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Using dynamic transit times and StorAge Selection (SAS) functions to explore nitrate export from small agricultural catchments

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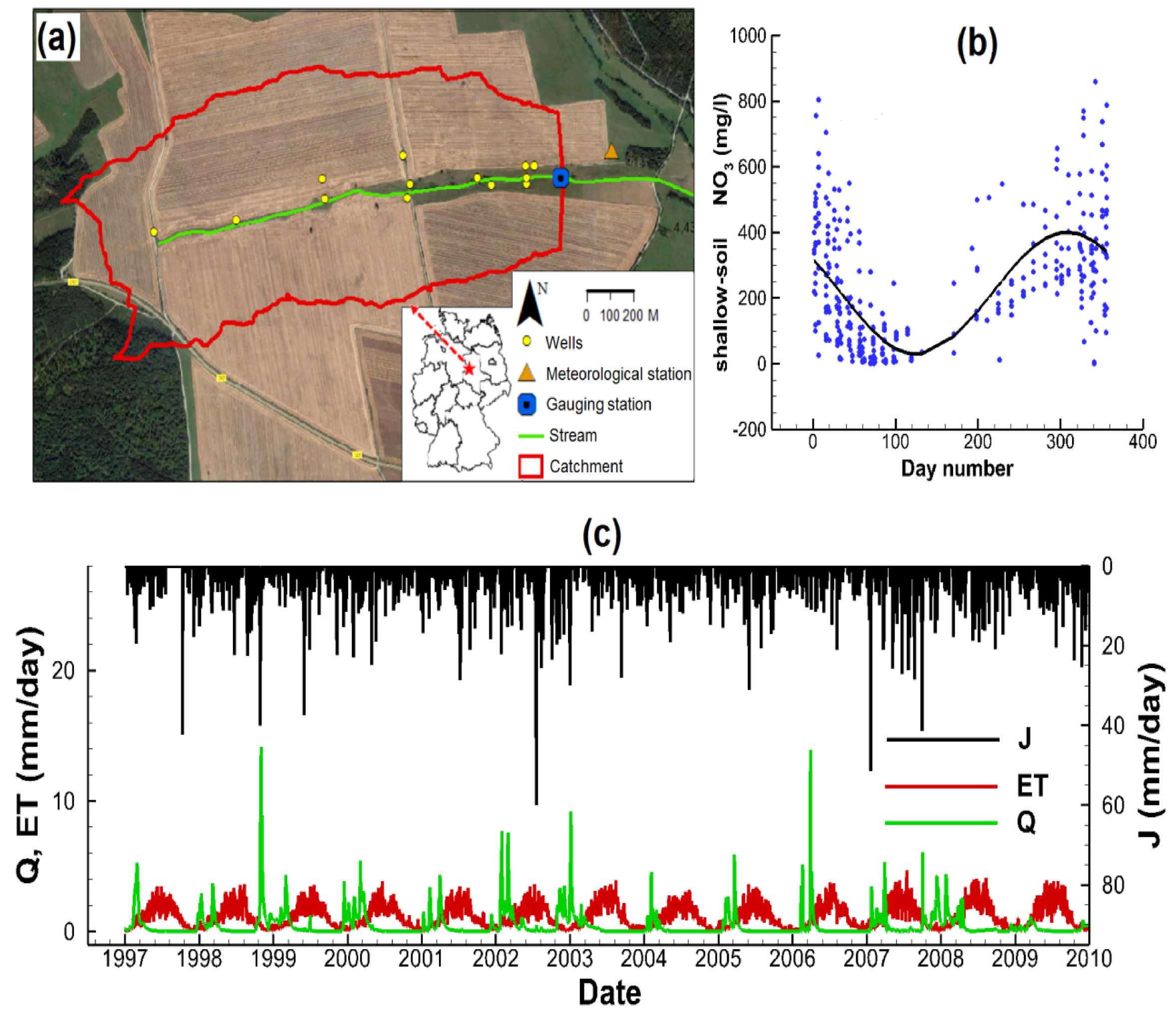
1 Background and Objectives

- Mechanistic transport models at catchment scale challenging
- Transit time distribution based models as potential alternative
- StorAge Selection (SAS) functions to define age distribution and concentration in catchment outflow (Q)
- **Objective I**: test SAS-function based nitrate export model
- **Objective II**: explore NO_3 export dynamics for different catchment types using SAS-function based model → scenarios

