Water Quality in a Changing Climate: Insights from a Deep Learning Approach

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Chesapeake Bay Program month seminar Integrated Trends Analysis Team

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Water Quality issue tends to be overlooked in climate risk assessment

nature reviews earth & environment https://doi.org/10.1038/s43017-023-00

Review article

Check for up

Global river water quality under climate change and hydroclimatic extremes

Michelle T. H. van Vliet[1], Josefin Thorslund[1,2], Maryna Strokal[3], Nynke Hofstra[3], Martina Flörke[4], Heloisa Ehalt Macedo[5], Albert Nkwasa[6,7], Ting Tang[8], Sujay S. Kaushal[9], Rohini Kumar[10], Ann van Griensven[6], Lex Bouwman[11,12] & Luke M. Mosley[13]

"… River water quality generally deteriorates under **droughts** and **heatwaves** (68% of compiled cases), **rainstorms** and **floods** (51%) and under long-term climate change (56%)."

Forecasting capabilities will become increasingly important.

https://www.science.org/content/article/europe-s-deadly-floods-leave-scientists-stunned

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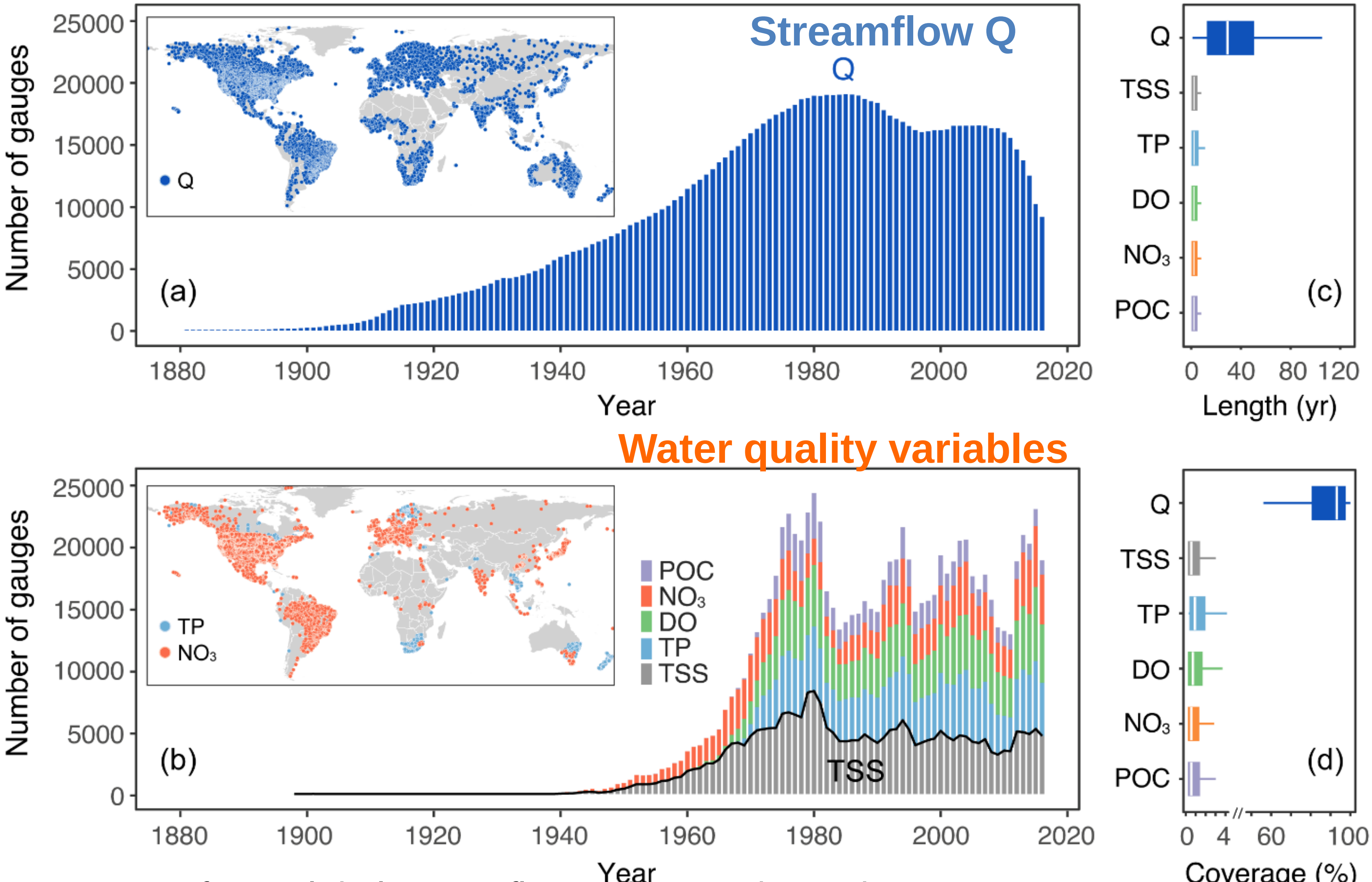
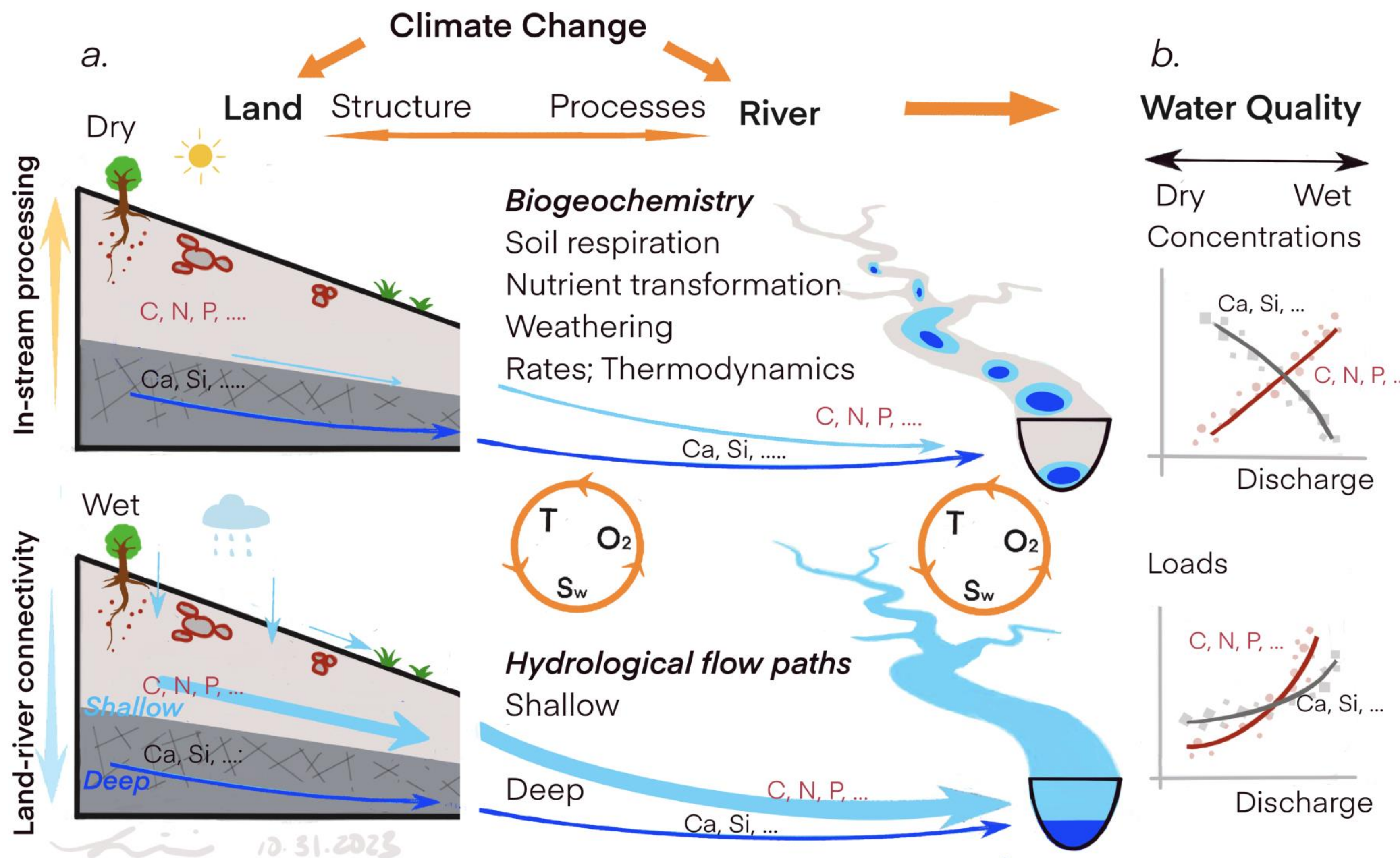
The Data Scarcity Challenge



Data from Global Streamflow Indices andMetadata Archive (GSIM); Global River Water Quality Archive (GRQA)

Process Complexity Challenge



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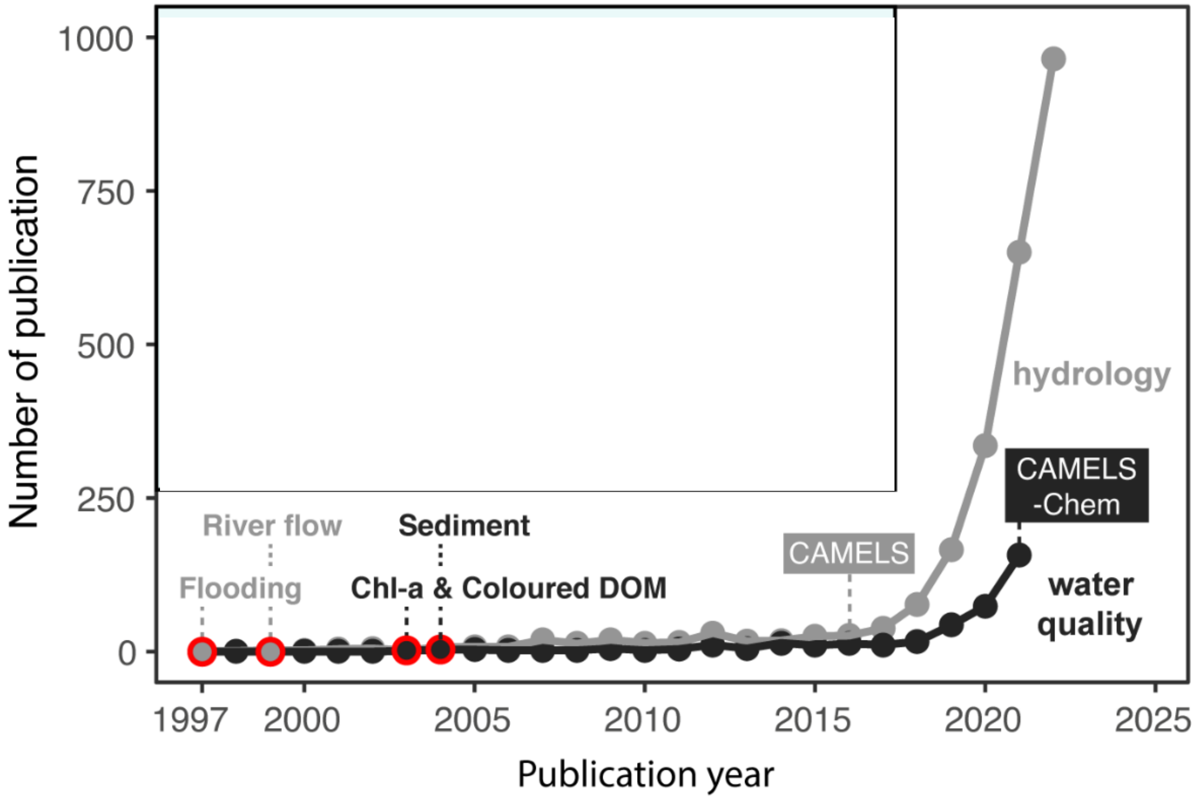
Li et al., in press

Deep Learning Models to the Rescue?



DL applications in hydrology have exploded;
Its applications in water quality is lagging behind.

