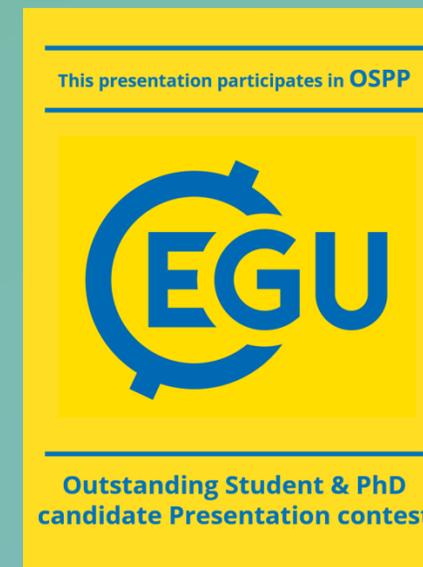


# EGU 2022 DISPLAY MATERIAL

Wed, 25 May 2022



Improving the identifiability of Transient Storage Model parameters to explore process information in solutes breakthrough curve

Enrico Bonanno (1, 2), Günter Blöschl (2), Julian Klaus (3)

- 1) Catchment and Eco-Hydrology Group, Luxembourg Institute of Science and Technology, Belvaux, Luxembourg;
- 2) Institute of Hydraulic and Water Resources Engineering, Vienna University of Technology, Vienna, Austria;
- 3) Institute of Geography, University of Bonn, Bonn, Germany

[bonanno@hydro.tuwien.ac.at](mailto:bonanno@hydro.tuwien.ac.at)

## Why do we care?

 Solute transport  
in streams 

Where does the water go?

# Why do we care?

Solute transport  
in streams

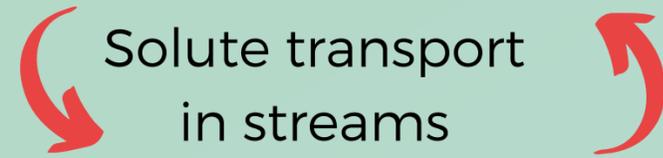
Where does the water go?



Control stream water quality in  
river network

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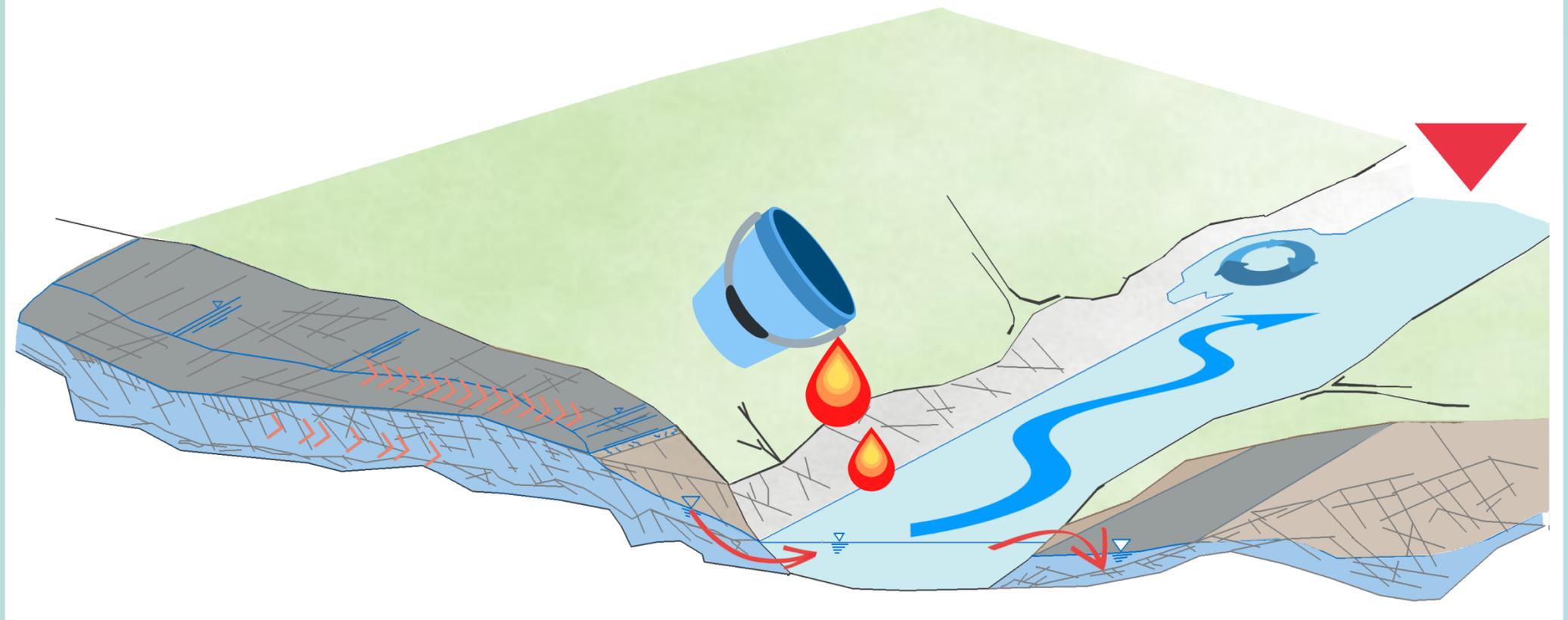


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## How do we experimentally study solute transport in streams?



