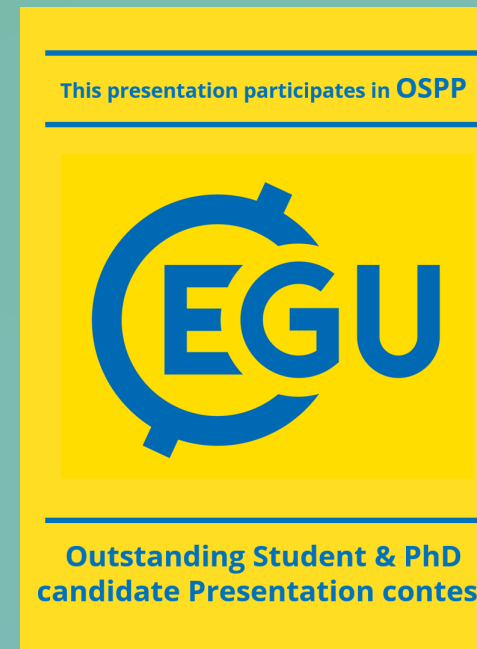


EGU 2022 DISPLAY MATERIAL

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

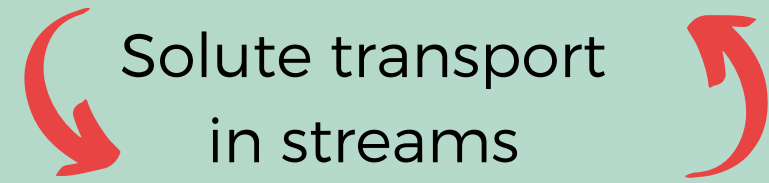
bonanno@hydro.tuwien.ac.at

LUXEMBOURG
INSTITUTE OF SCIENCE
AND TECHNOLOGY



Vienna Doctoral Programme on
Water Resource Systems

Why do we care?

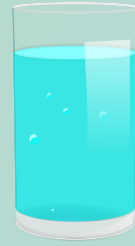


Where does the water go?

Why do we care?

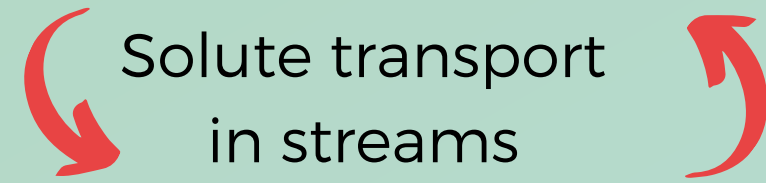
Solute transport
in streams

Where does the water go?

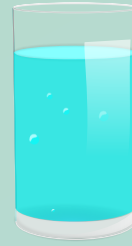


Control stream water quality in
river network

Why do we care?

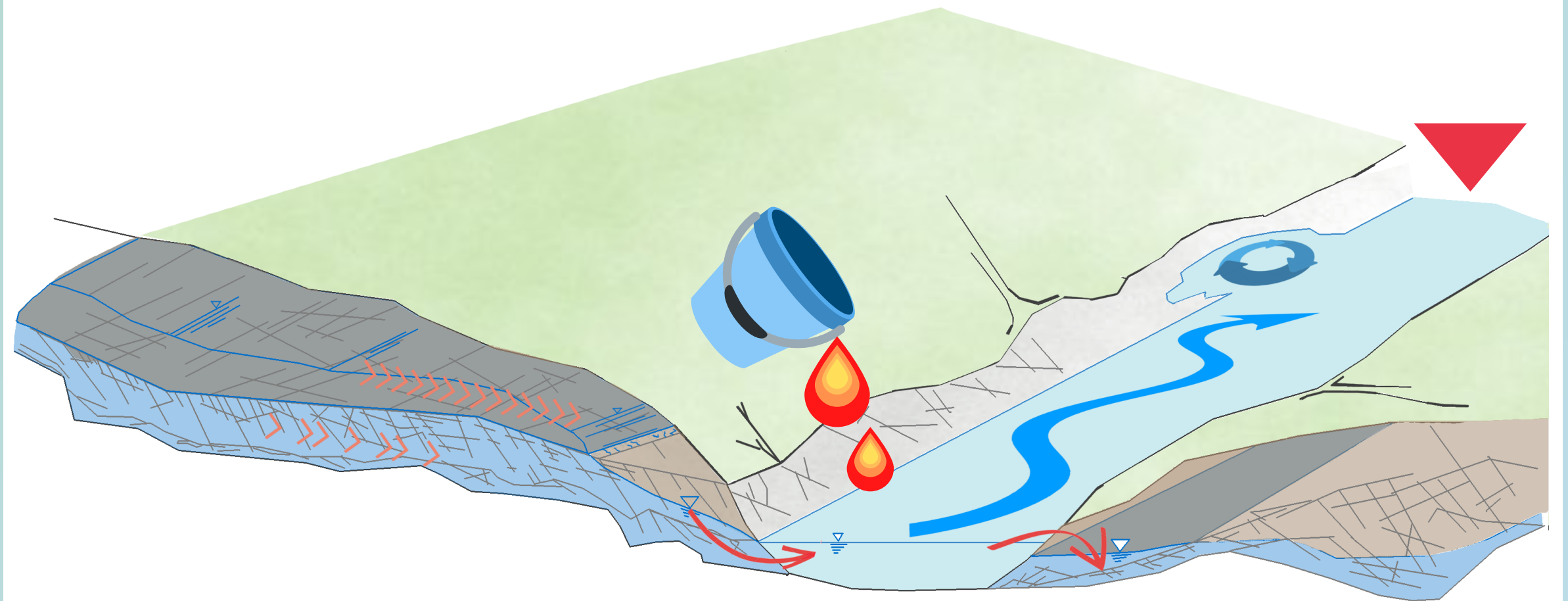


Where does the water go?



Control stream water quality in
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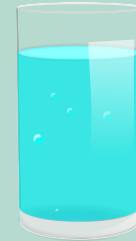
How do we experimentally study solute transport in streams?



Why do we care?

