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Delineating Groundwater-Surface Water Exchange Flux Using Temperature-Time Series Analysis Methods

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ABSTRACT: Groundwater-surface water interactions can play a crucial role in river-, riparian and wetland management. Their delineation and quantification at various spatial and temporal scales has become an important aspect in the study of contaminant transport and attenuation processes at the groundwater-surface water interface. One of the main parameters of interest is the groundwater-surface water exchange flux, which provides indications regarding stream-aquifer connectivity, the local flow regime as well as hydrogeological properties of the streambed. One of the methods to assess vertical exchange flux is through the analysis of temperature time-series. In this paper we delineate vertical exchange flux from temperature-time series collected at a Belgian River by comparing established numerical and analytical techniques with a novel approach. Results indicate a spatial variability of vertical fluxes over two orders of magnitude at the site.

INTRODUCTION

Over the last two decades the study of groundwater-surface water interaction has become increasingly popular. One major interest has been the delineation and quantification of exchange flux between aquifers and rivers. This information can be used to investigate the hyporheic flow regime (Buss et al., 2009) or assess the behavior of contaminant plumes within the hyporheic zone (Conant et al., 2004), i.e. the saturated transition zone between surface water and groundwater compartments that develops its specific physical and biogeochemical characteristics from active mixing of waters from both compartments (Krause et al., 2009).
Magnitude and direction of exchange flow are influenced by a variety of factors such as river-aquifer connectivity, i.e. gaining, losing or disconnected (Woessner, 2000), streambed morphology, stream channel planform and geometry, hydraulic properties of aquifer and streambed sediments, climatic conditions as well as anthropogenic factors such as near stream pumping or land use. These factors can interact on three distinct scales, the (i) the sediment scale, (ii) the reach scale and (iii) the catchment scale and are able to create a heterogeneous subsurface causing temporal and spatial variability in exchange flows.
Total exchange flow can commonly be divided into hyporheic exchange flow (HEF), i.e. stream water entering the hyporheic zone somewhere upstream and leaving it at some point downstream, and groundwater-surface water exchange flow, i.e. flow across the hyporheic zone (Hannah et al., 2009). In general, a separation of both flow types is difficult as this would usually require a hydraulic characterization of the subsurface and subsequent modeling so detailed that it is beyond the scope of most scientific studies. So far most studies consider vertical exchange flux (VEF) as a good substitute for groundwater-surface water exchange flux, especially in gaining/losing rivers with low horizontal intrabed velocities.
Exchange fluxes can be quantified in the field directly by seepage meter measurements (Rosenberry and LaBaugh, 2008) or indirectly by applying heat as a tracer (Anderson, 2005) and measuring temperatures within the riverbed (Essaid et al., 2008). In this study we use heat as a tracer to quantify the VEF at the Slootbeek, a small Belgian river. To estimate fluxes we make use of a newly developed method called LPML used to extract the frequency information contained in collected temperature-time series data. For one location we compare results obtained with the LPML to those obtained with established models as well as with seepage meter measurements. Afterwards we look at the spatial variability in vertical exchange flux and discuss future research possibilities.

METHODOLOGY

Study Site

Fieldwork was carried out at a small stretch of the Slootbeek, a category three lowland river and tributary to the Aa in Northern Flanders, Belgium, which is part of the Nete catchment (Fig. 1). At the study site, the Slootbeek riverbed comprised a mixture of gravel and sand near locations ML169 and ML193, while at the other locations indicated in Fig. 1 a larger part of the riverbed was formed by organic matter. Average channel width was 3.20 m and average flow velocity in the middle of the river amounted to 0.2 ms^{-1}. River stage ranged during the observation period from 0.15 m to 0.95 m due to climate influences as well as land use and irrigation practices on the nearby fields. Average discharge could roughly be estimated as 0.4 m^3s^{-1}. The local aquifer is described by Anibas et al. (2011) as consisting of heterogeneous sand layers with local clay inclusions. The lower boundary is formed by the Boom clay aquitard at about 80 m below surface where the Slootbeek flows into the Aa River. Aquifer hydraulic conductivities vary locally but average at 10 md^{-1}.

