The fate of disinfection byproducts precursors in Ashokan Reservoir

2025 Catskill Environmental Research & Monitoring Conference

SHARED GROUND: COLLABORATIVE APPROACHES TO CATSKILL ENVIRONMENTAL RESEARCH

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DISCOVERY LODGE, BELLEAYRE MOUNTAIN

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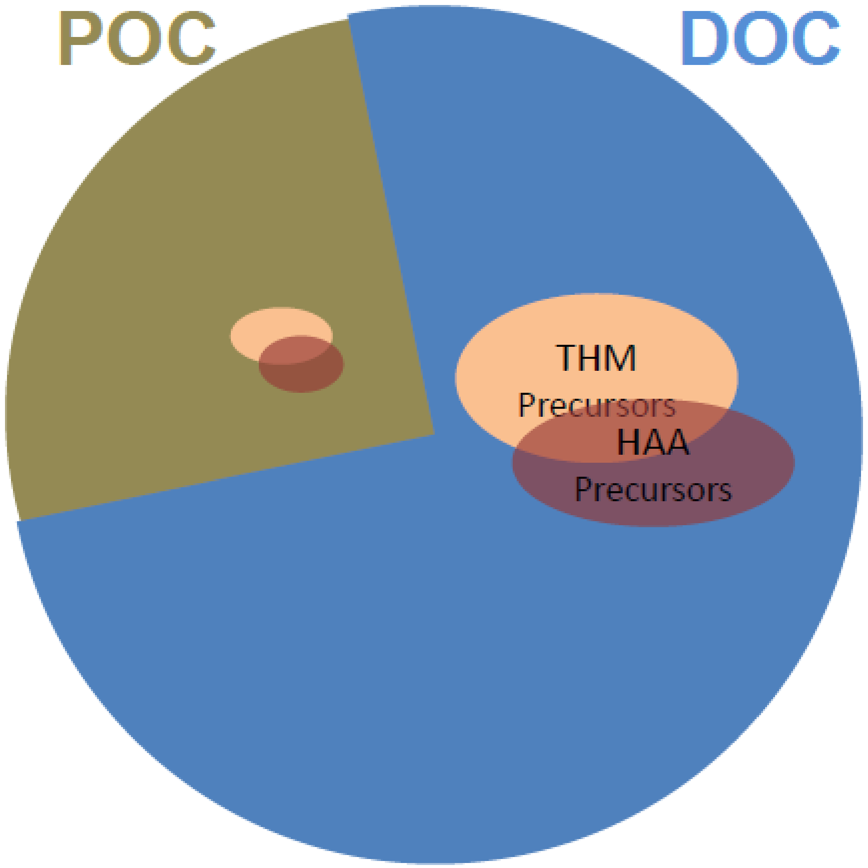
Outline

- What are precursors and where do they come from?
- Requirements for precursors modeling
- Model setup for Ashokan Reservoir
- Data review
- Results
- Key takeaways

Disinfection Byproducts (DBPs) Precursors



- A fraction of the TOC pool reacts to form DBPs
- The relative amounts vary
- Source of this fraction varies

NOM = POM + DOM

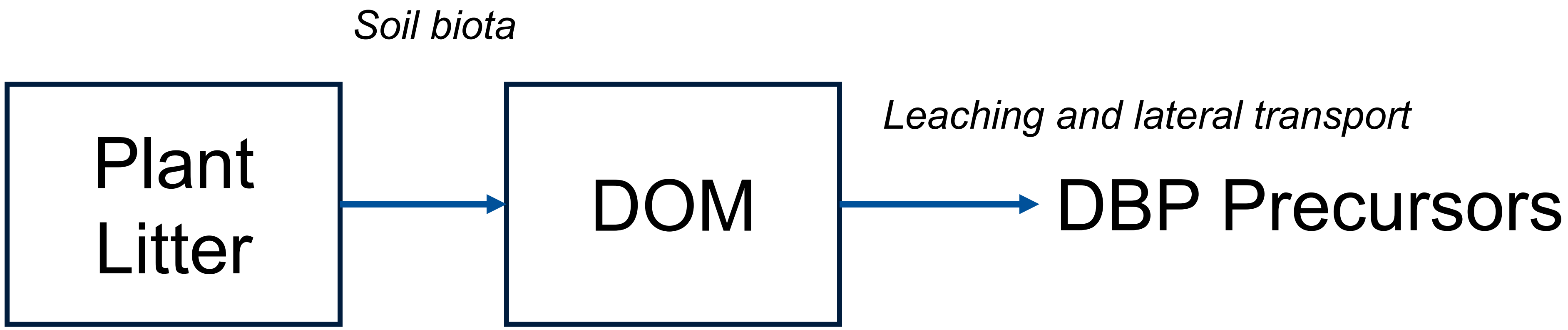
TOC = POC + DOC

THM = Trihalomethanes

HAA = Haloacetic Acids

source: Kraus et al. (2011); USGS

Simplified Representation



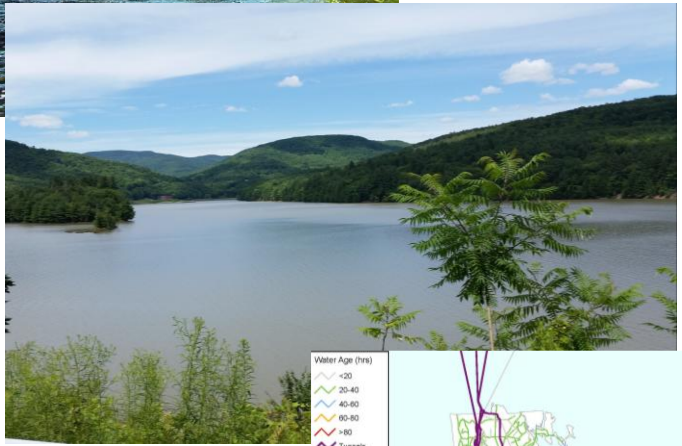
Conceptual Model of DBP Formation Potential

