

Analysis of temperature time series to estimate direction and magnitude of water fluxes in near-surface sediments

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The application of heat as a hydrological tracer has become a standard method for quantifying water fluxes between groundwater and surface water. Typically, time series of temperatures in the surface water and in the sediment are observed and are subsequently evaluated by a vertical 1D representation of heat transport by advection and dispersion. Several analytical solutions as well as their implementation into user-friendly software exist in order to estimate water fluxes from the observed temperatures. The underlying assumption of a stationary, one-dimensional vertical flow field is frequently violated in natural systems. Here subsurface water flow often has a significant horizontal component. We developed a methodology for identifying the geometry of the subsurface flow field based on the variations of diurnal temperature amplitudes with depths. For instance: Purely vertical heat transport is characterized by an exponential decline of temperature amplitudes with increasing depth. Pure horizontal flow would be indicated by a constant, depth independent vertical amplitude profile. The decline of temperature amplitudes with depths could be fitted by polynomials of different order whereby the best fit was defined by the highest Akaike Information Criterion. The stepwise model optimization and selection, evaluating the shape of vertical amplitude ratio profiles was used to determine the predominant subsurface flow field, which could be systematically categorized in purely vertical and horizontal (hyporheic, parafluvial) components.

Analytical solutions to estimate water fluxes from the observed temperatures are restricted to specific boundary conditions such as a sinusoidal upper temperature boundary. In contrast numerical solutions offer higher flexibility and can handle temperature data which is characterized by irregular variations such as storm-event induced temperature changes and thus cannot readily be incorporated in analytical solutions. There are several numerical models that simulate heat transport in porous media (e.g. VS2DH, HydroGeoSphere, FEFLOW) but there can be a steep learning curve to the modelling frameworks and may therefore not readily accessible to routinely infer water fluxes between groundwater and surface water. We developed a user-friendly, straightforward to use software to estimate water FLUXes Based On Temperatures- FLUX-BOT. FLUX-BOT is a numerical code written in MATLAB that calculates time variable vertical water fluxes in saturated sediments based on the inversion of measured temperature time series observed at multiple depths. It applies a cell-centered Crank-Nicolson implicit finite difference scheme to solve the one-dimensional heat advection-conduction equation (FLUX-BOT can be downloaded from the following web site: <https://bitbucket.org/flux-bot/flux-bot>). We provide applications of FLUX-BOT to generic as well as to measured temperature data to demonstrate its performance.

Both, the empirical analysis of temperature amplitudes as well as the numerical inversion of measured temperature time series to estimate the vertical magnitude of water fluxes extend the suite of current heat tracing methods and may provide insight into temperature data from an additional perspective.