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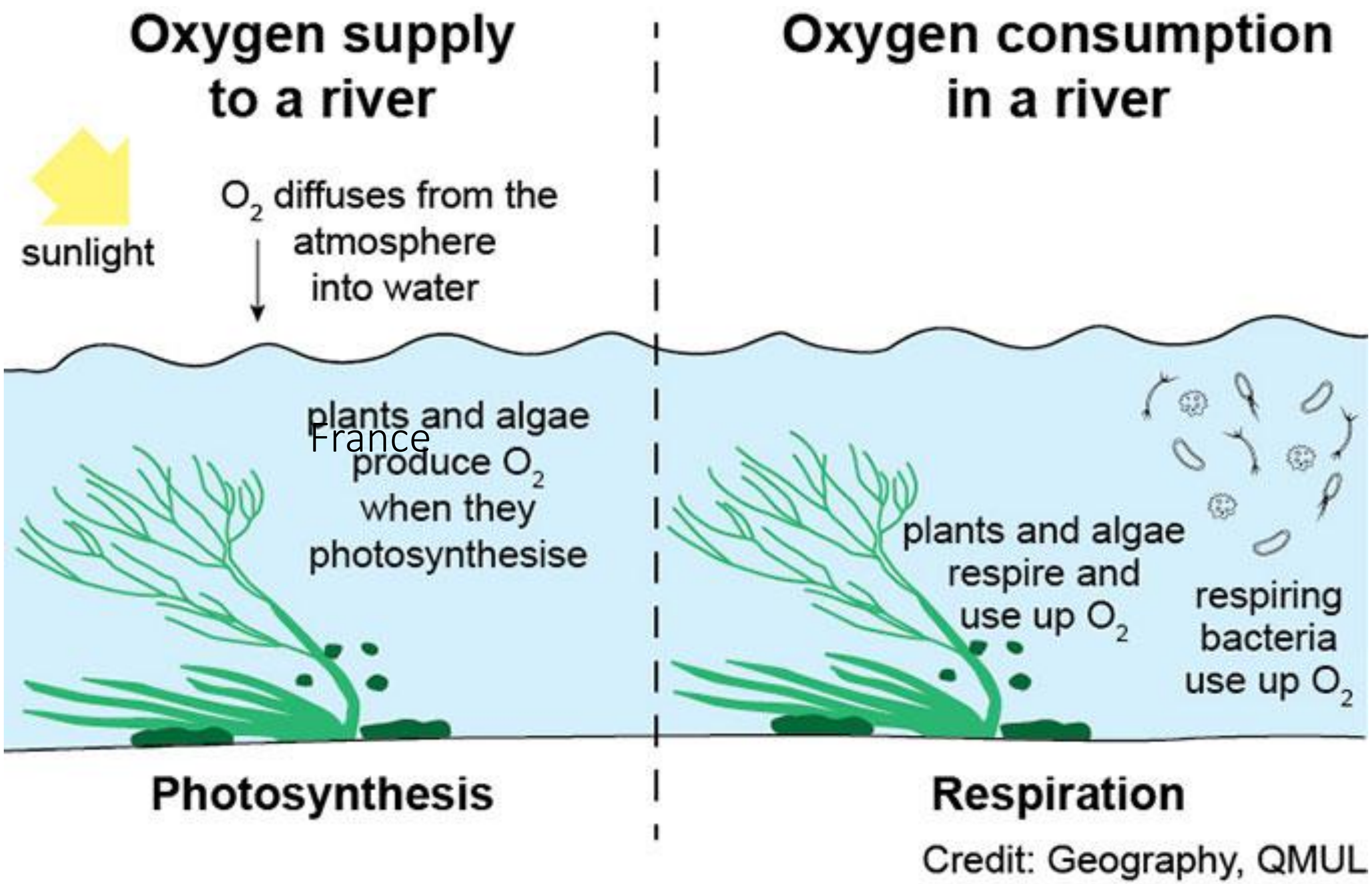
Zhi et al., accepted

Dissolved Oxygen (DO):
sun light, water flow, and temperature

Bernhardt et al., 2017



https://www.qmul.ac.uk/chesswatch/water-quality-sensors/dissolved-oxygen/

Deoxygenation is less expected in rivers than in oceans + lakes.

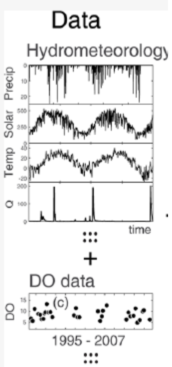
Environmental Science & Technology
pubs.acs.org/est
Article

From Hydrometeorology to River Water Quality: Can a Deep Learning Model Predict Dissolved Oxygen at the Continental Scale?

Wei Zhi, Dapeng Feng, Wen-Ping Tsai, Gary Sterle, Adrian Harpold, Chaopeng Shen, and Li Li*

Cite This: https://dx.doi.org/10.1021/

ACCESS | Metrics & M



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nature water

Article https://doi.org/10.1038/s44221-023-00038-z

Temperature outweighs light and flow as the predominant driver of dissolved oxygen in US rivers

Received: 15 May 2022

Accepted: 30 January 2023

Published online: 09 March 2023

Check for updates

nature climate change

Article https://doi.org/10.1038/s41558-023-01

Widespread deoxygenation in warming rivers

Received: 16 April 2022

Accepted: 4 August 2023

Published online: 14 September 2023

Check for updates

Wei Zhi [1,2], Christoph Klingler [3], Jiangtao Liu [1] & Li Li [1]

Deoxygenation is commonly observed in oceans and lakes but less expected in shallower, flowing rivers. Here we reconstructed daily water temperature and dissolved oxygen in 580 rivers across the United States

LSTM model:

- What is the utility of deep learning models in water quality modeling?
- When do models perform well?

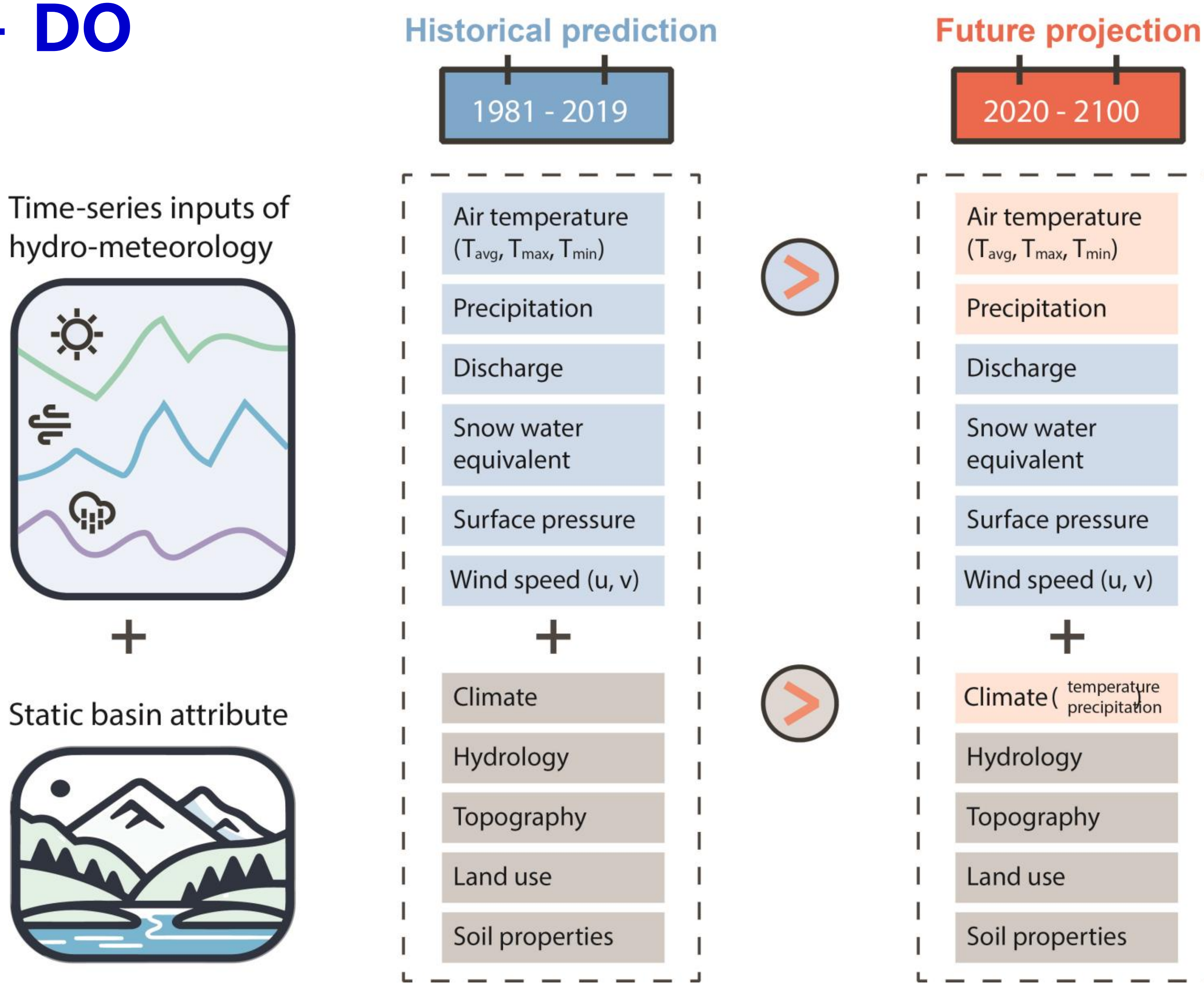
T and DO dynamics:

- How have T and DO changed in a warming climate?
- What are the drivers of DO?

US + Central Europe (~800 sites)
1980 – 2020;
T + DO

DayMet

GAGESII

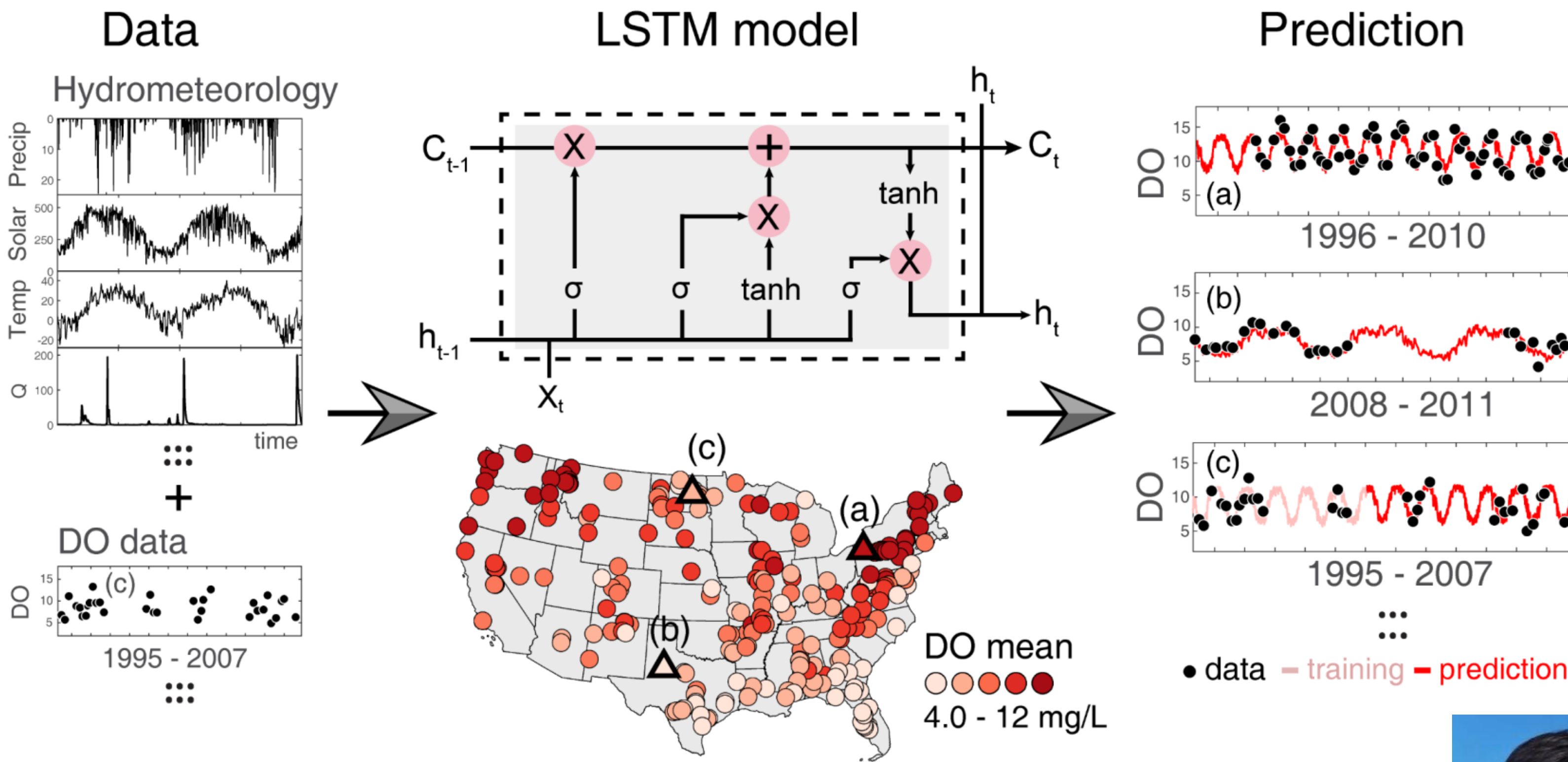


Deep Learning Models to Reconstruct "Data"

