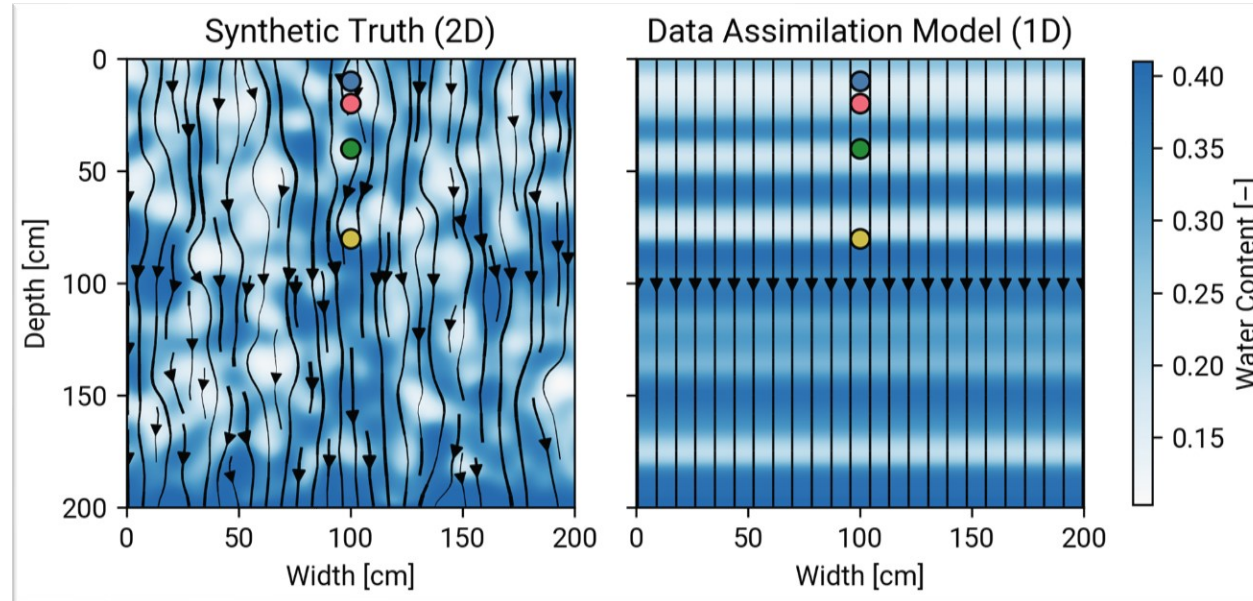


Predicting Solute Transport in Soil Water Flow with Estimated, Effective Material Properties

[Lukas Riedel](#), Hannes H. Bauser, Robert Maiwald, & Santiago Ospina De Los Ríos

Previous study (Bauser et al. 2020):

