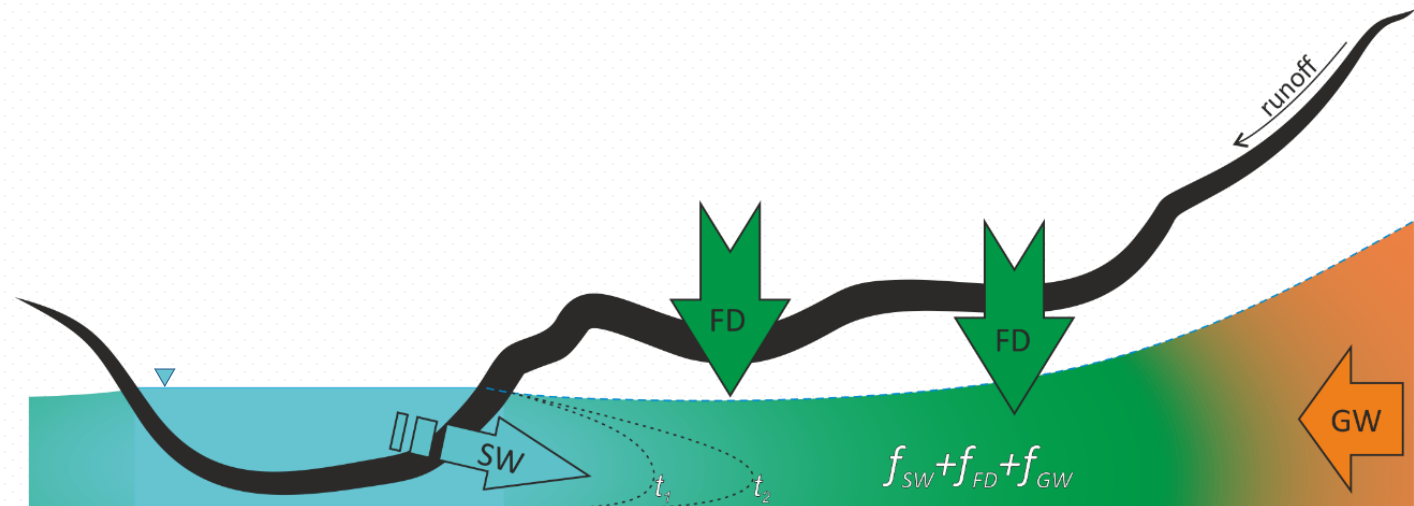


Spatio-temporal variations of high-degree mixing spots in a floodplain (assessed with a hydraulic mixing cell method)

Nogueira, G. E. H.
Schmidt, C.
Partington, D.
Brunner, P.
Fleckenstein, J. H.

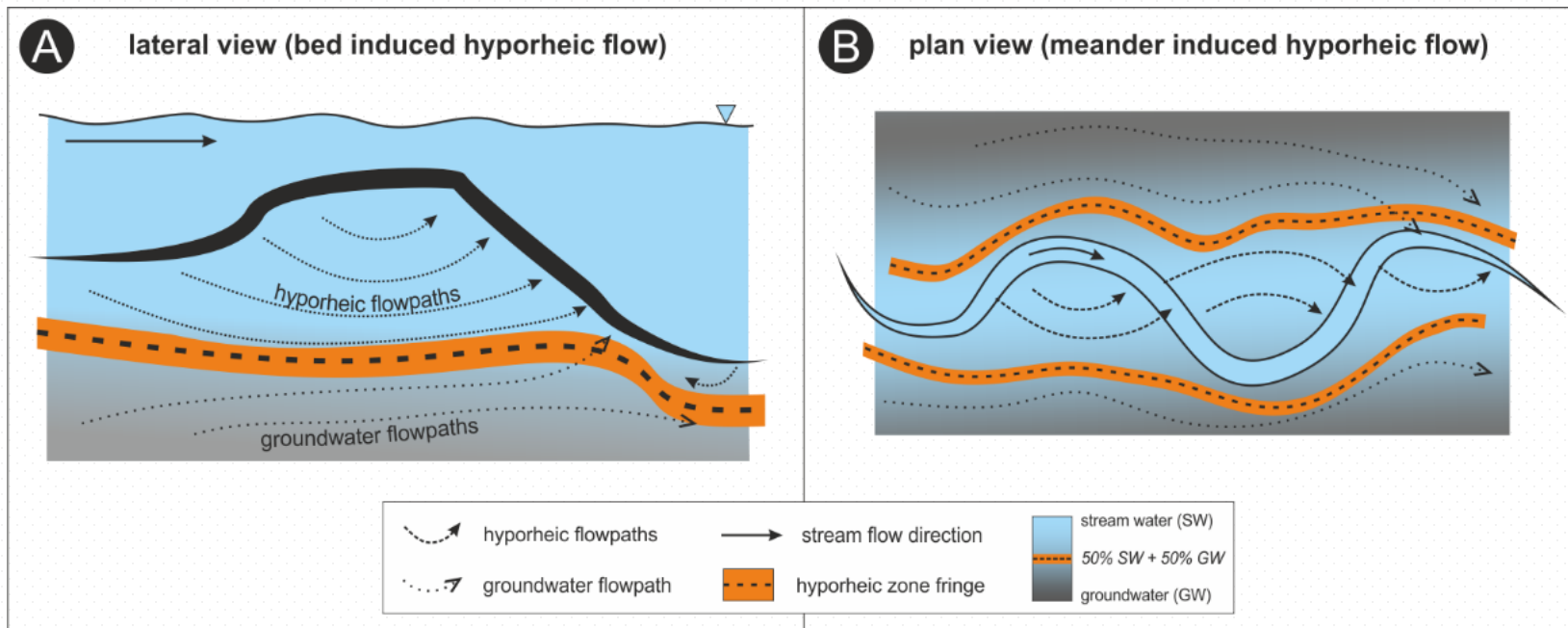


Why is mixing important?

Floodplain: mixing of different water sources, such as infiltrating stream water (SW); floodplain (rain/recharge, *FD*); and local flowing groundwater (GW).

Different solutes get in contact: higher potential for turnover of **groundwater-borne solutes** (e.g., NO_3^-).

Thus, mixing dynamics can control reactive potential of groundwater-borne solutes.



What has been done? What do we know?

- Directly quantification of mixing-dependent-denitrification below streambed: **Hester *et al.* (2013, 2014, 2019), Trauth *et al.* (2015), Trauth & Fleckenstein (2017)**
- Dynamics of the perihel zone (surficial fringe of HZ): **Berezowski *et al.* (2019)**
- Mixing and biogeochemical processes: **Jones *et al.* (2014), Stegen *et al.* (2016)**
- Mapping of different water sources at the floodplain (geostatistical/end-member models): **Lessels *et al.* (2016), Traut *et al.* (2018), Biehler *et al.* (2020)**
(time-labor demanding, may not capture full dynamics of processes)

What do we want to achieve?

- estimate different water sources at the floodplain and their variations;
- quantify and assess controls of (high-degree) mixing spots at the floodplain;
- assess their changes due to transient hydrological boundary conditions.

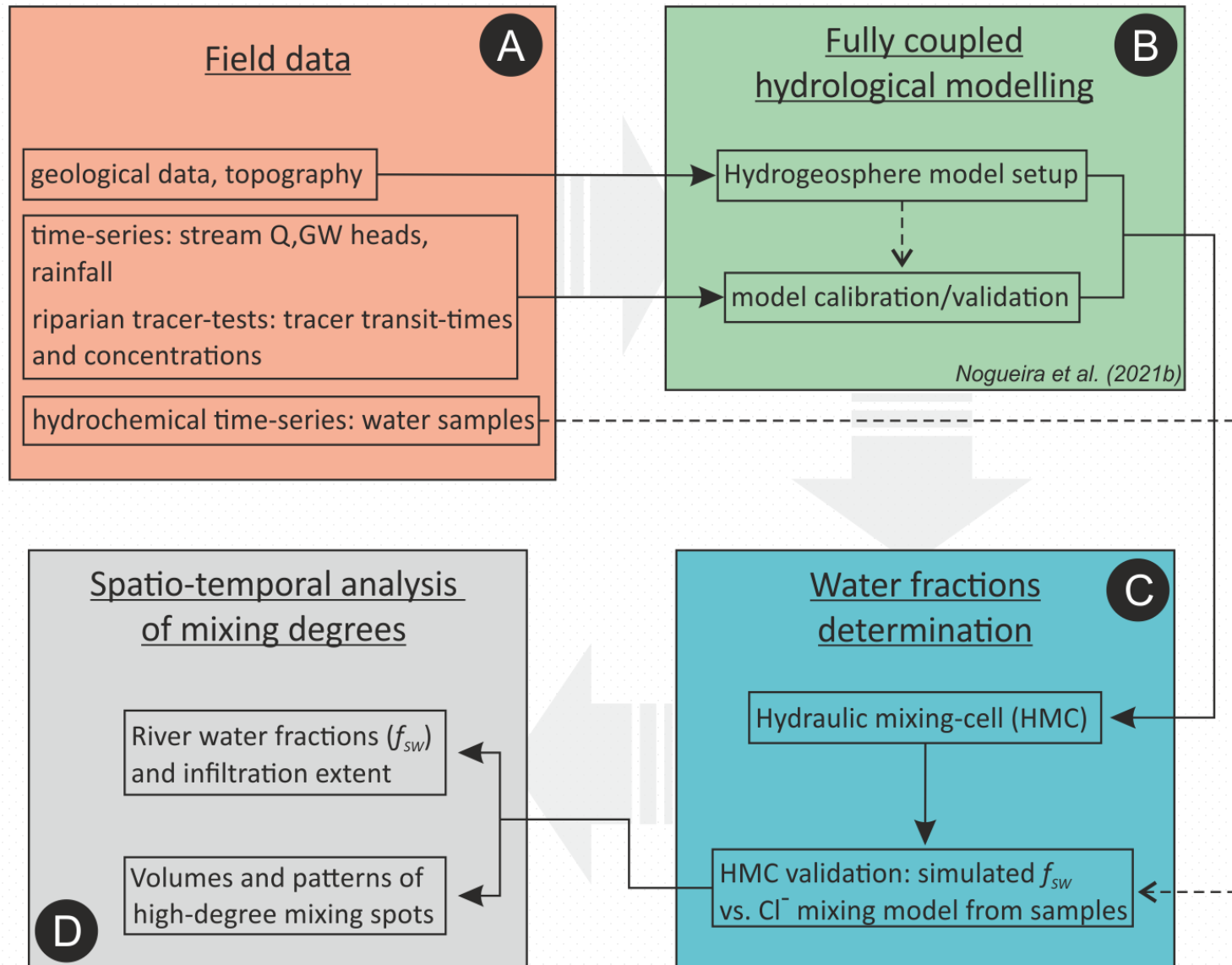
How?