## Why do we care?

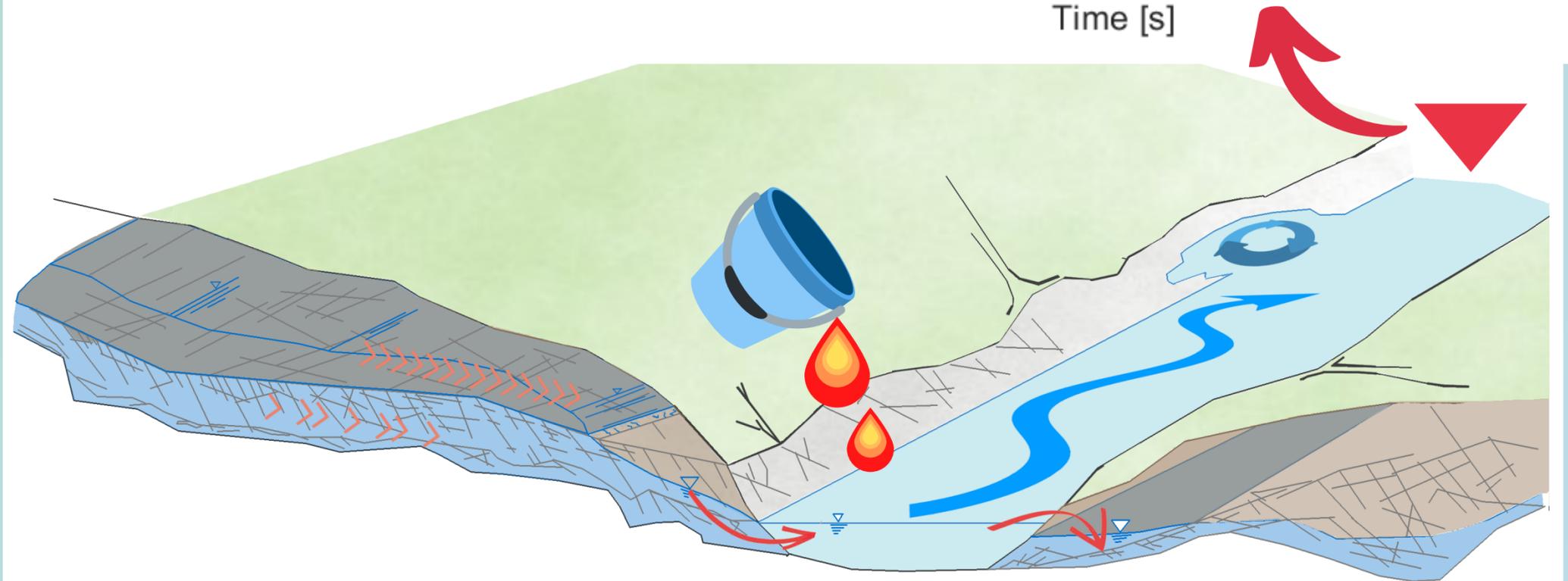
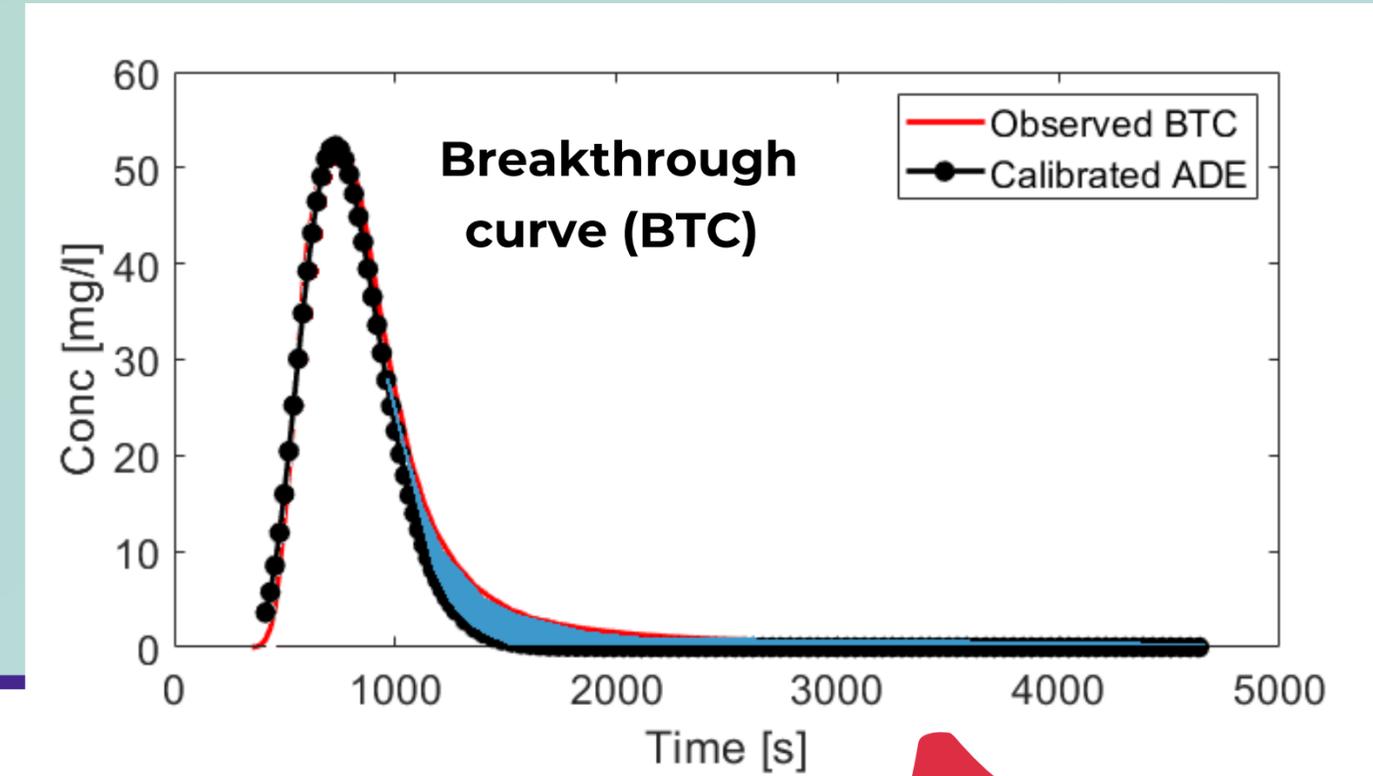
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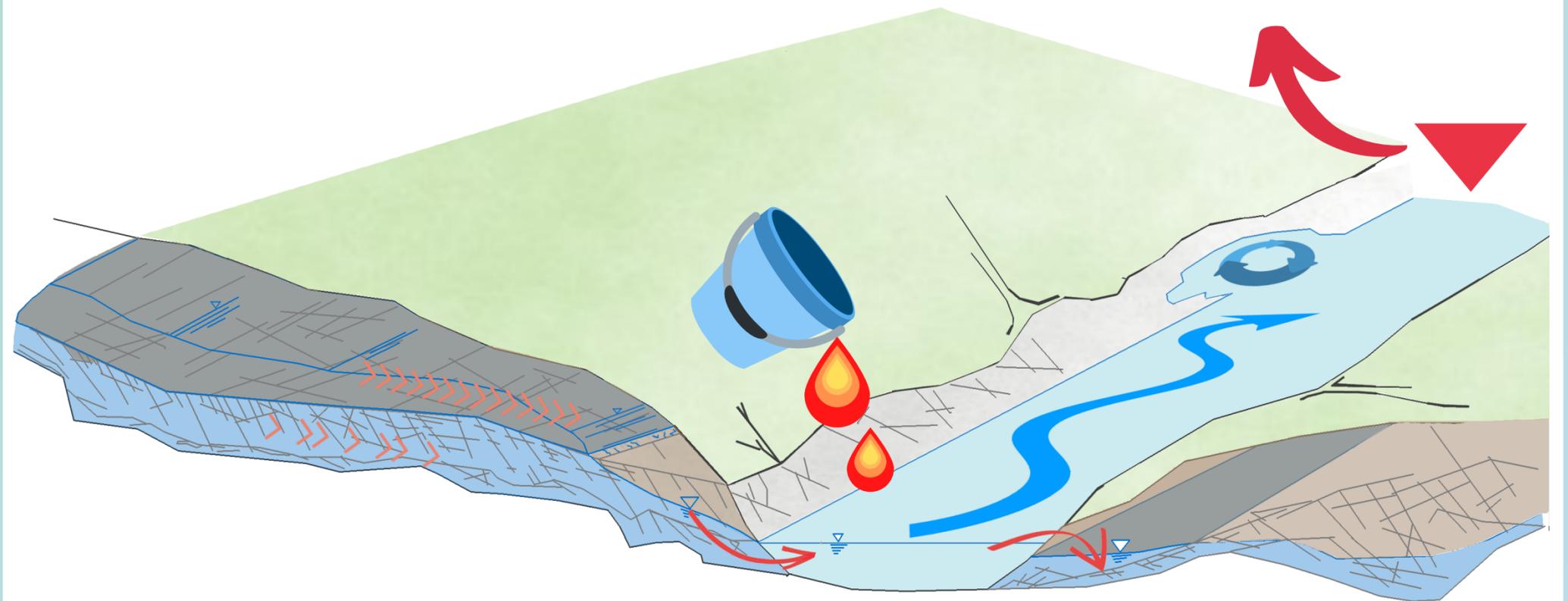
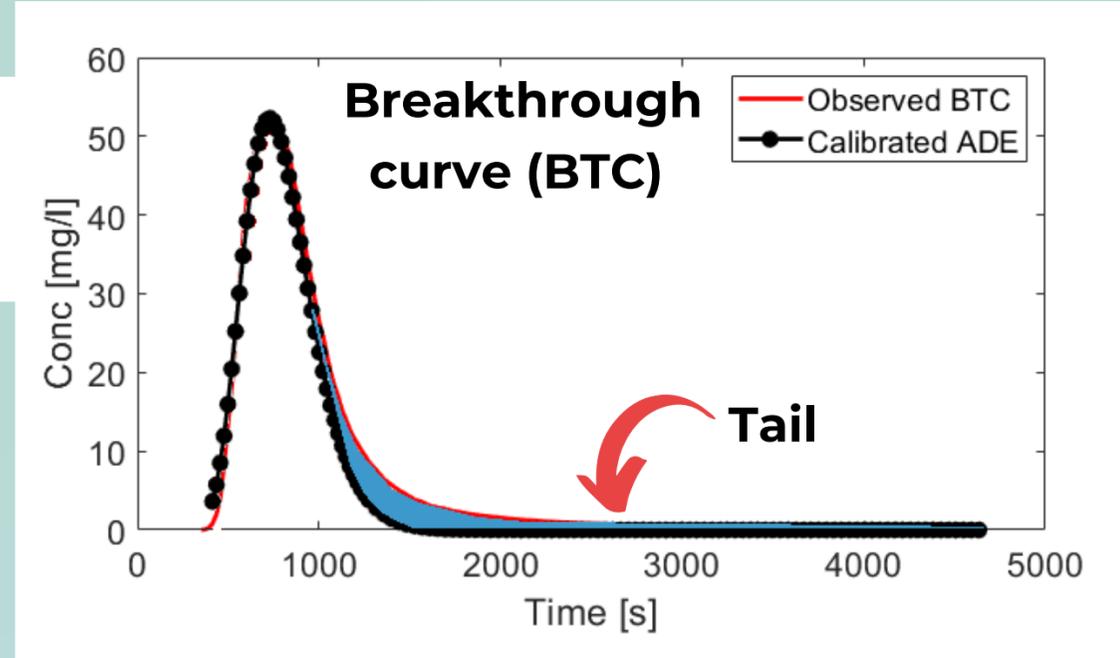
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Advection Dispersion Equation