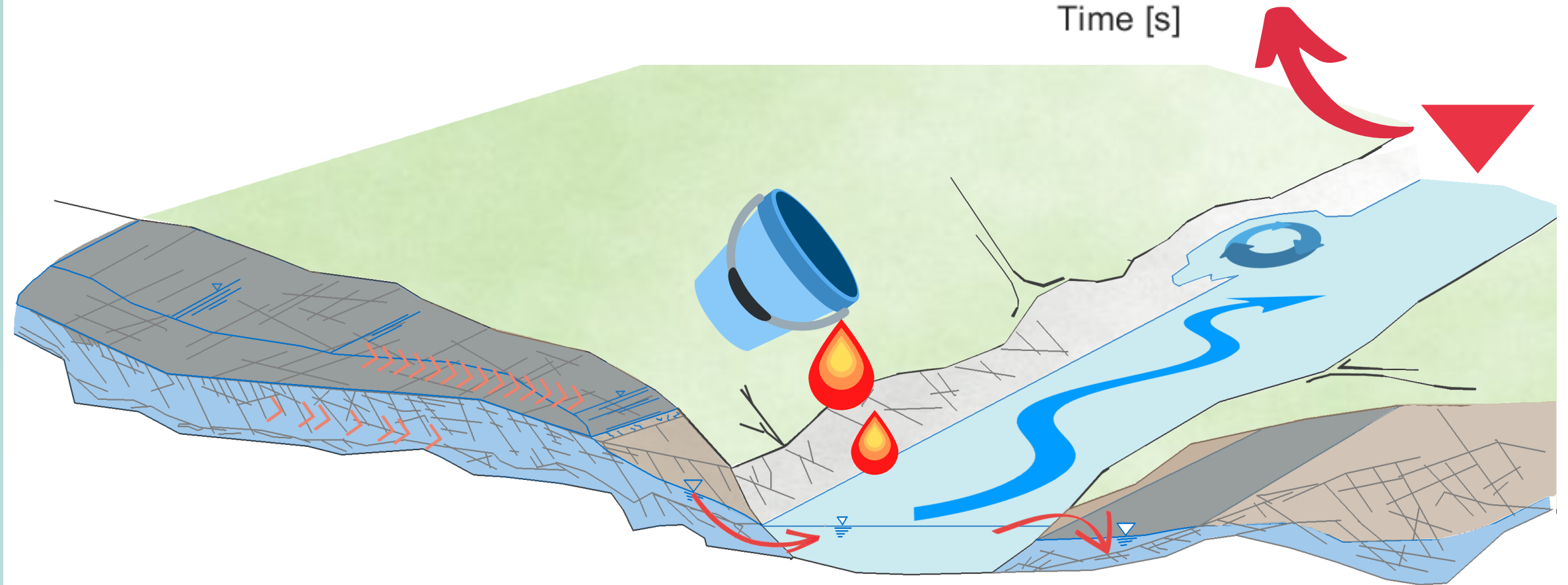
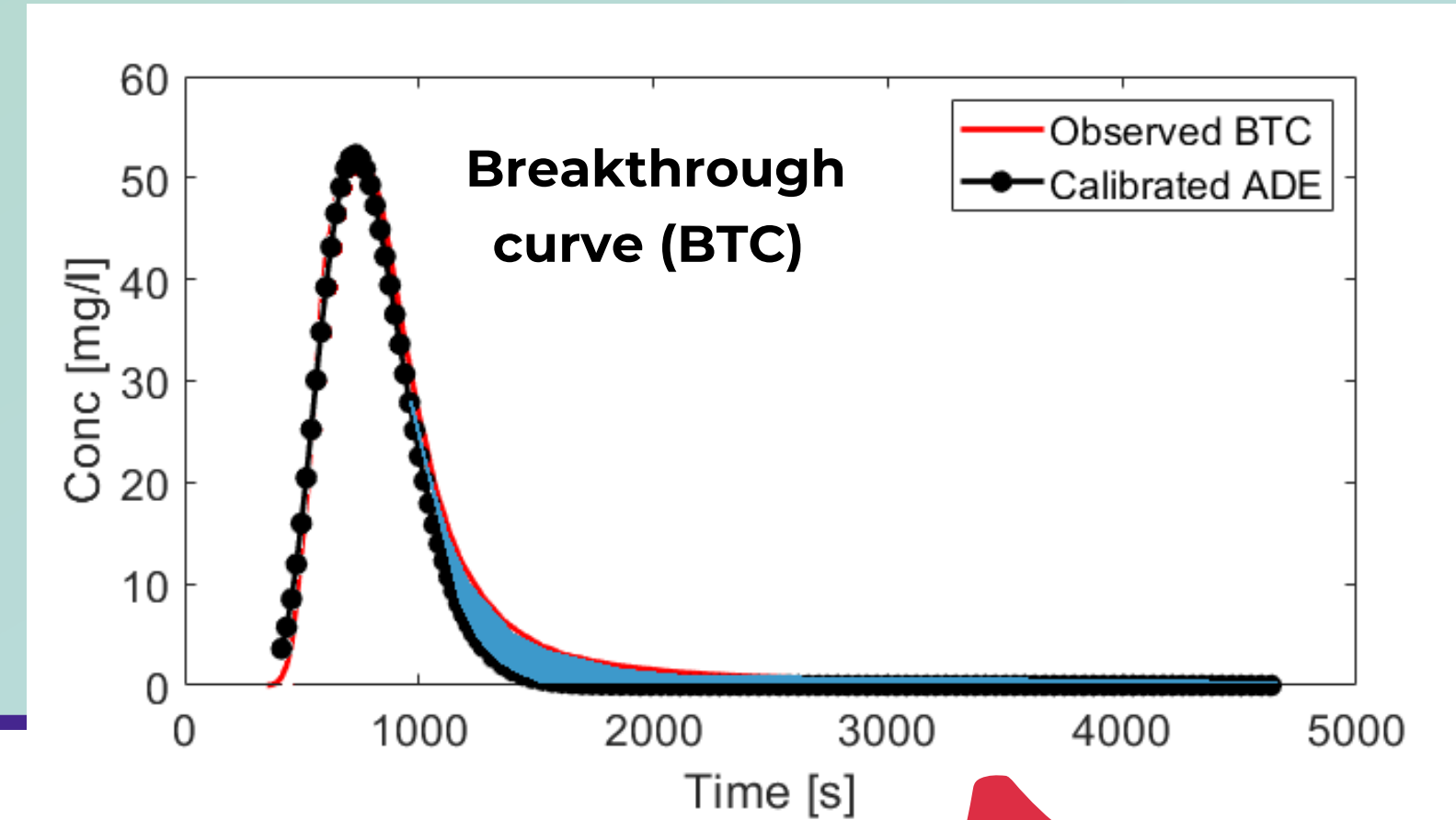
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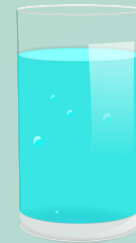
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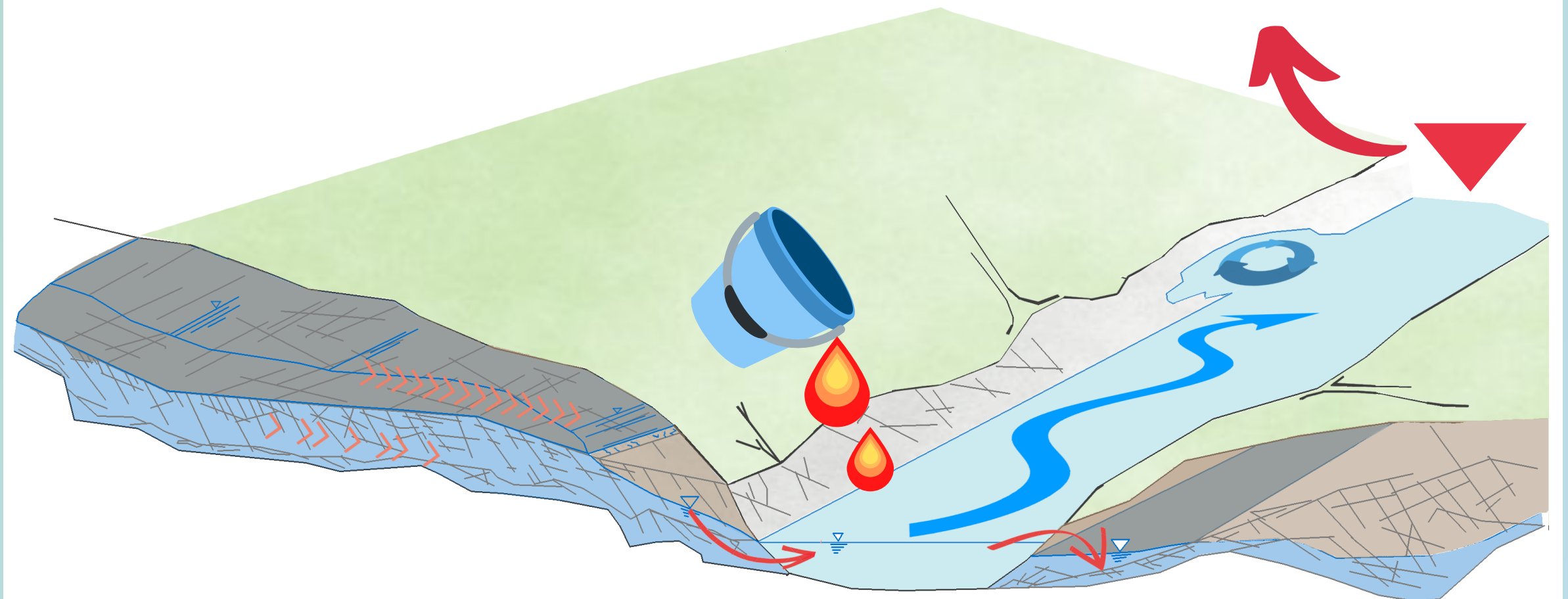
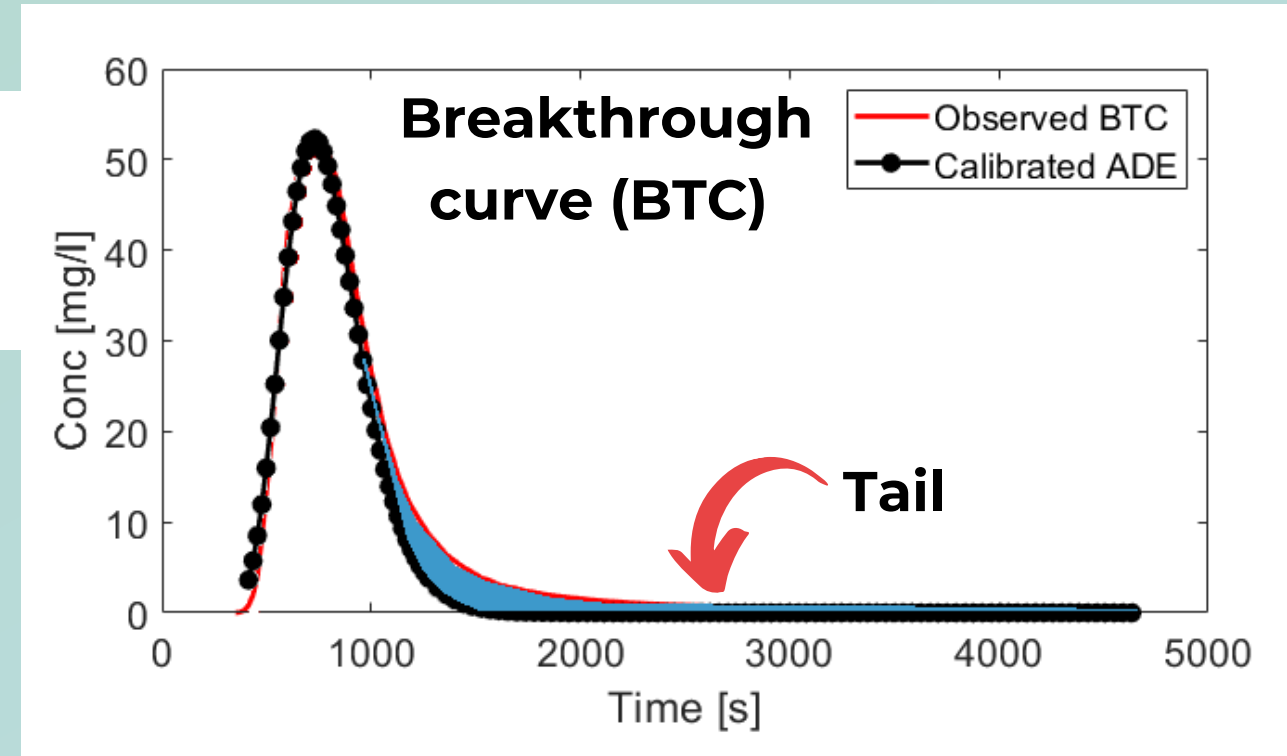
How do we experimentally study solute transport in streams?

