Validating modeled atmospheric deposition timeseries with observed long-term records across the U.S.

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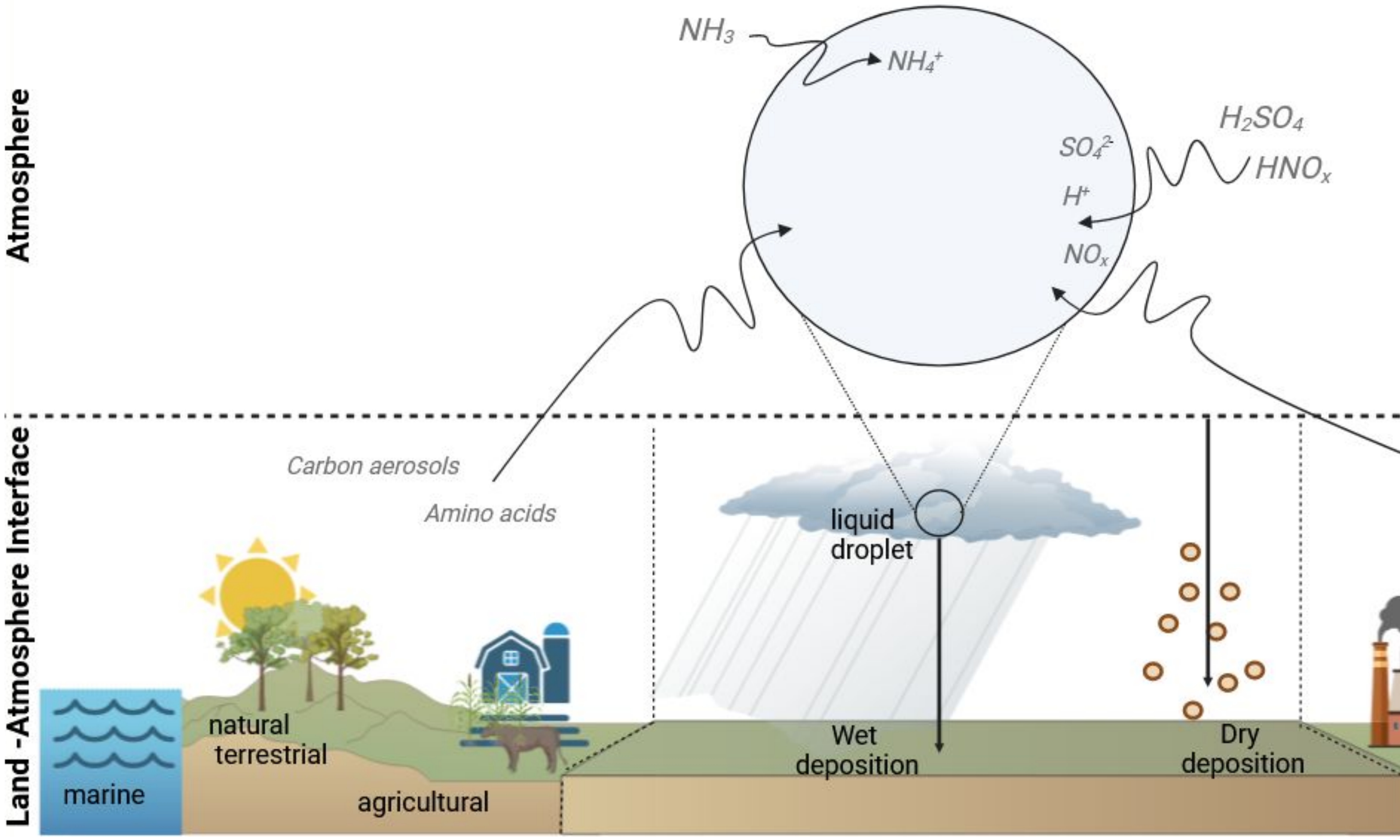
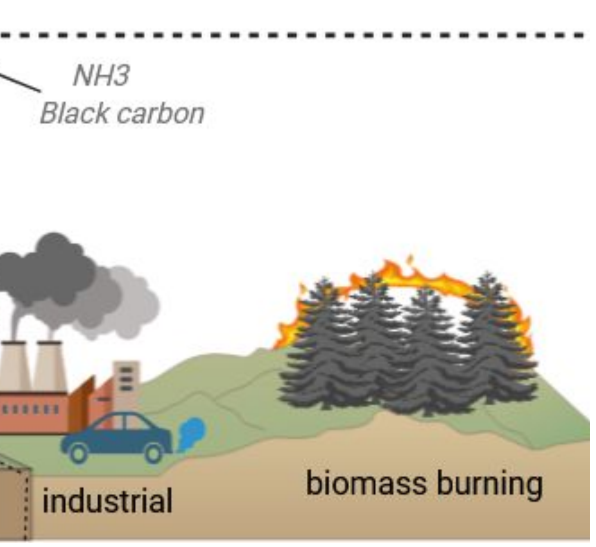
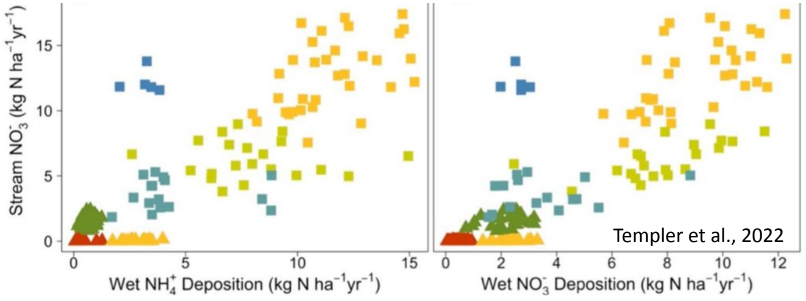
Atmospheric deposition is a main mechanism for the loss of aerosols and chemicals back to the land surface