2 Reference catchment and field data



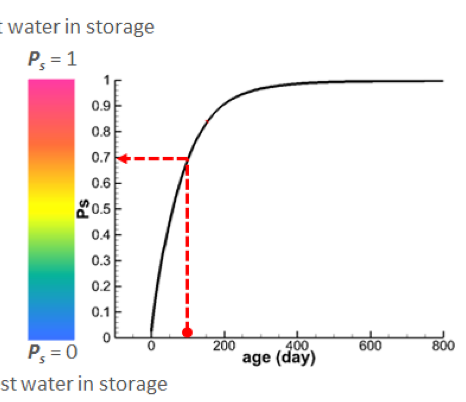
a) Schäfertal catchment in Central Germany (1.44 km²)
b) Nitrate percolation below root zone (from lysimeter data)
c) Precipitation (J), evapotranspiration (ET) and discharge (Q)

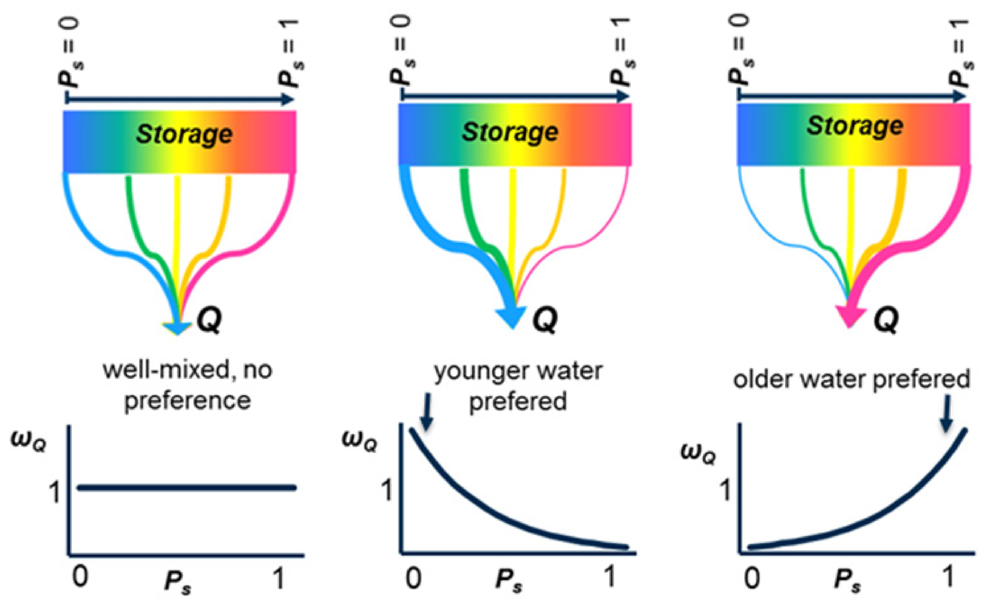
3 StorAge Selection (SAS) functions

fractional SAS-functions: define age distribution of water released from catchment storage via Q and ET

$$\omega_Q(Ps, t) = \frac{TTD}{RTD}$$

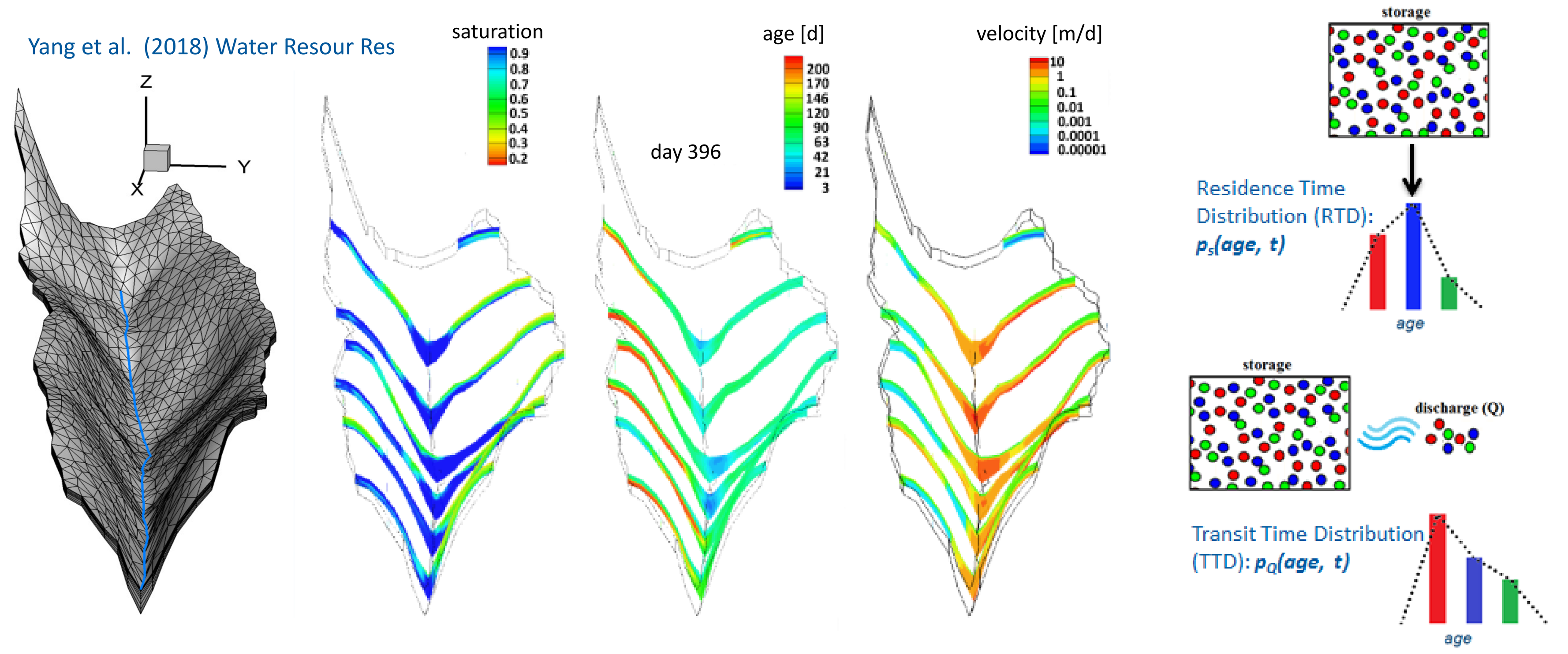
Transformation of absolute *Age* into cumulative RTD P_s [0 - 1]





