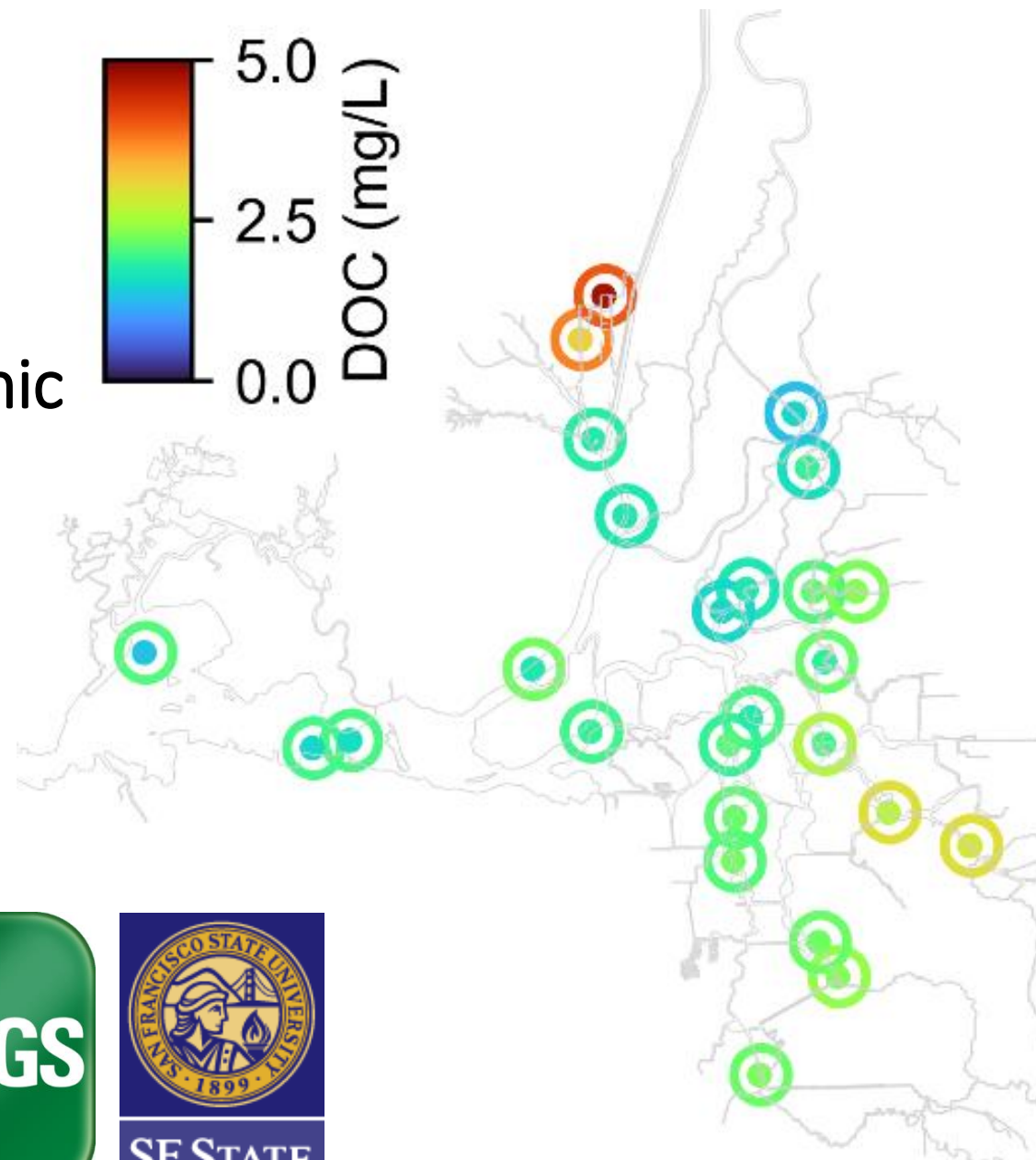


Tracer-Based Dissolved Organic Carbon (DOC) Modeling

Edward Gross, Rusty Holleman, Tamara Kraus, Brian Bergamaschi, Matt Young, Wim Kimmerer

September 2024



Original Research Goals (UCD project)

Goal:

“...combine modeled transport and biogeochemical observations to estimate net rates of nutrient cycling and primary production across habitat types and time-periods.”

- Original focus on Cache Slough Complex
- Quantify relative contributions of different Dissolved Organic Carbon sources
- Quantify contribution of DOC to food web
 - Labile DOC enters food web
- Other uses of work
 - DOC is a precursor to disinfection by-products formed during water treatment

Biogeochemical Modeling Approaches

Option 1: Box model

- Fast, simple
- Ignore or drastically simplify transport

Option 2: Coupled hydrodynamics and biogeochemistry

- Transport affects transformation
- Slow

Option 3: Tracer-based Lagrangian model

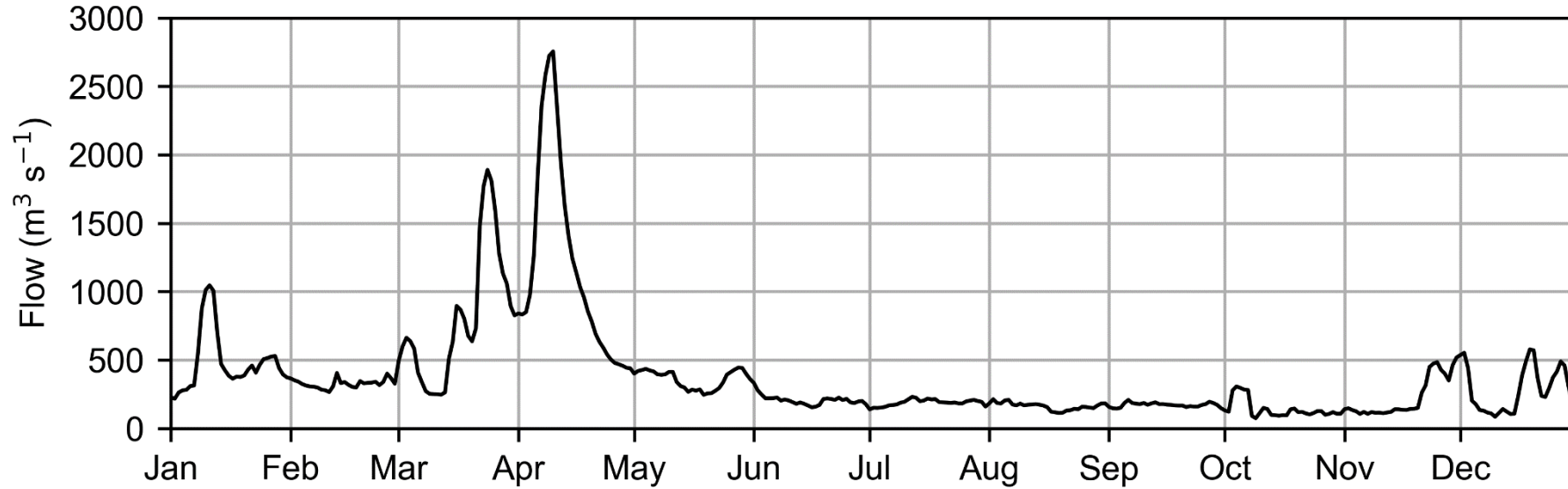
A box model where “the box is moved around by the hydrodynamics.”

Why Use Extremely Fast Models?

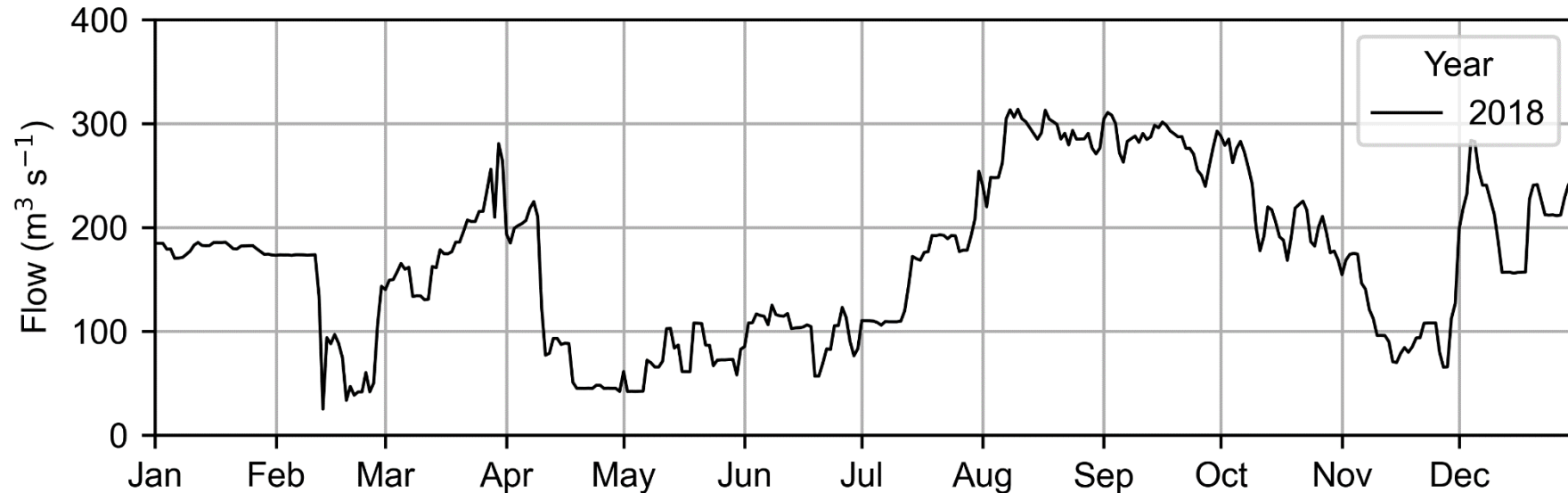
- Appropriate equations not known *a priori*
 - Justifiable level of complexity depends on how well parameters can be constrained
- Biogeochemical rate parameter values uncertain
 - May vary spatially and seasonally
- Contributions of individual sources uncertain
- Can quantify uncertainty using Bayesian inference

2018 Flow Conditions (Below Normal)

Net Delta Outflow



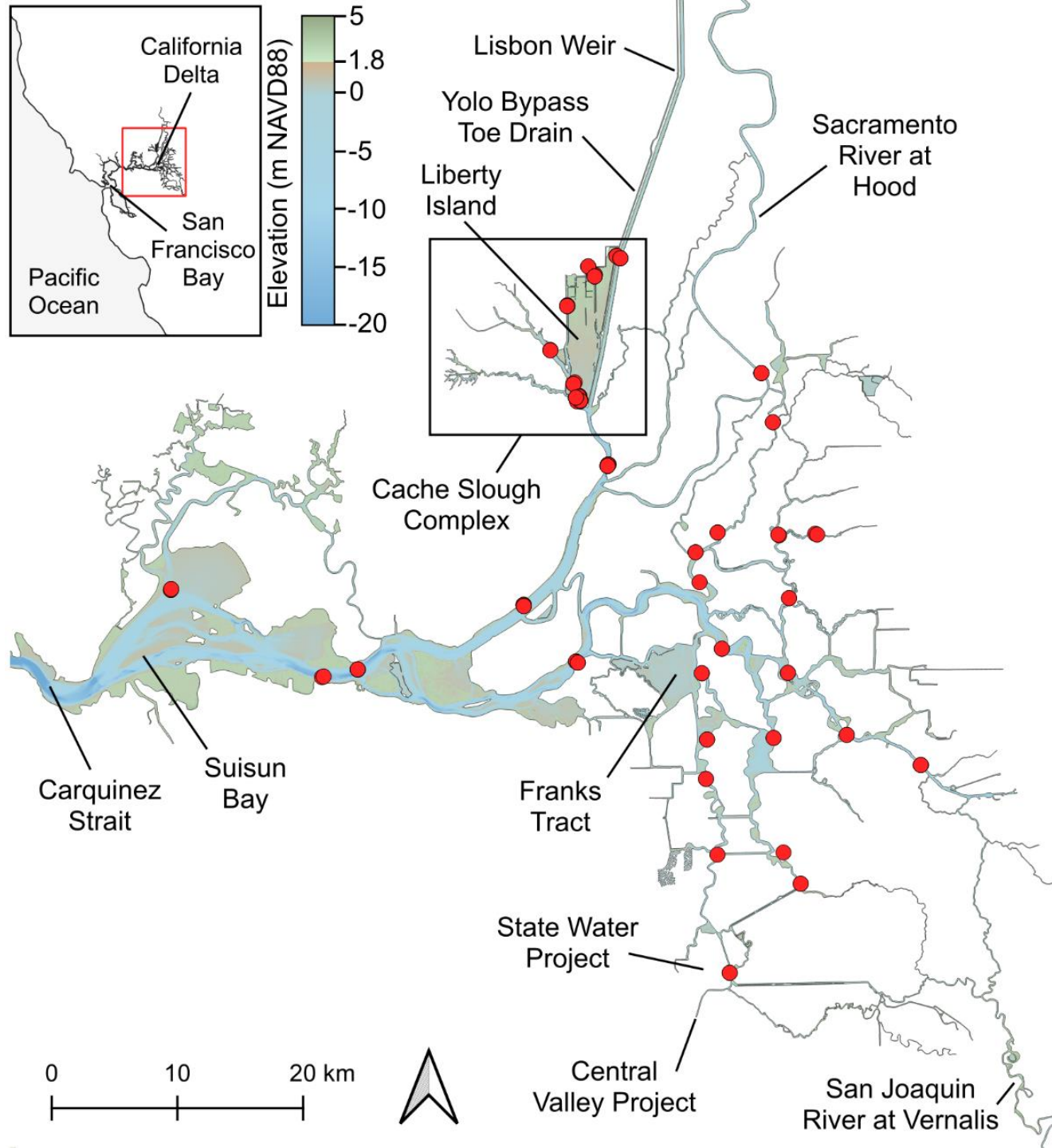
Diversion Flow



DOC Data Sources for Jul-Oct 2018

- USGS discrete sampling during underway cruises - **Calibration**
 - 94 discrete samples from July through October 2018
 - 63 discrete samples for “whole Delta” cruises
 - 31 discrete samples for NDFA (Cache Slough Complex) cruises
 - 53 discrete samples in French Island and Little Hastings Tract (“AV” study) – **Not used**
- DWR Municipal Water Quality Investigations (MWQI) samples
 - Discrete samples – **Validation (not shown)**
 - 139 discrete samples from July through October 2018 at discrete monitoring stations
 - Real Time Data and Forecasting stations
 - Hood and Vernalis - **Boundary Conditions**
 - Toe Drain data - **Boundary Condition**
 - Banks and Jones pumping plants observations - **Validation**