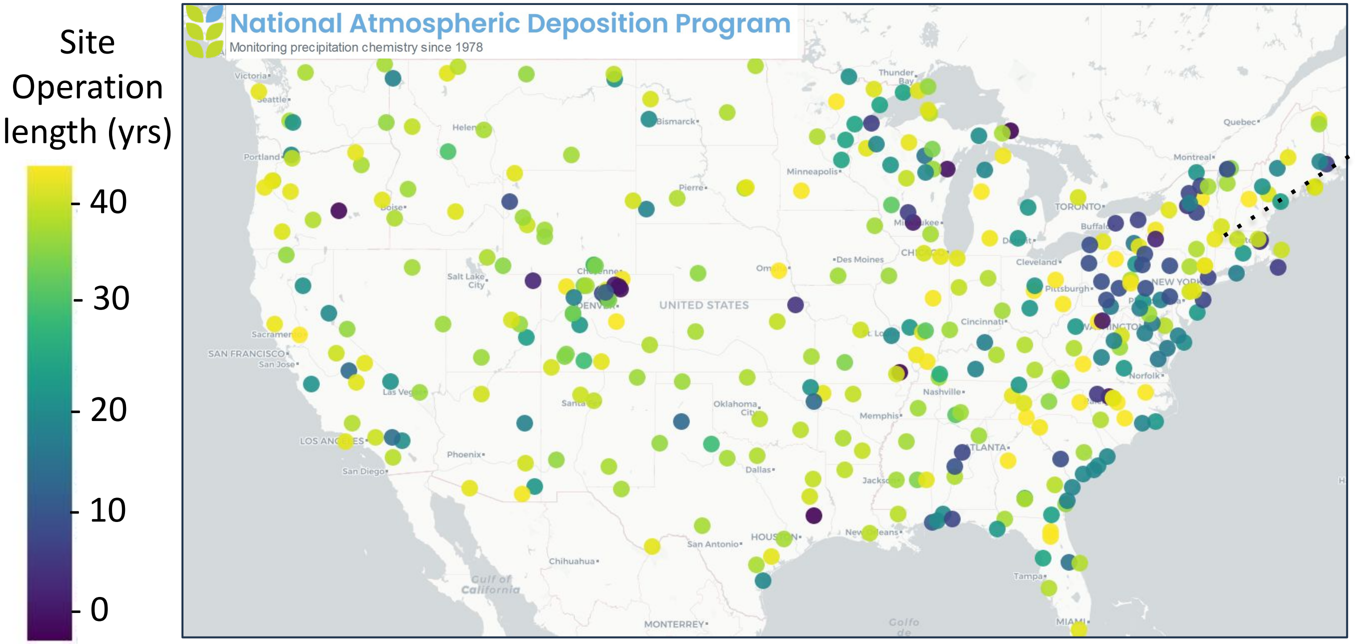
Wet deposition chemistry influences biogeochemical cycles



created in BioRender

Long-term records of wet deposition

- The National Atmospheric Deposition Program National Trends Network (NADP NTN) provides a long-term record of precipitation chemistry
- Collect weekly composite deposition samples from 391 sites across the U.S.
- Records extend back to the 1980's