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)

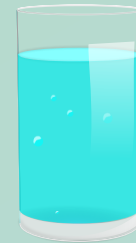
Advection dispersion Equation is non able to correctly describe the observed tracer transport in stream channels due to pronounced tail of the BTC



Why do we care?

Solute transport
in streams

Where does the water go?



Control stream water quality in
river network

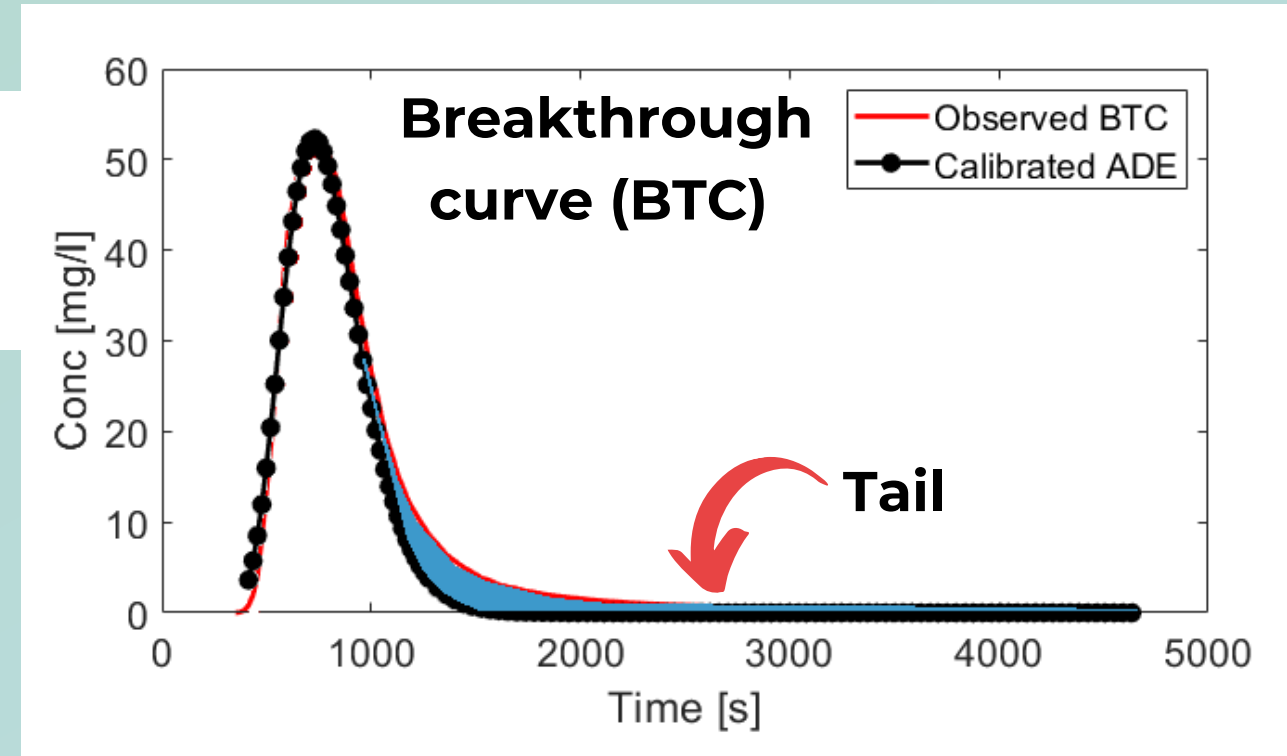
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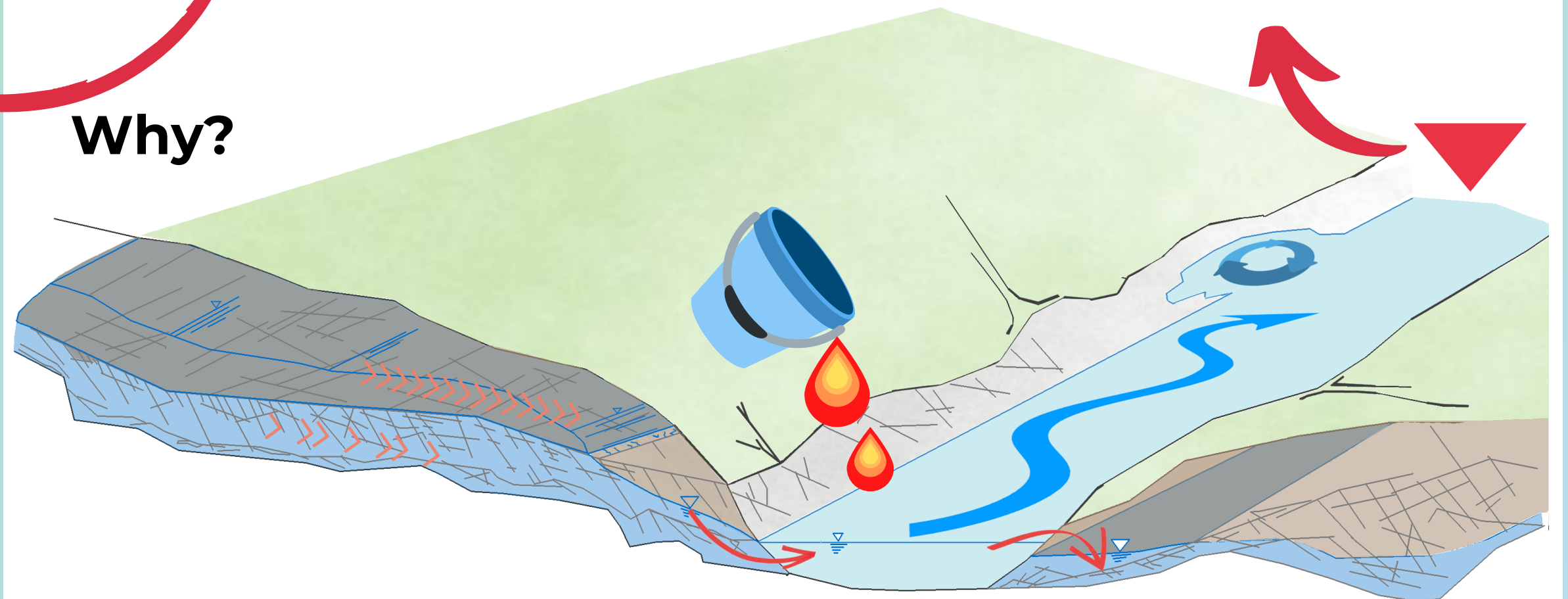
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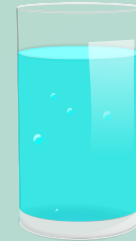
Why?



