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Extended principle component analysis - a useful tool to understand processes governing water quality at catchment scales

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Water quality of ground and surface waters in catchments is typically driven by many complex and interacting processes. While small scale processes are often studied in great detail, their relevance and interplay at catchment scales remain often poorly understood. For many catchments, extensive monitoring data on water quality have been collected for different purposes. These heterogeneous data sets contain valuable information on catchment scale processes but are rarely analysed using integrated methods. Principle component analysis (PCA) has previously been applied to this kind of data sets. However, a detailed analysis of scores, which are an important result of a PCA, is often missing. Mathematically, PCA expresses measured variables on water quality, e.g. nitrate concentrations, as linear combination of independent, not directly observable key processes. These computed key processes are represented by principle components. Their scores are interpretable as process intensities which vary in space and time. Subsequently, scores can be correlated with other key variables and catchment characteristics, such as water travel times and land use that were not considered in PCA. This detailed analysis of scores represents an extension of the commonly applied PCA which could considerably improve the understanding of processes governing water quality at catchment scales. In this study, we investigated the 170 km^2 Ammer catchment in SW Germany which is characterised by an above average proportion of agricultural (71%) and urban (17%) areas. The Ammer River is mainly fed by karstic springs. For PCA, we separately analysed concentrations from (a) surface waters of the Ammer River and its tributaries, (b) spring waters from the main aquifers and (c) deep groundwater from production wells. This analysis was extended by a detailed analysis of scores. We analysed measured concentrations on major ions and selected organic micropollutants. Additionally, redox-sensitive variables and environmental tracers indicating groundwater age were analysed for deep groundwater from production wells. For deep groundwater, we found that microbial turnover was stronger influenced by local availability of energy sources than by travel times of groundwater to the wells. Groundwater quality primarily reflected the input of pollutants determined by landuse, e.g. agrochemicals. We concluded that for water quality in the Ammer catchment, conservative mixing of waters with different origin is more important than reactive transport processes along the flow path.