Combine field-data and a fully-coupled flow numerical model (HGS);

+

The spatio-temporal tracking of water parcels and their composition with a hydraulic mixing cell (HMC).

2.Methods – HGS-HMC method



A) Field data acquisition

B) HGS flow model setup and calibration/validation
(*Nogueira et al. – under review*)

C) 1) HGS-HMC for tracking water parcel sources and composition (in each model cell and time-step);
2) HMC validation (f_{sw} x F_{RIV} on wells);

D) Spatio-temporal analysis of water fractions and mixing at the floodplain

2.Methods – HGS-HMC method

HMC - *Hydraulic mixing cell* (Partington et al., 2011, 2013)

- Water fractions calculated according to water fluxes and exchanges (based on flow solution - does not require any extra parameters)
- Predefined water sources/regions (e.g., rain, stream water, groundwater, seawater).
- Usually, all model nodes are initialized with an artificial “initial” fraction of 1.

Sources’ fractions mixed according to volumes of different water fluxes into/out of a cell. For a time t and a fraction w within cell i :

$$f_{i(w)}^t = \underbrace{\left(\frac{V_i^{t-1}}{V_i^t} - \frac{\sum_{j=1}^m V_{ij} \Big|_{t-1}^t}{V_i^t} \right)}_{\text{water fraction } w \text{ leaving cell } i \text{ to cell } j} f_{i(w)}^{t-1} + \underbrace{\frac{\sum_{j=1}^n V_{ji} \Big|_{t-1}^t}{V_i^t}}_{\text{water fraction } w \text{ flowing from cell } j \text{ to cell } i} f_{j(w)}^{t-1}$$

↑
water fraction w
at cell i
water fraction w
leaving cell i to cell j
water fraction w
flowing from cell j to cell i

with m sinks and n sources for cell i

Predefined HMC water sources

- Stream water (f_{SW})
- Groundwater (f_{GW}) + Floodplain water (f_{FD}) (water coming from model top)
- Initial groundwater (f_{GWi}) ← “warm-up” period to flush it out prior analyses

HMC validation

Comparison of simulated f_{SW} with calculated stream water fraction (F_{RIV}) from Cl^- mixing model

$$F_{RIV} = \frac{[Cl_{obs}^-] - [Cl_{GW}^-]}{[Cl_{SW}^-] - [Cl_{GW}^-]}$$

HMC fractions integration

$$V_w = \frac{\sum_{p=1}^P f_w}{V_{tot}} \times 100\%$$

2.Methods – HGS-HMC method

Mixing degrees (d)

$$d = 1 - \left[\frac{\sqrt{(1/2 - f_{sw})^2 + (1/2 - (f_{GW} + f_{FD}))^2}}{(\sqrt{2}/2)} \right]$$

$d=1$ (“perfect mixing”) = equal HMC water fractions within a cell

high-degree mixing spot (d_h) = $d \geq 0.75$

High-degree mixing spots (d_h) integration

$$V_{d_h} = \frac{\sum_{p=1}^P d_h}{V_{tot}} \times 100\%$$

HGS flow paths extraction and transit-times calculation

Based on transient velocity-fields and particles positions (TecPlot+MatLab)
 Particles released at the streambed and floodplain ($\approx 1,300$ per time-step)

Predefined HMC water sources

- Stream water (f_{sw})
- Groundwater (f_{GW}) + Floodplain water (f_{FD}) (water coming from model top)
- Initial groundwater (f_{GWi}) ← “warm-up” period to flush it out prior analyses

HMC validation

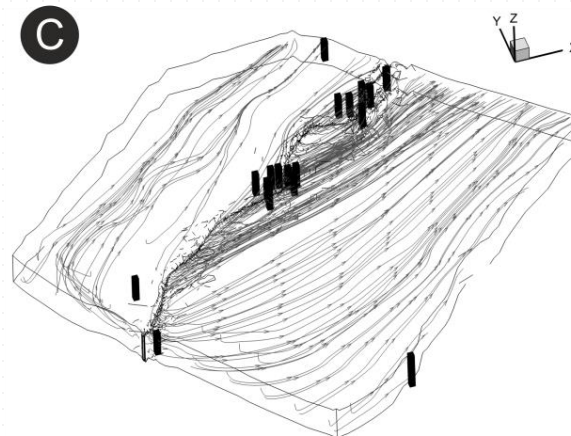
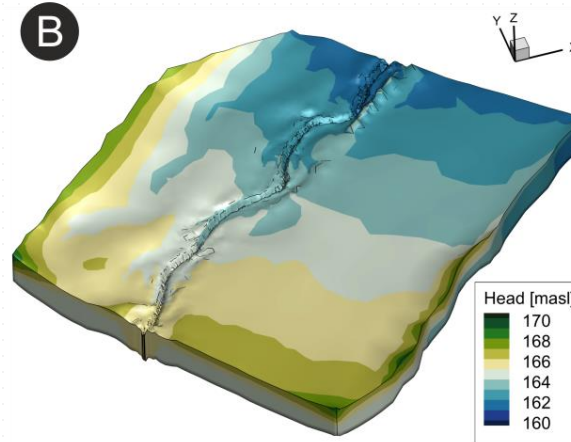
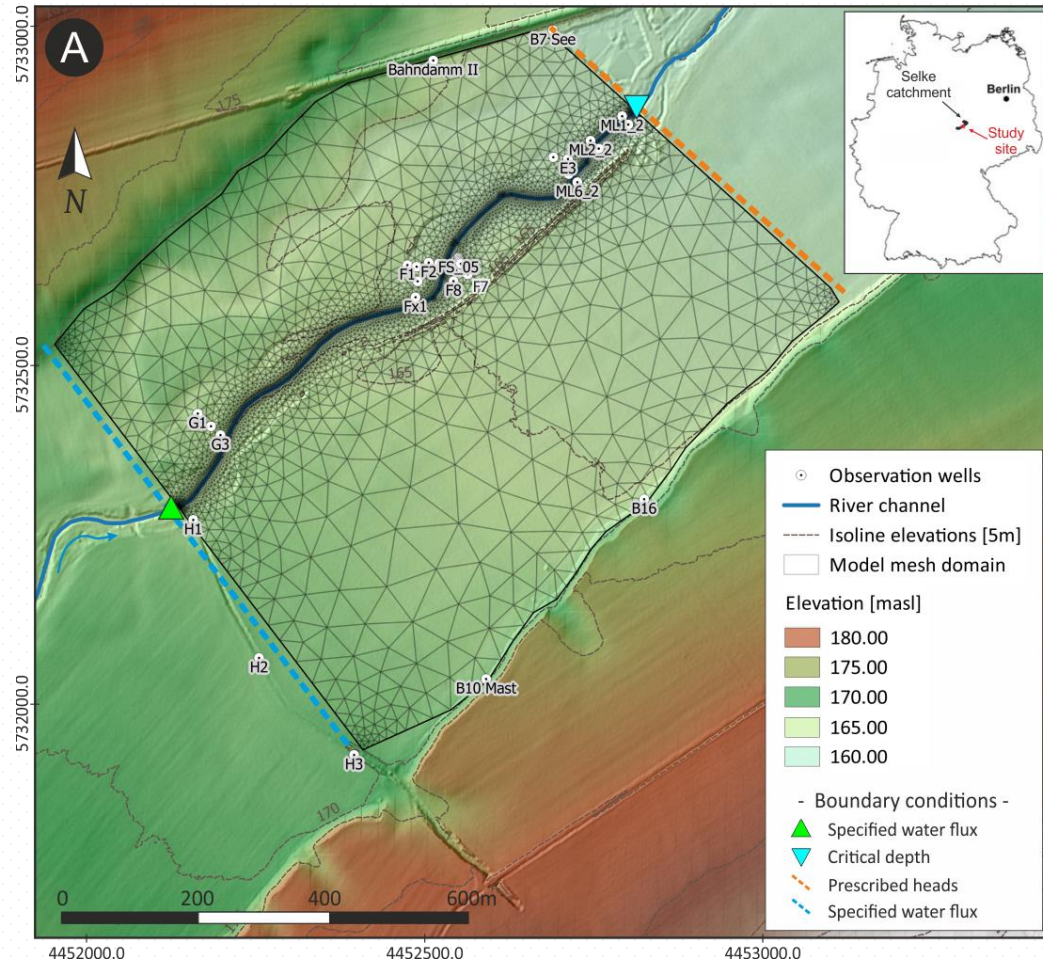
Comparison of simulated f_{sw} with calculated stream water fraction (F_{RIV}) from Cl^- mixing model