Why do we care?

Solute transport
in streams

Where does the water go?



Control stream water quality in
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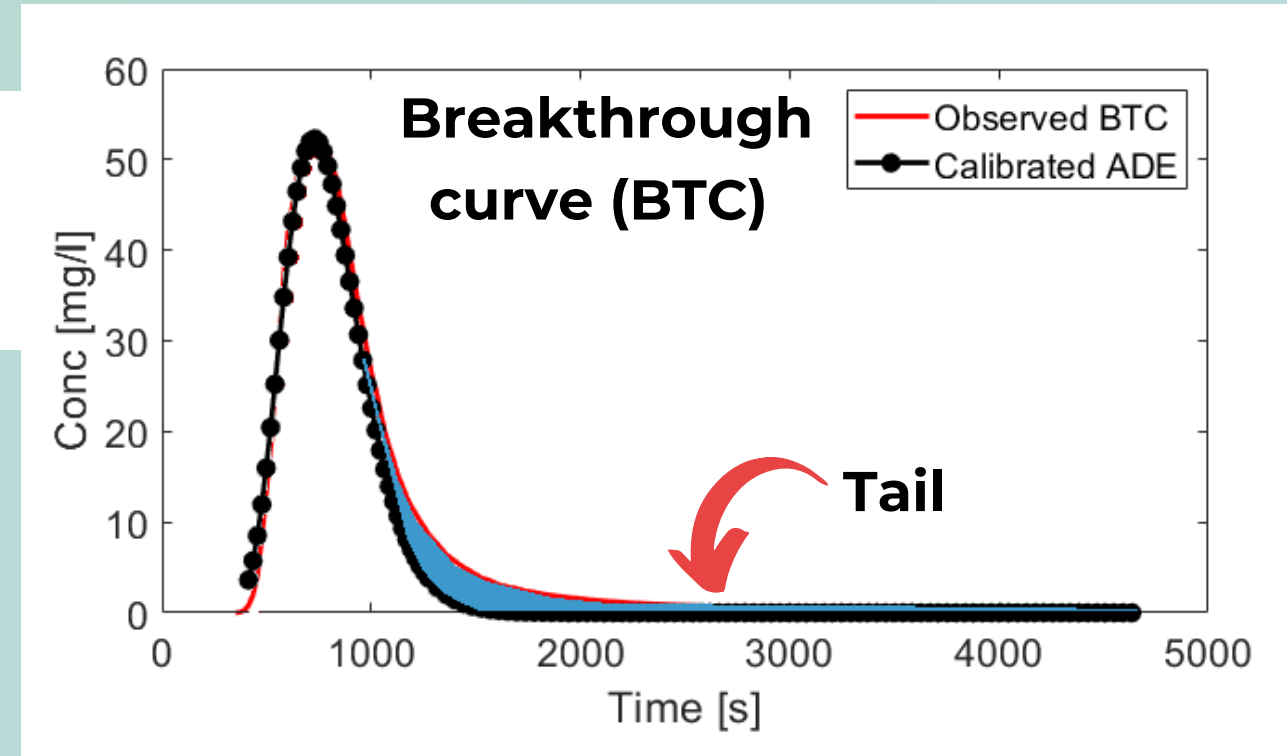
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Taylor (1921, 1954)

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



The stream is not a pipe!

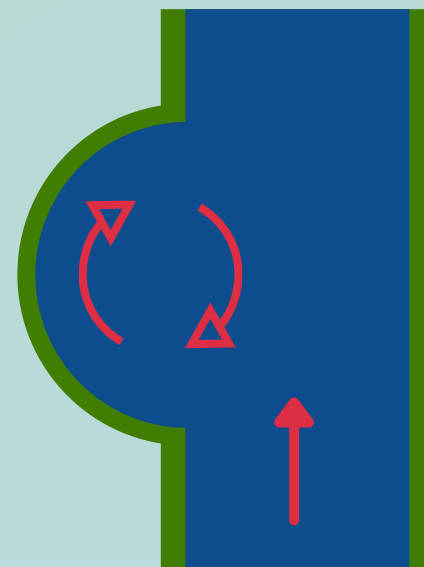
Bencala (1993)

Hydrologic exchange with:

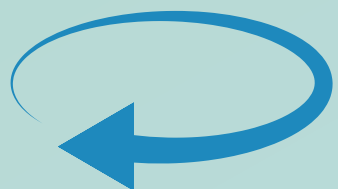


In-stream
sediments

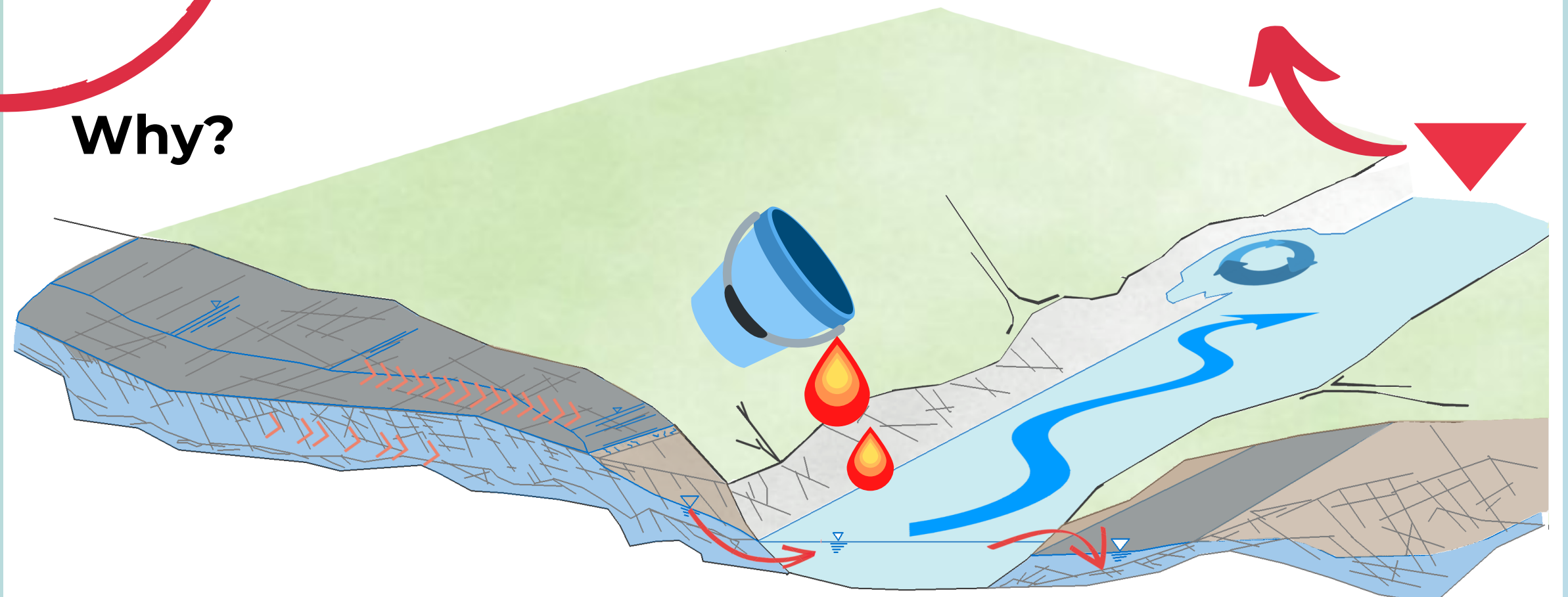
Pools



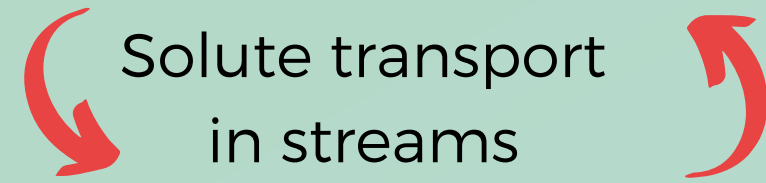
SW-GW
exchange



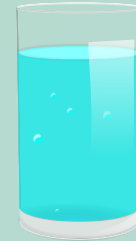
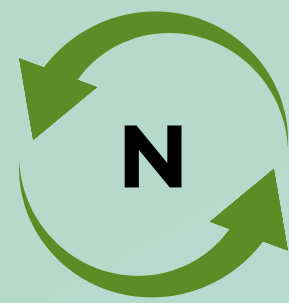
Why?



