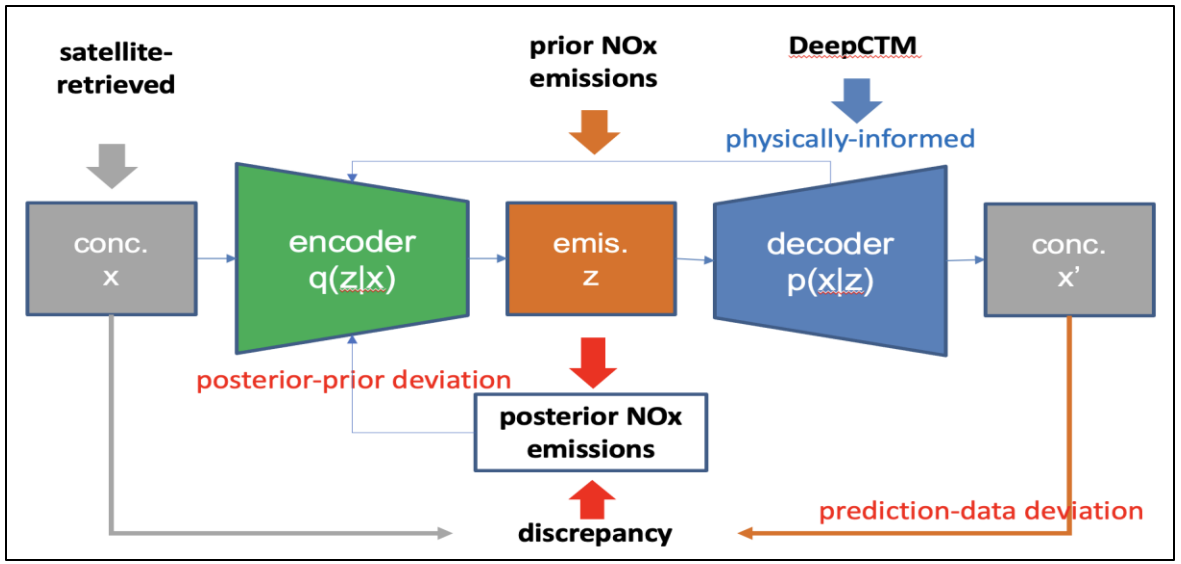
- **T2**: -2K
- **others**: -20%

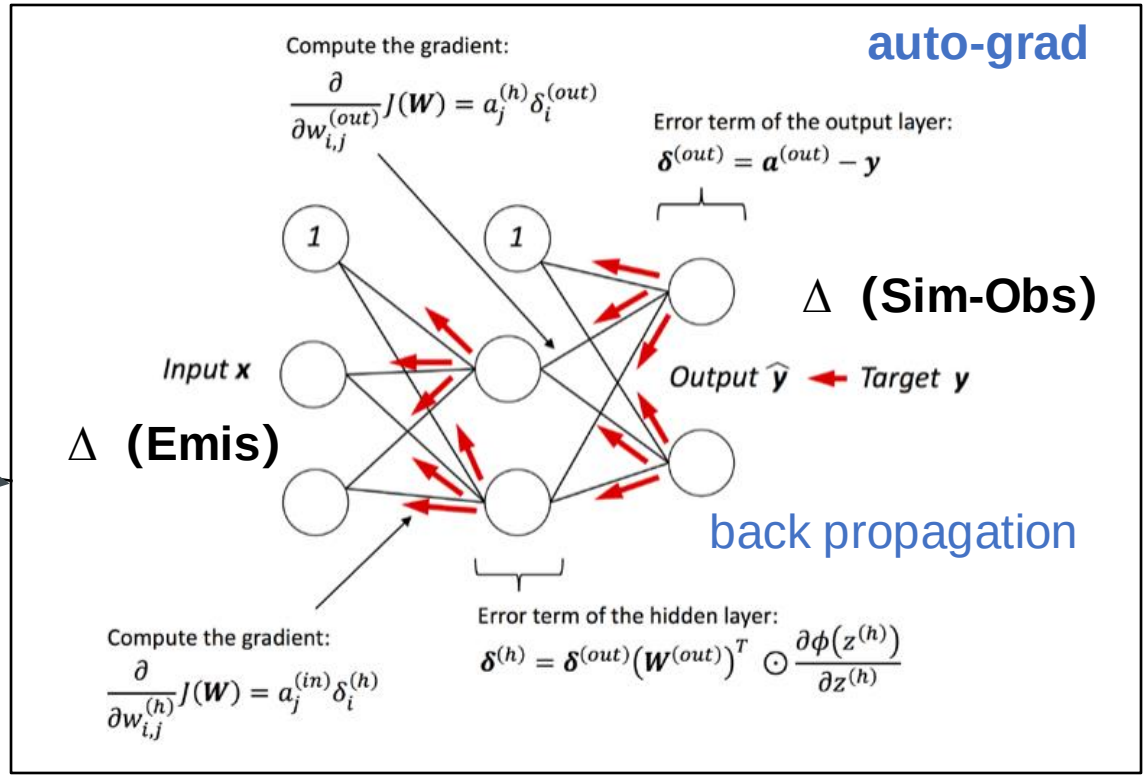
- NH_3 concentration is contributed by NH_3 emissions (Enh3) and initial NH_3 condition (Inh3)
- **Met variables** will modulate the NH3 concentration sensitivity to NH3 emissions
- DeepCTM exhibits high efficiency in identifying the dominant factor to photochemical formation

Variational AutoEncoder (VAE): Top-down Emissions



Variational AutoEncoder (VAE) *(Xing et al., ES&T, 2022)*





- Based on emission-concentration relationship from DeepCTM, we can accurately estimate the differences of emissions
- Because of the in-depth knowledge over various impactors (emissions, meteorology, initial conc.), we can proportionally correct the emissions only.

