A PRACTICAL GUIDE ON THE USE OF DIURNAL TEMPERATURE SIGNALS TO QUANTIFY SURFACE WATER-GROUNDWATER EXCHANGE

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Temperature is a powerful tracer to estimate vertical flows in the hyporheic zone. Temperature time series can be used to obtain estimates of fluid flux, and techniques can be employed to extend these estimates into plan-view flux maps. Key advantages of the use of heat as a tracer include that sensors are inexpensive, and that data can be collected and interpreted without the need for laboratory analyses. While the collection of temperature data is relatively straightforward, several factors influence the reliability of flux estimates. Sensor precision and deployment are particularly important in estimates of upwelling. The analysis of temperature time series data involves complex steps including signal processing, and the selection of the optimal analytical solution. A brief synthesis of diurnal temperature signal based methods is presented, providing details on optimal sensor selection and deployment, data requirements, and an overview of the available analytical solutions and computing tools.

1 BACKGROUND

Heat is an attractive tracer to determine fluid exchange between surface water and groundwater, because: 1) temperature variations in streambed (also lakebed, wetland) materials are naturally occurring, 2) robust and inexpensive sensors to measure temperature in saturated porous media are widely available, 3) field installation of equipment is inexpensive and straightforward, and 4) time series of flux estimates can be obtained without expensive and time consuming laboratory analyses [1].

Flux estimates can be obtained through the use of analytical solutions based on the assumptions of a sinusoidal surface temperature signal and steady 1-dimensional flow in homogeneous media. These diurnal signal methods (e.g. [2, 3]) determine the vertical flux between two temperature sensors based either on amplitude ratios (A_r) or phase lag ($\Delta\phi$) between the two time series, or through the simultaneous use of both ($A_r\Delta\phi$) (Fig. 1a).

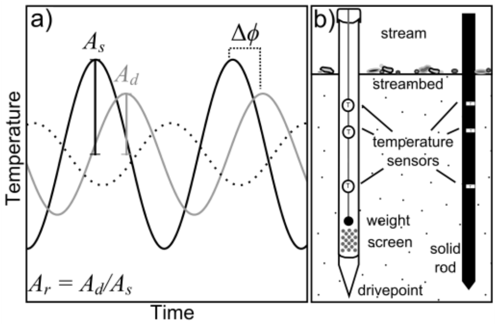

Figure 1: a) Hypothetical temperature time series, where A_r and $\Delta\phi$ are determined for the top sensor pair (*d* and *s* denote deep and shallow sensor respectively), and b) two instrumentations of the streambed. Adapted from [2].

While the assumptions of analytical solutions are rarely met in the field (e.g. temperature signals are non-sinusoidal, flows are multi-dimensional and porous media properties are heterogeneous), a number of studies have demonstrated that reliable flux estimates are possible (e.g. [4, 5, 6]). Additionally, methods are available to upscale point measurements to through paired use of these point-in-space fluxes, and spatial point-in-time mapping of streambed temperatures, to produce detailed plan view flux maps [7, 8].

Several complex steps are required to calculate fluxes from diurnal temperature signals, including the extraction of the sinusoidal component from raw temperature signals (to determine A_r and $\Delta\phi$), and the calculation of fluxes using iterative solutions. Computing tools (e.g. [9, 10]) have been central in the rapid adoption of heat as a tracer of surface water-groundwater interaction, as they incorporate methods to address these complexities for the user. However, there are still several important factors that must be taken into consideration in order to obtain reliable flux estimates. The choice of temperature sensors, their temperature resolution, how they are deployed, and the frequency of the measurements can all influence the quality of flux estimates. The user must also choose from several analytical solutions, which have differing requirements of thermal parameters in order to perform calculations. Our objective is to provide guidance on both data collection and data analysis to maximize the potential for reliable flux estimates from temperature time series.

2 CONSIDERATIONS FOR SITE INSTRUMENTATION

Two potential configurations for deployment of temperature sensors are shown in Fig. 1b, where temperature sensors are either suspended from a cable in a drivepoint (left), or are embedded in notches cut into a rod (right). With the drivepoint configuration, the temperature sensors are not in direct contact with the streambed sediments. However, the benefit of this approach is that relatively large sensors (>100 mm in length) can be easily accommodated. The alternative approach with the solid rod allows the sensors, typically held in place with tape (e.g. see [11]) and/or with silicon sealant (e.g. [7]), to be in close contact with the streambed sediments. However, this design is better suited to smaller sized sensors (<20 mm maximum diameter).

