

# **Quantifying surface water-groundwater exchange using temperature profile inverse modelling at a riparian wetland**

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## **Abstract**

Second Creek is a manoomin (wild rice) stream located on the Iron Range in northeast Minnesota which has been impacted by mining pollution. In order to understand how mining-derived sulfate affects biogeochemical cycling at Second Creek, surface water-ground water exchange must be quantified because it controls geochemical gradients in the sediment. We employed inverse temperature profile modeling to estimate hyporheic flux at the site. The Second Creek study site is a riparian wetland where low hyporheic flux is expected. Streambed temperature profiles were measured at three locations across a transect of the site spanning from the main stream channel to the flanking wetland area over the summer of 2016. The data were collected using low-cost, open-source vertical temperature profilers and “ALog” data loggers. The USGS model 1DTempPro was applied to the temperature data, along with co-located head data at each location to estimate hydraulic conductivity across the transect. The sediment thermal parameters used in the model were constrained based on the sediment bulk density, which is strongly controlled by soil organic content. The estimated hydraulic conductivity values were applied to the measured head gradients to generate time series of hyporheic flux at the transect for the summer. Results showed spatial variability in both hydraulic properties and hyporheic flux. Across the transect, flux was upward toward the surface water for nearly the entire summer, though the magnitude of the flux varied dynamically in response to variable weather conditions and one flux reversal occurred following a strong late-summer storm event.

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## **Introduction**

The impact of mining on water quality in Minnesota's iron range is a contentious topic. Elevated sulfate concentrations are present in the lakes and streams of the area due to runoff from mining operations (Ng et al., 2017 (a)). Concern that elevated sulfate levels in the surface water would negatively impact manoomin (wild rice) growth has prompted in depth studies of geochemical processes in aquatic ecosystems (Pastor el al., 2017; Myrbo et al., 2013; Ng et al., 2017 (a); Yourd 2017).

The work in this study is a continuation of the work done of (Yourd, 2017) and (Ng et al. 2017, (a) ), who investigated the effect of hydrologic conditions on sulfur cycling in stream sediment. Their study focused on a stream called Second Creek which is located in northeastern Minnesota on the iron range. More information on the study site is presented in the Study Site section.

This study addresses the need identified in (Yourd, 2017) for a reliable constraint on hydrologic flux at the Second Creek site. This constraint is necessary because the geochemical gradient in the hyporheic zone where manoomin is rooted is controlled by hydrologic flux (Hayashi & Rosenberry 2002; Kurtz et al. 2007). The inverse temperature profile modelling technique was employed using data collected in the summer of 2016 to better constrain the hyporheic flux at the site.

## Study Site



Figure 1: Second Creek Study Site. Yellow X's indicate the location of each temperature probe and collocated piezometer. From west to east, each location is referred to as the west wetland, west streambed, and the center streambed.

The second creek site is a riparian wetland. The main stream channel is 2-3 meters wide and surrounded by 20-30 meters of wetland. The main channel is 1-2 meters deep. The site is underlain by glacial outwash and till. At the surface the sediment is extremely heterogeneous and has a high fraction of organic matter. Sources of surface water to the stream include mining tailings basins which cause elevated sulfate levels in the channel. During the summer months, manoomin and submergent macrophytes grow in the main channel of the stream, and the densely vegetated wetlands contain grasses, sedges, and shrubs. (Yourd, 2017)

## Methods

The quantity of interest in this study is vertical hydrologic flux in the streambed of Second Creek. Hydrologic flux through porous medium is described by Darcy's law, presented here:

$$q_z = -K \frac{dh}{dz} \quad (1)$$

$q_z$  is the vertical hydrologic flux.  $K$  is the hydraulic conductivity which describes the medium's ability to let water flow through.  $\frac{dh}{dz}$  is the gradient of head between the aquifer and the surface water. In hydrologic studies the head gradient is can be measured in the field so the main challenge is quantifying hydraulic conductivity. Hydraulic conductivity is an extremely variable quantity. It can range over many orders of magnitude for a single medium. Inverse temperature profile modelling was employed to constrain  $K$  so that hydrologic flux can be calculated.

### Inverse Temperature Profile Modelling

The inverse temperature profile method uses temperature as a tracer to infer the movement of water through the aquifer - surface water interface. At the Second Creek site the surface water temperature fluctuates diurnally as it is heated by the sun and subsequently cools overnight. The surface water temperature fluctuation propagates down into the hyporheic zone where the surface water comes into contact with groundwater. The mixing of surface and groundwater in the streambed damps out the diurnal temperature signal. In addition to signal attenuation, the signal is also shifted in time. This phenomenon is demonstrated in figure 2.