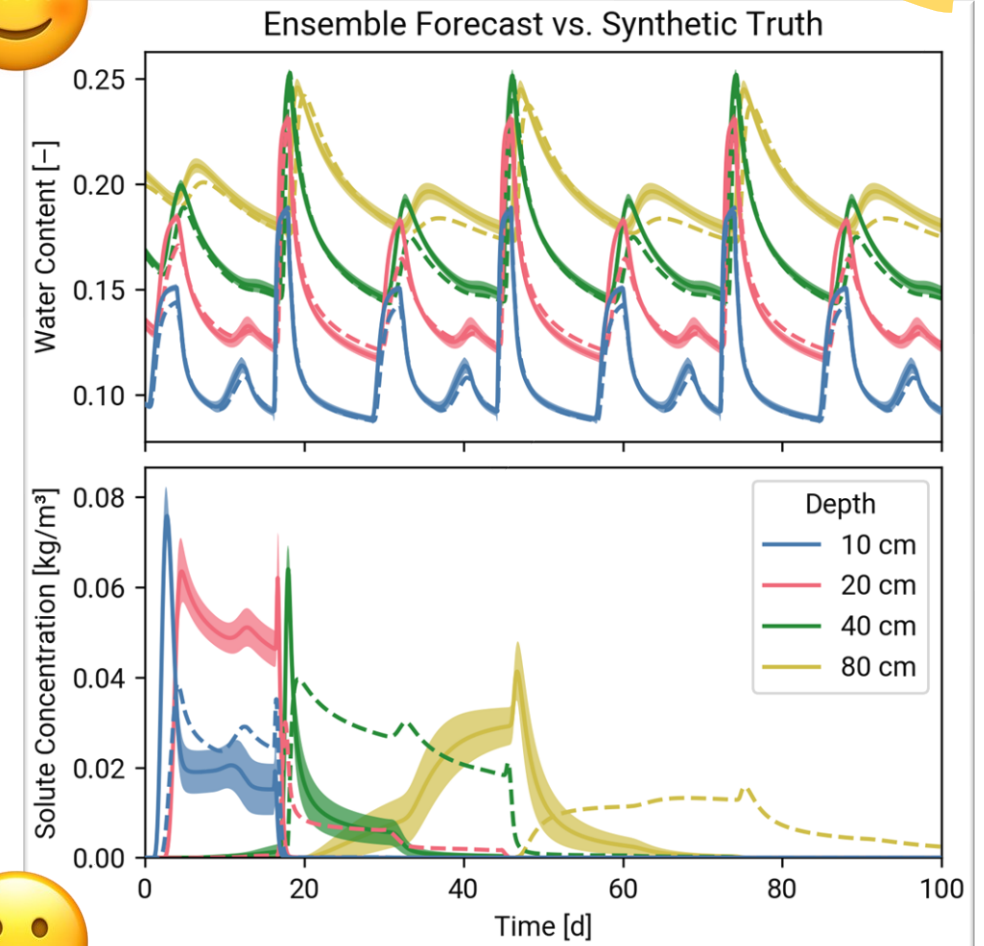
- Estimate effective material properties of 1D model based on water content measurements of 2D synthetic truth
- **Effective description of soil water flow dynamics**



This study:

- Add solute concentration and run ensemble forecast with estimated 1D model