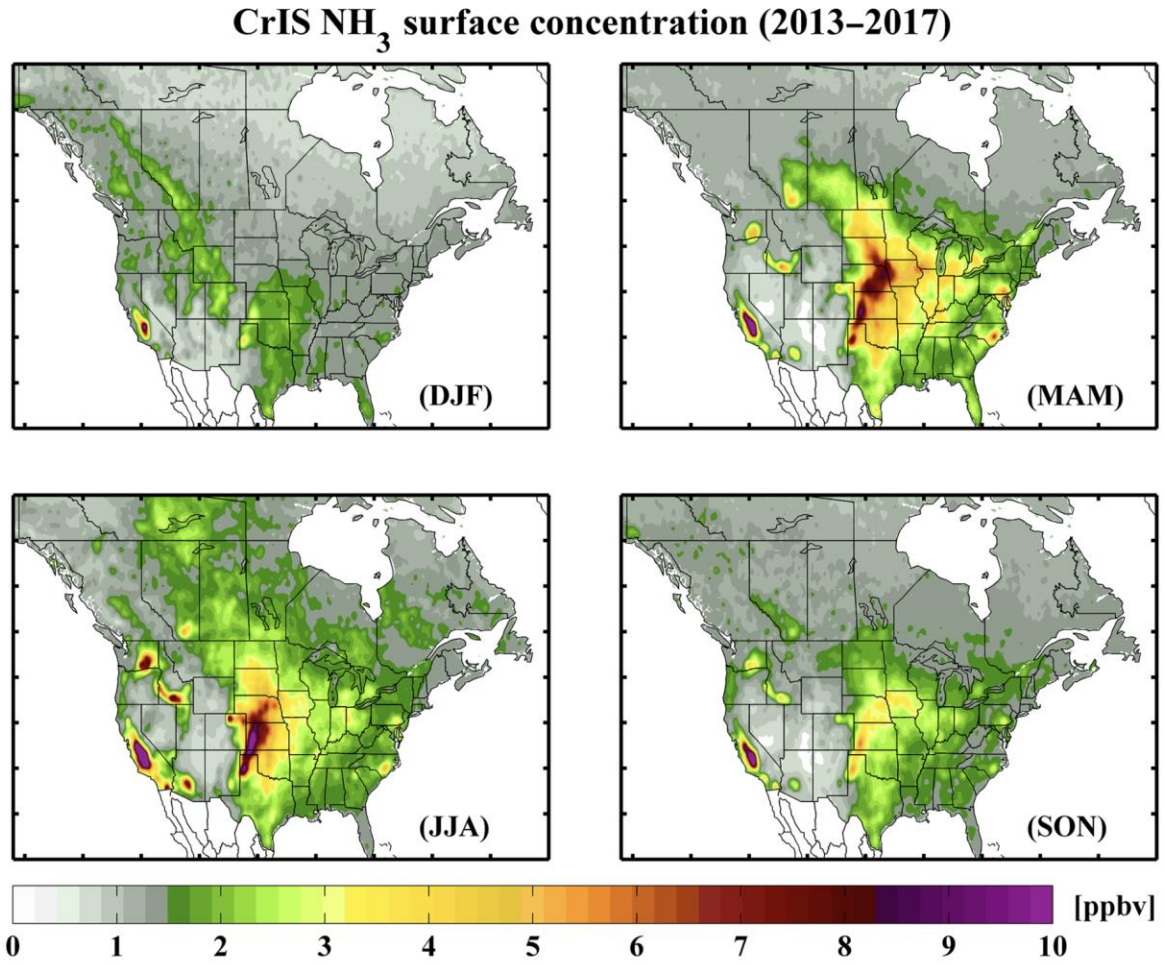
CrIS Fast Physical Retrieval (CFPR) Algorithm for NH_3

(Shepard et al., 2020)

	Satellite	Spatial Resolution (km^2)	Spatial Coverage	Temporal Coverage	Retrieved Quantity	Comments
NH_3	Cross-track Infrared Sounder **(CrIS)** (2012-2038)	14 (diameter)	Global	Twice a day CrIS-SNPP @ ~13:30 (**day**) ~1:30 (night) CrIS-NOAA20@ ~14:25 (**day**) 2:25 (night)	Profile level volume mixing ratio values (ppbv)	• Limited vertical resolution • Version 1.6 • Shephard et al., ACPD, 2020 • CFPR CrIS SNPP : May 2012 to May 2021 • CFPR CrIS NOAA : March 2019 to present