Litter Biochemical Groups	DBP Formation Potential
❑ Sugars, starches	Low
❑ Proteins	Moderate
❑ Hemicelluloses	Low
❑ Cellulose	Low-Moderate
❑ Fats & waxes	Low
❑ Lignin	High

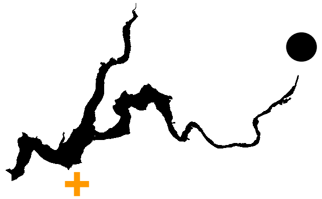
Increasing Recalcitrance

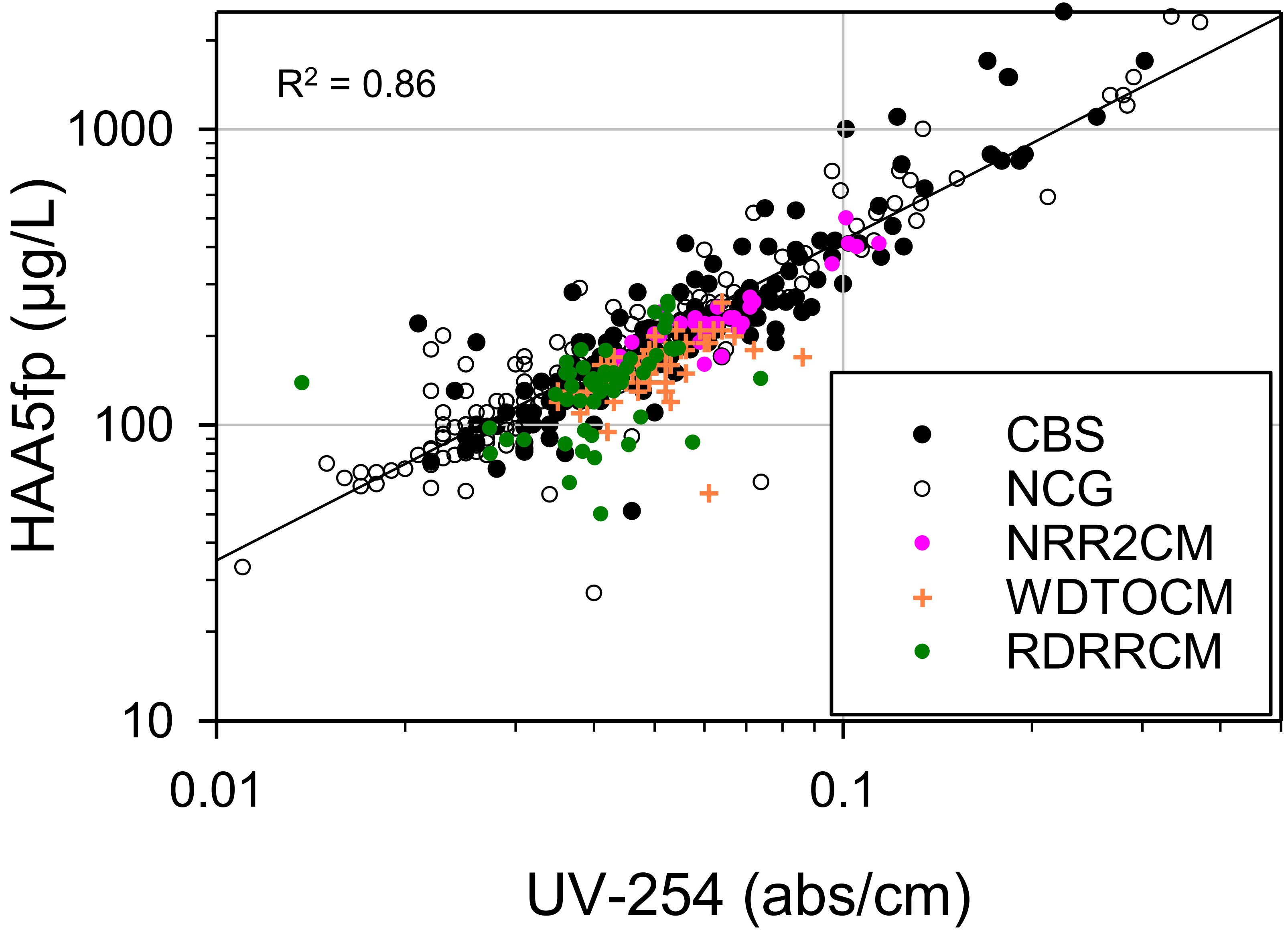
Modeling DBPs: Forest to Faucet

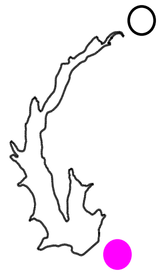
- What to model?
  - Measurable accurately, frequently, and fundamentally linked to DBPs
  - Precursors and their proxies [TOC, DOC, FDOM, UV absorbance at 254 nm wavelength, or some other wavelengths, UV254:DOC (aromaticity), UV250:UV365 (molecular size), spectral slope]
  - TTHMfp, HAA5fp
- How to model?
- Do we have the data to build (formulate) and test models?