Long Short-Term Memory, LSTM

Intensive hydrometeorology data

Temporal filling:
consistent daily DO



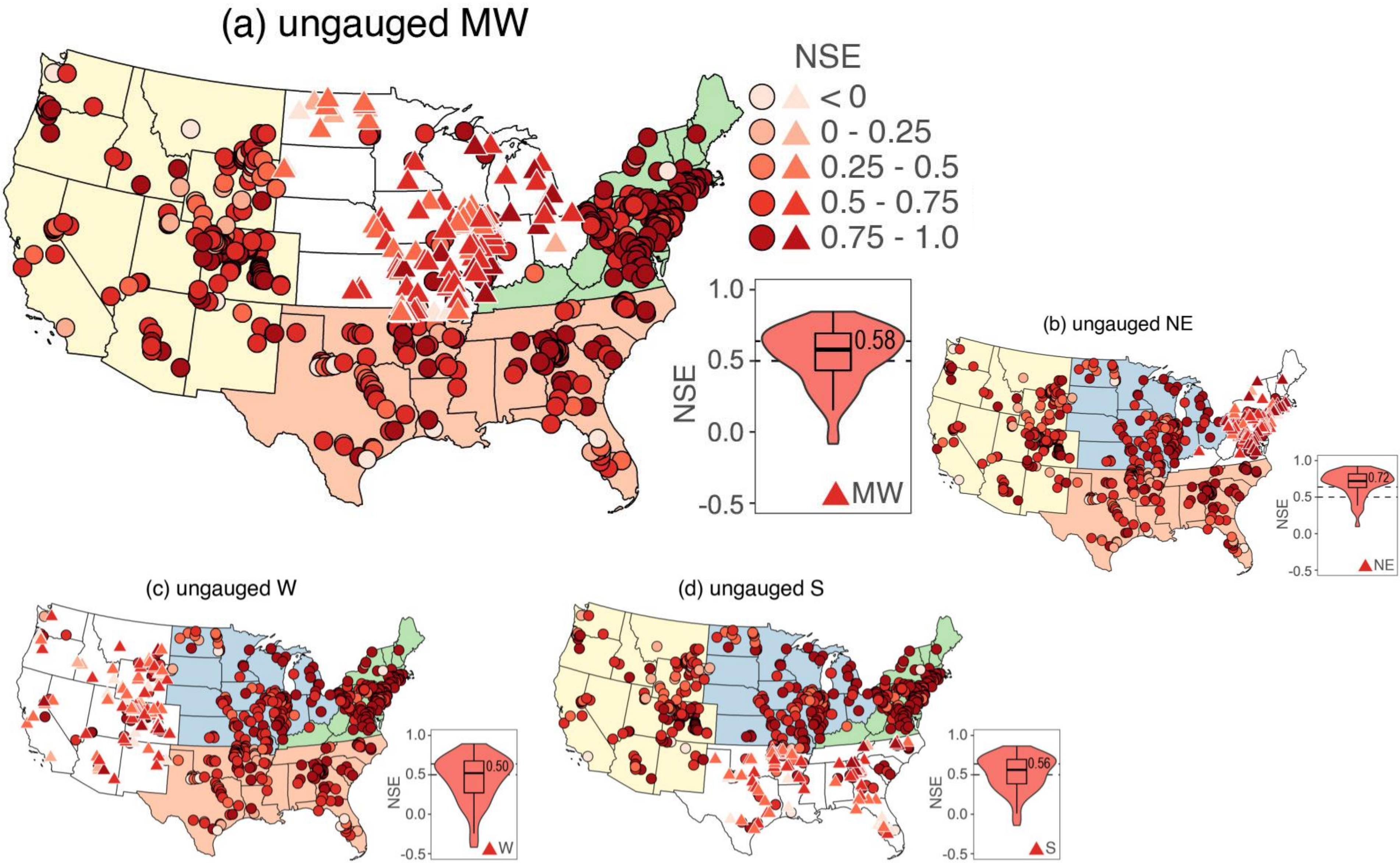
\+

\+ **Basin attributes**

Scarcely measured DO data

Zhi et al., ES&T, 2021. From hydrometeorology to river water quality

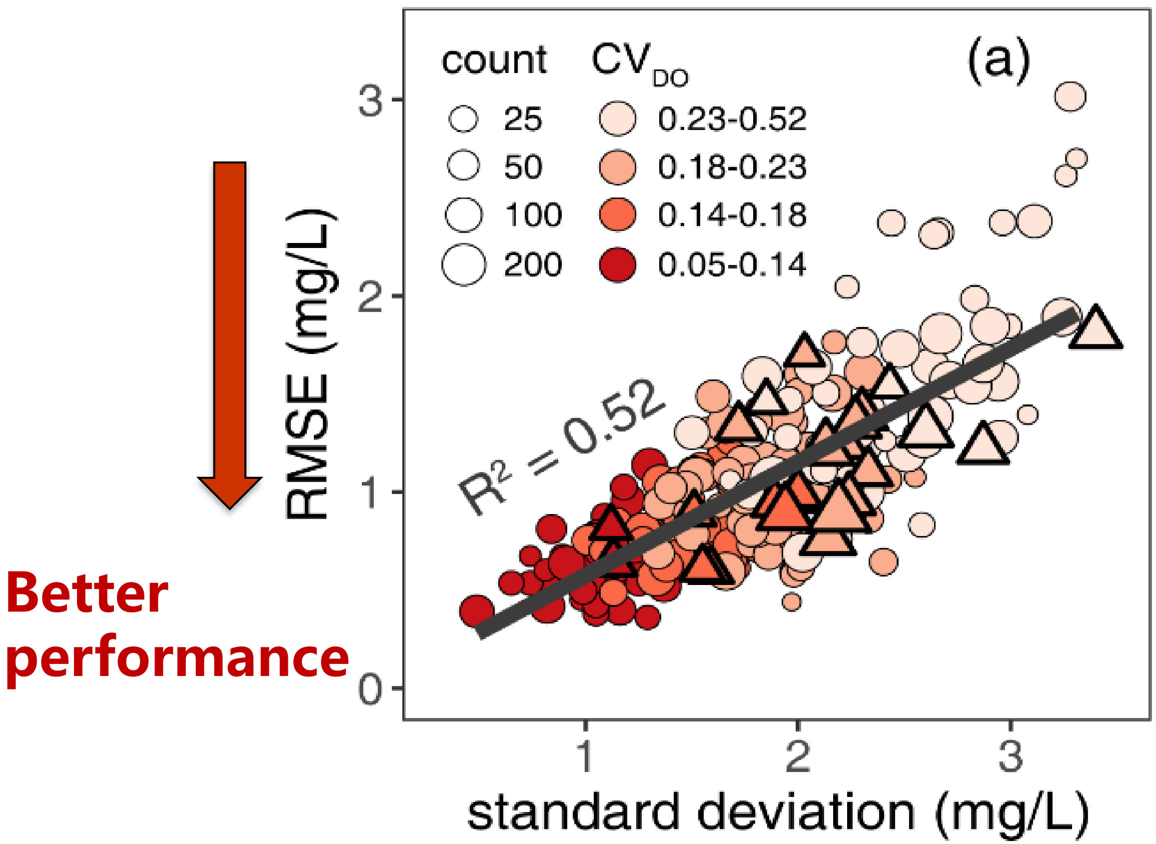
Spatial Filling: Prediction in chemically-ungauged Basins

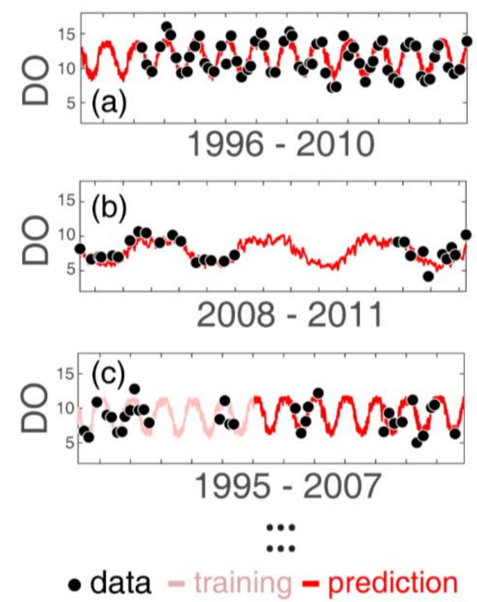


Zhi et al., Nature Water, 2023, Temperature outweighs light + flow …

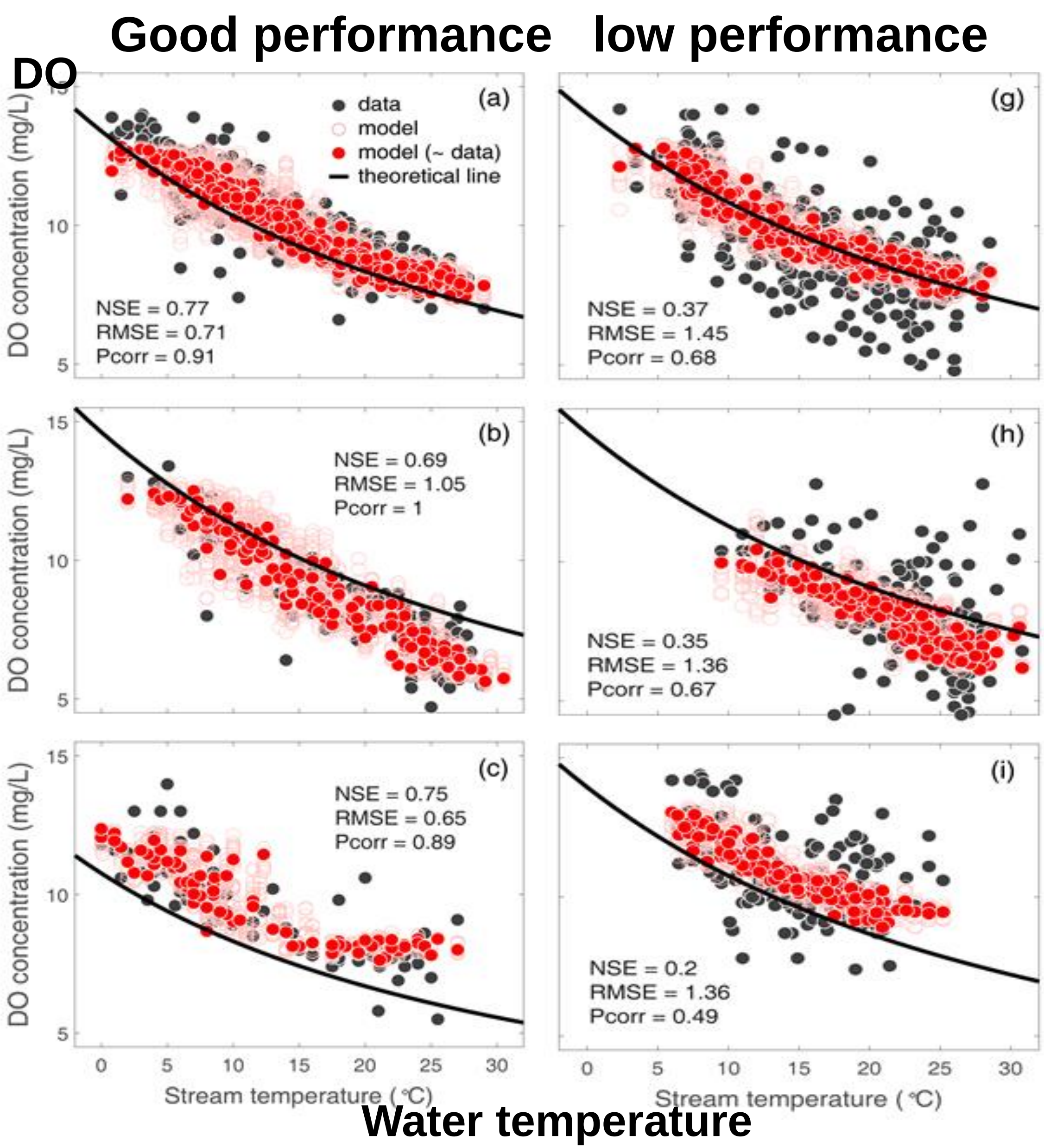
When do models do well?

More data ~~→~~ better model performance?





The model does better in basins with low DO variations.