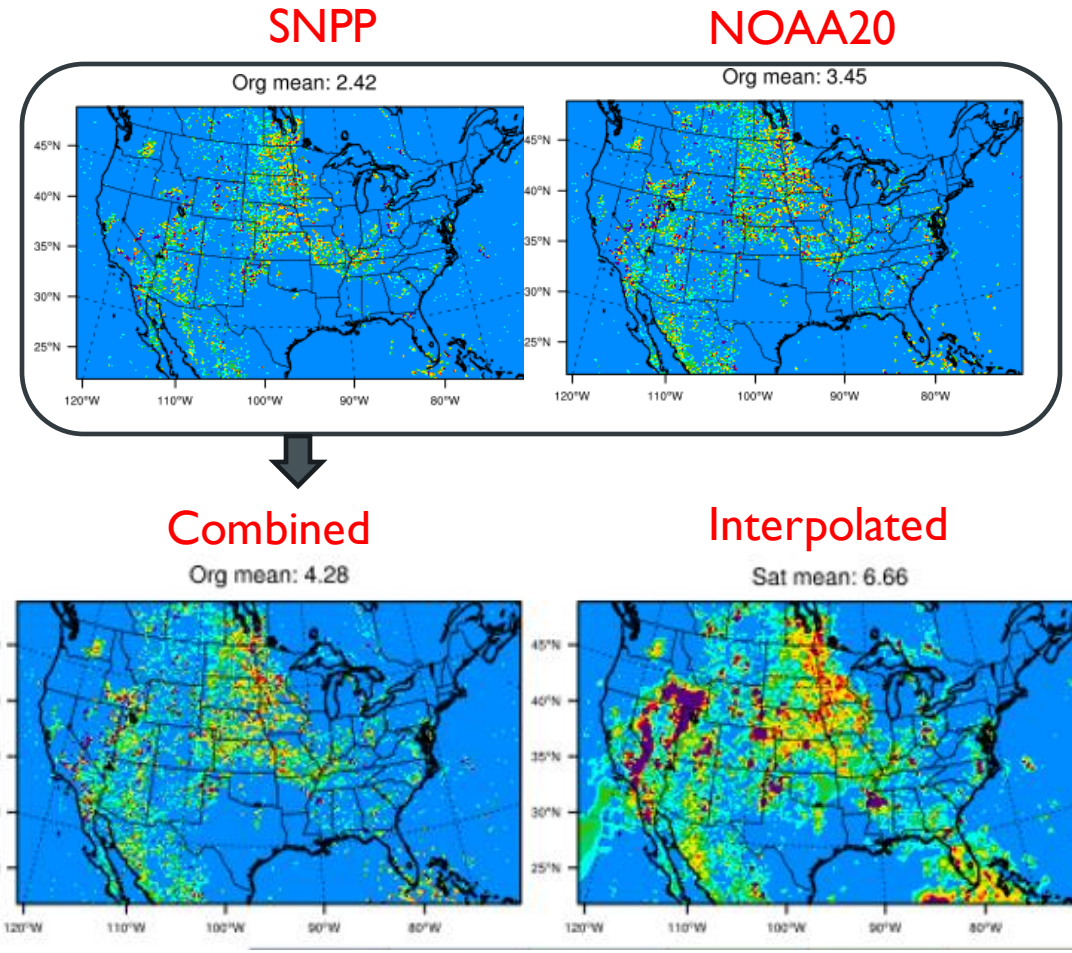
- CrIS is most sensitive to NH_3 between 950 and 700 mb (~0.5 to 3 km) with minimum 0.3 ppbv detectability
  - Not equally sensitive in the vertical and varies from profile-to-profile
  - Surface retrieved values are driven by sensitivity in the boundary layer
- CFPR has been validated with U.S. AMoN (Ammonia Monitoring Network) and other ground–based FTIR (Fourier Transform Infrared) spectroscopy observations to determine the errors
  - AMoN: CrIs ~15% higher with a good correlation of r ~ 0.8 and a slope of 1.02
  - FTIR: CrIs ~30% higher (SD~40%)
- Applications to data assimilations, data fusion and model-based emissions inversions for Confined Animal Feeding Operation (CAFO) facilities located remotely.