$$F_{RIV} = \frac{[Cl_{obs}^-] - [Cl_{GW}^-]}{[Cl_{sw}^-] - [Cl_{GW}^-]}$$

HMC fractions integration

$$V_w = \frac{\sum_{p=1}^P f_w}{V_{tot}} \times 100\%$$

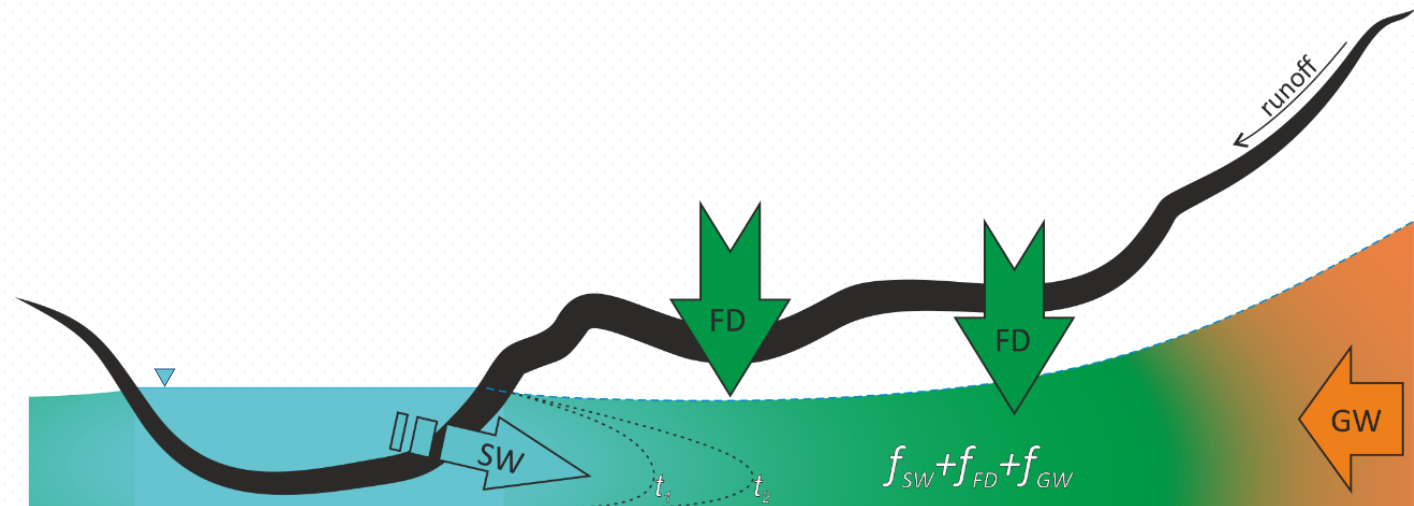
2.Methods – Case study and numerical model



Application of a pre-calibrated flow model (period 2017-2019) for a transient simulation between 2013-2016.

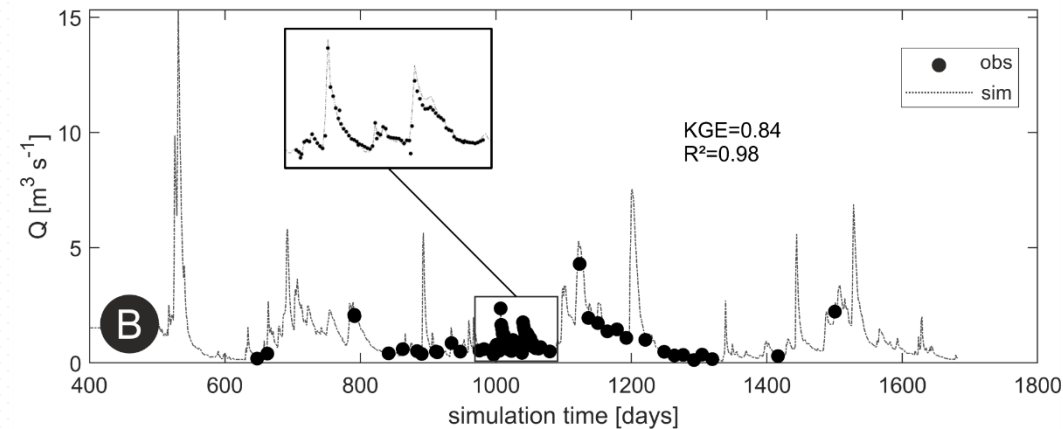
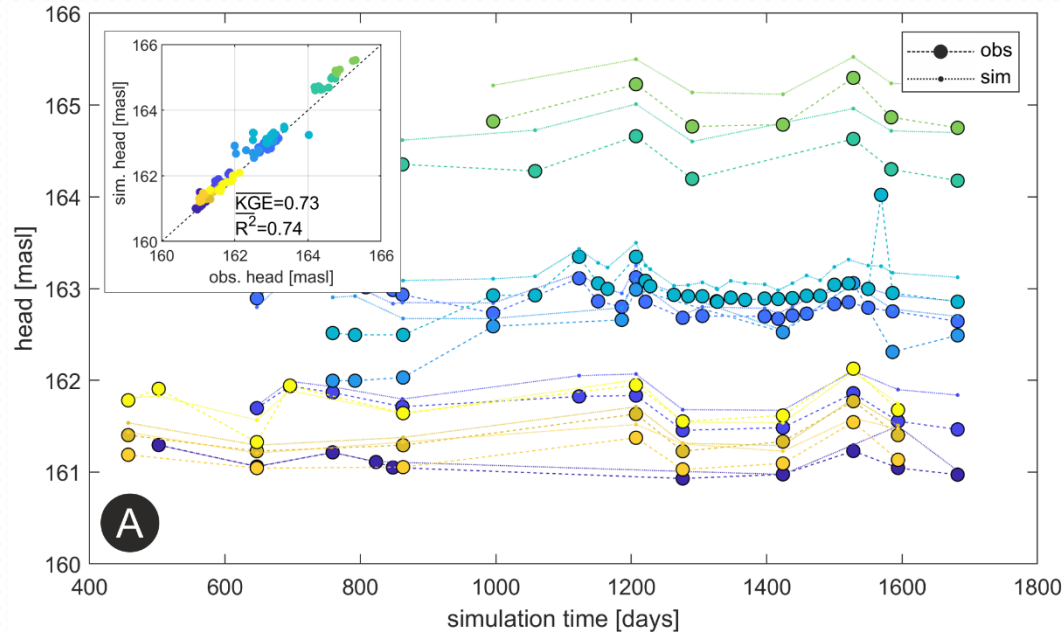
- Adjustment of flow boundary conditions
- & no additional calibration

3.Results



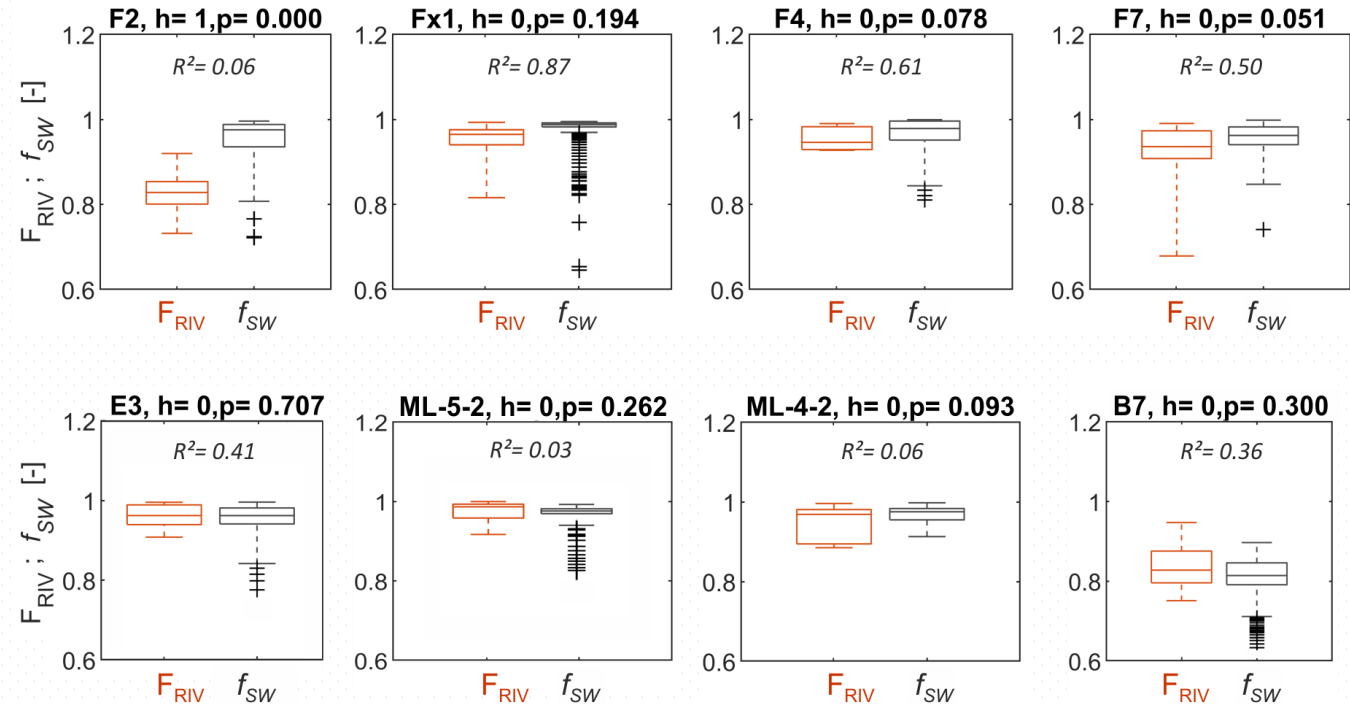
3.Results – Model/framework validation

HGS - flow



C

HMC - hydrochemistry



Calculated F_{RIV} and simulated f_{SW}

Wilcoxon-Test for groups medians ($h=0$, p -value); Correlation coefficient (R^2)