The model generally can learn the theory of DO solubility;

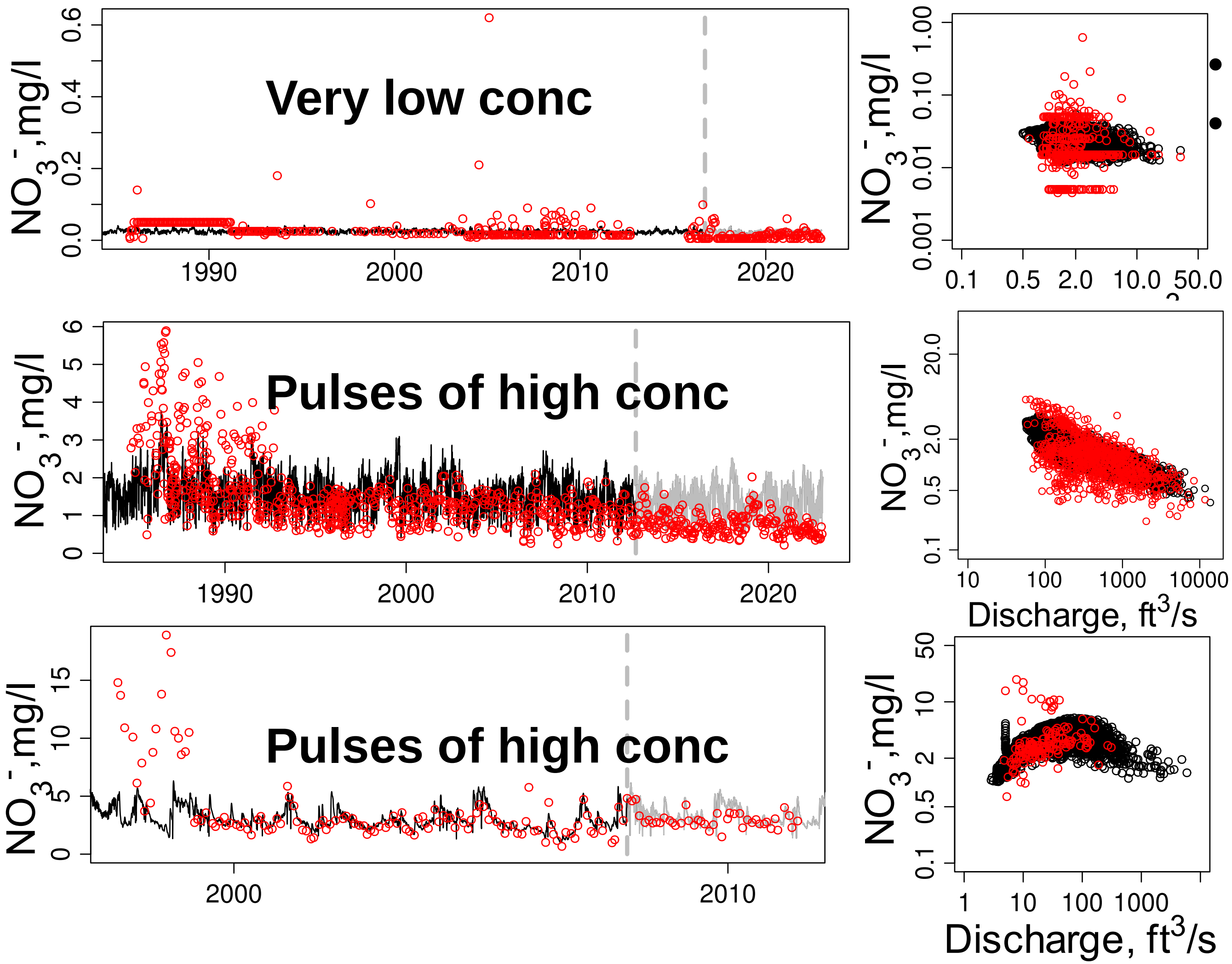
The model does better at sites with low DO variation.

Zhi et al., ES&T 2021

When Do Models Perform Poorly?

NO_3

- **Less data;**
- **Depends on land processes > hydrometeorology**



Relevance to climate extremes?

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LSTM model:

- What is the utility of deep learning models in water quality modeling?
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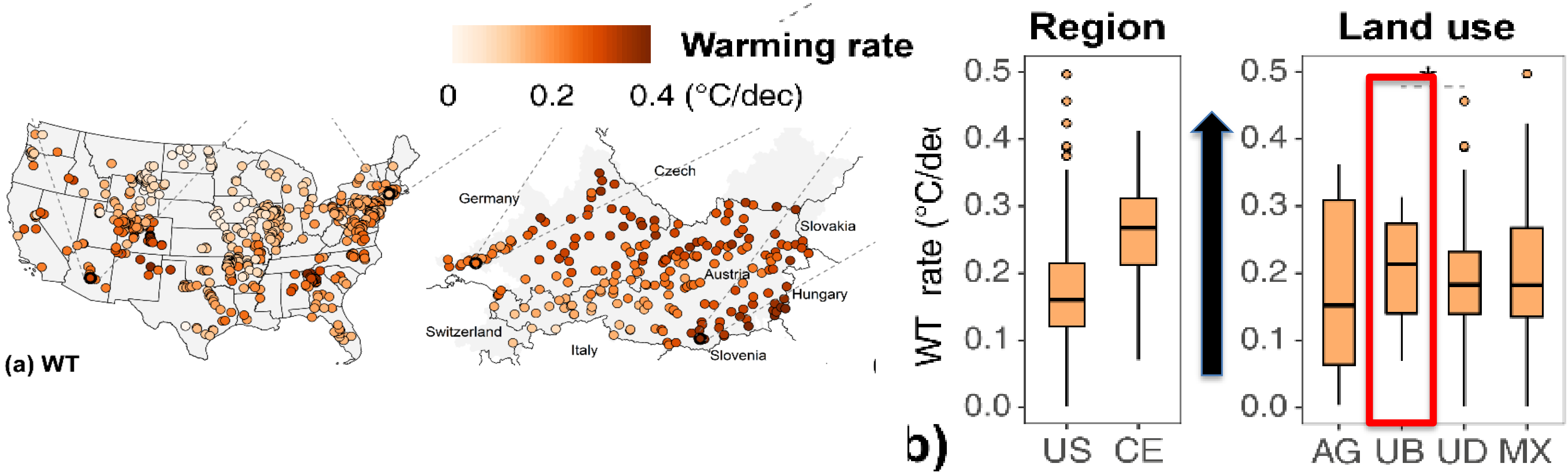
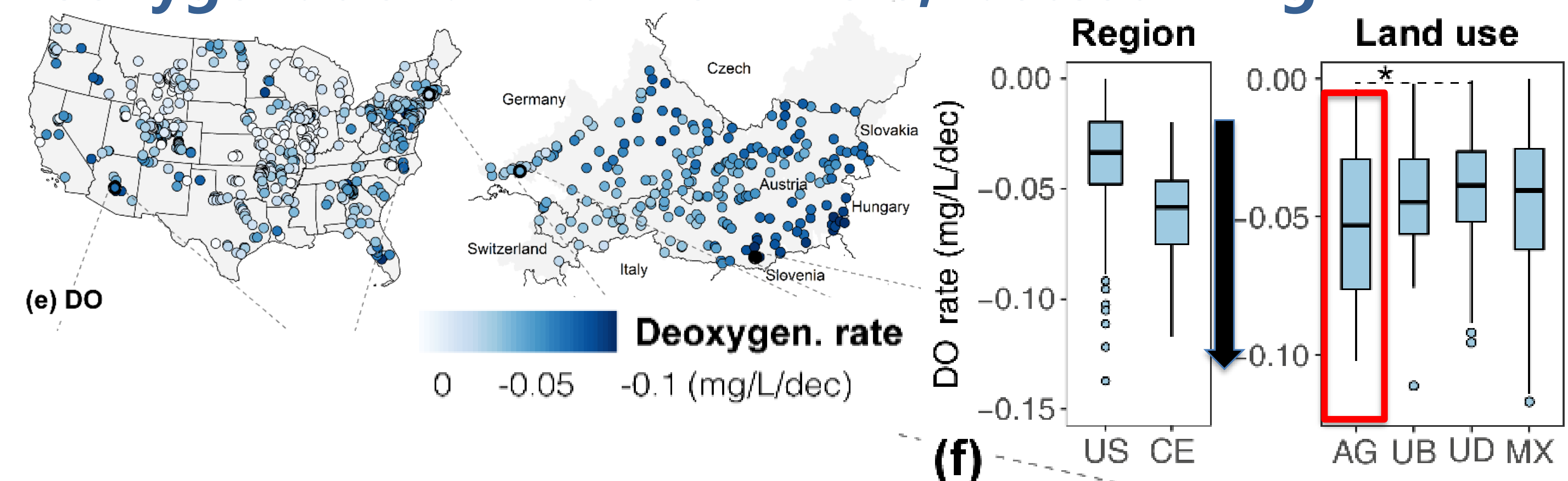
T and DO dynamics:

- What is the historical trend and future projection of T and DO in a warming climate?
- What is the predominant driver of DO?

Warming: fastest in urban, slowest in Ag

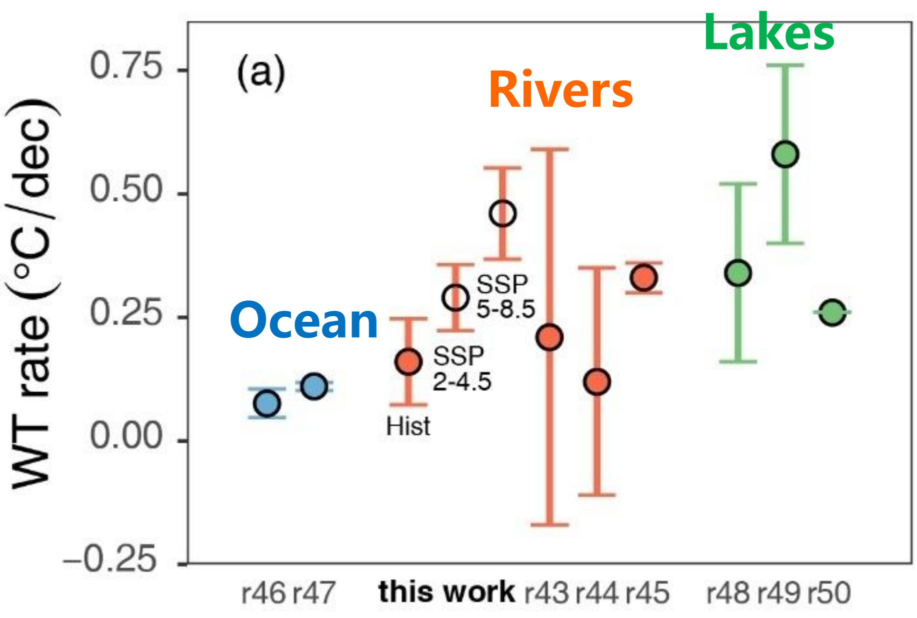


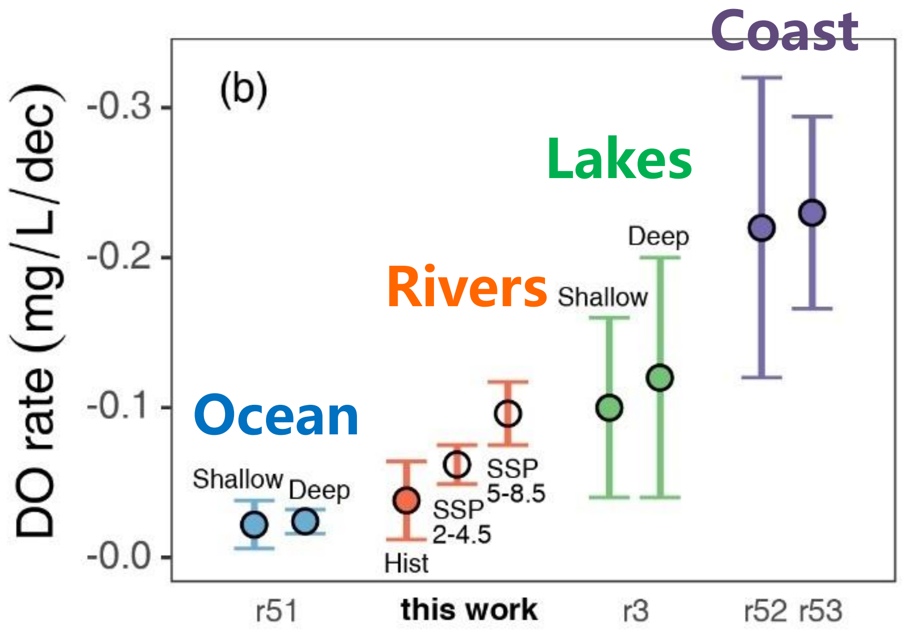
Deoxygenation: > 70% of rivers, fastest in Ag