NH_3 CrIs CFPR Spatiotemporal Patterns

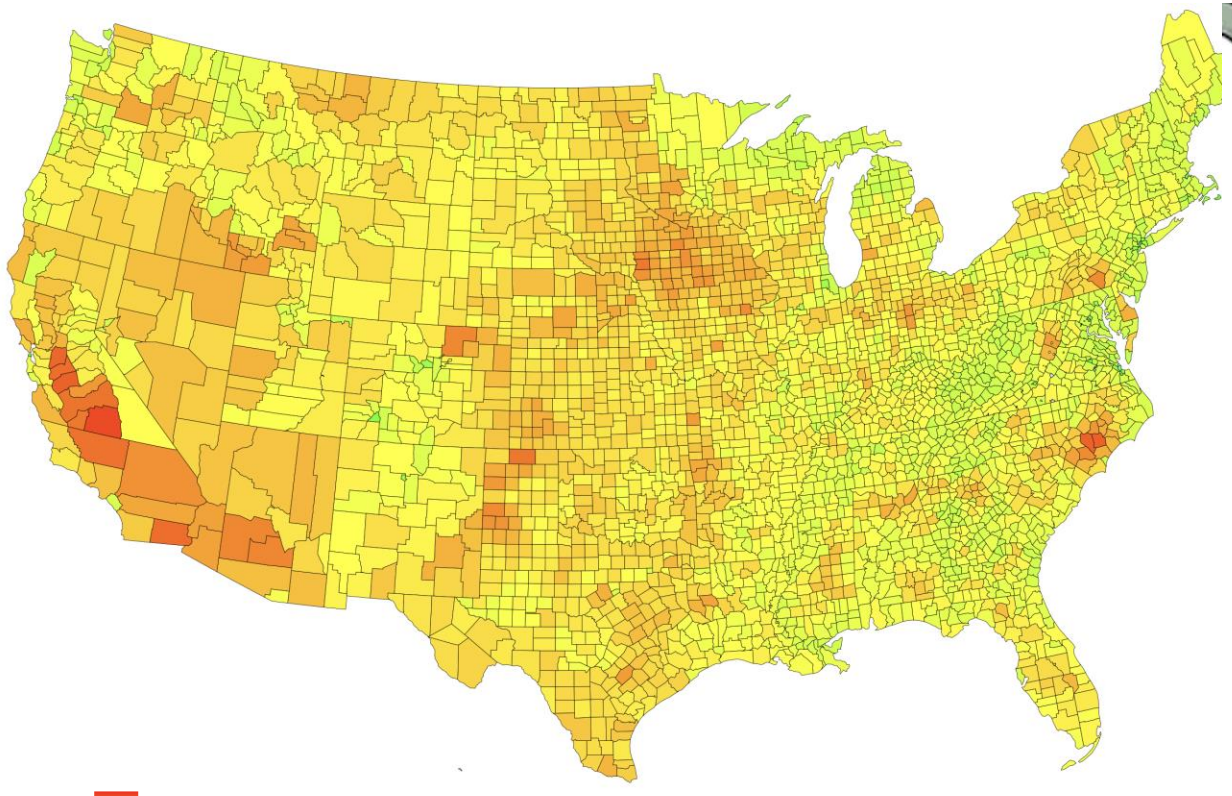


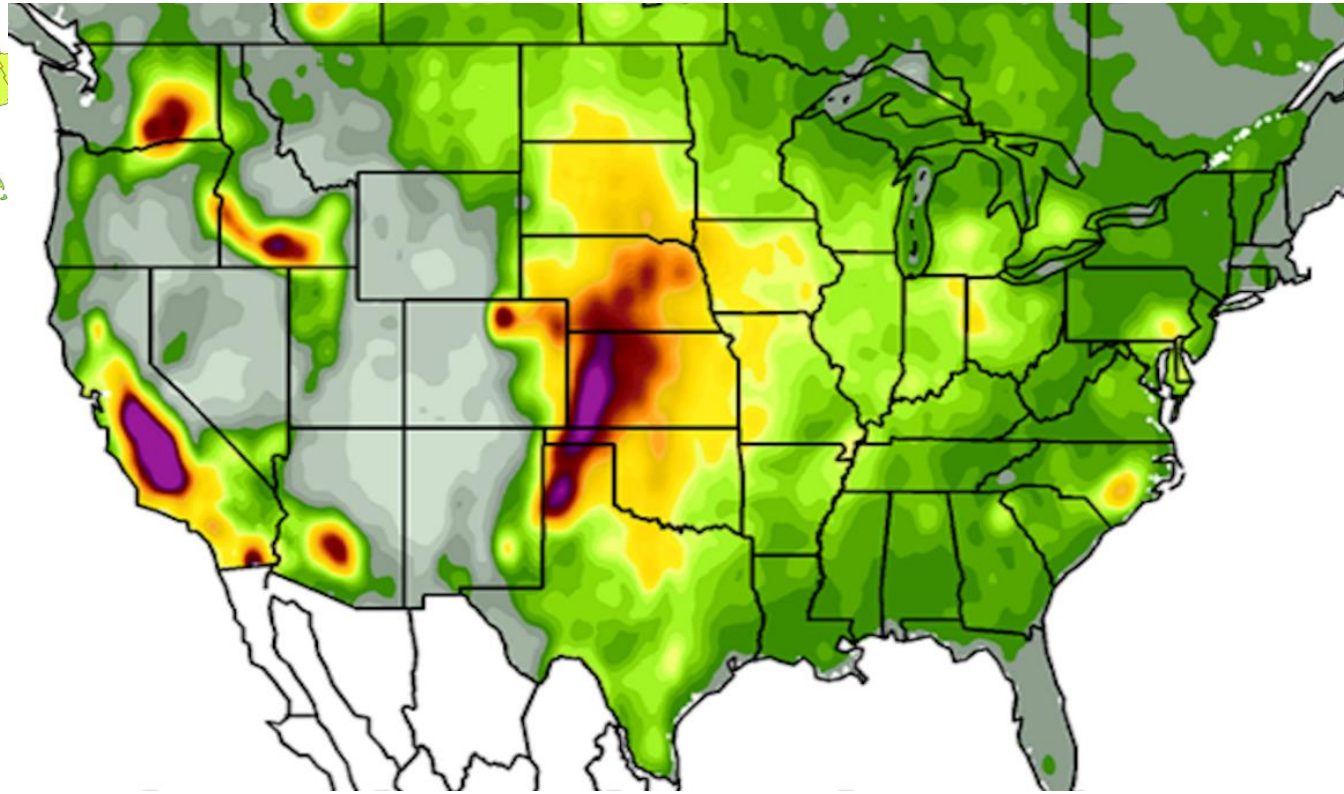
(Shepard et al., 2020)

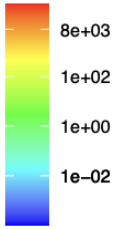
NOAA Satellites Surface NH_3 Measurements



