Marie Skłodowska-Curie

Innovative Training Network

"HypoTRAIN"

Hyporheic Zone Processes – A training network for enhancing the understanding of complex physical, chemical and biological process interactions

Grant Agreement No. 641939

Deliverable D5.3

Model-based evaluation of joint datasets

Dissemination Level of Deliverable:

PU	Public	**X**
CO	Confidential, only for the members of the consortium (including the Commission Services)	

Model-based evaluation of joint datasets

In the course of the first HypoTRAIN joint field experiment (June 2016) at River Erpe, a reach-scale micropollutant attenuation study was implemented. Surface water samples were collected at three different stations downstream of the waste water treatment plant outflow covering a 4.7 km reach. The samples were analysed for a set of highly abundant and relevant micropollutants by a direct injection-ultra performance liquid chromatography tandem mass spectrometry method developed at Stockholm University (Posselt et al., *in preparation*). In addition Boron and other cations concentrations were measured by ICP-OES analysis serving as a conservative waste water-derived tracer for solute transport. Nitrate and sulfate were measured by ion chromatography. Electrical conductivity, water temperature and discharge were measured continuously at each station and precipitation, solar radiation and air temperature data were provided by a close-by weather station. Hence, a large dataset with high spatial and temporal resolution was derived including detailed analysis of the water samples and comprehensive measurement of background data. In a simplified hourly water parcel approach - using Boron as a reference compound - degradation rate constants were calculated (Jaeger and Posselt et al., *in preparation*). In a second step the one-dimensional transport with inflow and storage model (OTIS; Runkel, 2000) will be applied to the concentration time-series and estimated flow and reaction parameters will be compared to calculated ones. Additionally, water retention times along the river system were estimated using a non-parametric deconvolution of electrical conductivity records that were collected at high temporal resolution (5 minutes) at different sections.

In the second HypoTRAIN joint field experiment (June 2017) at the University of Birmingham a mesocosm-study on the drivers of micropollutant attenuation was conducted. In total, 24 recirculating flumes of different microbial diversity and different extent of hyporheic flow were injected with a set of micropollutants and their concentration was monitored during the course of three months. Background data, such as water and air temperature and solar radiation, water oxygen content and electrical conductivity were recorded. Microbial community composition was analyzed from sediment samples at different time points. A salt tracer was injected at the end of the experiment resulting in dilution curves that track different intensities of pore water-surface water exchange. Hence, also here a comprehensive dataset was derived enabling us to understand drivers and the fate of the target pollutants under semi-controlled conditions. Different models were applied to the dataset.

- The concentration curves were fitted to first-order kinetic functions to calculate the dissipation half-lives. A central composite face design was chosen as the experimental design to estimate the influence of the two variables microbial diversity and hyporheic exchange flow on the half-lives of the compounds. The half-lives were fitted to a second-order surface response model to estimate linear and non-linear effects of the variables.

- A mass balance model (Mutz et al., 2007) was used to calculate the hyporheic exchange flow in each single flume. The salt tracer dilution curve was fitted to the mass balance equation to derive the vertical flow rate. In addition exchange volume and the residence time was estimated.

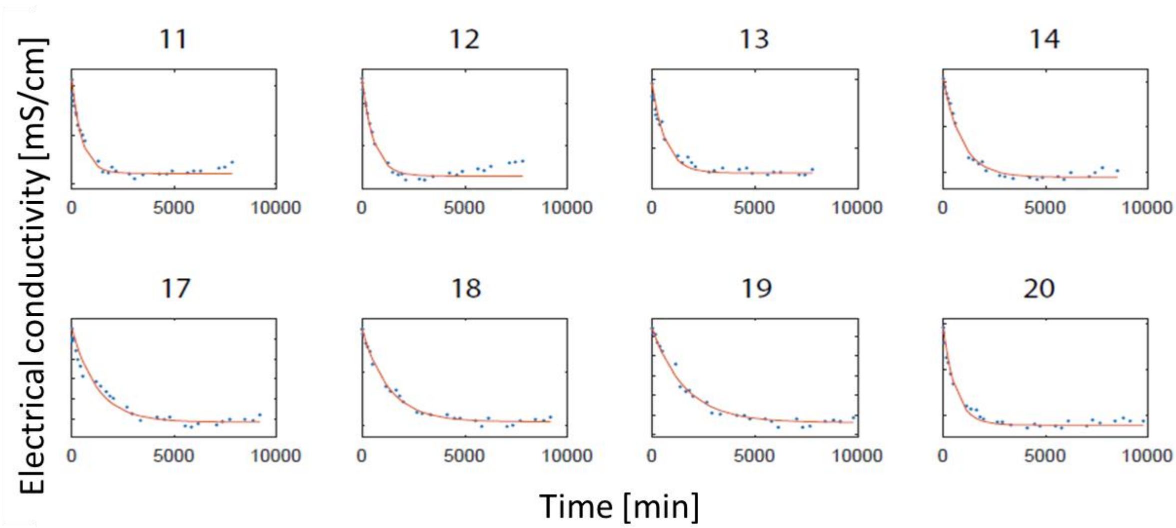

Figure 1. *Fitting salt tracer dilution curves of individual flumes (11-14 and 17-20) to a mass balance equation to obtain exchange flux, exchange volume and residence time.*

- Finally, various measurements and pore-water concentrations from a single ripple experiment, equipped with three pore water samplers along the flow paths were also simulated in a 2D homogeneous flow and transport model using COMSOL Multiphysics. Using this we derived the hyporheic exchange fluxes and residence time distribution within a single ripple. Moreover, we extended the model to study the transport of oxygen using Damkohler Number for different timescales of oxygen consumption. We also aim to model reactive transport of nutrients and micropollutants on a cm-scale to have an intricate understanding of hydrodynamic and transport characteristics of hyporheic zones in this mesocosm study.

References:

Mutz, M., Kalbus, E., Meinecke, S., 2007. Effect of instream wood on vertical water flux in low-energy sand bed flume experiments. Water Resour. Res., 43(10).

Runkel, R.L., 2000. Using OTIS to model solute transport in streams and rivers. USGS Fact Sheet: FS-138-99.