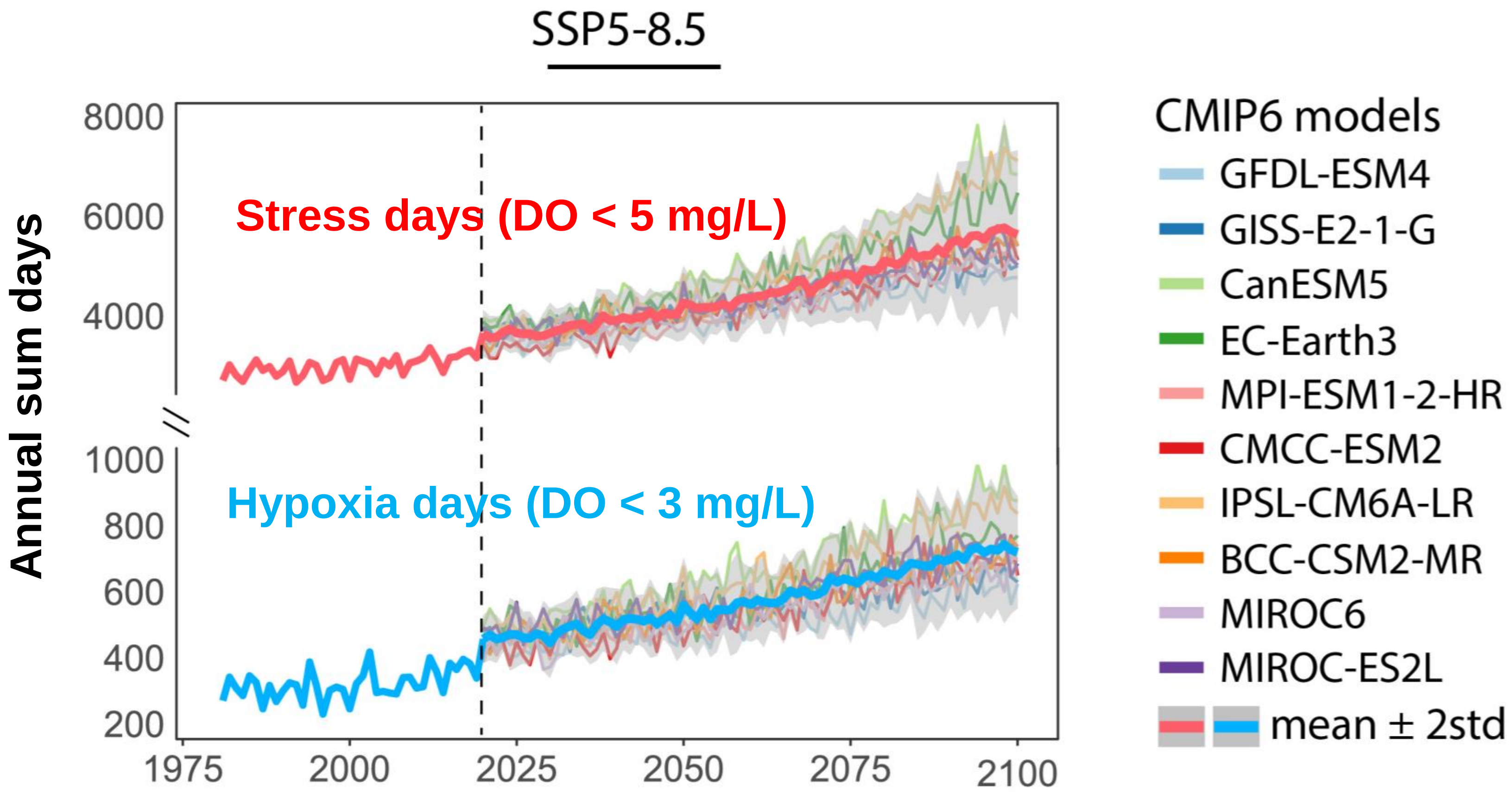
Zhi et al., 2023, Nature Climate Change

Rivers warm up and deoxygenate faster than oceans but slower than lakes and coastal areas.

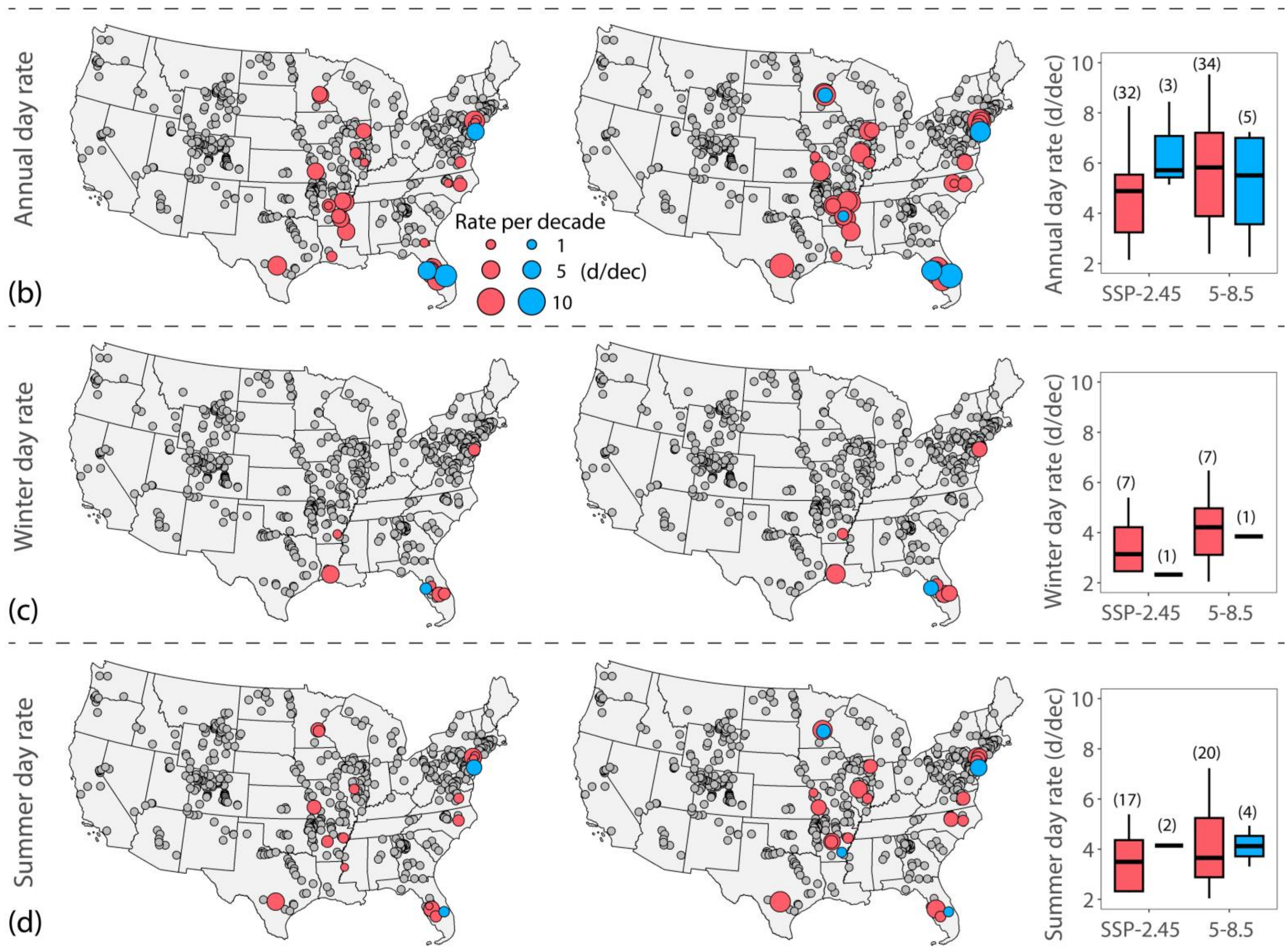




Zhi et al., 2023, Nature Climate Change



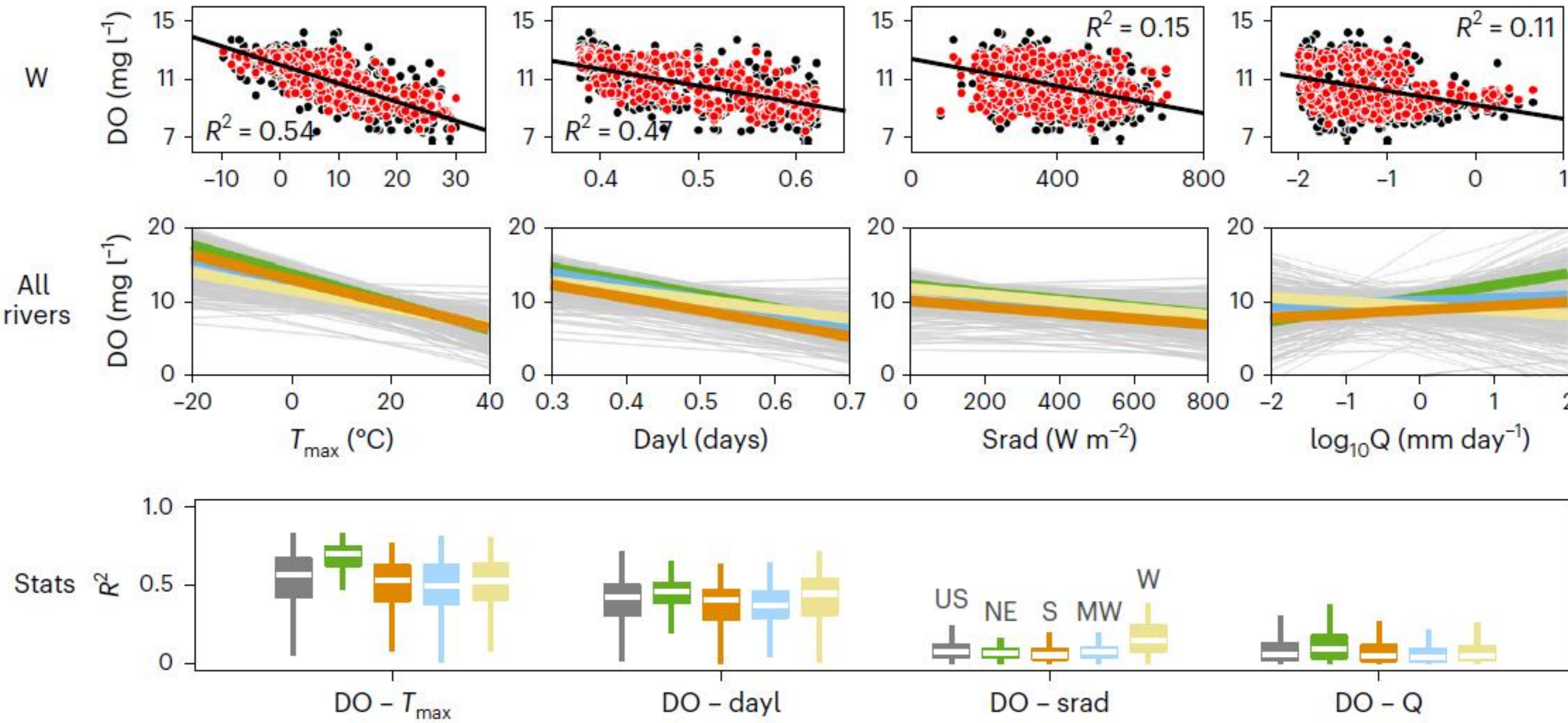
Stress and hypoxia days will continue to increase



Data from grab samples during daytime
Likely underestimate stress and hypoxia days

T is the primary driver

T_{max} > Day Length + Radiation > Flow



Zhi et al., Nature Water, 2023

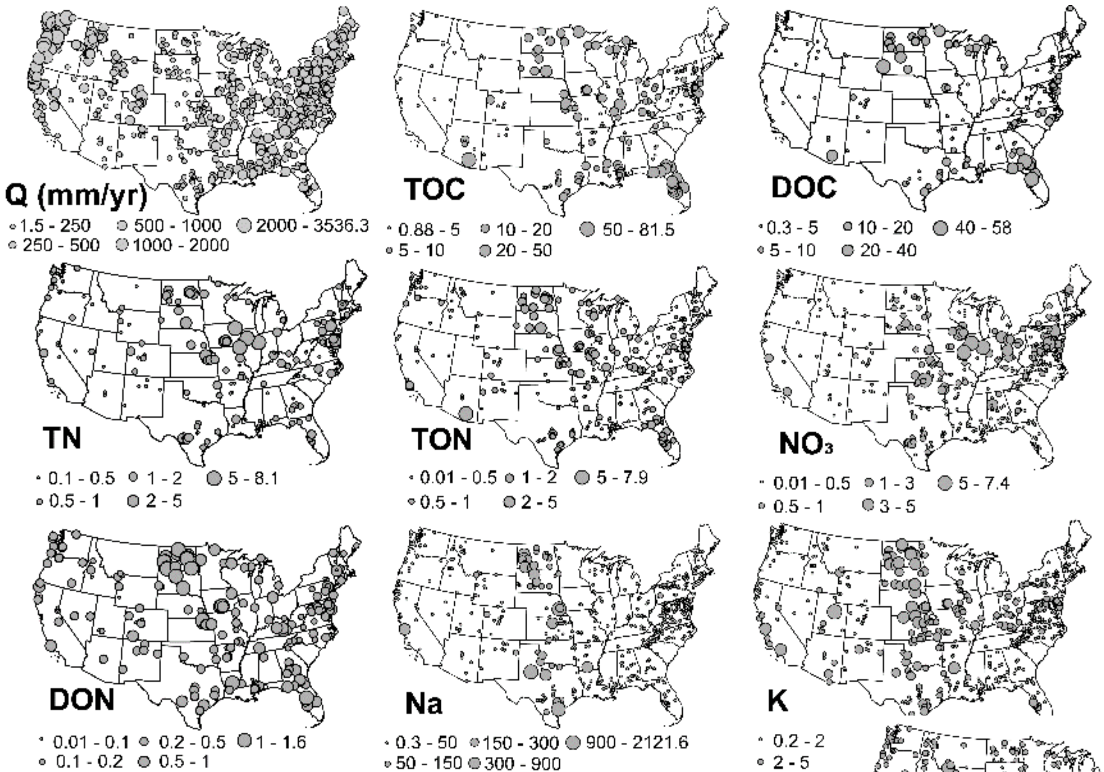
What about other solutes with less data?

