Assessing vertical water flux between groundwater and surface water at the River Tame Hyporheic Zone SWITCH Test Site using temperature time series

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ABSTRACT

Implementation of recent legislation coupled with the potential attenuation of contaminants in the groundwater-surface water exchange zone has sparked a global push to further our understanding of the complex geochemical, biological and hydrological processes occurring within the hyporheic corridor. Temperature time series analysis has been used increasingly to characterise water movement between rivers and groundwater. In this study temperature time series data collected from a multilevel temperature probe installed at the SWITCH (Sustainable Water Management Improves Tomorrow's Cities Health) Hyporheic Zone (HZ) test site, Birmingham, has been used to examine the vertical movement of water between the River Tame and the underlying hyporheic sediments. A method of temperature time series analysis was developed using a thermal analogue of the Ogata-Banks solution (1961) to the one dimensional advection dispersion equation for solute transport. Visual Basic (VB) language was used to write a simple program which solves the modified Ogata-Banks solution and uses superposition of step functions to simulate temperature signatures at selected depths. Vertical flux estimates obtained from this method were comparable to average flux values obtained from numerical modelling of the riverbed using the software package VS2DI, and Darcy based flux estimates. It is proposed that this semi-analytical method provides a simple and easy to apply method of temperature time series analysis, providing averaged estimates of vertical flux and thermal properties.

ACKNOWLEDGEMENTS

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1 INTRODUCTION

1.1 Research Context

Over the last few decades the interaction of river and aquifer systems has become an increasingly studied element of hydrogeology (Winter *et al*., 1998; Brunke & Gonser, 1997; Woessner, 2000; Sophocleous, 2002; Smith *et al*., 2008). One of the main drivers for this upturn in research has resulted from a need to understand the processes that occur in and around the surface-subsurface exchange zone which surround rivers and streams in order to better equip ourselves to deal with recent legislation (European Commission, 2000; EA, 2002). Further interest has also grown through an ever increasing need to improve the quality of our surface and subsurface waters and the ability of the hyporheic zone to act as a natural attenuation zone or barrier to protect groundwater or surface water from the migration of contaminants (Durand *et al*., 2008). The potential attenuation capacity within the hyporheic zone stems from the enhanced biological and geochemical conditions that are fostered by the blending of surface and subsurface flow. However, the complex interplay of hydraulic, geochemical, and biological processes at various scales makes delineating and characterising the hyporheic corridor extremely difficult (Brunke & Gonser, 1997; Woessner, 2000; Conant Jr., 2004; Poole *et al*., 2008).

In an attempt to understand hyporheic processes, it is paramount to accurately describe and characterise the nature of flow within the subsurface sediments. Forming part of the surge in hyporheic research, temperature propagation within hyporheic sediments has been found to be useful in characterising the movement of water and chemicals in the subsurface. As a result, the use of temperature time series data to investigate the interaction of surface and ground waters has grown significantly in recent times (Lapham, 1989;

Silliman & Booth, 1993; Constantz & Stonestrom, 2003; Conant Jr., 2004; Keery *et al*., 2007; Scmidt *et al*., 2007; Essaid *et al*., 2008).

1.2 Previous Studies

The connection between the propagation of heat and water movement through sediments has been studied for the last century. Bouyoucos (1915) looked at the thermal migration of moisture from regions of high temperature to regions of low temperature and reported that there is an optimum moisture content for the maximum movement of water under a fixed temperature gradient. Suzuki (1960) presented a method for estimating the rate of water movement through soil based on a formula relating water propagation rate to the subsurface temperature profile.

Stallman (1963) provided equations for the coupled flow of heat and groundwater, suggesting groundwater velocity in the vertical plain may be estimated using temperature profiles from within the subsurface. A solution to these equations was provided by Bredehoeft & Papadopolus (1965) who produced a set of type curves to calculate ground water velocity from subsurface temperature profiles, in a one-dimensional, vertical, steady flow system. Stallman (1965) also provided an analytical solution to the flow problem presented in Suzuki (1960) based on a sinusoidal temperature fluctuation of constant amplitude at the surface and constant and uniform percolation rate normal to land surface through a homogeneous medium.

In a more recent publication, Silliman & Booth (1993) were able to use temperature time series to locate areas of surface water inflow and groundwater outflow in a stream in northern Indiana. Based on this study, Silliman *et al.* (1995) used an extension of the solution provided by Stallman (1965) to estimate downward flux in sediments within an order of magnitude.

An empirical relationship was developed by Conant Jr. (2004) to compare temperature data measured below a streambed with hydraulic data obtained from minipiezometers, which related thermal and hydraulic data, allowing the computation of flux rates using only temperature data.

Hatch *et al.* (2006) presented a method of calculating seepage rates within a streambed using phase shift and amplitude attenuation of oscillating streambed temperature signals. Using calculations based on equations developed by Stallman (1965), they were able to compute estimates of vertical water flux which varied over time, providing validation by comparison with numerical simulations. In a related approach, Keery *et al.* (2007) proposed a method of determining groundwater flux by utilising Dynamic Harmonic Regression signal processing techniques to extract the diurnal component of a temperature time series, and combining this with an analytically extended version of the Stallman (1965) solution to the one-dimensional heat flow equation, producing a time series of seepage fluxes. In this research, flux values derived from the analytical method were compared with flux estimates taken from field measurements and yielded promising results.

Schmidt *et al.* (2007) presented another method of calculating groundwater discharge over the reach and sub-reach scales using the analytical solution of the one dimensional steady-state heat-diffusion-advection equation provided by Turcotte & Schubert (1982). Their analytical model results were compared to observed temperature data and numerical model results, showing that with only limited input of thermal parameters and temperature data, it is possible to deliver reasonable estimates of flux within riverbed sediments.

The publications discussed above generally use temperature time series analysis to derive information about flux direction or magnitude. However, there are numerous methods which can be applied to utilise heat as a tracer to estimate flux within hyporheic sediments. A summary of examples of the application of the heat tracer method is provided by Constantz &

Stonestrom (2003), with a more recent update in applications and developments provided by Constantz (2008).

1.3 The SWITCH project

The University of Birmingham has been carrying out research to improve understanding and characterise the behaviour of surface and subsurface water interactions within the urban hyporheic zone. As part of the EC Framework 6 SWITCH (Sustainable Water (management) Improves Tomorrows' Cities' Health) research programme, the University of Birmingham has designed and implemented a monitoring network on a 200m reach of the River Tame, Birmingham. The city of Birmingham itself has been designated a 'Demonstration City' as part the international SWITCH programme. The site, referred to as the Hyporheic Zone (HZ) test site, has been subject to a number of sampling campaigns in addition to extensive monitoring to investigate the dynamic interactions of groundwater and surface water in an urban environment as well as to assess the chemical attenuation capacity of the hyporheic zone (Durand *et al.*, 2008). Full details of the SWITCH project in Birmingham as well as the development and design of the HZ test site can be found in Durand *et al.* (2008) and Cuthbert *et al.* (In Press). The basis for the current study was borne from a gap in understanding and analysis of temperature propagation through the hyporheic sediments beneath the River Tame at the SWITCH HZ test site. All temperature time series and hydraulic data used in this project were provided by Dr. Mark Cuthbert of the University of Birmingham, and are summarised in Cuthbert *et al.* (In Press). Data was collected both before and during the course of this study as part of the ongoing monitoring at the SWITCH HZ test site.

1.4 Aims and Objectives of the Present Study

This main aim of this project was to assess the vertical flux within streambed sediments of the hyporheic zone at the SWITCH HZ test site, Birmingham, using temperature time series analysis. Key objectives to achieving this were to:

- Examine the nature of thermal flux through the riverbed sediments
- Assess the magnitude, direction and variation of water flux in the riverbed over time using temperature time series analysis and thermal modelling
- Compare flux estimates derived from temperature time series analysis with flux calculations derived from other methods
- Assess the impact of high flow events and pump tests on the temperature profile within the riverbed
- Ascertain the usefulness of temperature time series analysis in delineating water flux at the SWITCH site
- Determine what other information may be derived from temperature time series analysis at the SWITCH site

1.5 Study Approach

In order to achieve the objectives set out in Section 1.4, a number of activities were undertaken. These activities were subject to review as the project developed with more promising aspects of the project being pursued. The activities included:

- Examination of relevant published literature on using heat as a tracer in hyporheic sediments
- Assimilation of the required data for the present study from the extensive dataset gathered from the ongoing SWITCH research project

- Analysis of data gathered to assess the nature of temperature oscillation at the surface and propagation within the hyporheic sediments
- One dimensional analytical modelling using river temperature time series as a top boundary to examine:
  - variation in vertical flux over time
  - influence of high flow events e.g. storm events
  - effects of borehole pumping on flux
- Development of a numerical model to compare and contrast with analytical model results
- Comparison of modelled flux estimates with Darcy based values obtained using hydraulic data from the SWITCH HZ test site

2 FIELD SITE

2.1 Site Location

The River Tame, a tributary to the River Trent, is located to the south of the Trent Catchment, flowing eastwards through north Birmingham and continuing through the West Midlands conurbation before joining the River Trent. The HZ test site is situated on a 200m reach of the River Tame, approximately 10 km north of the University of Birmingham, where the river flows through an industrial estate to the north of Birmingham City Centre, near Witton (Figures 1 & 2). The boxed 'study area' in Figure 1 denotes an area which has been extensively researched by the University of Birmingham over the last few years as part of the SWITCH research project and other research activities (Ellis *et al.*, 2007; Ellis & Rivett, 2007; Rivett *et al.*, 2008; Durand *et al.*, 2008; Cuthbert *et al.*, In Press).