Why do we care?



Where does the water go?



Control stream water quality in
river network

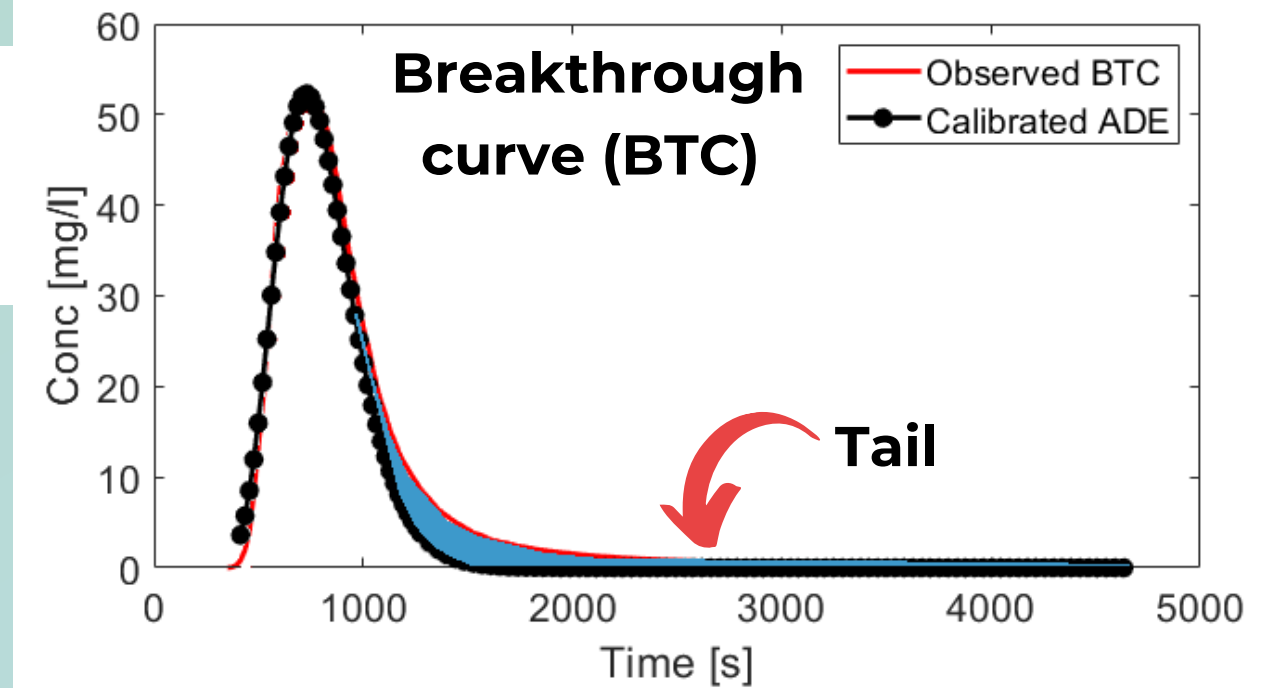
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Advection Dispersion Equation

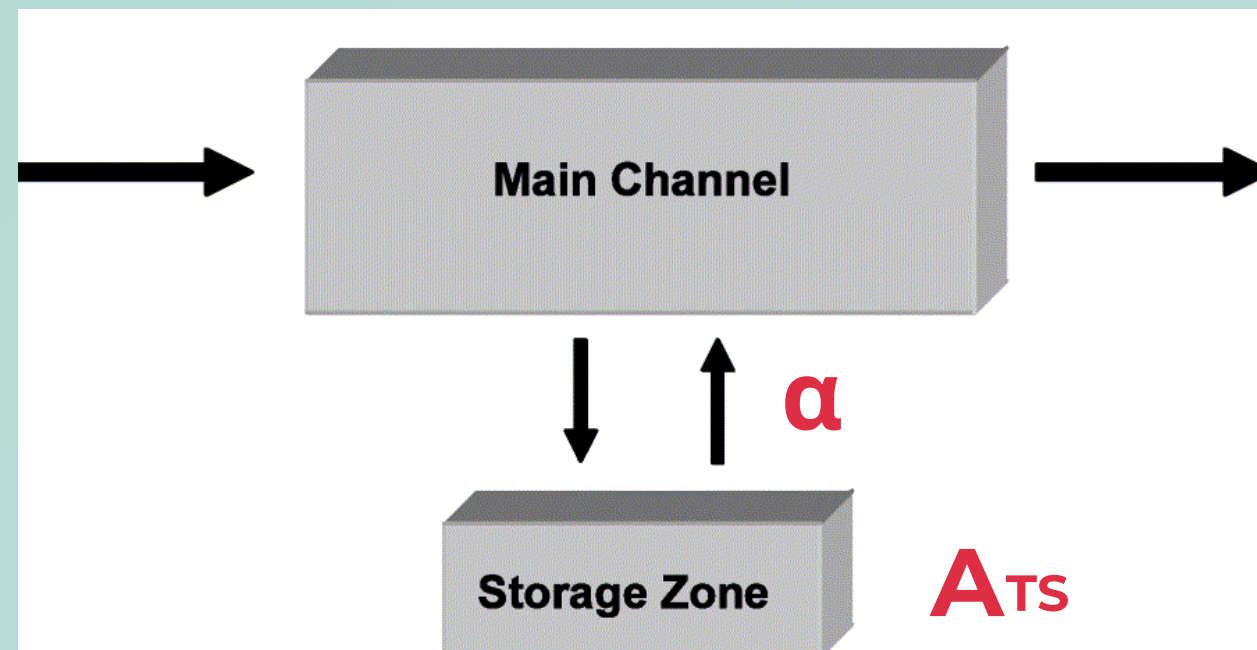
$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + \frac{1}{A} \frac{\partial}{\partial x} \left(AD \frac{\partial C}{\partial x} \right)$$

Transient storage model (TSM)