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + \frac{1}{A} \frac{\partial}{\partial x} \left( AD \frac{\partial C}{\partial x} \right)$$

Taylor (1921, 1954)

Advection dispersion Equation is non able to correctly describe the observed tracer transport in stream channels due to pronounced tail of the BTC



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Solute transport  
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Where does the water go?



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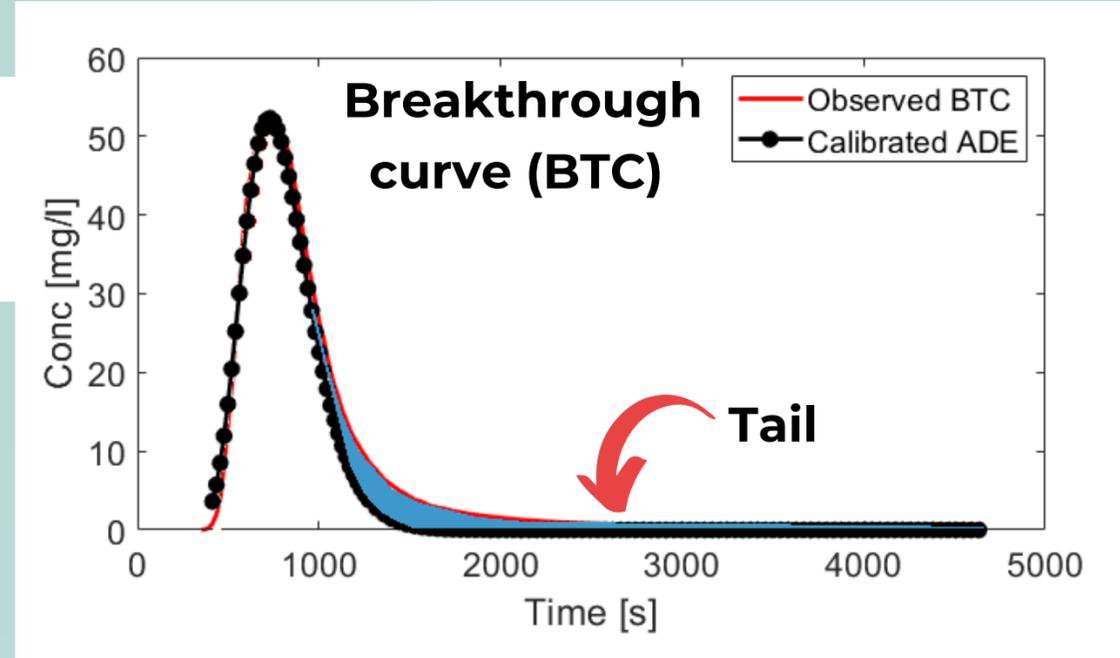
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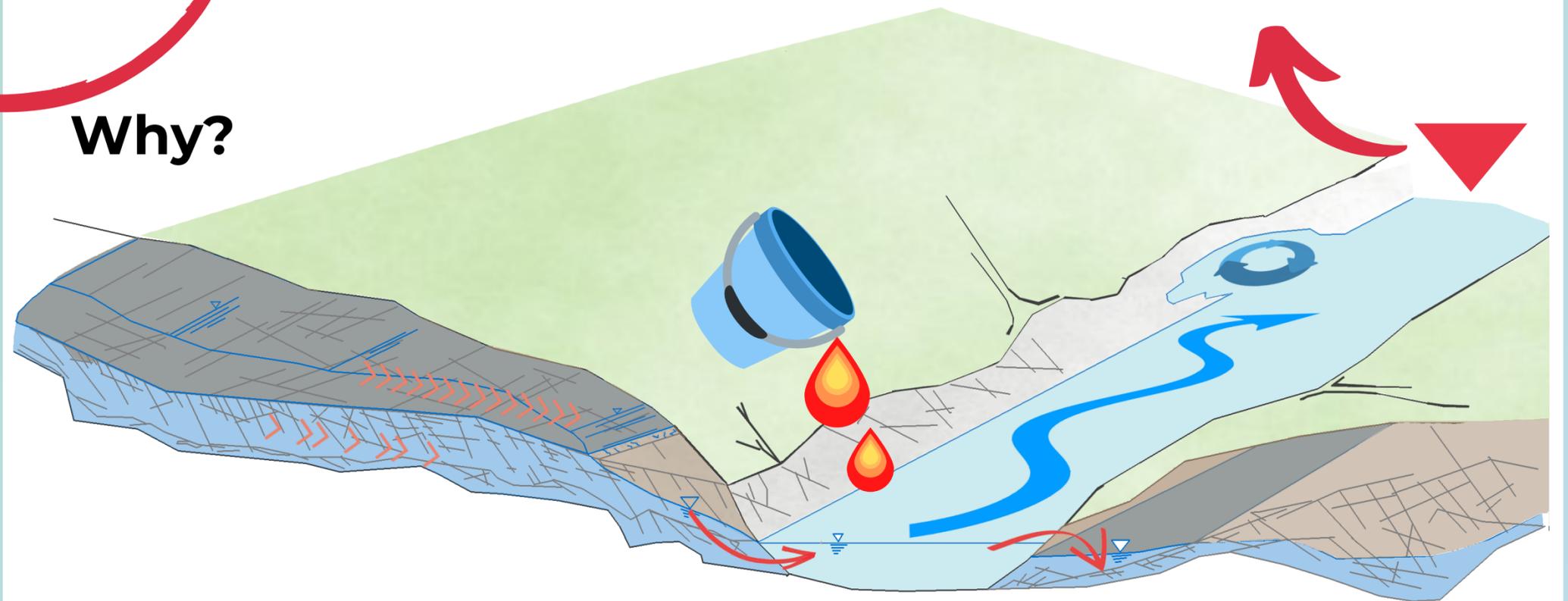
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Why?