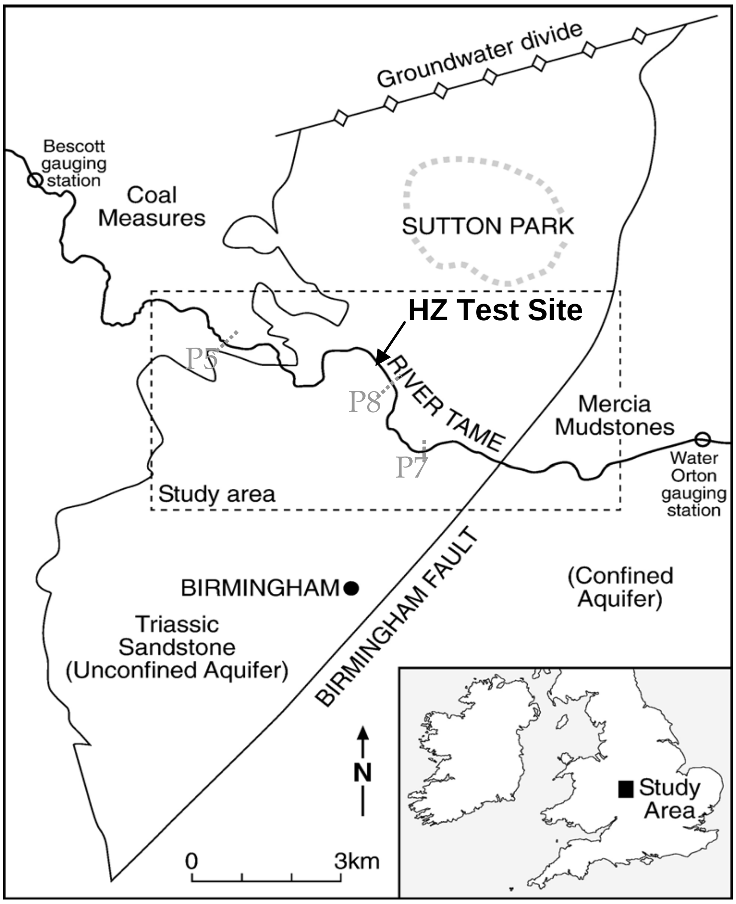

Figure 1: Map of Birmingham, showing the location of the Hyporheic Zone (HZ) test site on the unconfined aquifer of Triassic Sandstone. The boxed region shown is the study area researched by Ellis & Rivett (2007), with transects P5, P7 and P8 being used in previous research. (From Durand *et al.*, 2008**)**

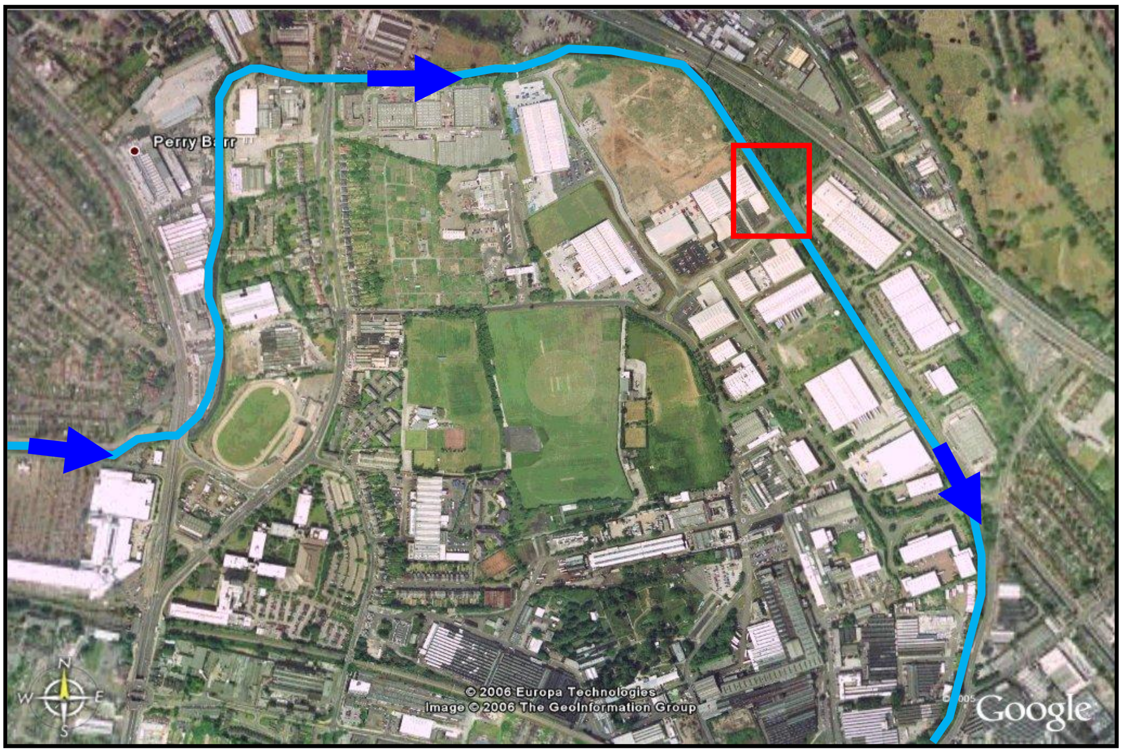

Figure 2: A satellite photograph (obtained from Google Earth) of a section of the River Tame showing the HZ test site (boxed area). (Modified from Cuthbert *et al.*, In Press)

2.2 Geological and Hydrogeological Setting

The River Tame flows eastward over coal measures to the north west of Birmingham City Centre, then over Triassic Sandstones, which form an unconfined aquifer beneath the city, and subsequently over Mercia Mudstones which are confining to the east of central Birmingham. The transition between the Triassic Sandstones and Mercia Mudstones is marked by the Birmingham Fault, which runs south west to north east (Figure 3). The HZ test site is located on the Triassic Sandstones and is underlain by around 7m of river terrace alluvial deposits. Underlying this is approximately 100m of fine to medium grained, horizontally bedded Kidderminster Formation Sandstone (Durand *et al.*, 2008). The alluvial deposits are typically wide varying in nature with sands, gravels, silts, clays and organic material juxtaposed, giving a highly heterogeneous near channel and subsurface environment. Within the HZ test site the River Tame is predominantly under gaining conditions with outflow from the underlying unconfined sandstone aquifer (Ellis *et al.*, 2007).

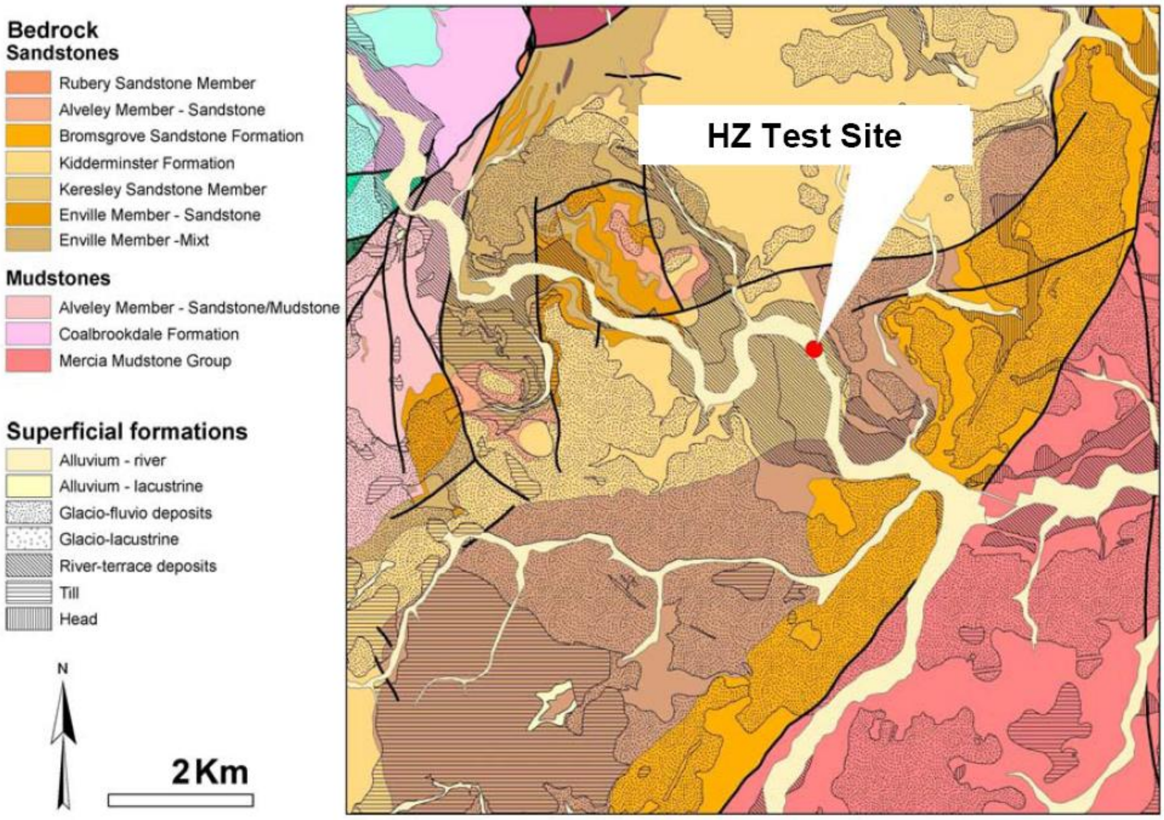

Figure 3: Geology of the Birmingham area showing the Hyporheic Zone (HZ) test site. (From Durand *et al.*, 2008)

The river itself has been substantially modified, and is almost completely straight along the length of the HZ test site (Figure 2), with made ground lining the river as it flows south east through the industrial estate.