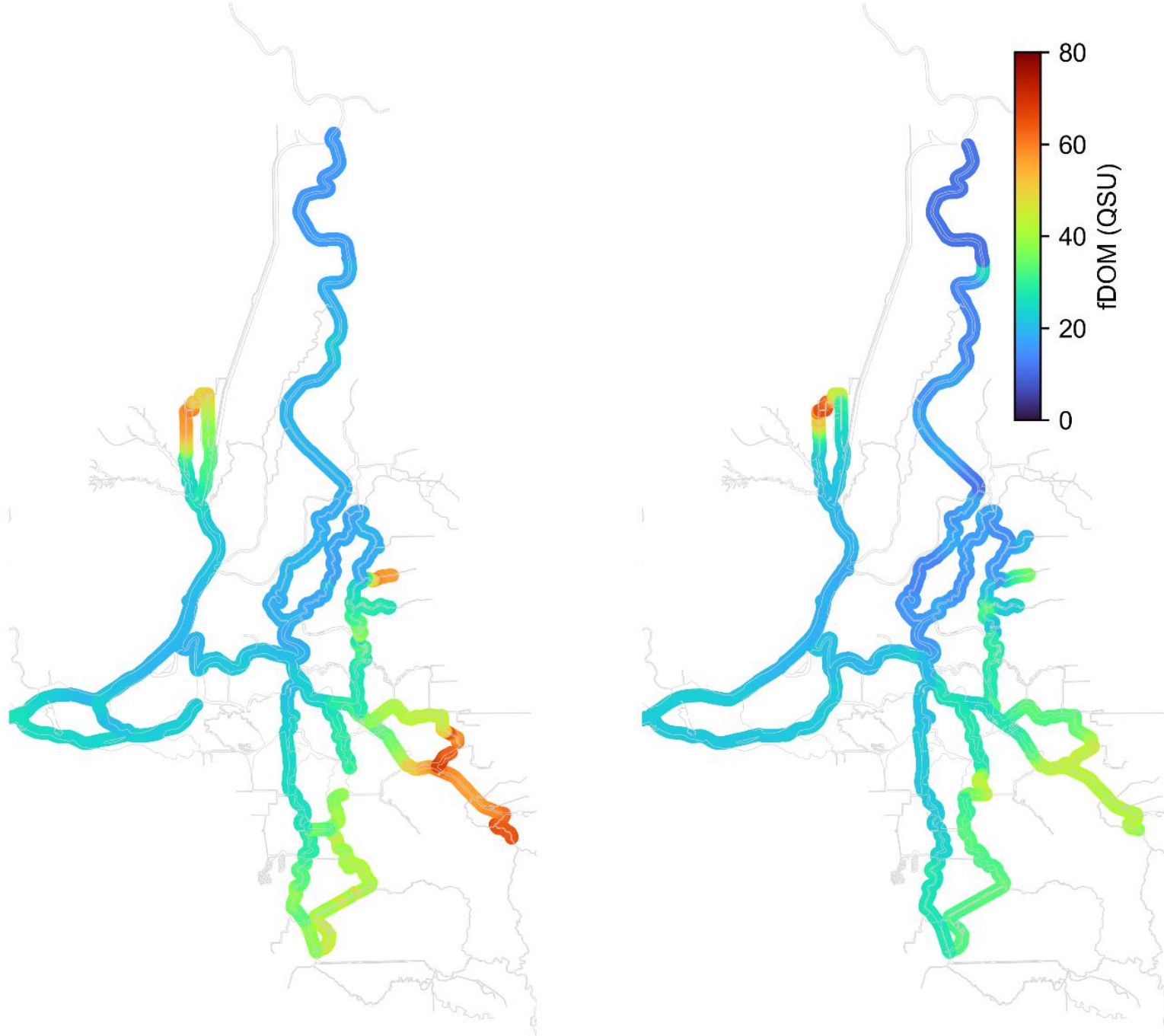
USGS discrete DOC
sampling locations in
study period of Jul-Oct
2018



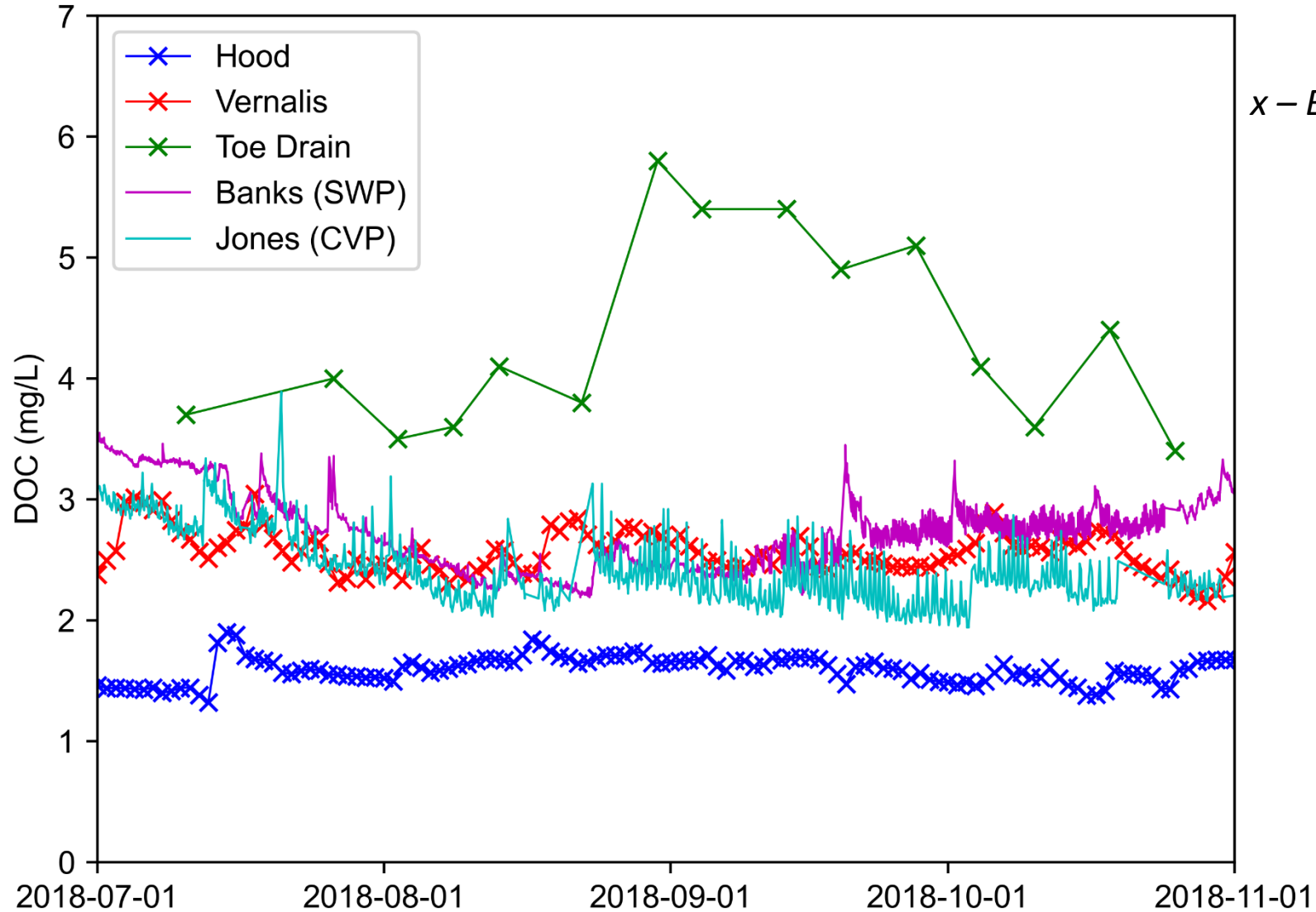
USGS high-speed
mapping fDOM
Observations

July 24-26, 2018

October 17-19, 2018

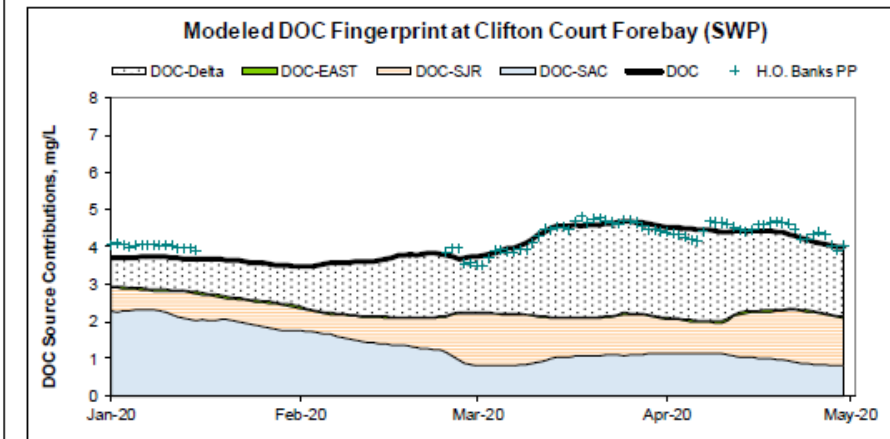
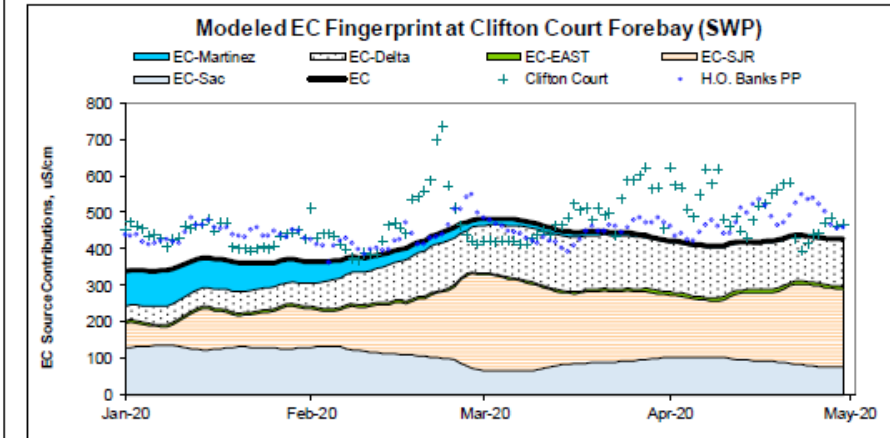
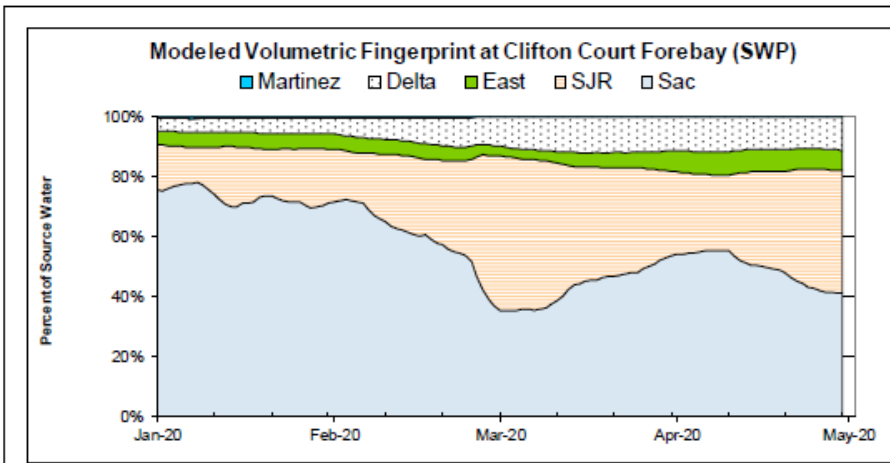


DWR MWQI Real Time Data and Forecasting (RTDF)



Previous DOC Modeling Work

- Used DSM2-QUAL tracers for fingerprinting of sources
- Utilized measured incoming DOC concentrations
- Compared with DOC observations
- Estimated contributions from individual sources at diversions
- MWQI investigations summarized in Hutton et al. 2022



Review

The Municipal Water Quality Investigations Program: A Retrospective Overview of the Program's First Three Decades