$P_s = 0$: youngest water in storage
$P_s = 1$: oldest water in storage

4 Mechanistic reference model (HydroGeoSphere + PARTRACE)



velocity fields (HGS) → random-walk particle tracking (PARTRACE) – water ages → SAS-functions

5 Formulation of SAS-function based nitrate export model

age master equation (Botter et al. (2011) Geophys Res Lett)

Δ (age of storage) — water removal by Q and by ET — aging

$$\frac{\partial s(T,t)}{\partial t} = -Q(t)\cdot p_Q(T,t) - ET(t)\cdot p_{ET}(T,t) - \frac{\partial s(T,t)}{\partial T}$$

Δ (solute mass) — solute mass removal by Q and by ET — aging — first-order decay

$$\frac{\partial C_S(T,t)s(T,t)}{\partial t} = C_S(T,t)\left[Q(t)\cdot p_Q(T,t) + \alpha ET(t)\cdot p_{ET}(T,t)\right] - \frac{\partial C_S(T,t)s(T,t)}{\partial T} - \lambda\cdot C_S(T,t)s(T,t)$$

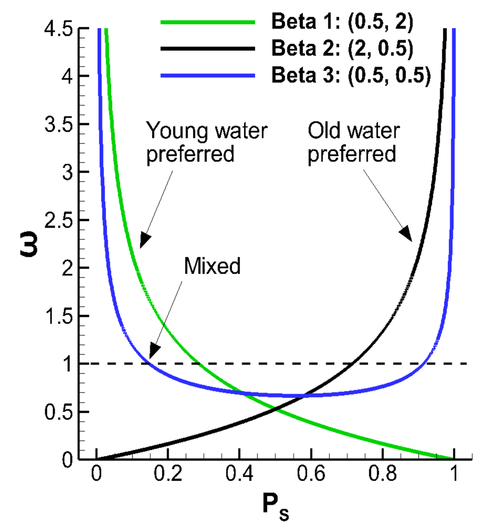
solute mass balance equation (following: Queloz et al. (2015) Water Resour Res)

solute concentration in Q by integration $C_Q(t) = \int_0^\infty C(T,t)p_Q(T,t)dT$