2.3 The Hyporheic Zone Test Site

An extensive array of piezometers, multilevel samplers and automatic pressure transducers has been installed as part of the monitoring network at the HZ test site (Figure 4). In addition an extraction borehole has been drilled on the north east side of the river, 5m from the riverbank and to a depth of approximately 14 m below the river level, as part of the SWITCH research project. The data used in this study was taken from: a multilevel temperature probe (P+005-1T), installed downstream of the borehole; piezometers; two divers which recorded head data, one located approximately 30m upstream and one located approximately 30m

downstream of the extraction borehole; a diver located in the extraction borehole which recorded head and temperature data during ambient conditions and pumping tests. It should be noted that a long term pump test was carried out at the SWITCH HZ test site which started on the 18th of December 2008 and continued until 29th May 2009, during which the borehole was pumped continuously at approximately 135-140 l/min (Cuthbert, M., personal communication, 2009). The full monitoring network and location of samples taken is shown in Figure 4. A thorough description and explanation of the monitoring network at the HZ test site is given in Durand *et al.* (2008) and a report of data collected thus far from the site is given by Cuthbert *et al.* (In Press). An explanation of the method of installation, fabrication and construction of the multilevel samplers and piezometers is provided by Rivett *et al.* (2008).

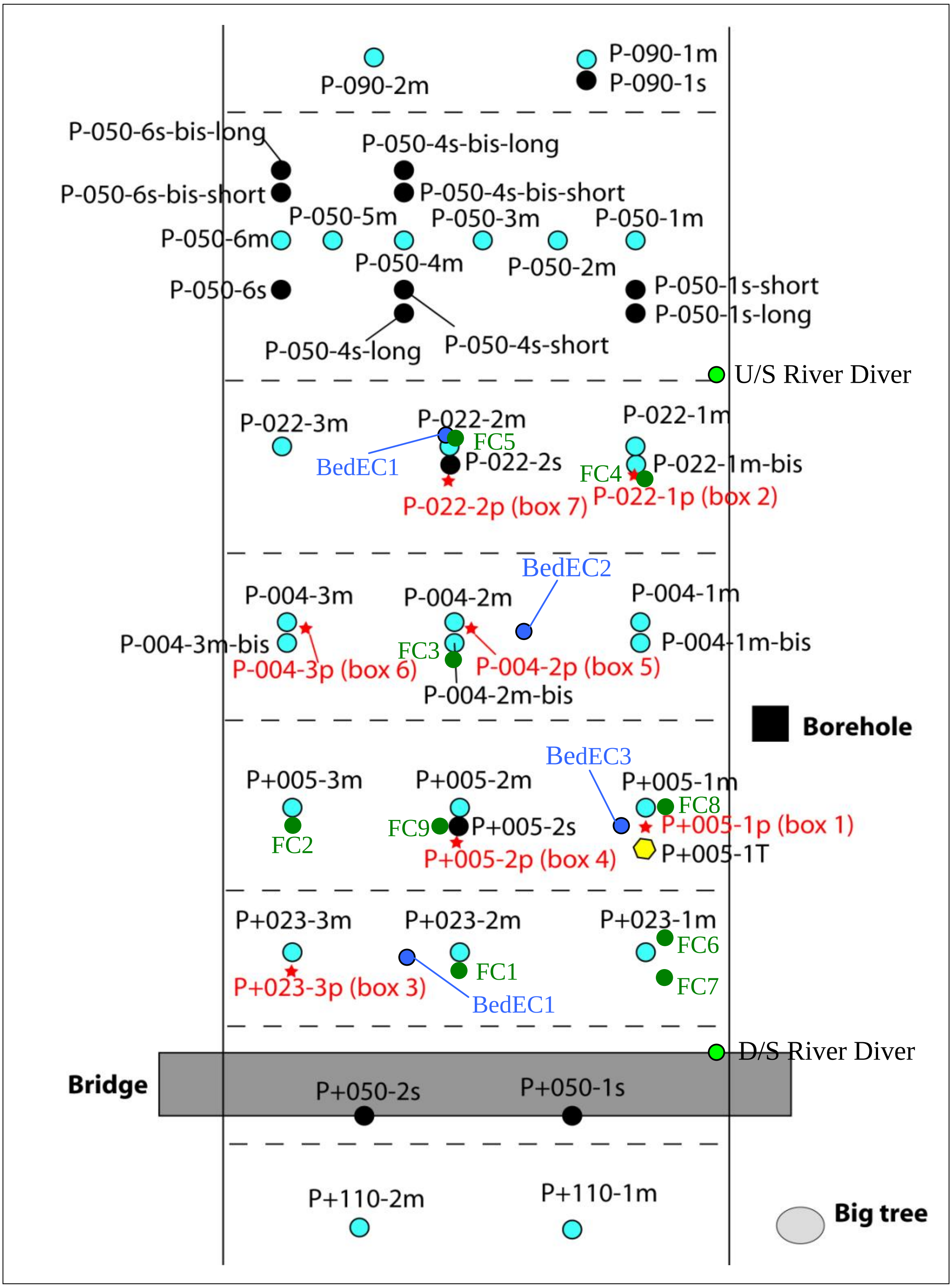

Figure 4: Schematic diagram of the monitoring network and sample sites at the HZ test site. Naming convention: P is for point; + or – indicate location upstream or downstream of the extraction borehole respectively; 3 digits represent distance of cross-section from borehole in metres, followed by hyphen; 1 digit represents order in the considered cross-section, 1 being closest to the riverbank on which the borehole is located; 1 letter represents type of measurement: multilevel (m), simple piezometer (s), pressure transducer (p), temperature device (T); any supplementary data e.g. replacement installation (-bis), -short or –long. 'BedEC' represents an electrical conductivity probe installation, with a digit representing the order of installation. 'FC' represents the location of an extracted freeze core sample with a digit representing the order of sampling. 'U/S' and 'D/S' are shorthand for upstream and downstream respectively. (Modified from Cuthbert *et al*., In Press)

3 DATA

3.1 Temperature Measurement and Collection

The multilevel temperature probe was installed at the HZ test site by the University of Birmingham as part of the SWITCH project. It is located approximately 5m downstream of the extraction borehole and is compiled of a vertical array of 4 thermistors which were positioned at depths of 0.09m, 0.185m, 0.285m and 0.395m within the streambed. The thermistors were connected to a Hobo datalogger which was set to record temperature measurements at each depth at 5 minute intervals, with the ability to log up to 44000 measurements. The datalogger was placed into a protective OtterBox™ which could be safely submerged in the river and secured via a stainless steel rope tether attached to a stainless steel rod, which was driven into the riverbed (Cuthbert *et al.*, In Press). The logger operates by recording changes in voltage measured by the thermistors at each level within the streambed. The thermistors were calibrated at the University of Birmingham before being installed at the HZ test site. The divers located upstream (U/S) and downstream (D/S) of the extraction borehole, recorded river water temperature, also at 5 minute intervals.

Calculated temperature data already available from previous research was provided by Mark Cuthbert, while raw data recorded during the course of this project was downloaded to a laptop during field work at the HZ test site and exported in CSV (comma-separated values) file format. The raw voltage data from the datalogger was then imported into a simple spreadsheet in order to apply a linear conversion calculation to produce the observed temperature time series. These conversion calculations were carried out according to the same procedure applied to produce the already available temperature data.

3.2 Temperature Data

The data collected ranges from August 2008 to June 2009. The time series is not completely continuous and breaks in the data set can be seen due to various circumstances such as logger malfunction, or simply poor weather making retrieving the data impossible. Figures 5 and 6 below show the temperature time series data collated for this study. A copy of the temperature time series data used for this study is given in Electronic Appendix A