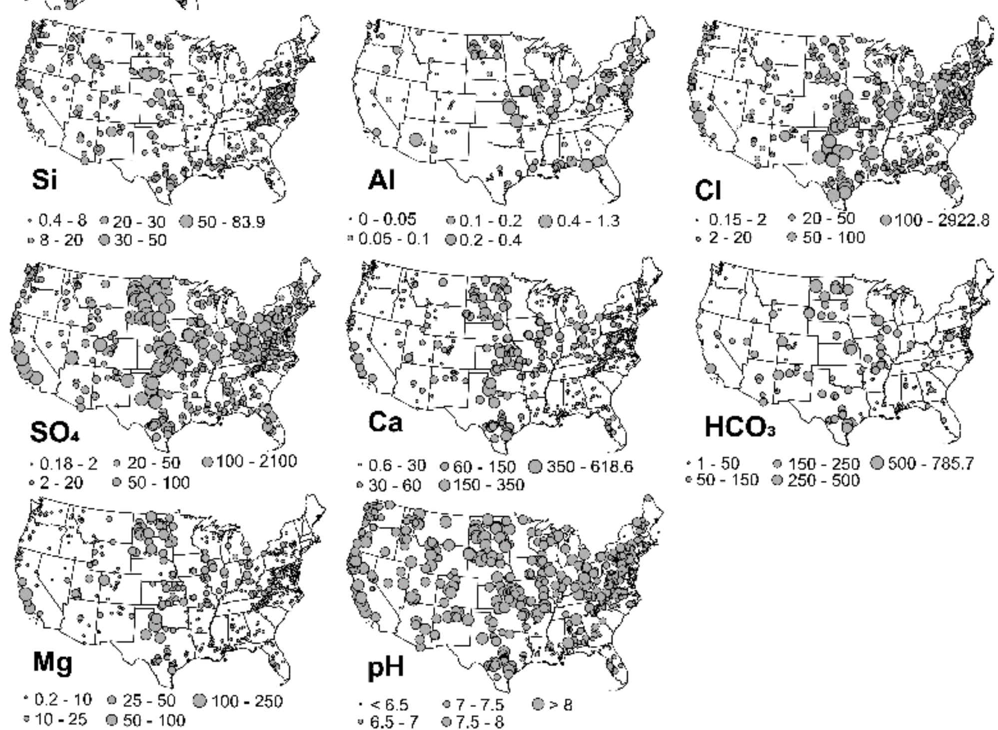
How does climate affect other solutes?

Li et al., 2022. Climate Controls on river chemistry, Earth’s Future

Sterle et al. CAMELS-Chem dataset: HESS, 2024

Minimally-Impacted sites (least human perturbation)



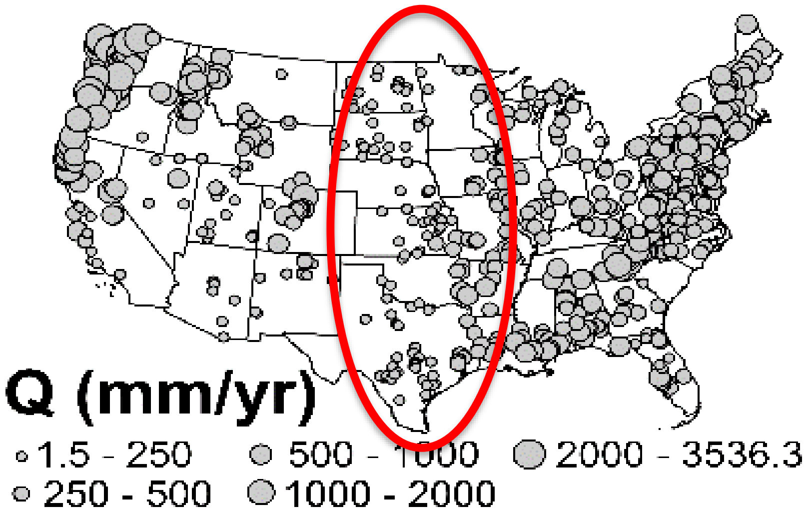


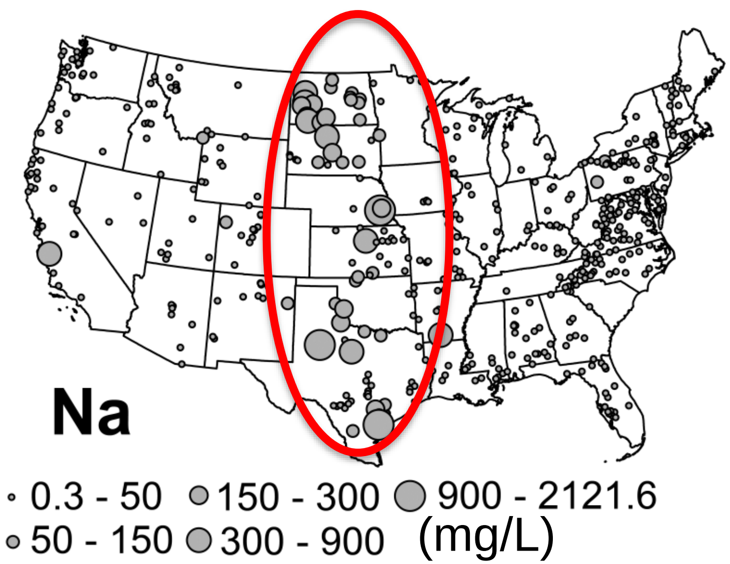
Mean, long-term conc for 16 solutes

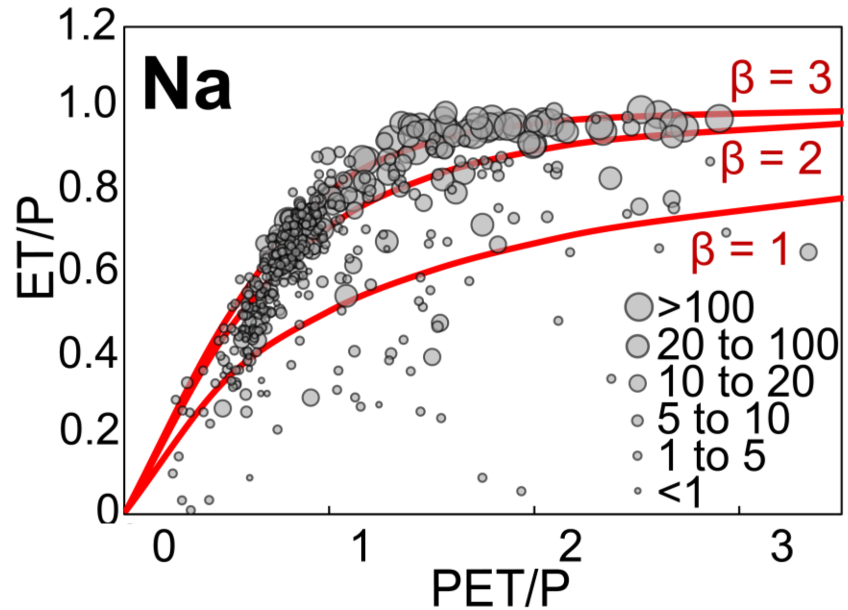
Universal pattern: higher conc. in arid climates

Li et al., 2022. Climate Controls on river chemistry, Earth's Future

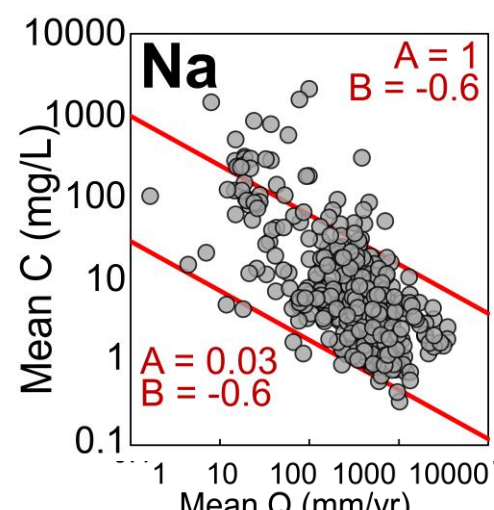
Na: higher in arid climates





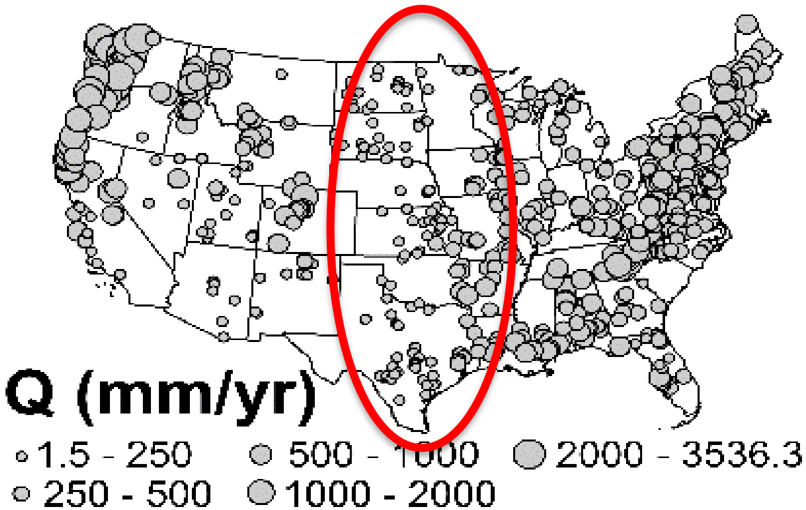


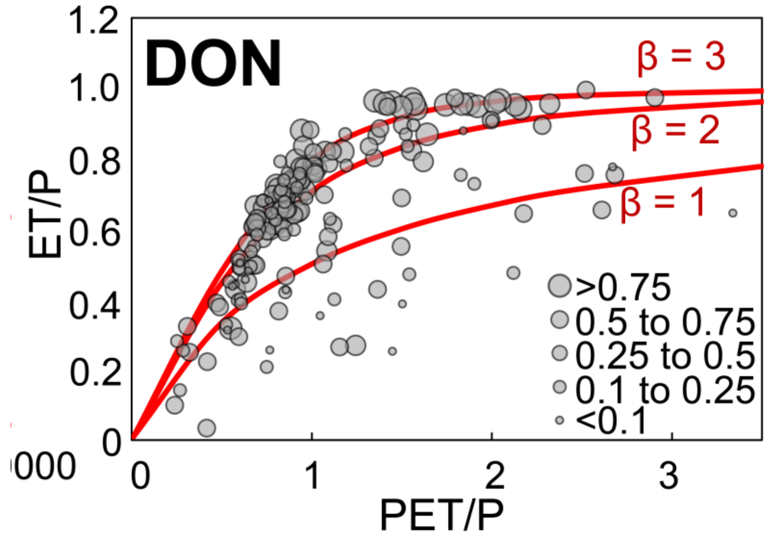
Aridity increase, Conc. increase

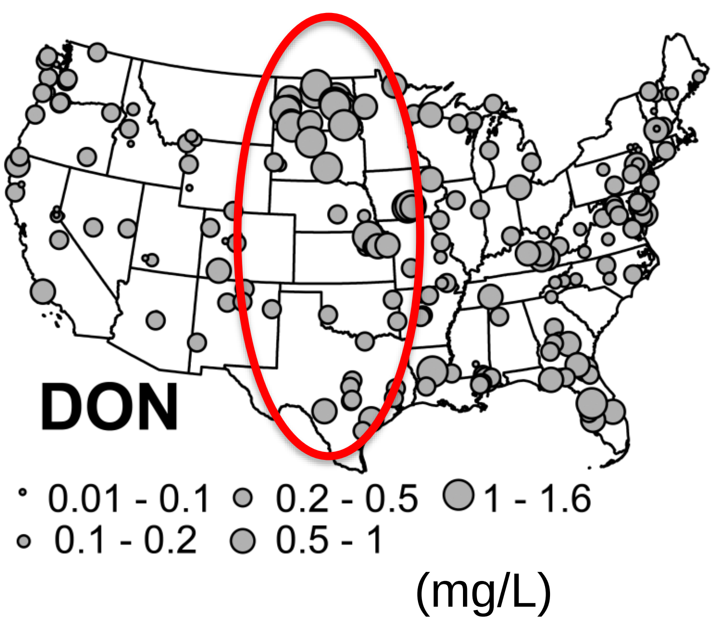


Li et al., 2022. Climate Controls on river chemistry. Earth's Future

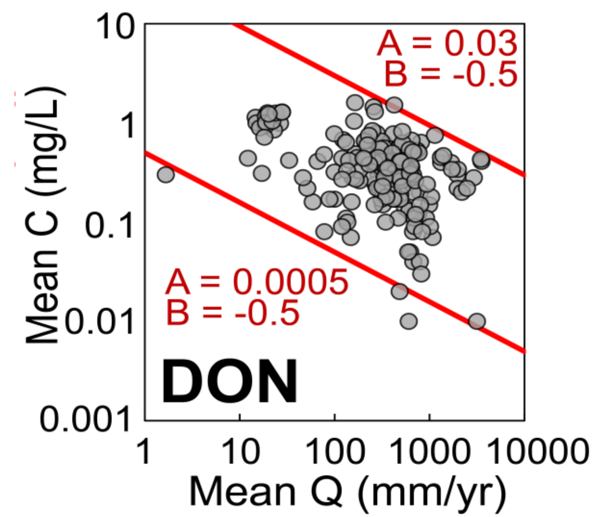
Dissolved Organic Nitrogen (DON): higher in arid climates