UV254 a good proxy for DBPfp and Precursors:
Data from Reservoirs Inflow-Outflow

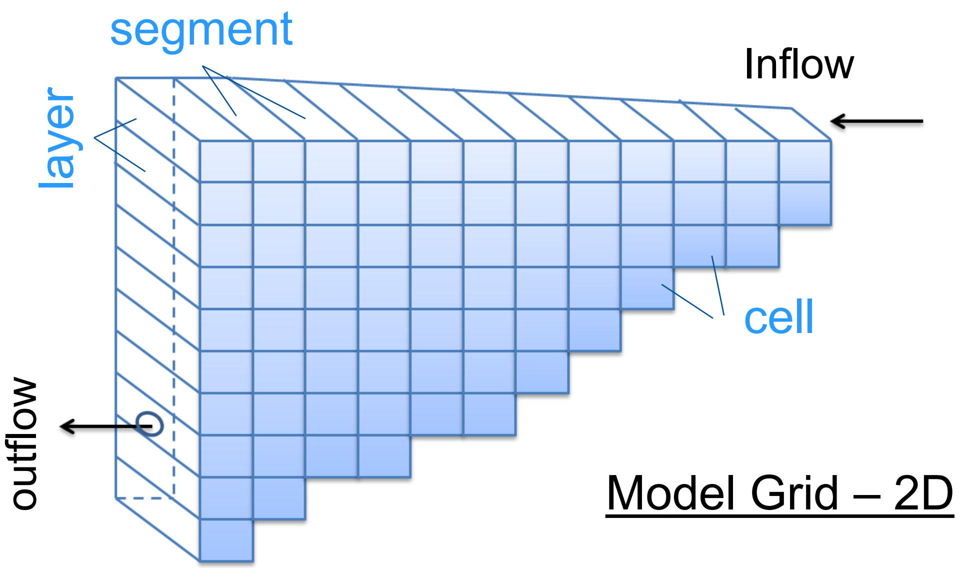






Reservoir Model CE-QUAL-W2 (W2)

- Transport, mixing, biogeochemical processes
- Not an empirical model
- Based on conservation of momentum, heat, mass
- Spatial complexity: 2D
- Temporal complexity: dynamic, sub daily time-step
- Data requirements and state variables
  - Temperature
  - UV_{254}



Model Setup

Configuration
Bathymetry
No. of Inflows
No. of Outflows

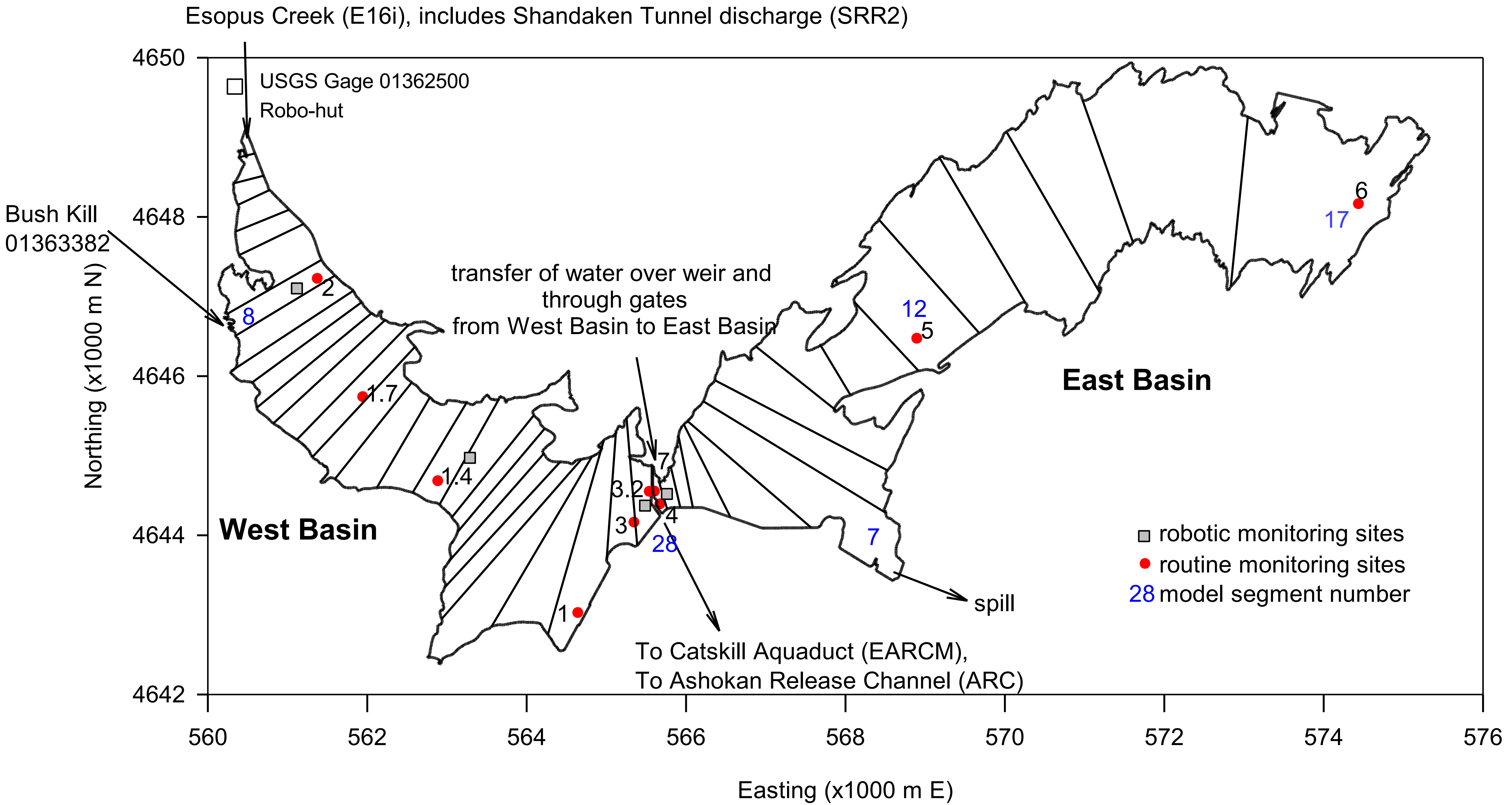
Process Parameters (*e.g.*)
Eddy Diffusivity
Sediment Oxygen Demand
Many others