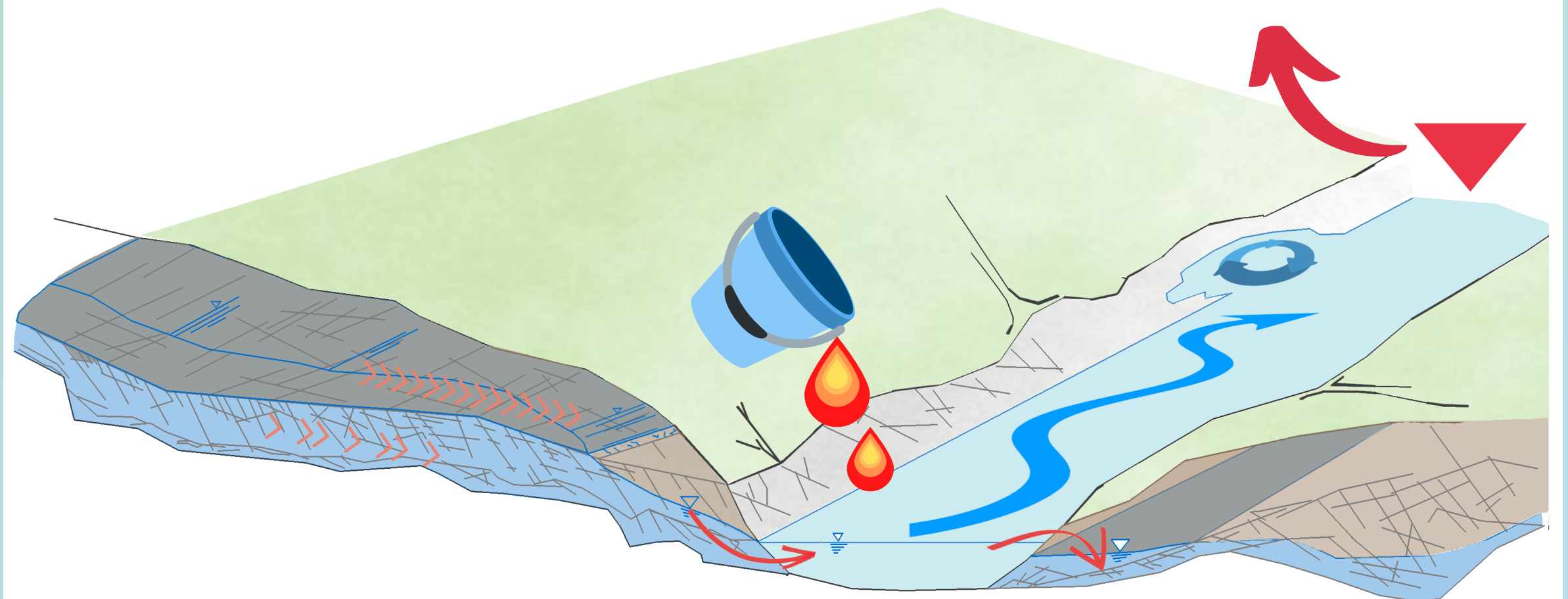
$$\begin{cases} \frac{\partial C}{\partial t} + \frac{Q}{A} \frac{\partial C}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(AD \frac{\partial C}{\partial x} \right) + \alpha (C_s - C) \\ \frac{dC_s}{dt} = \alpha \frac{A}{A_s} (C - C_s) \end{cases}$$



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?



Where does the water go?



Control stream water quality in river network

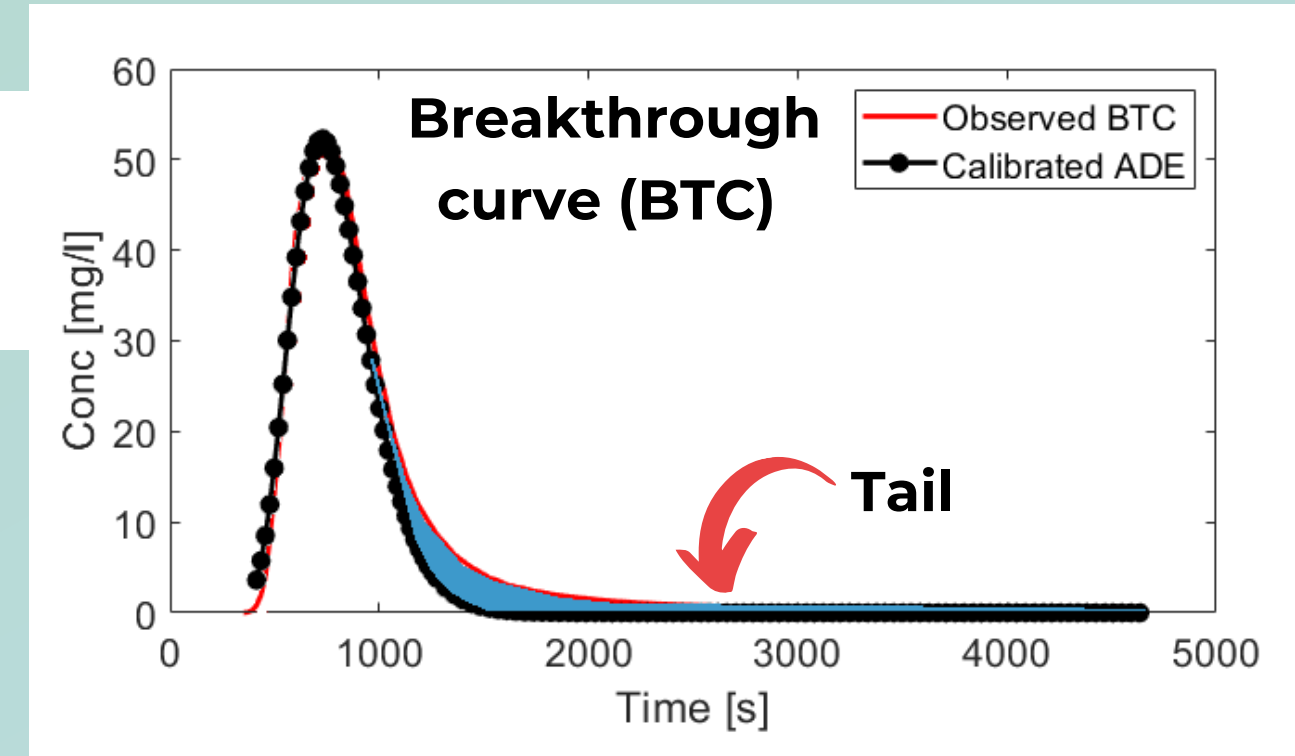
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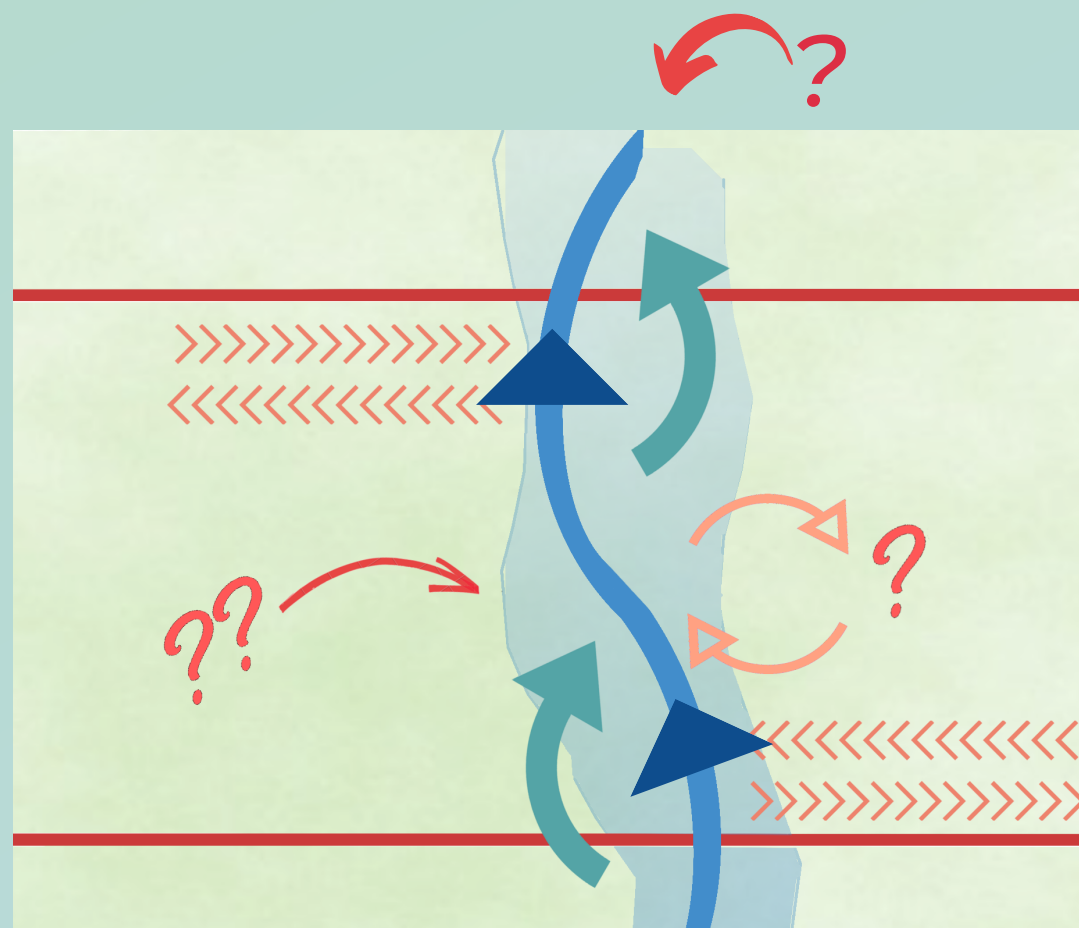
Despite what we know

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**



Non-identifiability in TSM

That's not a small detail...