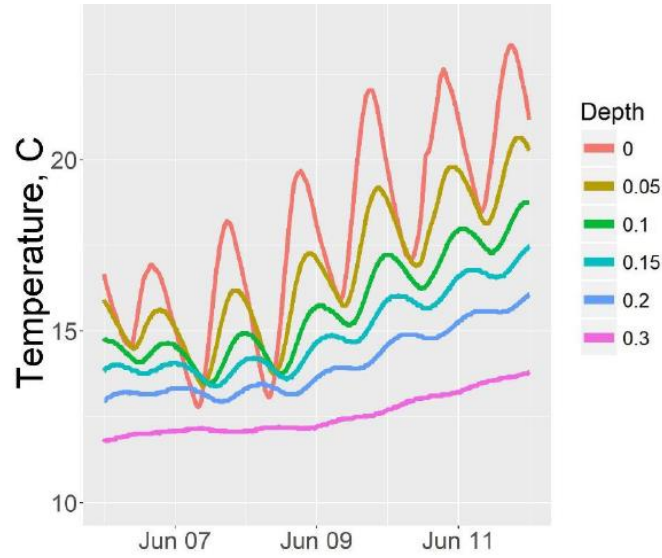


Figure 2: Sample streambed temperature profile from Second Creek. Surface water exhibits the strongest diurnal fluctuations. The diurnal fluctuations are almost entirely damped out at 0.3 m depth. The diurnal signal is also phase shifted at depth.

The magnitude of signal attenuation that occurs is related to the direction of water flow in the streambed. In a gaining stream, the signal will damp out at a more shallow depth than in a losing stream where infiltrating surface water carries the temperature signal with it. The phase lag at depth is controlled by the time which the signal takes to propagate, which is similarly dictated by hydrologic flux.

One dimensional propagation of heat through a porous medium is well understood and described by the heat diffusion equation:

$$(\lambda_s + q_z \alpha C_w) \frac{\partial^2 T}{\partial z^2} - q_z C_w \frac{\partial T}{\partial z} = \frac{\partial T}{\partial t} (\phi C_w + (1 - \phi) C_s) \quad (2)$$

The meaning of each variables in this equation is listed in Appendix 1.



The inverse temperature profiling method uses the top and bottom temperature readings of an observed temperature profile as boundary conditions to find a solution of the heat diffusion equation. The observed profile and the synthetic profile are then compared. The parameters such as  $q_z$ , which were used to develop the synthetic profile can be adjusted and compared again. This process can be performed iteratively until the profiles match to a desired tolerance. The adjustment of the input parameters in this manner allows estimation of the true parameter value.

There are a variety of software available to perform inverse temperature profile modelling. The USGS software 1DTempPro (Kockh et al., 2015) was chosen for this study because it is the only GUI based inverse temperature profile modelling software that uses a numerical solution to the heat diffusion equation. 1DTempPro also offers the most complete solution to the diffusion equation by including the dispersion term which is left out of some models. 1DTempPro is capable of automated estimation of hydraulic conductivity in a streambed when it is given the physical properties of the streambed, a temperature profile time series, and a collocated head gradient time series. . In this study 1DTempPro was used to estimate hydraulic conductivity at all three temperature probe locations.

## **Data Collection**

To inform the inverse model, temperature and head data was collected during the summer of 2016. The temperature probes were 1 inch PVC tubing with 6 thermistors attached. The probes were inserted into the stream or wetland sediment such that the top thermistor was approximately at the sediment-water interface, and the bottom thermistor was located at approximately 30-40cm depth below the sediment-water interface, with most sensors clustered within the top 10 cm, which corresponds to the manoomin root zone. (Yourd, 2017). Temperature readings were

logged at 15 minute intervals to capture diurnal and seasonal temperature variability at the site. Two probes collected data from June to August and one collected data from June to October. The location of the probes is indicated in figure 1.

Head data was collected using three piezometers and a stream gauge. The piezometers and temperature probes were collocated. Pressure transducers in each piezometer and the stream gauge collected pressure data for the entire summer. The data loggers used in this study were low cost, open source loggers developed by Northern Widget LLC. (Wickert, 2014)

One gap in the stream gauge data exists from 7/25/16 to 8/1/16. The stream gauge went dry during this period. The gauge was relocated in the stream channel during field work on 8/1/2016.