Field Work

Seven multilevel temperature measuring devices (sticks) from UIT, Germany, were installed at locations indicated in Fig. 1. These sticks consisted of polyoxymethylene, in which several stainless steel temperature sensors were embedded. In our study we used a sensor configuration according to Fig. 2C to record temperatures in 10 minute intervals over several months during 2012. River stage was monitored with a cera mini diver from Schlumberger. Additionally, two piezometers were installed into the riverbed and equipped with mini divers to record temperatures and pressures as shown in Fig. 2A. Groundwater temperature and level (around 1 m below surface) were monitored at the right riverbank. Vertical fluxes were also directly measured by means of three seepage meters (Fig. 1 and 2B) that were self-made based on discussions in Rosenberry (2008). Seepage meter measurements took place over several days.

Modeling

The general heat transport equation is often solved together with fluid flow (and contaminant transport) using complex physics-based coupled numerical models such as Hydrogeosphere (Therrien et al., 2010). These models can optimize hydraulic and thermal properties of the subsurface and represent complex fluid flow and heat transport patterns. A much simpler method is the quantification of the vertical exchange flux component only, assuming simultaneous vertical 1D non-isothermal advective-dispersive heat transport through a homogeneous saturated medium (Stallman, 1965), which can be represented by the following partial differential equation (PDE):

$$\frac{\partial T}{\partial t} = \frac{\kappa}{\rho c}\frac{\partial^2 T}{\partial z^2} - q_z\frac{\rho_w c_w}{\rho c}\frac{\partial T}{\partial z} \quad (1)$$

T [Θ] represents the temperature of the subsurface dependent on position z and varying over time t [T], q_z [LT^{-1}] is the specific discharge or flux along the z-direction, c_w and c [$L^2T^{-2}\Theta^{-1}$] are the specific heat of the fluid and the fluid-rock matrix, respectively, while ρ and ρ_w [ML^{-3}] represent the density of the respective fluid-rock matrix and the fluid. Whereas variations in ρ_w and c_w in most hydrological settings can be considered negligible, ρc as the bulk volumetric heat capacity of the fluid-rock matrix strongly depends on sediment characteristics. D [L^2T^{-1}] denotes the effective thermal diffusivity (Rau et al., 2012b) and is in most literature sources described by

$$D = \frac{\kappa}{\rho c} + \psi|q_z| \quad (2)$$

with κ [$M^1L^1T^{-3}\Theta^{-1}$] as the bulk thermal conductivity representing the combined thermal conductivity of fluid and solid. The parameter ψ [L] is the thermal dispersivity and its importance for the determination of D is subject to on-going scientific debate (see e.g. Anderson, 2005; Rau et al., 2012a). Its influence definitely increases with increasing exchange fluxes. In this study we considered it negligible. Analytical solutions to (1) have been developed e.g. in Schmidt et al. (2007) for thermal steady-state conditions as well as in Hatch et al.(2006), Keery et al. (2007) or Onderka et al. (2013) for transient conditions. Some of these have been integrated into automated software routines such as Ex-Stream (Swanson and Cardenas, 2011) or VFLUX (Gordon et al., 2012).

In our study we modeled temperature measurements taken over a 90-day period (17 February – 16 May 2012) using the frequency response contained in the temperature data considering the sensor on top of the riverbed (Fig. 2C red circle) as the input signal that is (non)-linearly transported through the porous medium. For that we use the LPML, a newly developed method (Vandersteen et al., in preparation) that first determines the frequency responses using a local polynomial method, followed by a dedicate Maximum Likelihood estimator. Equation 1 can be re-written as the following PDE where the different parameters α, β and γ are constant.

$$\frac{\partial^2 T}{\partial z^2} + \alpha \frac{\partial T}{\partial z} + \beta T + \gamma \frac{\partial T}{\partial t} = 0 \qquad (3)$$

