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Physically Constrained Storage Age Selection (SAS) Functions: Benchmarking SAS-based Simulations of Catchment Nitrate Export

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StorAge Selection (SAS) functions describe how catchments selectively remove water of different ages in storage via discharge, providing insights into subsurface flow paths and solute export behavior. SAS-based models have been used to study conservative and reactive solute exports and are typically calibrated against in-stream solute concentrations. However, as the simulated transit times in these models are not explicitly linked to physical processes, questions remain regarding the consistency of SAS-derived transit times with transit times derived from physically based model. To evaluate the validity of transit times obtained from SAS-based models such as the conceptual mHM-SAS model (Nguyen et al. 2021), we employ the 3D physically-based model HydroGeoSphere coupled with particle tracking. The physically based model coupled with particle tracking can explicitly simulate catchment water storage dynamics, spatial heterogeneity in subsurface flow and solute transport pathways, water ages, and transit time distributions (TTDs). We hypothesize that both modeling approaches are expected to reproduce comparable nitrate concentration dynamics and concentration–discharge relationships at the catchment outlet, but may differ in water age compositions due to conceptual differences between the models. Through this comparison, we can evaluate the capabilities and limitations of mHM-SAS model to simulate catchment-scale nitrate export and clarify the conditions under which the mHM-SAS model may be sufficient for rapid prediction of concentrations in heterogeneous agricultural catchments. Overall, this study demonstrates that particle-tracking-based SAS functions derived from a physically based model can provide a robust benchmark for evaluating the physical consistency of calibrated SAS-based models.

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