pH

Ca^{2+}

Mg^{2+}

Na^{+}

K^{+}

SO_4^{2-}

Cl^{-}

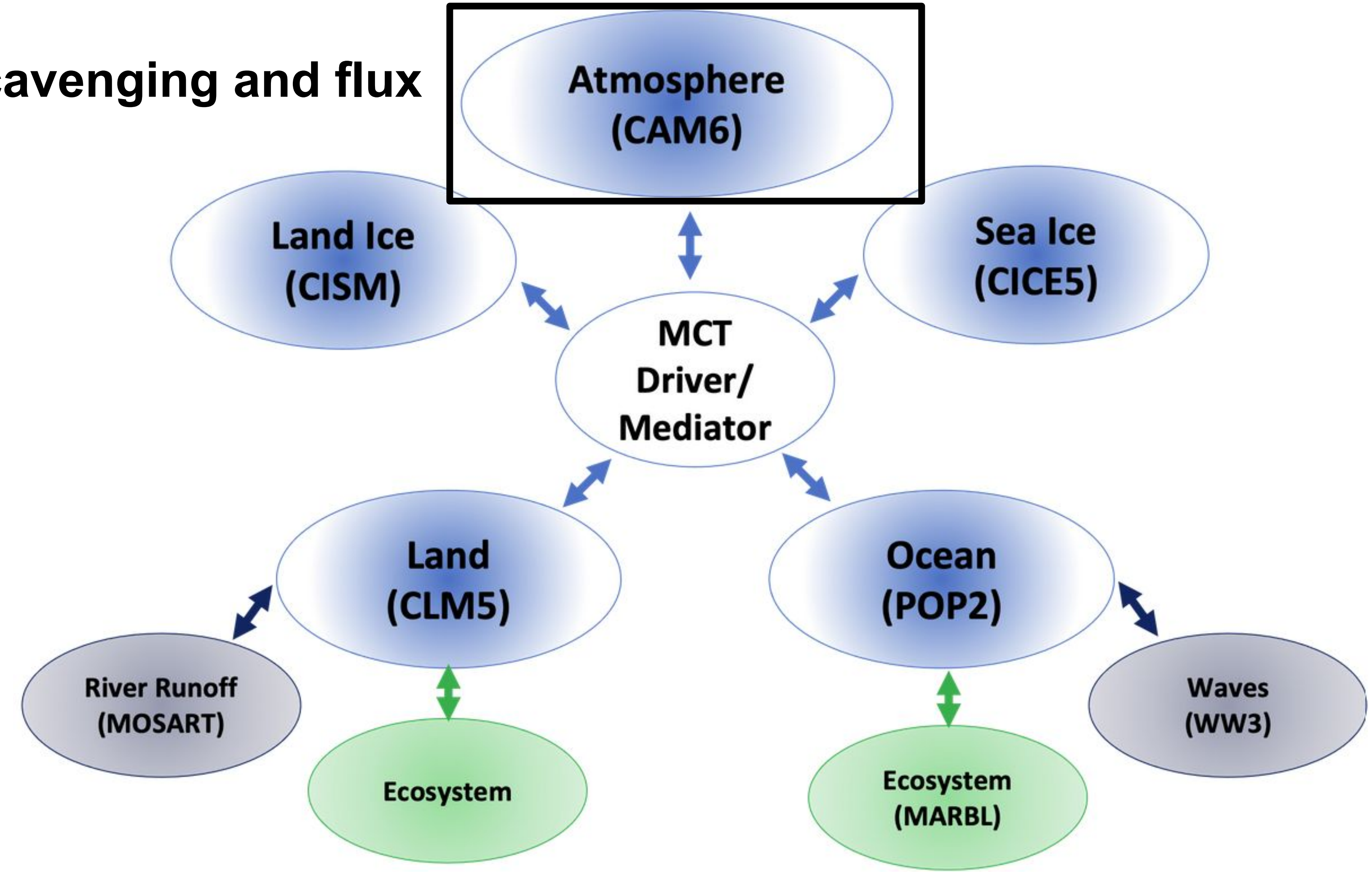
NO_3^{-}

NH_4^{+}

Samples are **wet-only composite** collected on ~7-day window

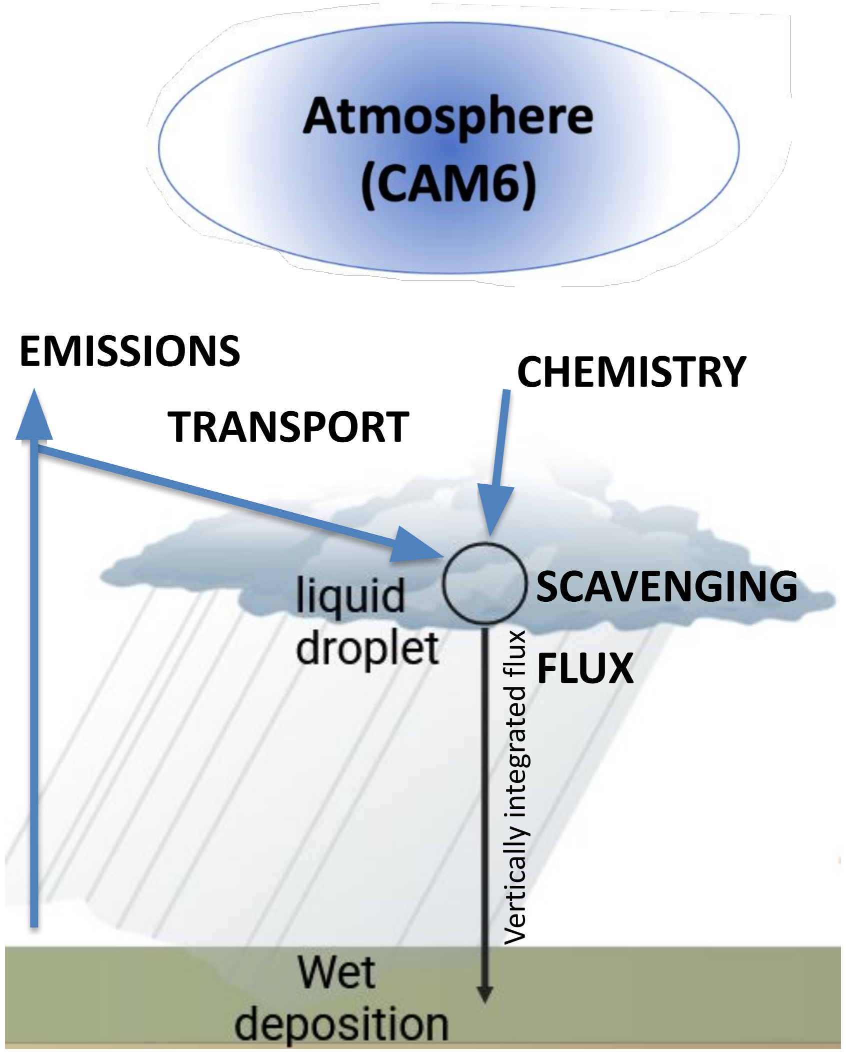
Modeled wet deposition chemistry and flux in CESM

scavenging and flux

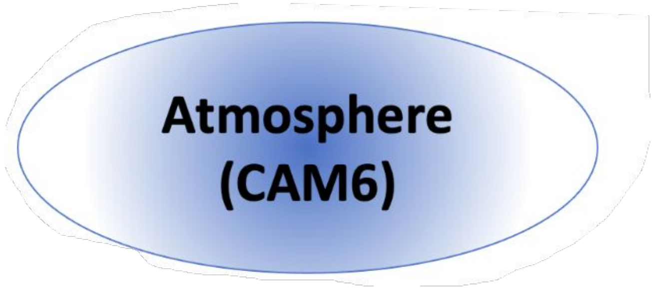


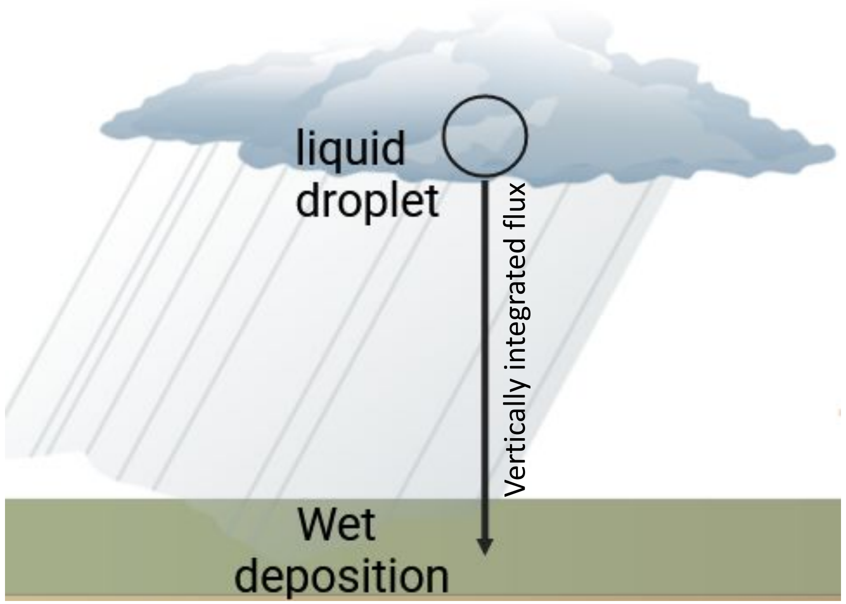
https://ncar.github.io/CESM-Tutorial/notebooks/intro/components.html

Wet deposition parameterization in CAM6



Wet deposition parameterization in CAM6



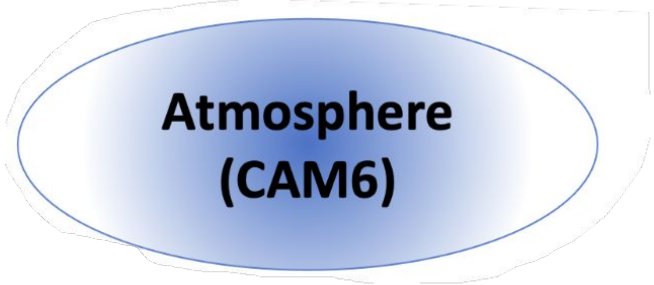


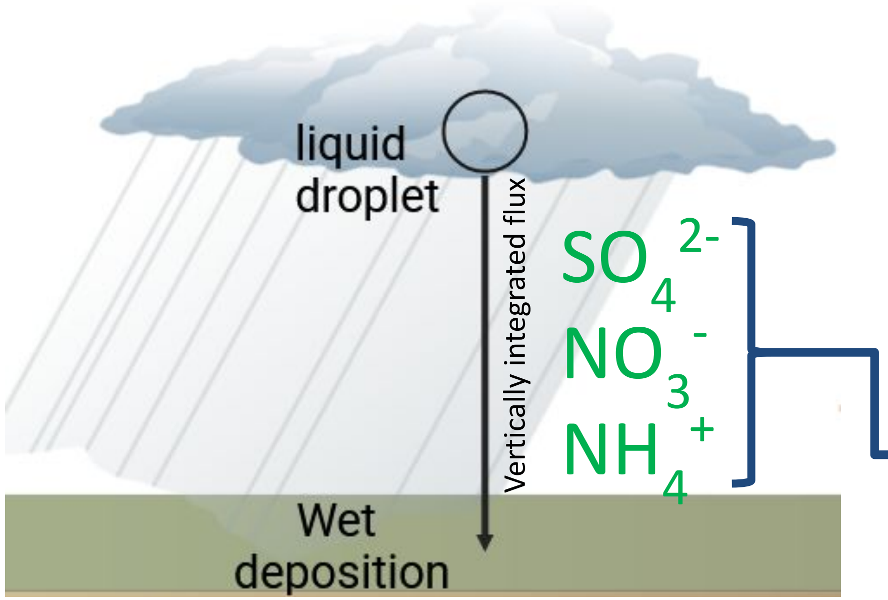
- Considers in-cloud and below-cloud scavenging rates and solubility factors of aerosol and chemical species

- Wet removal is modeled based on a simple first order loss process and effective Henry's Law
    - *solubility factor * scavenging coefficient * precipitation rate*
    - *solubility of gas is determined by Henry's Law*
    - *varies based on particle size*

References: (Barth et al., 2000, Neu and Prather 2012, Lamarque et al., 2012)