The response of the system to a steady-state periodic excitation $T\,(0,t) = \Re(e^{j\omega t})$ can be represented as $T(z,t) = \Re(G(z,\omega)e^{j\omega t})$ with $G(z,\omega)$ as the frequency response from the input at the upper boundary. This frequency response function is extracted applying a local polynomial method (Pintelon et al., 2010) that uses the randomness of the input data and the spectral smoothness of the transient part $Tr(\omega)$ to separate $G(\omega)$, $Tr(\omega)$and the additive circular-complex normal noise. Applying a local polynomial method provides us with $G(\omega)$ and its uncertainty $\sigma_G^2(\omega)$, which allows for the development of an output error model that is equivalent to a Maximum-Likelihood estimator. Maximum Likelihood estimates are be obtained using nonlinear least squares minimization techniques such as Gauss-Newton or Levenberg-Marquardt optimization methods (Fletcher, 1980). As such, parameters α, β and γ in (3) can be optimized and their uncertainties can be determined. Combining equations 1-3, vertical exchange flux and thermal conductivity can then be deduced using $\hat{q}_z = \frac{\hat{\alpha}}{\hat{\gamma}} \frac{\rho c}{\rho_w c_w}$ (4) and $\hat{\kappa} \leftrightarrow -\frac{c\rho}{\hat{\gamma}}$ (5).

The LPML was implemented in MATLAB 2011b® (The MathWorks, Inc., Natick, Massachusetts, USA) and its applicability to solve (1) and provide meaningful flux estimates was tested on data from all seven locations shown in Fig. 1. For location ML169 we also compared fluxes obtained by using the LPML to those obtained with VFLUX applying the method after Keery et al. (2007) and using only information from sensors two (on top of riverbed) and eight (lowest), as the latter method cannot incorporate information from more sensors simultaneously. Also, LPML results were compared to estimates obtained with the modeling software STRIVE (Anibas et al., 2009; Soetaert et al., 2002) that contains both a numerical solver after Lapham (1989) and an analytical solver after Stallman (1965).

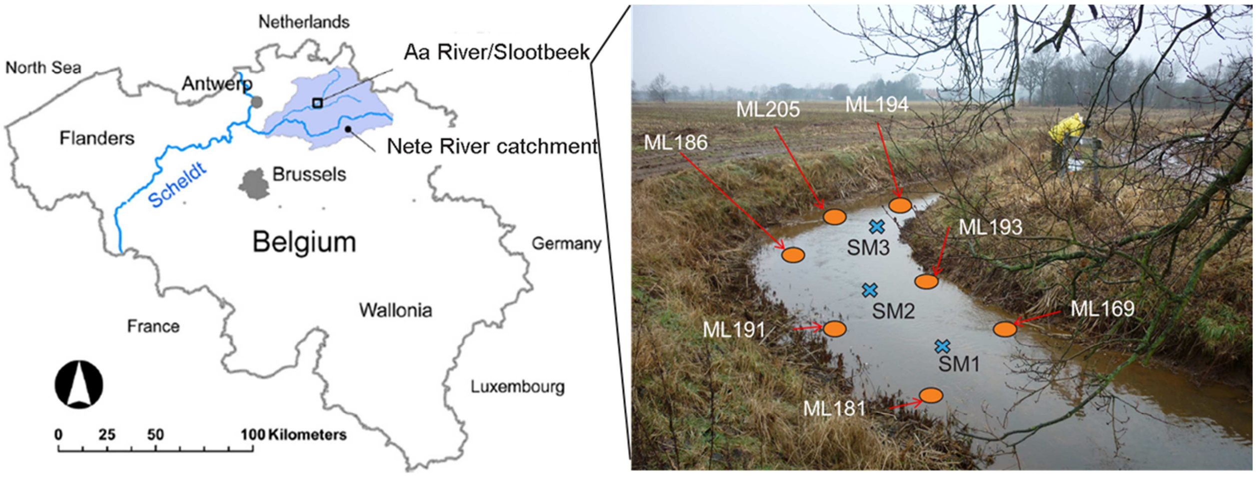

Figure 1: Slootbeek field site near Aa River. Right side roughly shows locations of temperature sensors (ML) and seepage meters (SM). At locations SM1 and SM3 piezometers as shown in Figure 2B were also installed. Left side was adapted after Anibas et al., 2011.