# Why do we care?

Solute transport in streams

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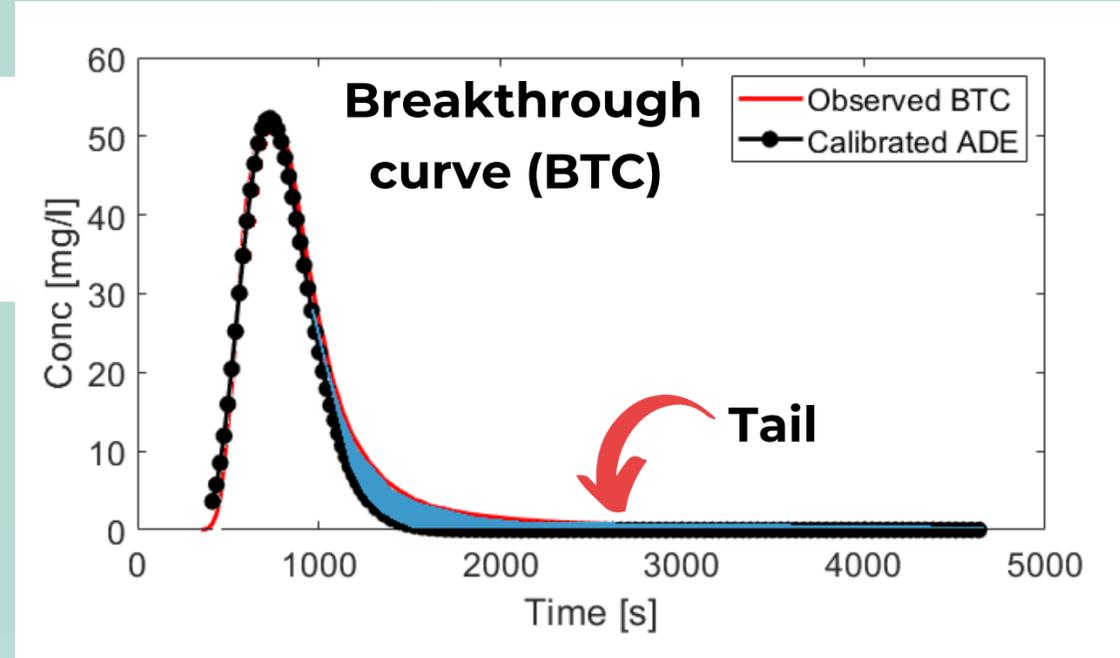
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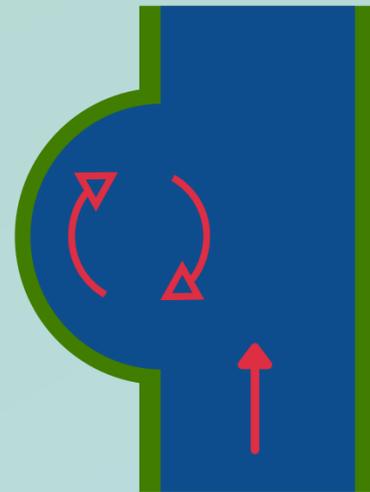
**The stream is not a pipe!**  
Bencala (1993)

Hydrologic exchange with:

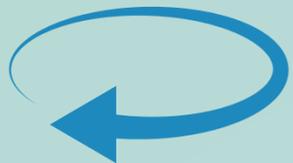


In-stream sediments

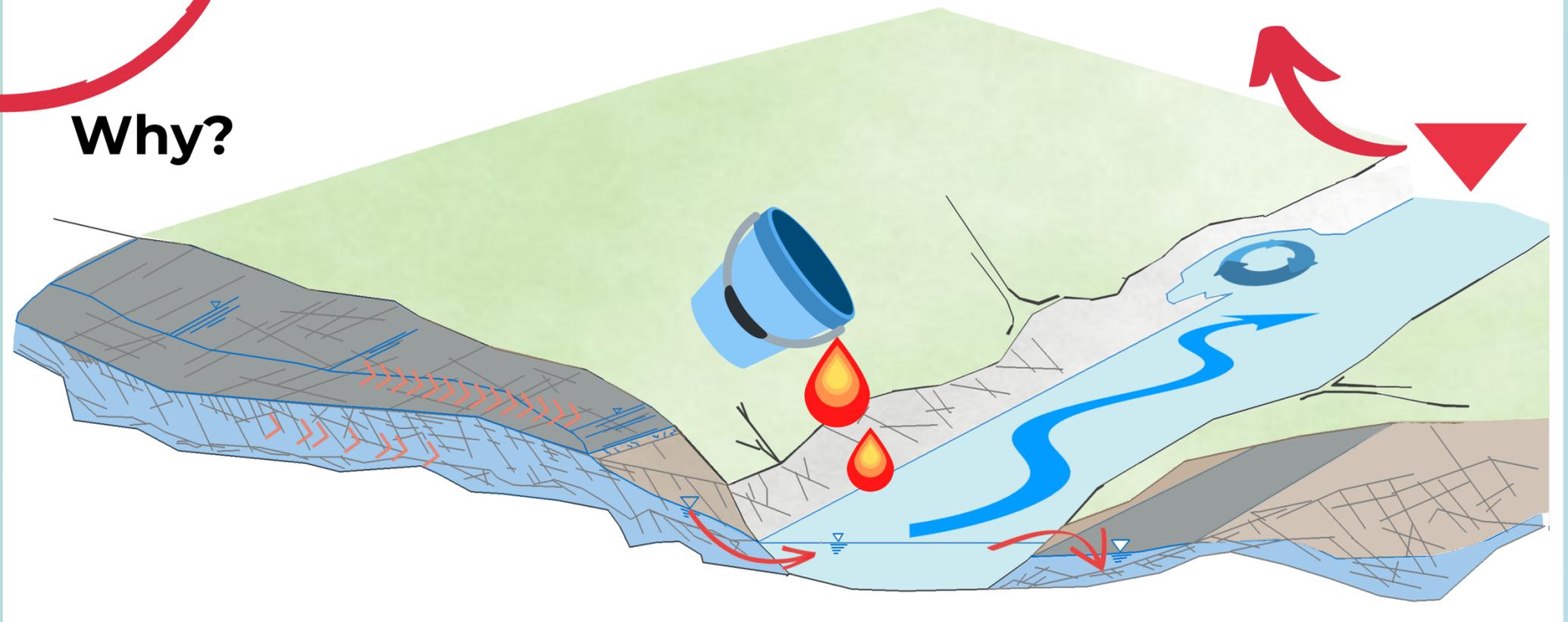
Pools



SW-GW exchange



**Why?**



# Why do we care?

Solute transport in streams

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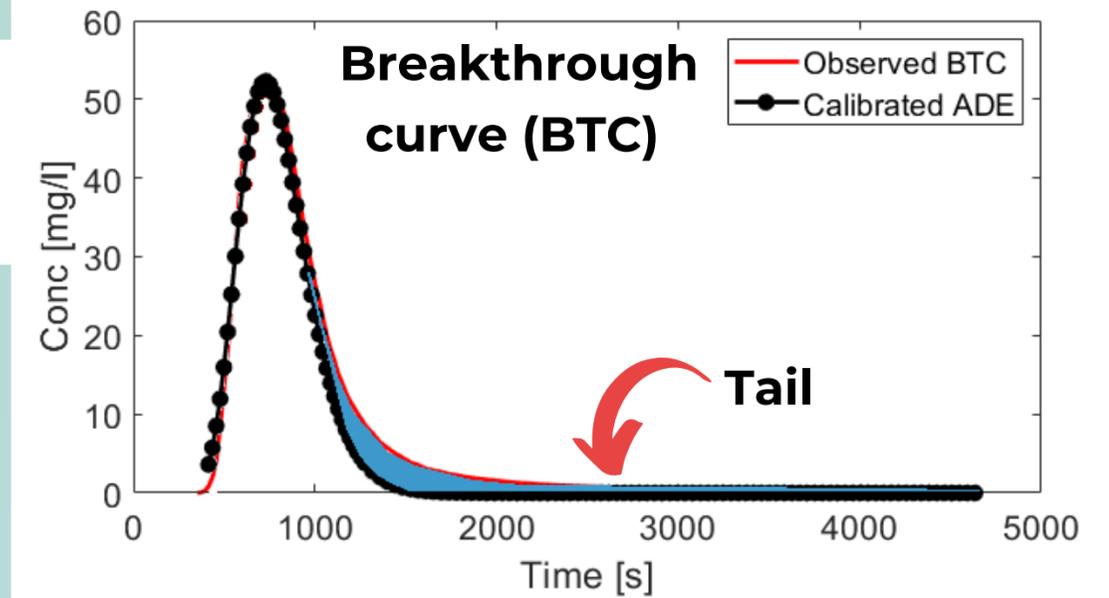
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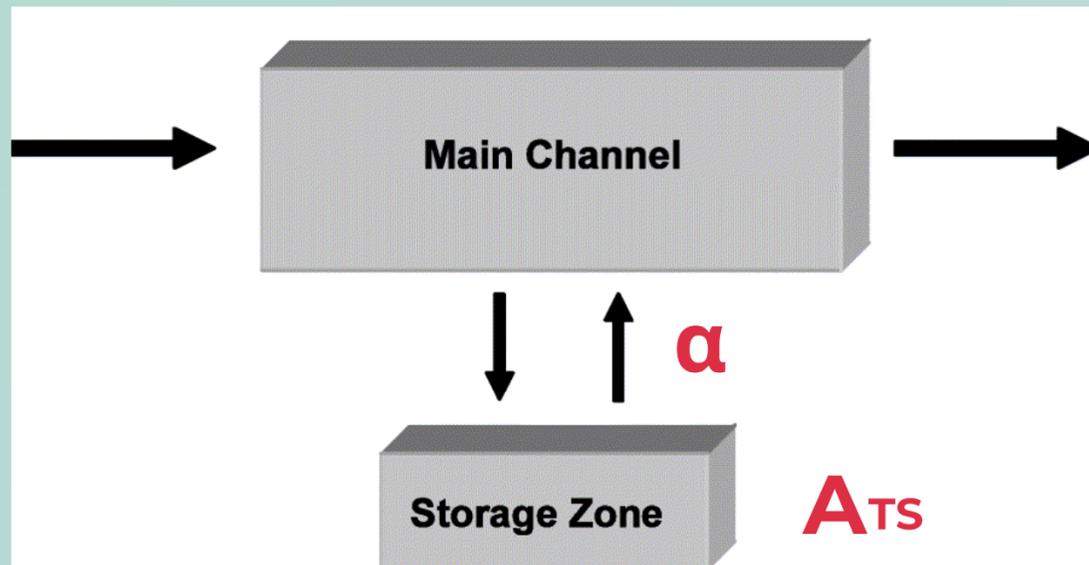
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Transient storage model (TSM)

