Supporting Information for "Effect of topographic slope on the export of nitrate in humid catchments"

Jie Yang[1], Ingo Heidbüchel[2,4], Chunhui Lu[1], Yueqing Xie[3], Andreas Musolff[2],

and Jan H. Fleckenstein[2,4]

Contents of this file

[1]State Key Laboratory of

Hydrology-Water Resources and Hydraulic

Engineering, Hohai University, Nanjing,

China

[2]Helmholtz-Zentrum für Umweltforschung

GmbH - UFZ, Department of Hydrogeology,

Leipzig, Germany

[3]School of Earth Sciences and

Engineering, University of Nanjing,

Nanjing, China

[4]Hydrologic Modeling Unit, Bayreuth

Center of Ecology and Environmental

Research (BayCEER), University of

Bayreuth, Bayreuth, Germany

1. Text S1

2. Figures S1-S3

Additional Supporting Information (Files uploaded separately)

1. Captions for Datasets S1 to S7

Introduction

The supporting information includes: Text S1, Figure S1-S3, Captions for Datasets S1-S7

Text S1. Numerical tracer experiments to calculate TTDs

To calculate the transit time distributions (TTDs) for Q and ET for the cross-sectional aquifers, numerical tracer experiments were performed with the numerical transport solution using the finite-element method in HydroGeoSphere. We assumed that inert tracers of uniform concentration existed in precipitation, therefore the fluxes of the tracers were applied to the land surface as a third-type (Cauchy) boundary condition for transport modeling. Tracer can exit the aquifer with outfluxes (Q and ET), neglecting the evapo-concentration effect associated with ET.

We considered a 200 years period for tracer experiments, which was sufficient to ensure convergence of computed residence/transit times. The 200 years were partitioned into 2400 periods of one-month intervals Δt. A different tracer was used for each of the periods resulting in a total of 2400 distinct tracers. The tracers were assumed to be injected at the beginning of their associated period t_0^i. The advective-dispersive multi-solutes transport was simulated using HydroGeoSphere. Longitudinal and transverse dispersivity values were 8 m and 0.8 m, respectively. The first 199 years of the simulation period were used as a spin-up phase. The last year was used for actual observation and computation

of TTDs. Because the climate (boundary) conditions were identical for each year, the transport simulation was actually performed only for the first 12 tracers (covering the course of year), based on which the results for the other 2388 tracers can be reproduced. In this way, the breakthrough curves for the mass fluxes of the tracers in Q, ET, and for the stored mass of the tracers in the aquifer were determined. For a specific time t, the TTD for Q (or ET) was computed by calculating the mass fraction of each tracer in Q (or ET), using:

$$p_{Q/ET}(T,t) = \frac{F^i(t)}{\Delta t \sum F^i(t)} \qquad (1)$$

where $F^i(t)$ is the mass flux of the tracer i in Q/ET at time t, $\sum F^i(t)$ is the sum of the mass flux of all tracers in Q/ET. T is the transit time that equals t - t_0^i for tracer i. Similarly, the age distribution of storage was computed by calculating the mass fraction of each tracer stored in the aquifer, using:

$$p_S(T,t) = \frac{M^i(t)}{\Delta t \sum M^i(t)} \qquad (2)$$

where $M^i(t)$ is the mass of the tracer i stored in the subsurface at time t, $\sum M^i(t)$ is the total mass of all tracer stored in the aquifer. Based on the TTDs, the (mean) age and young water fraction of the Q/ET can be calculated using:

$$T_{Q/ET}(t) = \int_0^\infty p_{Q/ET}(T,t)T dT \qquad (3)$$

$$YF_{Q/ET}(t) = \int_0^{90days} p_{Q/ET}(T,t)dT \qquad (4)$$

where $T_{Q/ET}(t)$ and $YF_{Q/ET}(t)$ are the age and young water fractions of Q (or ET), respectively. Note that both of them are time-variant and their temporal mean, e.g., annual mean values, can be further calculated.
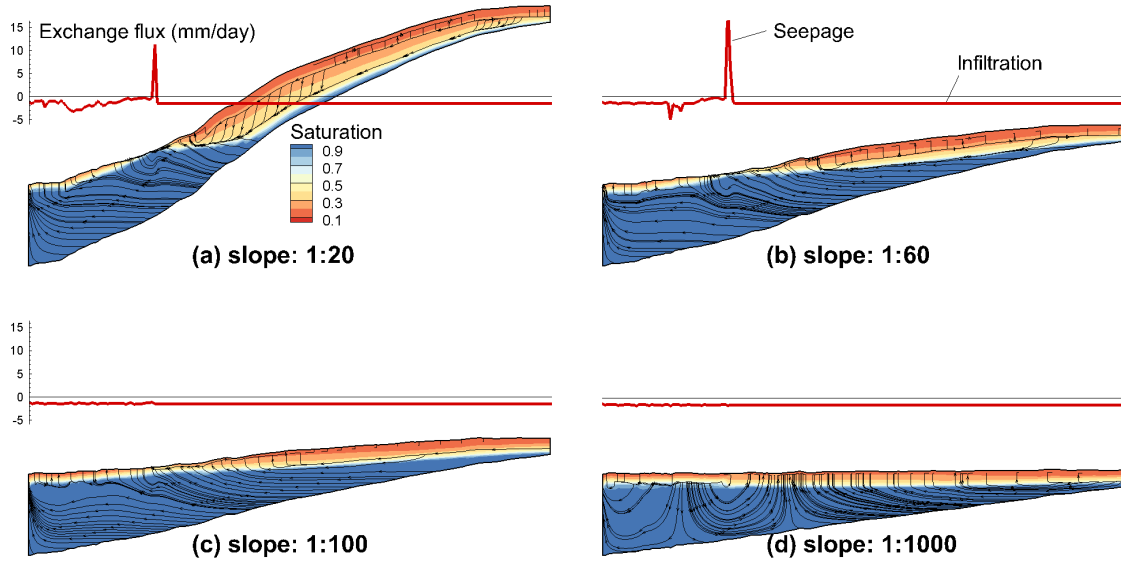