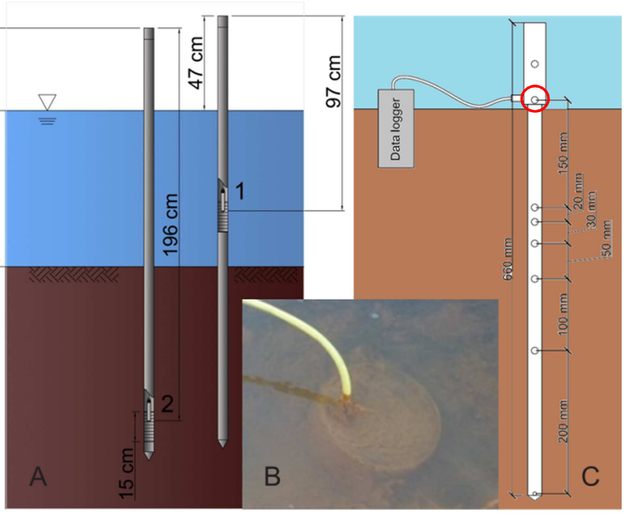

Figure 2A: Piezometer installed at location SM1. Location SM3 was equipped with a similar one. 2B: Picture of one of the self-made seepage meters used. 2C: Sensor configuration used for this study. Red circle indicates reference sensor on top of riverbed.

RESULTS

Riverbed temperatures ranged from 6.4°C to 15.4°C over the 90-day period and all ML measurement locations. Average temperatures at ML194 and ML205 are about 1°C above those of other locations. For all locations time-series profiles are similar to that of ML169 (Fig. 3), with highly fluctuating surface water temperatures and decreasing temperature fluctuations with increasing riverbed depth. Using the ML169 temperature time-series data we calculated vertical exchange fluxes with the LPML and compared them to estimates obtained with STRIVE and VFLUX (Table 1). When using the information of all sensors simultaneously results obtained with the LPML (-52.3 mmd-1)are of the same order of magnitude as those obtained with STRIVE. However, if only information from sensors two and eight is used the flux estimated with LPML is reduced to only -2.9 mmd^{-1} while VFLUX even provides a small positive flux indicating losing conditions.

Additionally, the LPML was used to estimate fluxes for all other ML locations and results were compared to direct flux measurements by seepage meters (Table 2). As can be seen, fluxes estimated with the LPML vary from -19.4 mmd^{-1} for location ML193 to -648.5 mmd^{-1} for location ML186. For all flux estimations in this study thermal conductivity was fixed to κ = 1.8 Wm^{-1}K^{-1} and volumetric heat capacities were chosen as ρc = 2.90 x 10^{6} Jm^{-3}K^{-1} and $\rho_w c_w$ = 4.2 x 10^{6} Jm^{-3}K^{-1}. Results of seepage meter measurements also vary by one order of magnitude with location SM1 showing the smallest fluxes and similar values as obtained with the LPML at nearby locations ML 169, ML181 and ML193. In general, flux estimates from seepage meters and those applying the LPML are in good agreement. LPML results also indicate less groundwater inflow into the river at its right bank (ML169, ML193, ML194) than at its left bank (ML181, ML186, ML191, ML205).

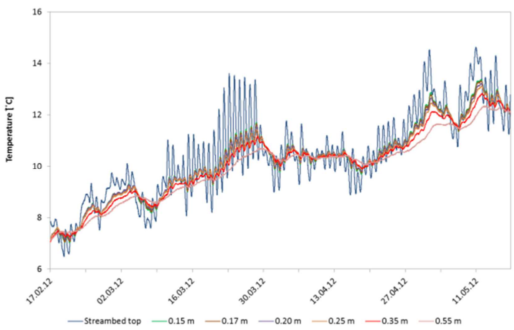

Figure 3: Temperature time series for location ML169 at various depths.

Table 1. Flux estimates for location ML169 using different models.

Parameter	Unit	STRIVE (numerical)	STRIVE (analytical)	VFLUX[b]	LPML[c]	LPML[c] stdev
q_z[a]	mmd^{-1}	-23.3	-35.9	17.8	-52.3/-2.2	0.86/1.67

[a]Negative sign = flow from aquifer to river

[b]Solution after Keery et al., 2007 used.

[c]First value represents flux estimate with all 7 sensors used, second value with sensors 1 and 7 only to compare it to VFLUX estimate.

