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An uncertainty inclusive un-mixing model to identify tracer non-conservativeness

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Sediment fingerprinting is being increasingly recognised as an essential tool for catchment soil and water management. Selected physico-chemical properties (tracers) of soils and river sediments are used in a statistically-based 'un-mixing' model to apportion sediment delivered to the catchment outlet (target) to its upstream sediment sources. Development of uncertainty-inclusive approaches, taking into account uncertainties in the sampling, measurement and statistical un-mixing, are improving the robustness of results. However, methodological challenges remain including issues of particle size and organic matter selectivity and non-conservative behaviour of tracers – relating to biogeochemical transformations along the transport pathway. This study builds on our earlier uncertainty-inclusive approach (FR2000) to detect and assess the impact of tracer non-conservativeness using synthetic data before applying these lessons to new field data from Ireland.

Un-mixing was conducted on 'pristine' and 'corrupted' synthetic datasets containing three to fifty tracers (in the corrupted dataset one target tracer value was manually corrupted to replicate non-conservative behaviour). Additionally, a smaller corrupted dataset was un-mixed using a permutation version of the algorithm. Field data was collected in an 11 km2 river catchment in Ireland. Source samples were collected from topsoils, subsoils, channel banks, open field drains, damaged road verges and farm tracks. Target samples were collected using time integrated suspended sediment samplers at the catchment outlet at 6-12 week intervals from July 2012 to June 2013. Samples were dried (<40°C), sieved (125 μm) and analysed for mineral magnetic susceptibility, anhysteretic remanence and iso-thermal remanence, and geochemical elements Cd, Co, Cr, Cu, Mn, Ni, Pb and Zn (following microwave-assisted acid digestion). Discriminant analysis was used to reduce the number of tracer numbers before un-mixing.

Tracer non-conservativeness results showed that the predictions of median source contributions were negatively affected whereas uncertainty was only marginally impacted by the corrupted tracer. Improvement of uncertainty resulted from increasing the number of tracers in both the perfect and corrupted datasets. FR2000 was capable of detecting non-conservative tracer behaviour within the range of mean source values, therefore, it provided a more sensitive screening technique than assessing target values against source data. Non-conservative behaviour was identified in field data however only at a significant degree of corruption. Whilst further testing is required to determine the impact of individual and combined uncertainty components on synthetic, controlled experiments and field data, this study provides a framework for future assessment of uncertainty in un-mixing models.