Boundary Conditions
Meteorological Data
Inflow
Inflow Temperature
Inflow Concentrations
Outflow

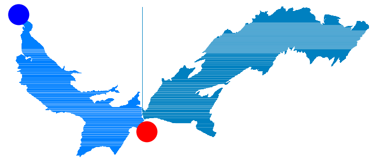
Initial Conditions (t = 0)
Water Surface Elevation
In-reservoir Temperature
In-reservoir Concentration
Ice thickness

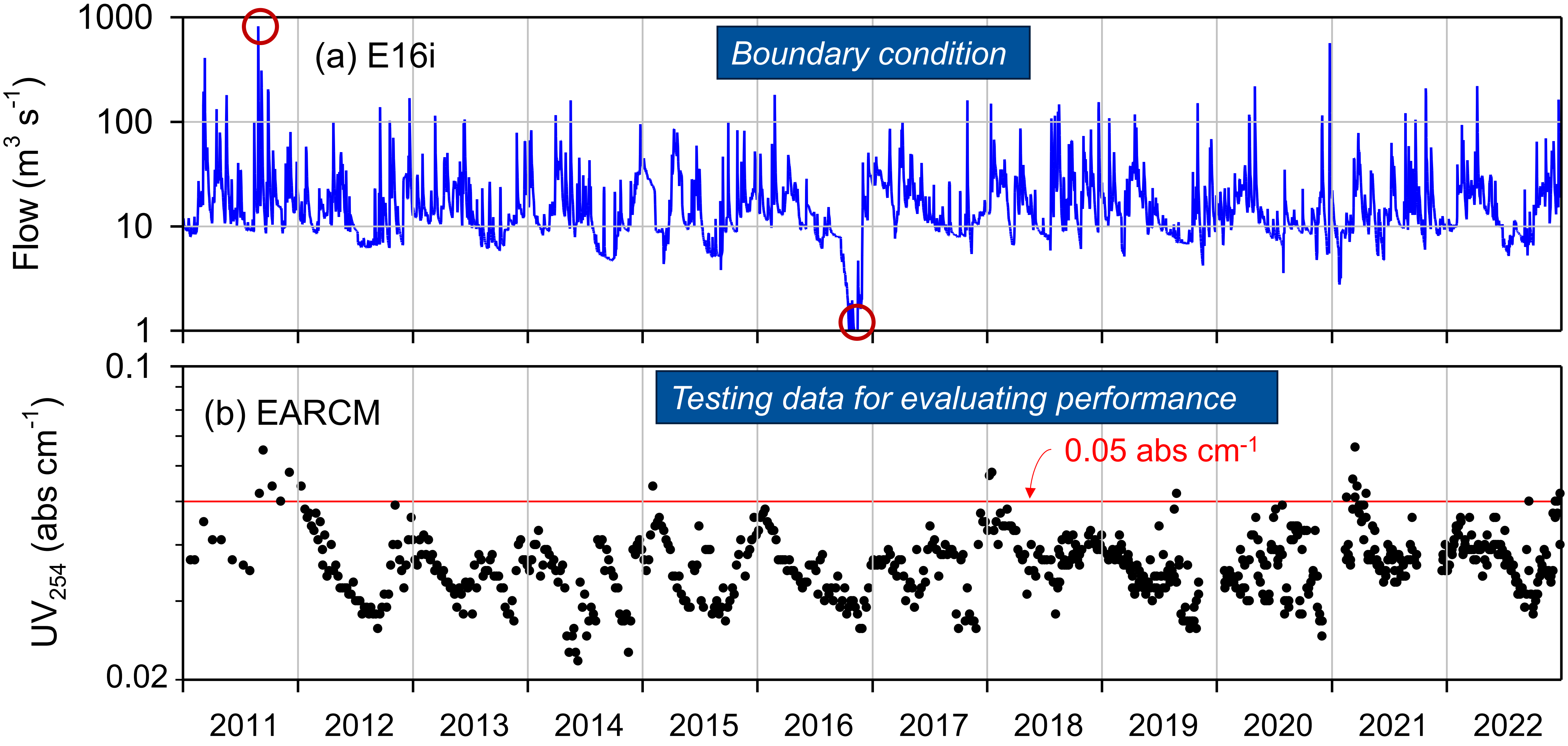
Testing Data
Water Surface Elevation
In-reservoir Temperature
In-reservoir Concentration
Ice thickness
Outflow Temperature
Outflow Concentration
Hydrodynamic Variables