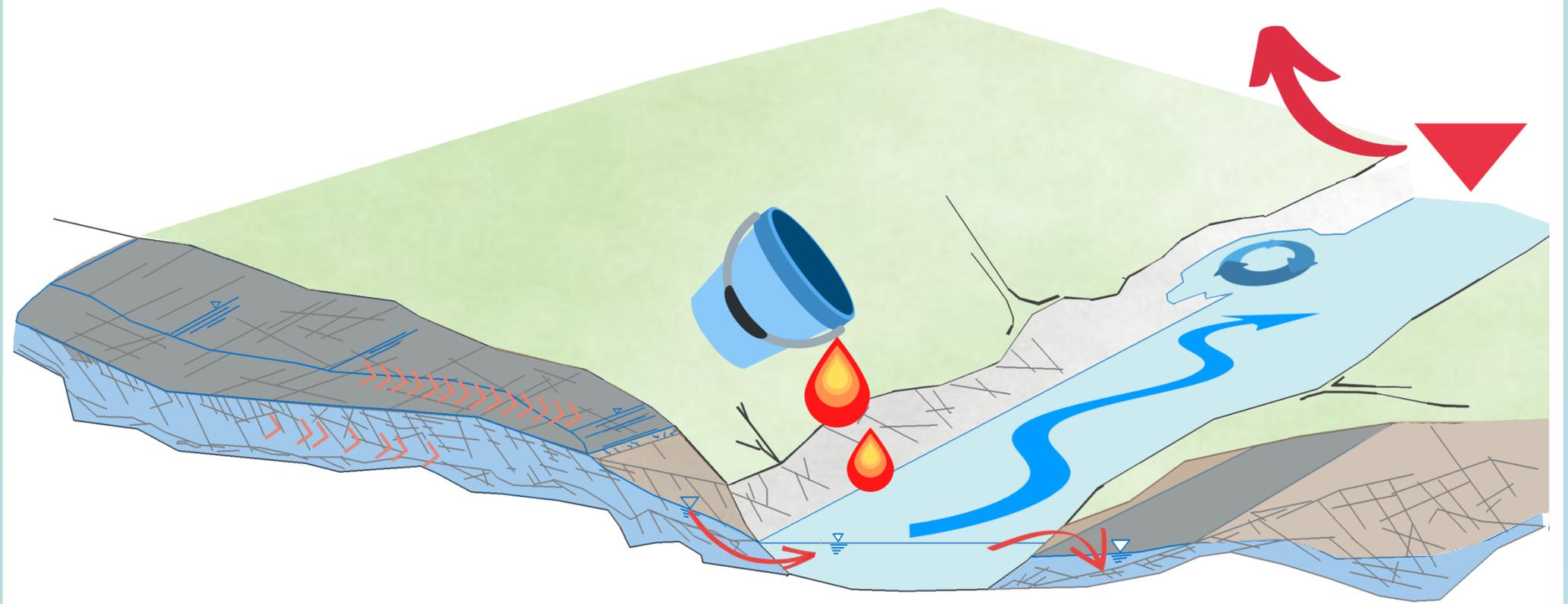
$$\begin{cases} \frac{\partial C}{\partial t} + \frac{Q}{A} \frac{\partial C}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left( AD \frac{\partial C}{\partial x} \right) + \alpha (C_s - C) \\ \frac{dC_s}{dt} = \alpha \frac{A}{A_s} (C - C_s) \end{cases}$$



We can model the hydrologic exchanges that cause solute delay in the stream channel



Bencala (1983) and Bencala and Walters (1983)