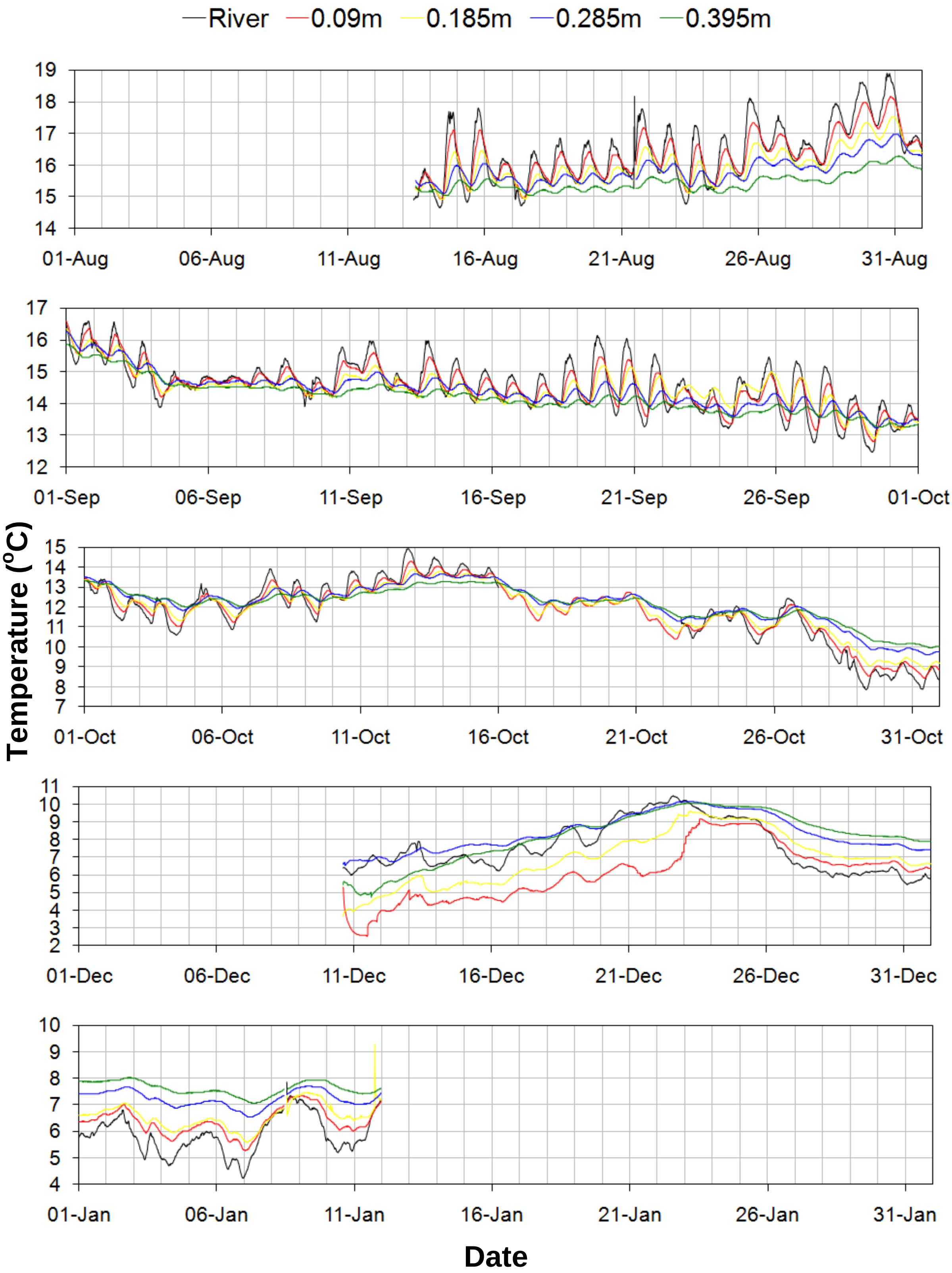

Figure 5: Temperature time series data August 2008 to January 2009. Time series includes river temperature from river divers and temperature signal from the 4 depths monitored by the multilevel temperature probe installed at the HZ test site. Nb. no data was available for November 2008.

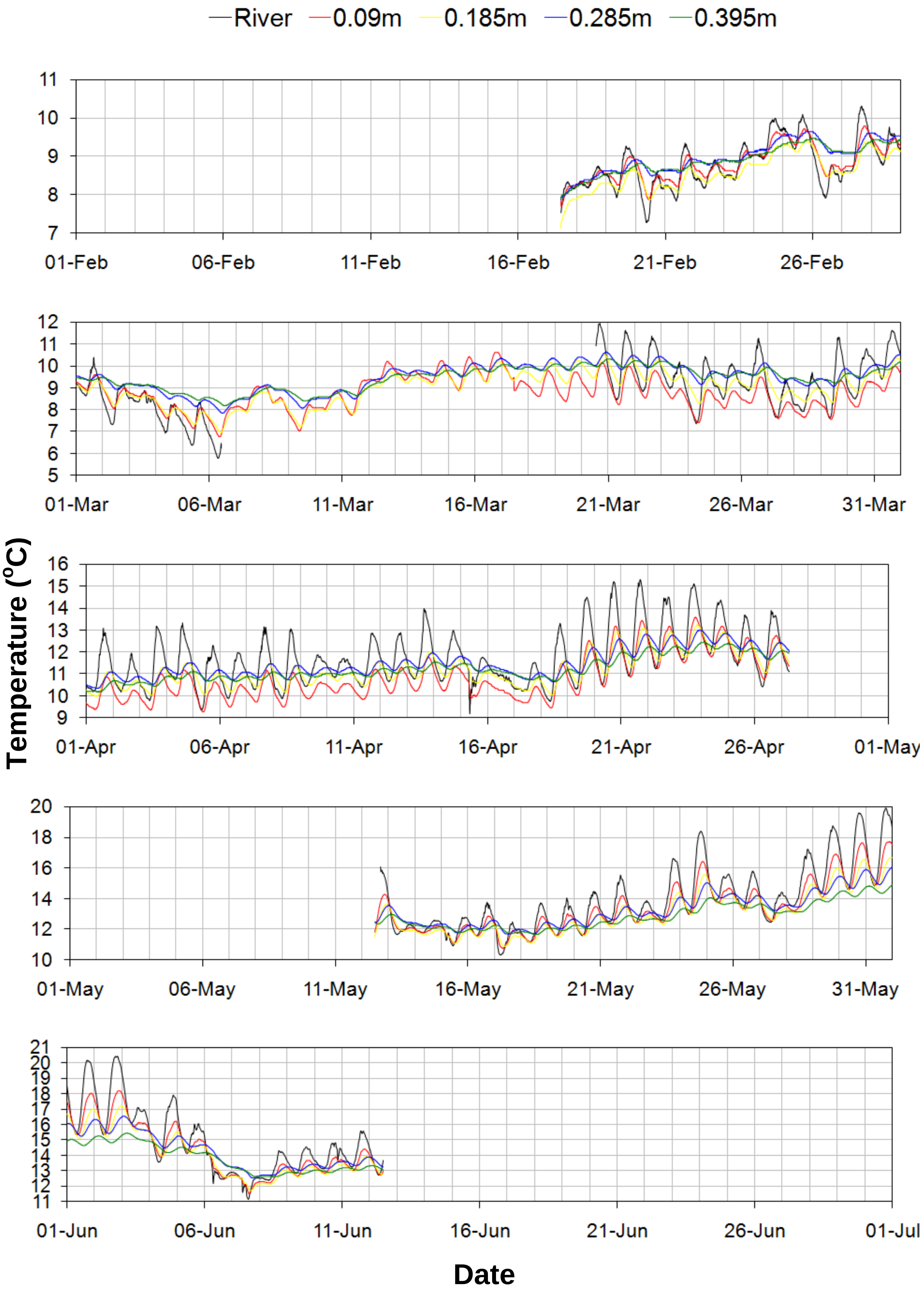

Figure 6: Temperature time series data February 2009 to June 2009. Time series includes river temperature from river divers and temperature signal from the 4 depths monitored by the multilevel temperature probe installed at the HZ test site.

3.3 Head Data

Time series of river level data was available via the river divers installed upstream and downstream of the extraction borehole and is shown in Figure 7. The datum for the site the cover plate for the extraction borehole and its elevation estimated at 96m AOD (Cuthbert *et al.*, In Press). A copy of the river head time series data used for this study is given in Electronic Appendix A.