Wet deposition parameterization in CAM6





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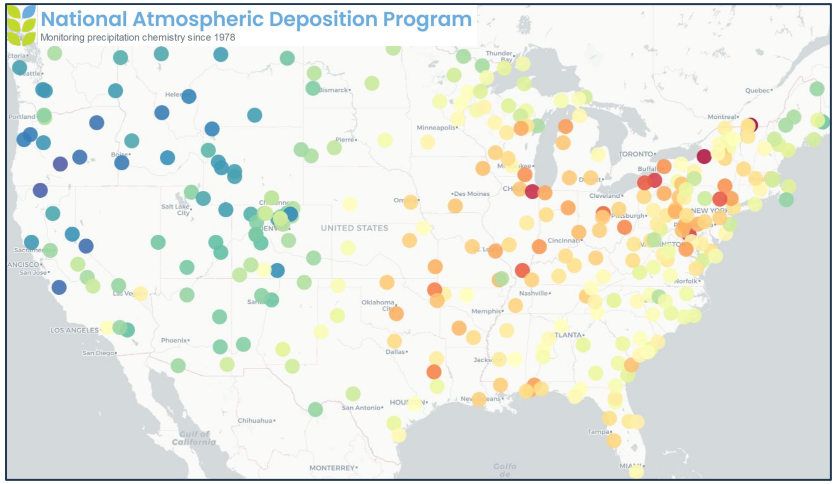
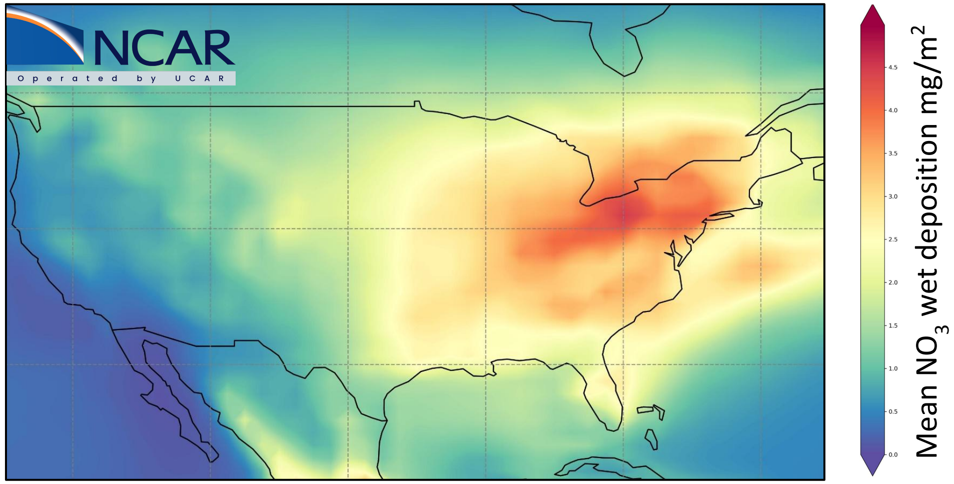
Previous validation of wet deposition modeled outputs is limited

Objective: assess the accuracy of CAM6 modeled wet deposition over CONUS

Approach: pair CAM-chem modeled and NADP observed wet deposition records of SO_4^{2-}, NO_3^-, and NH_4^+ from 2002-2022





Analyses:

(1) identify potential sources of error between modeled and observed solutes
(2) determine where modeled deposition parameters perform acceptably

Global model run of CESM2 & CAM6

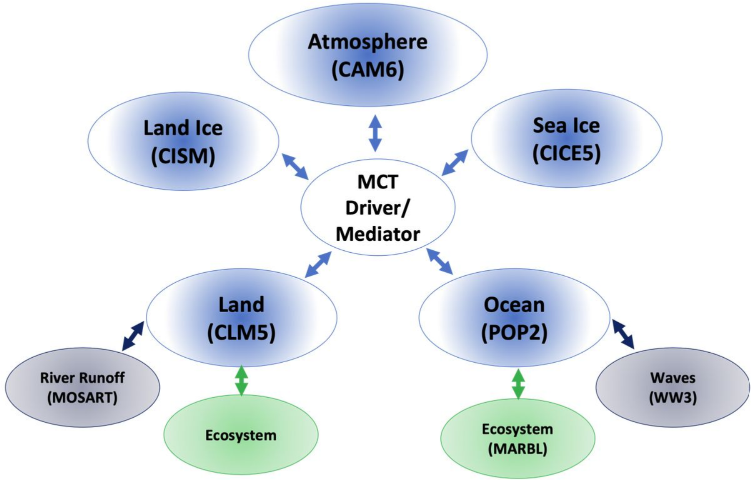
- CESM2.2 CAM-chem as Boundary Conditions
  - DOI: 10.5065/XS0R-QE86
- Full chemistry 2002-2022
- $0.92^{\circ} \times 1.25^{\circ}$ horizontal resolution
- 32 level vertical resolution
- MOZART T1 Chemistry (Emmons et al., 2020; Tilmes et al., 2019)

•Specified dynamics: MERRA2 nudged at 10%

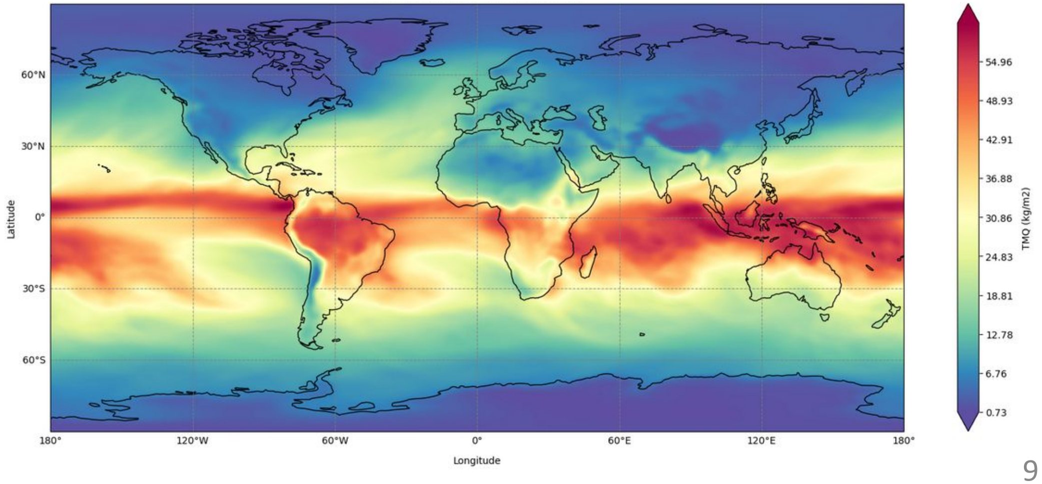
•Emissions:

- Anthropogenic – CAMS (Granier et al., 2019)
- Fire – QFED (Darmenov et al., 2015)
- Biogenic – online MEGAN scheme (Guenther et al., 2012)