199

© IWA Publishing 2002 | Journal of Hydroinformatics | 04.3 | 2002

WATER RESOURCES RESEARCH, VOL. 49, 1184–1188, doi:10.1002/wrcr.20103, 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,^{1,3}
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^{1,2} , Adam Ward³ , J. L. A. Knapp^{4,5} , P. J. Blaen^{6,7} , M. J. Kurz^{8,9} ,
J. D. Drummond¹⁰ , J. P. Zarnetske¹¹ , D. M. Hannah⁶ , C. Mendoza-Lera^{12,13} ,
N. M. Schmadel^{3,14} , T. Datry¹² , J. Lewandowski¹⁵ , A. M. Milner⁶, and S. Krause^{6,7} 

Non-identifiability in TSM

That's not a small detail...

Since α 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. Knapp¹  and Christa Kelleher² 

¹Department of Environmental Systems Science, ETH Zurich, Zurich, Switzerland, ²Department 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-indentifiable?

Definition of the parameter range

Is it the first
TSM iteration?

Yes

No

Define the parameter range from ADE
results and literature (Table 1)Use identifiability analysis results
of the previous iteration

Does global identifiability analysis indicate the parameter is identifiable?

 v A D

Yes

No

 α A_{TS}

Yes

No

Does dynamic identifiability analysis indicate
parameter identifiability on the BTC tail?New parameter
range defined from
top 10% of the
resultsNew parameter
range with
increased
min/max values

No

Yes

New parameter range
defined from the 90%
confidence limits on
the BTC tail

Sampling

Parameter sampling via LHS
(115000 parameter sets)

Simulation

Solve TSM via OTIS for
each parameter setSave
results

Yes

No

Identifiability analysis

Global identifiability analysis

Param. vs RMSE

Param. dist.

Reg. sens. An.

Param. ident.

Dynamic identifiability analysis

Likelihood plot

Information content plot

Are all the parameters identifiable?

Our approach

For every BTC:

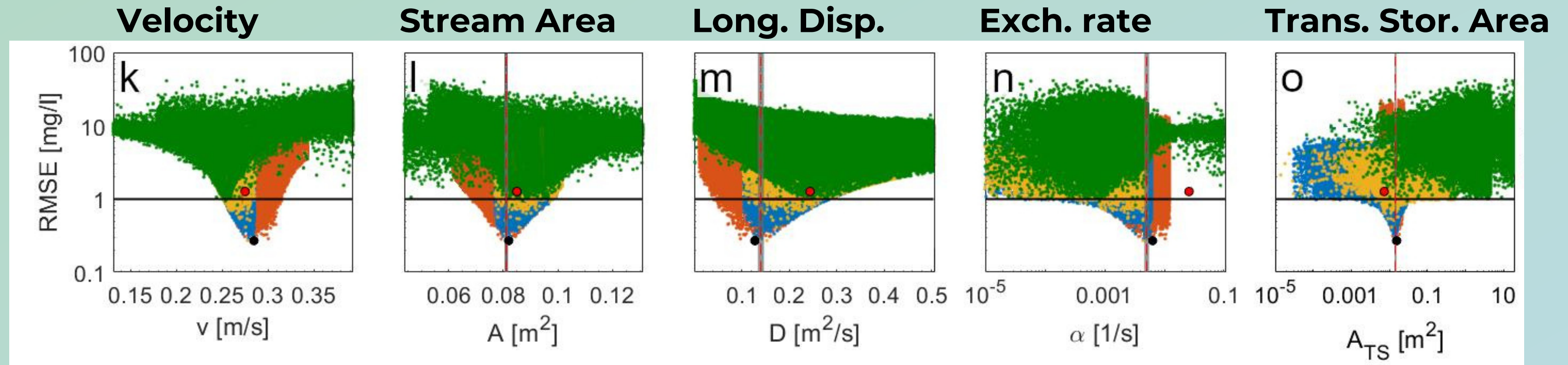
We start defining the parameter range from:
Literature and ADE modelling OR results from
previous iteration

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

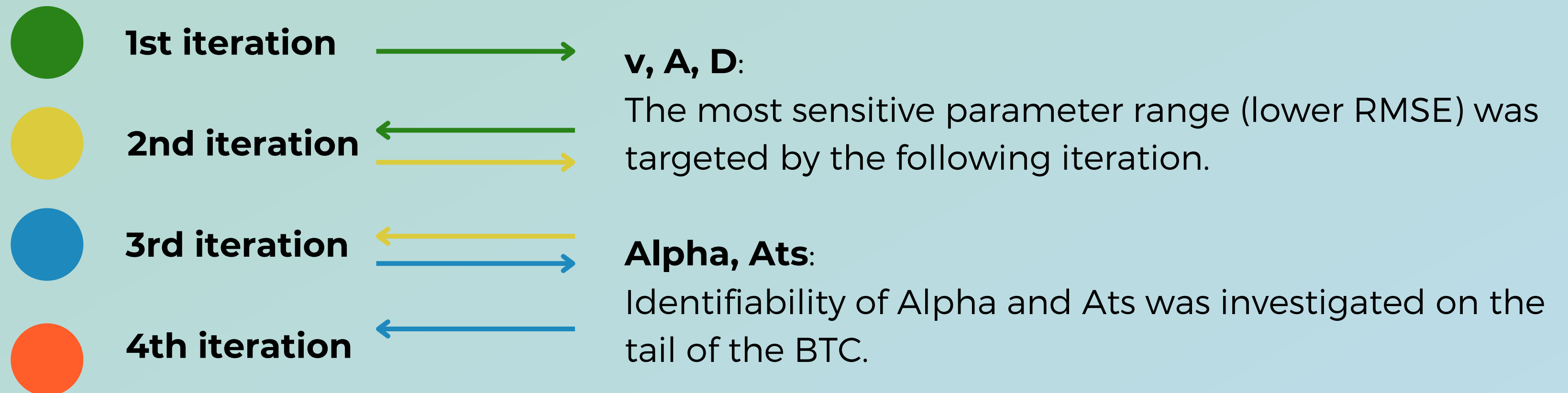
We run TSM and perform global parameter
sensitivity analysis and dynamic sensitivity analysis

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.