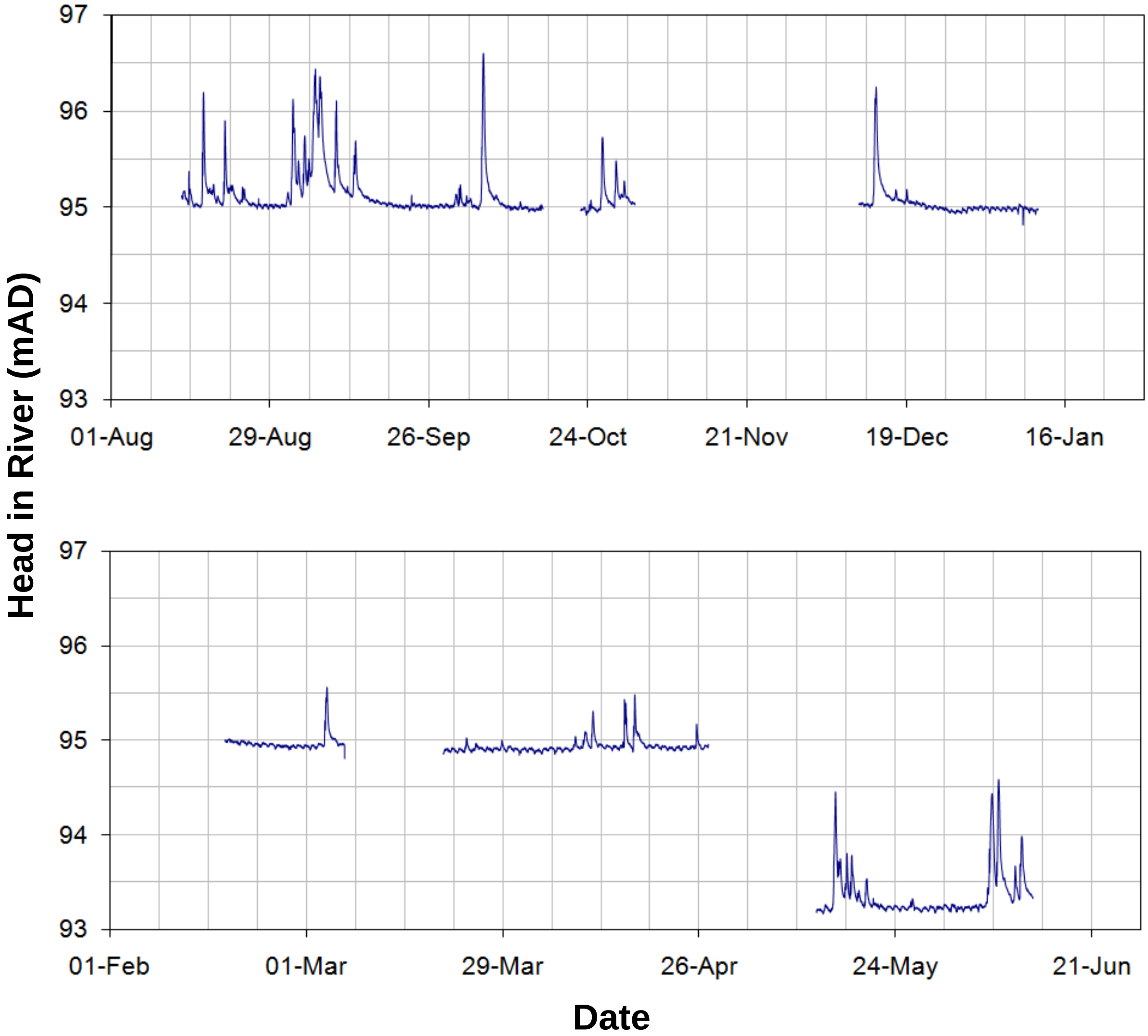

Figure 7: Time series for head in the River Tame at the HZ test site for the August 2008 to June 2009

4 ANALYTICAL MODELLING

4.1 Introduction

Analytical solutions have been used in many studies and in many formats to estimate the vertical flux in hyporheic sediments. The decision to use analytical modelling was based on the uncertainty of thermal and hydraulic parameters for the HZ test site. This would also cultivate a broader understanding of the thermal behaviour of the system.

As discussed in Section 1.2, the Stallman (1965) solution for one-dimensional heat transfer through a homogeneous medium at constant flux and sinusoidal surface temperature oscillation has been used in numerous studies to analyse temperature time series data. The solution provided by Stallman (1965) allows the calculation of a vertical flux based on sinusoidal temperature oscillation at the surface or top boundary. However, this assumption of a sinusoidal oscillation of temperature does not accurately reflect real temperature time series data. Moreover method described by Hatch *et al.*, (2006) and Keery *at al.*, (2007) require some form of pre-processing of the data to delineate phase shifts or extract diurnal temperature signals from the observed time series. In order to more accurately analyse temperature time series data directly using observed river temperature data in an analytical model, a different solution had to be sought from the Stallman (1965) methods described in Section 1.2. A method was required to analytically model temperature propagation within the riverbed using time-varying surface temperatures as a top boundary condition. Thus, a solution was sought to analyse the temperature time series data ‘as given’.

4.2 Ogata-Banks Solution (1961) and Thermal Analogue

The one-dimensional form of the solute transport equation (Equation 1) describes changes in concentration of non-reactive dissolved contaminants in a saturated homogeneous and

isotropic medium under steady state and uniform flow conditions at time, *t* and distance *l*, from a source (Hiscock, 2004):

$$\frac{\partial C}{\partial t} = D_l \frac{\partial^2 C}{\partial l^2} - \bar{v}_l \frac{\partial C}{\partial l} \qquad (1)$$

Where: *C* is concentration

t is time

D_l is the hydrodynamic dispersion coefficient in the longitudinal direction

l is distance from source

$\bar{v}_l$ is velocity of groundwater which is positive in the longitudinal direction

Ogata and Banks (1961) provided an analytical solution to the one dimensional advection-dispersion equation above:

$$\frac{C}{C_0} = \frac{1}{2}\left[erfc\left(\frac{l - \bar{v}_l t}{2\sqrt{D_l t}} \right) + \exp\left(\frac{\bar{v}_l l}{D_l} \right) erfc\left(\frac{l + \bar{v}_l t}{2\sqrt{D_l t}} \right) \right] \qquad (2)$$

where: *t* is time

l is distance from source

C_0 is the constant concentration at the source

C is the concentration at time t, and distance l from source

D_l is the dispersion coefficient in the *l* direction

erfc is the complementary error function

$\bar{v}_l$ is the groundwater velocity in the *l* direction

This solution was designed to look at contaminant concentration down gradient from a constant source at a distance, x, and a time, t. This solution is a step function requiring an input of concentration and has the following boundary conditions:

$C(l, 0) = 0 \qquad l \geq 0$

$C(0, t) = 0 \qquad l \geq 0$

$C(\infty, t) = 0 \qquad l \geq 0$

Temperature propagation through sediments is generally dominated by heat transport via advection (heat transported by moving water) and conduction through the solid, fluid and gas phase of the sediment. Following from this, it is possible to describe one-dimensional heat transfer through a vertical column of saturated sediment with constant flux using an equation analogous to Equation 1 (Keery *et al*., 2007):

$$\frac{\partial T}{\partial t} = \frac{k_e}{\rho c}\frac{\partial^2 T}{\partial z^2} - q\,\frac{\rho_w c_w}{\rho c}\frac{\partial T}{\partial z} \qquad (3)$$

where: T is temperature

t is time

z is depth

q is flux (positive in z direction)

k_e is the effective thermal conductivity of the saturated material

ρ is density of the saturated material

c is specific heat of saturated material

ρ_w is the density of water

c_w is the specific heat of water

By using the Ogata-Banks (1961) solution, concentration profiles within a saturated medium can be calculated. Analogously, thermal profiles can be computed by using a thermal analogue of Ogata-Banks (1961) solution. To achieve this, the solute transport terms of the Ogata-Banks (1961) solution (Equation 2) are substituted for their thermal counterparts i.e. the corresponding terms in equations 1 and 3:

$$\frac{T}{T_0} = \frac{1}{2}\left[erfc\left(\frac{z - q\,\frac{\rho_w c_w}{\rho c}\,t}{2\sqrt{\frac{k_e}{\rho c}\,t}} \right) + \exp\left(\frac{q\,\frac{\rho_w c_w}{\rho c}\,z}{\frac{k_e}{\rho c}} \right) erfc\left(\frac{z + q\,\frac{\rho_w c_w}{\rho c}\,t}{2\sqrt{\frac{k_e}{\rho c}\,t}} \right) \right] \qquad (4)$$

where the respective terms are the same as that described for Equation 3 and erfc is the complementary error function. Substituting the equations for bulk volumetric heat capacity of the saturated sediment (*VHC*):

$$VHC = \rho c \qquad (5)$$

volumetric heat capacity of water (VHC_w):

$$VHC_w = \rho_w c_w \qquad (6)$$

and thermal diffusivity (α):

$$\alpha = \frac{k_e}{\rho c} \qquad (7)$$

into Equation 4:

$$\frac{T}{T_0} = \frac{1}{2}\left[erfc\left(\frac{z - q\dfrac{VHC_w}{VHC}t}{2\sqrt{\alpha t}} \right) + \exp\left(\frac{q\dfrac{VHC_w}{VHC}z}{\alpha} \right) erfc\left(\frac{z + q\dfrac{VHC_w}{VHC}t}{2\sqrt{\alpha t}} \right) \right] \qquad (8)$$

As can be seen from Equation 8, the solute transport terms in the Ogata-Banks (1961) solution of the advection-dispersion equation are replaced by their respective thermal analogues: velocity is replaced by flux multiplied by the ratio of volumetric heat capacity of water to the bulk volumetric heat capacity of the saturated sediment with the water flux in the vertical (*z*) direction, and the hydrodynamic dispersion coefficient is replaced by thermal diffusivity.

Referred to as the 'modified Ogata-Banks solution' hereafter, this produces a one dimensional step function for heat flow through a homogeneous system which can be used to make a semi-analytical model for conduction and advection of heat using superposition of step functions to calculate the vertical flux through a medium. The principle of superposition can be applied simply by adding surface temperature changes (i.e. changes in river temperature) to an initial temperature condition at depth *z*, with each individual surface temperature variation being input into Equation 8 (or Equation 4) above. The fluctuations in surface temperature mark time steps in the model, which form a time and temperature varying top boundary condition for the solution. The output from modified Ogata-Banks solution after each surface temperature fluctuation (or time step) is added in a stepwise fashion to the set initial temperature condition at depth *z*, resulting in a given temperature at time *t* and depth *z*. Therefore, it is possible to calculate the temperature at a given depth and time providing values are input for the required thermal and physical variables, appropriate initial conditions can be set, and the oscillation of surface temperature is known. This semi-analytical method requires a time series of surface temperature for the top boundary condition

at z = 0, which can differ at the start of each individual step. Using this step function allows variation in amplitude of temperature oscillations over time, thus providing a direct method of analysing a time-variant real system.

4.3 Implementing the Ogata-Banks analytical model

A method utilising the modified Ogata-Banks solution was designed and written using Visual Basic (VB) language. The design had to allow the input of the required parameters and the computation of a temperature time series at a specified depth using a semi-analytical approach. The program was required to calculate the temperature profile using the modified Ogata-Banks solution over a set period of time which would then allow thermal parameters and flux to be calibrated against observed data. Once calibrated the model would provide average flux values and thermal parameters over a selected period of time. Prior to VB programming, the method of superposition described in the previous section was tested in a spreadsheet format simply by adding up successive rows to a set initial condition within the spreadsheet. This allowed the method to be tested and calculations to be checked before programming began.