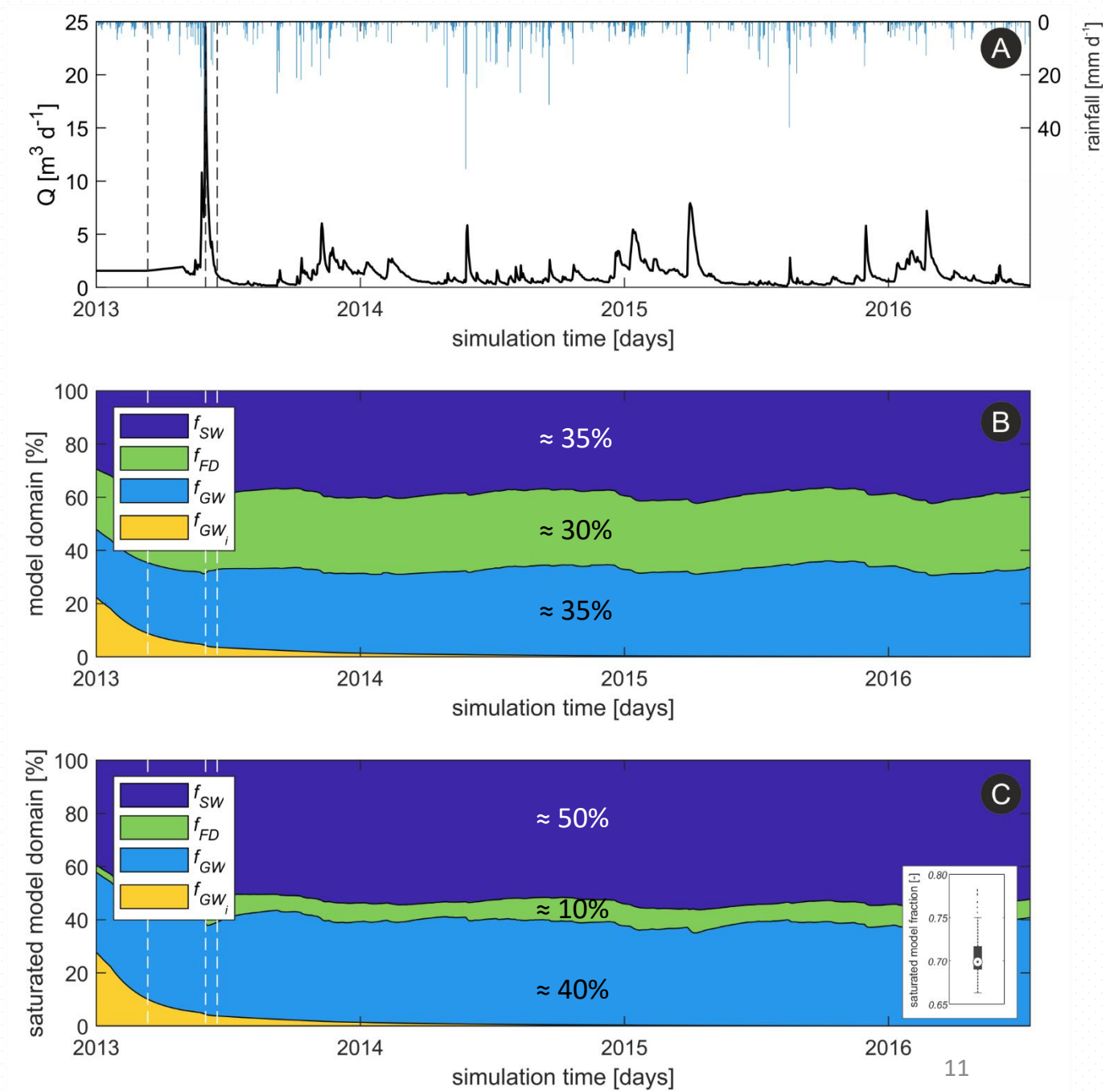
Acceptable differences since a rigorous calibration to hydrochemical data was not our goal

3.Results – Temporal variation of HMC fractions

(B) HMC fractions for the entire domain

HMC results : water origin (*not the water content!*)

(C) HMC fractions for the fully-saturated domain



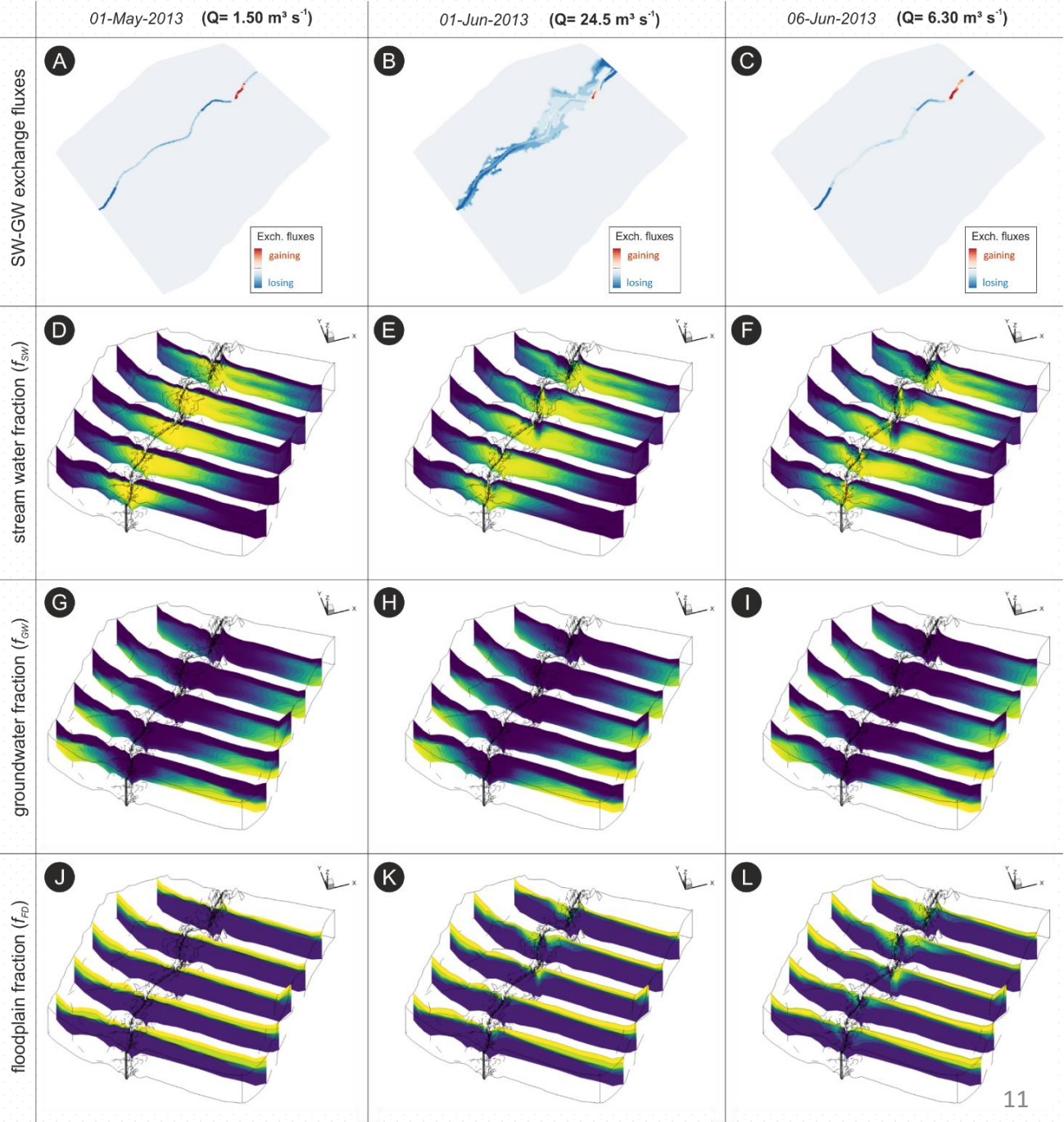
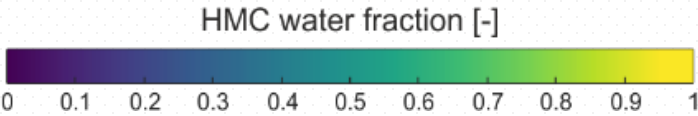
3.Results – Spatial distribution of HMC fractions

(A-C) SW-GW exchange patterns

(D-F) stream water (f_{SW})

(G-I) groundwater (f_{GW})