•Output: daily averages



CAM-chem Total Precipitable Water, January 2002



Merging modeled and observed wet deposition

1) Unit conversions

Model $\frac{kg}{m^2}$ → $\frac{mg}{m^2}$ ← ***Observed*** $\frac{mg}{L}$ * precipitation depth (mm)

desired unit is areal flux of solute

Merged dataframe

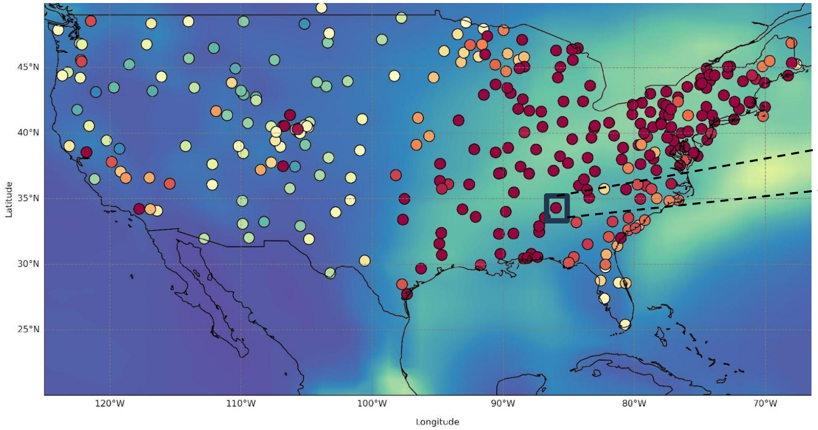
333 sites

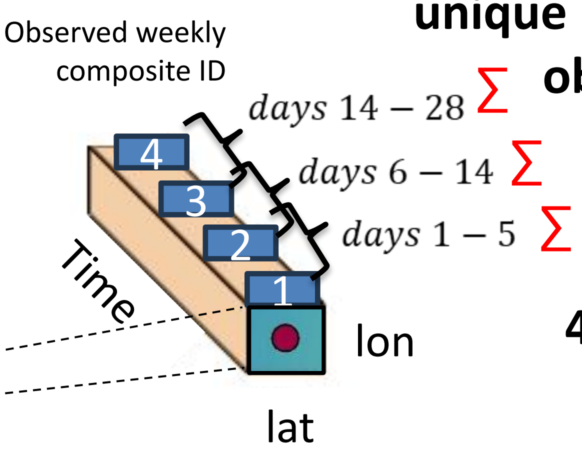
585 observations per site

183,000 total observations (x 3 vars)