- **No effective description of solute transport dynamics**

*soil water flow
dynamics
≠
solute transport
dynamics*



Estimating Effective Material Properties

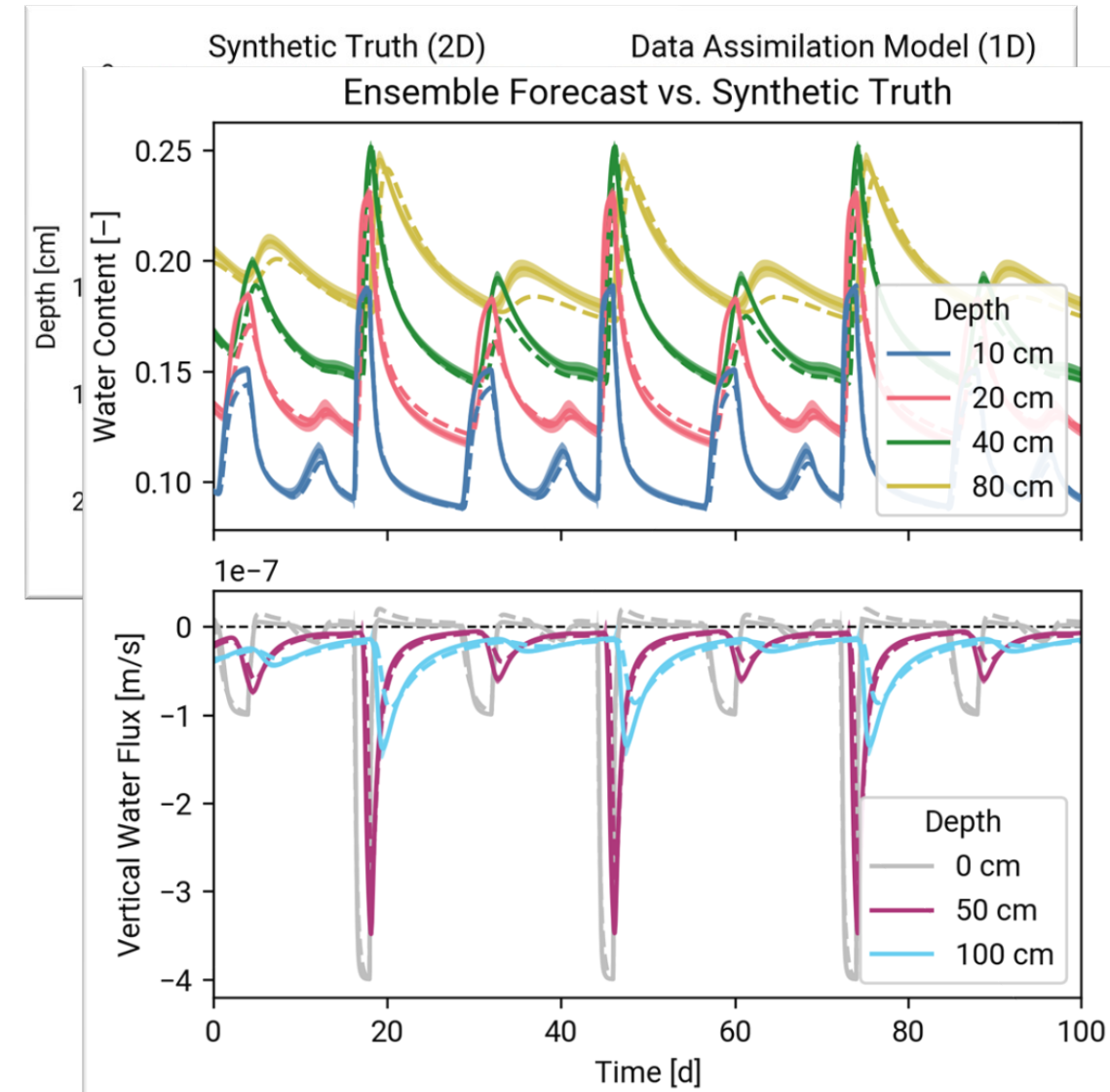
Bauser et al. (2020): <https://doi.org/10.1002/vzj2.20040>