(J-L) floodplain water (f_{FD})

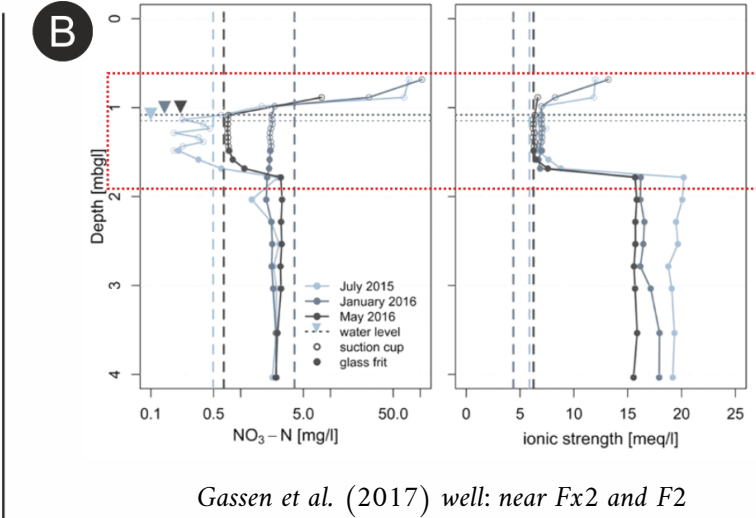
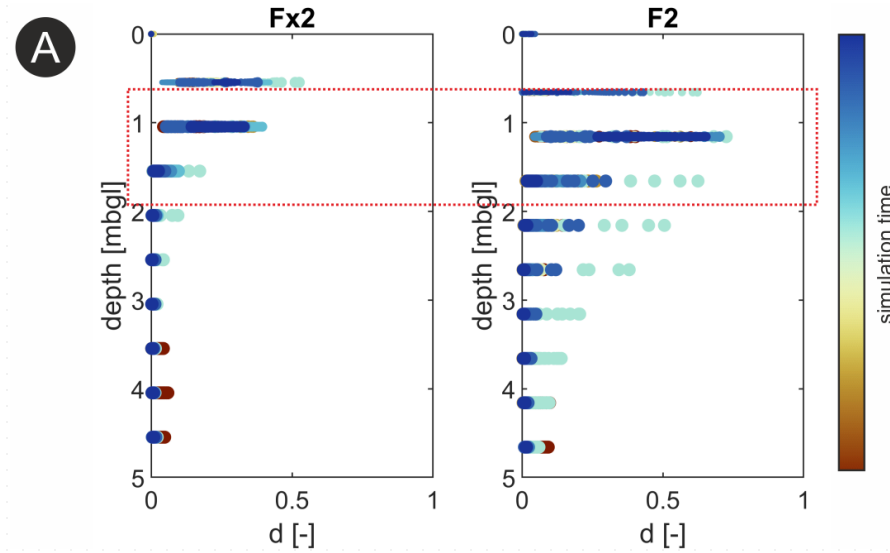


3.Results – Mixing degree: vertical variation

(A) Mixing degrees vs. wells' depths

(B) NO_3^- concentration and ionic strength for a high-resolution obs. well (Gassen *et al.*, 2017)

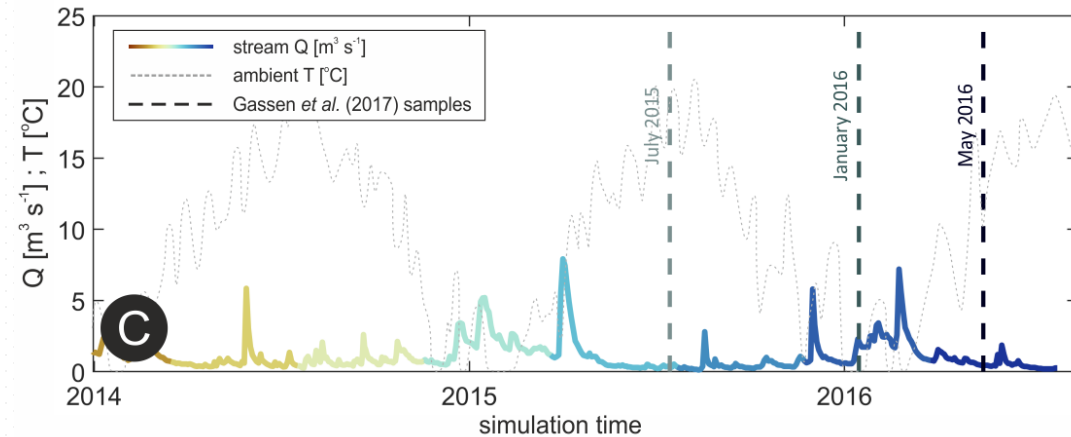
(C) Stream Q and sampling of Gassen *et al.* (2017)



Key point:

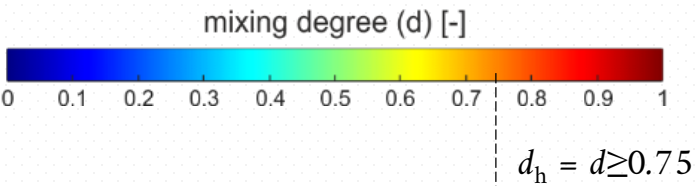
FD- NO_3^-
+
SW-DOC

High NO_3^- “mixing-turnover”
(temperature controlled)



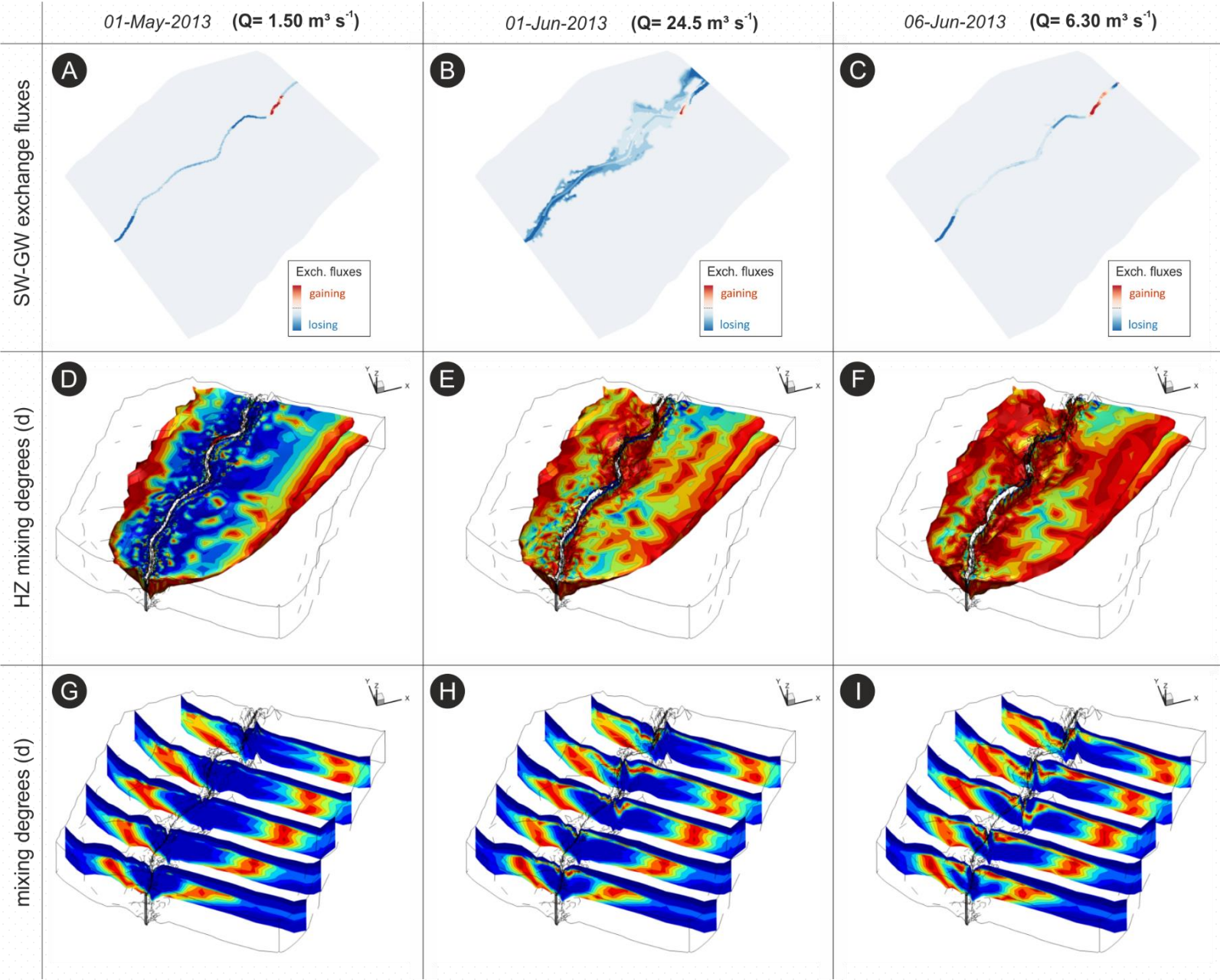
3.Results – Mixing degree: spatial distribution

(A-C) SW-GW exchange patterns;
(D-F) mixing degrees within the HZ ($f_{SW} \geq 0.5$),
(G-I) mixing degrees on the entire domain.