Ashokan Reservoir Model



Review of Data





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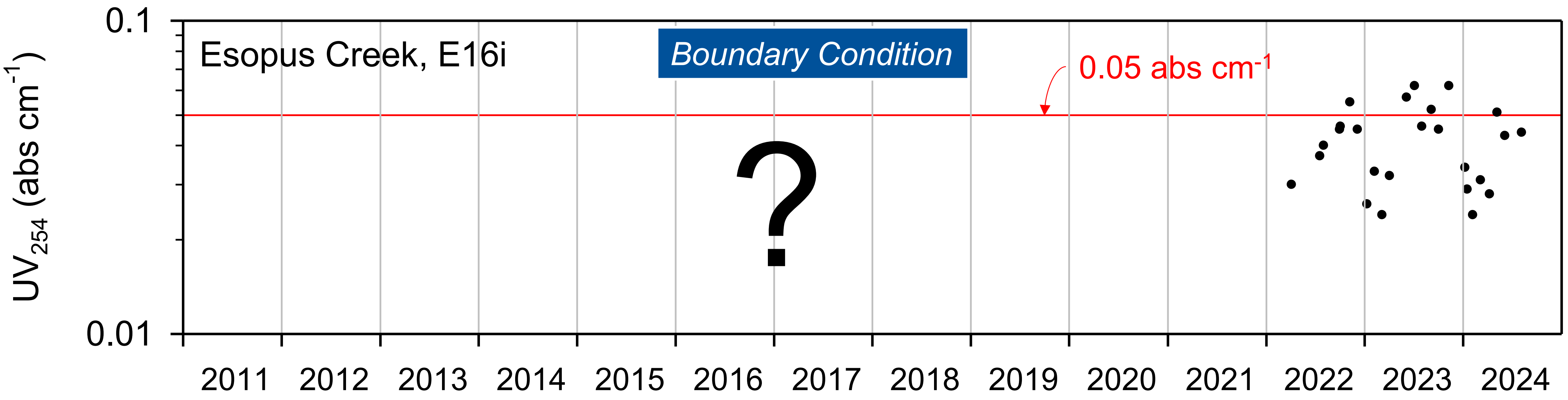
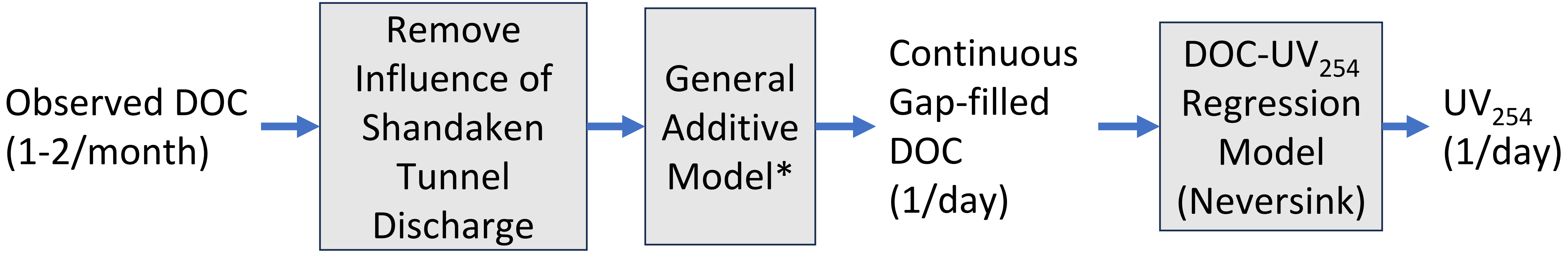


