UFZ HELMHOLTZ Zentrum für Umweltforschung

# Modeling Catchment Scale Nitrate Export using the StorAge Selection Functions

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## ➢ *Water age & solute dynamics at the catchment scale*

- Catchments store and release water of different ages.

- The age of a water parcel has big implications for understanding flow and transport mechanisms (Botter et al., 2011; Sprenger et al., 2019).

- The water-age based concept, the formulation of transport by transit time distributions (TTDs), has been emerging as a useful tool for understanding catchment-scale solute export (Sprenger et al., 2019).

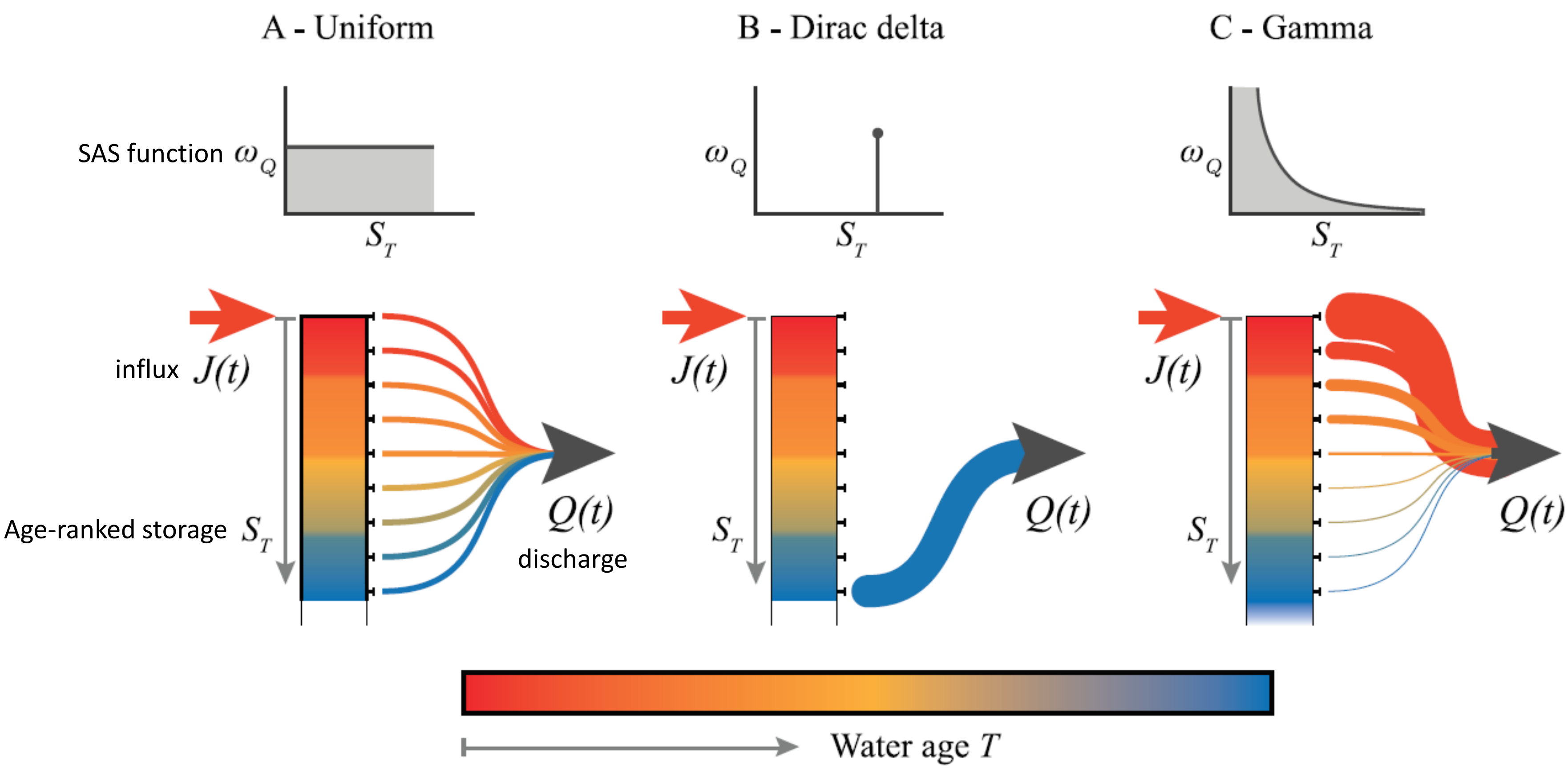
## *Formulation of transport by transit time distributions*

- TTD-based models have been used to explore solute export at the catchment scale, including nitrogen legacy (Ilampooranan et al., 2019; van Meter et al., 2018; 2017).

- These models assume that TTDs are time-invariant.

- Experimental data and numerical studies have indicated that TTDs (e.g., for discharge) are time-variant for many hydrological systems (Yang et al., 2018a; Kaandorp et al., 2018; Rodriguez et al., 2018; Kim et al., 2016; van der Velde et al., 2012).

## *Formulation of transport with SAS-based approach*




Concept of the SAS-based approach (Harman et al., 2015)

- *Formulation of transport with SAS-based approach*

  - StorAge Selection (SAS) function is a transformed TTD function.

  - SAS functions have a clearer physical meaning and are more stable in time, easier for parameterization than TTDs (van der Velde et al., 2012)

  - SAS functions could be combined with storage-discharge functions to provide a coherent framework for describing both velocity and celerity transport mechanisms (Harman et al., 2019; Hrachowitz et al., 2016)

*Spatial heterogeneity of catchment characteristics and large scale testing have not been addressed with the SAS-based model.*

- *Research objectives*

  - Introducing a new model, allowing a distributed representation of soil nitrogen dynamics and a spatially implicit representation of subsurface transport pathways based on the SAS-based approach.

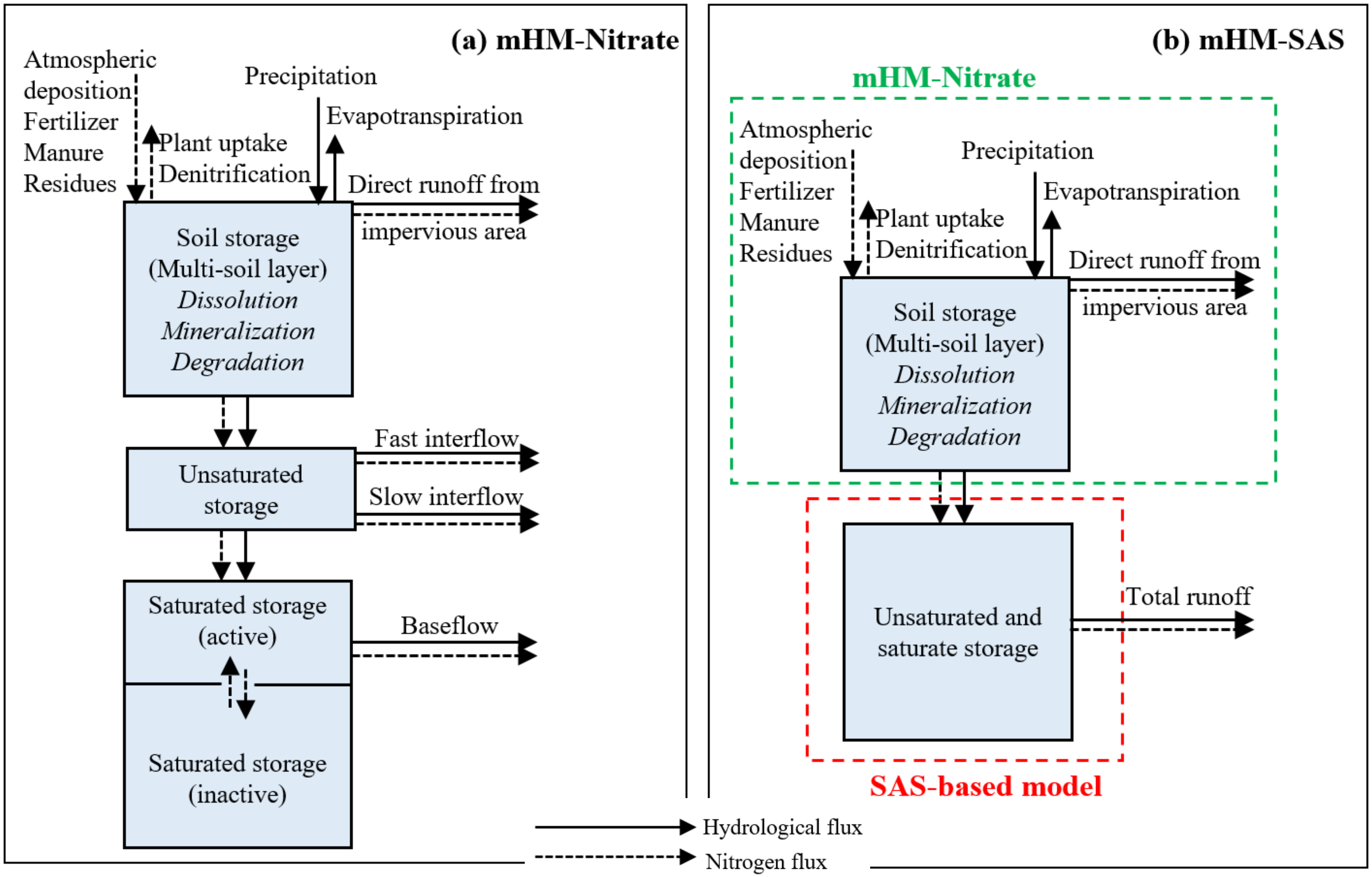
  - Validating the proposed model at a mesoscale catchment with heterogeneous characteristics.

## ➢ *mHM-Nitrate model*

- a grid-based water quality (nitrate) model (Samaniego et al., 2010; Kumar et al., 2013; Lindström et al., 2010; Yang et al., 2018b).
- accounts for spatial heterogeneity in land use management practices (fertilizer/manure application, crop rotation).
- has a simple subsurface nitrate transport module (no denitrification below the root zone, inadequate representation of celerity-driven transport).

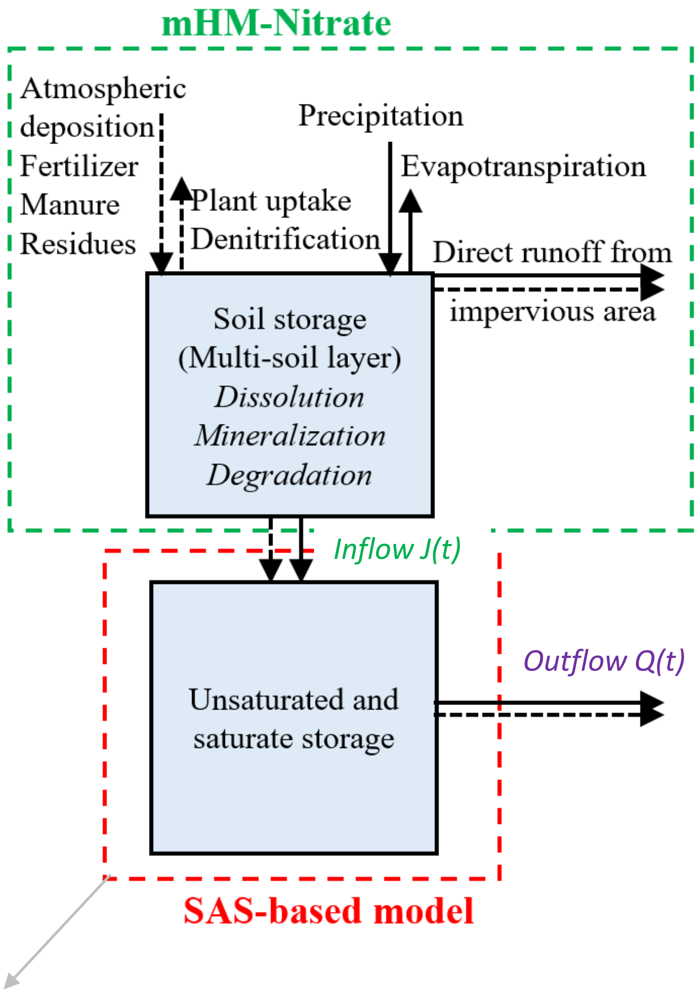
→ Replace the subsurface transport module with the SAS-based concept

## ➢ *mHM-Nitrate model vs. proposed mHM-SAS model*




Conceptual model of (a) the mHM-Nitrate model and (b) the proposed mHM-SAS model at a grid cell level

## ➢ *mHM-SAS model*




### Master equation for the SAS compartment

*changes of the water volume in storage with age $\leq T$* — *inflow* — *outflow* — *aging*

$$\frac{\partial S_T(T,t)}{\partial t} = J(t) - Q(t) \cdot P_Q(T,t) - \frac{\partial S_T(T,t)}{\partial T}$$

$P_Q(T,t)$: *TTD of discharge*

### Solute (nitrate) concentration at the outlet

$$C_Q(t) = \int_0^{\infty} C_J(T,t) \cdot p_Q(T,t) \cdot exp(-\frac{T}{t_{12}}) \cdot dT$$

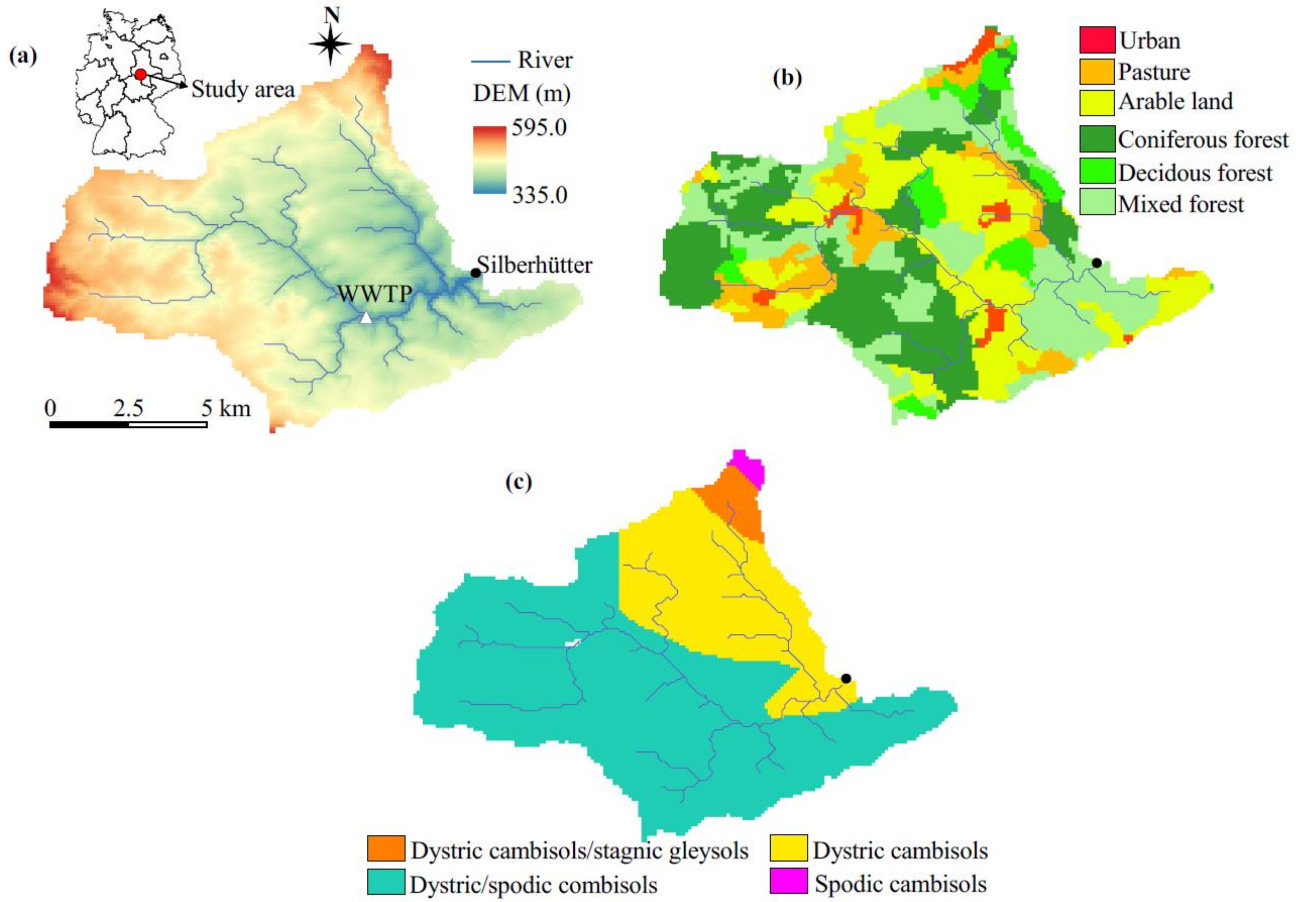
$p_Q(T,t)$: *TTD of discharge*; $t_{12}$: *Half life of nitrate*

$$P_Q(T,t) = \Omega_Q(P_S(T,t),t)$$

$P_S(T,t)$: *normalized age-ranked storage*; $\Omega_Q$: *SAS function*

SAS compartment: unsaturated and saturate zone below the root zone over the whole catchment

## ➢ *Study area*




Location of the upper Selke with (a) the digital elevation model (DEM), (b) land use/land cover map, and (c) soil map. The catchment outlet is indicated by a black dot.

- *Study area*

  - Catchment area: 100 $km^2$ (61% forest, 36% agricultural)
  - Main crops: winter wheat, triticale, winter barley, rye, rapeseed, corn.
  - Fertilizer/manure application rate: 130 – 190 kg N/ha/yr
  - Strong seasonality in runoff regime
  - Chemodynamic C(nitrate)-Q relationship

## ➢ *Representation of the time-variant SAS functions*

- Two-parameter beta function $beta(P_S, a, b)$

- Two beta functions are used to characteristics of the time-variant SAS functions: $beta_{wet}(P_S, a_{wet}, b_{wet})$, and $beta_{dry}(P_S, a_{dry}, b_{dry})$

- The wet and dry periods are defined based on the following factor:

$$r_t = \frac{\sum_{i=t-n}^{t} J_i}{\sum_{i=t-n}^{t} Q_i}$$

Inflow to the SAS compartment ($J_i$)

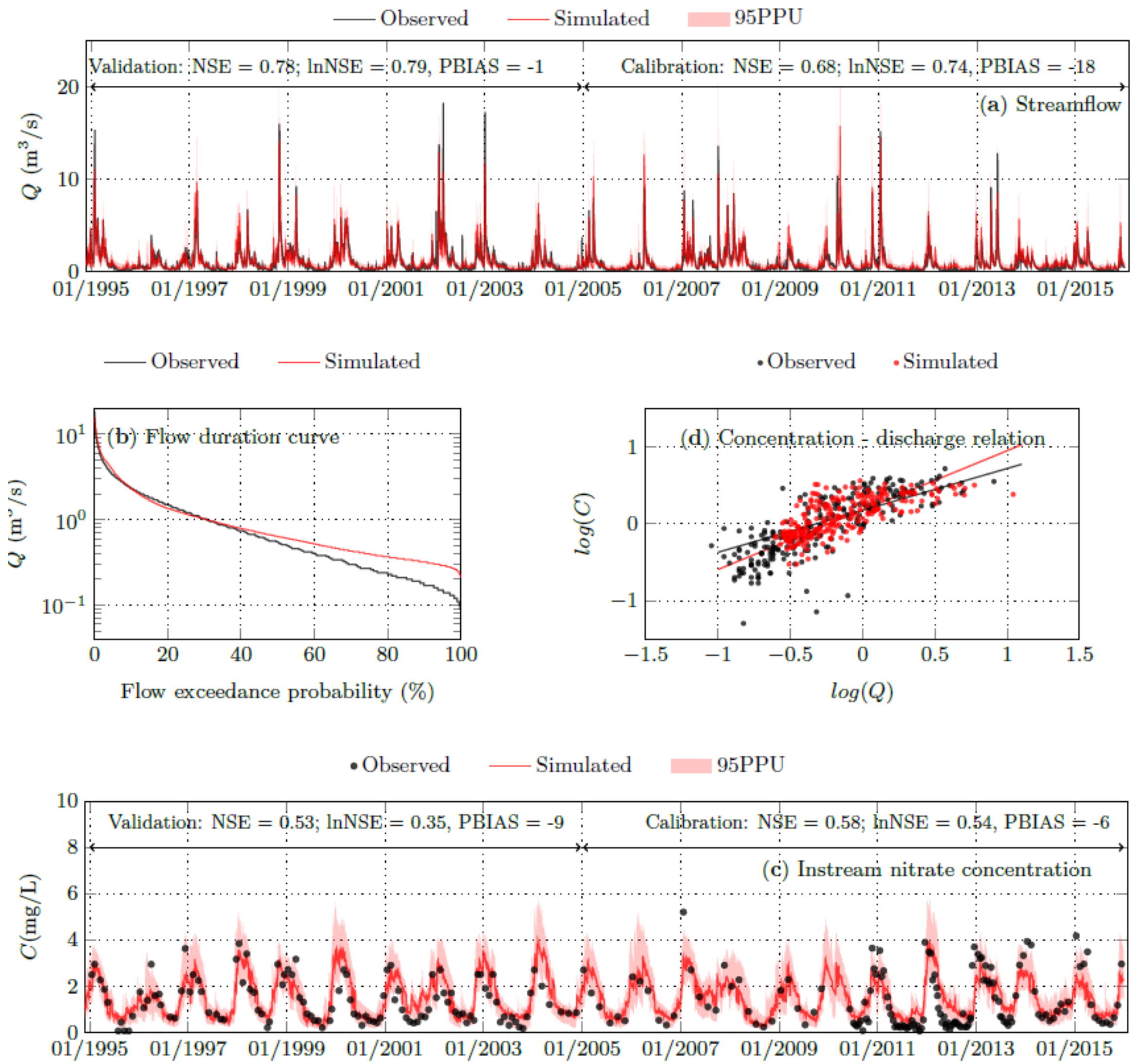
Outflow ($Q_i$)

n: number of time steps

$r_t \geq 1 \rightarrow wet \rightarrow beta_{wet}$ : *Young water selection preference*

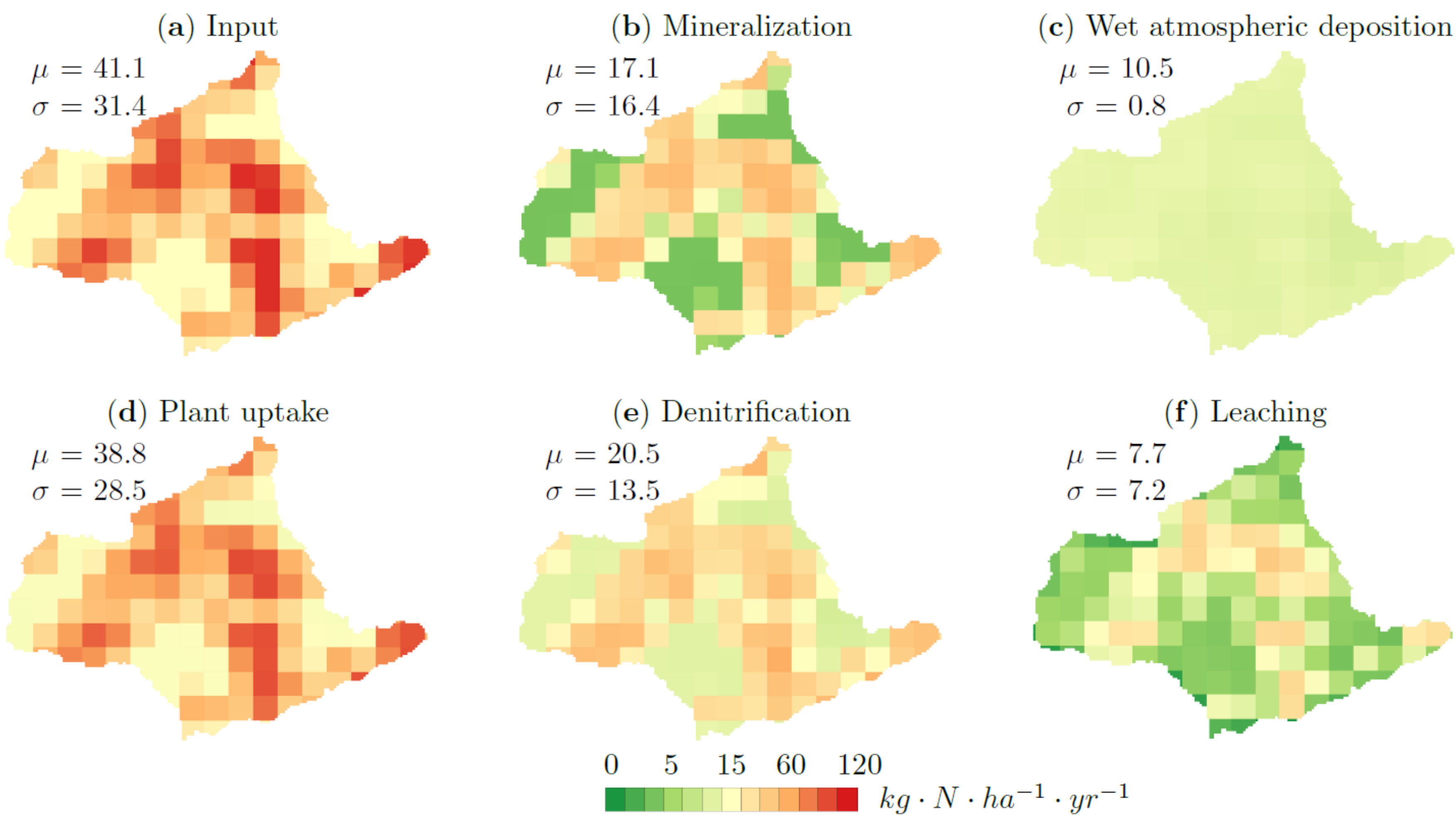
$r_t < 1 \rightarrow dry \rightarrow beta_{dry}$: *Old (and young) water selection preference*

➢ *Simulated discharge and in-stream nitrate ($N-NO_3$) concentration at Silberhütter*

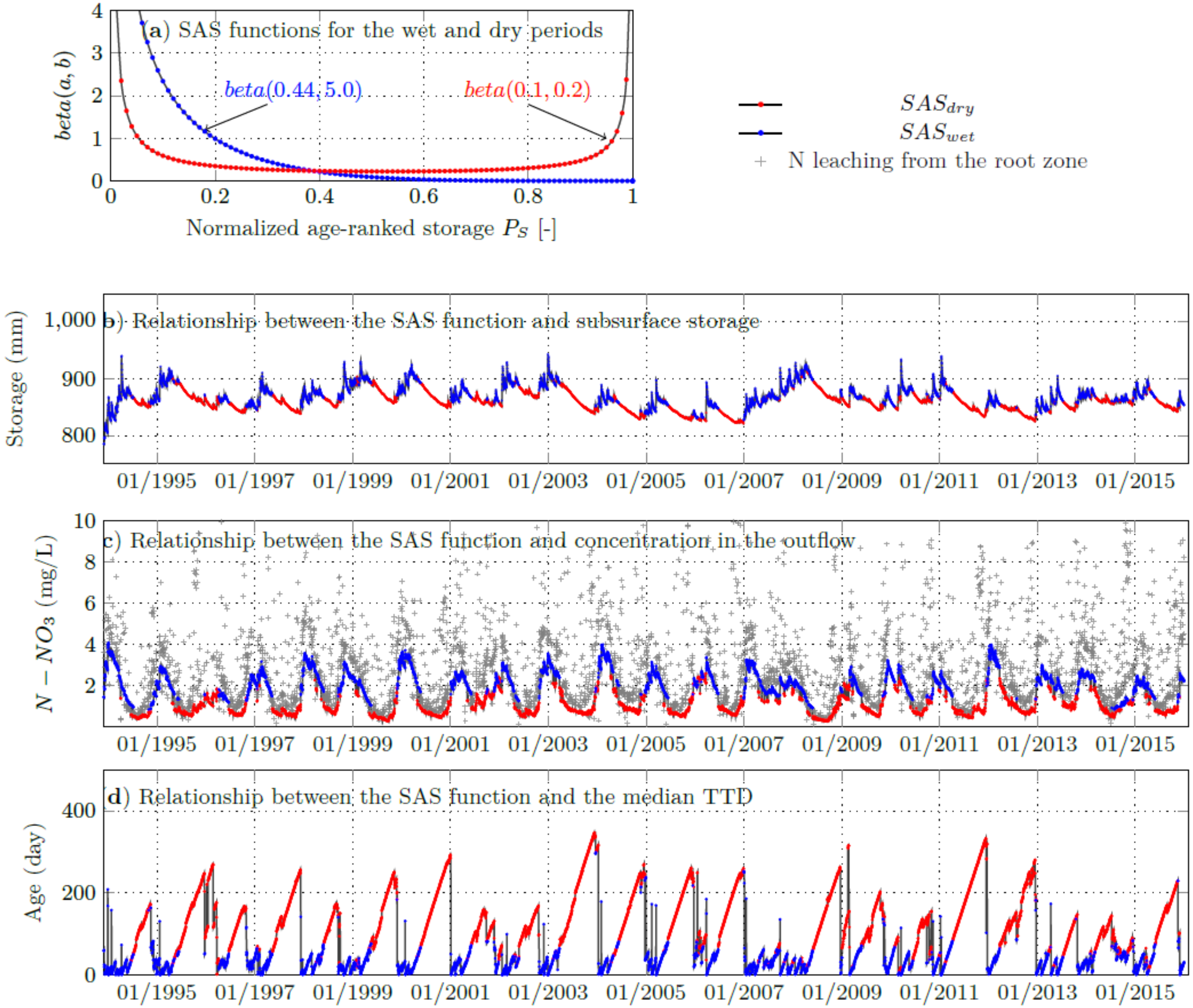



half life of nitrate = 134 days

## ➤ *Simulated spatial nitrogen dynamics within the root zone*



➢ *SAS functions –subsurface storage – nitrate concentration – median TTD of discharge*



- Denitrification below the root zone should be accounted for.
- Discharge and in-stream nitrate concentration dynamics at the catchment outlet could be well represented by the proposed model
- The mHM-SAS model could provide explicit spatial information about soil nitrogen
- The mHM-SAS model can represent the relation between the SAS function, storage, and median TTD of discharge in a qualitative and reasonable manner.

- Outlook
  - Quantitative verification of the simulated travel time and spatial nitrogen dynamic within the root zone
  - Testing of the model for catchments with nitrogen legacy (velocity-driven transport)

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Thank you for your attention ☺

Questions and Suggestions are welcome