## Why do we care?

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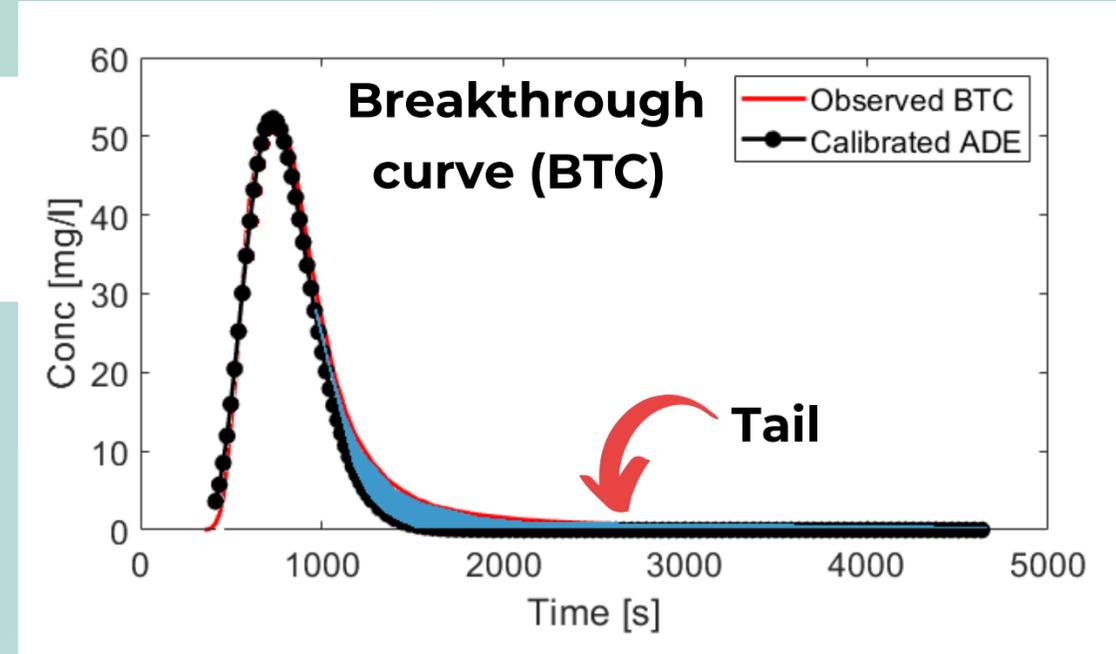
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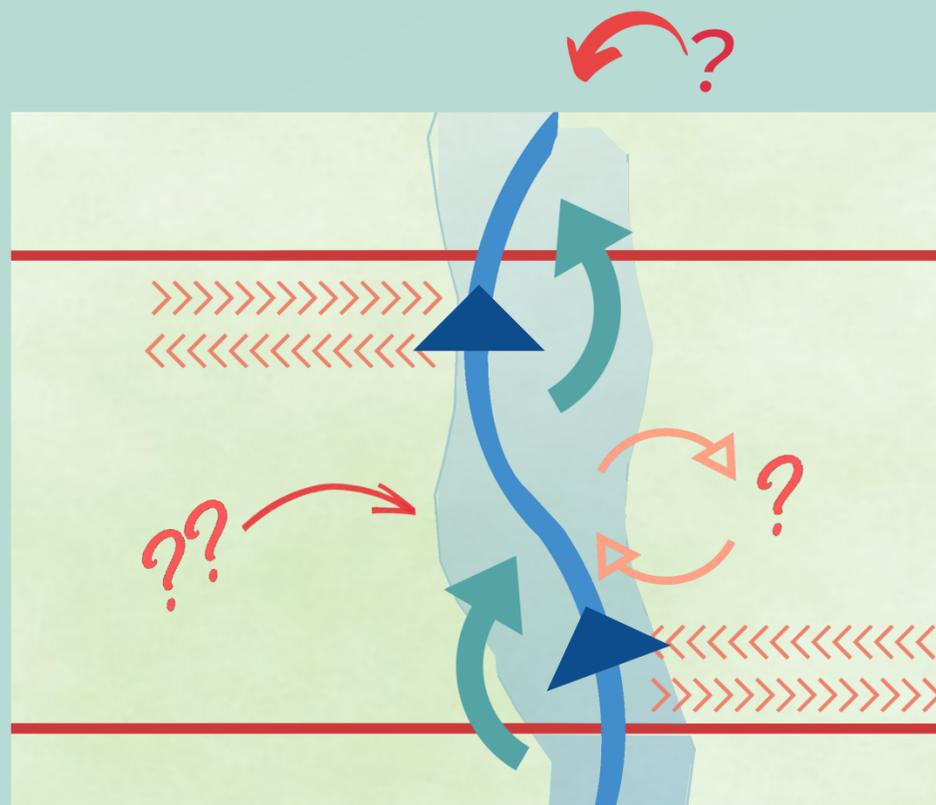
## Despite what we know

Do our modelling have a  
physical meaning?

We still have **inconsistent understanding** of water/solute exchange in the stream corridor;  
**We are uncertain about the information content of the measurement and what TSM parameter indicate** (Ward and Packman, 2019).

## Contradicting results

Interpretations of the physical phenomenon via TSM is based on few parameters, with no focus on their **uncertainty**, and **reliability** (Knapp and Kelleher, 2020) -> **Non-identifiability** 1



# Non-identifiability in TSM

That's not a small detail...

WATER RESOURCES RESEARCH, VOL. 49, 1184–1188, doi:10.1002/wrcr.20103, 2013

WATER RESOURCES RESEARCH, VOL. 49, 5290–5306, doi:10.1002/wrcr.20413, 2013

**Alpha and A\_TS  
are often non-  
identifiable!**

**Dynam  
model**

Thorsten **Influen  
on para  
stream**

Adam N.  
Received 9 A

**Identifiability of transient storage model parameters along a  
mountain st**

C. Kelleher,<sup>1,3</sup>  
Received 15 October

A software tool to assess uncertainty in transient-storage

**model Exploring Tracer Information and Model Framework  
Trade-Offs to Improve Estimation of Stream  
Transient Storage Processes**

Adam S. Ward  
Neil McIntyre

Christa Kelleher<sup>1,2</sup> , Adam Ward<sup>3</sup> , J. L. A. Knapp<sup>4,5</sup> , P. J. Blaen<sup>6,7</sup> , M. J. Kurz<sup>8,9</sup> ,  
J. D. Drummond<sup>10</sup> , J. P. Zarnetske<sup>11</sup> , D. M. Hannah<sup>6</sup> , C. Mendoza-Lera<sup>12,13</sup> ,  
N. M. Schmadel<sup>3,14</sup> , T. Datry<sup>12</sup> , J. Lewandowski<sup>15</sup> , A. M. Milner<sup>6</sup>, and S. Krause<sup>6,7</sup> 

# Non-identifiability in TSM

That's not a small detail...

Since  $\alpha$  and  $A_{TS}$  are uncertain and they are supposed to describe the tail of the BTC...

Shall we really keep looking at the tail?

Are we missing the focus?

Do we need to change our approach?

## Water Resources Research

COMMENTARY

10.1029/2019WR026257

Julia L.A. Knapp and Christa Kelleher  
contributed equally to this work.

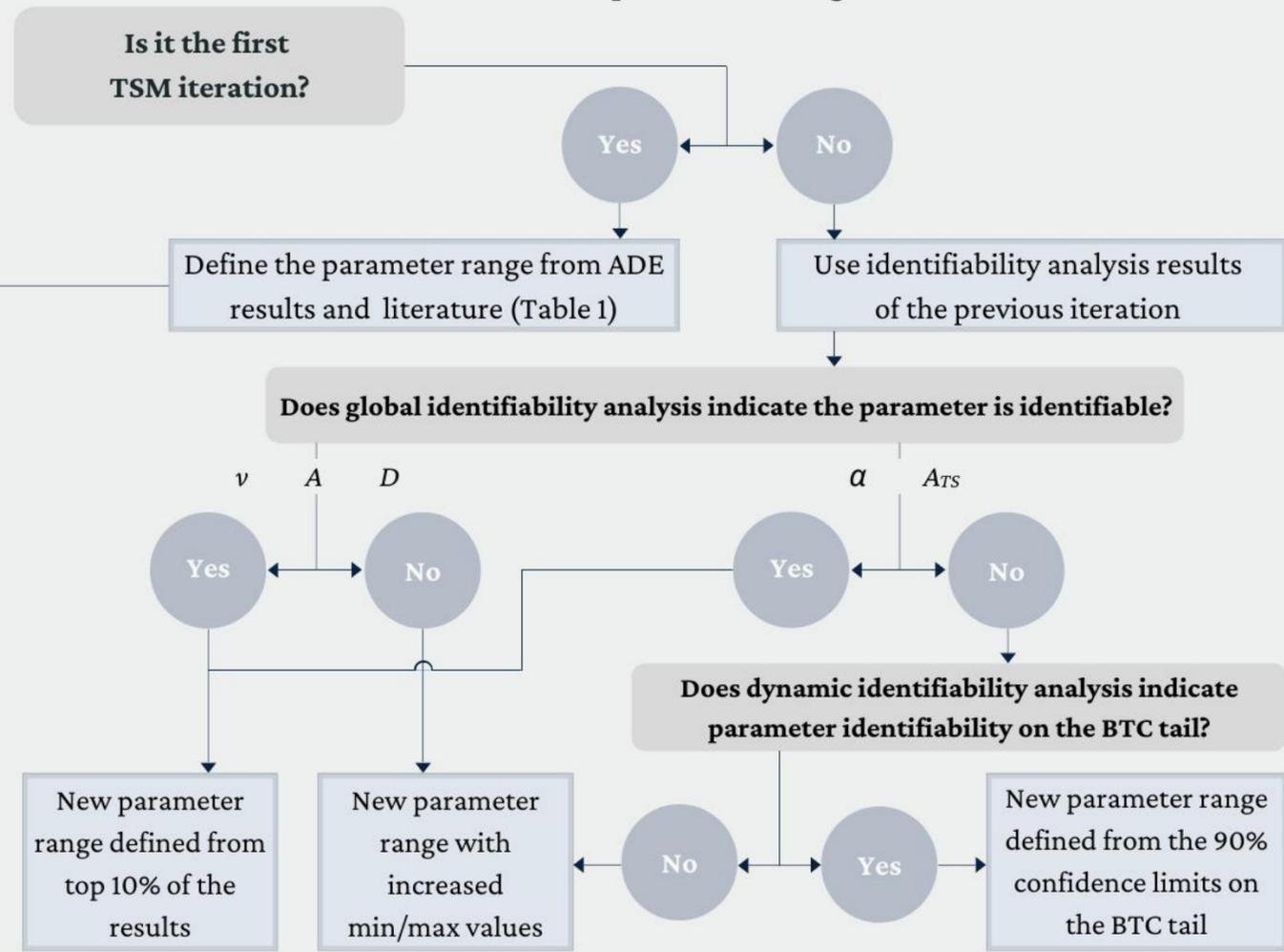
### A Perspective on the Future of Transient Storage Modeling: Let's Stop Chasing Our Tails