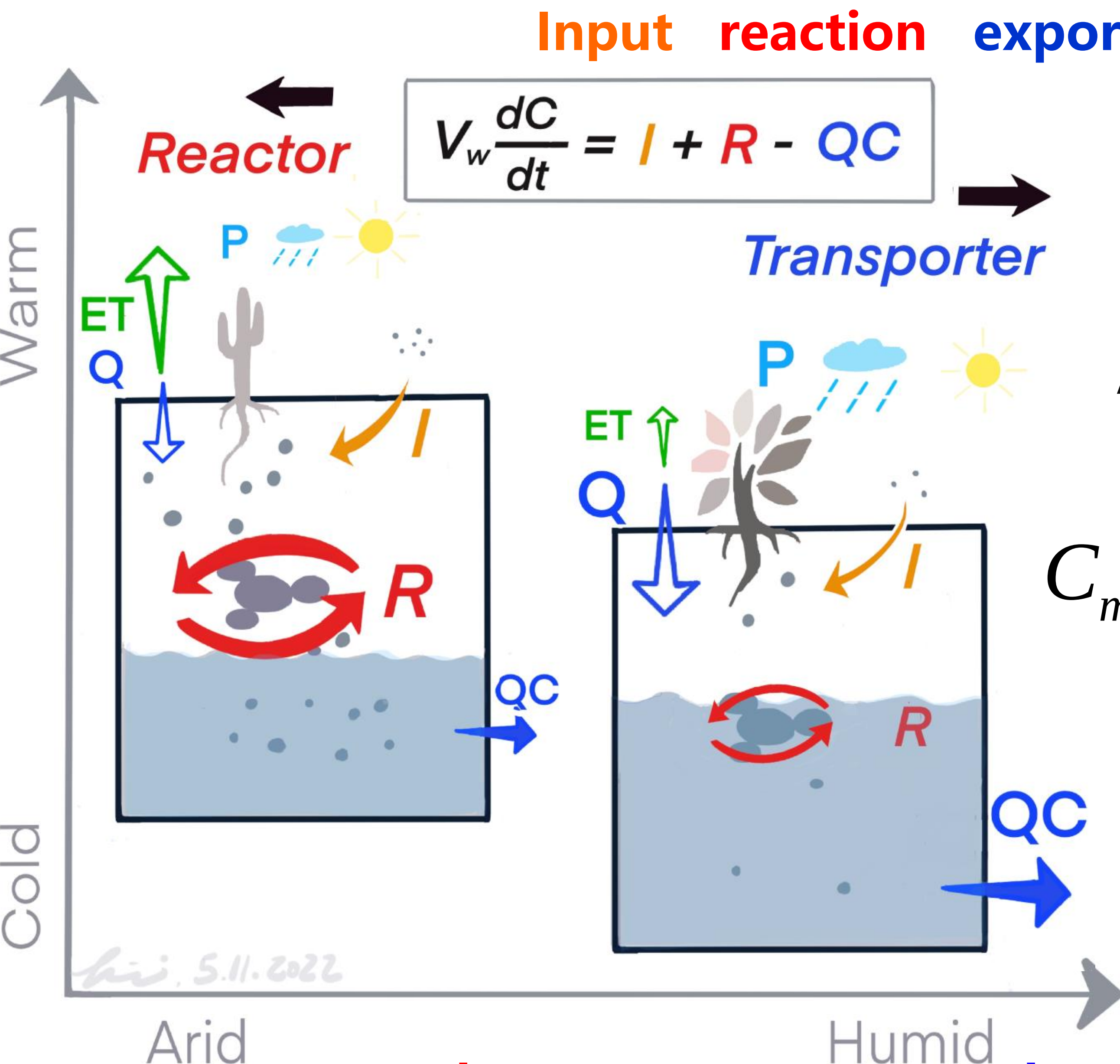




Aridity increase, Conc. increase



A Watershed Reactor Model



At steady-state:

$$C_m = \frac{R_m}{Q_m}$$

reaction

export

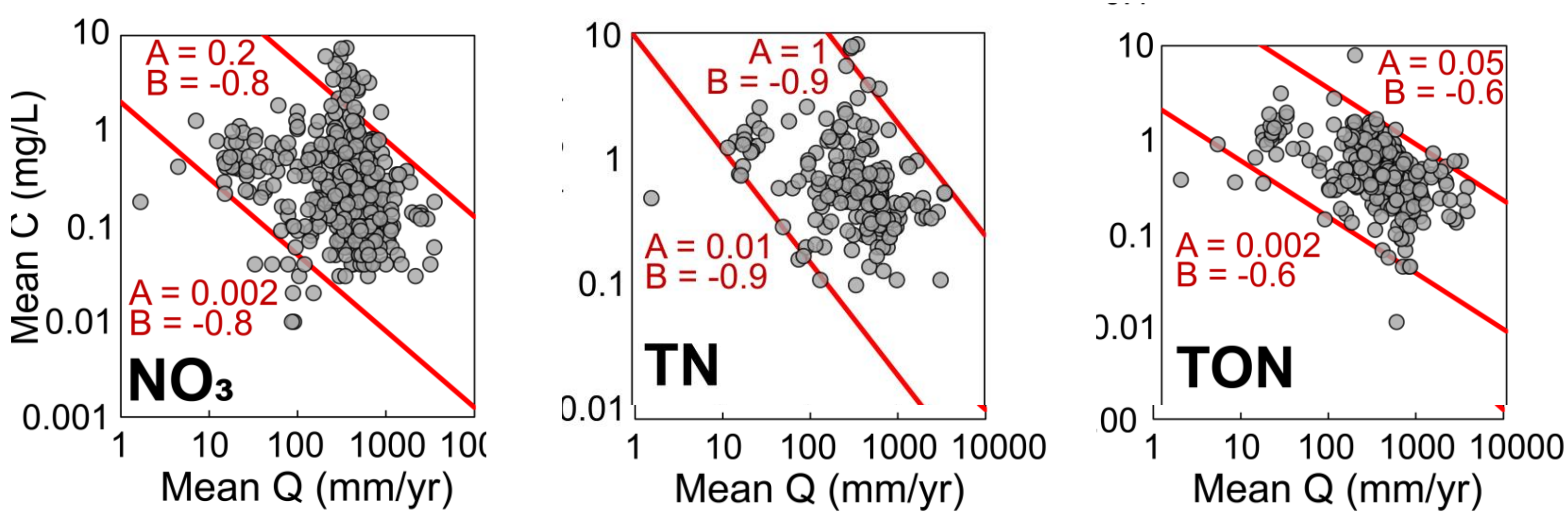
Less connected **More connected**

Long-term $C_m Q_m$ Relationships

$$C_m = \frac{R_m}{Q_m}$$

$$\boxed{C_m = A Q_m^{\,B},} \quad A = k_0 S_A f(T) \alpha_0^{\left(-\frac{n}{\beta_0}\right)}, \; B = \frac{n}{\beta_0} - 1$$

Rates **Sensitivity to water content**



....

More arid → higher conc; more humid → lower conc

As aridity increases, water quality will decline

Summary

- **Deep learning application in water quality is still growing**
- **Temporal and spatial data filling to reconstruct consistent data series**
- **More data do not mean better performance**
- **Consistent data → temporal trend + spatial analysis**
  - Urban rivers warm up fastest; ag rivers lose oxygen fastest
  - Rivers and streams warm up and lose oxygen faster than oceans and slower than lakes.
  - Temperature (> light> flow) is the predominant driver
- **High solute concentrations in more arid places**

Lots of Opportunities to Explore

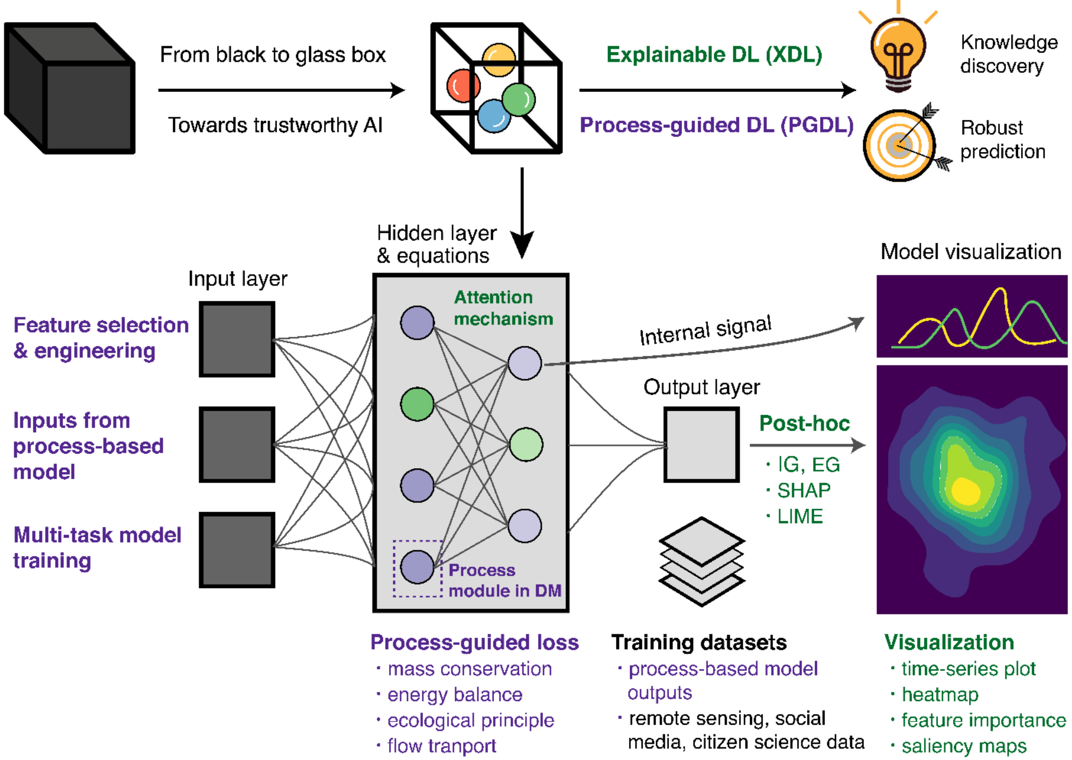
- **Data availability will still be the bottle neck!!!**
- **Interconnected water quality variables?**

  Master variables (T, pH, DO);

  Data-rich variables → data-scarce variables
- **Process-based + deep learning models**

  Neural ODE (Hoge et al., 2023); Differential modeling (Shen et al., 2023)
- **Explainable AI**

From Black Boxes to Glass Boxes



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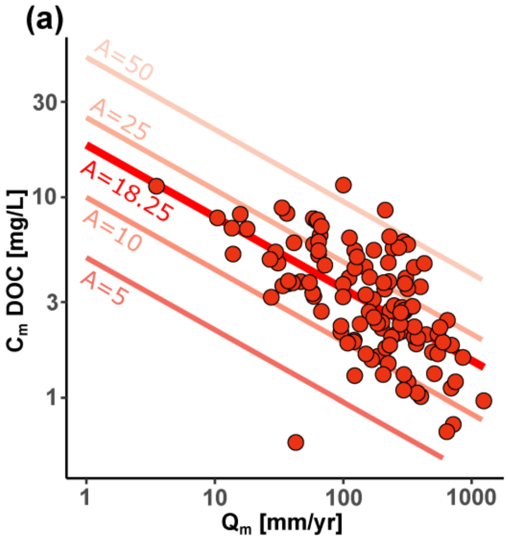
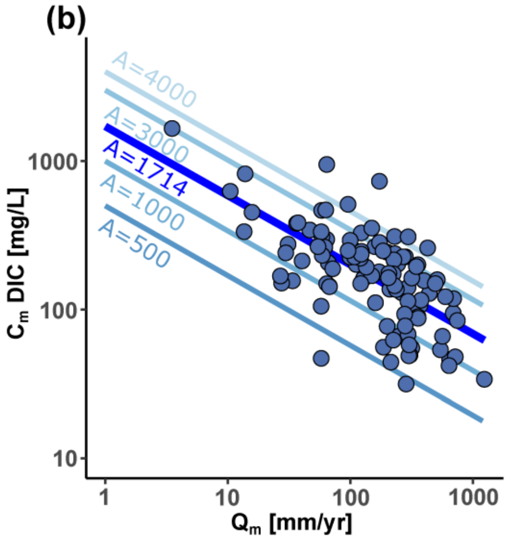
Climate has a major control,