Initially the program was written to investigate temperature at a single depth but was modified during initial calibration to allow up to four depths to be modelled on a single run. It was deemed sufficient to have a maximum of four depths as the data used in this study was taken from a multilevel probed which recorded temperature at four different depths. The program can, however, be easily adapted to look at more or less depths. This allowed increased efficiency in calibration by providing simulated temperature profiles at multiple depths.

The physical parameter inputs required by the program are simply the same as those required by the modified Ogata-Banks solution, although the model requires the input of 4

values of depth (z_1, z_2, z_3, z_4) in metres. Other inputs required include: a time series of surface temperature data in ^{o}C (as a top boundary condition); initial temperature condition at each depth of investigation in ^{o}C ; the observed temperature time series for each depth of investigation in ^{o}C (to allow a residual error statistics to be calculated and graphical comparison between model simulations and the observed data); the run time for the model in days (equal to the length of time of the observed temperature time series data); the size of each time step in minutes (in this study time steps of 5 minutes were used to mirror the intervals of the observed temperature time series).

Once the required inputs are set and a model run is initiated, the model first calculates the size of data array required for the whole simulation using the input run time. The model then computes the change in surface temperature at each time step. This change in surface temperature is used in the modified Ogata-Banks solution to calculate the change in temperature at each depth for the first time step, with these values being added to the initial temperature condition for that depth. This creates a new temperature for each depth after the first time step which is stored by the model for output at the end of the model run. For the next time step the model calculates a new temperature change at each depth for the end of that time step using the change in surface temperature during that time step. This is then added to the new temperature calculated for the first time step, which is again stored for output. This process is continued for all subsequent time steps until the model has completed the run. Residual errors and squared residual errors for each depth are then calculated for each time step using the simulated data and observed data input by the user. From this the program calculates mean square error (MSE) and the root mean square error (RMSE) of the residuals for each considered depth, as well as average MSE and RMSE values over all depths for the entire model run.

The program outputs a number of different values in numerical and graphical format to ease calibration of the model. Simulated temperature values calculated by the model at each depth are output numerically and are also displayed in a graphical format alongside the observed temperature time series at the surface and at each depth of investigation (Figure 8), providing a visual comparison by which to calibrate the model. In addition, the program numerically outputs residual error and squared residual error statistics for each time step and each depth. A graphical output of the squared residual error for each depth is also provided for the entire model run, again to assist in assessing the 'goodness of fit' of the model during each simulation. Values for MSE and RMSE for each considered depth are also output, with average MSE and RMSE values over all depths being output at the end of each model run.

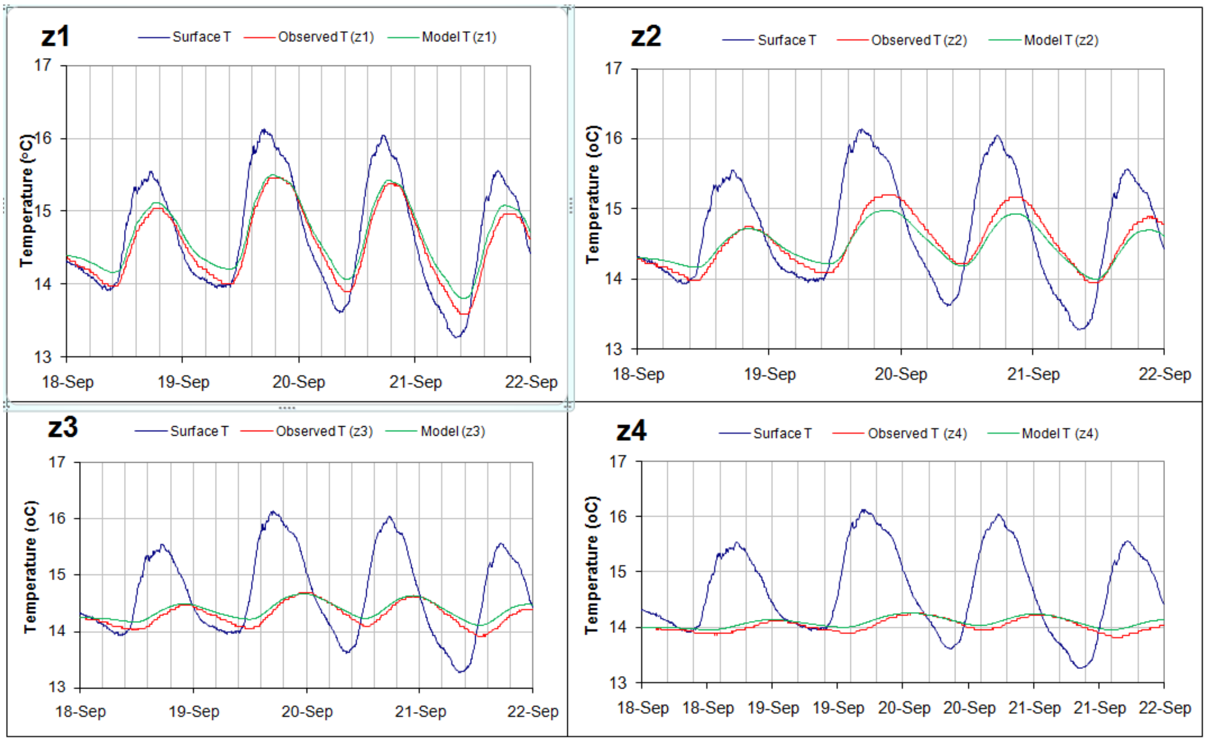

Figure 8: Example of graphical output from modified Ogata-Banks model (for period 19/09/08 to 21/09/08) showing surface temperature and simulated vs. observed temperature profiles. Depths: z1 = 0.09m, z1 = 0.185m, z1 = 0.285m, z1 = 0.395m

As shown in Equation 8, the modified Ogata-Banks solution only requires bulk thermal properties for saturated sediment. As a result it is possible to use this model simply by inputting thermal properties for bulk saturated sediment (as well as thermal properties for water). However, the option to compute a weighted arithmetic mean values for bulk density, bulk specific heat and bulk thermal conductivity was created, using the following standard equations:

$$\rho = \rho_r(1-n) + \rho_w n_{eff} + \rho_a(n - n_{eff}) \tag{9}$$

$$c = c_r(1-n) + c_w n_{eff} + c_a(n - n_{eff}) \tag{10}$$

$$k = k_r(1-n) + k_w n_{eff} + k_a(n - n_{eff}) \tag{11}$$

where: ρ is the bulk density of the saturated sediment

ρ_r is the density of the solid sediment

ρ_w is the density of water

ρ_a is the density of air or gas phase

c is the bulk specific heat of saturated sediment

c_r is the specific heat of the solid sediment

c_w is the specific heat of water

c_a is the specific heat of air or gas phase

k is the bulk thermal conductivity of the saturated sediment

k_r is the thermal conductivity of the solid sediment

k_w is the thermal conductivity of water

k_a is the thermal conductivity of air or gas phase

This option allowed values to be input for total porosity, effective porosity, density of solids and liquids, specific heat of solids and liquids and thermal conductivity of solids and liquids. This would allow either bulk estimates of thermal parameters for the sediment to be used or allow the input of defined thermal properties of different materials to be input, as well as porosity values in order to calculate the bulk properties. The option of adding in the required parameters to compute the effects of a gas phase were also available by changing the effective porosity of in the model. Although this option was simple to implement into the workings of the model, the thermal parameters and porosity values of the sediments under investigation were not known and as a result estimates of bulk properties of saturated sediments were use for calculation. The required and optional input parameters for the modified Ogata-Banks program developed for this study are given in Table 1.

This semi-analytical model is inherently flawed by the stepwise approach to calculating temperatures at depth by its inability to input a smooth time series of surface temperature, but providing the measurements are taken at high frequency the superposition of step functions approach can provide a realistic solution. Obviously the higher the frequency of measurement the more realistic the temperature profile input into the model and the greater the accuracy of the output. In this case measurements were recorded at five minute intervals which dictated the size of the time steps used in the model and was deemed sufficient for the purpose of this study. It should also be noted that the version of the modified Ogata-Banks program used here was developed specifically for this study but can be adapted easily for other similar studies using temperature time series data. A working version of the modified Ogata-Banks model is given in Electronic Appendix B.

Input Parameter	***Symbol***	***Units***	***Value if constant***	***Comment***
Bulk Porosity	n	-	-	Optional
Effective Porosity	n_{eff}	-	-	Optional
Density of Rock	ρ_r	kg m^{-3}	-	Optional
Density of Water	ρ_w	kg m^{-3}	999.2*	Required
Density of Air/Gas	ρ_a	kg m^{-3}	-	Optional
Bulk density of material	P	kg m^{-3}	-	Required (could be input manually or computed via weighted arithmetic mean using other optional parameters)
Specific Heat of Rock	c_r	J kg^{-1} K^{-1}	-	Optional
Specific Heat of Water	c_w	J kg^{-1} K^{-1}	4186*	Required
Specific Heat of Air/Gas	c_a	J kg^{-1} K^{-1}	-	Optional
Bulk Specific Heat of material	C	J kg^{-1} K^{-1}	-	Required parameter (could be input manually or computed via weighted arithmetic mean using other optional parameters)
Thermal Conductivity of Rock	k_r	W m^{-1} K^{-1}	-	Optional
Thermal Conductivity of Water	k_w	W m^{-1} K^{-1}	0.58*	Required
Thermal Conductivity of Air/Gas	k_a	W m^{-1} K^{-1}	-	Optional
Bulk Thermal Conductivity of material	K	W m^{-1} K^{-1}	-	Required parameter (could be input manually or computed via weighted arithmetic mean using other optional parameters)
Time Step	Δt	minutes	5	Required
Observation Depth up to 4 depths)	z_i	m	0.09, 0.185, 0.285, 0.395	Required
Initial Temperature (each observation depth)	T_0	^oC	Variable, dependent on dataset	Required
Surface temperature	T_i	^oC	Variable, dependent on dataset	Required
Run Time	-	days	Variable, dependent on dataset	Required

Table 1: Input parameters for the modified Ogata-Banks VB program. *Values are for water at 15^{o}C from Lal (2005)

4.4 Calibration Method

4.4.1 Stable periods

As there was a large dataset available for this study and average flux over a period was being calculated, only time periods of stable weather conditions were used for calibration, referred to as 'stable periods' hereafter. This allowed calibration of thermal parameters and flux values which could then be used to examine flux variation during storm events or pump tests. Ten periods of stable water level were selected from the dataset to calibrate from with a subset of three of these being used in the first instance as they also showed steady oscillation of surface temperature. The stable periods are shown in Table 2.

