



Modelling water quality in UK upland streams using high-frequency observations

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Nant Rhesfa (LI7) stream at Llyn Brianne basin

OVERVIEW:

- **High–frequency water quality** monitoring in upland Wales
- Novel **continuous-time transfer function modelling** of H^+ , DOC & $\text{NO}_3\text{-N}$ from rainfall
- Developing understanding of the relationship between catchment **hydrological functioning & biogeochemical response**
- Fundamental importance of sub-daily to sub-hourly observations

NERC DURESS project

Diversity in Upland Rivers for Ecosystem Service Sustainability

One of 4 UK national projects under NERC Biodiversity & Ecosystem Service Sustainability

Affect of **water quality (& quantity) variables on aquatic biodiversity** & visa versa



upland streams with/without affects of conifer plantation – resultant impact on ecosystem service delivery

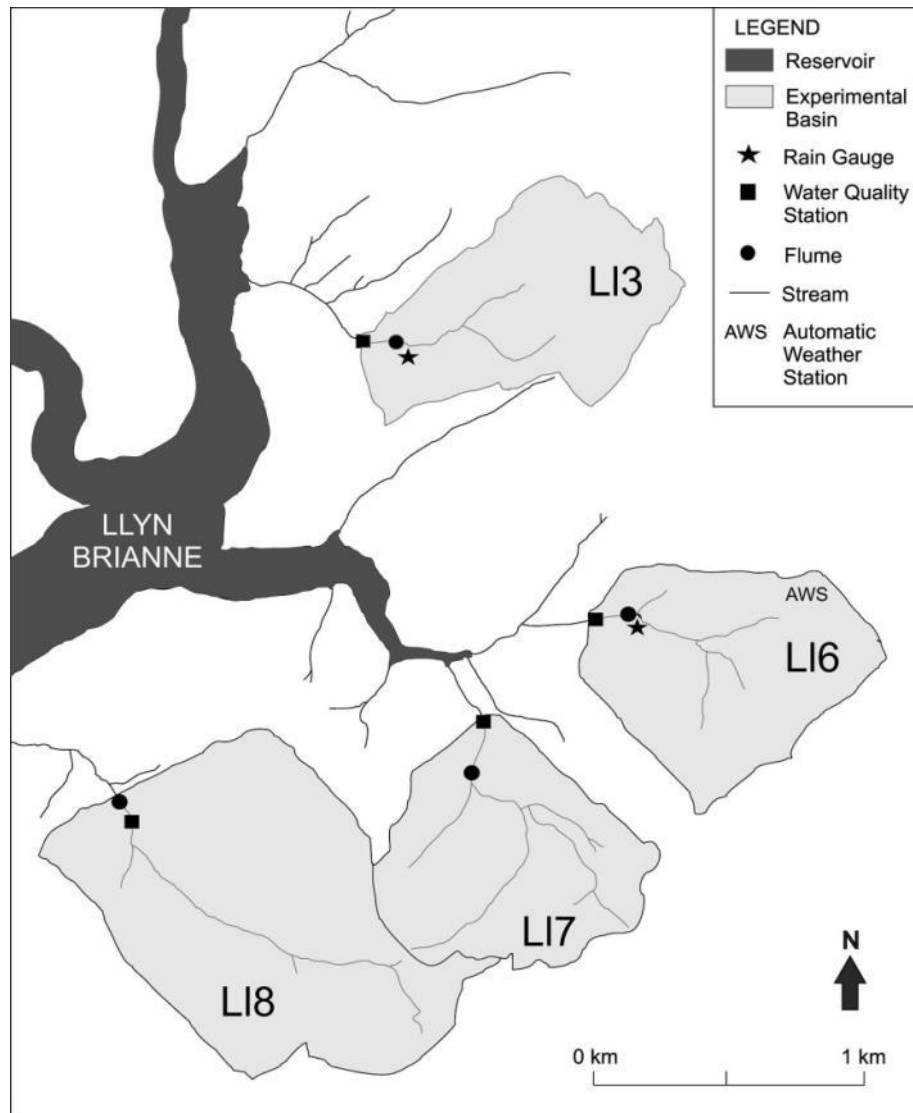
Necessarily inter-disciplinary project

Research / academic institutions e.g.:



Practitioners in water sector (in Wales) e.g.:





4 identically instrumented
micro-basins

Llyn Brianne
Upland Wales, UK

Typical upland land-uses

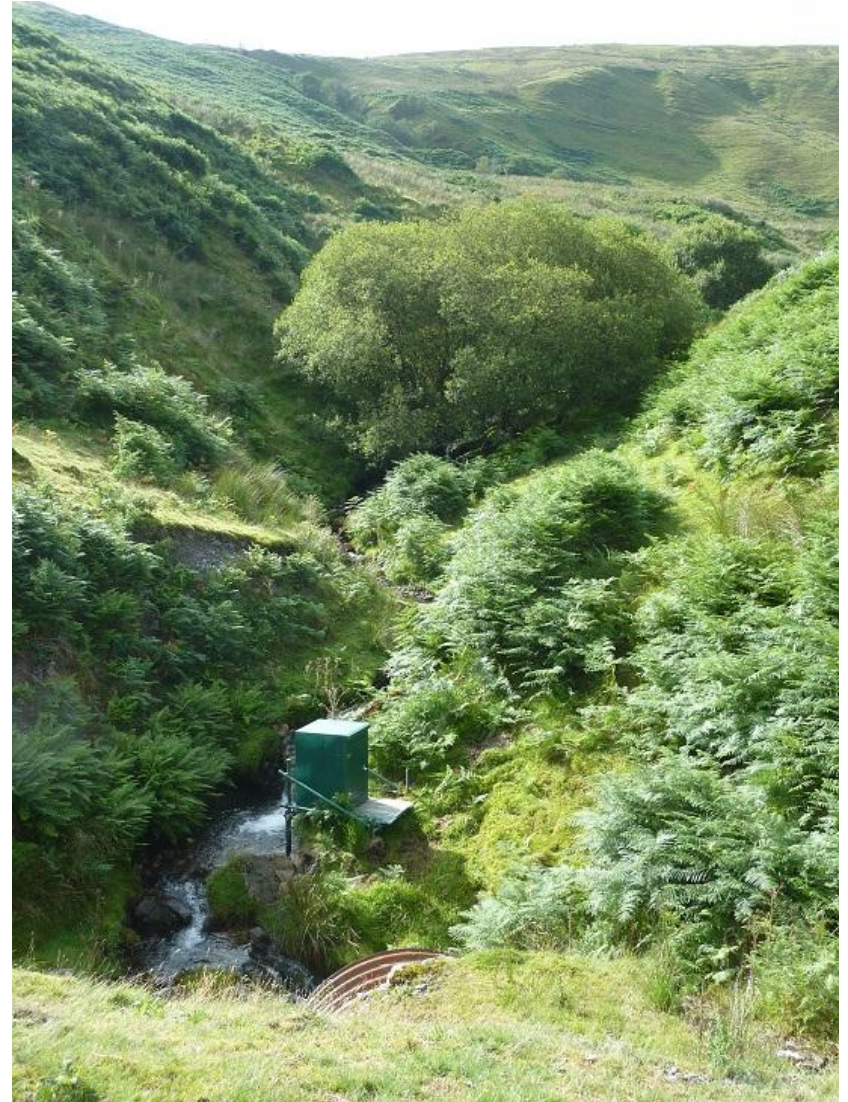
Improved moorland (x2)

Conifer plantations (x2)

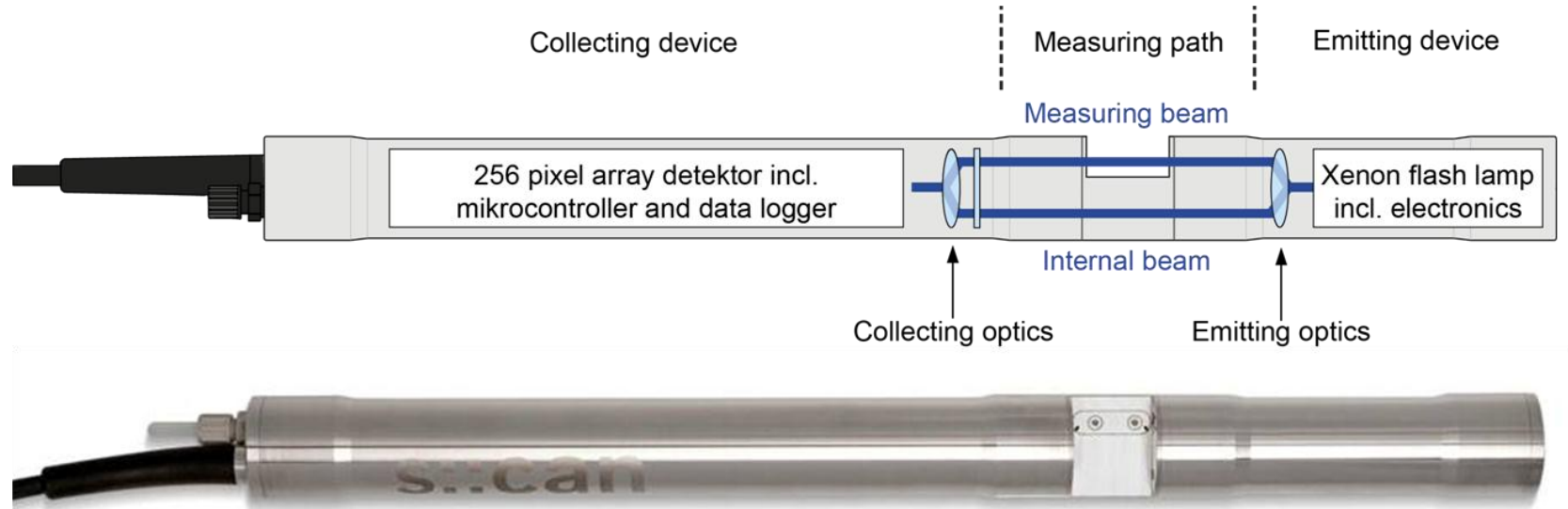
Hydrometric station (LI6)



Water quality station (LI7)



- High frequency (15-min continuous monitoring) using state-of-art water quality & hydrometric sensors e.g.



S::CAN spectrolyser (DOC, TOC, NO₃-N, turbidity, colour)

Accurate measurement of water quality variables now possible *in situ* (& cost effectively) following **sensor advances** (Hipsey & Arheimer 2013 *IAHS Publ* 361: 17-29)

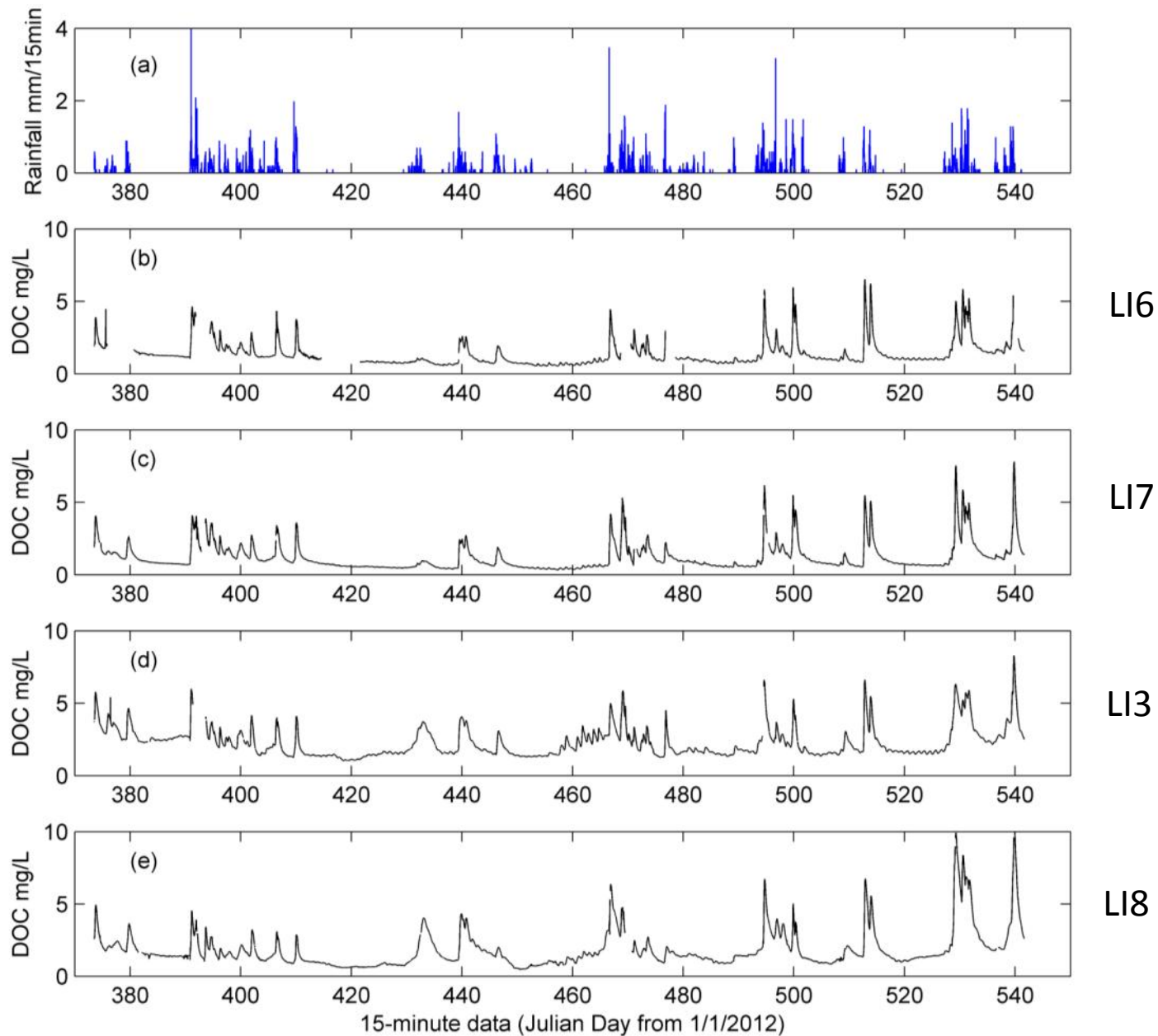


Digital differential pH probes
e.g., Hach DPS1

DOC conc.
time series

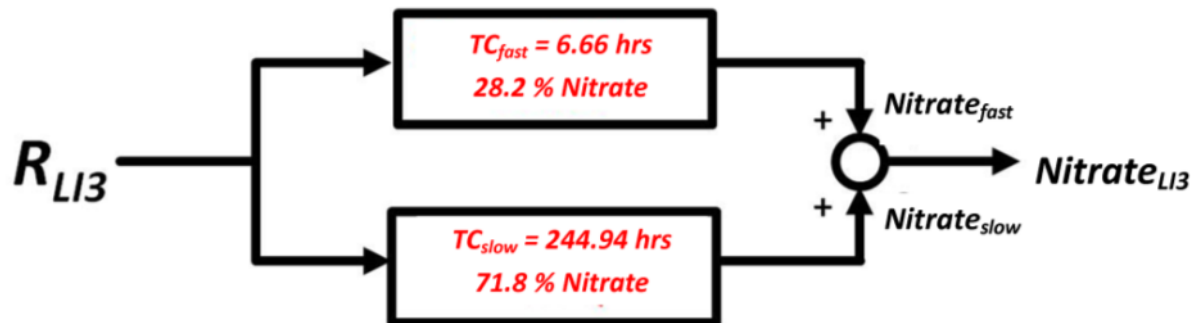
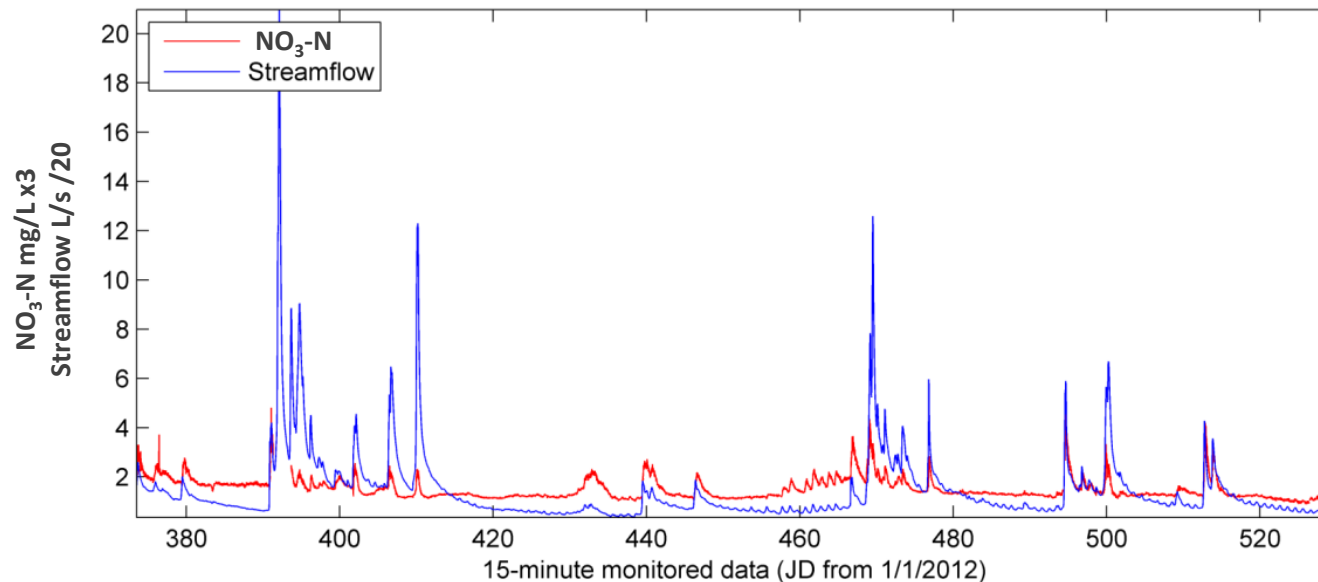
from Fig. 1

Jones,
Chappell &
Tych ES&T
(submitted)



High quality time-series of hydrochemistry

To develop understanding of catchment hydrological functioning from water quality time-series...



...need **high quality data** & numerical **tools capable of extracting** dominant dynamics

Requires high quality time-series of hydrochemistry & robust numerical methods

Numerical tools...

Some water quality time-series (often non-conservative variables) are **information rich** (e.g., H^+ , DOC) - methods available to **extract dynamics** contained e.g.,

RIVC

Refined Instrumental Variable Continuous-time
Box-Jenkins identification algorithm

Taylor, Pedregal, Young & Tych (2007) *Environ. Model. Software* 22: 797–814



Numerical tools...

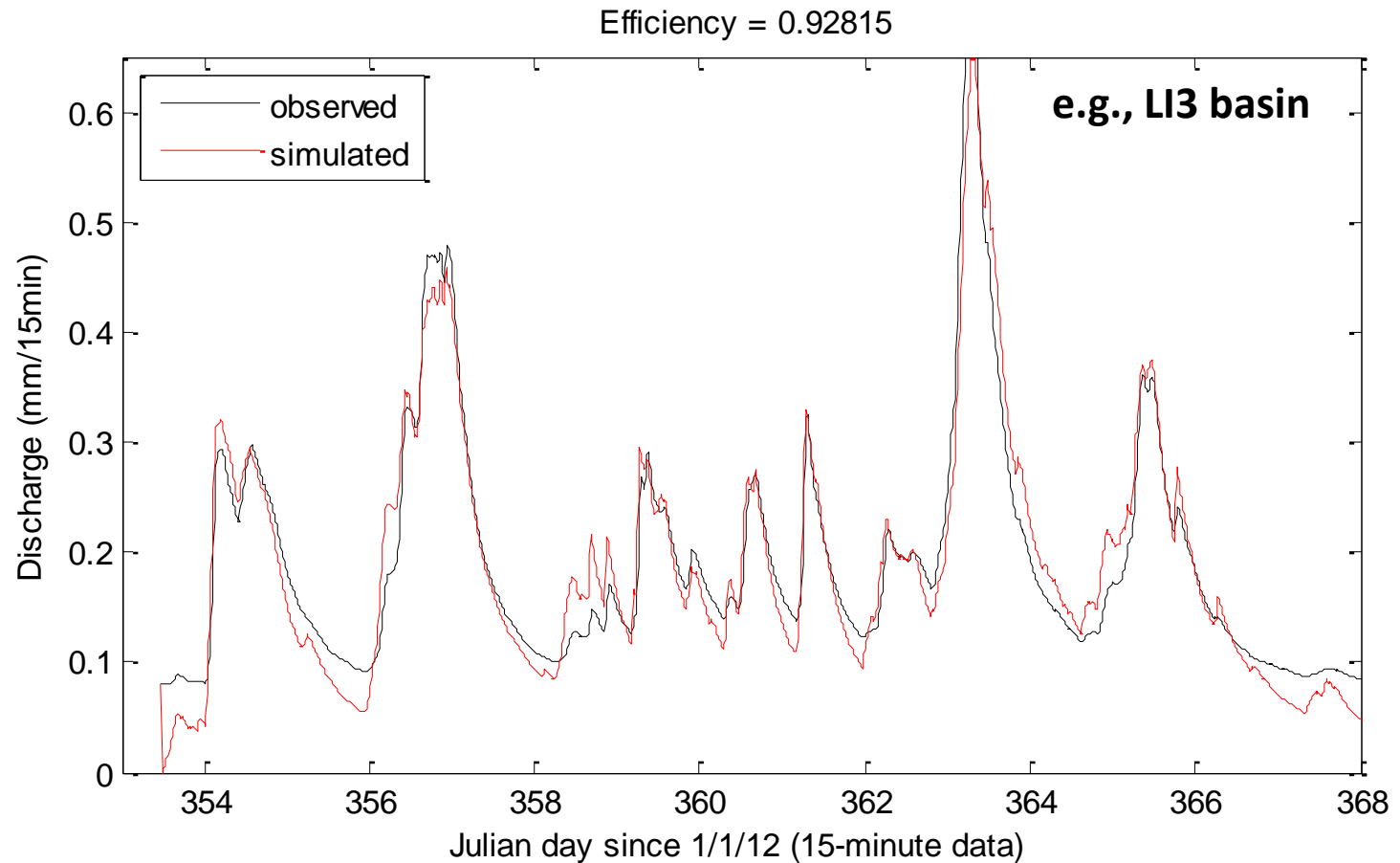
RIVC applied within a

Data-Based Mechanistic philosophy

- (1) Identification of many potential model structures, minimising prior assumptions about processes – that are often unknown (**'Data-Based'**)
- (2) Rejection of most using objective statistical & mathematical criteria (incorporating **'Principles of Parsimony'** via heuristic measures)
- (3) Rejection of further models that have no physical (e.g., hydrological) interpretation (**'Mechanistic'**) – giving models for testing against independent observations (e.g., dynamics within component flow paths)

rainfall-streamflow models identified **linear 2nd order CT-TFs***

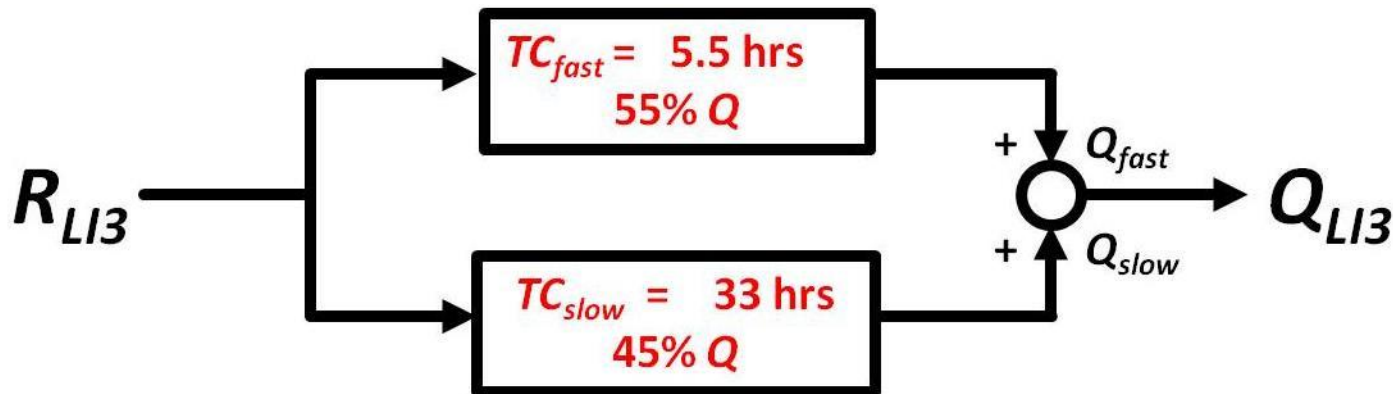
*given high efficiency, no marked drop in YIC, no complex roots etc



e.g., for LI3 basin (in winter)

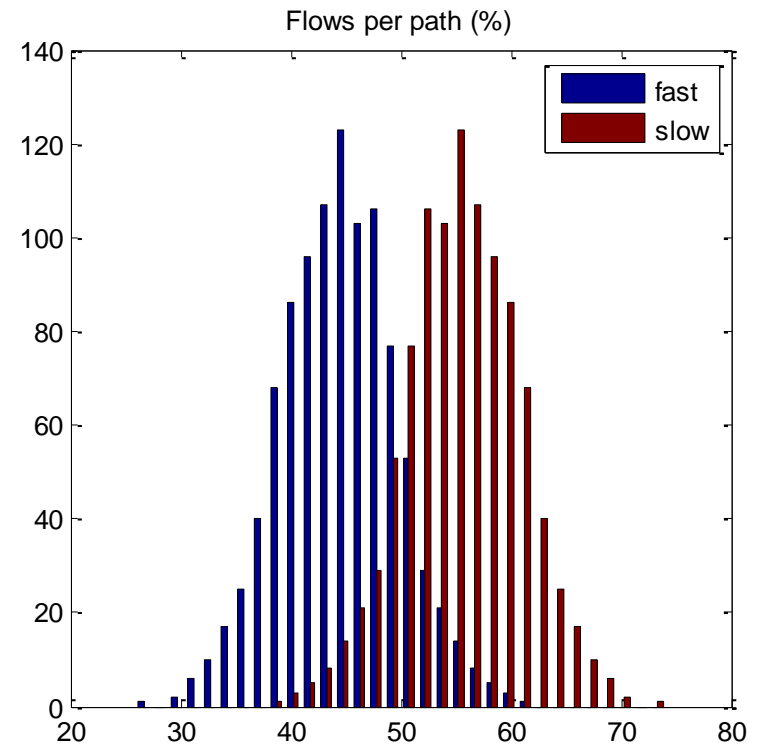
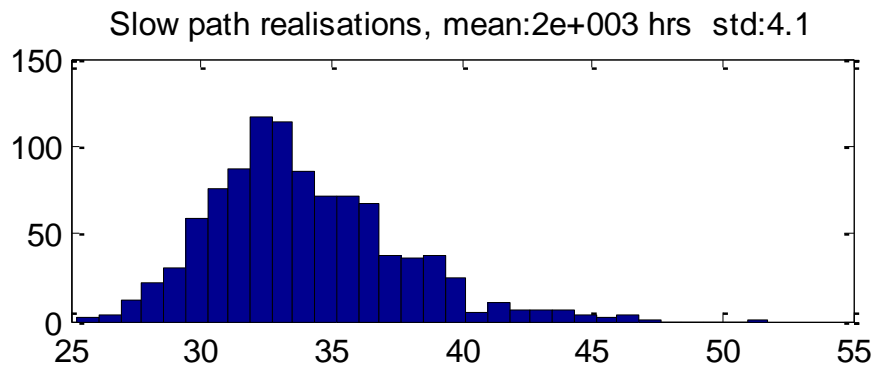
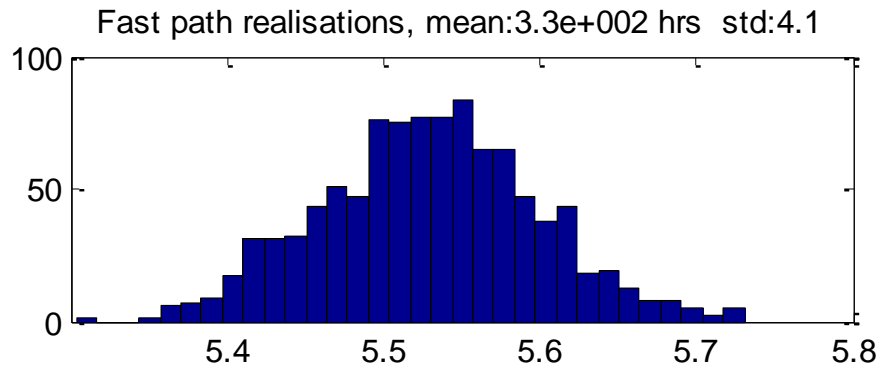
$$Q_{LI3} = \frac{0.0248s + 0.0003}{s^2 + 0.0527s + 0.0003} e^{-s1} R_{LI3\&6} \quad s = \frac{d}{dt}$$

Decomposition of 2nd-order rainfall-streamflow model to **two parallel pathways** usually considered to have most robust physical interpretation (via **Dynamic Response Characteristics**, DRCs)



Uncertainty in DRCs (1000 Monte Carlo realisations) – allow **DRC comparison**

e.g., for LI3 basin



li3qmodel3_tj2.m (Fig. 70 & 73)

Comparison of model characteristics between catchments

e.g., TC (time constant)

TC	Dominant runoff process associated	Flow path reference
5 mins	overland flow (infiltration-excess primarily)	Chappell <i>et al.</i> (2006)
2.9 hrs	shallow subsurface flow from a hillslope	Chappell <i>et al.</i> (1990)
100 hrs	fracture flow in Lower Devonian slate	Chappell & Franks (1996); Birkinshaw & Webb (2010)
107 dys	deep pathway through a chalk aquifer	Ockenden & Chappell 2011

from Jones & Chappell (2014) Hydrology Research doi: 10.2166/nh.2014.155

5.5 hrs(45%)
33 hrs (55%)

L13

0 0.25 0.5 1 Kilometers

2.4 hrs (45%)
25 hrs (55%)

L16

3.7 hrs (30%)
35 hrs (70%)

L18

L17

3.3 hrs (43%)
36 hrs (57%)

**Time constant (TC)
of hydrometric
responses are similar**

**Basins behave similarly
despite land use**

e.g., presence of a
slower 25-35 hr
component (in winter
response)

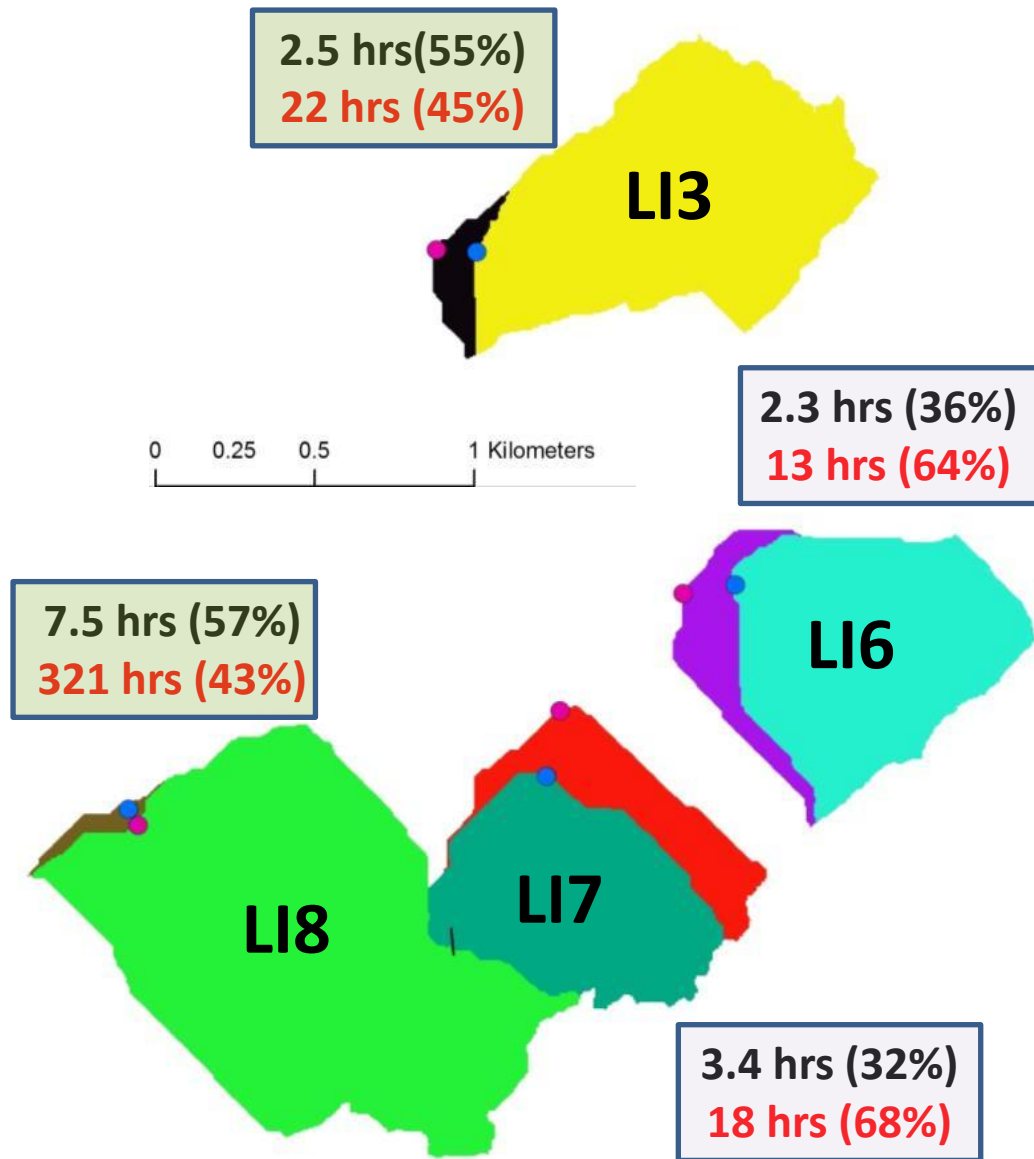
Source?

Deep soil pipes path

Drift (C) path

Rock-fracture path

Compare rainfall-streamflow response between nearby basins



Rainfall-H⁺ load models identified: **linear 2nd order CT-TFs** optimal

Residence times of H⁺ load response to rainfall (TC)

Faster response than rainfall-streamflow

'Exhaustion' or ion exchange effect?

except mature conifer (LI8)

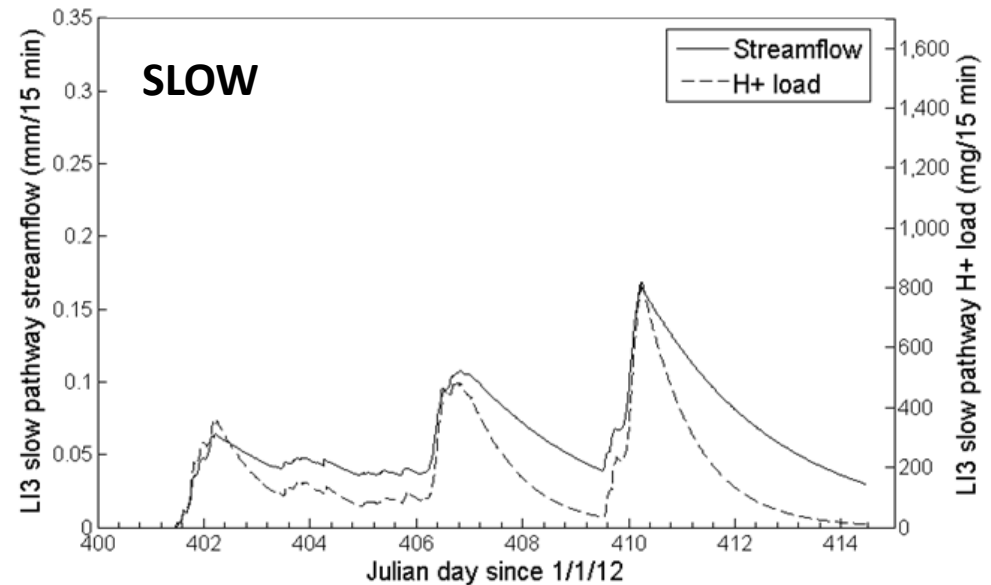
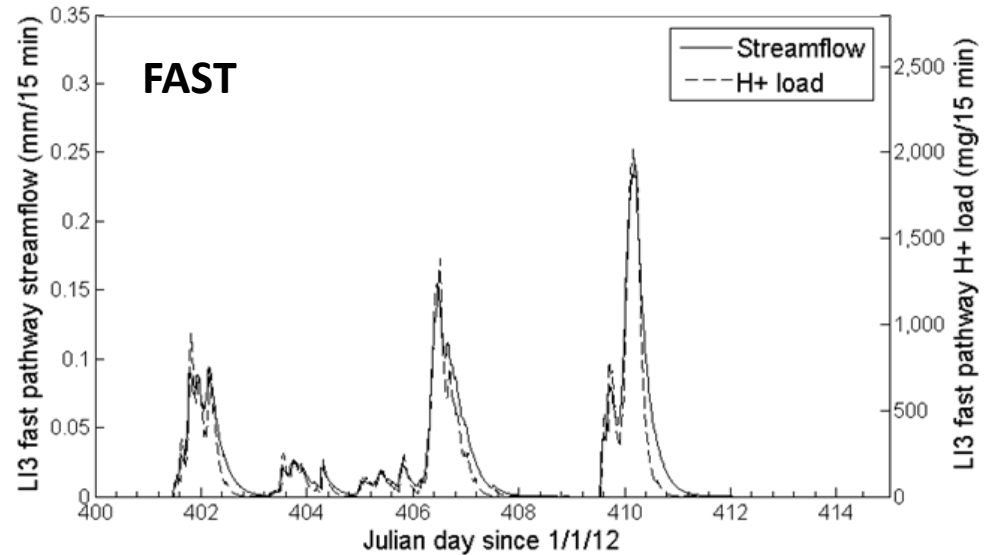
Compare rainfall-streamflow response with rainfall-H⁺ response

Also shown in model
simulated data

e.g.,
Identified components of
Rainfall-streamflow (—)
Rainfall- H^+ load (- -)
LI3 models

from Jones & Chappell (2014)
Hydrology Research doi:
10.2166/nh.2014.155

**H^+ path exhausted faster
than hydrometric response
path (LI3, LI6, LI7) – flow
path implications?**



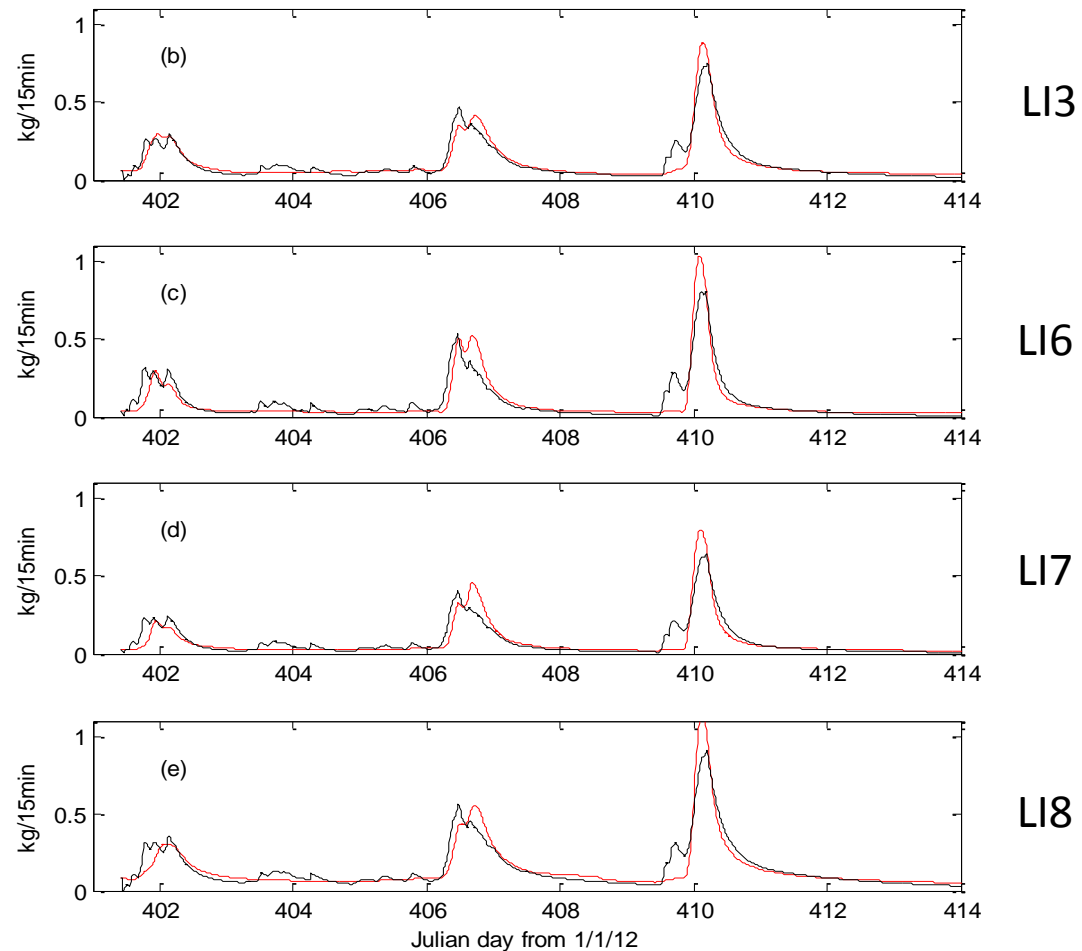
Compare rainfall-streamflow response with rainfall- H^+ response

Obtain similar **linear 2nd order CT-TF models** for rainfall-DOC load

—
observed DOC

—
simulated DOC

*from Jones,
Chappell & Tych
(2014) ES&T
submitted*



Simulated DOC load from rainfall

**How realistic are
component path
proportions &
dynamics
identified from
whole-basin
responses?**

*Next phase
of independent
observation &
modelling of
component flow
paths*

e.g., hydrometric & H^+
response in natural
soil pipes, fracture
flow, soil pathways



Observe & compare hydrometric & water quality response of component paths

Key message:

interpretation only possible if can avoid **under-sampling** water quality time-series

e.g. LI3

Rainfall-streamflow fast TC = 5.13 hrs

Rainfall-H⁺ load fast TC = 2.50 hrs

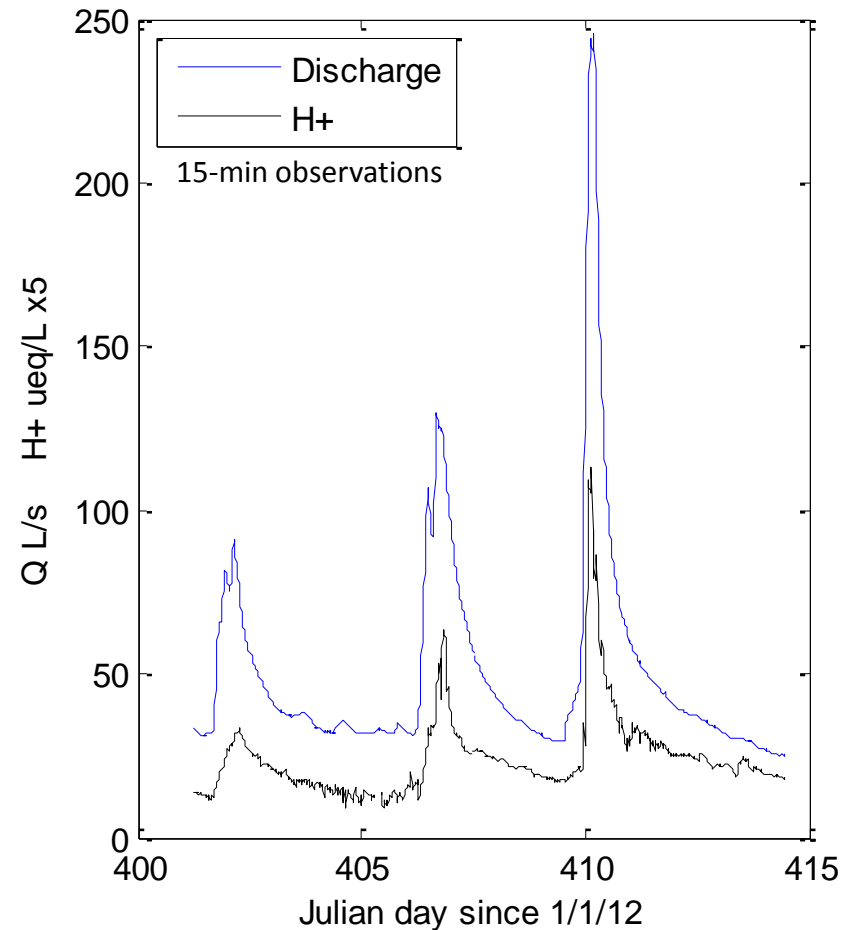
Time Constants (TCs) from li3q8.m

Minimum sampling for H⁺ load

Nyquist-Shannon: fast TC/2 = 75 mins

Young (2010 *BHS*)*: fast TC/6 = **25 mins**

*Young, P. 2010. The estimation of continuous-time rainfall-flow models for flood risk management. In: *Role of Hydrology in Managing Consequences of a Changing Global Environment*. BHS, Newcastle



Interpretation only plausible if sampling has been sufficient given the dynamics

Thank you - any questions?



Further information

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