Data Assimilation Task

- Ensemble Kalman filter (EnKF) estimates soil hydraulic properties and small-scale heterogeneity based on synthetic water content measurements
- Employ one-dimensional model with reduced representation of heterogeneity within EnKF

Results

- Soil water flow dynamics can be reasonably replicated, but hinge on the accuracy of boundary conditions
- Estimated material properties are effective for the 1D model but deviate from true properties

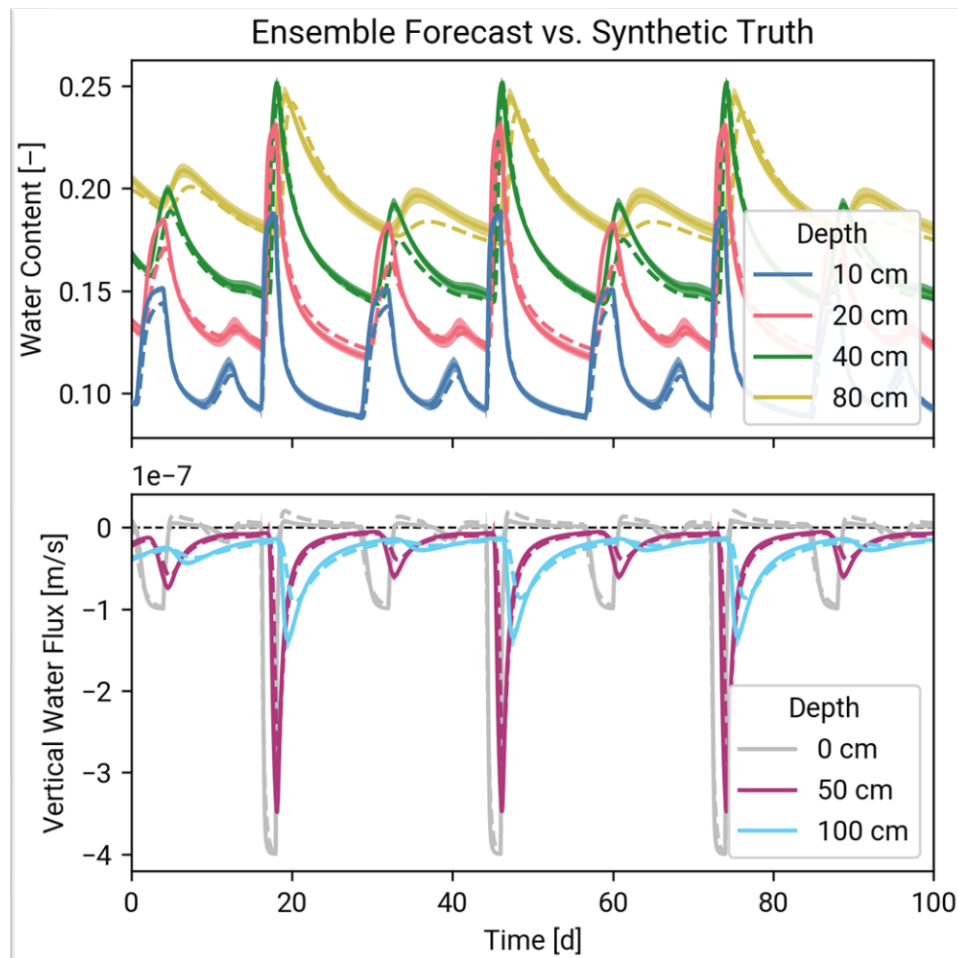


Ensemble Forecast with Passive Solute Transport

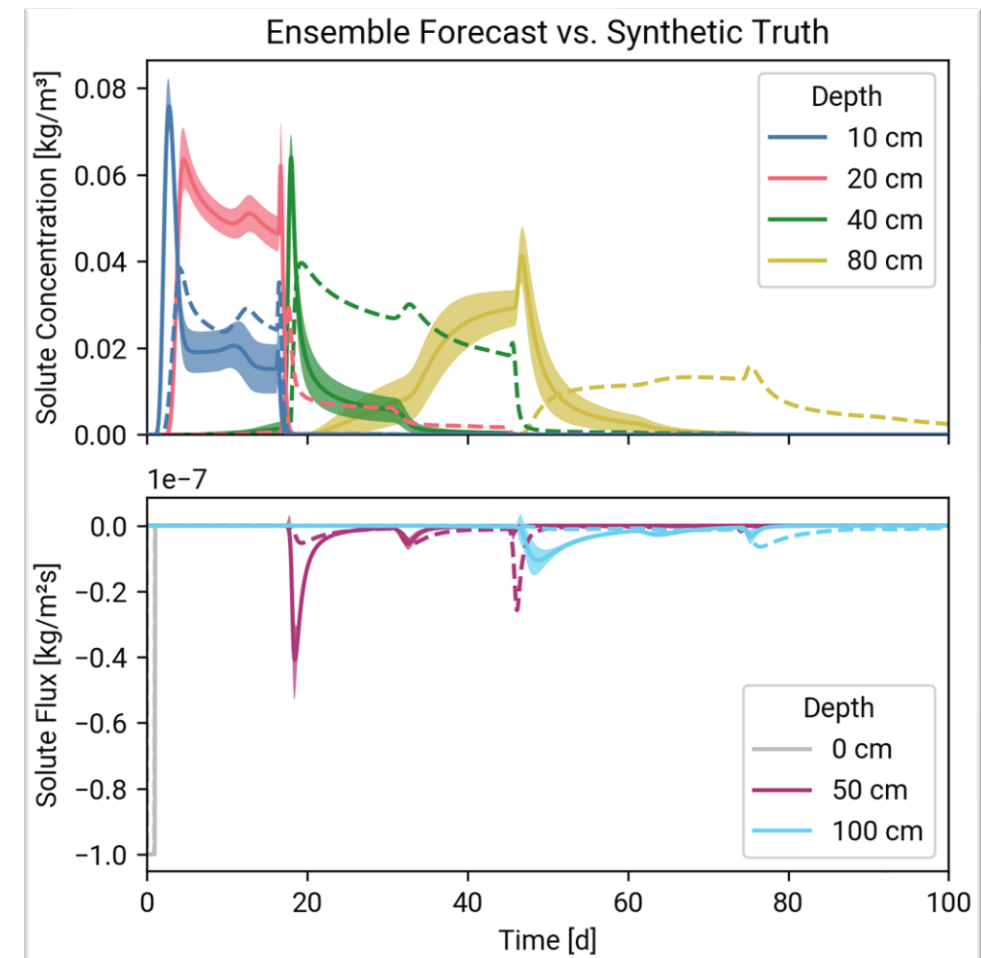
All simulations conducted with DORiE: <https://doi.org/10.21105/joss.02313>