The elevation of the top of casing for the transducers and stream gauge were surveyed 10/1/16. The depth to each transducer was also measured.

Atmospheric pressure data was provided by \_\_\_\_\_ (Crystal, who provided this data, I recall that it was a state of MN study?) Site precipitation data was acquired from the nearest weather station located in Embarrass, MN 10 miles north of the site.

The atmospheric pressure was subtracted from the pressure readings made in each piezometer and the stream gauge. The elevation of each transducer was calculated from the surveyed elevation and measured depth for each transducer. The elevation of each transducer was used to convert the pressure measurements into hydraulic head measurements based on a consistent datum across all of the piezometers.

The elevation of the stream gauge before it was moved on 8/1/16 was not surveyed so a correction factor was applied to the data from the first half of summer. The correction factor was determined by imposing the assumption that the average head difference ( $\Delta h$ ) between each piezometer and the stream gauge was constant throughout the summer. This was accomplished by shifting the 6/1 – 7/25 portion of each  $\Delta h$  time series by the difference between the average  $\Delta h$  for 8/1- 10/1 and average  $\Delta h$  for 6/1 – 7/25.

### **Model input parameter estimation**

To compute a synthetic solution to the heat diffusion equation, 1DTempPro requires information about the physical properties of the streambed. Specifically, porosity, thermal conductivity, and saturated heat capacity. Porosity was measured in (Myrbo, 2013). The remaining physical properties were estimated based on methods in (Farouki, 1986).

The streambed is composed of a mixture of siliclastic sediments and organic matter (SOM). The sediment at Second Creek is extremely heterogeneous, as show in figure 3.



Figure 3: Second Creek wetland sediment (left) and streambed sediment (center, right).  
(Yourd, 2017)

In order to make a reasonable estimation of the thermal parameters of the site sediment some simplifying assumptions were required. The first simplifying assumption was that the sediment was composed entirely of two endmembers, siliclastic material and soil organic matter. The second simplifying assumption is that the streambed is homogenous across all of the temperature probe locations. Both of these assumptions are justified during model sensitivity analysis in the results and conclusions section.

The percentage, by mass, of soil organic matter and siliclastic minerals present in the sediment was calculated using the following expressions

$$\rho_b = x_{si}\rho_{si} + x_{som}\rho_{som} \quad (3)$$

$$1 = x_{si} + x_{som} \quad (4)$$

The value for dry bulk density ( $\rho_b$ ) was established in (Myrbo, 2013). The values for  $\rho_{som}$  and  $\rho_{si}$  were sourced from (Farouki, 1986). This calculation resulted in a sediment makeup of 90% SOM and 10% siliclastic material. High organic content is expected at Second creek, and this value is supported by the images above where many of the sediment samples appear to contain entirely SOM. In order to extend to our second assumption (heterogeneity) an 80% SOM - 20% siliclastic split was chosen to better generalize the conditions at the site.

Using the fraction of SOM and siliclastic material, the thermal properties of the streambed can be estimated by the following methods from (Farouki, 1986).

Sediment Thermal conductivity,  $\lambda$

$$\lambda_{max} = x_{si}\lambda_{si} + x_{som}\lambda_{som} \quad (5)$$

$$\lambda_{min} = \frac{x_{si}}{\lambda_{si}} + \frac{x_{som}}{\lambda_{som}} \quad (6)$$

Saturated heat capacity,  $C$

$$C_{max} = (1 - \theta)x_{Si}C_{Si} + (1 - \theta)x_{Som}C_{Som} + \theta C_{H_2O} \quad (7)$$

$$C_{min} = \frac{(1 - \theta)x_{Si}}{C_{Si}} + \frac{(1 - \theta)x_{Som}}{C_{Som}} + \frac{\theta}{C_{H_2O}} \quad (8)$$

This method bounds the thermal parameter with an upper and lower limit. Values for  $\lambda_{Si}, \lambda_{Som}, C_{Si}, C_{Som}$  and  $C_{H_2O}$  were found in Farouki (1986). Validity of the resulting parameter range is discussed in the sensitivity analysis portion of the results and conclusions section.