2017 NEI NH_3 Emissions from Agricultural Sector

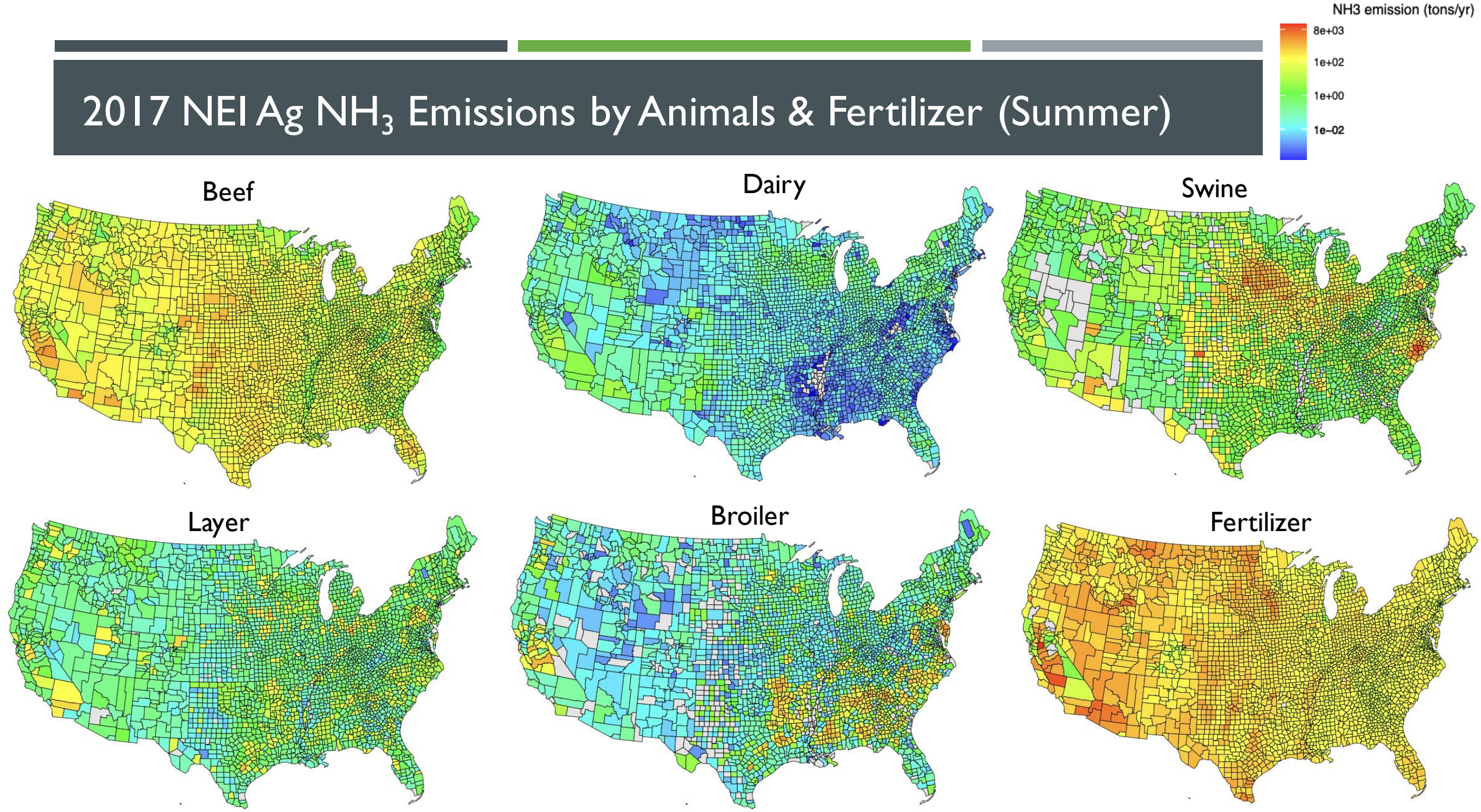




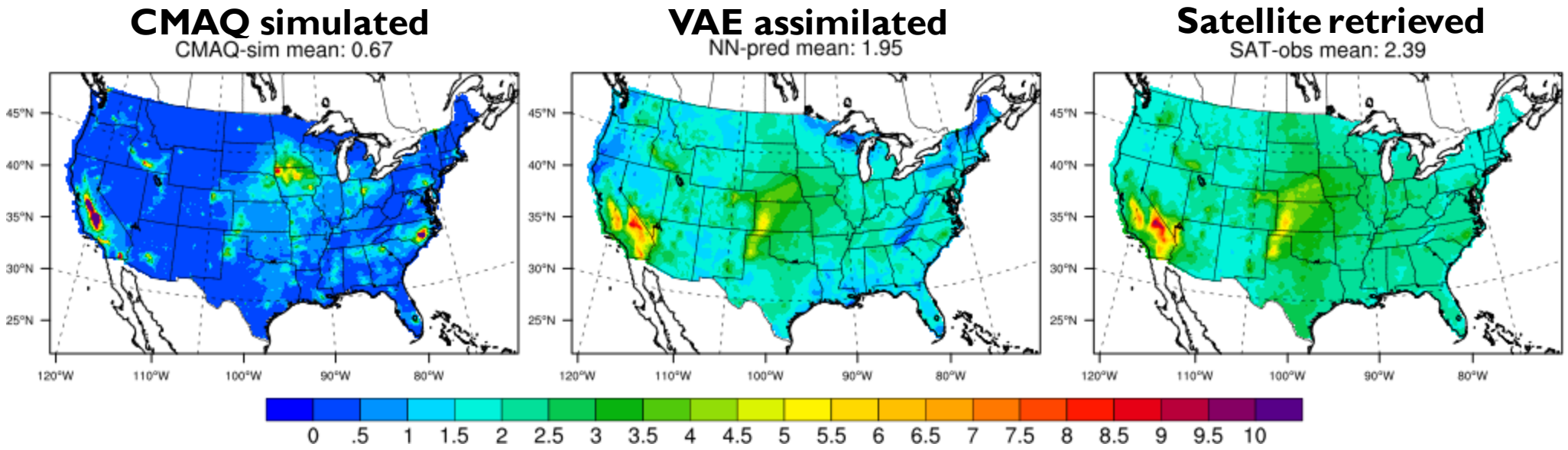


Agricultural Sector: Fertilizer + Animals (Beef, Dairy, Swine, Broiler, Layers, Sheep, Horses, and Goats)

