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

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1 Estimation of vertical water fluxes (FLUX-BOT)

The application of heat as a hydrological tracer has become a standard method for quantifying water fluxes between groundwater and surface water. Here, we present a new computer code (FLUX-BOT) that was developed to estimate vertical water fluxes from measured temperature profiles. Flexibility in the temperature boundary conditions allows for better representation of measured temperatures and enables the direct use of all natural temperature condition without the need of any data pre-processing (e.g. curve fitting, frequency analysis).

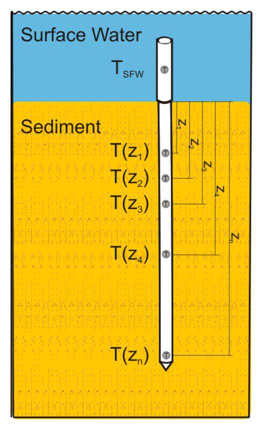
Method:

FLUX-BOT uses a numerical solver of the one dimensional conduction equation. The program automates the entire workflow to calculate vertical water fluxes from raw temperature time series and, thus, provides a handy and flexible tool to allow analysis of transient vertical exchange fluxes in saturated porous media.The automated time-varying functionality of FLUX-BOT (24 hours windows or greater) and the automated uncertainty assessment are features not available in established one-dimensional numerical models [1].

Code availability:

FLUX-BOT is distributed as open source code. The most up to date version can be downloaded from the following web site: **https://bitbucket.org/flux-bot/flux-bot.**

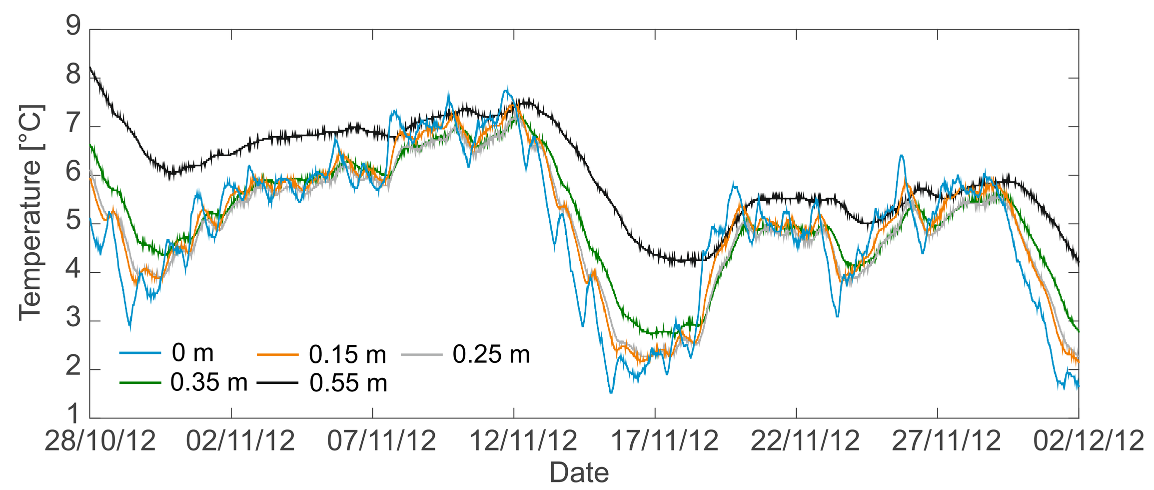
Temperature probe setup and data structure:



Time	0	z_1	z_2	z_3	z_4	....	z_n
t_1	$T_{SFW}(t_1)$	$T(z_1,t_1)$	$T(z_2,t_1)$	$T(z_3,t_1)$	$T(z_4,t_1)$	....	$T(z_n,t_1)$
t_2	$T_{SFW}(t_2)$	$T(z_1,t_2)$	$T(z_2,t_2)$	$T(z_3,t_2)$	$T(z_4,t_2)$	....	$T(z_n,t_2)$
....	....	....	....	....	....	....	....
t_m	$T_{SFW}(t_m)$	$T(z_1,t_m)$	$T(z_2,t_m)$	$T(z_3,t_m)$	$T(z_4,t_m)$	....	$T(z_n,t_m)$