The last parameter needed for the forwards model is dispersivity. This parameter depends on the scale of the problem. A range of dispersivity values were considered based on (Zheng & Bennet, 2002). The validity of the range is analyzed in the sensitivity analysis portion of the results and conclusions section.

## Results and Conclusions

The estimates of hydraulic conductivity at each temperature probe were obtained using 1DTempPro. They are presented in Table 1. The user specified parameter values for these estimations are presented in table 2. The validity of the estimated hydraulic conductivity values is explored in the sensitivity analysis section.

<u>Location</u>	<u>Hydraulic conductivity, m/d</u>
West wetland	0.07
Stream west	0.04
Stream center	0.18

Table 1: Hydraulic conductivity estimates from the 1DTempPro inverse model. Model inputs include head and temperature time series and the parameter values in table 2.

<u>Parameter</u>	<u>Value</u>
$\theta$	0.51
$\lambda$	0.56 w/(m°C)
$C$	$2.44 \times 10^6 \text{ J/(m}^3 \text{ °C)}$
$\alpha$	0.1 m

Table 2: 1DTempPro inverse model inputs for hydraulic conductivity estimation.

These hydraulic conductivity values were plugged in to Darcy's law with the head gradient time series for each probe to generate a time series of vertical hydrologic flux at each location. The hydrologic flux time series are presented in figure 3. The time series are plotted with precipitation data from the Embarrass, MN weather station to help visualize the relationship between precipitation and hydrologic flux