Period	***Comment***
24/08/08 – 30/08/08	stable water level
14/09/08 – 17/09/08	stable water level and steady temperature fluctuation
18/09/08 – 21/09/08	stable water level and steady temperature fluctuation
11/10/10 – 15/10/08	stable water level and steady temperature fluctuation
25/12/08 – 30/12/08	stable water level
01/01/09 – 07/01/09	stable water level
09/01/09 – 11/01/09	stable water level
21/02/09 – 28/02/09	stable water level
29/03/09 – 07/04/09	stable water level
19/04/09 – 24/04/09	stable water level

Table 2: Period of stable river level and/or temperature used for calibration of the modified Ogata-Banks program

Manual calibration of the modified Ogata-Banks model using these datasets was carried out using the numerical output of error statistic and the graphical output of the simulated data to test goodness of fit with the observed data. Calibration was performed using the bulk density, bulk thermal conductivity and bulk volumetric heat capacity, with q = 0. The aim was to minimise the RMSE error between the modelled temperatures and observed temperature, and accurately simulate the observed temperature profile at each depth. After calibrating to find the best average volumetric heat capacity and thermal conductivity only,

flux was introduced to attempt to improve the calibration. Thus, for each period a calibrated set of parameters was established as well as a best fit flux *q*.

4.4.2 Storm episodes and pumping test

The parameters obtained for each stable period provided a parameter range to use for analysis of flux during storm events and during the period where the long term pumping test at the HZ test site was stopped. Data from six high flow events between August 2008 and April 2009 were used to assess the impact of increased head in the river, in particular to investigate the possibility of recognising flow reversals using temperature time series data to analyse any change in vertical flux direction. To assess if there was any flux change during storm events, calibrated thermal parameters from the nearest stable period were input into the model and kept constant, while flux was varied until a best fit was achieved. A similar method was used to examine any impact on the subsurface temperature profile or modelled vertical flux when the long term pumping test at the HZ test site, which had been pumping since 18/12/08, was stopped. The period prior to the pump being switched off (21/05/09 to 28/05/09) experienced a relatively stable water level, and as such was used to calibrate the model prior to examining the time immediately after the pump was stopped. The six storm events and the period leading up to and directly after the cessation of pumping at the HZ test site are shown in Table 3.

Period	***Scenario***
01/09/08 – 12/09/08	High water level
04/10/08 – 06/10/08	High water level
25/10/10 – 27/10/08	High water level
12/12/08 – 14/12/08	High water level
02/03/09 – 04/03/09	High water level
14/04/09 – 16/04/09	High water level
21/05/09 – 05/06/09	Pumping period – long term pumping test ceased on 29/05/09)

Table 3: Periods used to assess the effect of storm events and borehole pumping on thermal profile and vertical flux direction

4.5 Results

4.5.1 Modelled flux during periods of stable river level

The calibrated thermal parameters and modelled vertical flux values for the selected stable periods using the modified Ogata-Banks solution are shown in Table 4.

Period	***Bulk Volumetric Heat Capacity x10^6 (J m^{-3} K^{-1})***	***Thermal Conductivity (W m^{-1} K^{-1})***	***Thermal Diffusivity x10^{-6} (m^{2}s^{-1})***	***Vertical Flux positive in downward direction x10^{-6} (ms^{-1})***	***Average RMSE from Ogata-Banks Model***
24/08/08 – 30/08/08	2.25	4	1.78	-3.6	0.185
14/09/08 – 17/09/08	1.82	3	1.65	0.2	0.079
18/09/08 – 21/09/08	1.63	3	1.85	-2.1	0.107
11/10/08 – 15/10/08	1.75	2.5	1.43	-0.4	0.070
25/12/08 – 30/12/08	1.65	2.5	1.52	-0.5	0.128
01/01/09 – 07/01/09	1.26	1.6	1.27	0.6	0.133
09/01/09 – 11/01/09	2.3	1.9	0.83	-1.2	0.066
21/02/09 – 28/02/09	1.6	2.5	1.56	-0.4	0.056
29/03/09 – 07/04/09	1.6	2.3	1.44	-0.8	0.137
19/04/09 – 24/04/09	1.5	2.3	1.53	-1.1	0.172

Table 4: Calibrated flux and thermal parameter values for the modelled stable periods

During the calibration process there were several unusual or anomalous profiles at certain depths which showed a considerable increase in residual error in comparison to other depth profiles during that period. In these instances calibration was based on fitting a simulated thermal profile to those depths which showed comparable behaviour. For several periods (18/09/08 to 21/09/08, 09/01/09 to 11/01/09 and 21/05/09 to 24/05/09) the temperature profile for 0.185m depth displayed noticeably larger than average residuals when compared to the residual errors for other depths during these periods.

4.5.2 Modelled flux during storm episodes

The results from the modified Ogata-Banks model when used to analyse flux variation during periods of increased flow are shown in Table 5.

Period	***Approx. Increase in River Head (m)***	***Bulk Volumetric Heat Capacity x10^6 (J m^{-3} K^{-1})***	***Thermal Conductivity (W m^{-1} K^{-1})***	***Thermal Diffusivity x10^{-6} (m^{2}s^{-1})***	***Vertical Flux positive in downward direction x10^{-6} (ms^{-1})***	***Average RMSE from Ogata-Banks Model***
01/09/08 – 12/09/08	1.4	2.25	4	1.78	1.1	0.133
04/10/08 – 06/10/08	1.5	1.75	2.5	1.43	1.5	0.563
25/10/10 – 27/10/08	0.7	1.75	2.5	1.43	0.5	0.320
12/12/08 – 14/12/08	1.25	1.65	2.5	1.51	1.9	0.376
02/03/09 – 04/03/09	0.6	1.6	2.5	1.56	2.8	0.327
14/04/09 – 16/04/09	0.6	1.5	2.3	1.53	1.8	0.313

Table 5: Calibrated flux and thermal parameter values for the modelled storm flow periods

As can be seen from the modelled values of flux during high flow events, there is a consistent indication that vertical flux direction is reversed. Downwards flux values seen in Table 5 indicate substantial inflow to the hyporheic sediments but the residual errors from the model during such storm episodes are also relatively high in comparison to those residuals from modelled stable periods. These high residuals hint at something further with regards to the system during flow reversals resulting from increased river levels, which cannot be simulated by using such a simplified model. In particular, the period from 4/10/08 to 06/10/08 saw one of the highest increases in river level, an increase of approximately 1.5m. Although the model indicates a change in flow, the residual errors in this model run were substantially higher than the average errors, indicating that there is a limit within this model for quantifying the impact of storm episodes and that the observed data is perhaps showing a lateral component of flux and/or the thermal properties are being influence by flow reversal.

4.5.3 Modelled flux during and after pumping test

Calibrated thermal parameters and modelled flux values before and after the pumping test was stopped using the modified Ogata-Banks solution are shown in Table 6.

Period	***Bulk Volumetric Heat Capacity x10⁶ (J m⁻³ K⁻¹)***	***Thermal Conductivity (W m⁻¹ K⁻¹)***	***Thermal Diffusivity x10⁻⁶ (m²s⁻¹)***	***Vertical Flux positive in downward direction x10⁻⁶ (ms⁻¹)***	***Average RMSE from Ogata-Banks Model***
21/05/09 – 24/05/09	1.33	2.2	1.65	-0.26	0.131
25/05/28 – 28/05/09	1.65	2.5	1.52	-0.5	0.299
29/05/09* – 31/05/09	1.49	2.5	1.68	-0.8	0.208
01/06/09 – 05/06/09	1.49	2.5	1.68	-1.4	0.236

Table 6: Calibrated flux and thermal parameter values for the period before and after pumping of the extraction borehole at the HZ test stopped. *indicates day when pump was stopped

The modelled flux values for the two modelled periods prior to pumping are relatively similar. They indicate a small upward flux from the hyporheic sediments. However, after the pump is switched off there is a steady but clear increase in vertical flux. Figure 9 shows a graph of the squared residual errors for this entire period, showing the temperature profile before and after pumping, using average thermal parameters and flux values for the two modelled periods leading up to the pump being switched off. It can be seen from this that when the pump is switched off on the 29/05/08, a definite increase in residual error in the model starting on 29/05/08 and gradually increasing over the subsequent few days. The model residuals from the two deepest levels of the temperature probe (0.285m and 0.395m) show a continual increase in upwards flux over the days immediately after the pumping test, a response which is not mirrored as strongly in the upper two temperature profiles (0.09m and 0.185m), although an increase in upwards flux relative to the period before pumping stopped was estimated for all depths. The issues experienced in fitting thermal profiles at 0.09m and 0.185m with those observed at 0.285m and 0.395m might be as a result of the pumping test being stopped, but the more evidence would be required to support this conclusion.