Paul H. Hutton¹, Sujoy B. Roy^{1,*}, Stuart W. Krasner² and Leslie Palencia³

DOC Model Formulation Components

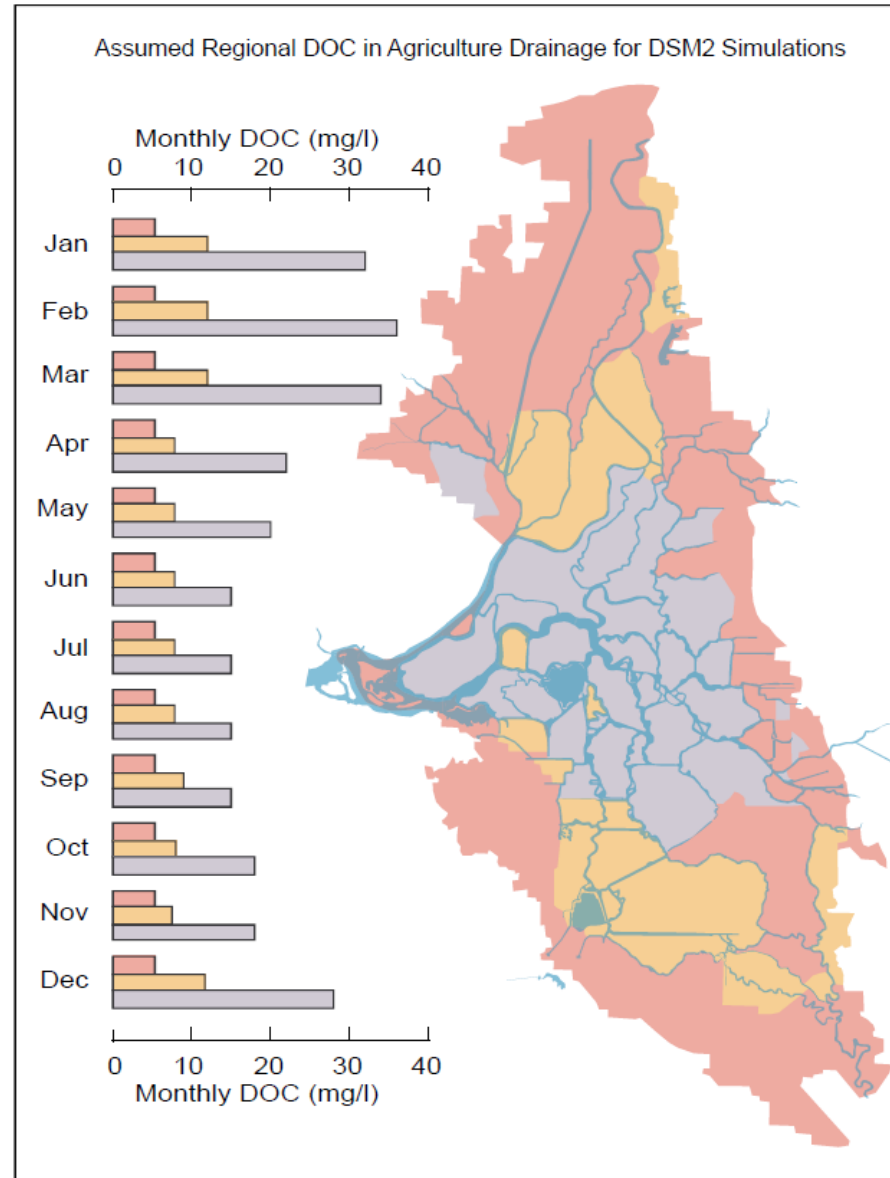
- 7 DOC Sources
 - Water sources (5)
 - Sacramento River
 - San Joaquin River
 - Agricultural returns (DICU)
 - Yolo Bypass Toe Drain
 - All other freshwater to the Delta
 - Plant sources of DOC inside model domain (2)
 - Marsh plants
 - Aquatic vegetation
- Two fractions
 - Refractory
 - Labile

Components added in this study are in red

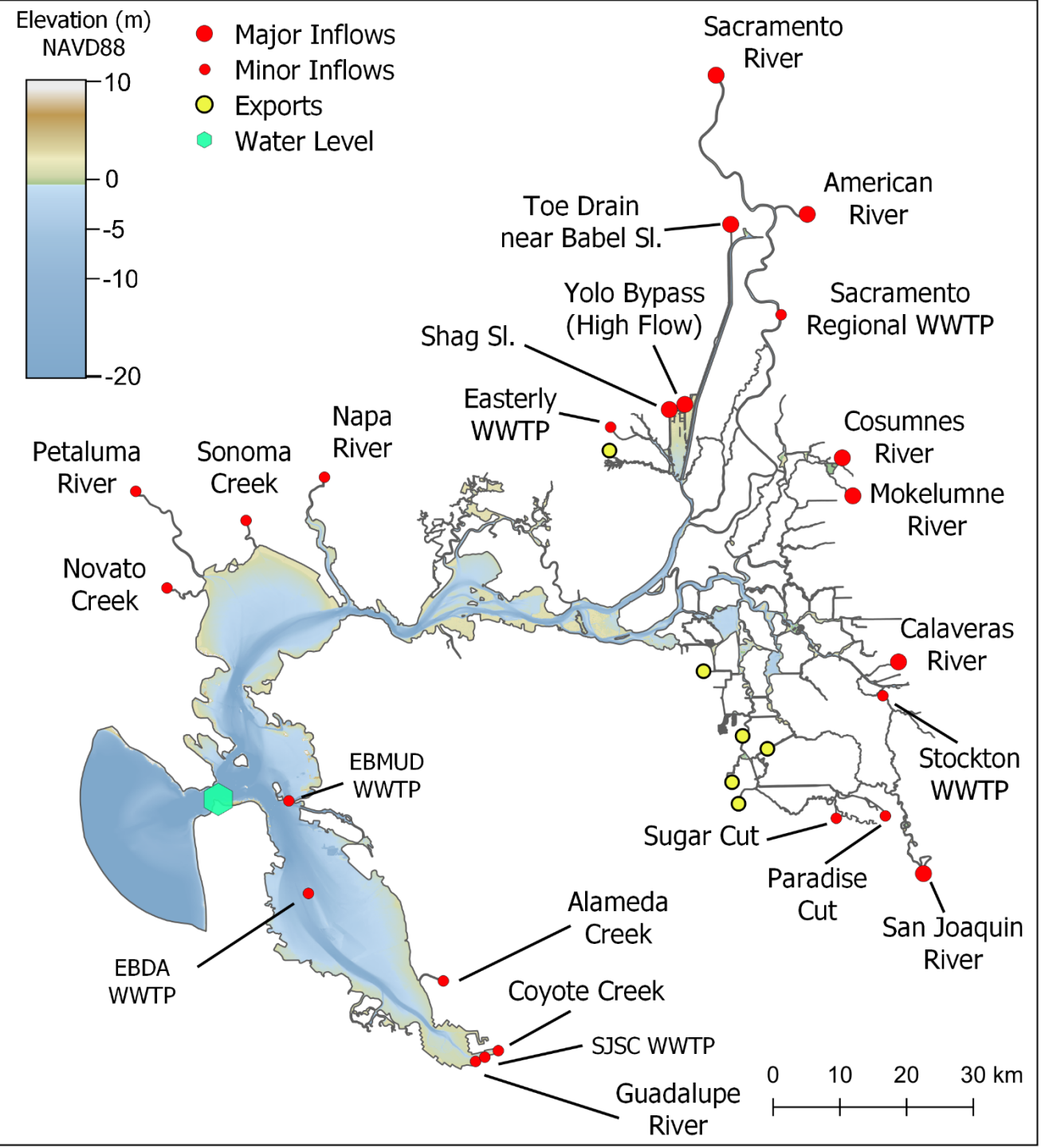
Novel Aspects of Our Work

- **Fast** offline model
 - ~0.6 milliseconds on laptop computer
 - Bayesian inference using ~200,000 model runs completed in ~2 minutes
- Using **age tracers** to account for time lag between time of entry of “source water” and arrival at observation point
- Using age tracers in DOC **decay** terms
- Accounting for **marsh and aquatic vegetation** contributions
- Using **Bayesian Inference** to identify confounding and uncertainty of parameters
- After fitting to DOC, comparing to high spatial resolution **fDOM** data

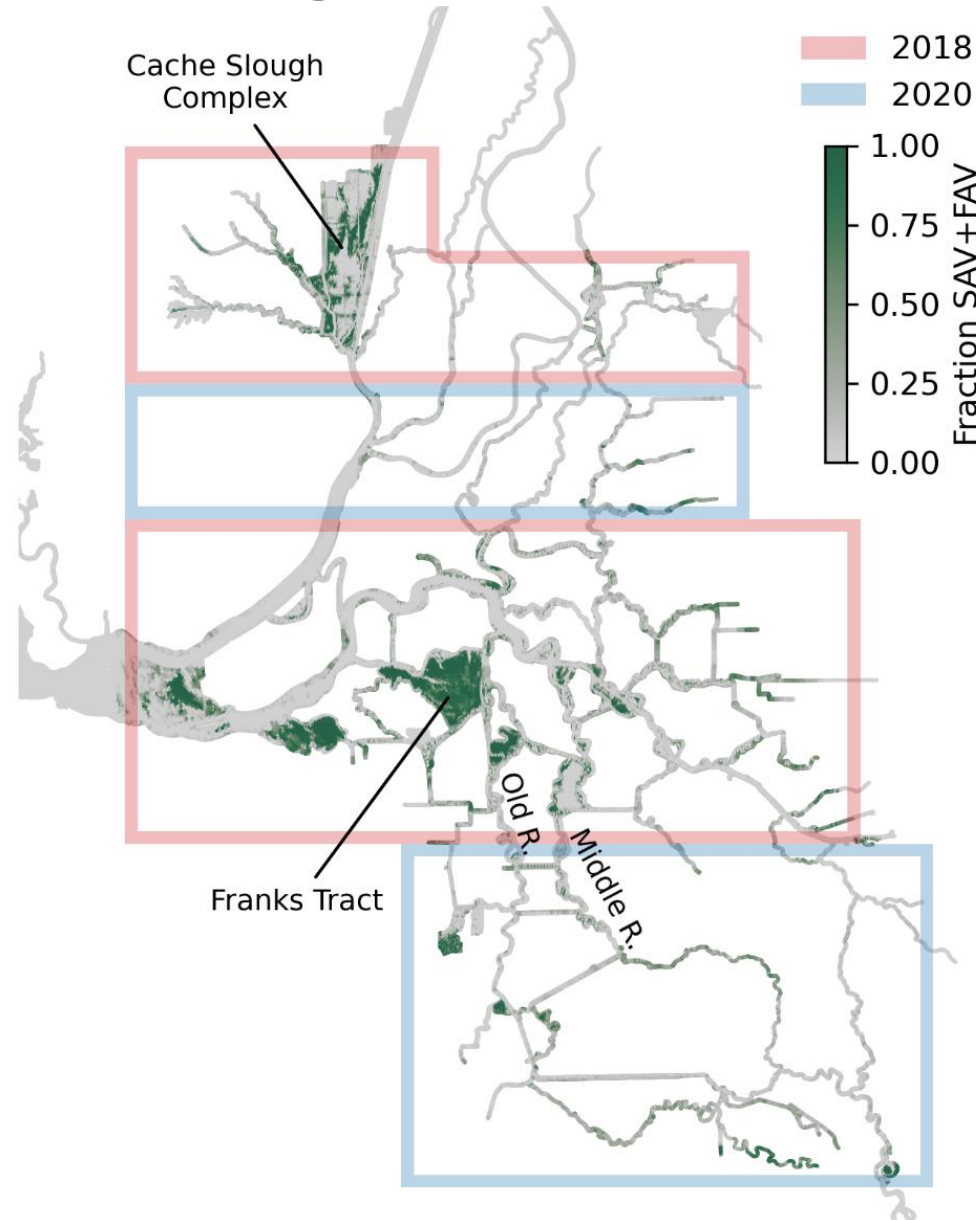
Approach Does NOT (yet) Use Variable Ag. DOC