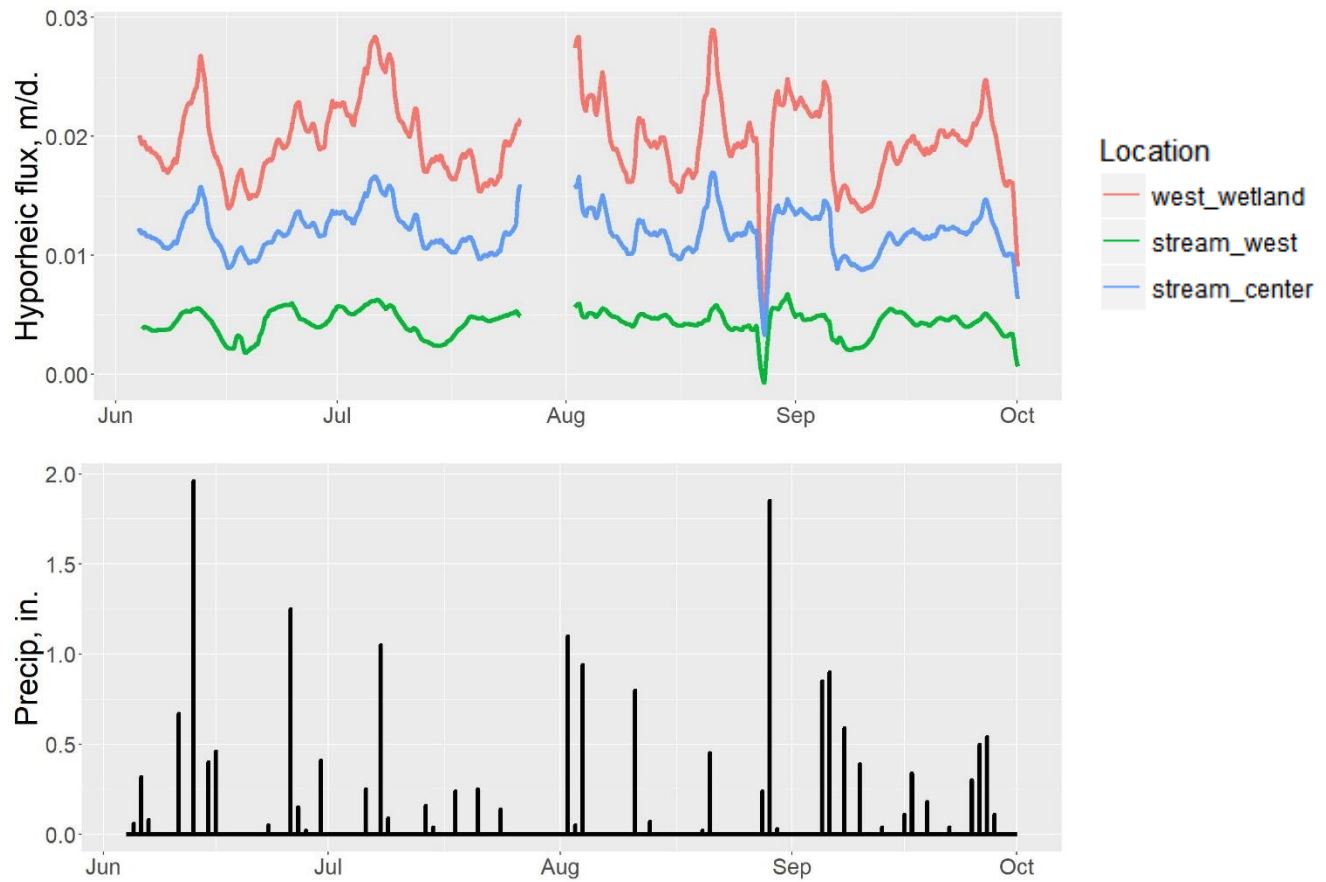


Figure 3: Vertical hyporheic flux and precipitation at Second Creek for summer 2016. Positive values indicate upwards flux. Large storm events appear to control hydrologic flux at the site, though the exact mechanism is uncertain.

The highest hydraulic conductivity and flux occur in the west wetland, followed by the stream center and the west stream channel. This is counterintuitive, as we originally expected the wetland area to have the smallest flux. There are several possible explanations for this discrepancy. First, the site sediment is highly heterogeneous which suggests that the hydrologic flux is equally heterogeneous. It is possible that the wetland temperature probe was placed in a region that facilitated higher flux while the stream probes were located in lower flux regions. Another possible explanation is that flow at the wetland probe has a significant horizontal

component, violating the assumption of 1DTempPro that hydrologic flux is entirely in the vertical direction. This explanation has merit because the head in the wetland sediment was consistently higher than the head at the base of the stream which suggests that the water in the wetland sediment could have a significant component of flow velocity towards the stream.

The direction of vertical flux across the transect is upwards for the entire summer except for one brief flux reversal in late August. The magnitude of vertical hydrologic flux over the summer is variable. The flux magnitude appears to be linked with precipitation. Major changes in flux magnitude occur following large rain events. Sometimes these rain events increase the upward flux magnitude, indicating that the rainfall initiates a base flow event. In other cases, rain events are followed by decreased upwards flux, or even downwards flux, indicating that the rainfall runs off into the surface water quickly. A possible explanation for this discrepancy is that the precipitation data was collected from a weather station that is 10 miles north of the study site so it is possible that during these storm events the stream and the weather station don't experience the same meteorological conditions. The streams response to the storms could be related to the proximity of the storm to the stream. For example, a distant storm would be more likely to trigger a large prolonged base flow event, and a storm that occurs near second creek could cause a rapid rise in surface water levels, resulting in an immediate decrease in upwards flux or even downwards flux. Another possible explanation for the varied response to storm events could be seasonal changes in vegetation in the region. More study is required to determine which of these explanations have merit.



## Sensitivity analysis

This section is dedicated to evaluating the quality of the model results and the model's dependency on the hand estimated thermal parameters. To investigate this the inverse model was run over the possible range of parameters estimated for dispersivity, thermal conductivity, and heat capacity. The inverse model was run as each parameter was varied over its range while the rest of the parameters were held at the values in table 2. The resulting value of K for each of these model runs is presented in figure 4. The goodness of fit between the model's final synthetic profile and the observed temperature profile is qualitatively demonstrated by the size of each point in figure 4.