500,000 datapoints for validation

2) Select nearest grid cell to observed site latitude x longitude

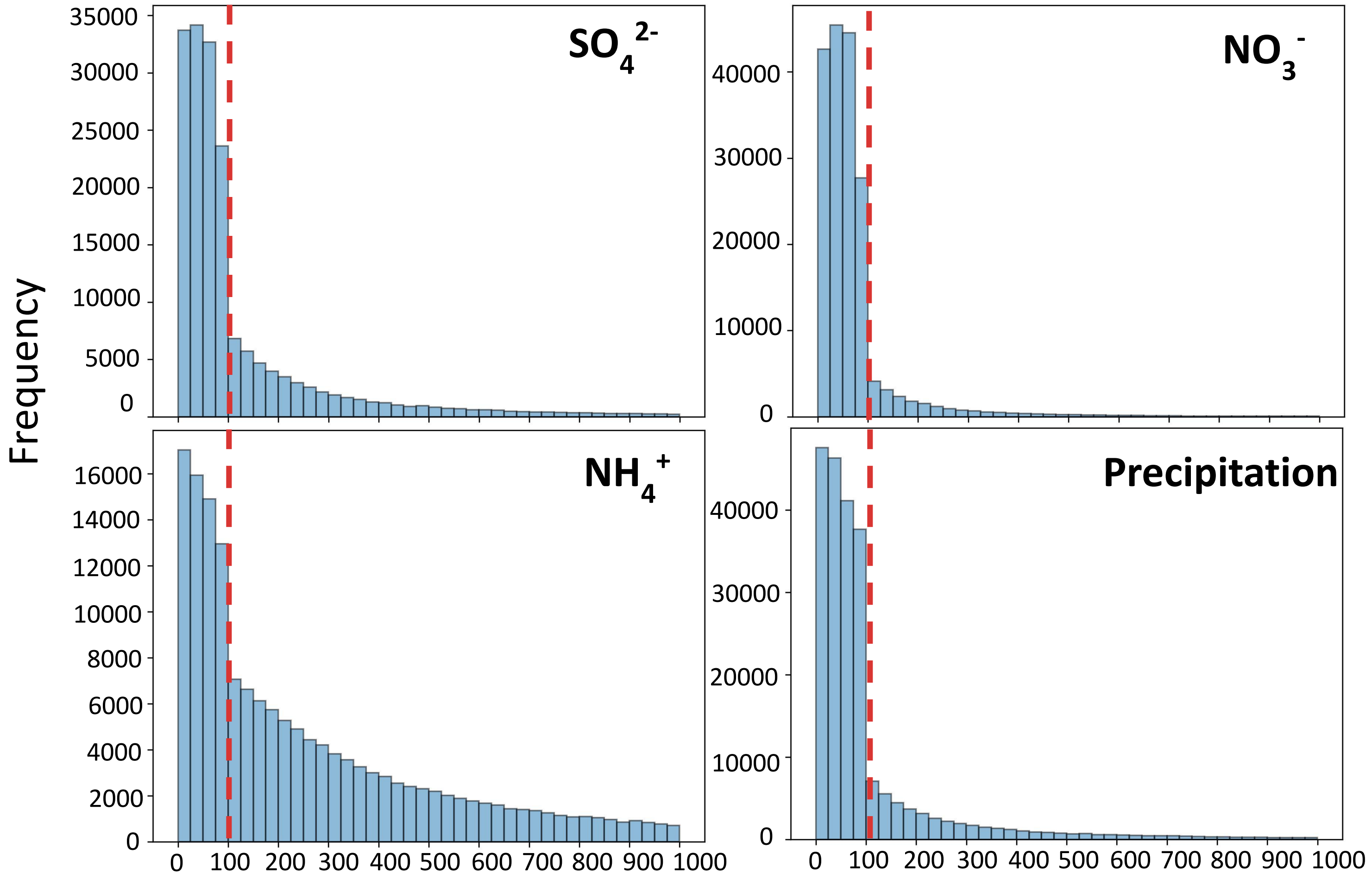




3) Assign modelled data unique id # corresponding to observed sample

4) Sum daily modeled data to irregular sampling dates

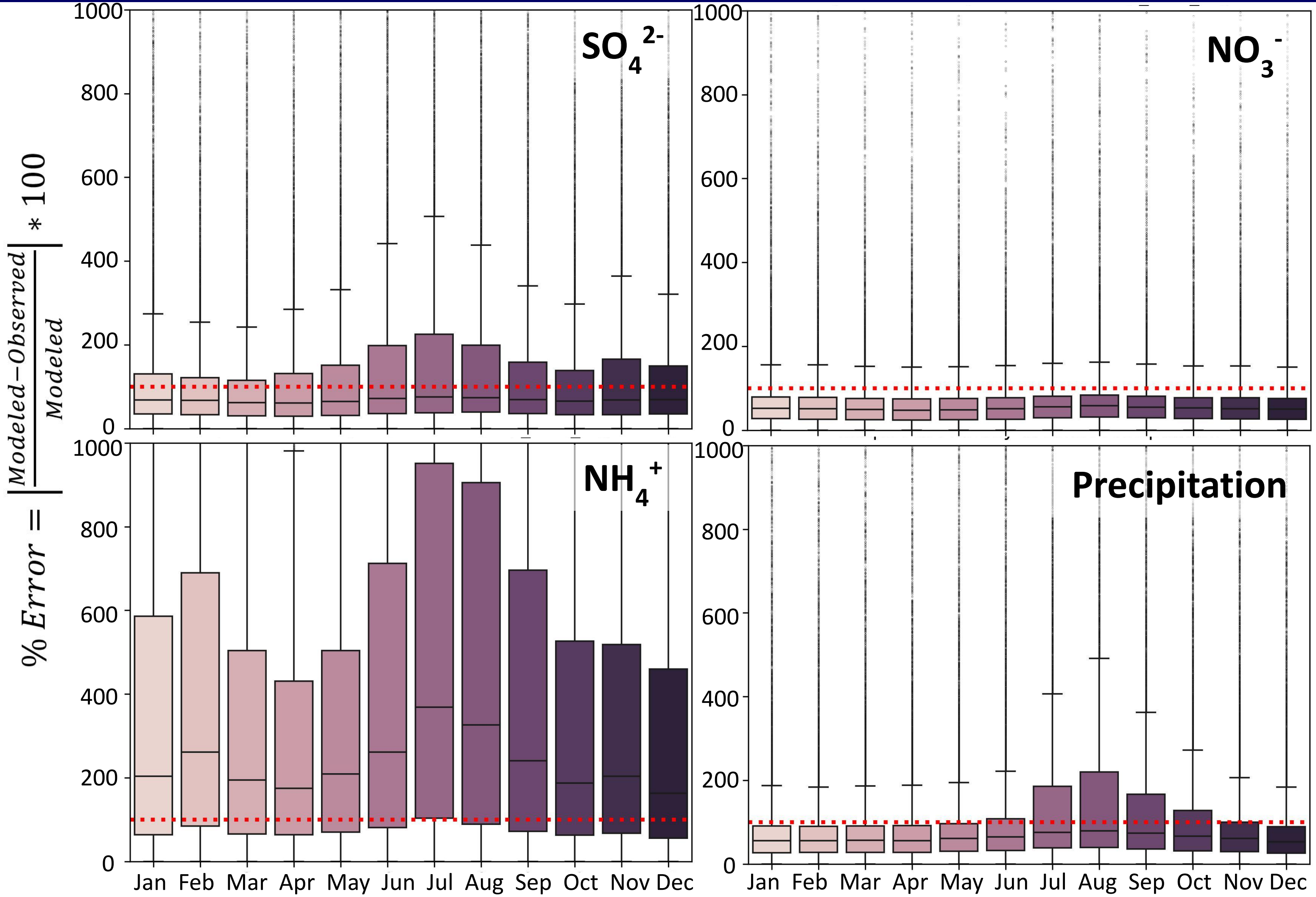
Percent error between modeled and observed wet deposition



Merged dataframe
333 sites
585 observations per site
183,000 total observations (x 3 vars)
500,000 datapoints for validation

$$\%\ Error = \left|\frac{Modeled - Observed}{Modeled}\right| * 100$$

Percent error between modeled and observed wet deposition



Merged dataframe
333 sites
585 observations per site
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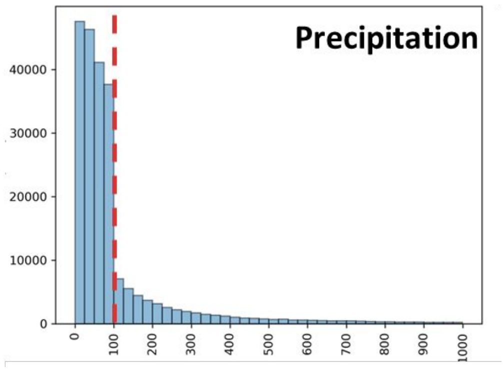
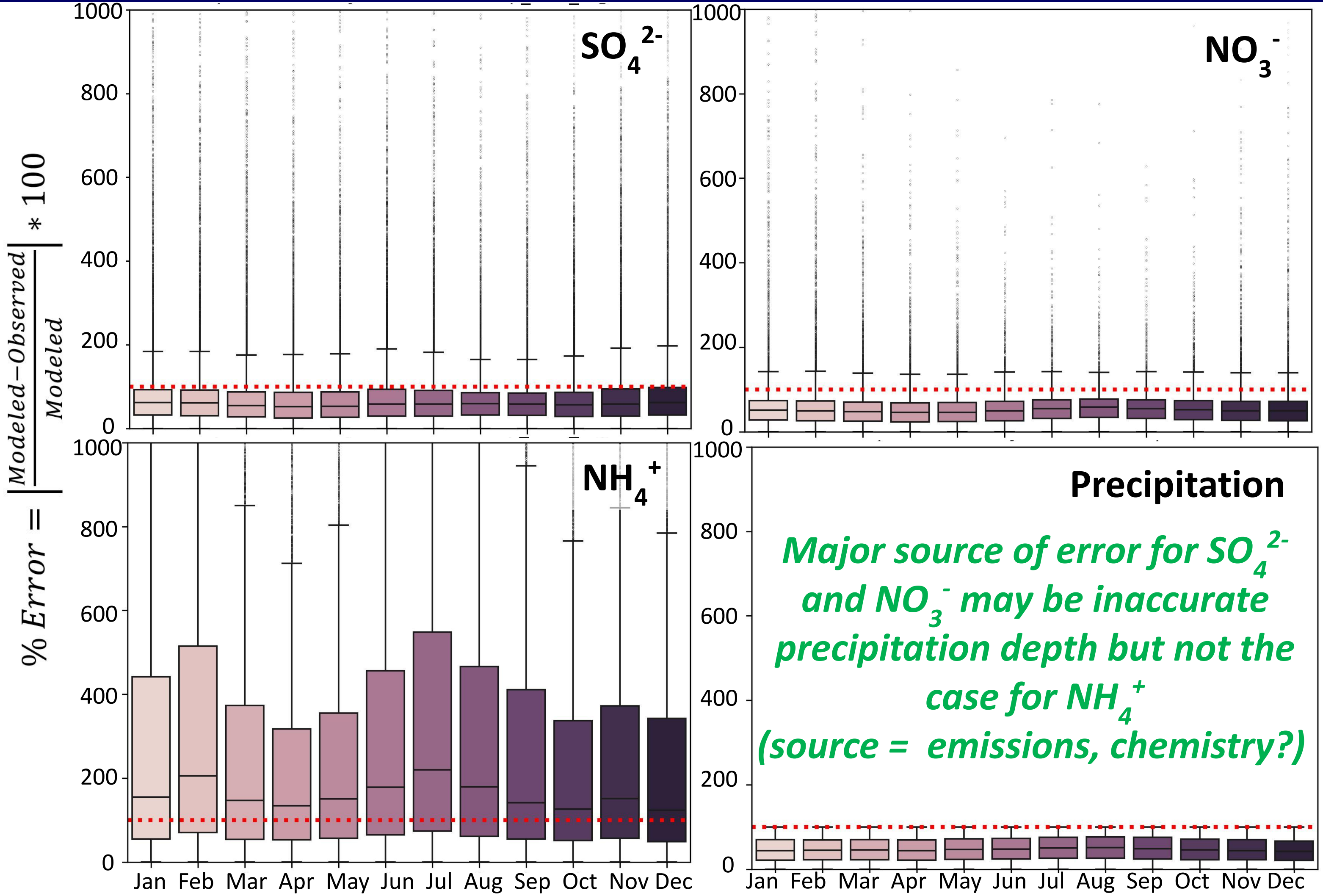
What are potential sources of error between modeled and observed solutes?