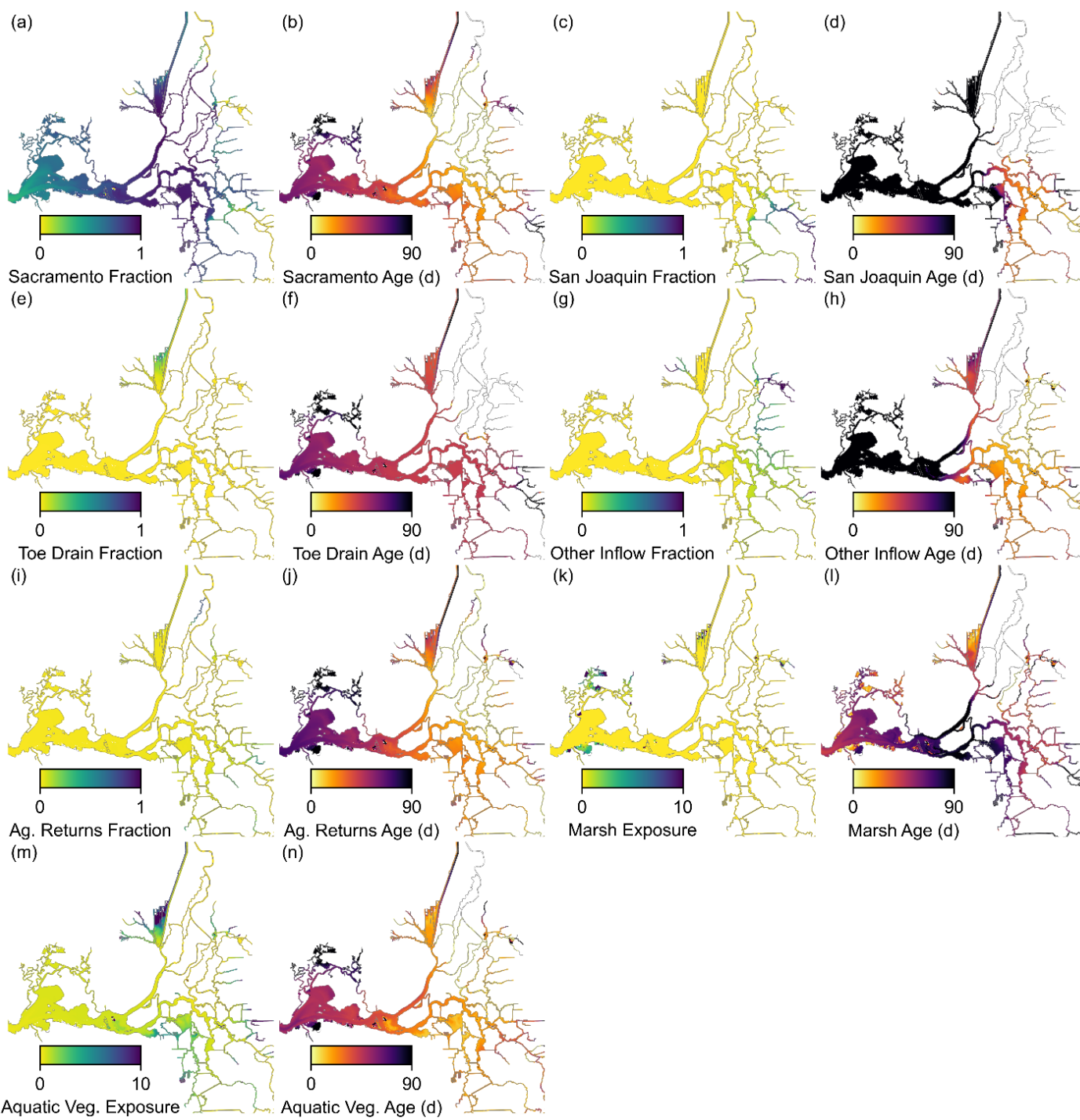
RMA San Francisco Estuary UnTRIM Boundary Conditions



Aquatic Vegetation Distribution



Data from Khanna et al. 2022

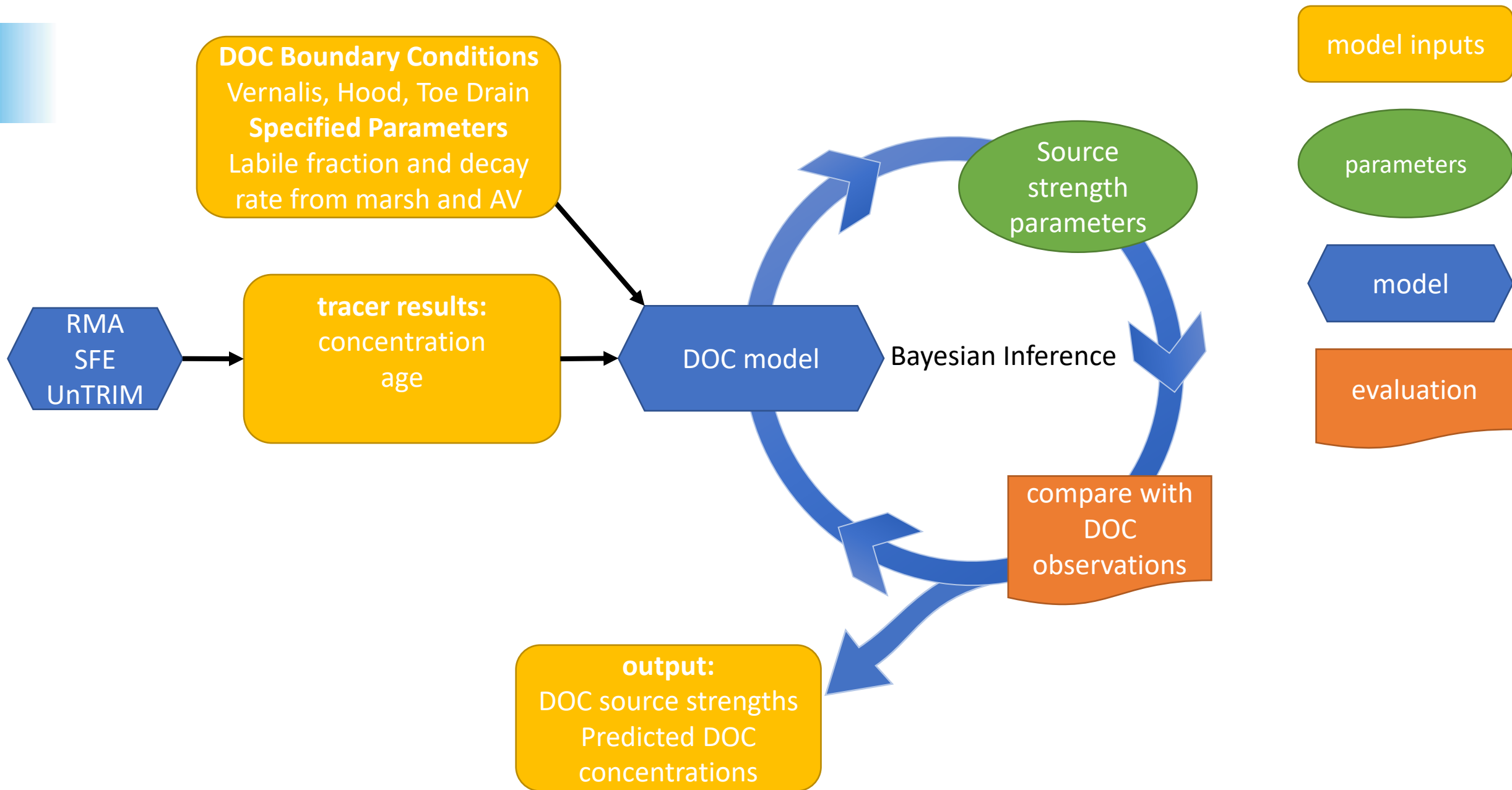


DOC Governing Equations Including Labile Fraction

- Sources with known concentration: Sacramento, San Joaquin, Toe Drain
 - $D_x(t) = D_{in,x}(t - a_x)(1 - f_x + f_x * e^{-ka_x})$ for $x = s, j, t$
 - Incoming time-varying concentration known (measured)
- Unknown concentrations: other freshwater (o), agricultural returns (a)
 - $D_x(t) = D_{in,x}(1 - f_x + f_x * e^{-ka_x})$ for $x = o, a$
 - Incoming concentration **unknown**, assumed constant
- DOC concentration from inflows as volume-weighted average
 - $D_w(t) = C_s D_s(t) + C_j D_j(t) + C_t D_t(t) + C_f D_f(t) + C_a D_a(t)$
 - Average by source concentration (which sum to 1)
- Add marsh (m) and aquatic vegetation (v) contributions
 - $D_x(t) = S_x C_x(1 - f_x + f_x * e^{-ka_x})$ for $x = m, v$
 - S_x is **unknown** source strength (mass/area*time)
 - f is fraction labile

Specified Parameters

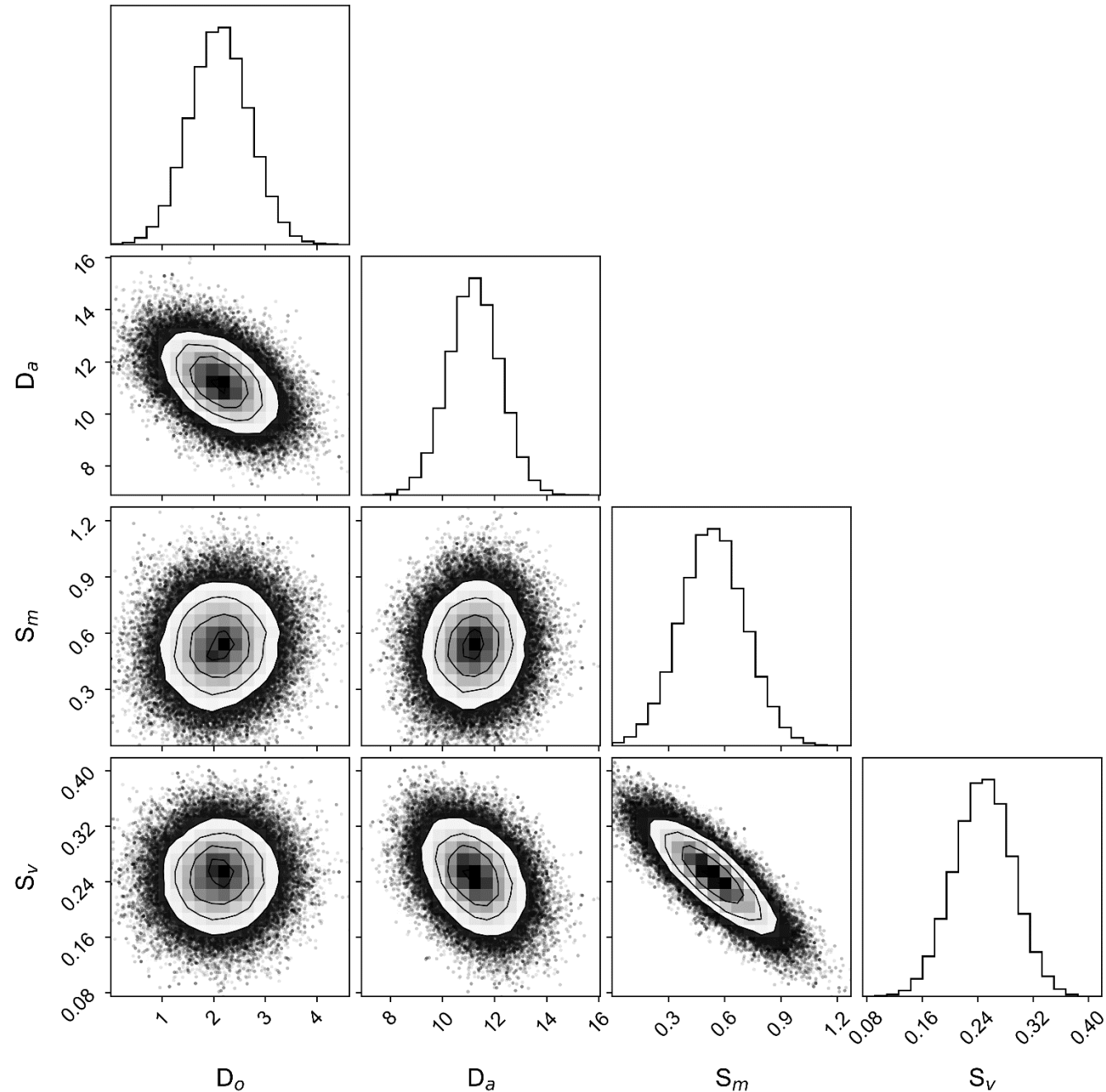
- Fraction labile and decay rate based on Stepanauskas et al. 2005
 - Samples incubated over two weeks and to estimate “DOC bioavailability”
 - We assumed 90% of labile material transformed in those two weeks
 - Decay coefficient $k = 0.164 \text{ d}^{-1}$
 - Used summer samples only (values in paper are averaged across seasons)
 - Labile fractions:
 - Sacramento River: $f_s = 0.150$ (based on samples from Hood)
 - San Joaquin River: $f_j = 0.128$ (based on samples from Vernalis)
 - Toe Drain: $f_t = 0.091$ (based on samples from Shag Slough)
 - Other: $f_o = 0.128$ (based on samples from Vernalis)
 - Ag returns: $f_a = 0.085$ (based on samples from Twitchell Island)
 - Marsh: $f_m = 0.057$ (based on samples from Brown’s Island)
 - Aquatic vegetation: $f_m = 0.143$ (based on samples from Franks Tract)



