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Localisation of processes governing water quality in mesoscale catchments

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An important method to study water and solute fluxes in mesoscale catchments is the identification of dominant hydrological processes from catchment scale observations such as streamflow records of water quality. For an explicit spatial and temporal representation of these identified processes in catchment models, as a second step, one needs to analyse spatio-temporal patterns of these identified processes. While process identification including analysis of temporal dynamics is usually performed using, e.g., hydrograph separation via end member mixing analysis, detection of spatial patterns is typically missing. Consequently, the location of identified processes within a catchment and its relation with landscape properties such as soil, geology and landuse often remains poorly understood. In this study, monthly water samples of major cations and anions, and organic pollutants such as pesticides, pharmaceutics and polycyclic aromatic hydrocarbons from 12 streamflow sampling sites within a 170 km^2 catchment in SW Germany were analysed using principle component analysis. For principal component analysis, observed time series of water quality variables at different sampling site were expressed as a linear combination of a number of independent processes, i.e. a set of uncorrelated variables called principal components. First, four principle components (PC) were extracted that explained 92 % of the observed spatial and temporal variance of the observed solutes, with all measured variables being also well represented by these four PCs. These PCs were interpreted as dominant processes governing water quality using component loadings, which are correlations between PCs and the original observed water quality variables. In a second step, PC values for all records, i.e. projections of the observations in the four dimensional PC space that can be interpreted as process intensities, were correlated with landscape attributes such as landuse, soil and geology for a buffer area along the stream up to the particular sampling point. Using this analysis, we localized main processes governing water quality in the catchment, i.e. waste water effluents and mineral weathering, and associated landscape features.