XXXVIII IAH Congress

Groundwater Quality Sustainability Krakow, 12–17 September 2010

Extended Abstracts

Editors: Andrzej Zuber Jarosław Kania Ewa Kmiecik





University of Silesia Press 2010



abstract id: 285

topic: 2

Groundwater and dependent ecosystems

2.3

Interactions of surface and ground waters

title: Uncertainty of vertical streambed seepage rates under realistic field conditions using diel temperature fluctuations

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keywords: groundwater, surface water, connectivity, heat modelling, temperature

INTRODUCTION

Groundwater and surface water are connected and form one single resource. Sustainable water management requires knowledge of direction and magnitude of flow between streams and aquifers. The use of heat as a tracer promises to be an alternative to traditional methods, such as seepage meters, successive stream gauging and hydrometric methods. Flow through streambeds has been shown to vary greatly on a temporal and spatial scale (e.g. Schmidt et al. 2007; Keery et al. 2007; Essaid et al. 2008). Analytical solutions to the 1D conductive convective heat flow equation have been developed to estimate streambed fluxes (Stallmann 1965; Silliman et al. 1995; Hatch et al. 2006; Keery et al. 2007). In particular, the method devised by Hatch et al. (2006) is based on the analysis of the thermal response to the diurnal temperature signature recorded at two depths in the streambed. The direction and magnitude of vertical flow velocity distinctly impacts on thermal response at depth, causing variable amplitude damping and shift of phase (Hatch et al. 2006). Testing of this method with field data provided interesting unresolved artefacts in the flow results. These are large fluctuations of flow that could not be ascribed to hydraulic changes, and large deviations between velocities derived by either analysing the amplitude ratio or the phase shift (Rau et al. 2010).

Theoretically, deviations in flow velocities between measurement locations can be caused by natural variability in physical parameters introducing non-uniqueness into the analysis. It has been noted that the thermal conductivity of the streambed is generally well constrained and is not a function of grain size unlike the hydraulic conductivity (Blasch et al. 2007). This suggests a possible advantage of quantifying flow using heat as tracer compared to traditional Darcy type investigations. However, the heat method still requires estimates of a number of streambed properties before results can be calculated. Investigation of how parameter uncertainty impacts on calculated flows is required to estimate the overall uncertainty of the heat method. This paper quantifies the uncertainty in the calculated velocity using the method by Hatch et al. (2006) related to the widest range of physical parameters reported in the literature. Furthermore, numerical simulations confirm that the reduction in dimensionality (1D) is an important limitation to the method.

METHODOLOGY

The basic equations that relate amplitude ratio (AR) and phase shift (PS) of two vertical temperature time series to vertical water velocity are derived from an analytical solution to the conductive convective heat transport equation with sinusoidal boundary condition (Hatch et al. 2007):

$$AR = \frac{A_2}{A_1} = \exp\left(\frac{\Delta z}{2 \cdot \kappa_e} \cdot \left(\upsilon - \sqrt{\frac{\alpha + \upsilon^2}{2}}\right)\right) \text{ and } PS = t(P_2) - t(P_1) = \frac{P \cdot \Delta z}{4 \cdot \pi \cdot \kappa_e} \cdot \left(\sqrt{\frac{\alpha - \upsilon^2}{2}}\right)$$

with $\alpha = \sqrt{\upsilon^4 + \left(\frac{8 \cdot \pi \cdot \kappa_e}{P_i}\right)^2}$, $\kappa_e = \frac{\lambda_f^n \cdot \lambda_s^{(1-n)}}{\rho \cdot c}$, $\rho \cdot c = n \cdot \rho_f \cdot c_f + (1-n) \cdot \rho_s \cdot c_s$
and $\upsilon = v_f \cdot \frac{\rho_f \cdot c_f}{\rho \cdot c}$

Parameters are: *AR* and *PS* are amplitude ratio and phase shift between two temperature time series; κ_e is effective thermal diffusivity; κ_f and κ_s are thermal conductivity of water and solid; κ_e is the effective thermal diffusivity; *n* is porosity; v_f is the vertical water velocity; ρ_f and c_f are density and heat capacity of the water, and ρ_s and c_s are density and heat capacity of the solids; and ρ and *c* are density and heat capacity of the saturated sediment-fluid system; Δz is the vertical spacing between temperature measurement points. The physical properties of water are accurately known.

Analytical and numerical simulations were performed in order to clarify the impact of streambed physical parameter uncertainty and the field condition of horizontal flow on this 1D vertical method. The study focuses on two major aspects, the impact of: 1) natural variability in streambed parameters (solid thermal conductivity, solid heat capacity, solid density, porosity and dispersivity), and 2) directional flow and directional heat propagation which can be caused by thermal dispersivity.

For 1) a Monte Carlo analysis was performed: a min/max range for values derived from literature (e.g. Schön 1996; Schärli & Rybach 2001; Maqsood 2004; Markle et al. 2006; Markle & Schincariol 2007; Chen 2008; Smits 2010) was defined for each thermal parameter. The ranges are: solid thermal conductivity: $1 < \lambda_s < 4.5$ W/mK; solid heat capacity: $650 < c_s < 1,550$ J/kgK; solid density: $2,500 < \rho_s < 3,200$ kg/m³; porosity: 0.1 < n < 0.5. The mechanism of thermal dispersion was discarded from the uncertainty investigation because it is not well understood and statistical details are not available. This limits the uncertainty results to systems where conduction is dominant over convection, as is best described by the dimensionless particle related thermal Peclet number (Koch and Brady 1984; Anderson 2005)

$$Pe = \frac{\rho_f \cdot c_f}{\lambda_f} v_f d_p$$

The investigation is based on the following assumptions: a) the investigated streambed parameters are in general normally distributed, b) parameters are independent from each other, c) ranges as found in literature represent approx. 95% of values found in the field, which corresponds to the area between $\mu \pm 2\sigma$ under the normal distribution. Although field site specific samples of above thermal parameters exhibit normality (e.g. Markle et al. 2006), a general statistical distribution of streambed thermal parameters is unknown and therefore the statistical normal distribution is forced.