Bayesian Analysis

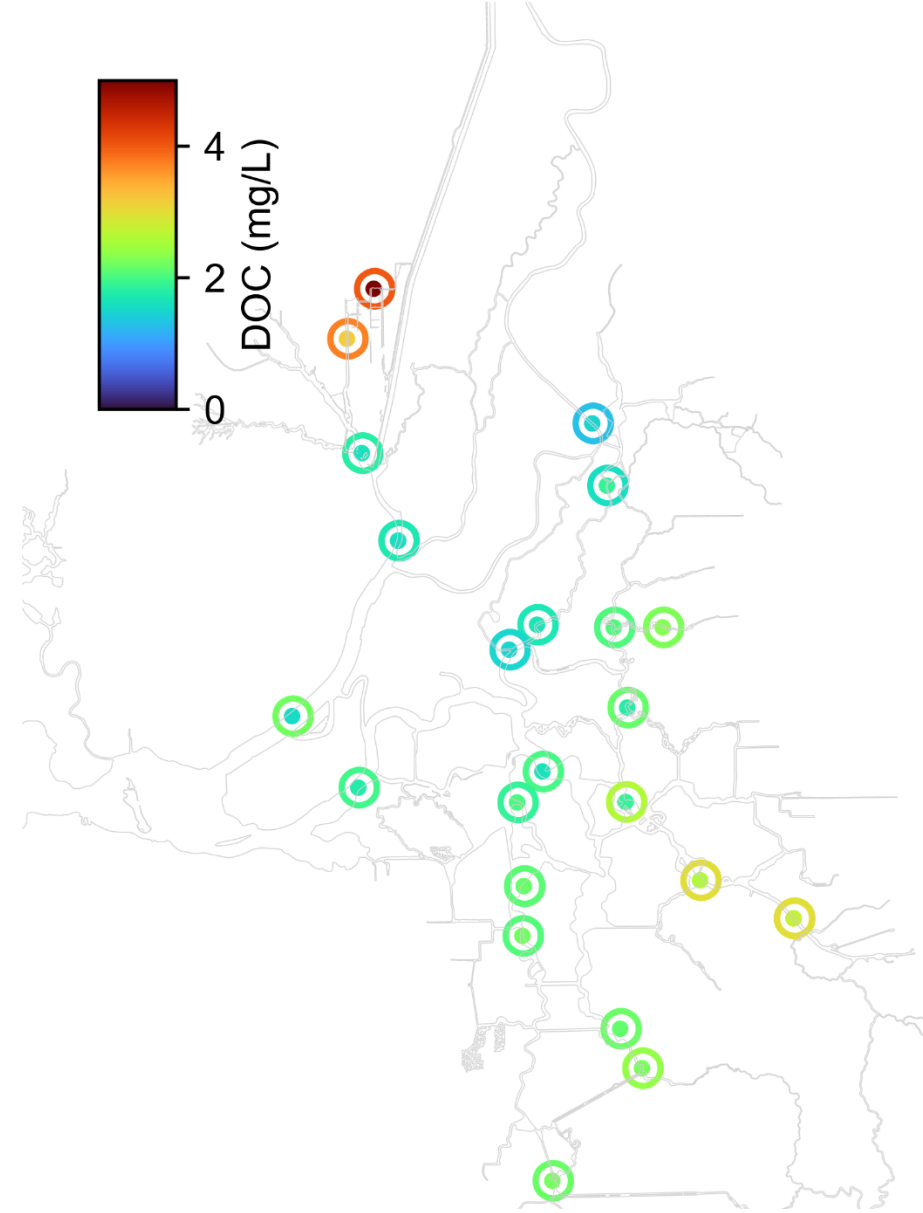
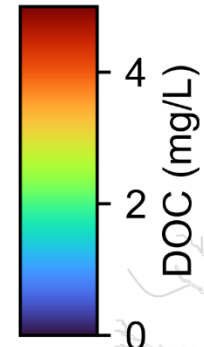
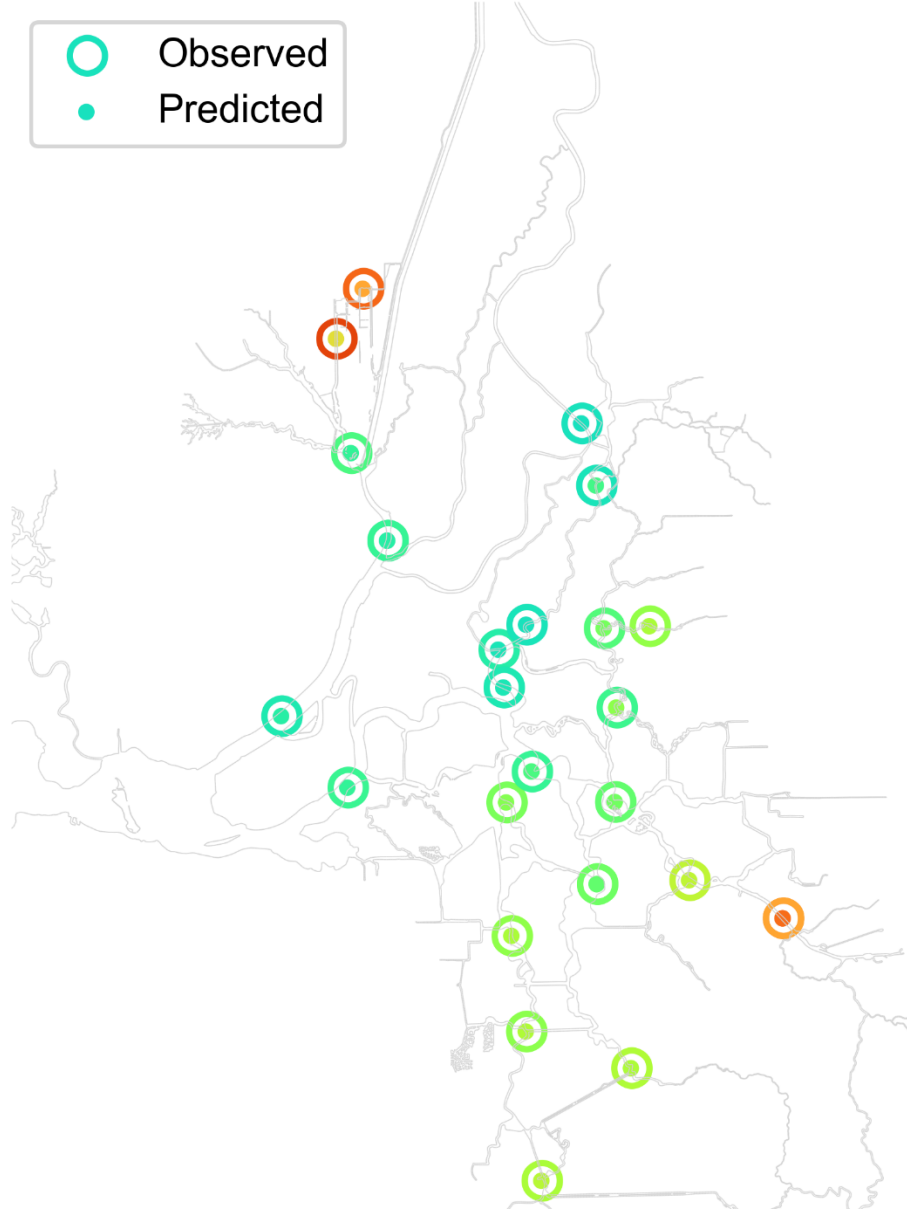
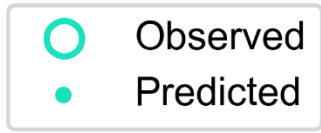
Parameter	Description	MLE	Interquartile Range		Units
D_o	Other inflows	2.058	1.725	2.498	mg L ⁻¹
D_a	Ag. returns	11.249	10.541	11.876	mg L ⁻¹
S_m	Marsh source	0.522	0.421	0.651	g m ⁻² d ⁻¹
S_v	SAV/FAV source	0.250	0.220	0.277	g m ⁻² d ⁻¹

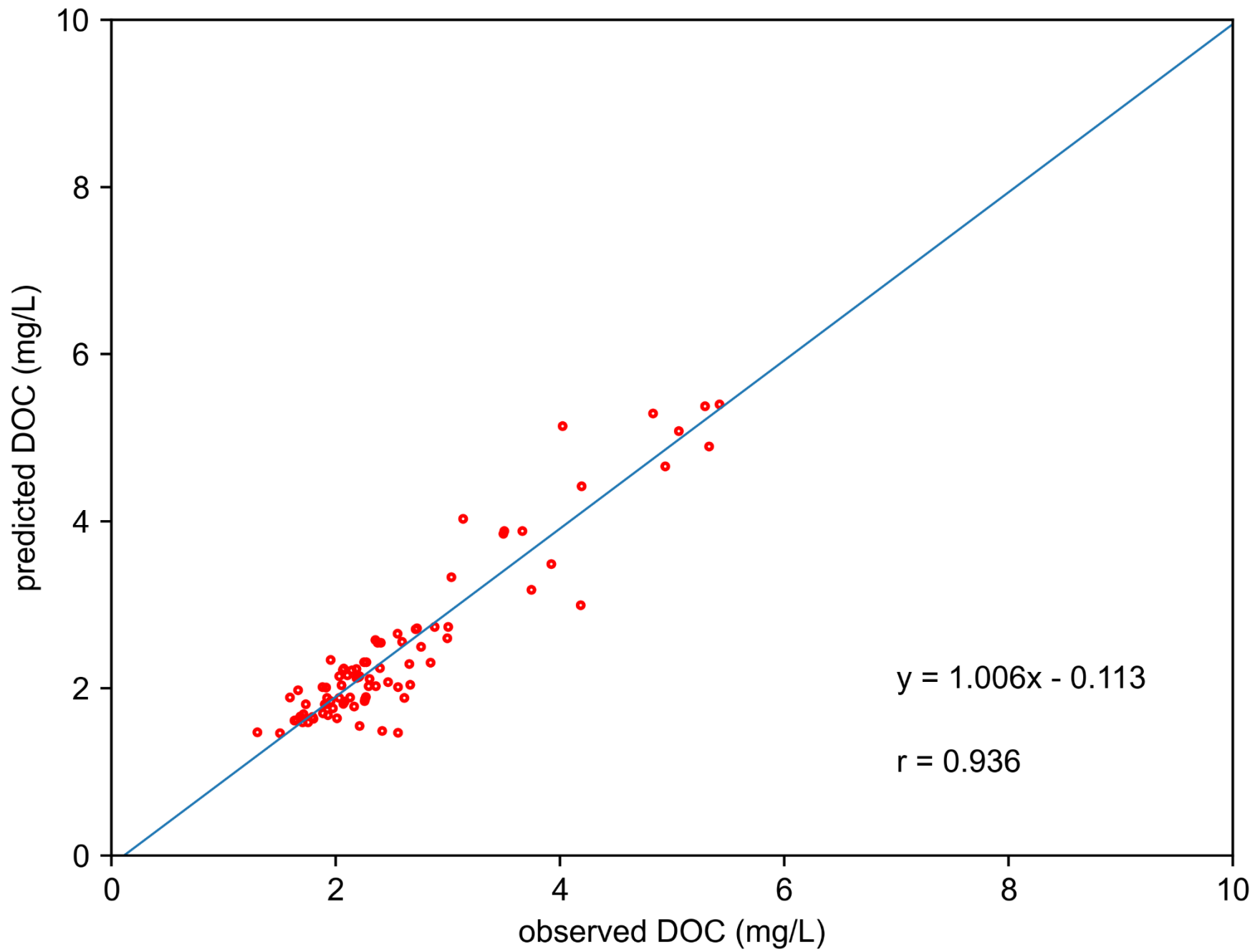
- Corner plot indicates that
 - Marsh and AV contributions are strongly confounded
 - “Other flows” and agricultural return contributions are significantly confounded