Julia L.A. Knapp<sup>1</sup>  and Christa Kelleher<sup>2</sup> 

<sup>1</sup>Department of Environmental Systems Science, ETH Zurich, Zurich, Switzerland, <sup>2</sup>Department of Earth Sciences,  
Syracuse University, Syracuse, NY, USA

How can be sure of physical interpretation of TSM parameters if Alpha and  $A_{TS}$  are non-identifiable?

Definition of the parameter range



# Our approach

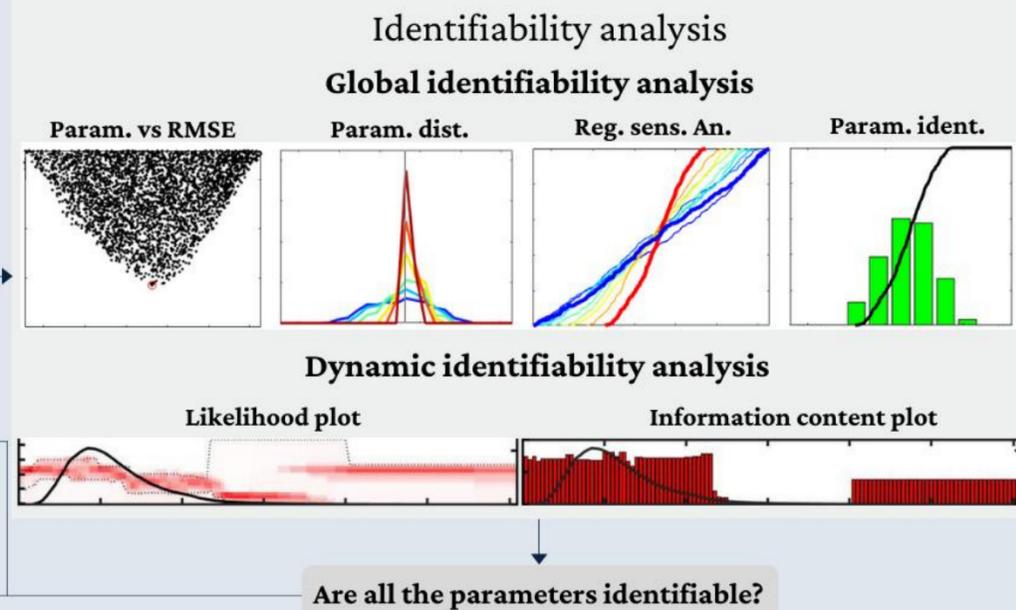
For every BTC:

We start defining the parameter range from: Literature and ADE modelling OR results from previous iteration

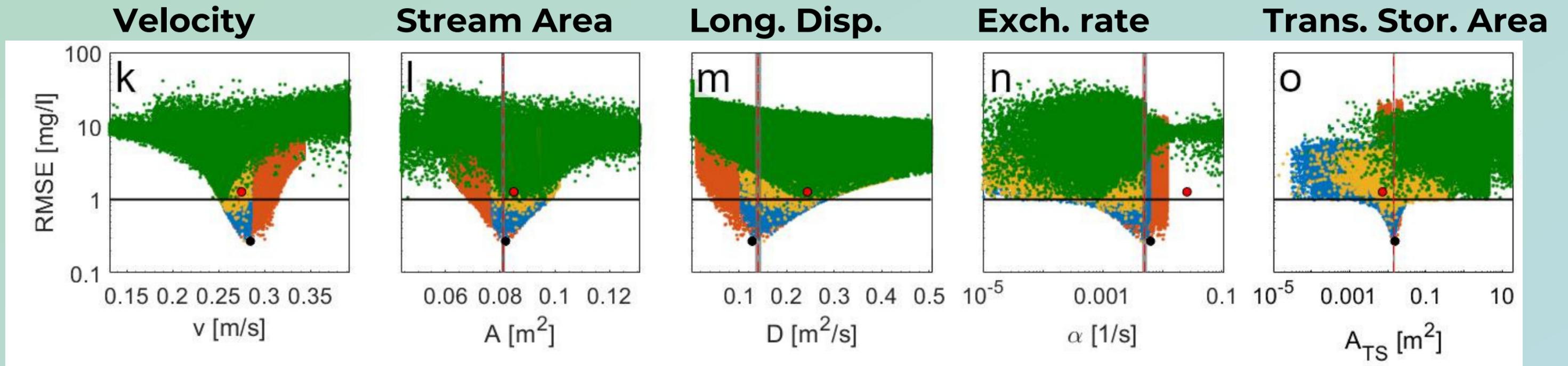
We sample from the parameters' space 115'000 parameter sets via Latin Hypercube Sampling

We run TSM and perform global parameter sensitivity analysis and dynamic sensitivity analysis

We use these results to define the most sensitive parameter space and, for Alpha and A\_TS, their identifiability range on the tail of the BTC



# Results



Each iteration included 115'000 parameter sets.



**1st iteration**



**v, A, D:**



**2nd iteration**



The most sensitive parameter range (lower RMSE) was targeted by the following iteration.



**3rd iteration**



**Alpha, A<sub>ts</sub>:**

Identifiability of Alpha and A<sub>ts</sub> was investigated on the tail of the BTC.



