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

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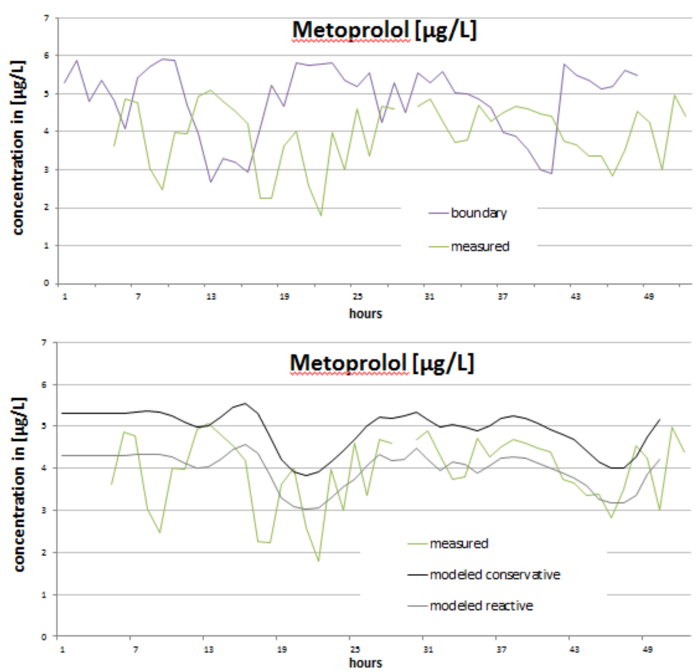
Integrated reactive transport models

Dissemination Level of Deliverable:

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

Integrated reactive transport models for the fate of micropollutants during the passage of the hyporheic zone

Excess nutrient and pharmaceuticals are significant concerns regarding drinking water pollutions and eutrophication of aquatic ecosystems. Hyporheic zones are recognized as a unique ecosystem providing vital functions (e.g. organic carbon oxidation, nitrification and denitrification) which might be related to the attenuation and degradation of organic micropollutants. In order to assess the fate of micropollutants in hyporheic zones, fully coupled physically based models which numerically describe how water, heat and reactive solute transport from stream to hyporheic zones under various flow conditions, bedform morphology and sediment properties are created. The models can be used to instruct field experiment design and also provide opportunities to identify processes that are unnoticed from field observations. The hydraulic component, which is the driver of all the transport processes, is numerically tested under different surface forcing and channel geomorphological conditions. Further, the heat transport is coupled to the flow model due to its important role on influencing hyporheic exchange rate by controlling pore water viscosity and density, as well as reaction rates in many of the biogeochemical reactions occurring in hyporheic zones. With all the major physical processes accounted, integrated reactive transport models can be used to predict the fate of micropollutants under various hydraulic and geomorphological conditions present in the complex natural systems.



Hydraulic parameters obtained from parameter estimation of the EC curves			Fixed
Main channel first-order decay coefficient	Λ [/s]	5.90E-6	Fitted
Storage zone first-order decay coefficient	ΛS [/s]	5.6E-6	Fitted
Residual sum of squares: 27.0; Residual standard deviation: 0.77			

Figure 1 *top: Time series of metropolol concentration at station 1 (purple) and 2 (green) on April 11-13th 2016. Bottom: “theoretical conservative concentration curve at station 2 calculated from transport parameters obtained from fitting electrical conductivity curves with OTIS (black). Fitting the theoretical conservative curve to the observed concentrations to obtain a first-order decay coefficient (grey).*

Micropollutant attenuation data obtained in the first HypoTRAIN joint field experiment at River Erpe in Berlin, Germany (Jaeger and Posselt et al. *in preparation*) were implemented in the OTIS model for one-dimensional transport with inflow and storage (Runkel, 2000). Intrinsic fluctuations in electrical conductivity caused by waste water treatment plant dynamics are used to trace the conservative solute transport and derive estimates for dispersion, travel times and transient storage parameters. In a second step, the transport parameters are applied to concentration time series of reactive micropollutants (eg. metoprolol, diclofenac, valsartan) and thus enabled the estimation of reaction parameters, such as first-order decay and sorption in the main channel and in the transient storage zone (Figure 1). The field investigations have been conducted in different sections and repeated in different seasons. The model was applied to all resulting datasets.

References:

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