Rocky Mountains regional scale

Dissolved Organic Carbon (DOC) **Inorganic Carbon (DIC)**

$$C_m = AQ_m^{\ B}$$

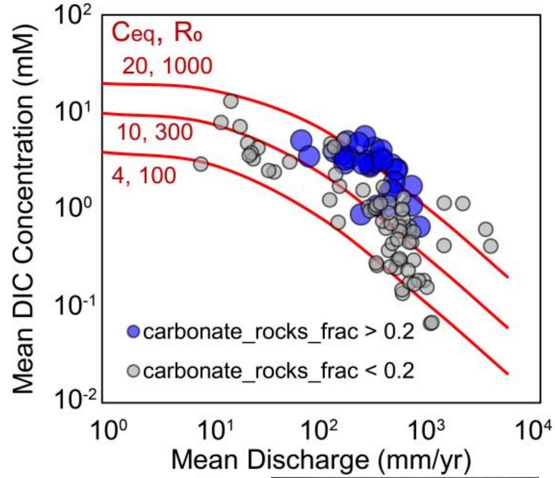




Kerins and Li, 2023; Stewart et al., 2022

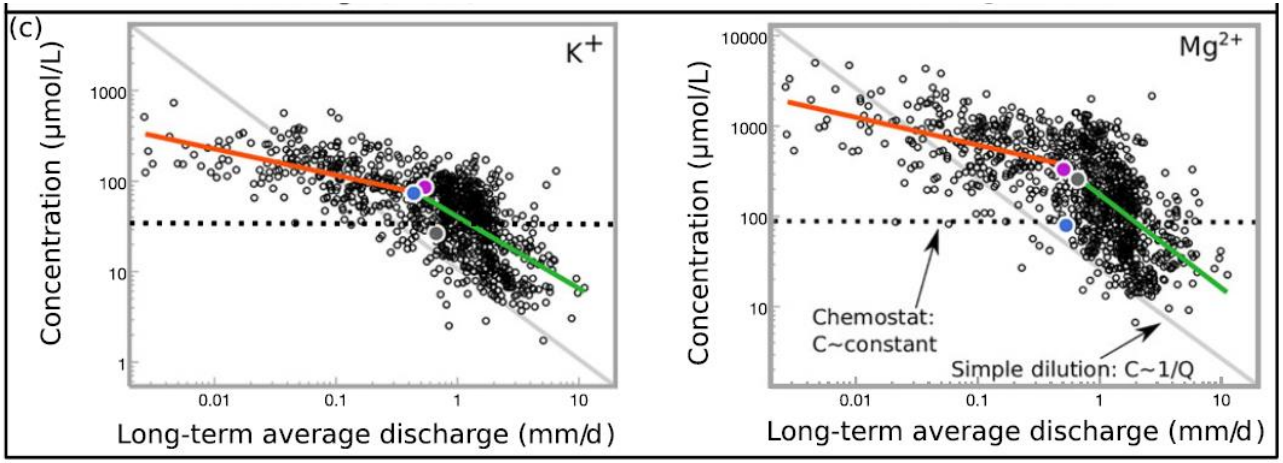
Contiguous United States

DIC



$$C_m = \frac{C_{eq} R_0}{Q_m C_{eq} + R_0}$$

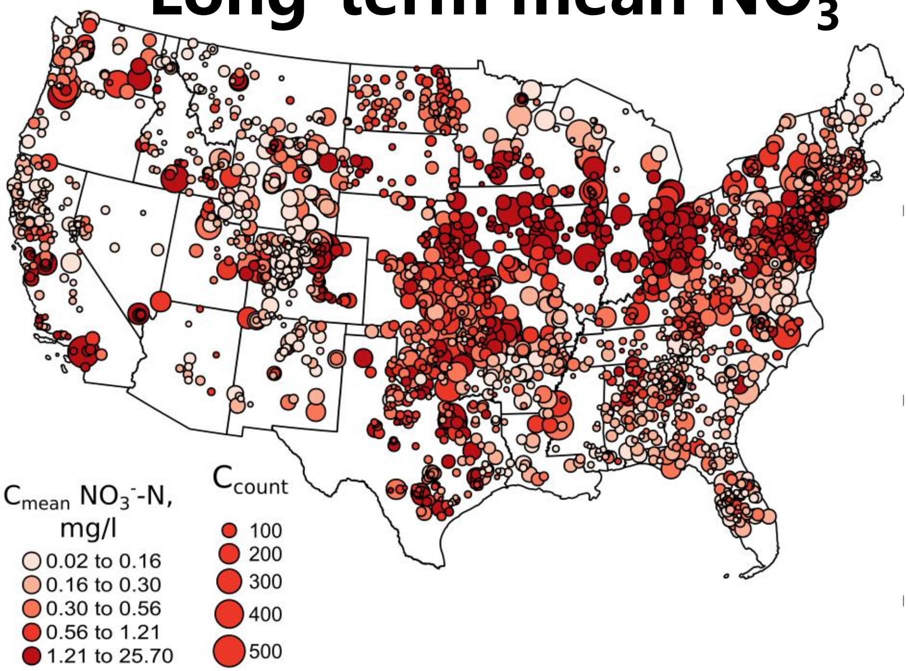
Global Scale

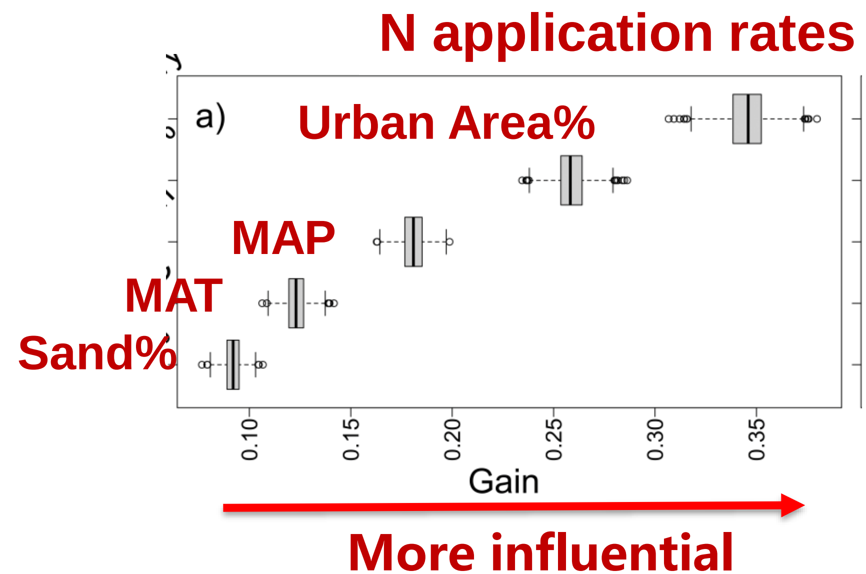


Godsey et al., 2019

… but human stressors are more influential

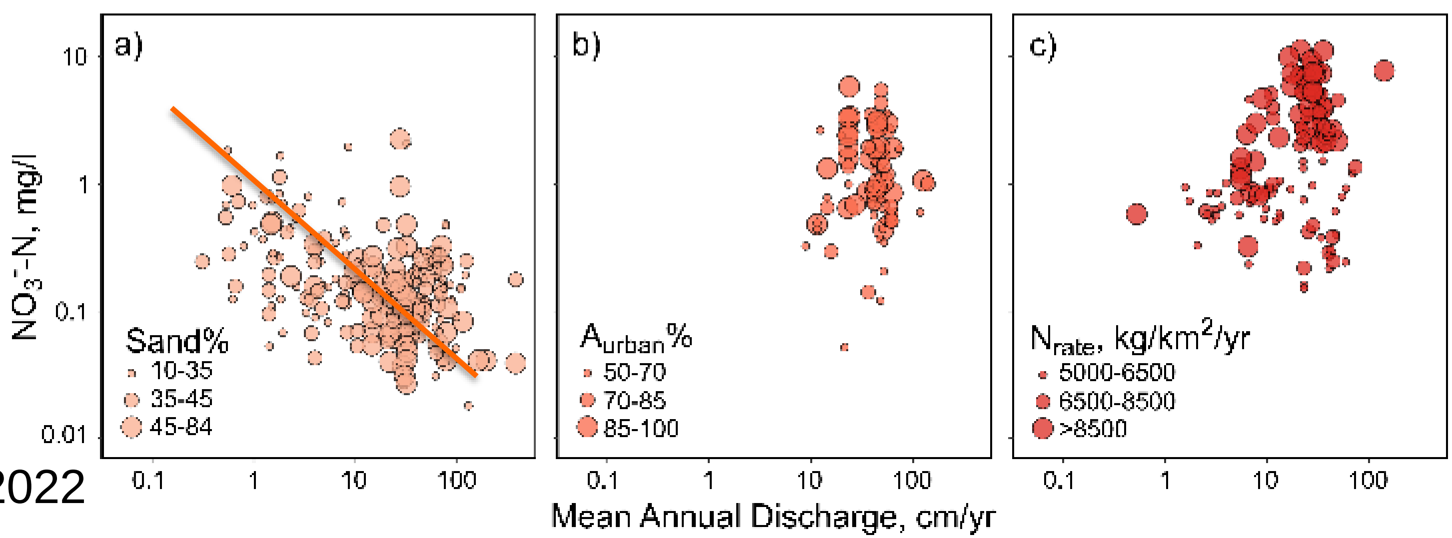
Long-term mean NO_3





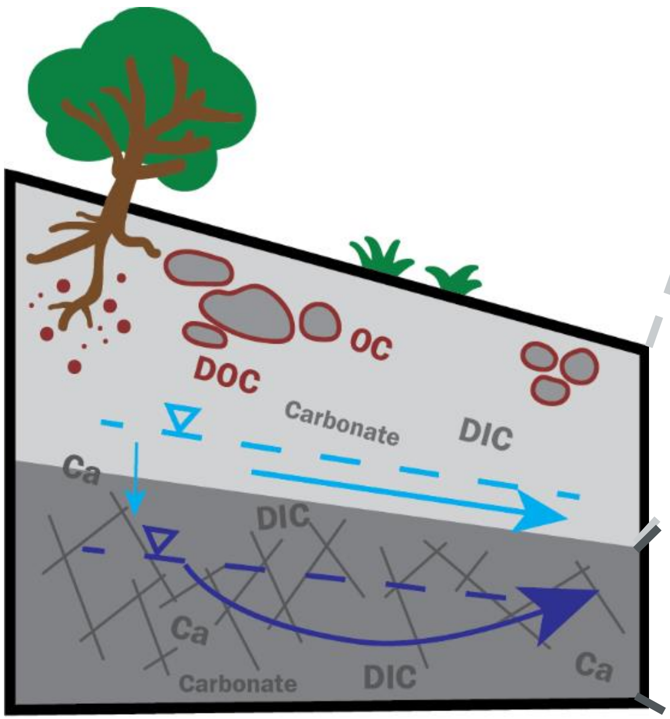
Sadayappan et a., 2022

Undeveloped **Urban** **Agriculture**



2. Illuminating the black box: Biogeochemistry

Reactions in shallow + deep zones
using BioRT-HBV model, a watershed Reactive Transport Model



Shallow Zone Reactions:

Soil Respiration + C decomposition:

$OC_{(s)}$ + roots → DOC + DIC

Carbonate Weathering:

$Carbonate_{(s)}$ ←→ Ca^{2+} + DIC

Deep Zone Reactions:

Deep Respiration + C decomposition :

$OC_{(s)}$ + DOC → DIC

Carbonate Weathering:

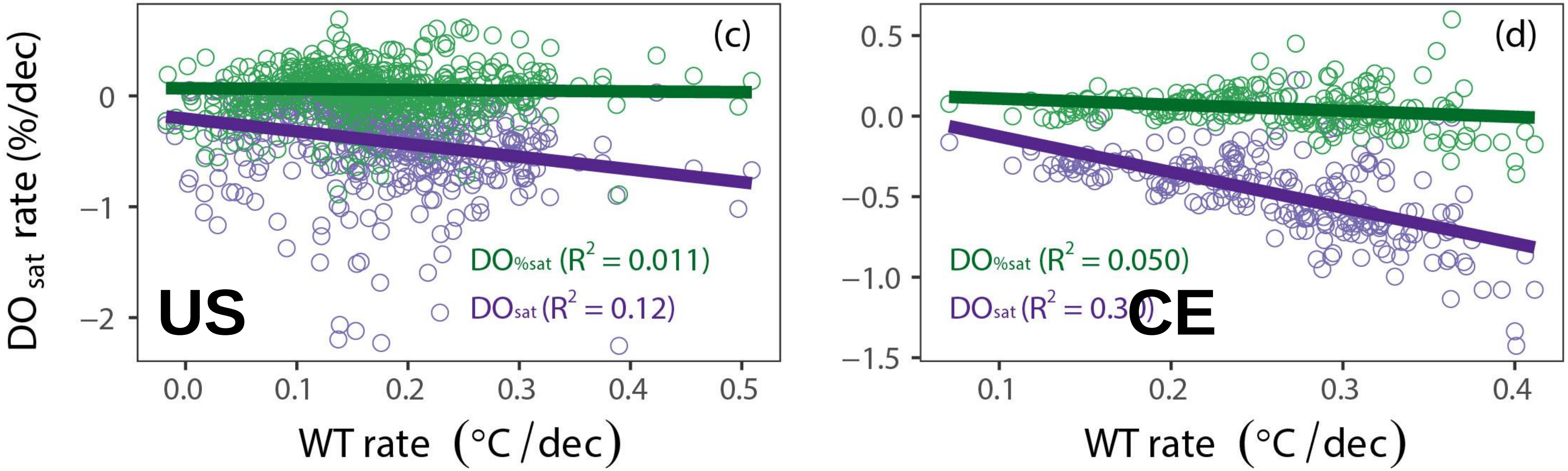
$Carbonate_{(s)}$ ←→ Ca^{2+} + DIC

Example reactions from Sleepers Rivers, Stewart et al., in preparation

Sadayappan et al., BioRT-HBV model, in preparation

After normalizing T influence, other factors come into play.

$DO_{\%sat}$ change does not depend on WT change



DO_{sat} change depends on WT change

PennState