The above parameter ranges were used to create a large number of random values according to the assumptions. For a measurement spacing of 0.15m, amplitude ratios (AR) and phase shifts (PS) dependent on velocities between -10 m/d (downward flow) and +10 m/d (upward flow) were synthesised using the computed statistical variability for each individual parameter fixing all others to the respective mean values. Furthermore, the computations were repeated allowing for variability in all parameters. The velocity from the synthesised AR and PS values were then re-interpreted using parameter mean values as would be done for temperature field data with unknown streambed properties. The deviation from the real velocity value was calculated, and upper/lower probability of non-exceedence (90%) was computed for the velocity deviations. These calculated confidence limits can be plotted against the original velocity in order to

reveal the impact of individual and combined statistical parameter uncertainty on the AR and PS estimates over the entire range of vertical flow velocities.



Figure 1. Setup of the numerical heat transport model used to investigate the effect of horizontal flow components on the results of the 1D analytical method.

For 2, a 2D vertical slice of a streambed was set up (Fig. 1) in the numerical code VS2DH (Healy 1996). Temperature boundary conditions were: diel sinusoidal temperature change at the top and constant temperature at both sides as well as the bottom. Flow boundary conditions were: a constant downward flow component and ten simulations of increasingly higher horizontal flow (expressed as ratio of horizontal to vertical velocity V_h/V_z between 0 and 2). Five observation points at depths of 0.15, 0.3, 0.45 and 0.6 m recorded temperature time series. For each model run, the thermal dispersivity was restricted to 10% of the largest spacing. The last temperature peak of the top boundary condition in combination with each depth response was taken to calculate the vertical velocity using amplitude ratio and phase shift according to the method by Hatch et al. (2006).

RESULTS & DISCUSSION

The results of the Monte Carlo analysis using the above analytical models illustrate that the AR and PS estimates exhibit different statistical distributions, with the AR results being skewed as a result of the non-linear model (Fig. 2).

Generally, the downward velocity estimates are less affected by parameter variability than upwards flow. The major impact by variation in thermal properties is on the AR results and caused by the thermal conductivity in particular for upwards flow. Uncertainty in streambed solid density is the parameter of least impact (Fig. 2).



Figure 2. Lower and upper 90% non-exceedence limits for velocity deviations, a result of combined streambed thermal parameter variation, as function of vertical flow velocity.

For downward flow, solid density and porosity have the least effect on the results, whilst thermal conductivity and heat capacity distort results much more severely. Overall, there is a 90% probability that estimates are within 25% of the real vertical flow rate when mean literature thermal streambed parameter values are used (Fig. 3). The PS solution should be avoided at small or zero velocities because of its divergent nature (Hatch et al. 2007).



Figure 3. Lower and upper 90% non-exceedence limits for velocity deviations, a result of combined streambed thermal parameter variation, as function of vertical flow velocity.

In hydrogeology, hydrodynamic thermal dispersivity is mathematically described in terms identically to solute dispersivity, an approach that is disputed (Anderson 2005). Theoretical and experimental investigations on the issue of thermal dispersion in general porous media have been comprehensively reviewed (Kaviany 1995). Even though there is a lack of experimental data for thermal transport under slow flow rates, theoretical investigations suggest that the effective thermal conductivity term is much less dependent on the fluid velocity when conduction is dominant, meaning thermal Peclet numbers $Pe_t < 1$. It appears that the hydrodynamic thermal dispersivity has no or little impact in this case so that uncertainty results are limited to conduction dominant conditions. Theoretically, this is given for velocities that are slower than 10 m/d when the mean grain size of the streambed does not exceed 1.2 mm. However, more research is needed especially for different grain size distributions as found in streambeds.

Numerical modelling under 2D flow conditions revealed that thermal dispersivity can introduce deviation between the AR and PS results when horizontal flow is present in the streambed (Fig. 4).



Figure 4. Numerical modelling results showing the potential impact on the AR and PS velocity estimates of thermal dispersivity in simulations with a horizontal flow component.

The directional impact of thermal transport can significantly alter the phase derived velocity results depending on the magnitude of horizontal flow (Lautz 2010), and on the measurement spacing. In comparison, the amplitude derived results vary less when the direction of flow changes from vertical, and they do not show much dependence on the measurement spacing.

CONCLUSION

The outcome of this investigation highlights that caution must be applied when analytical methods are used to interpret diel temperature field measurements with the method devised by Hatch et al. (2006). Lacking knowledge of sediment thermal properties prior to velocity calculation can cause results with a 90% likeliness that velocity estimates can deviate by up to approx. 25% for systems with downward flow. However, this potential error can be decreased if the thermal properties are either directly measured or estimated e.g. from streambed mineral content. Unfortunately, these results are limited to conduction dominant conditions, because the mechanism of hydrodynamic thermal dispersivity is not well understood.

The numerical analysis suggests that deviations between amplitude and phase derived velocities can be caused by horizontal flow when there is significant thermal dispersivity. Systematic deviations between the AR and PS velocities can thus be used as an indication that significant horizontal flow may be present in the streambed. If that is the case vertical flow is generally overestimated. Nevertheless, this paper shows that analysis of diel temperature signatures can improve the understanding of streambed water exchange even when the streambed thermal parameters are estimated from literature values.

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2-vol. set + CD ISSN 0208-6336 ISBN 978-83-226-1979-0