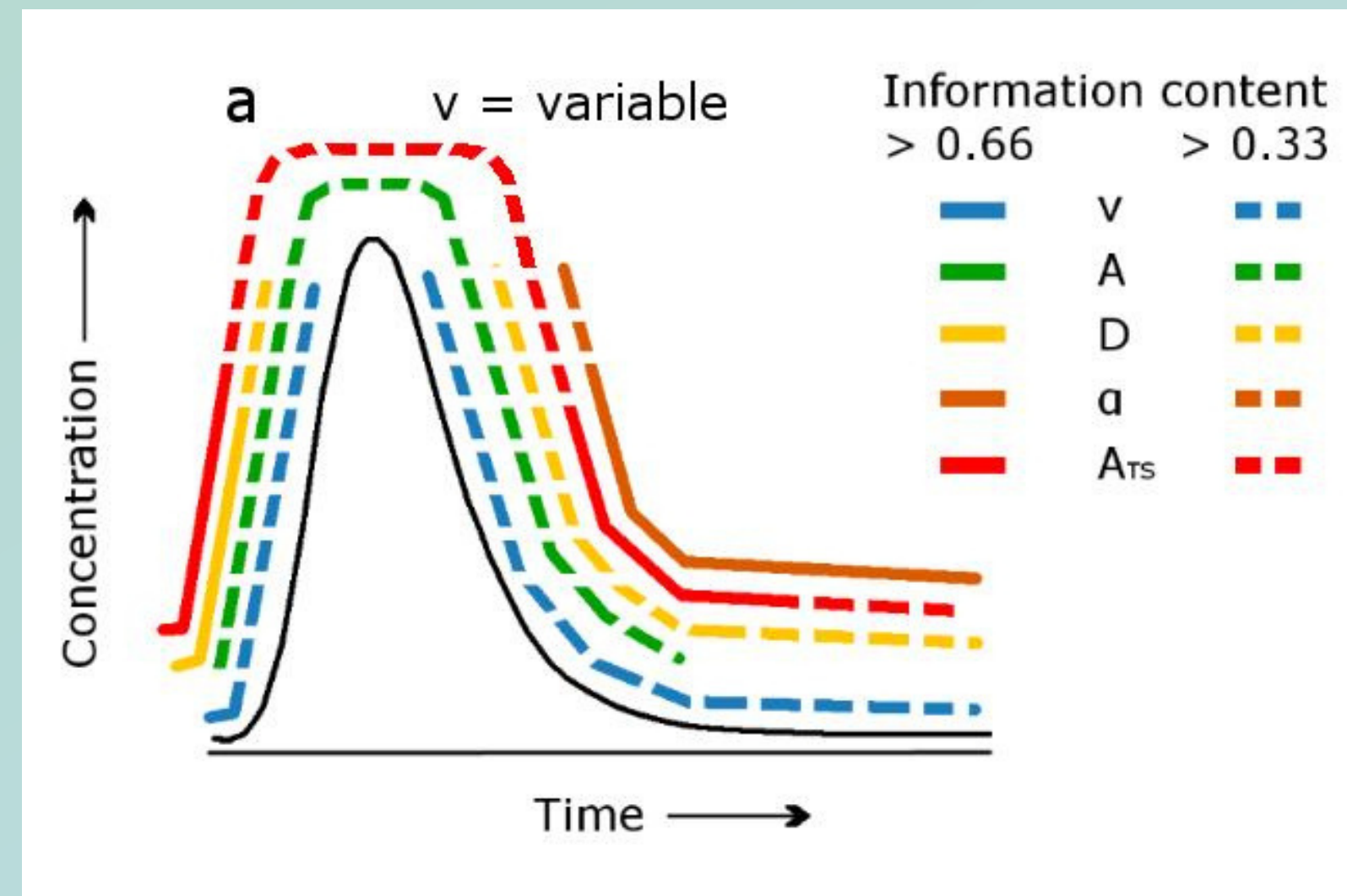


Conclusions

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

Conclusions

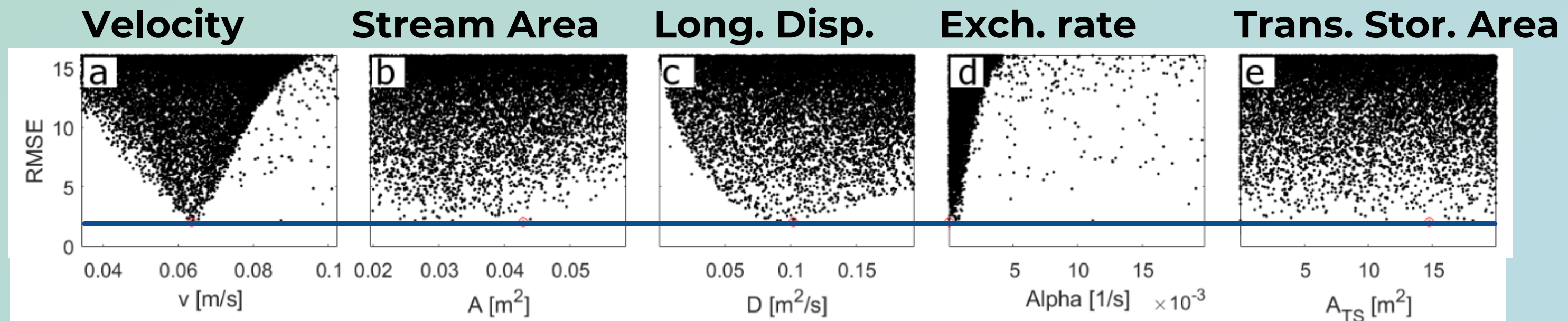
- 1) Studying the identifiability of Alpha and A_{TS} on the tail of the BTC was pivotal to improve identifiability of TSM parameters;
- 2) When identifiable, the TSM parameters control solute arrival-time and solute retention in stream channels;



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;

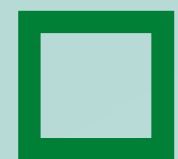


Conclusions

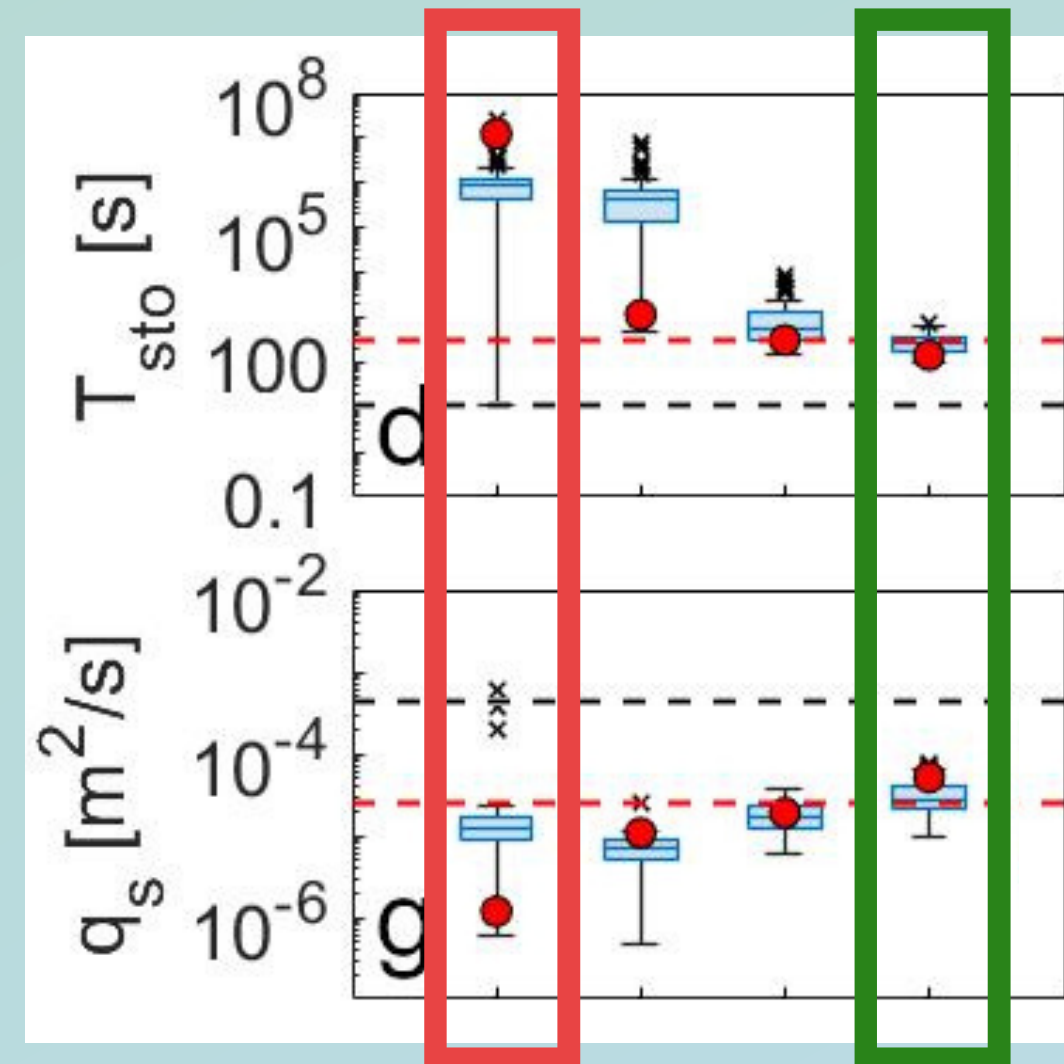
- 1) Studying the identifiability of Alpha and A_TS on the tail of the BTC was pivotal to improve identifiability of TSM parameters;
- 2) When identifiable, the TSM parameters control solute arrival-time and solute retention in stream channels;
- 3) The TSM mimics the ADE when one or more transient storage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