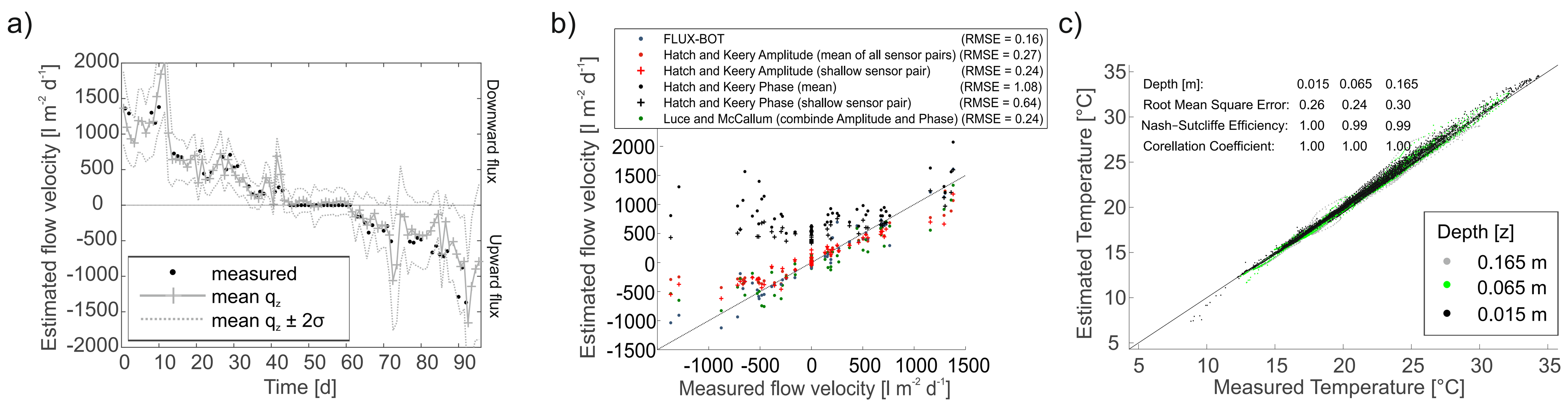
e.g.:

Time	0	0.15	0.20	0.25	0.35	0.55
01.01.2011 00:00:00	15.71	16.22	16.05	16.05	15.95	15.88
01.01.2011 00:10:00	...	...	...	...	...	...



FLUX-BOT requires at least three temperature timeseries measured in a vertical profile and estimations of the thermal diffussivity of the saturated sediment

Application and verification (sand box experiment under controlled hydrological conditions [2]):



- **Accurate estimates of vertical water fluxes (a, b)**
- **Time variable vertical flux estimates for long time series and a wide range of temperature boundary condition**
- **The goodness of fit can be derived immediately by comparing measured and modeled temperatures (c)**

2 Investigation of horizontal flux direction

Characterizing the flow conditions in the streambed can be challenging because of the complex, multi-dimensional flow patterns driven by time variable vertical hydraulic gradients and groundwater discharge. The identification of horizontal flow paths is essential to identify hyporheic exchange processes at the interface between river and groundwater Here, we present a methodology to analyse the geometry of subsurface water flux using vertical temperature profiles. The approach relies on changes in daily temperature amplitude between subsurface temperature sensors.Beyond the one-dimensional vertical exchange flow, major flow patterns could be identified and systematically categorised in purely vertical and horizontal (hyporheic, parafluvial) components.