Percent error between modeled and observed wet deposition



Merged dataframe

333 sites

585 observations per site

183,000 total observations (x 3 vars)

500,000 datapoints for validation

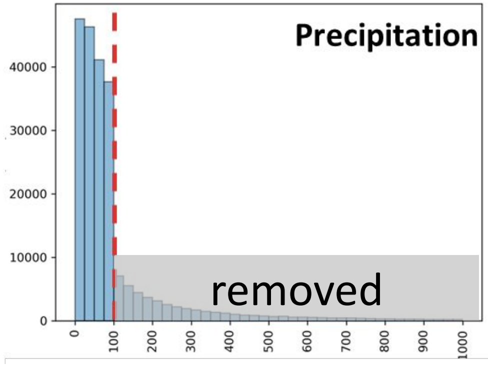
Clean precipitation dataframe

331 sites

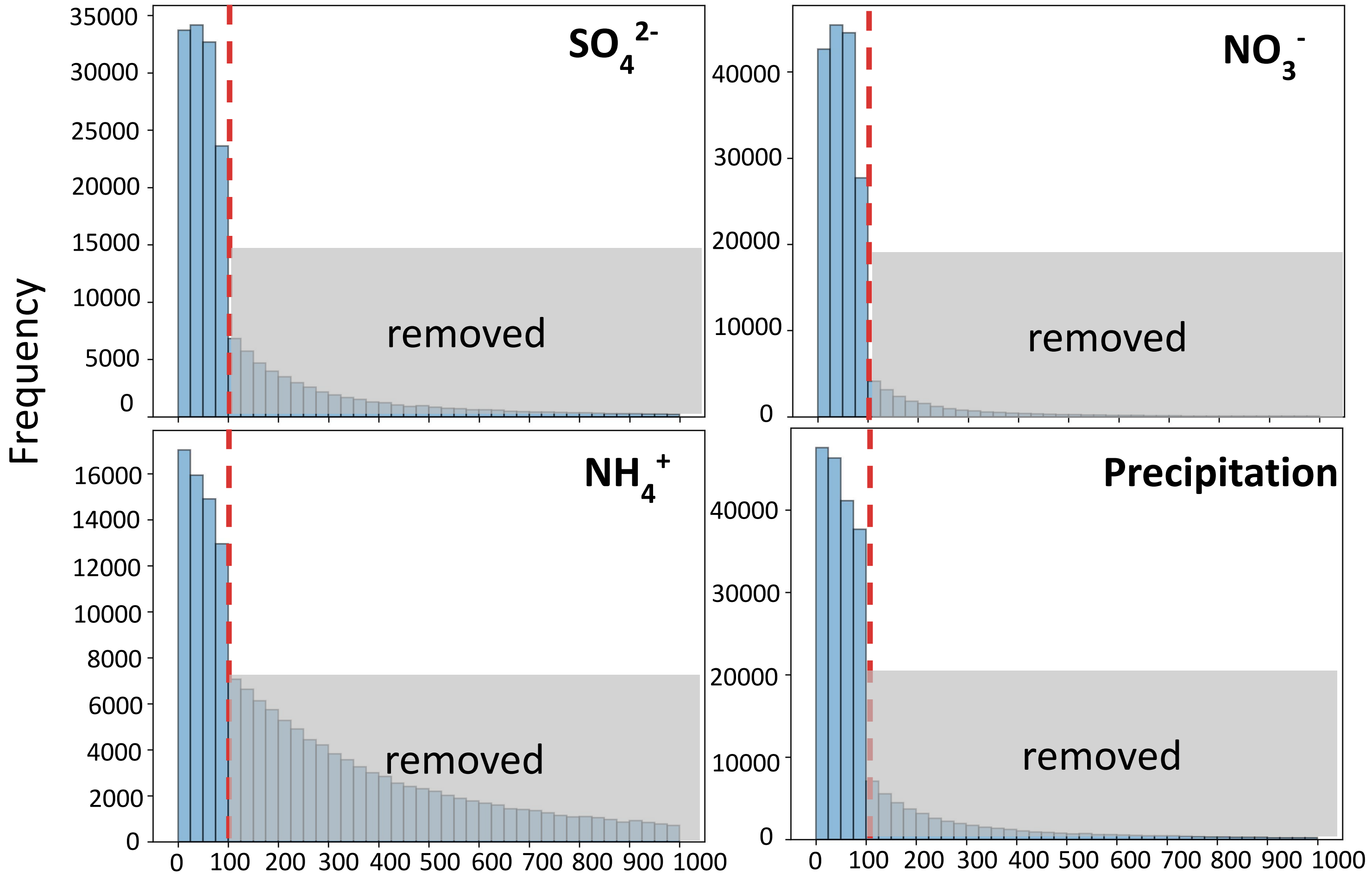
435 observations per site ↓ 25%

135,000 total observations (x 3 vars)

400,000 datapoints for validation



Percent error between modeled and observed wet deposition



$$\%\ Error = \left|\frac{Modeled - Observed}{Modeled}\right| * 100$$

Merged dataframe

333 sites

585 observations per site

183,000 total observations (x 3 vars)

500,000 datapoints for validation

Clean precipitation dataframe

331 sites

435 observations per site ↓ 25%

135,000 total observations (x 3 vars)

400,000 datapoints for validation

Clean precip + chemistry dataframe

331 sites

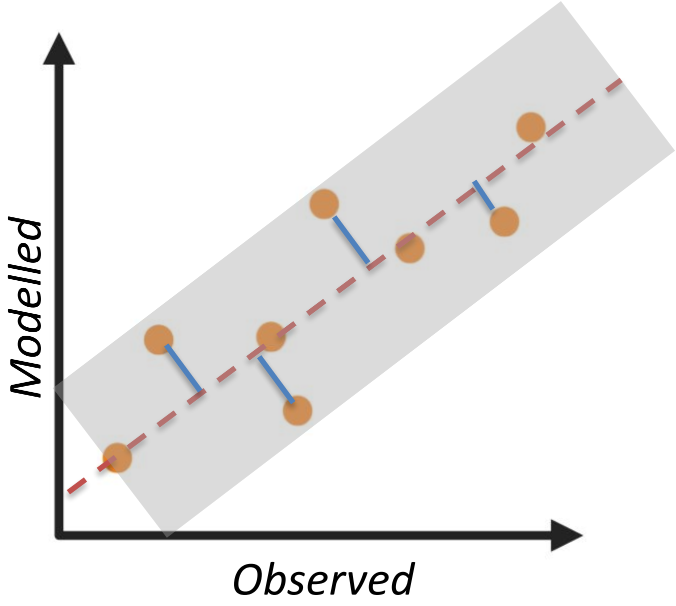
350 observations per site ↓ 20%

55,000 NH_4^+, 110,000 SO_4^{2-}, and 130,000 NO_3^- total observations

300,000 datapoints for validation

Where do modeled wet deposition parameters perform 'acceptably'?