Sensor spacing is an important consideration in field instrumentation, with the optimal spacing depending on the flow direction and magnitude. Examples of sensor spacing used varies across the literature with spacing of neighboring sensors ranging between 0.02 – 0.05 m (close, e.g. [7, 11]), ~0.1 m (typical, e.g. [4, 9]), and 0.3 m (large) [2]. Studies have shown that the Hatch *et al.* [2] and Luce *et al.* [3] methods produce the mean flux between the sensor pair (e.g. [4]). Using several sensor pairs allows the calculation of fluxes at a range of depths, building up a profile of flux with depth. With multiple sensors in a vertical array, the number of depth ranges over which fluxes can be estimated is $n(n-1)/2$, where n is number of sensors in a vertical array.

For cases of downwelling, the diurnal signal is transported into the streambed materials both by flowing water (advection) and conduction. For high downwelling cases (>1.5 m d^{-1}), A_r approaches unity for close sensor spacing, which can lead to erroneously unrealistic high flow rates. In order to obtain more accurate flux estimates for downwelling, a greater sensor spacing may be required. Sensor spacing can simply be increased by selecting data from different sensor pairs during the analysis of the temperature time series.

For cases of upwelling, the propagation of the diurnal temperature signal into the streambed is only driven by conduction [11]. The magnitude of upwelling and the thermal properties of the porous media will control how deep the diurnal signal will propagate. The depth where observable diurnal signals can no longer be observed (extinction depth) will depend on a number of factors including the amplitude of the temperature signal at the water-porous media interface, sensor resolution and thermal properties [11]. For upwelling on the order of ~ 1.0 m d^{-1}, the extinction depth will likely be less than 0.1 m. In cases where upwelling is expected, or flow direction is unknown, it is advisable for at least two sensors to be placed as close as possible to the surface to ensure that the diurnal signal can be observed, as analytical solutions by Hatch *et al.* [2] and Luce *et al.* [3] are only applicable where a diurnal signal is observable.

Another consideration with site instrumentation is the temporal resolution of temperature measurements. Streambed temperatures are typically recorded with a measurement every 10-20 min (e.g. [2, 7, 9]), although hourly temperature measurements have also been used [7]. Reliable flux estimates from $\Delta\phi$ methods are based on the accurate identification of the timing of peaks from the filtered temperature time series. Briggs *et al.* [11] suggest setting temporal resolution as fine as practically possible (this point is discussed further in Section 3 below), but also highlight that some signal processing methods make it possible to identify $\Delta\phi$ at higher resolution than the resolution of the raw data.

3 CONSIDERATIONS FOR SENSOR SELECTION

Important factors which come into consideration when selecting appropriate temperature sensors/data loggers include the size of the logger, temperature resolution, and data storage capacity. These factors can influence the accuracy of flux estimates, the flow settings in which they can be used, and the duration that loggers can be deployed. Examples of four commonly used temperature loggers are shown in Table 1.

Table 1. Examples of temperature sensors/data loggers

Manufacturer, sensor, model	Resolution (°C)	*T* range (°C)	Storage capacity (samples)	Height × width (mm)
Onset® TidbiT v2	0.02	-20 to 70	42 000	17 × 41
Thermochron® iButton DS1922L	0.5/ 0.0625	-40 to 85	8192 / 4096	6.4 × 17.4
Onset® HOBO Water Temperature Pro v2	0.02	-40 to 70	42 000	114 × 30
Vemco Minilog-II-T	0.01	-10 to 40	1 000 000	98 × 23

With sinusoidal based analytical solutions being based on the comparison of amplitudes or the phase lag between two temperature time series, temperature resolution is more important that absolute accuracy, provided the offsets in temperature do not vary significantly over a 24 hour period. Generally, the temperature loggers in Table 1 can record temperatures with sufficiently fine resolution to allow the calculation of fluxes. For example, the iButton sensor (Table 1) has a selectable resolution, which influences the number of samples that can be stored. It is advisable to use the 0.0625 °C setting, as 0.5 °C is too coarse for most situations on the depth scales considered in surface water- groundwater exchange.

As highlighted in Section 2, sensor spacing and vertical location are particularly important for detecting upwelling using temperature time series. With the requirement for close sensor spacing to detect upwelling fluxes, temperature sensors (such as the Onset® HOBO or Vemco Minilog sensors) with large physical size may not be appropriate [10]. However, larger temperature sensors typically have the added benefit of the ability to store greater amounts of temperature data. With the larger temperature sensors, knowledge of the position of the temperature sensor within the logger is important to accurately determine the sensor spacing in analyses.