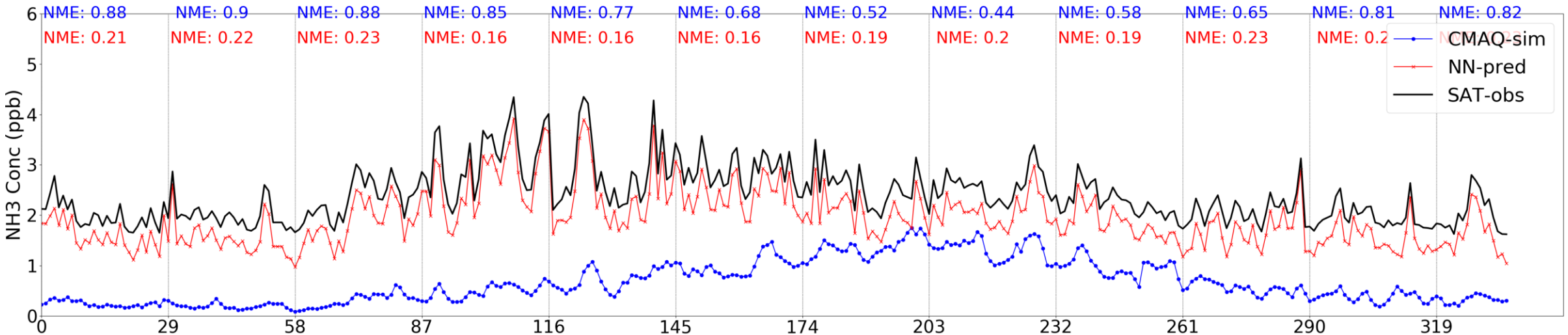
2017 NEI Ag NH_3 Emissions by Animals & Fertilizer (Summer)



Performance of VAE-assimilation (2019)

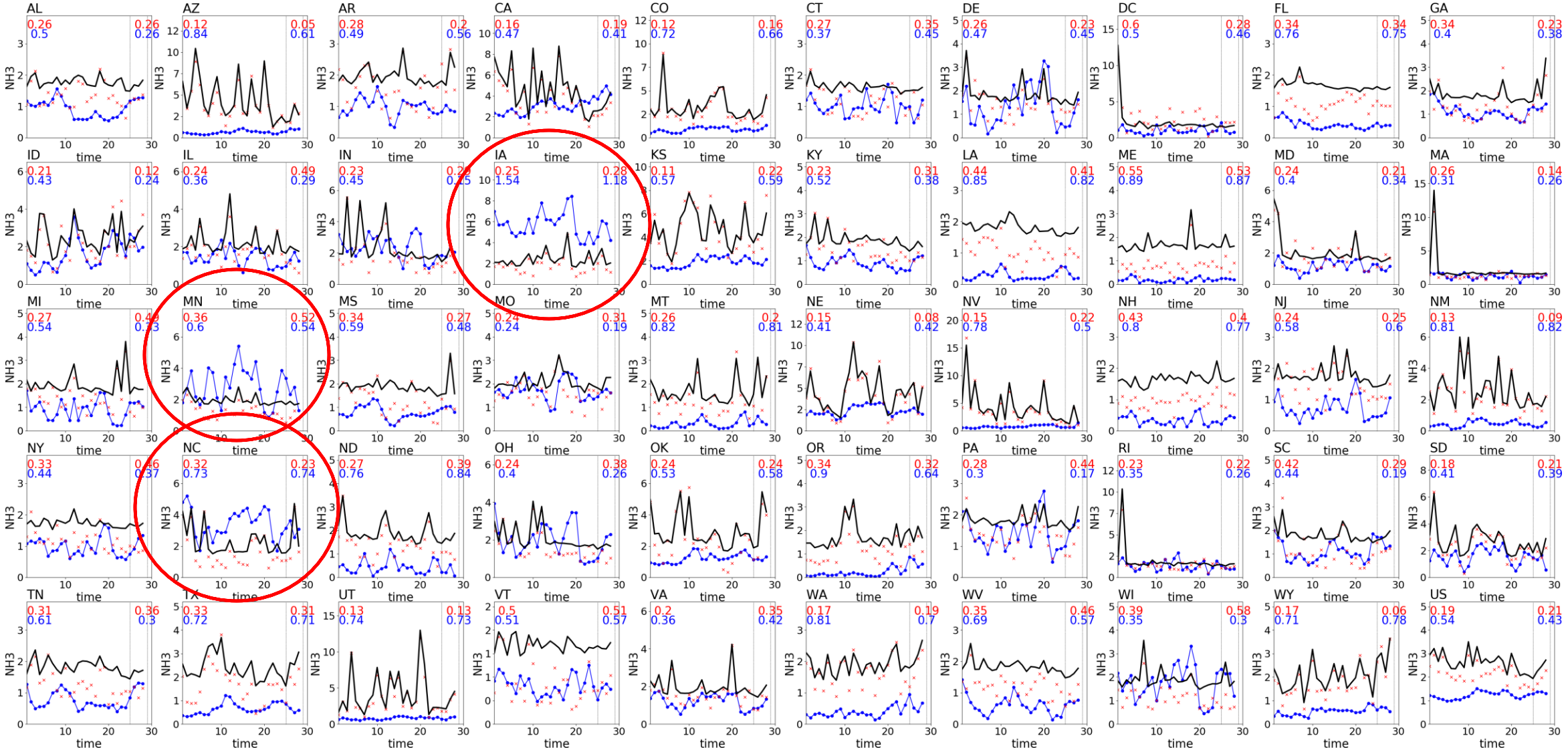


Annual mean surface NH_3 concentration (2019)