Figure S1. The distribution of saturation, flow paths, and exchange fluxes between surface and subsurface for the simulated cross-sections in the dry season, with topographic slope (a) 1:20, (b) 1:60, (c) 1:100, and (d) 1:1000. The black lines are the flow paths. The red curves describe exchange fluxes (along the cross-sectional profiles), positive values indicate seepage to the land surface and negative values indicate infiltration to the subsurface.
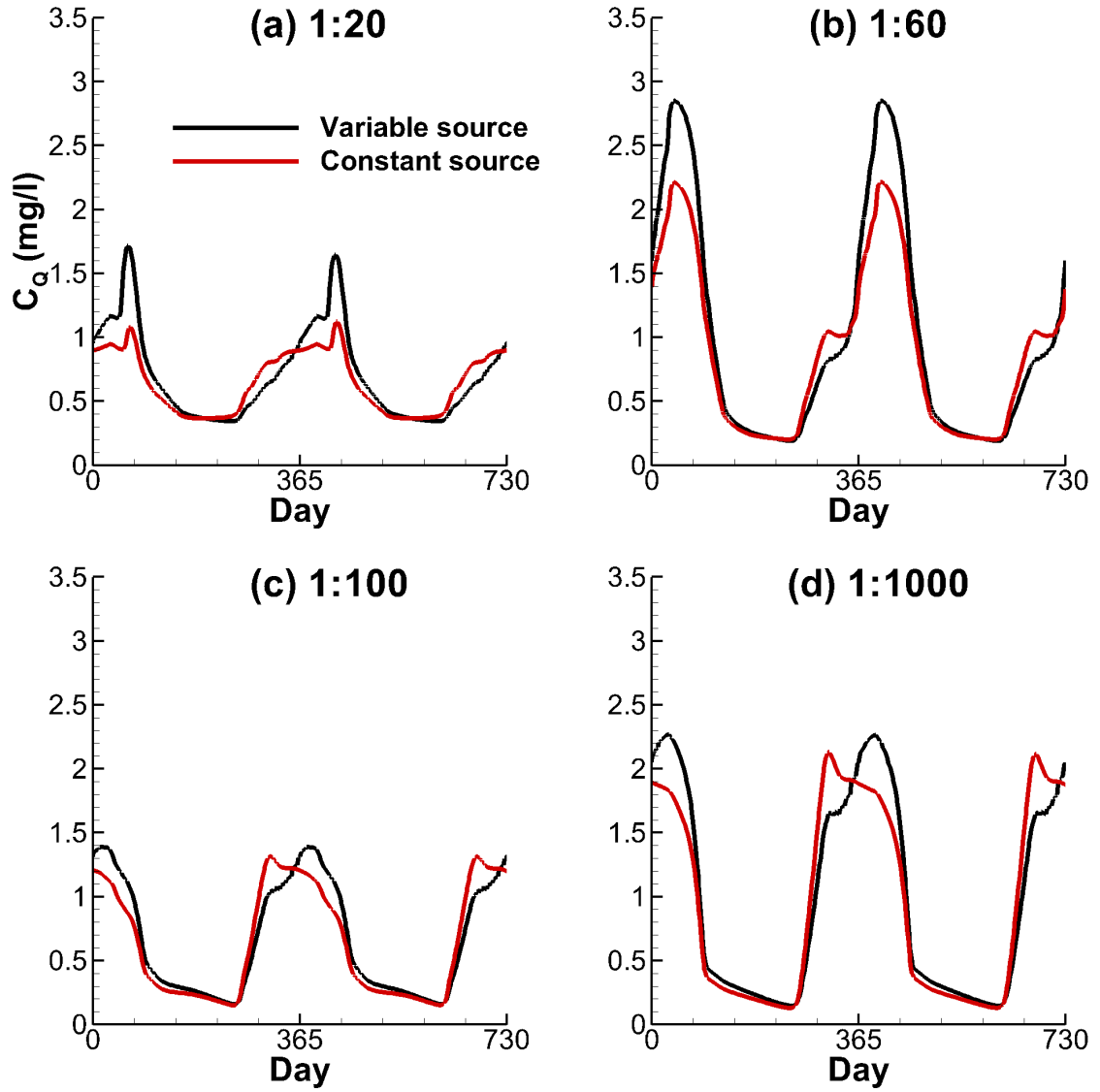
Figure S2. Simulated in-stream nitrate concentration C_Q for cross-sections with topographic slope (a) 1:20, (b) 1:60, (c) 1:100, and (d) 1:1000.
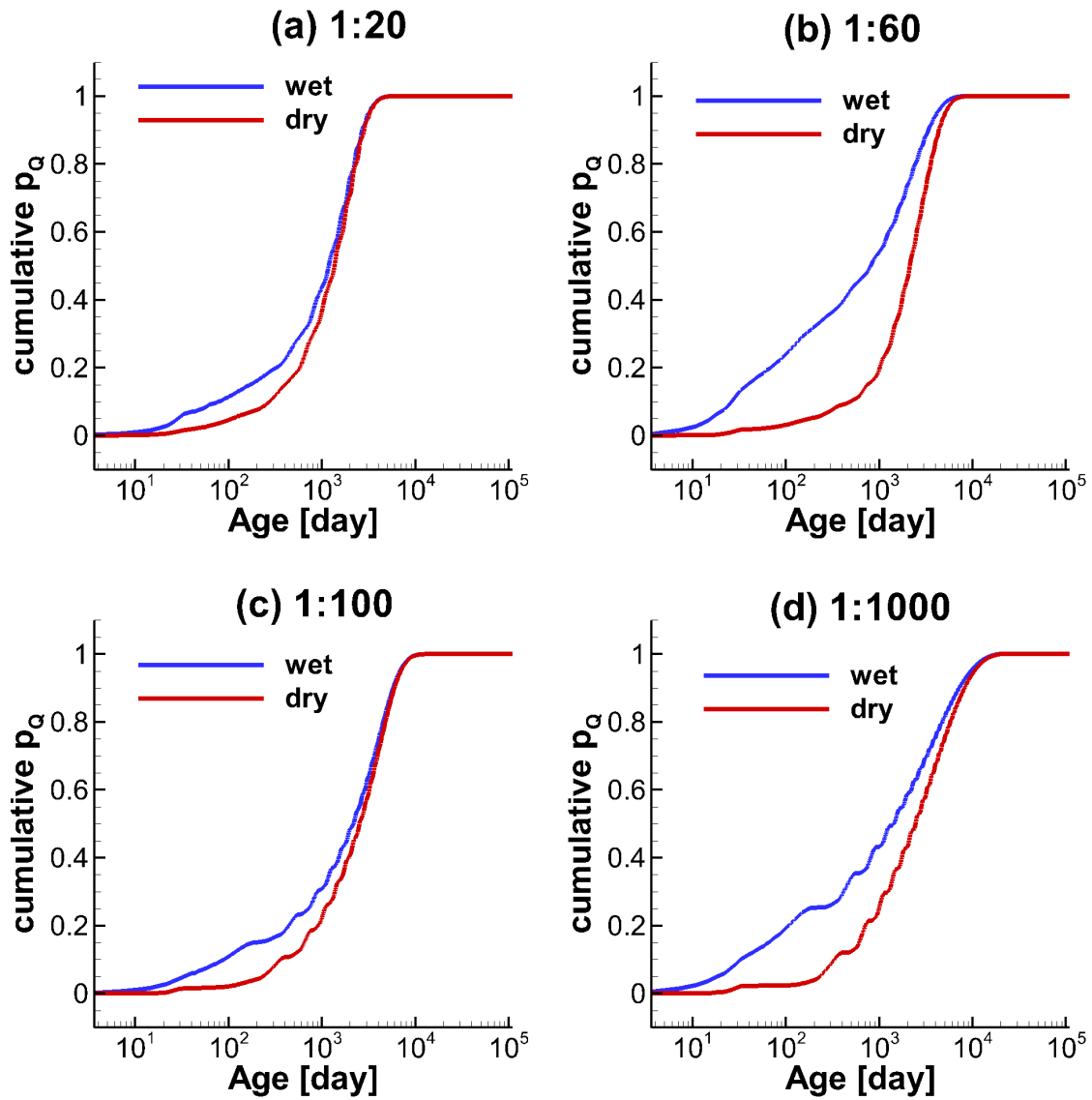
Figure S3.   The computed cumulative TTDs for Q during the wet season (February) and the dry season (September), for the cross-sections with topographic slope of (a) 1:20, (b) 1:60, (c) 1:100, and (d) 1:1000.

Data Set S1. Average precipitation for the year 2005.

Data Set S2. Daily potential ET for the year 2005, estimated by Yang et al. [2018].

Data Set S3. Monthly-averaged potential ET for the year 2005.

Data Set S4. Simulated Q, surface run-off, nitrate concentrations, water ages, young flow fractions using variable source concentrations for topographic slope 1:20 (Data for Figure 3). Data format is ready for Tecplot.

Data Set S5. Simulated variables (C_Q, T_Q, young flow fraction of Q, groundwater table depth, source contribution, and standard deviations) in response to various topographic slopes (Data for Figure 4 and 8). Data format is ready for Tecplot.

Data Set S6. The TTDs for Q in the wet period and dry period, for the cross-sections with topographic slope of (a) 1:20 (b) 1:60, (c) 1:100 and (d) 1:1000. Data format is ready for Tecplot.

Data Set S7. The model package with essential files (without HydroGeoSphere software) to reproduce the flow, transport and tracer experiments results for the cross-sectional aquifer with topographic slope 1:20. This data set is a ZIP file.