Thermochron® iButtons, in particular, are popular sensors due to their small size and relatively low cost. However it is important to note that iButtons are not waterproof, and therefore require special attention to prevent logger failure. Various approaches can be used to waterproof iButtons, including resin, wax, and waterproof tape. Another consideration that should be made before using iButtons is the fact that their relatively low data storage capacity may be restrictive. For example, with the 0.0625 °C resolution setting, and a temperature measurement every 15 minutes, iButtons can only be deployed for 42 days. If longer term data storage is required, either coarser temporal resolution or use of a sensor with a larger storage capacity is required.

4 ANALYTICAL METHOD SELECTION

There are numerous analytical solutions to provide flux estimates from temperature time series. One of the first was developed by Hatch *et al.* [2], who produced analytical solutions based on either A_r or $\Delta\phi$. The $\Delta\phi$ solution can only provide the magnitude of flux, and not the flow direction [2]. Several researchers have also identified that fluxes estimated from $\Delta\phi$ are either unreliable or have greater errors relative to the A_r method [e.g. 4, 11]. Rau *et al.* [6] identified that for highly transient flows, several signal processing methods produced erroneous $\Delta\phi$ output, providing one potential explanation for poor flux estimates from the $\Delta\phi$ method.

Benefits of the Hatch *et al.* [2] approach (and those similar) include that when poor $\Delta\phi$ output from filtering are produced, fluxes can still be provided from the use of A_r. However, the Hatch *et al.* [2] method requires an estimate of thermal conductivity of the saturated medium, which is not required in the Luce *et al.* [3] approach (and similar approaches), providing an additional source of uncertainty in the flux estimates.

The Luce *et al.* [3] combined $A_r\Delta\phi$ approach has several advantages over the Hatch *et al.* [2] approach. It does not require an estimate of thermal conductivity, reducing the uncertainty in flux estimates from uncertainty in thermal properties. Additionally, the Luce *et al.* [3] method can produce a time series of thermal diffusivity that only requires A_r and $\Delta\phi$, and no estimates of thermal properties. While this parameter is typically unknown, reasonable limits can be calculated from literature values. If thermal diffusivity output exceed realistic limits, it is likely that flux estimates are also inaccurate. However, the drawback of the Luce *et al.* [3] method is that it is reliant on accurate A_r *and* $\Delta\phi$ information. If filtering of temperature time series produces unreliable $\Delta\phi$ information, it is also likely that flux estimates from non-steady flows may be inaccurate.

The Hatch *et al.* [2] A_r method has been shown to be more reliable than the $\Delta\phi$ method by several authors (e.g. [4, 5, 11]). The combined $A_r\Delta\phi$ method produced similar results to the A_r method in losing conditions [4], with the added benefit of not requiring an estimate of thermal conductivity.

5 TIME SERIES AND DATA ANALYSIS CONSIDERATIONS

As analytical temperature time series methods are based on the assumption of sinusoidal temperature variations at the upper boundary, the sinusoidal component of the raw temperature series is typically identified via signal processing. This process is typically based on a Fourier transform, which can induce edge effects at the beginning and end of the time series (e.g. see [2]), or when a rapid change in flux rate occurs (e.g. see [5, 6]). To limit the influence of edge effects, it is generally recommended to omit the flux estimates from the first and last days of the calculated time series. However, some computer software tools employ techniques to limit the influence of edge effects. For example, VFLUX [9] pads the time series prior to signal processing, discarding the padded data once the process is complete, hence reducing the influence of any edge effects.

In cases where only short temperature time series are available (i.e. 1-3 days), the Ex-Stream computer package by Swanson and Cardenas [10] may be suitable. Ex-Stream uses a sinusoidal fitting process to raw temperature signals to determine A_r and $\Delta\phi$. This approach determines A_r and $\Delta\phi$ without any Fourier analyses, and therefore flux estimates can be obtained with time series as short as 24 hours.

Another important consideration is the thermal properties that are required to calculate fluxes from the temperature time series. There are several temperature time series analytical solutions (see Section 4 above), with varying requirements of thermal parameters. Uncertainties in thermal parameters produce uncertainties in flux estimates. For example, VFLUX includes Monte Carlo and sensitivity programs to determine the influence of the uncertainty in thermal properties on flux estimates.

6 SUMMARY

To maximize the accuracy of flux estimates, especially where the flow direction is not known *a priori*, it is generally advised: 1) that at least two closely spaced temperature sensors should be located as close as possible to the water-porous media interface, 2) to use several sensors with depth, 3) to select sensors that have high precision (in temperature), and 4) to ensure that temperature time series should be collected over several days to reduce the influence of edge effects in signal processing.

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