Identifying areas where the model predicts wet deposition well is important for further sensitivity studies on drivers of wet deposition



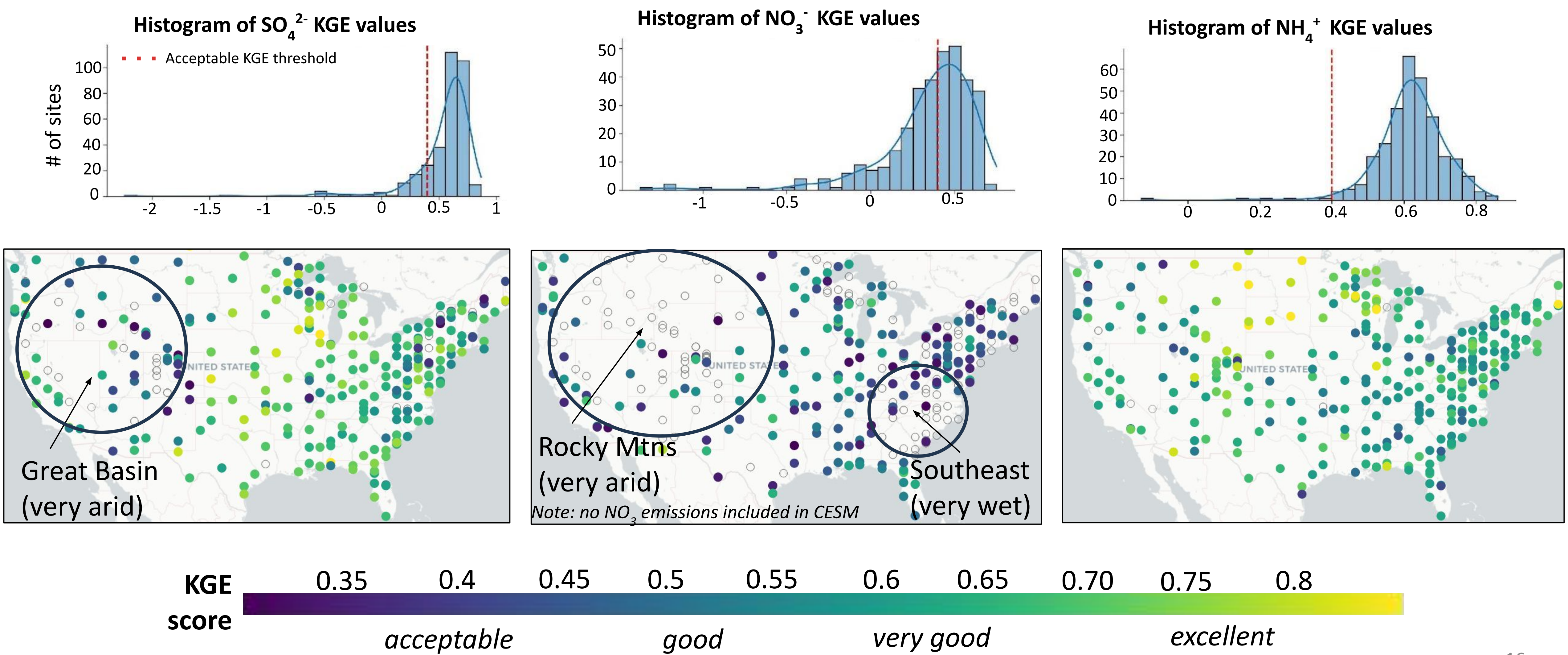
KGE (Kling Gupta Efficiency) Metric

- Combined correlation, bias and variability metric
  - R, R^2, RMSE, slope of regression
- Provides a comprehensive assessment of the model's ability to reproduce the observed variability
- Calculated this metric per site to understand spatial variability

KGE > 0.4 = **acceptable** model performance

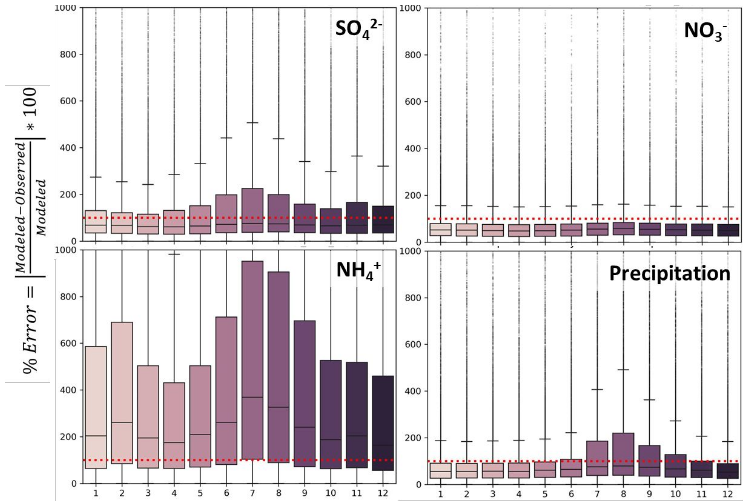
(*Reference*: Knoben et al., 2019)

Where do modeled wet deposition parameters perform 'acceptably'?

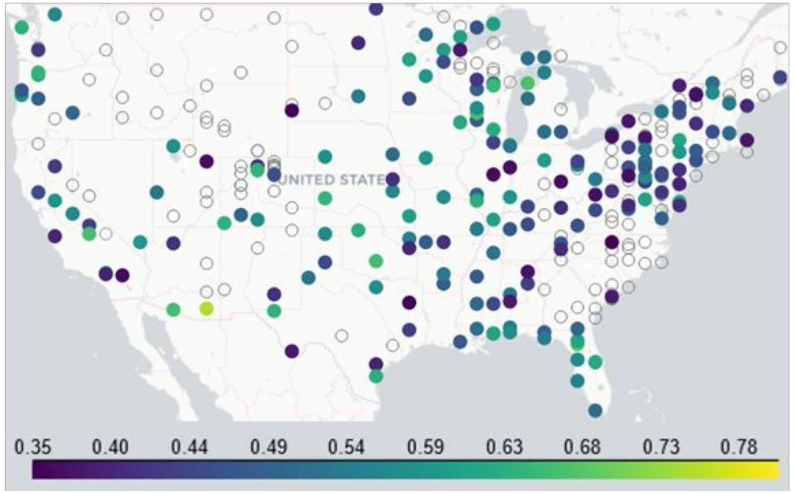


Key points and next steps

Major source of error for wet deposition SO_4^{2-} and NO_3^- may be inaccurate precipitation depth but error for NH_4^+ may be emissions or chemistry.



The model has more acceptable spatial performance for SO_4^{2-} and NH_4^+ while NO_3^- performs poorly in regions experiencing precipitation extremes.



Next Steps:

- Continue to evaluate error sources and develop “best practices” for using CAM-chem wet deposition data
- Validation of organic carbon and black carbon wet deposition solutes
- Assess differences in wet deposition accuracy between the Global model and MUSICA regionally refined over CONUS

Thank you!

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Questions?

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