Add solute concentration to first infiltration event

Water Flow



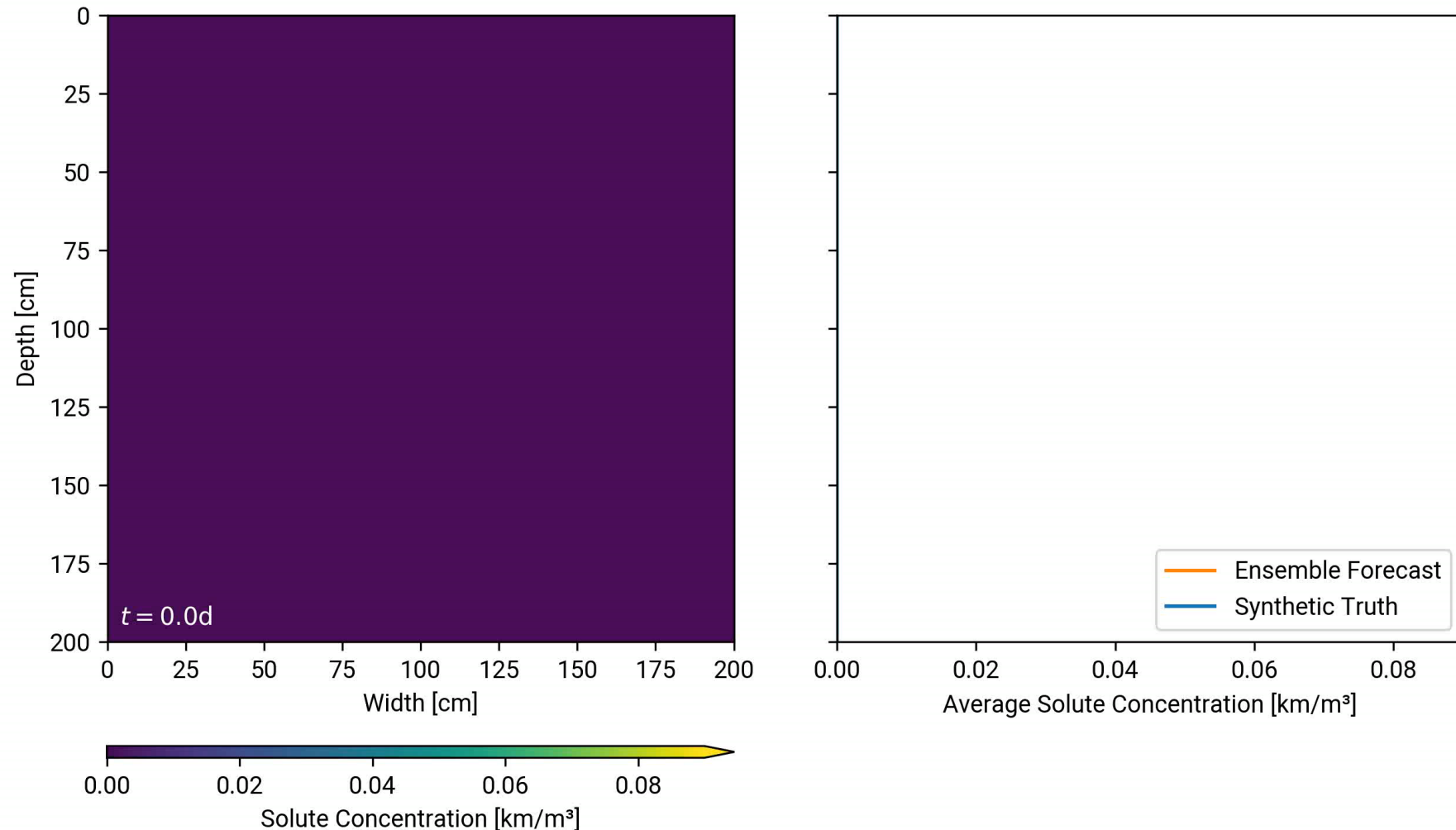
Solute Flow



Ensemble Forecast with Passive Solute Transport

All simulations conducted with DORiE: <https://doi.org/10.21105/joss.02313>

(Video also available as separate file)



Root Mean Squared Error (RMSE)