Table 2. Vertical exchange flux calculated for several locations at Slootbeek.

Location	q_z[a] mm d^{-1}	Method
169	-52.3	LPML
181	-174.4	LPML
186	-648.3	LPML
191	-164.6	LPML
193	-19.3	LPML
194	-24.1	LPML
205	-276.5	LPML
SM1	-31.4	Direct
SM2	-378.5	Direct
SM3	-656.5	Direct

[a]κ was fixed to 1.8 $Wm^{-1}K^{-1}$ while q_z was optimized

DISCUSSION

Measured riverbed temperatures at the Slootbeek vary by location and depth. In general, advective and diffusive processes act simultaneously, causing differences in signal penetration depth depending on the upper boundary temperature at the riverbed top. Although measurements were taken during winter and early spring time with no in-channel vegetation and little plant coverage along the river bank, thus avoiding local shade effects and lower T at the riverbed top, average temperatures vary by almost 2°C. These variations could have been caused by locally increased amounts of upwelling groundwater with warmer temperature or by heterogeneous riverbed sediments (sand and gravel, sandy loam, varying organic matter content) and riverbed morphology that bring about variations in heat transport parameters and determine sediment scale water movement (hydraulic conductivity, flow velocity).
Considering temperature data of the entire 90-day period, averaged exchange fluxes estimated with the LPML indicate a gaining stream, as do seepage meter measurements where seepage was collected in plastic bags over 20-30 min intervals and several days. However, additional investigations on the same data shown in Vandersteen et al. (in preparation) indicate alternating gaining and losing periods depending on the location and length of the data set used.
Furthermore, fluxes estimated with the LPML in this study are limited in the sense that they were obtained while thermal conductivity was constrained to κ = 1.8 $Wm^{-1}K^{-1}$. This value is generally representative for sandy soils (Stonestrom and Constantz, 2003) but especially at locations near SM3 a higher organic matter content was encountered that due to its often high porosity shows a higher volumetric heat capacity and thus a lower thermal conductivity. In Vandersteen et al. (in preparation) this issue is further addressed and the LPML is applied to estimate vertical exchange flux and thermal conductivity simultaneously. In general, flux estimates obtained with the LPML

coincide well with estimates obtained by other models. However, it has to be pointed out that flux estimates are dependent on the number of sensors used. This fact could lead to contradicting results as is the case with the LPML and VFLUX only using information from two sensors that alternatively show gaining or losing conditions albeit magnitudes of fluxes are close to zero. A larger number of sensors seems to improve estimates as uncertainties are reduced and flux results are closer to those obtained with seepage meters. Compared to transient methods that use only data with the frequency of one day and apply the amplitude ratios and phase shifts between two temperature sensors (Hatch et al., 2006; Keery et al., 2007) the LPML has the following advantages:

(i) It can make use of data from multiple frequencies and multiple sensors simultaneously.
(ii) The input signal can be non-linear or non-sinusoidal
(iii) The method provides uncertainties on the model as well as on the optimized parameters, using statistically-based Maximum-Likelihood modeling techniques without applying elaborate post-processing procedures (Shanafield et al., 2011).
(iv) LPML allows for a simultaneous optimization of fluxes and thermal conductivity under certain cases as discussed in Vandersteen et al. (in preparation).
(v) Computational efforts are minimal and the method is easy to use.

CONCLUSIONS AND FUTURE RESEARCH

In this work we calculated vertical exchange fluxes between a small reach of the Slootbeek and its connected aquifer using temperature time series using LPML. This method is a novel approach that makes use of the frequency response of the entire system to a known (non)-linear input signal at the riverbed top using a local polynomial functional model and a maximum likelihood estimator. For location ML169 fluxes estimates obtained with the LPML were compared to those obtained by other models and showed a good agreement. Estimates at six additional locations (Figure 1) show a spatial variability in fluxes ranging over two orders of magnitude on a scale of less than 50 m.
Future research will focus on estimating fluxes over different volumes (e.g. between sensors 1 and 2 or 1 and 3, etc.) at each location by assigning upper and lower boundary conditions. Additional temperature data can also shed more light on the temporal variability of fluxes in winter/spring and spring/summer periods.

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