Key point:

- Mixing mainly at the fringe of HZ, following Q events

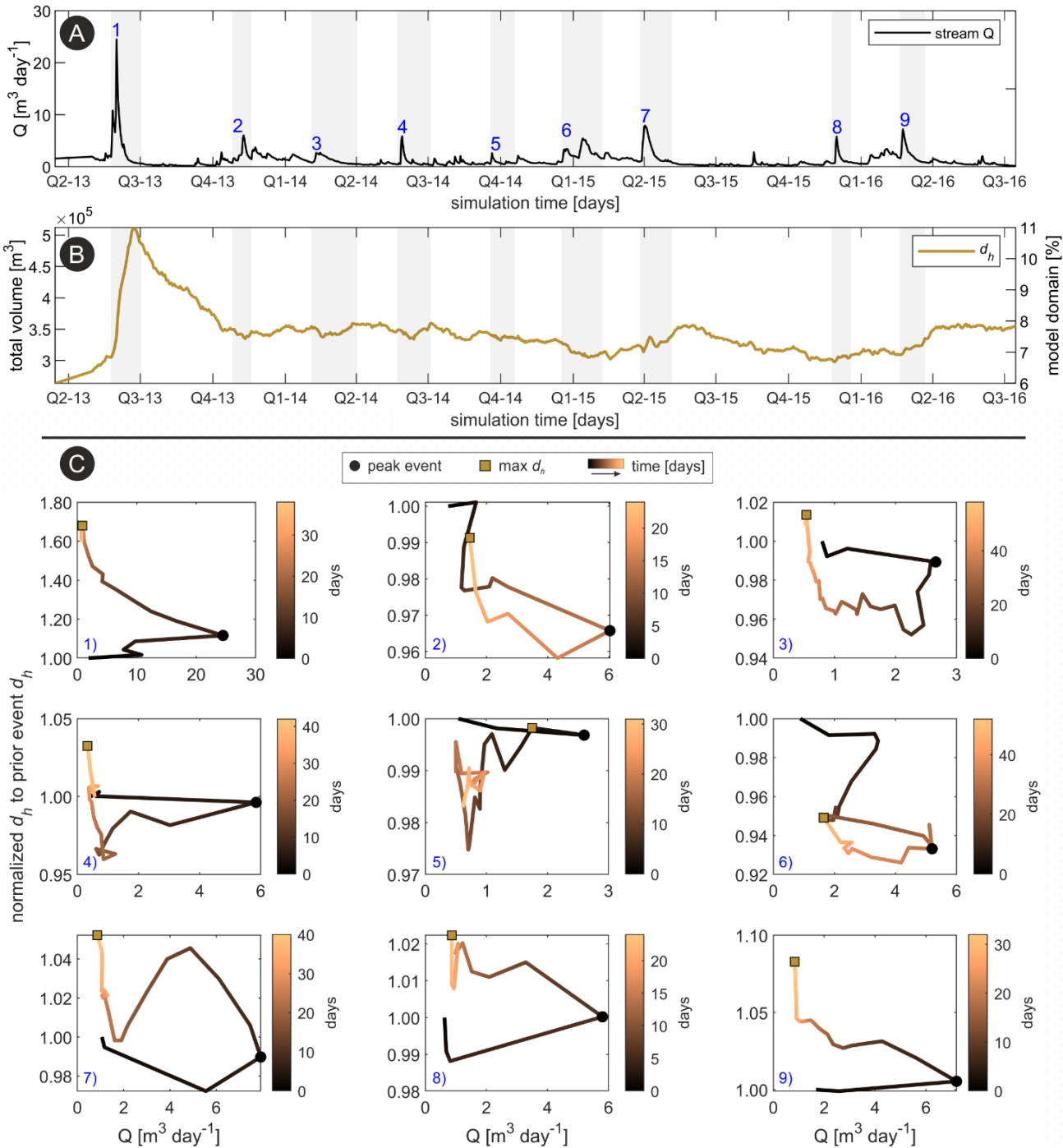


3.Results – Temporal variation of high-degree mixing spots (d_h)

(A) Selected discharge events

(B) Total d_h volume (and % of domain)

(C) Q vs. *normalized* d_h plots for selected discharge events



Key points:

- Q events increase overall d_h ($\approx 5\%$)

3.Results – Temporal variation of high-degree mixing spots (d_h)

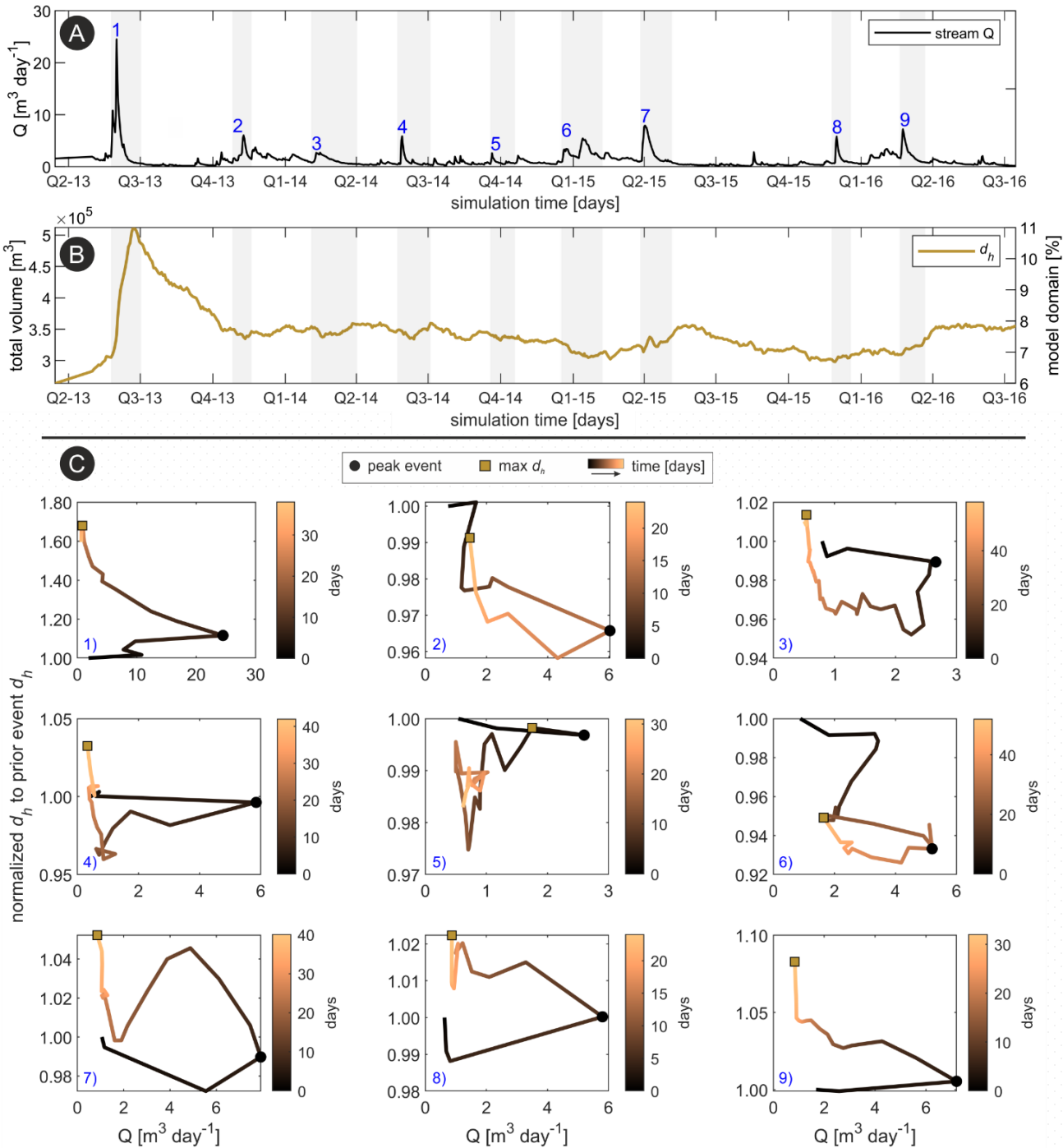
(A) Selected discharge events

Table 1 – Overall Spearman’s rank correlation between metrics of discharge events and the increasing of high-degree mixing spots (d_h) at the floodplain.