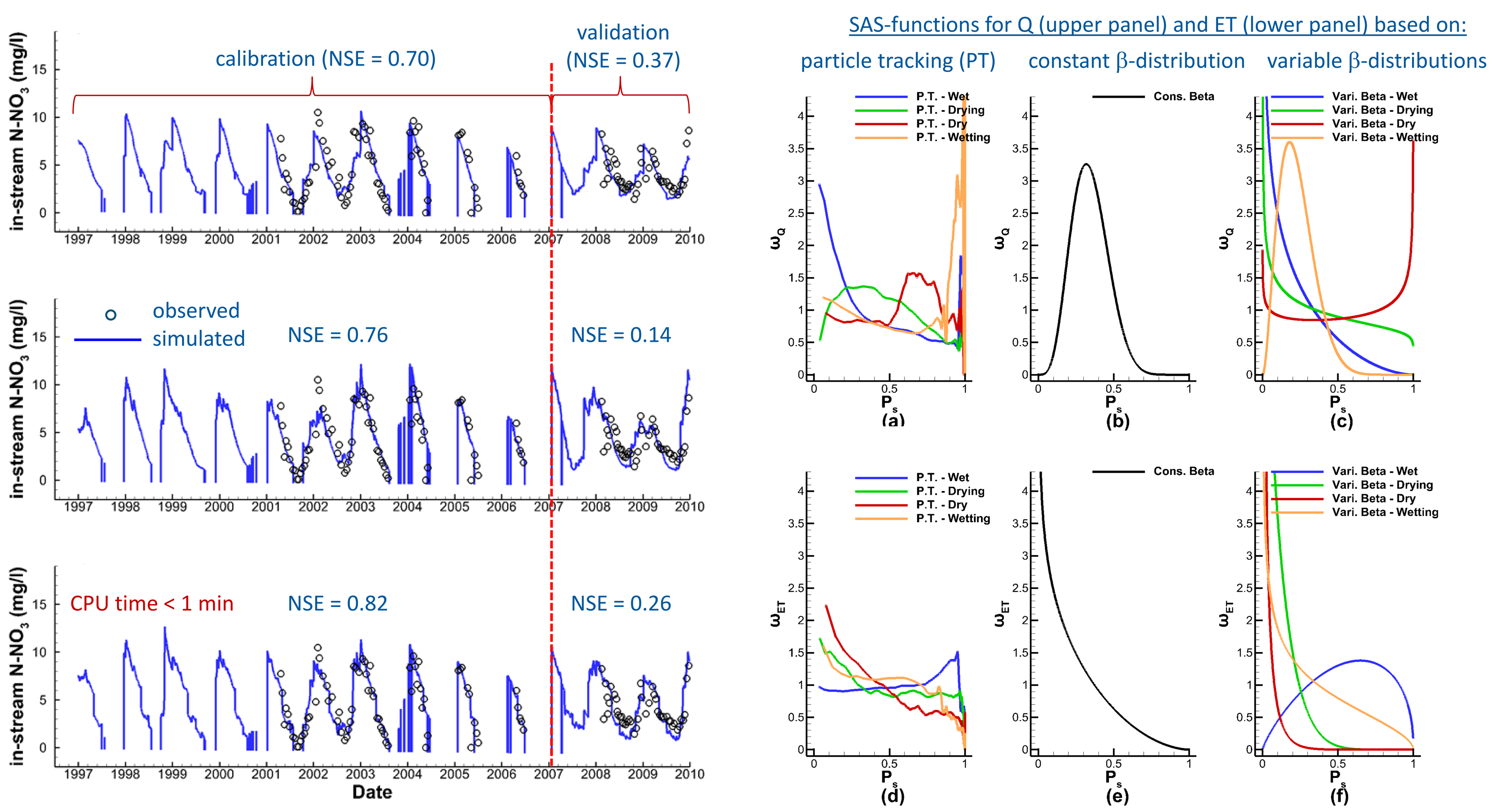
inverse model subject to:

Initial conditions: $S(0)$, $p_s(T,0)$, $C(T,0)$
Boundary conditions: $Q(t)$, $ET(t)$, $J(t)$, $C_{in}(t)$
$p_Q(T,t) = \omega_Q\ p_s(T,t)$ & $p_{ET}(T,t) = \omega_{ET}\ p_s(T,t)$
SAS-functions