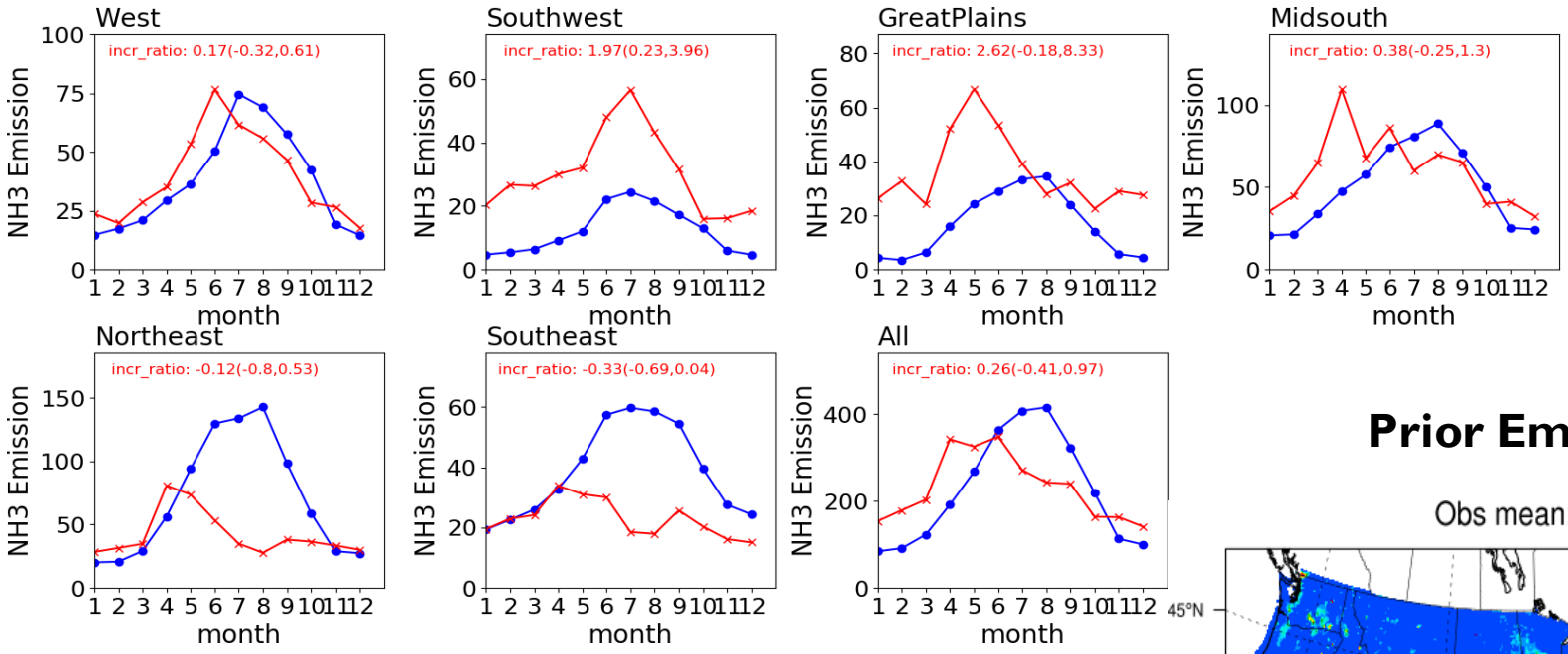


Performance of VAE-assimilation (June 2019)

Blue: CMAQ Simulation
Red:VAE-assimilation
Black: CFPR Satellite

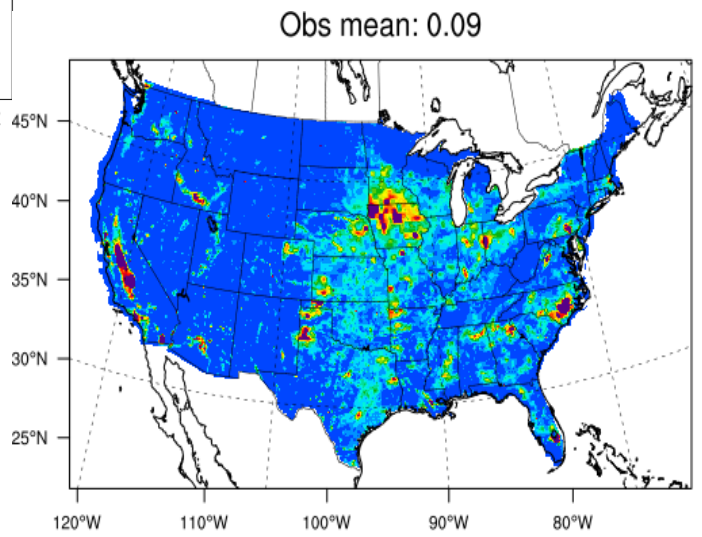


NH_3 Emissions Comparison (2019)