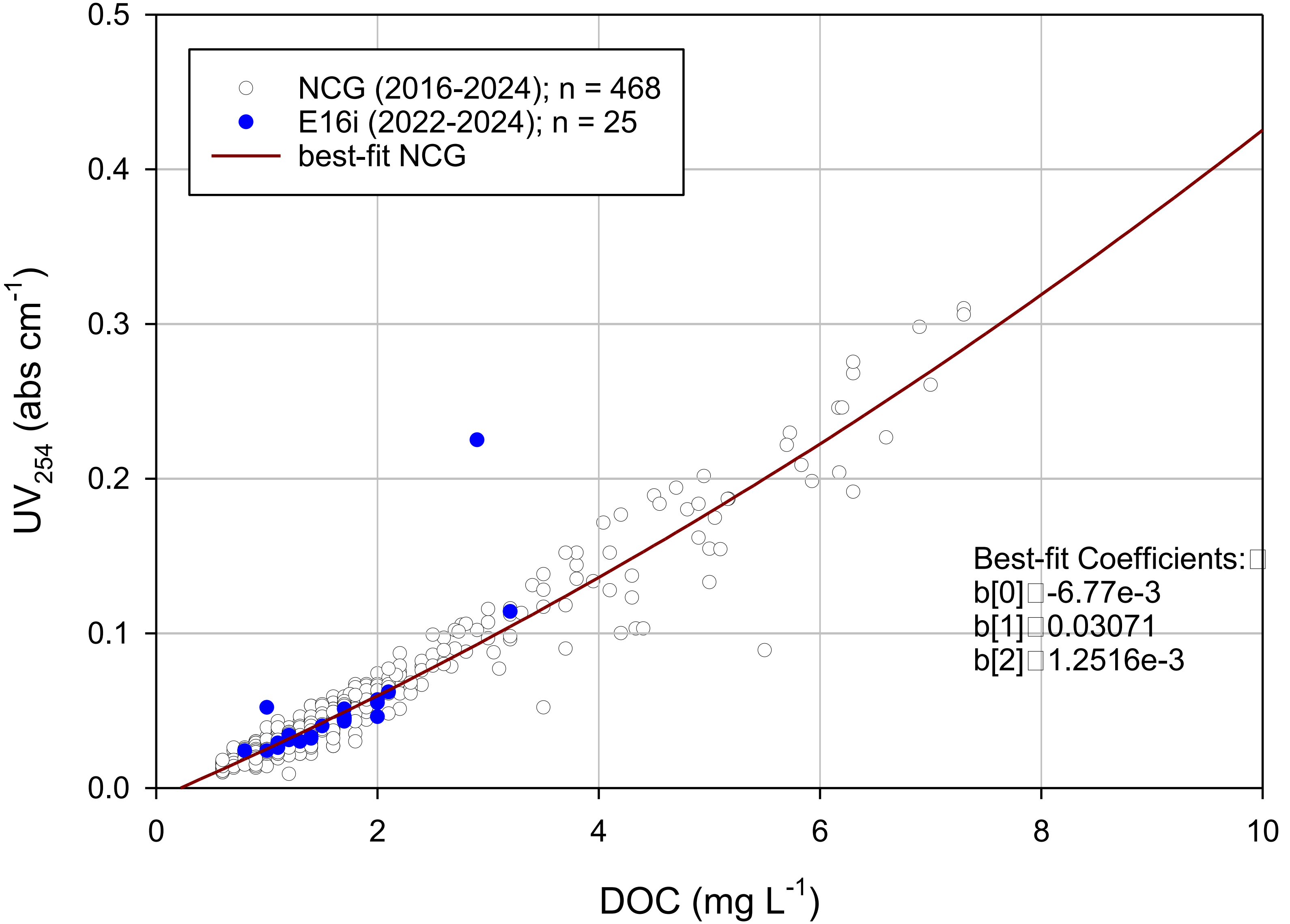
Estimating Esopus Creek UV_{254}



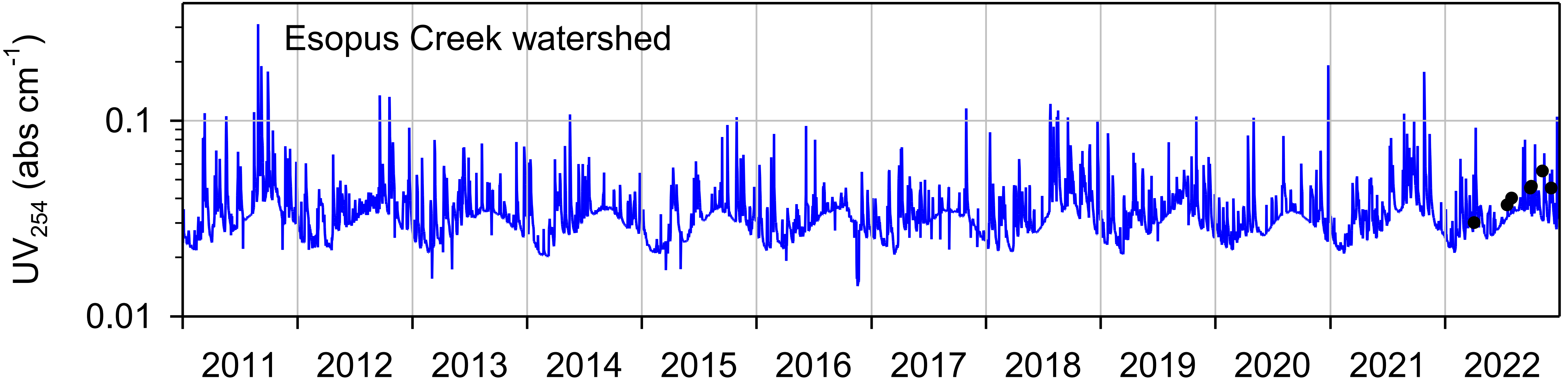
$$\ln\left(DOC_{esp}\right) = f_1\left(Q_{esp}\right) + f_2(Tn) + f_3(JD) + f_4(ADD) + \varepsilon$$

**Wang, K., Mukundan, R., Gelda, R. K., & Frei, A. (2025). Modeling dissolved organic carbon export from water supply catchments in the northeastern United States. Science of The Total Environment, 963, 178532. https://doi.org/10.1016/j.scitotenv.2025.178532*

DOC-UV_{254} Neversink Watershed (NCG)