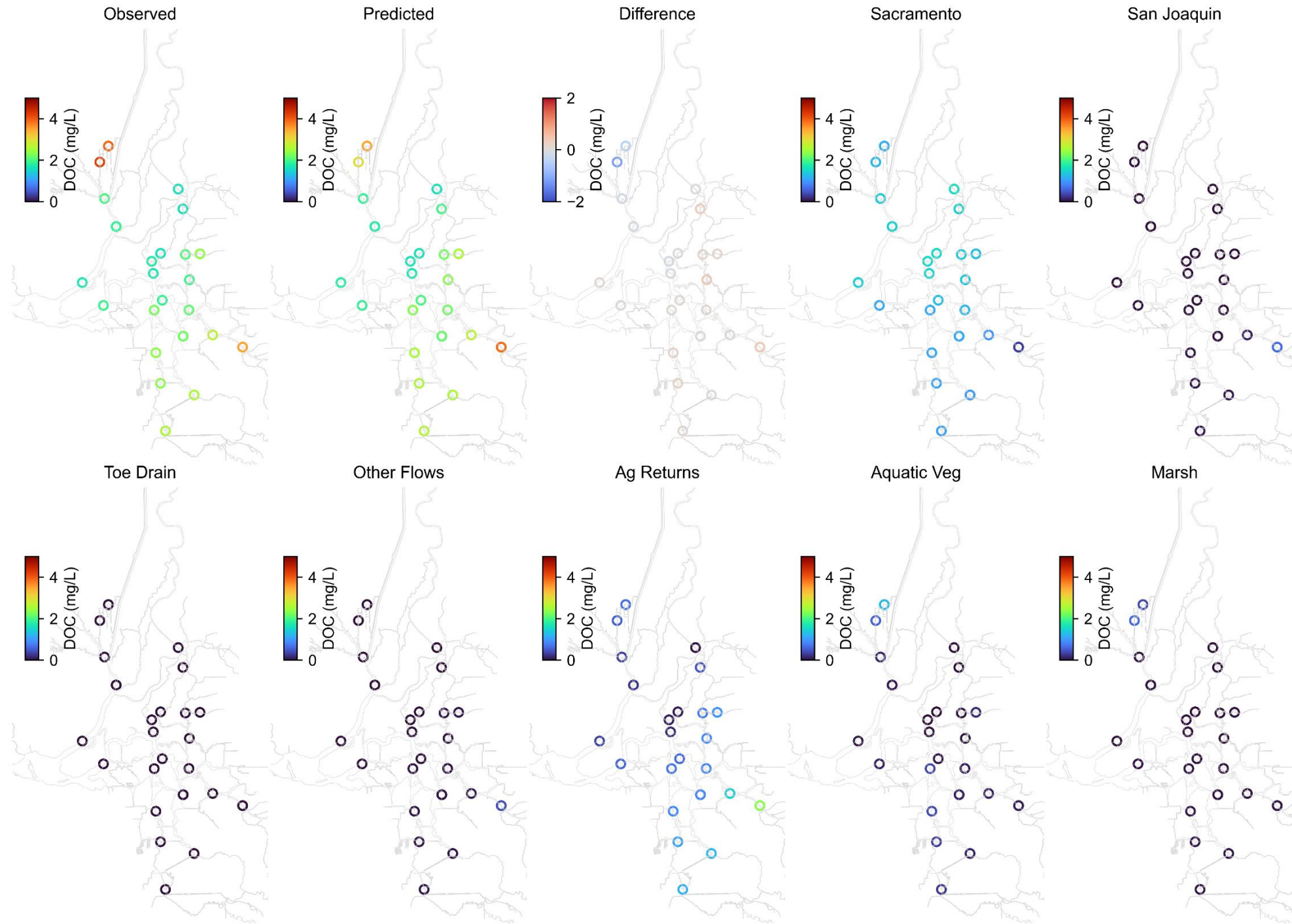
July 24-26, 2018

October 17-19, 2018

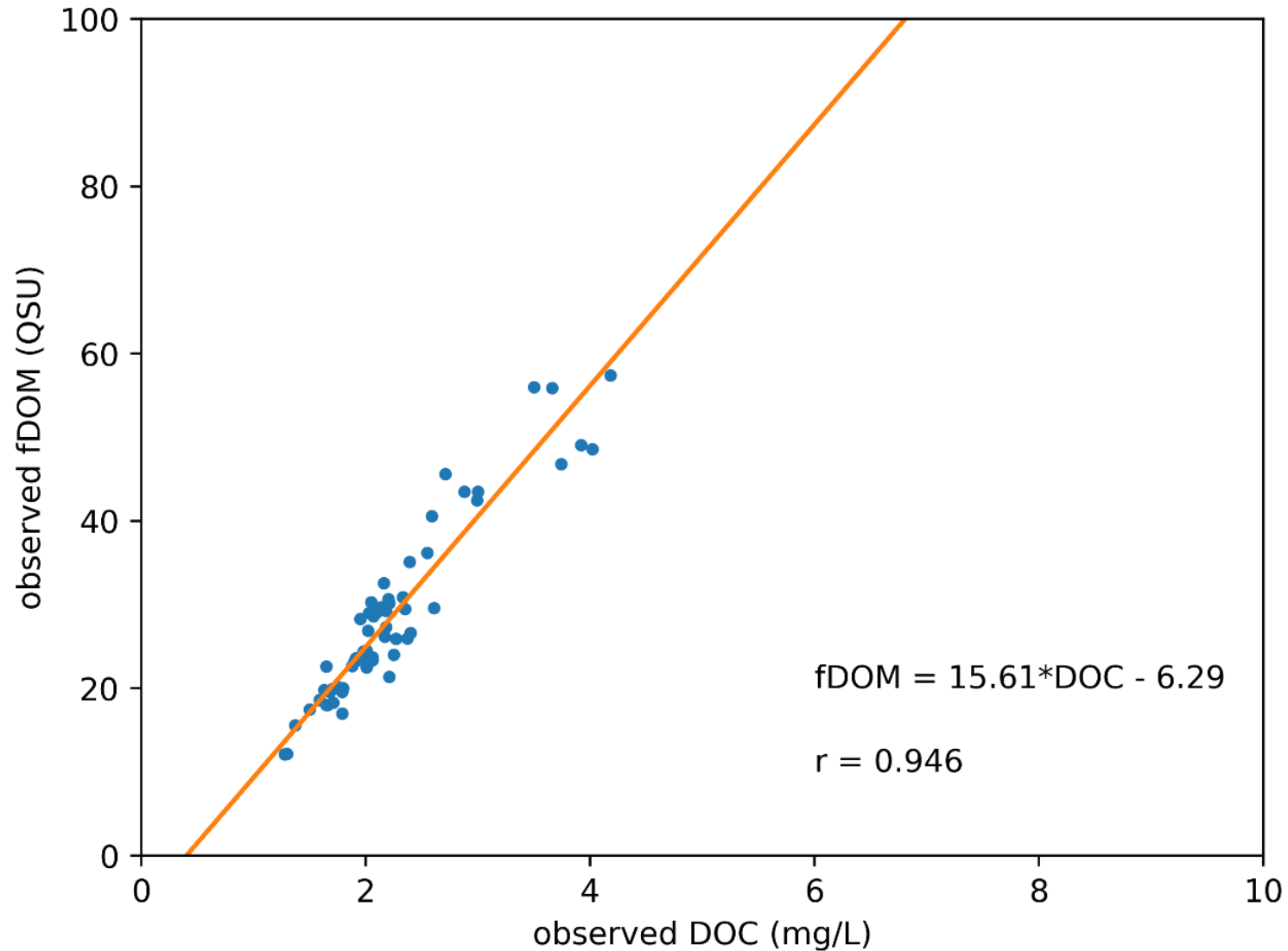


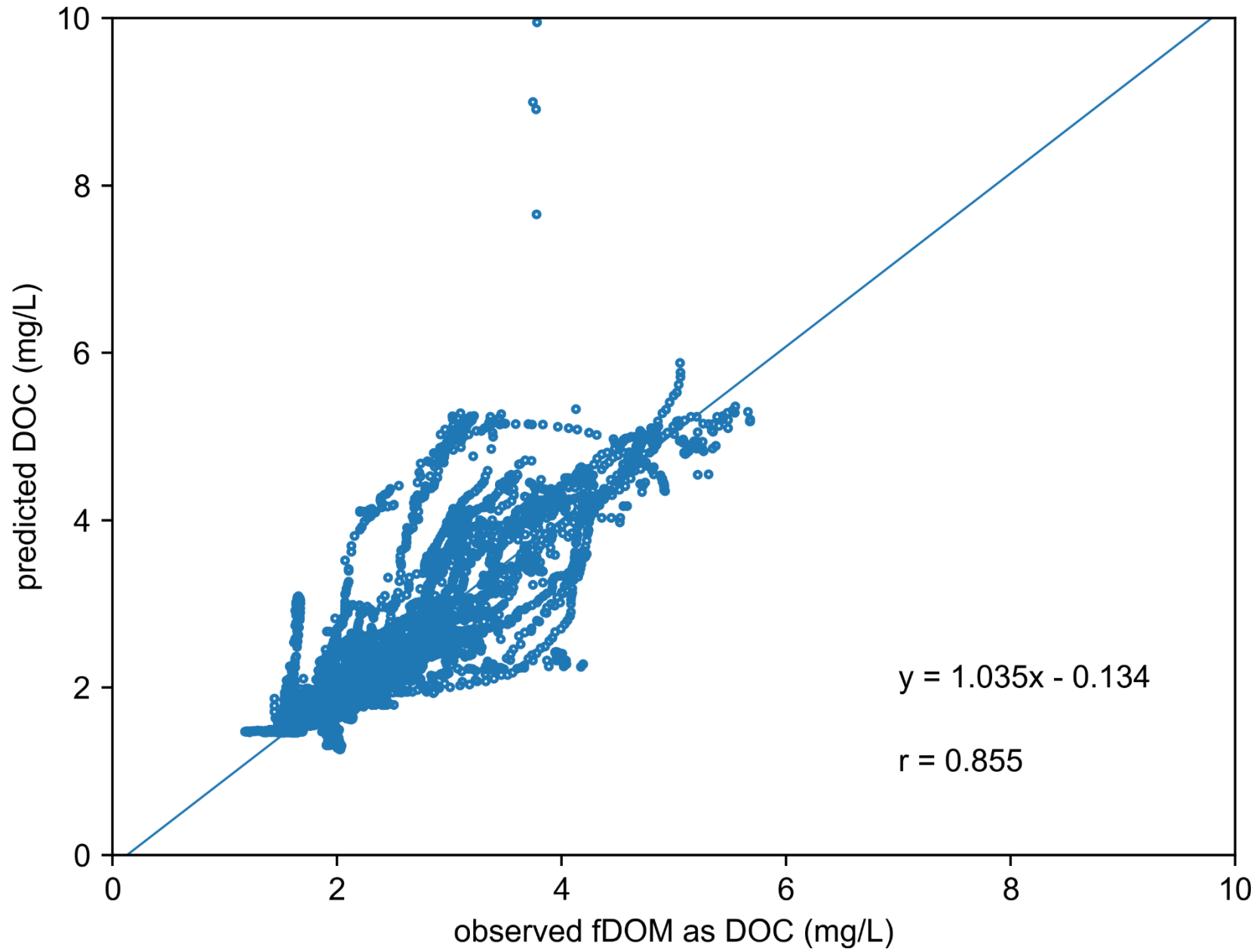


July 24-26
2018

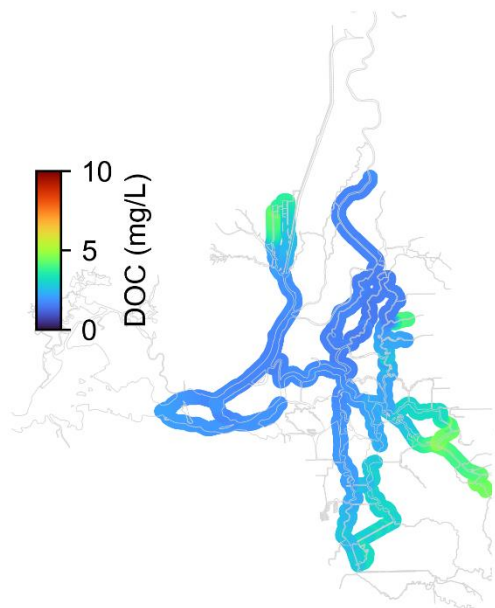


USGS High-Speed Mapping fDOM vs. Discrete DOC

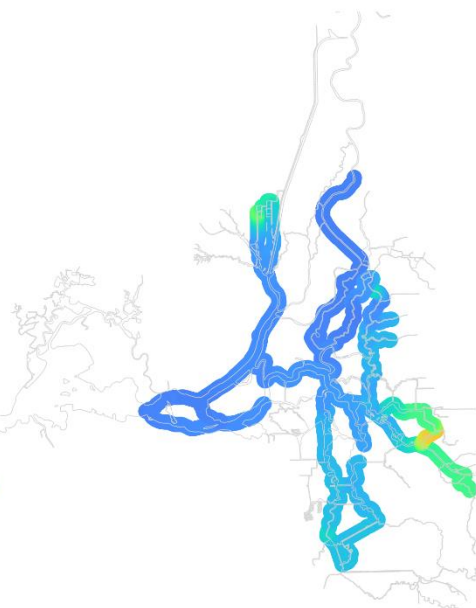




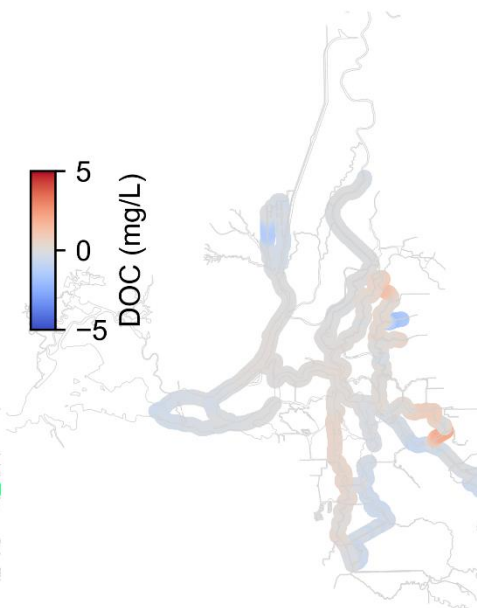
Observed fDOM as DOC



Predicted DOC



DOC Difference



Sacramento



San Joaquin



July 24-26, 2018
Ag Returns

Toe Drain



Other Flows



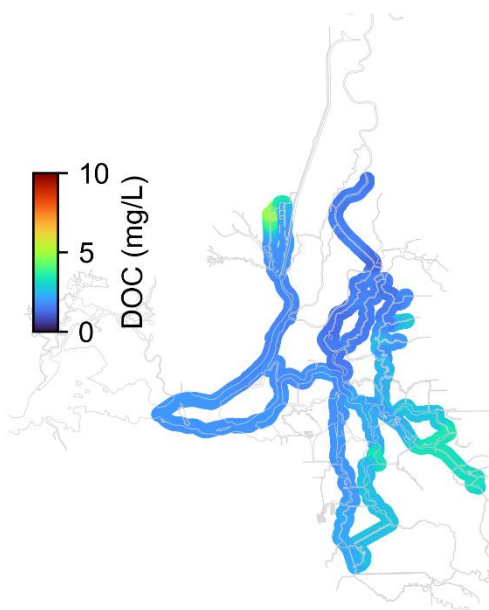
Aquatic Veg



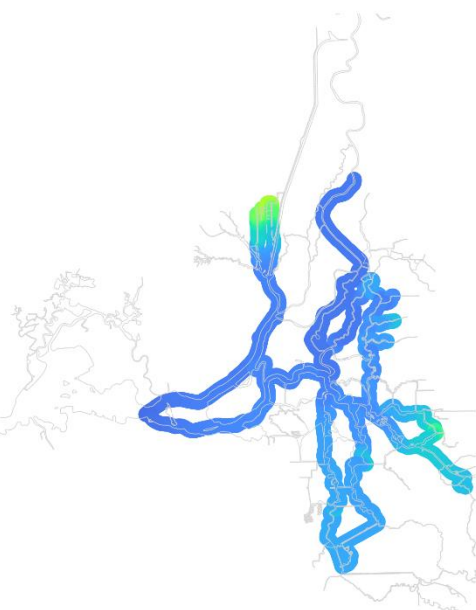
Marsh



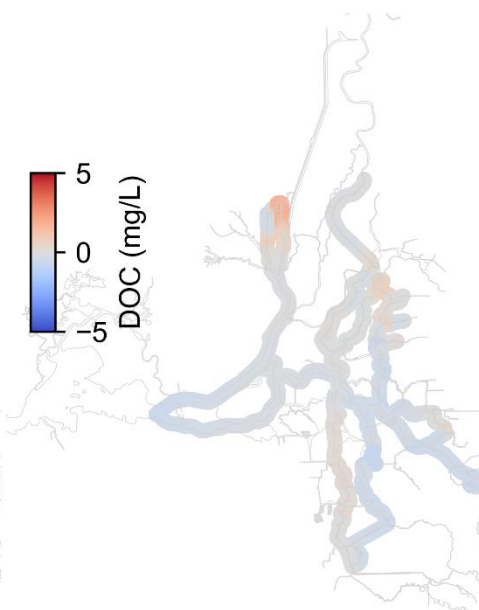