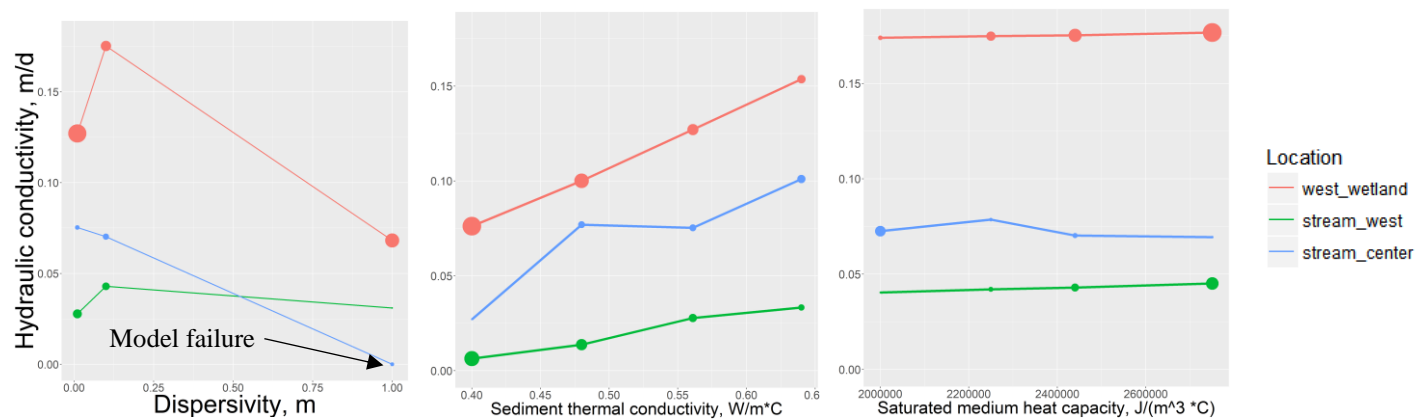


Figure 4: Inverse model sensitivity analysis results. The sensitivity of each hand estimated parameter was tested by running the inverse model over a range of input values and comparing the results.

## Dispersivity sensitivity

The inverse model sensitivity results show the strongest nonlinearity in the sensitivity to dispersivity. This nonlinearity can be explained by the complicated interdependence of dispersivity and flux magnitude. In Equation 2 the term that represents the transport of heat by dispersion is

$$q_z \alpha C_w \frac{\partial^2 T}{\partial t^2} \quad (9)$$

This term shows that the effect of dispersion grows both as flow velocity grows and as the dispersivity,  $\alpha$ , grows. Noting that  $q_z$  depends linearly on  $K$ , reasoning suggests that there is an inverse relationship between dispersivity and the estimated value of  $K$ . This relationship appeared in the sensitivity results above, however there appears to be an additional phenomenon occurring at middling dispersivity values. These data are not sufficient to fully illuminate this phenomenon. An interested reader is referred to (Rau et al., 2012) for further investigation of the significance of thermal dispersion.

The value of dispersivity also depends on the spatial scale that heat transport is taking place. (Zheng & Bennett, 2002). (Zheng & Bennet, 2002) states that for an investigations of this scale, dispersivity can be expected to vary between 0.01m and 1m. In this range,  $\alpha = 0.1\text{m}$  gave the best quality of fit between the synthetic temperature profiles and the observed profiles so this value was chosen to be the representative vertical dispersivity at the site.

## Thermal conductivity

The dependency of the inverse model results on thermal conductivity is fairly linear. This makes sense at our site because there is primarily upwards hydrologic flux. As thermal conductivity increases the diurnal surface water signal can propagate further into the streambed.

To match the observed temperature profile, upwards hydrologic flux must damp the diurnal signal thus increasing thermal conductivity results in an increased estimated hydraulic conductivity.

The thermal conductivity value  $0.56 \text{ W/(m}^{\circ}\text{C)}$  was chosen as the representative thermal conductivity of the sediment at the site. This value was chosen because it gave a good fit for all three temperature probes and, being in the middle of the range of possible values, helped average out heterogeneity at the site.

### **Saturated heat capacity**

The inverse model results appear to have no dependence on saturated heat capacity. The saturated heat capacity value that was chosen to be the representative value for the site was  $2.44 \times 10^6 \text{ J/(m}^3 \text{ C)}$ . The lack of sensitivity to this parameter gives us confidence in choosing this as the representative value.

### **Outro**

To summarize our findings, hydrologic flux at the site during the summer of 2016 was consistently upwards with variation in magnitude driven by precipitation. The results of this work have been used with reactive transport modeling to investigate the influence of hyporheic flux on biogeochemical cycling at Second Creek (Ng et al., 2017 (b)).

The results of this investigation could be expanded and improved by doing unique sediment parameter calibration for each temperature probe. This includes porosity and sediment content as well as thermal parameters. This could be achieved by careful sediment sampling and

analysis in the field or by employing a multiple parameter estimation routine. This work would help quantify heterogeneity at the site and identify potential biogeochemical hot-spots.

## Appendix 1 – Variable meanings for equation 2

<u>Symbol</u>	<u>Variable</u>
$K$	Hydraulic conductivity
$\varphi$	Porosity
$\lambda_s$	Saturated thermal conductivity
$C$	Sediment heat capacity
$C_w$	Heat capacity of water
$\alpha$	Dispersivity
$q_z$	Hyporheic flux
$T$	Temperature

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