Estimated Esopus Creek UV_{254}



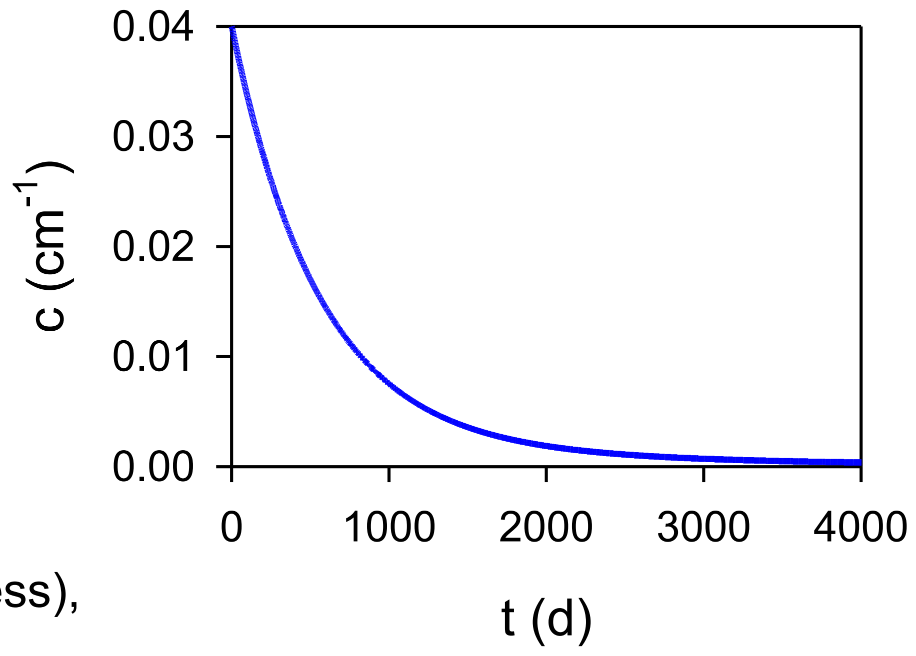
Model Kinetics

CE-QUAL-W2
UV-254

Testing period
2011-2022

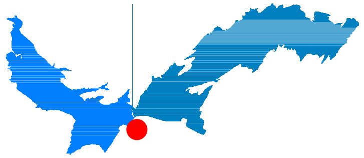
$$\frac{dc}{dt} = -k\theta^{(T-20)}\frac{c}{c+k_s}c$$

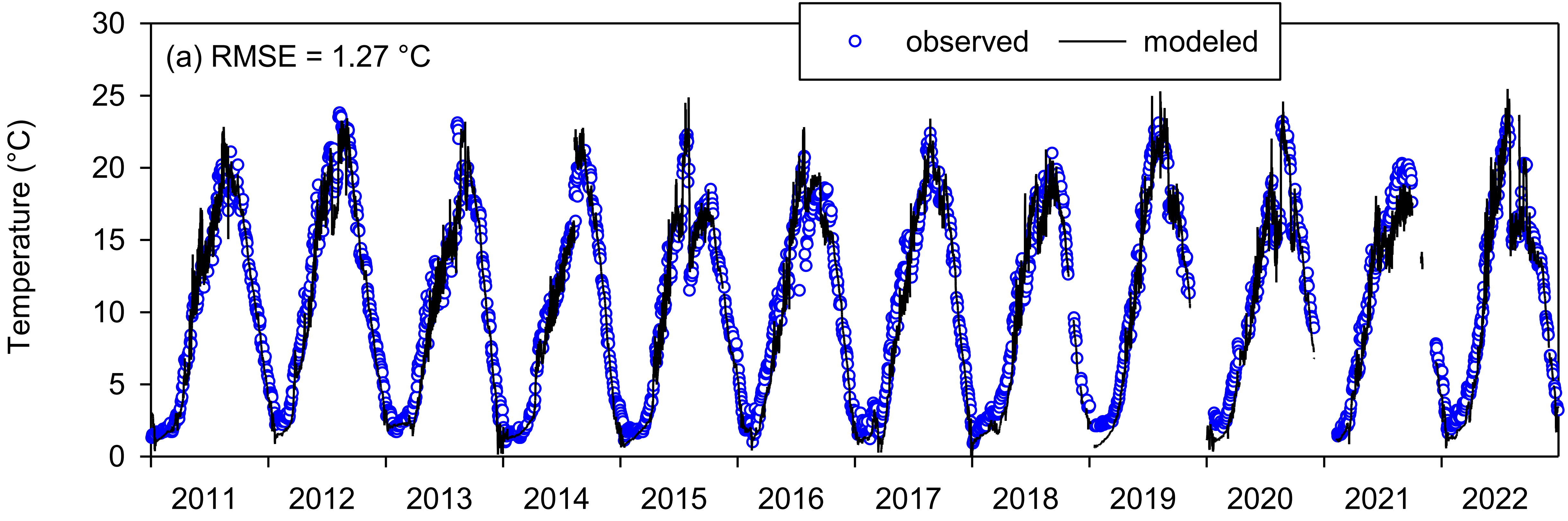
where,
c = UV_{254} concentration (cm^{-1}),
t = time (d),
k = net first-order rate of change (d^{-1}),
θ = temperature correction multiplier (dimensionless),
T = water temperature (°C),
k_s = half-saturation constant (cm^{-1})



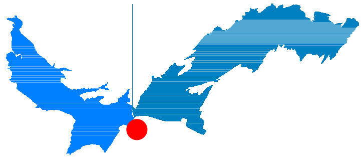
Calibration: net loss rate = – 0.002 d^{-1}, θ = 1.024, T = 15°C, k_s = 0.001 cm^{-1}