Observed fDOM as DOC



Predicted DOC



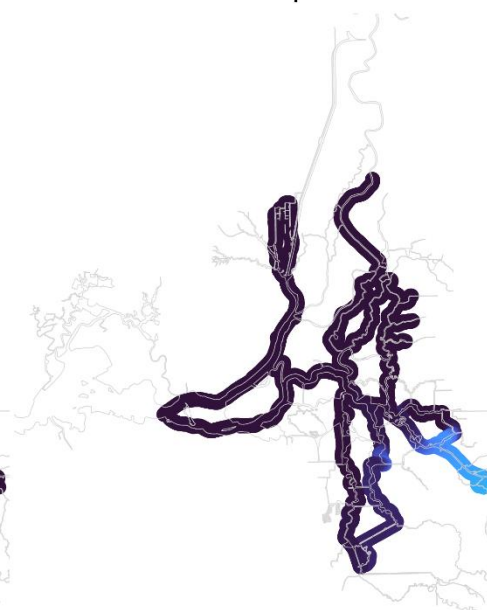
DOC Difference



Sacramento

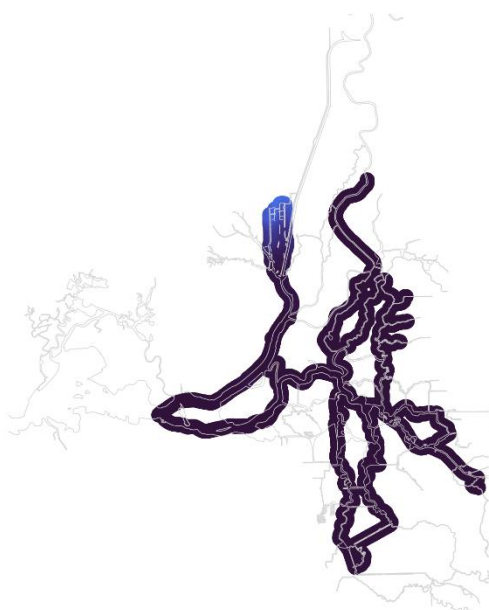


San Joaquin

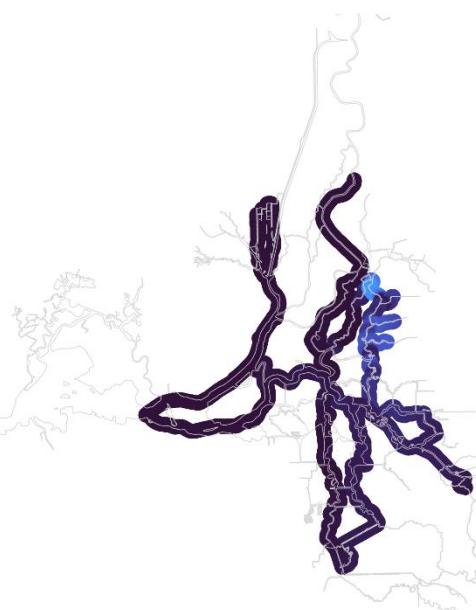


October 17-19, 2018
Ag Returns

Toe Drain



Other Flows



Aquatic Veg



Marsh



August 23, 2018 (Before North Delta Flow Action)

Observed

Predicted

Difference

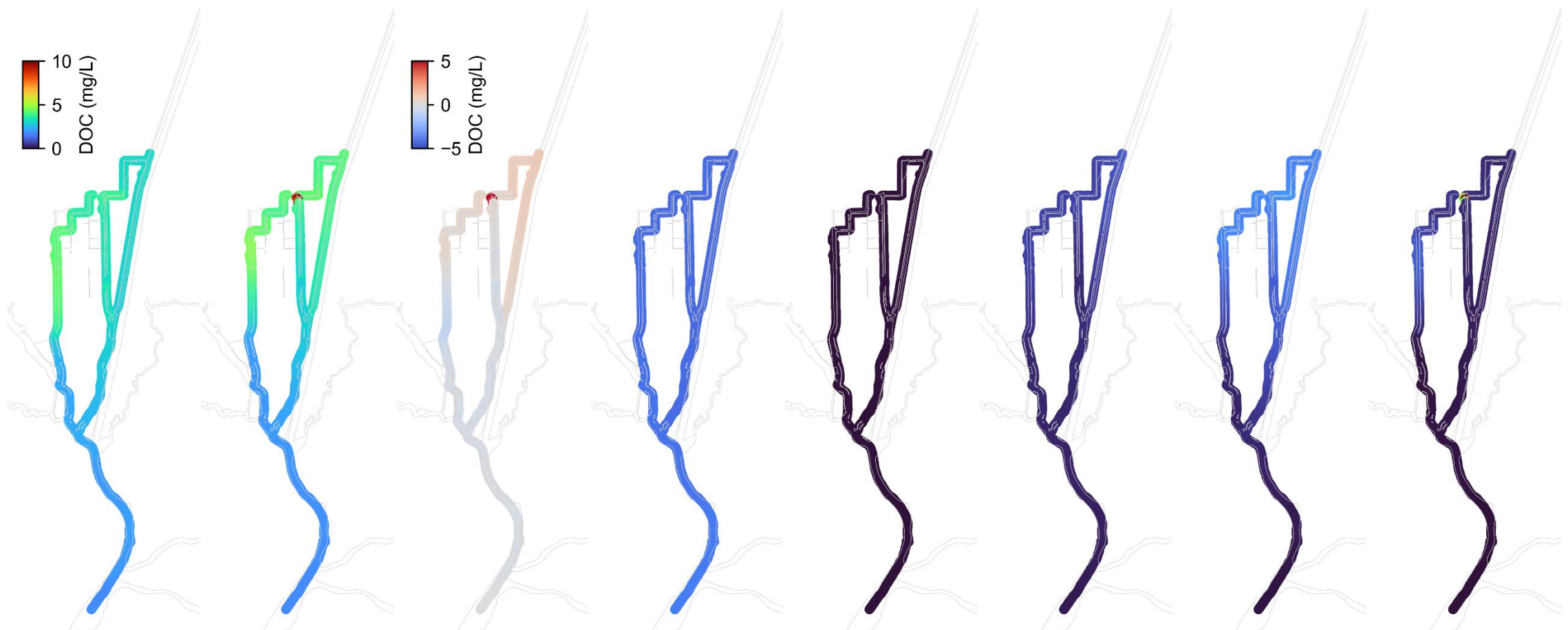
Sac

Toe

Ag

AV

Marsh



September 5, 2018 (During North Delta Flow Action)

Observed

Predicted

Difference

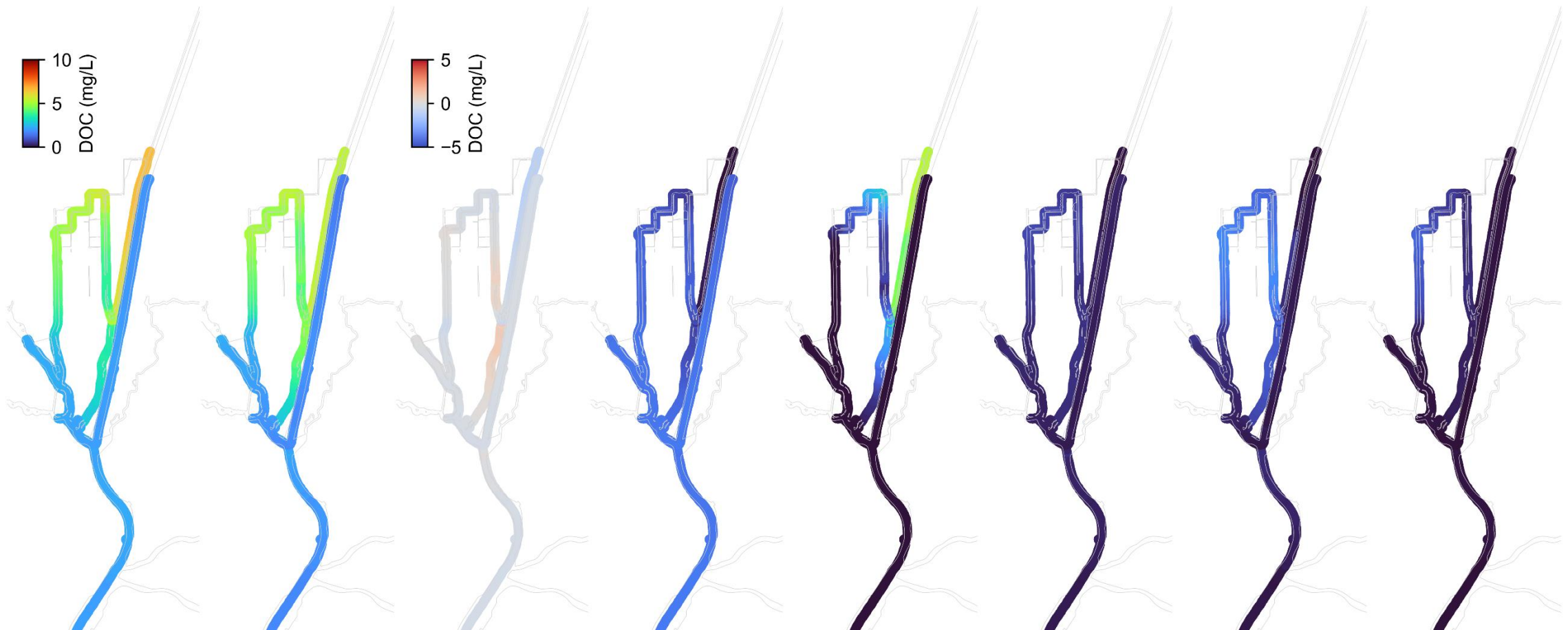
Sac

Toe

Ag

AV

Marsh



October 4, 2018 (After North Delta Flow Action)