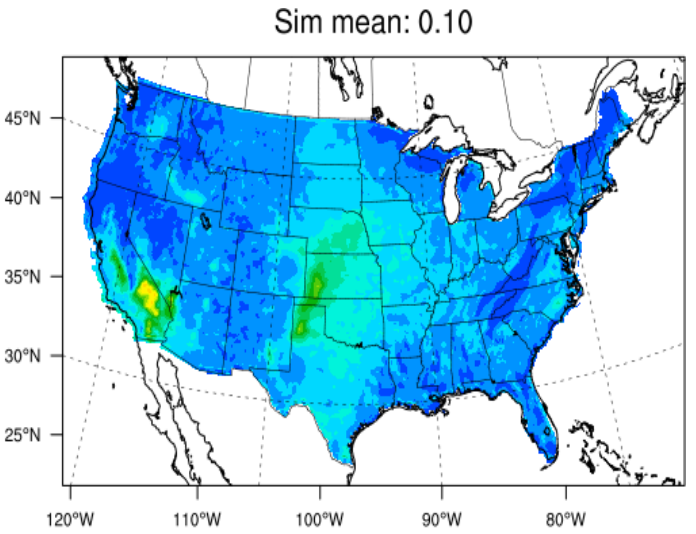


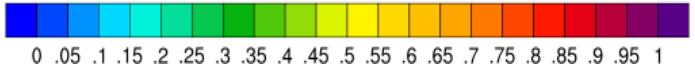
- Indicating that the significant differences over the Great Plains and Southwest regions

Prior Emissions



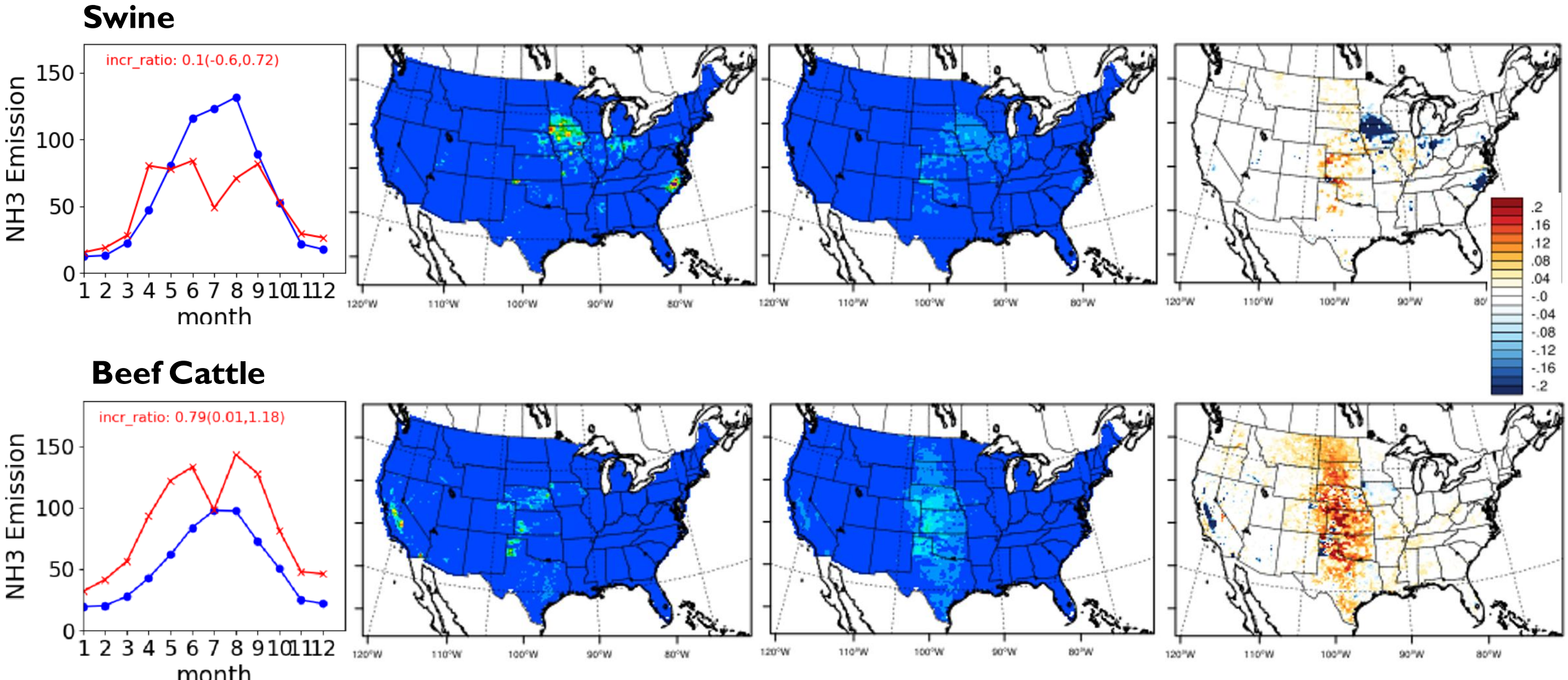
Posterior Emissions





- Important to utilize the spatial and temporal coverages from the CrIs NH_3
- **<u>Relatively</u>** underestimated NH_3 from Beef vs overestimated NH_3 from Swine

Sector-level NH_3 Emissions Comparison (2019)



Findings

- A significant amount of surface NH_3 concentrations changes by location and time/dates
- Requires a better spatiotemporal representation of NH_3 from livestock wastes
- DeepCTM/VAE performed well in capturing the spatial and temporal differences of NEI Livestock Waste NH_3 against the observations
- Identified the sector-level (anima-specific) NH_3 differences for the calibrations of animal-specific NEI Emissions from the Farm Emissions Model used in NEI development
- Swine and Beef Cattle shows the lack of spatiotemporal representations
  - **Swine**: *Overestimations* of NH_3 over the areas in Iowa and NC (most swine-dense area)
  - **Beef**: *Underestimation* of NH_3 over the areas in TX, KY, CO, NE, SD, ND, and MT, while the *overestimation* occurred over CA.
    - Regional farm management practices input to the FEM need an update to address this issue.

Thank you!

ACKNOWLEDGEMENT

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- USEPA
- Korea National Institute of Environment Research