SAS-functions defined by β-distributions: $f(x,a,b) = x^{a-1}\cdot(1-x)^{b-1}$



6 Results – nitrate concentrations in Q and SAS-functions



7 Results – mass removal, reactivity, mean transit times

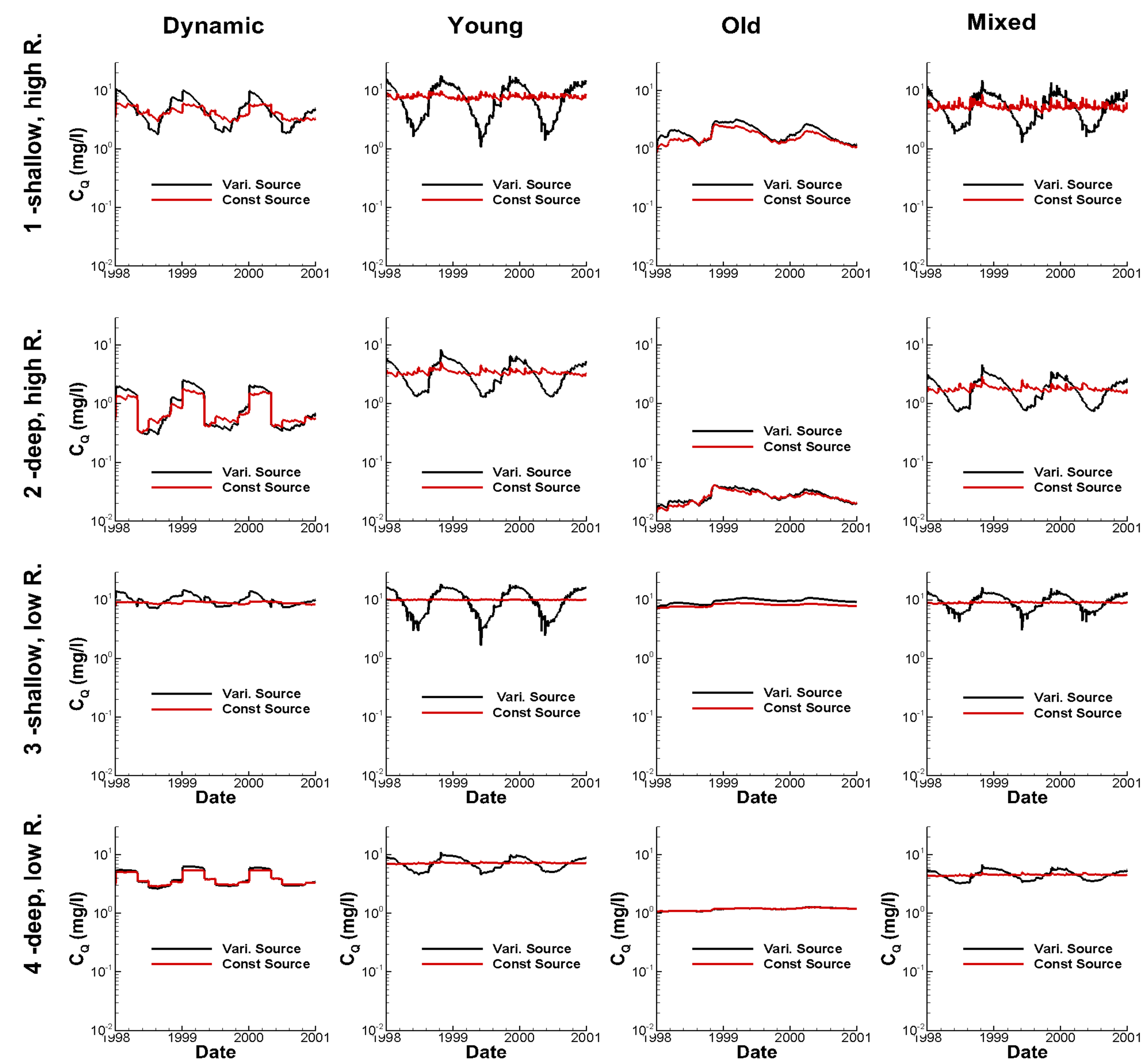
Summary statistics for the different models:

	PT-model	constant β	variable β
NSE (calibration)	0.70	0.76	0.82
NSE (validation)	0.37	0.14	0.26
Mass removal by reactions [kg/ha/year]	37.0	34.7	34.8
Mass export by discharge [kg/ha/year]	11.5	12.9	13.0
Half-life time reaction [days]	126.1	79.6	84.1
Mean T_Q [days]	296.9	122.3	219.6
Mean T_{ET} [days]	288.3	143.4	247.7

- Model fits and mass balances similar between models
- Reaction rates and mean ages of Q and ET quite different
- Constant β-model produces younger mean Q and ET
- Variable β-model reproduces seasonal shifts in selection preference well

8 Scenario simulations – different catchment types

Differing in: age preference (**AP**), reactivity (**R**), aquifer depth (**AD**), source variability (**SV**)*



9 Conclusions – „take home messages"

- Observed NO_3-concentrations in Q reasonably reproduced by SAS-models
- Modeling suggests denitrification as a significant mass removal process
- Seasonal shifts in SAS-functions needed to match water ages from PT-model
- Interplay between AP, R, AD and SV*(8) controls saisonal NO_3-variability in Q
- NO_3-concentrations in Q alone may not fully constrain SAS-based inverse model

References:

Yang, Heidbuechel, Musolff, Reinstorf, Fleckenstein (2018) Exploring the Dynamics of Transit Times and Subsurface Mixing in a Small Agricultural Catchment, Water Resour Res, 54(3)

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