Observed

Predicted

Difference

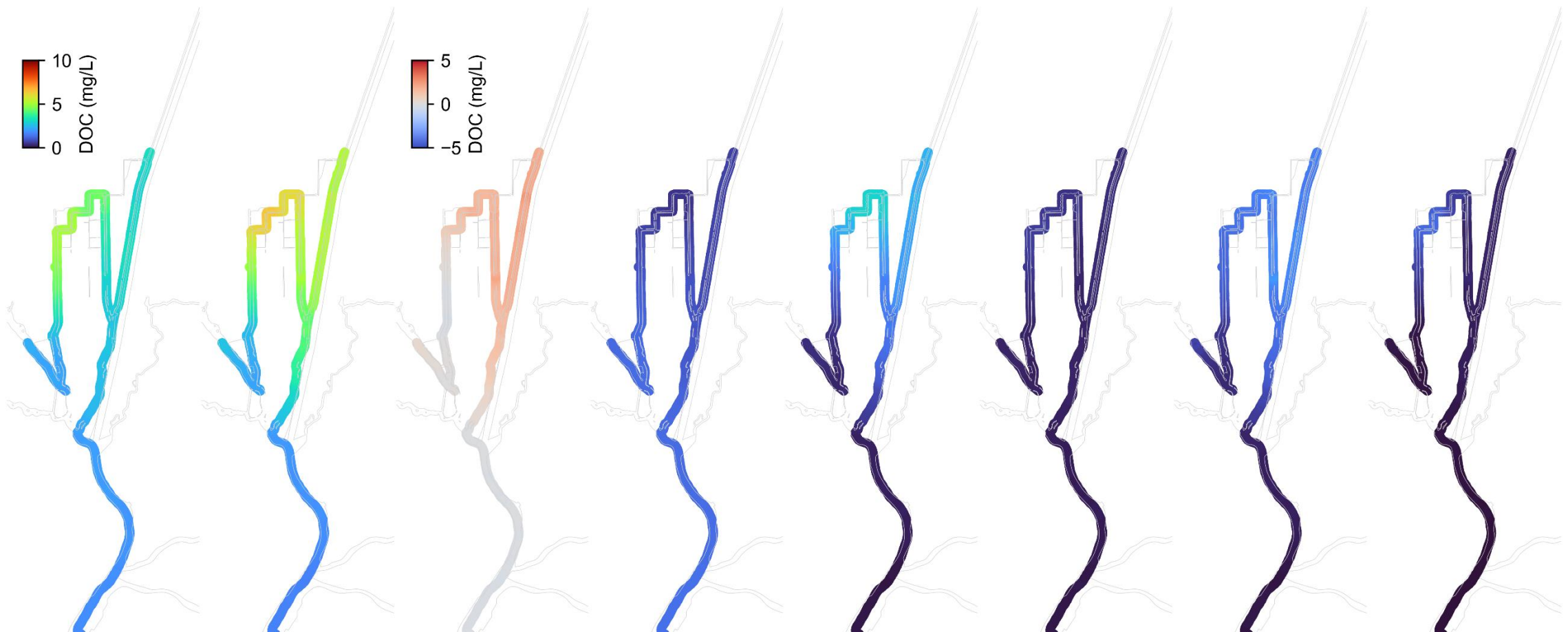
Sac

Toe

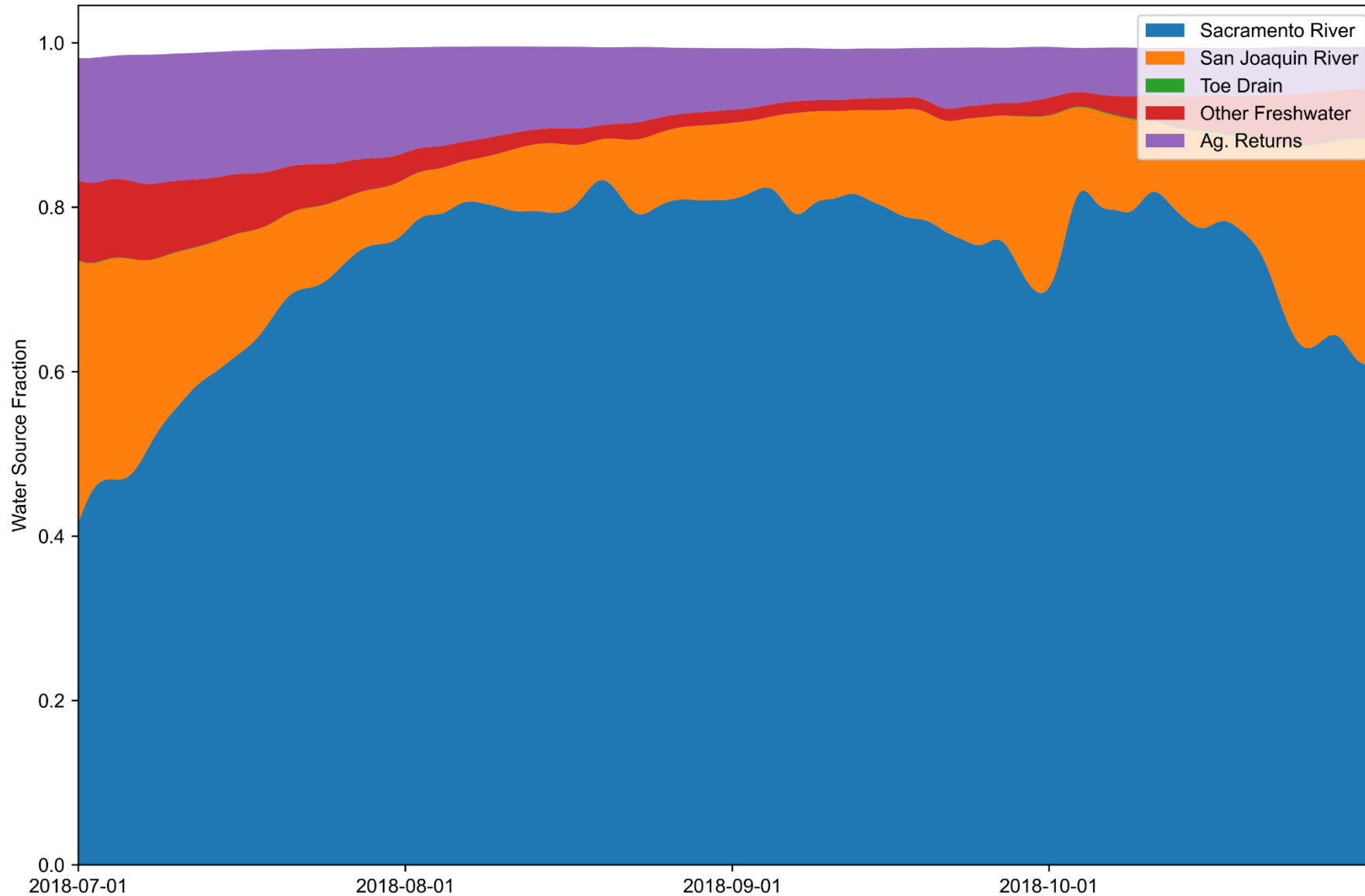
Ag

AV

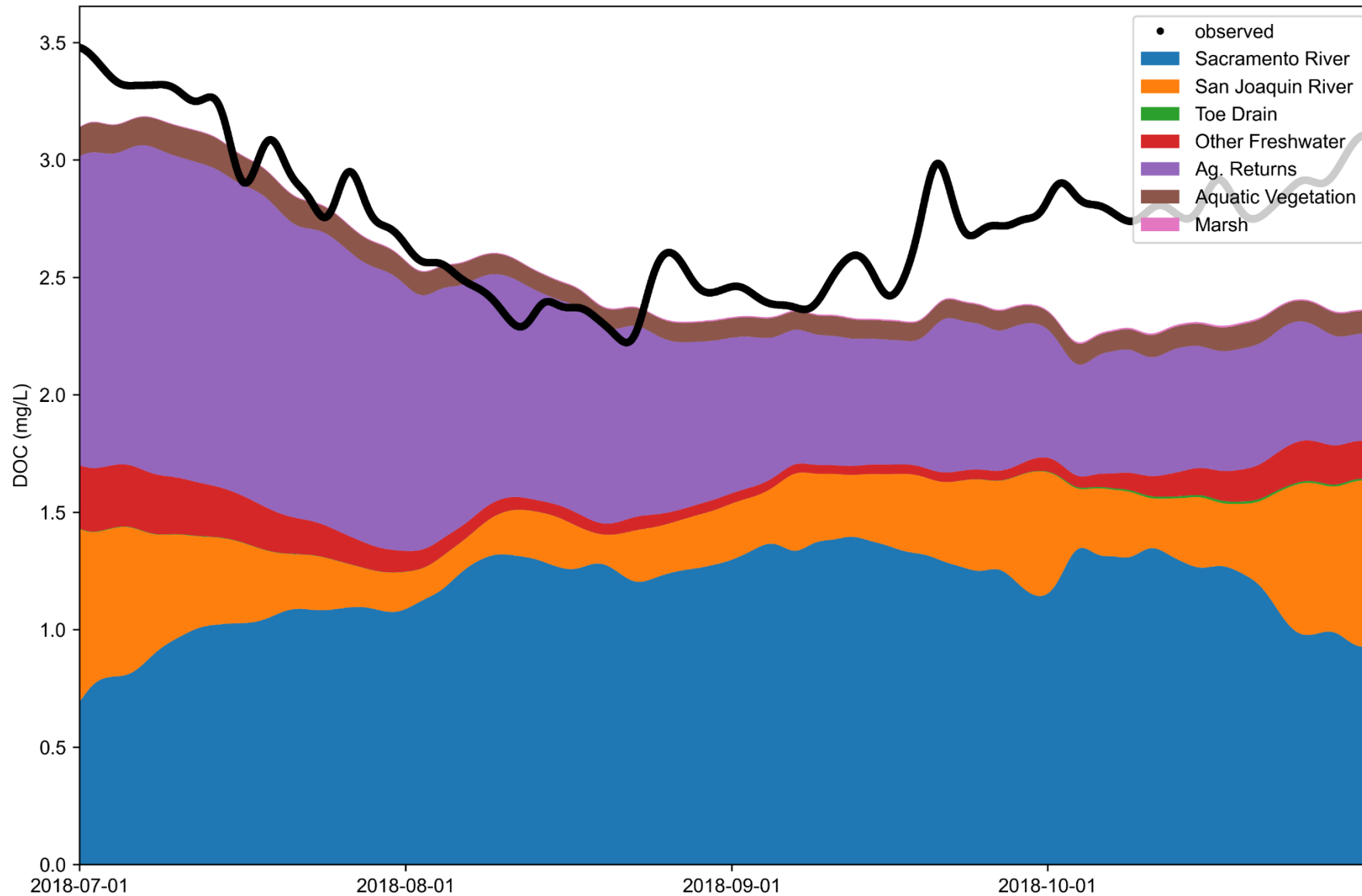
Marsh



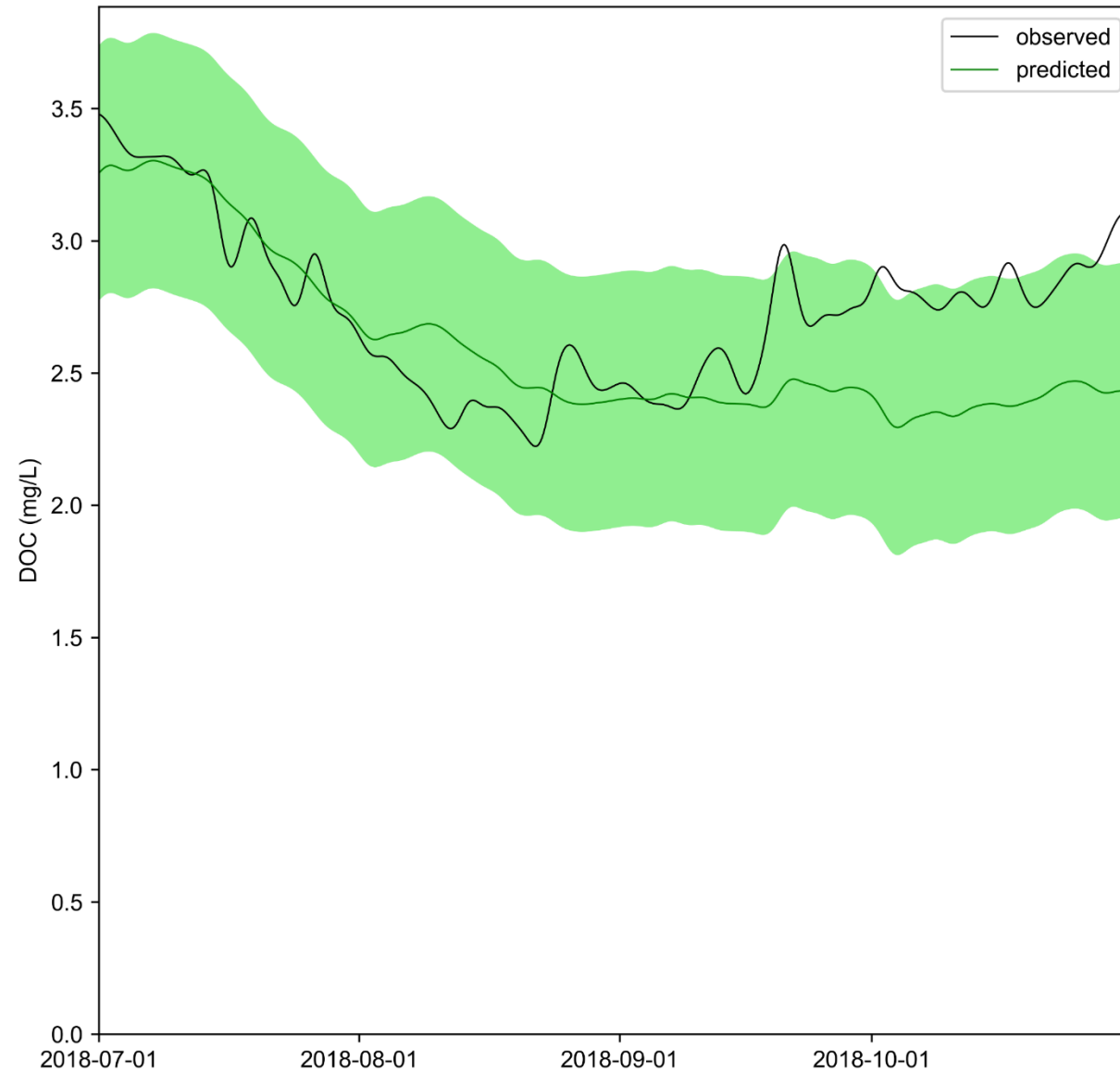
Banks (SWP) Fingerprint



Banks (SWP) DOC



Banks (SWP) DOC



Conclusions

- Can predict spatial and temporal patterns in DOC and fDOM with a simple model
- Aquatic vegetation and marsh sources are important in the Cache Slough Complex
- Results likely sensitive to spatial distribution of data points
- Effect of marsh and aquatic vegetation on food web uncertain
 - Our modeling does not quantify highly labile material that enters the food web close to these plant sources
- Possible extensions
 - Annual and multi-year simulations
 - Time varying unknown source strengths
 - Multiple categories of agricultural returns
 - Spatially variable concentration
 - Fit fraction labile and decay rate
 - May require additional observations to constrain well



Thank you!

Questions?

Funded by the California Department of Fish and Wildlife and the Delta Science Program