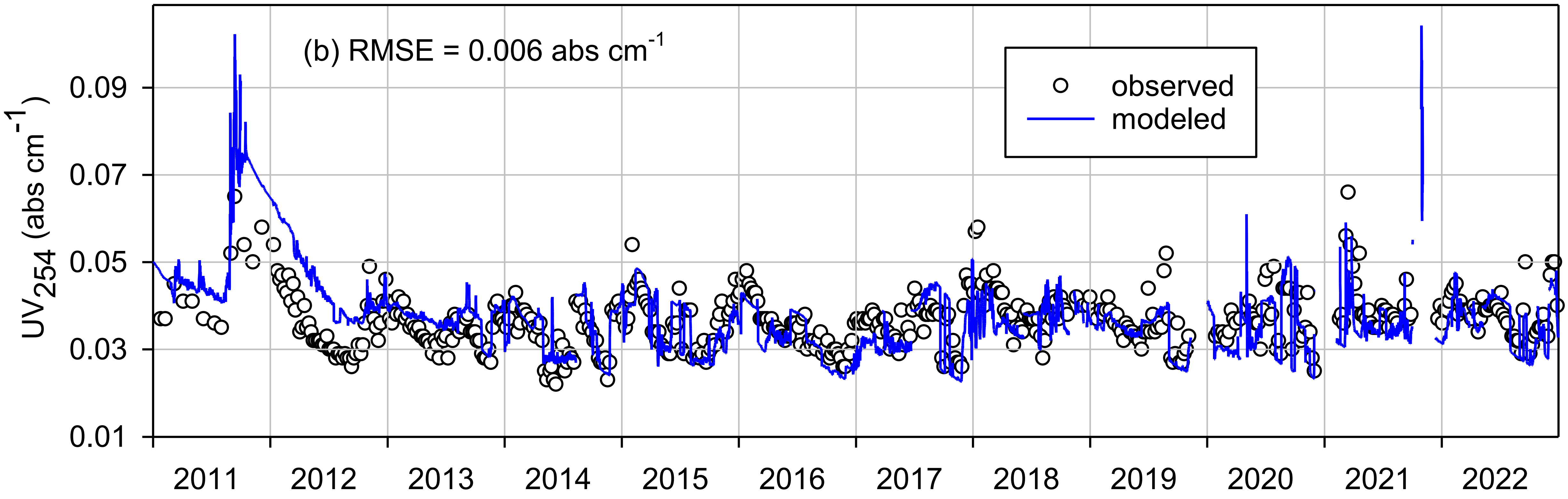
Model Performance Evaluation: site EARCM





Model Performance Evaluation: site EARCM





Key Takeaways

- UV_{254} is a good, model-able proxy of precursors
- In-reservoir UV_{254} can be modeled with a mechanistic model
- Hydrodynamics more important than kinetics
- First-order kinetics & largely refractory organics

Extra Slides

Regulated DBPs

- Some DBPs are classified as *probable/possible* carcinogens; other harmful health effects

- DEP monitors all regulated DBPs (9 total) in the two classes:
  - Trihalomethanes (THMs)
    - Total THMs (TTHM) = [$CHCl_3$] + [$CHBr_3$] + [$CHBrCl_2$] + [$CHBr_2Cl$]
    - MCL = 80 µg/l; compliance based on LRAA for individual sites; OEL = 80 µg/L

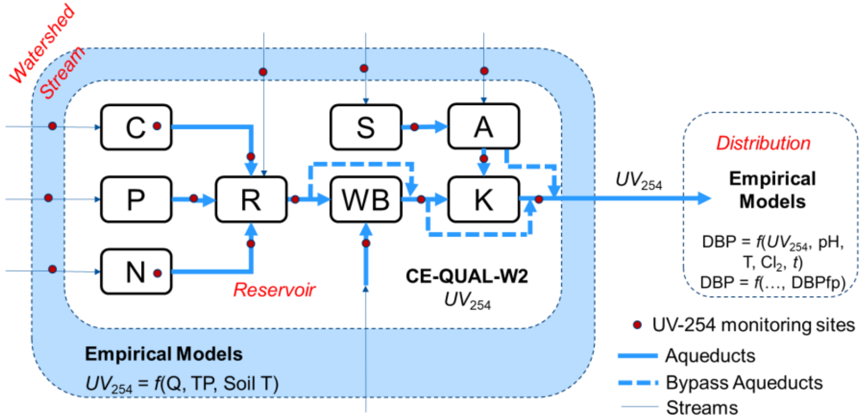
  - Haloacetic acids (HAAs)
    - HAA5 = [$ClCH_2COOH$] + [$Cl_2CHCOOH$] + [Cl_3CCOOH] + [BrCH2COOH] + [$Br_2CHCOOH$]
    - MCL = 60 µg/l; compliance based on LRAA for individual sites; OEL = 60 µg/L

[ ] most important compounds in NYC system

LRAA: Locational Running Annual Average = (PQ3+PQ2+PQ1+CQ)/4
OEL: Operational Evaluation Level = (PQ2+PQ1+CQ+CQ)/4
MCL: Maximum Contaminant Level

Next Steps

- ❑ Expand stream modeling to all major streams
- ❑ Test w2 models for UV-254 for other reservoirs
- ❑ Test stream and w2 models for the system
- ❑ Model distribution system



- ❑ Study on how to optimize *source operations & treatment* to minimize DBPs: precision Cl_2 dosing, selective withdrawal – minimum precursor levels, optimum temperature, optimum pH, hydraulic modeling to reduce water age

- ❑ Include UV-254, DBPfp, and DBP modeling in OST (Operation Support Tool)

System-wide UV_{254}