Analysis

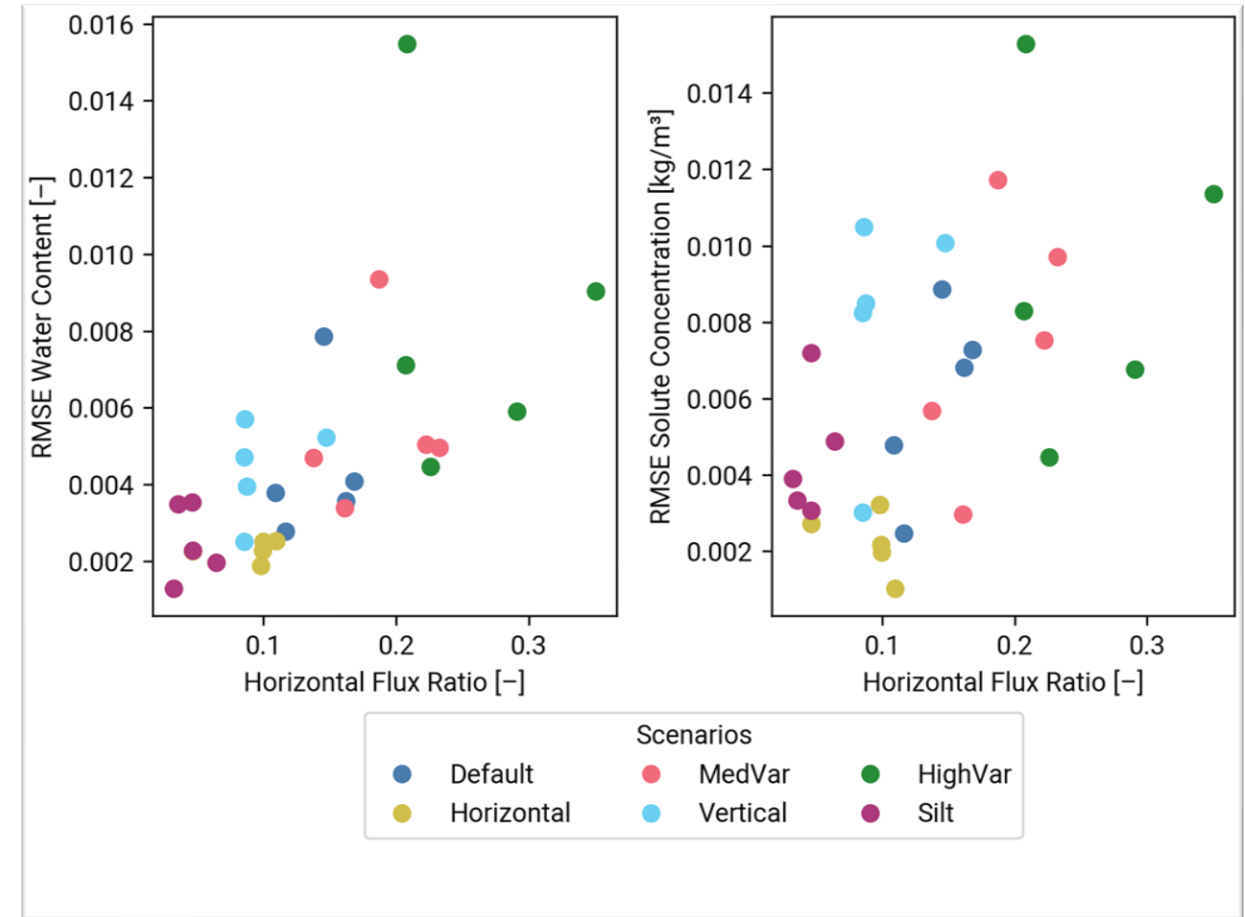
- Compare results based on average horizontal flux ratio (AHFR) of water flux:

$$\text{AHFR} = \frac{1}{N_t} \sum_t \frac{\langle j_{x,t} \rangle_z}{\langle j_{z,t} \rangle_z}$$

- Compute RMSE over all measurement locations and observation times

Results

- Solute concentration RMSE shows no clear tendency with AHFR
- Relative solute concentration RMSE much higher than relative water content RMSE



Nash-Sutcliffe Efficiency (NSE)