Method:

Stationary and vertical (1D) heat transport:

$$A_z(t) = A_0(t) \times e^{-a_1 z}; \rightarrow \ln(A_z(t)/A_0(t)) = -a_1 z; \; a_1 = f(q;\lambda;P); \; M > 0$$

Non stationary two dimensional heat transport [3]:

$$p(z) = \ln(A_z(t)/A_0(t)) = a_0 - a_1 z + a_2 z^2 + a_3 z^3 + \ldots \quad a_n z^{\bar{o}}$$

A_0: Amplitude of daily temperature oscillation at the river bottom (°C)
A_z: Amplitude of the corresponding Temperature oscillation at depth z (°C)
q: Flow velocity (l m^{-2} d^{-1})
λ: Thermal diffusivity (m^2 s^{-1})
P: Period of the temperature oscillation

Results:

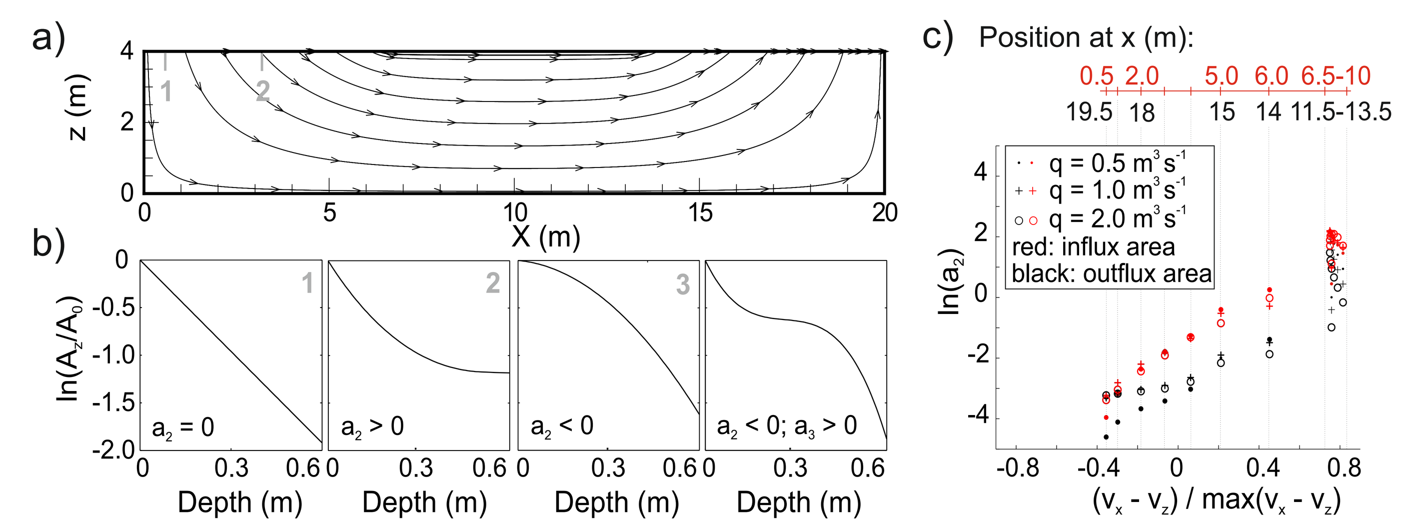


Figure: (a) Flow vectors idealising hyporheic exchange. Exchange flux range from vertically (v_z) dominated subsurface flow at the left hand side to horizontally (v_x) dominated subsurface flow at the centre of the domain; e.g. the horizontal flow component increases from the left to the centre of the domain;
(b) Simulated amplitude ratio profiles for flow field and positions shown in (a);
(c) Relation between dominant flow direction and polynomial coefficient a_2

- **Deviation from stationary 1D heat transport result in non-linearity in $\ln(A_z/A_0)$**
- **Non-linearity in $\ln(A_z/A_0)$ can be described by higher order polynomials**
- **Polynomial parameter a_2 is independent of the magnitude of the exchange flux and the sediment thermal properties, and captures the normalised difference between horizontal and vertical flux**

Application:

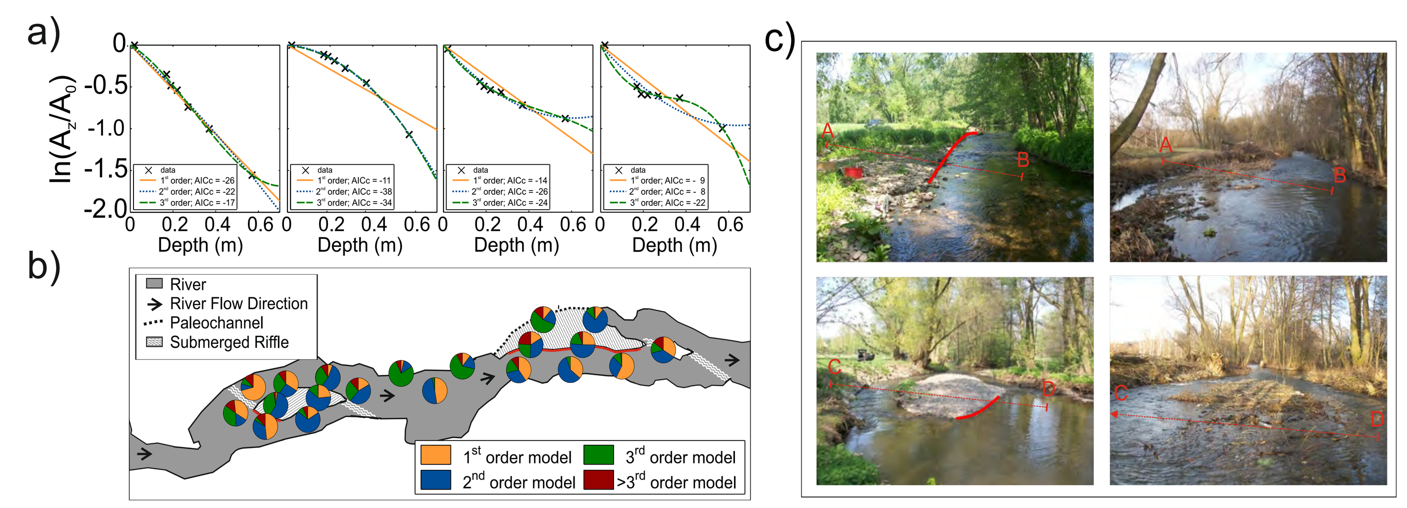


Figure: (a) Experimental amplitude ratio profiles, fitted model set and corres-ponding performance measures;
(b) Schematic showing relative freq-uency of best supported model for the entire observation period from June 2011 until July 2013 in a losing reach of a gravel bed river (Selke). Position of the pie diagrams correspond to the measurement location;
(c) Photographs of the point bar (top) and the in-stream gravel bar (bottom) during low ($q = 0.25$ m^3 s^{-1}, left) and high ($q = 3.60$ m^3 s^{-1}, right) river discharges.

- **Polynomials (p(z)) of 1st to 3rd order are clearly identified as best supported model concerning model residuals and model complexity**
- **River groundwater exchange flux at the head, crest and tail of the geomorphological structure is characterized by a strong horizontal advective component**

References: 1] Munz, M., Oswald, S. E., and Schmidt, C. (2011): Sand box experiments to evaluate the influence of subsurface temperature probe design on temperature based water flux calculation, Hydrol Earth Syst Sc, 15, 3495-3510, 2011.
2] Munz, M., and Schmidt, C. (2017): Estimation of vertical water fluxes from temperature time series by the inverse numerical computer program FLUX-BOT. Hydrol. Process., doi: 10.1002/hyp.11198.
3] Munz, M., Oswald, S. E., and Schmidt, C. (2016): Analysis of riverbed temperatures to determine the geometry of subsurface water flow around in-stream geomorphological structures, J Hydrol, 539, 74-87, 2016.

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