**4th iteration**



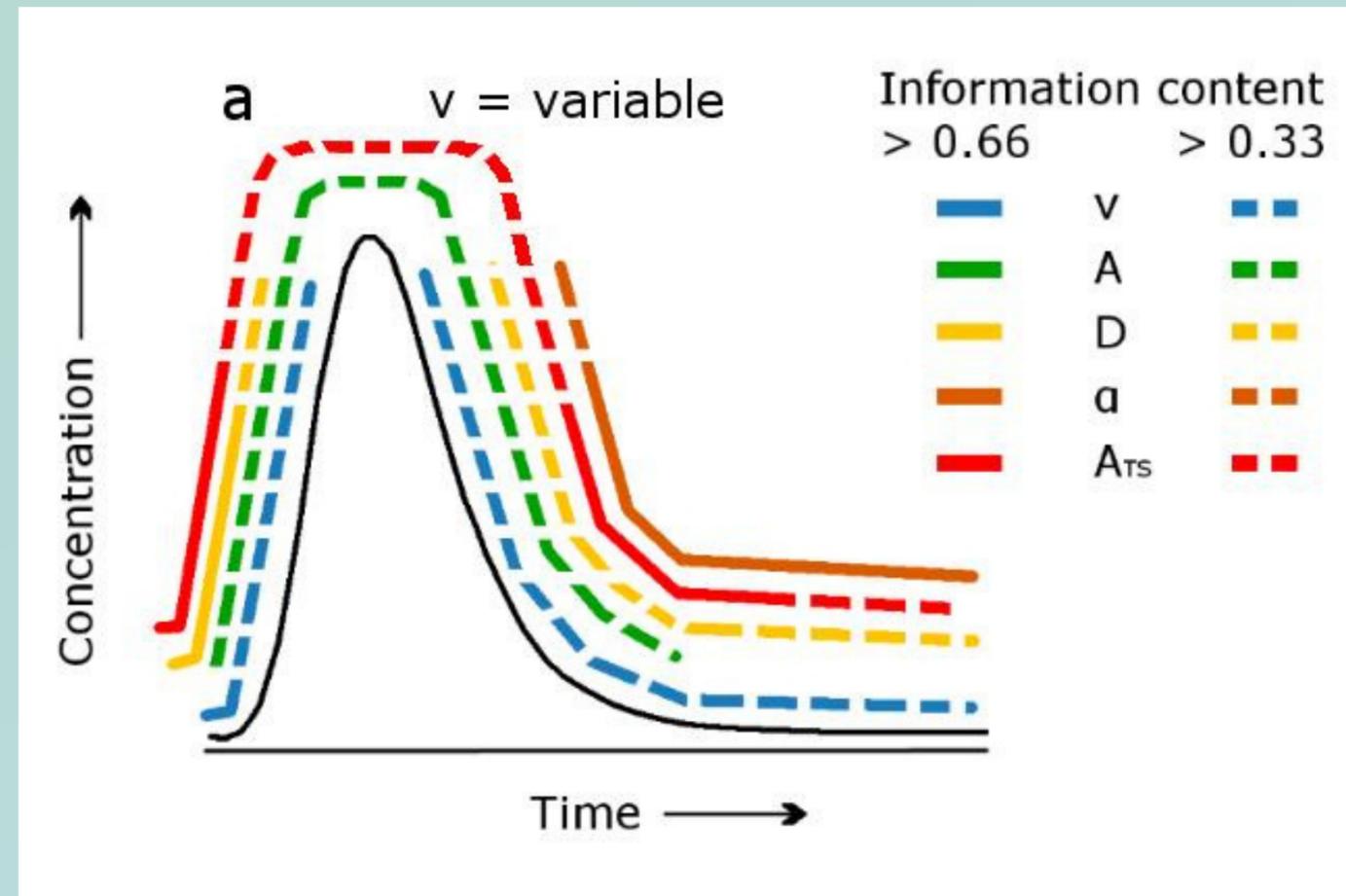
# Conclusions

1) Studying the identifiability of Alpha and A\_TS on the **tail** of the BTC was pivotal to improve identifiability of TSM parameters;

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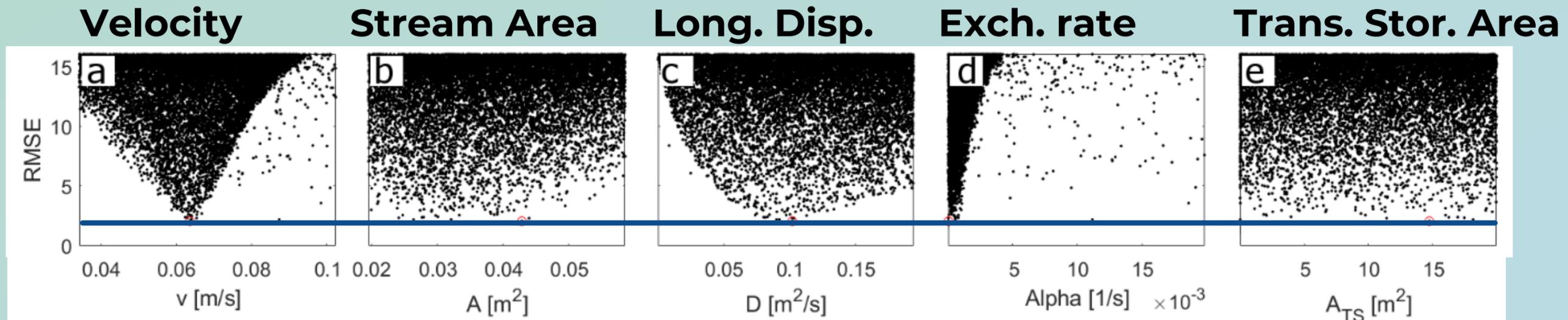
2) When identifiable, the TSM parameters control solute arrival-time and solute retention in stream channels;



Parameter influence on the BTC

# Conclusions

- 1) Studying the identifiability of Alpha and  $A_{TS}$  on the tail of the BTC was pivotal to improve identifiability of TSM parameters;
- 2) When identifiable, the TSM parameters control solute arrival-time and solute retention in stream channels;
- 3) The TSM mimics the ADE when one or more transient storage parameters is not-identifiable;

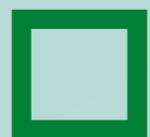


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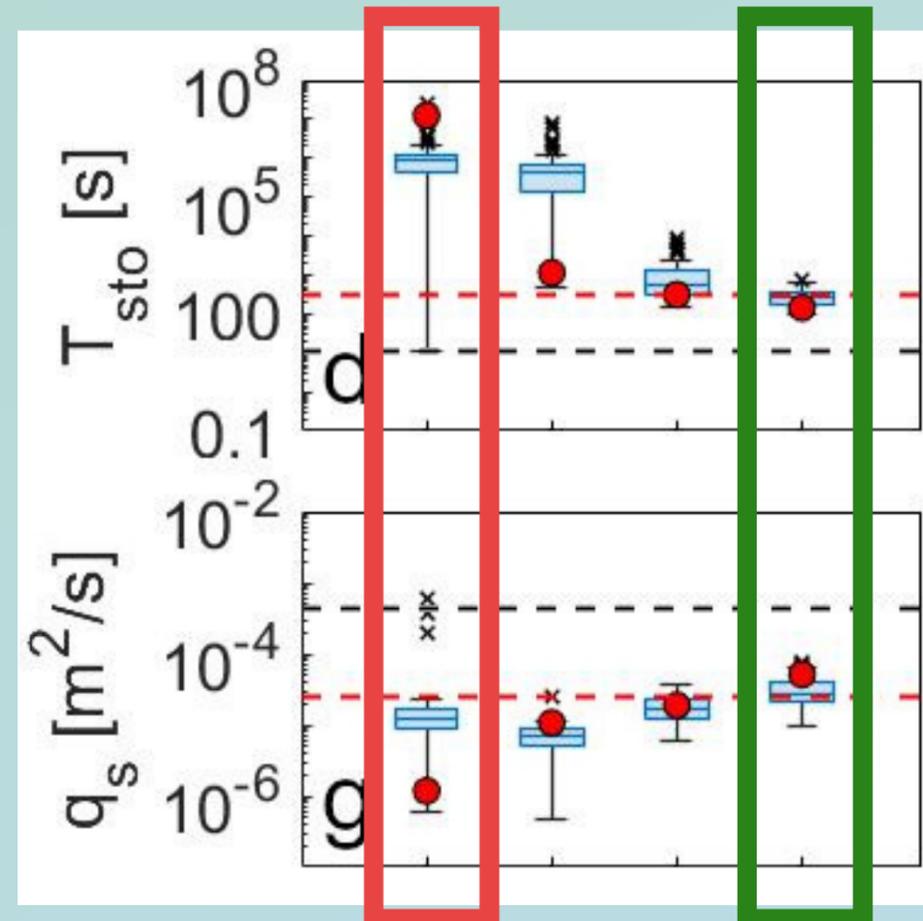
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- 2) When identifiable, the TSM parameters control solute arrival-time and solute retention in stream channels;
- 3) The TSM mimics the ADE when one or more transient storage parameters is not-identifiable;
- 4) Non-identifiable parameters result in wrong estimation of the metrics describing solute transport in stream.



Metrics results after the 1st iteration



Metrics results after the 4th iteration



$T_{sto}$  is the average time spent by a molecule in the transient storage zone (Thackston and Schnelle, 1970):  
 $T_{sto} = A_{TS}/(\alpha A)$

$q_s$  is the water flux through the storage zone per unit length of stream channel (Harvey et al., 1996):  
 $q_s = \alpha A$

# THANK YOU!

## EGU 2022 DISPLAY MATERIAL

Enrico Bonanno

Full paper under discussion at:  
<https://hess.copernicus.org/preprints/hess-2022-149/>

bonanno@hydro.tuwien.ac.at