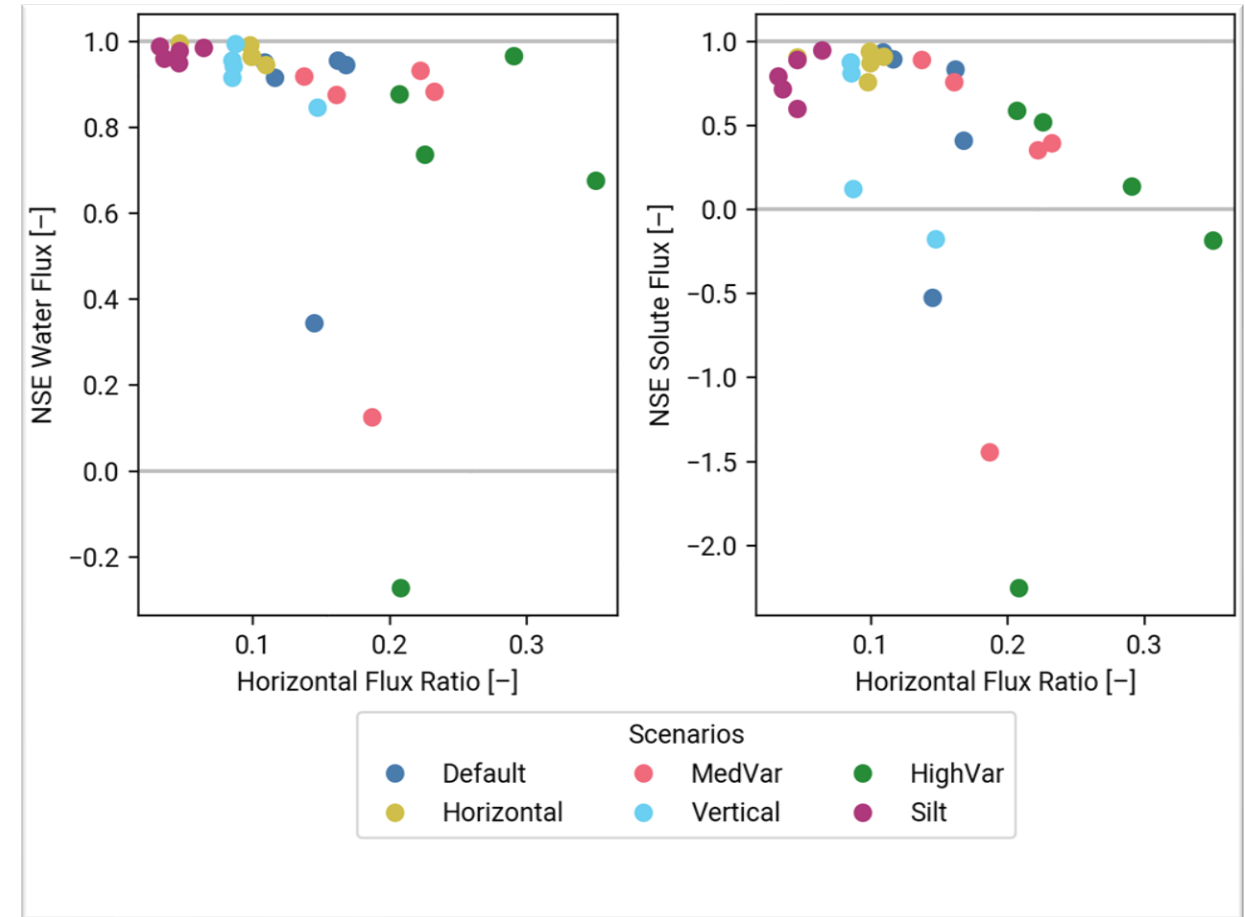
Analysis

- Compute Nash-Sutcliffe efficiency (NSE) of fluxes at a depth of 100 cm:

$$\text{NSE} = 1 - \frac{\sum_t^{N_t} [\bar{j}_t - j_t^*]^2}{\sum_t^{N_t} [j_t^* - \sum_t^{N_t} j_t^* / N_t]^2}$$

Results

- Solute flux NSE significantly worse than water flux NSE
- Estimated solute flux rarely is a better descriptor than average solute flux



Timing Differences

Analysis: Compute timing differences for 20% and 80% of cumulative solute flux

Results: Description of pulse tailing is worse than of pulse onset