Discharge events metrics	Correlation to increase in d_h
Event duration [days]	0.009
Time-to-peak [days]	0.305
Time-to-peak/event duration [-]	0.340
Peak prominence (ΔQ) [$\text{m}^3 \text{s}^{-1}$]	0.963
Lag between <i>peak-event</i> and peak d_h (after <i>peak-event</i>) [days]	
Min	1
Mean	14
Max	46
Spearman’s correlation between ΔQ and lag to peak d_h : 0.28	
Spearman’s correlation between event duration and lag to peak d_h : 0.66	

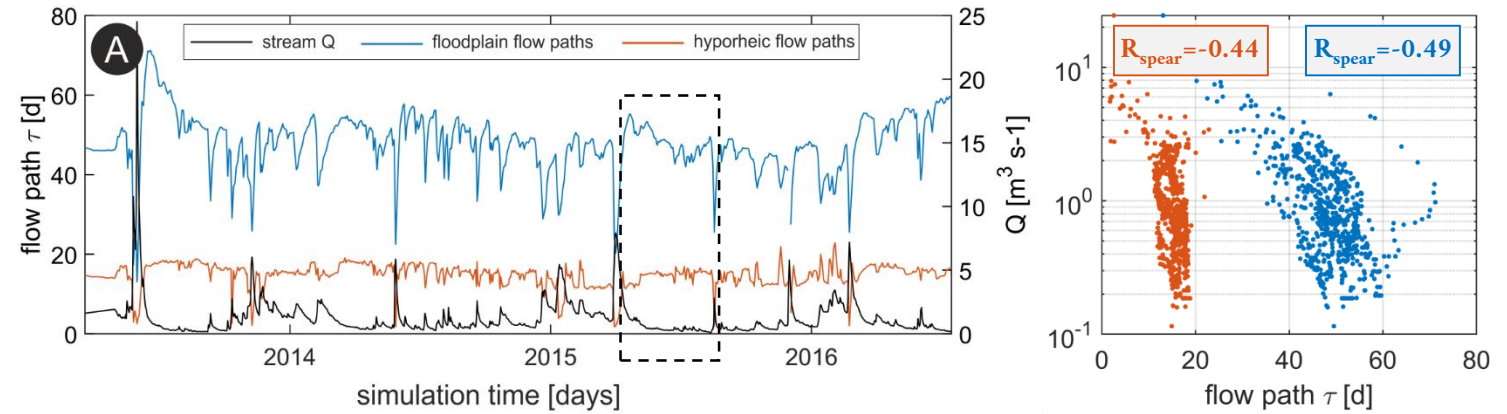
Key points:

- Q events increase overall d_h ($\approx 5\%$)
- Peak prominence has the strongest control on increasing d_h
- Event duration has the strongest control on lag between Q peak and d_h

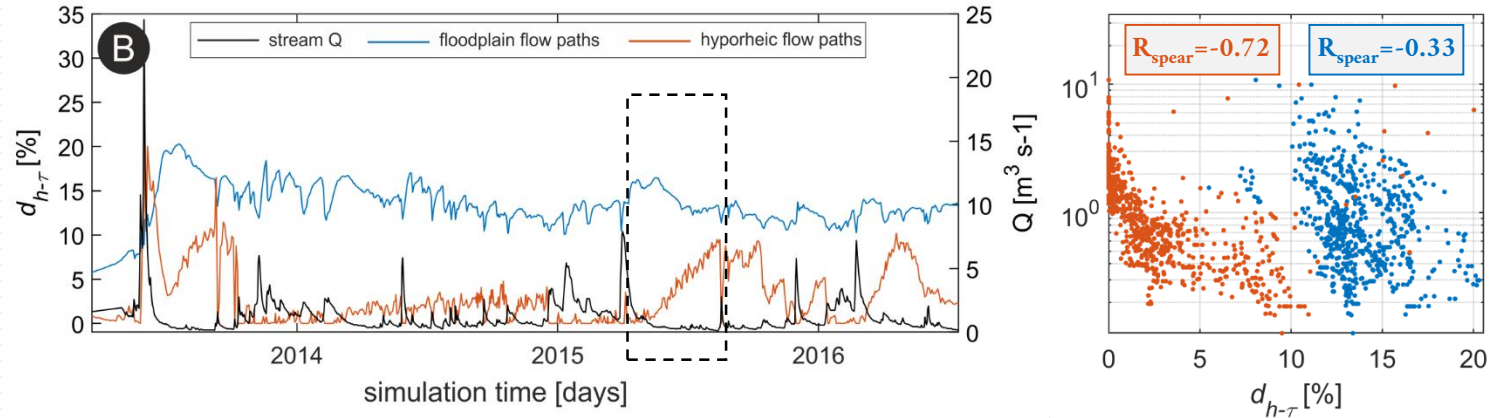


3.Results – Residence-time within high-degree mixing spots ($d_{h-\tau}$)

(A) Median flow path transit-times (flow path τ)



(B) Median residence-time within d_h zones ($d_{h-\tau}$) as a fraction of total flow path τ



Key points:

- Shorter transit-times during Q events (and also $d_{h-\tau}$)

- Hyporheic flow paths: greater $d_{h-\tau}$ during baseflow (slightly stronger gaining conditions -higher d_h)

opposite to floodplain flow paths

Take home messages

Key message 1:

- *HGS-HMC* is an easy-to-transfer (straight-forward) tool for tracking different water-sources and their contribution at the floodplain scale

Key message 2:

- (high) Mixing mostly at the lateral fringe of the HZ, and at the groundwater table interface (mainly after flooding events)

Key messages 3:

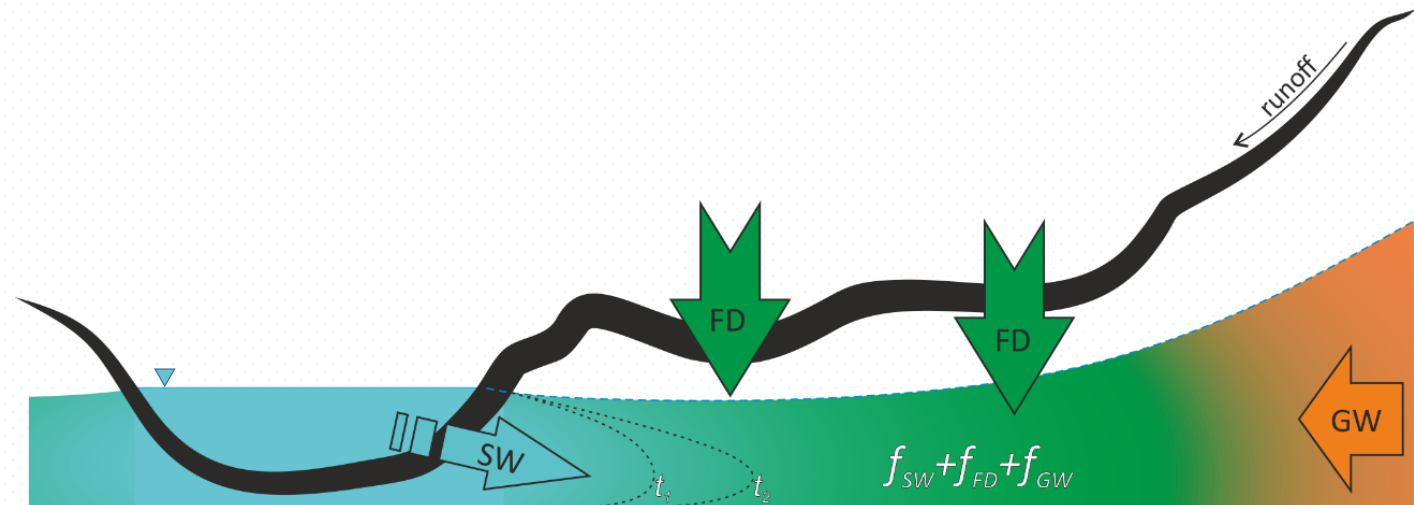
- Peak prominence has the strongest control on increasing mixing spots (on average 5% increasing, up to 50%)

Key message 4:

- Transit-times generally decrease during Q events (also does $d_{h-\tau}$); Discharge events seem to enhance “mixing-turnover” of groundwater-borne solutes at the floodplain more than at hyporheic regions.

Limitations:

- No simulation of reactions (or validation)
- No spatial distribution of HMC fractions within a cell
- Reliance on flow model solution



Something else?



Thanks for the attention! :]

Mixing degrees: a vector in w dimensions

The distance between a “perfect mixing” point (V_p)
and fractions in your node (V_n)

For 3 end-members (3D):

the perfect mixing:

$$V_p = [1/3, 1/3, 1/3]$$

the mixture:

$$V_n = [f_{SW}, f_{FD}, f_{SW}]$$

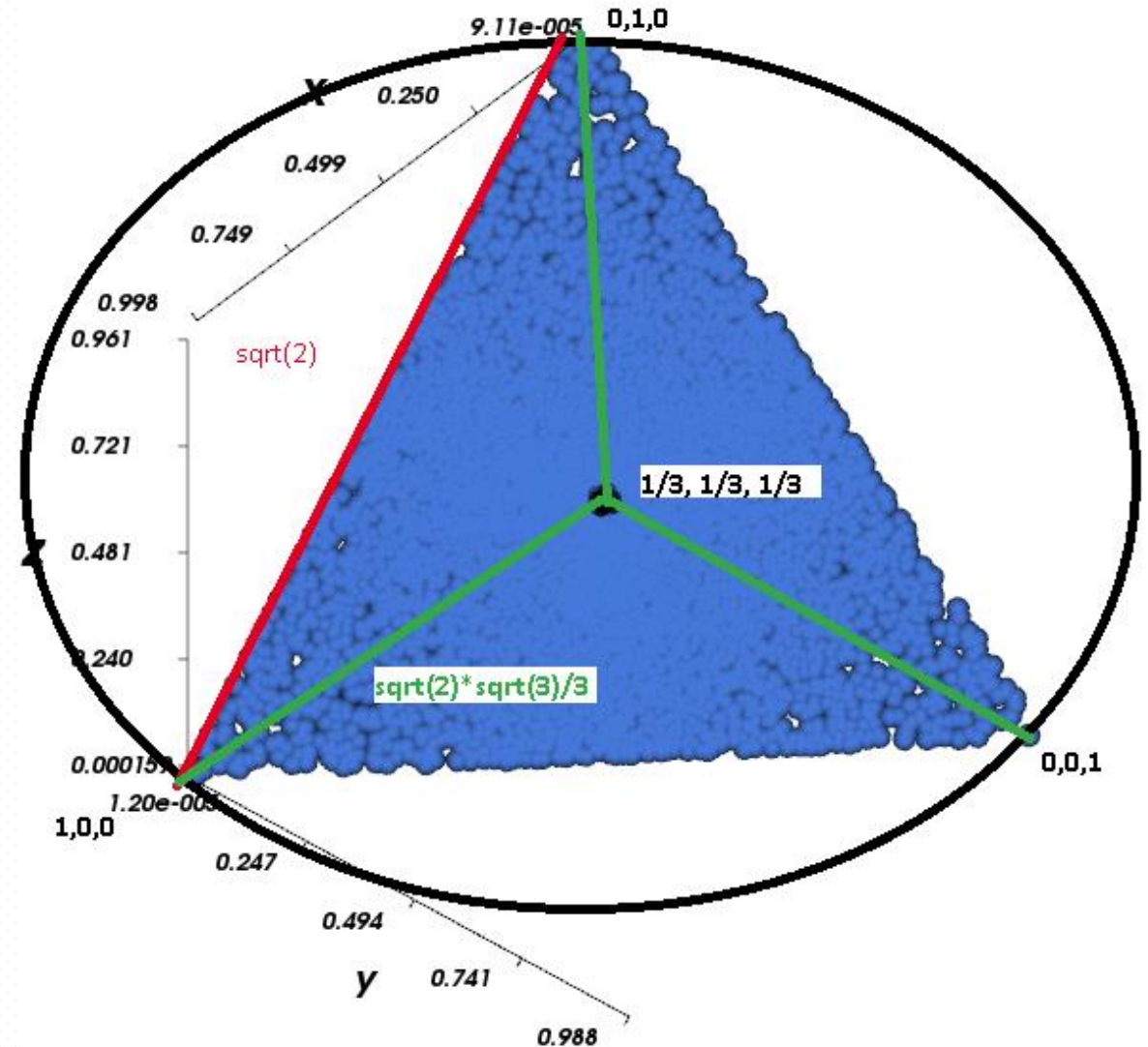
distance between the two vectors:

$$\text{dist} = \sqrt{(x_p - x_n)^2 + (y_p - y_n)^2 + (z_p - z_n)^2}$$

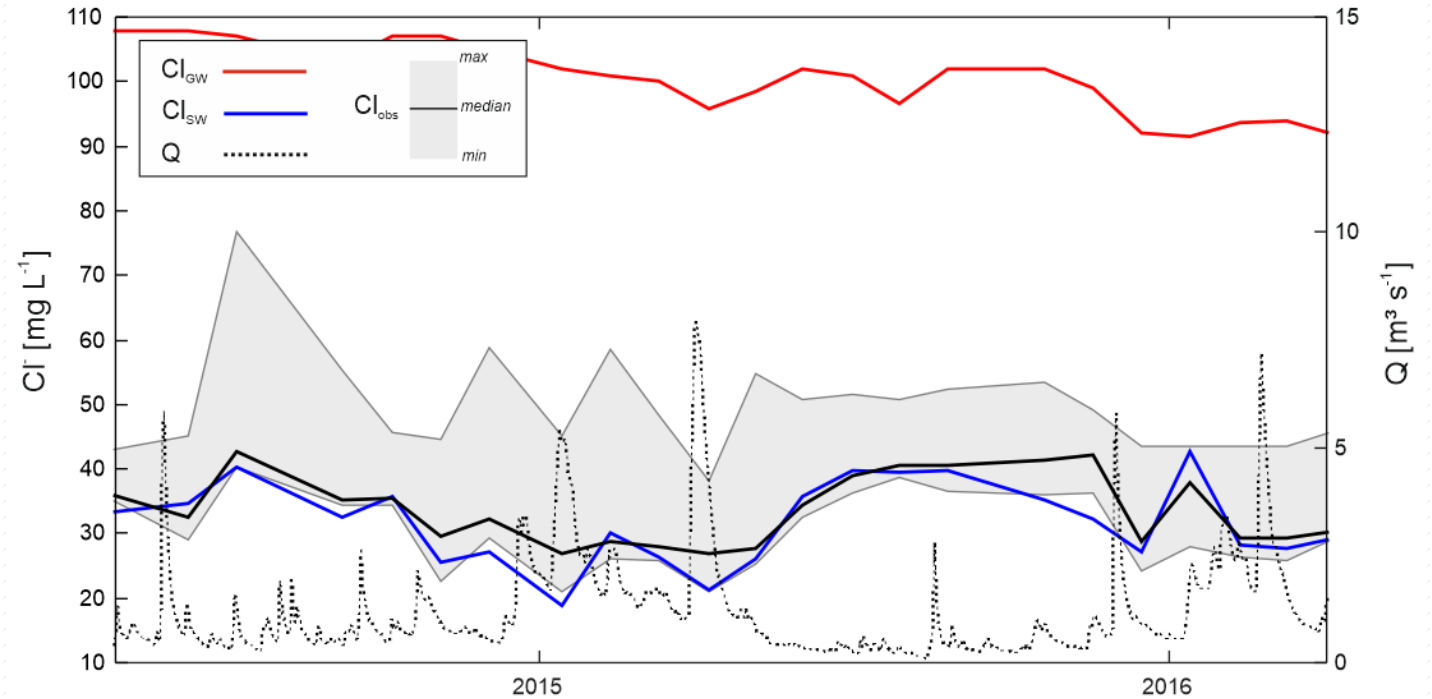
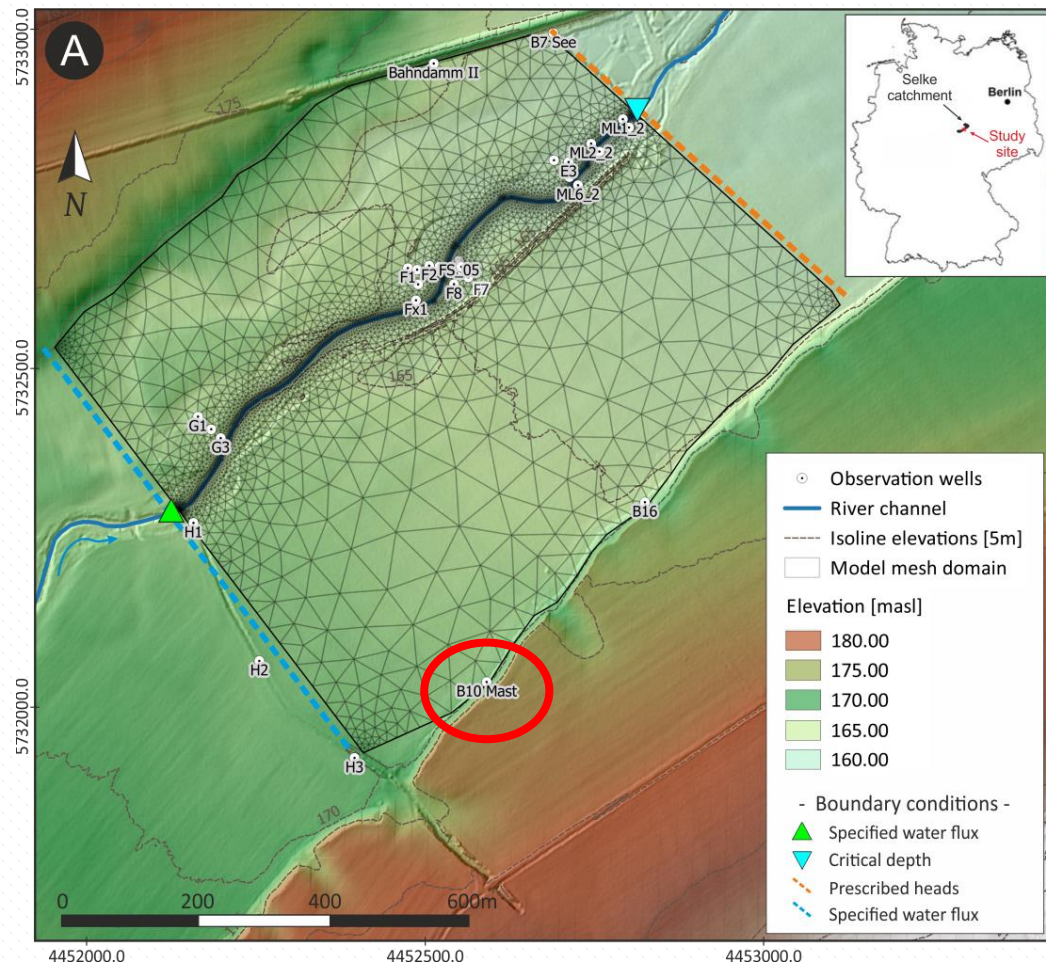
$$\text{max_dist} = \sqrt{2} \cdot \sqrt{3} / 3$$

$$d = 1 - \text{dist} / \text{max_dist}$$

$$d = 1 - \left[\frac{\sqrt{(1/w - f_1)^2 + (1/w - f_2)^2 + \dots + (1/w - f_w)^2}}{(\sqrt{2} \times \sqrt{w} / w)} \right] \quad \text{or} \quad d = 1 - \left[\frac{\sqrt{(1/2 - f_{SW})^2 + (1/2 - (f_{GW} + f_{FD}))^2}}{(\sqrt{2}/2)} \right]$$



Measured Cl^- concentrations for HMC validation



Measured Cl^- concentrations from groundwater *end-member* (Cl_{GW}), surface water *end-member* (Cl_{SW}), and observation wells (Cl_{obs}). Q is the stream discharge.

Flow paths, velocities and mixing degrees

Particles released at the streambed (≈ 300) and floodplain (1,000)

Release locations:

