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

A - Uniform

B - Dirac delta

C - Gamma

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

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

Changes of the water volume in storage with age \( \leq T \)

**Solute (nitrate) concentration at the outlet**

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

TTD of discharge

**Half life of nitrate**

\[
P_Q(T, t) = \Omega_Q(P_S(T, t), t)
\]

**Normalized age-ranked storage**

**SAS compartment:** unsaturated and saturate zone below the root zone over the whole catchment
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 km² (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 \(\text{beta}(P_s, a, b)\)

- Two beta functions are used to characteristics of the time-variant SAS functions: \(\text{beta}_{\text{wet}}(P_s, a_{\text{wet}}, b_{\text{wet}})\), and \(\text{beta}_{\text{dry}}(P_s, a_{\text{dry}}, b_{\text{dry}})\)

- 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
- Outflow
- \(n\): number of time steps

\(r_t \geq 1 \rightarrow \text{wet} \rightarrow \text{beta}_{\text{wet}}: \text{Young water selection preference}\)

\(r_t < 1 \rightarrow \text{dry} \rightarrow \text{beta}_{\text{dry}}: \text{Old (and young) water selection preference}\)
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

(a) Input

\( \mu = 41.1 \)

\( \sigma = 31.4 \)

(b) Mineralization

\( \mu = 17.1 \)

\( \sigma = 16.4 \)

(c) Wet atmospheric deposition

\( \mu = 10.5 \)

\( \sigma = 0.8 \)

(d) Plant uptake

\( \mu = 38.8 \)

\( \sigma = 28.5 \)

(e) Denitrification

\( \mu = 20.5 \)

\( \sigma = 13.5 \)

(f) Leaching

\( \mu = 7.7 \)

\( \sigma = 7.2 \)

0 5 15 60 120

\( kg \cdot N \cdot ha^{-1} \cdot yr^{-1} \)
SAS functions – subsurface storage – nitrate concentration – median TTD of discharge

(a) SAS functions for the wet and dry periods

\[ \text{beta} (0.44, 5.0) \quad \text{beta} (0.1, 0.2) \]

Normalized age-ranked storage \( P_s \) [-]

(b) Relationship between the SAS function and subsurface storage

(c) Relationship between the SAS function and concentration in the outflow

(d) Relationship between the SAS function and the median TTD

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• 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)
REFERENCES


Thank you for your attention 😊

Questions and Suggestions are welcome