Furthermore, during the period modelled between 25/12/08 and 30/12/08, shortly after the pump test was initiated, the residuals for depths of 0.185m, 0.285m and 0.395m showed a better fit when the flux was decreased, with the uppermost profile, 0.09m, having a better fit with a higher flux. The nature of this change in temperature profile and the flux estimates derived from modelling seem to indicate that the deeper sediments are hydraulically connected to the extraction borehole. It can also be argued that this is a sign of the hyporheic outflow from the riverbed sediments being subdued at depth by the pumping of the extraction borehole.

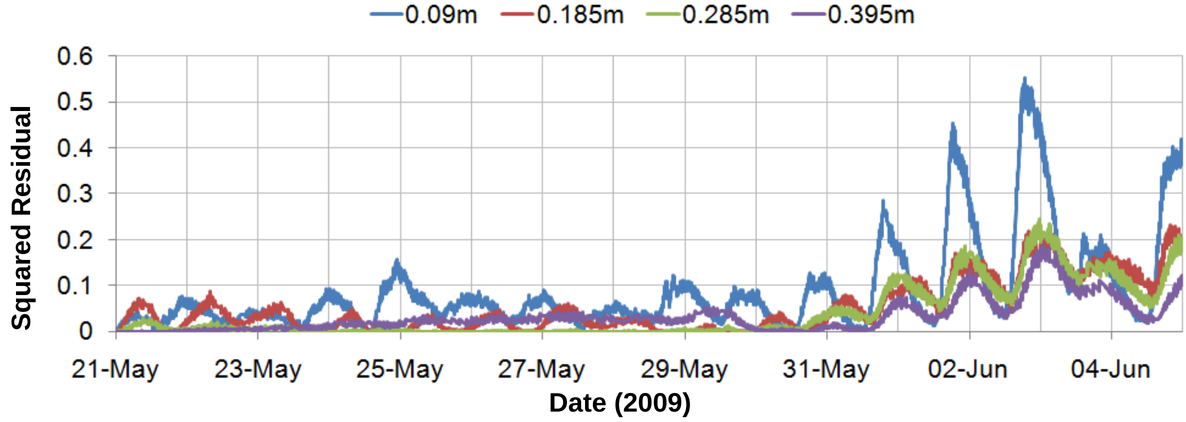

Figure 9: Graph of squared residuals from model run for period 21/05/09 to 05/06/09. Nb. Pump is switched off on 29/05/09

4.6 Sensitivity Analysis

Sensitivity analysis was carried out on the modified Ogata-Banks model by increasing and decreasing each input parameter by 20%. Figures 10 and 11 show the relative sensitivity of the model output to changes in magnitude of different parameters for periods where a low vertical flux was estimated and a period where high vertical flux was estimated. Sensitivity analysis was carried out on several modelled periods and indicated greatest sensitivity to variations in thermal conductivity. Sensitivity analysis also highlighted the relationship between uncertainty and the magnitude of estimated flux. In the case of lower fluxes the sensitivity of the model to changes in thermal parameters and flux is noticeably reduced relative to the sensitivity for higher fluxes. The implications of this are that for modelled flux values which are relatively low, the uncertainty in the estimates for flux and thermal properties is greatly increased. This is discussed further in Chapter 7.

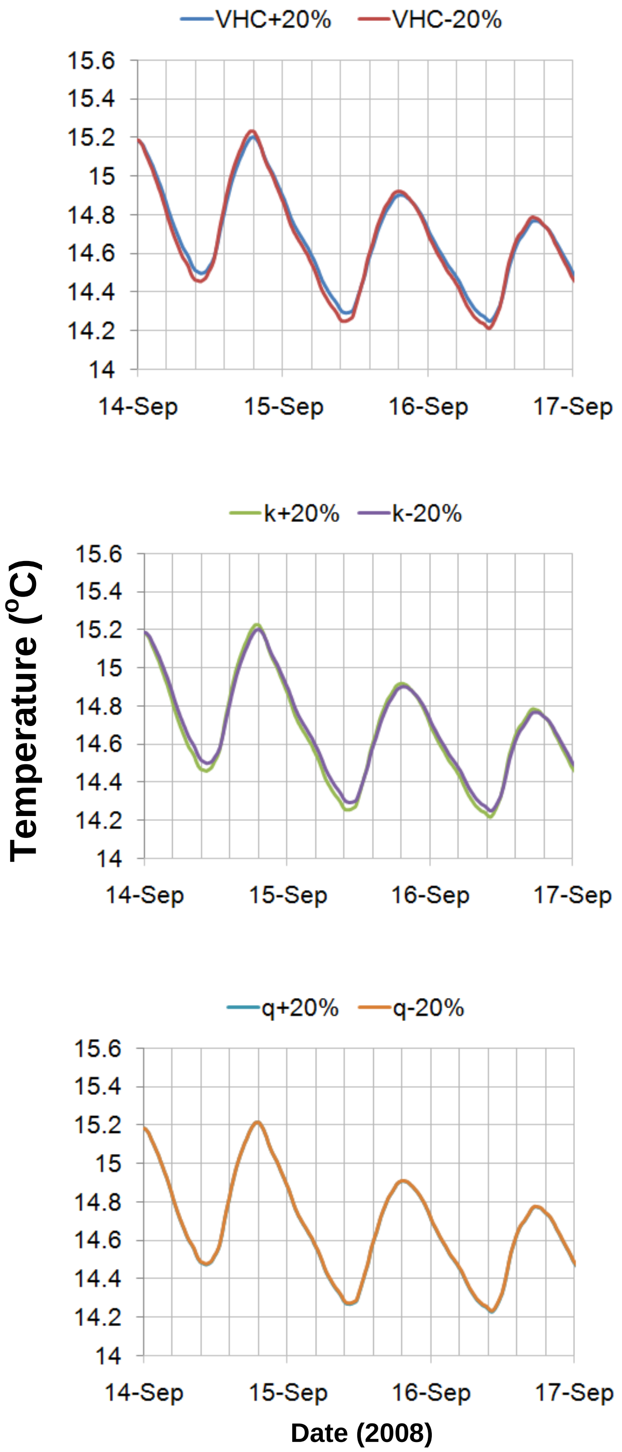

Figure 10: Sensitivity analysis for period 14/09/08 to 17/09/08 (low calibrated flux)

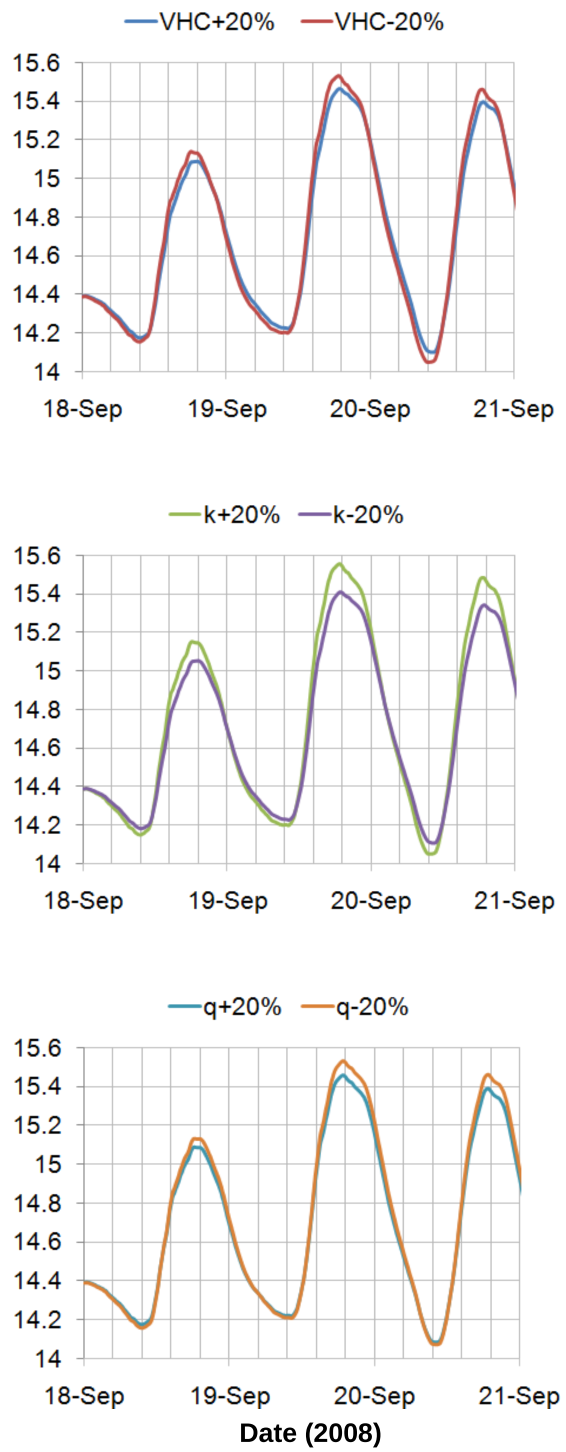

Figure 11: Sensitivity analysis for period 18/09/08 to 21/09/08 (high calibrated flux)

5 NUMERICAL MODELLING

5.1 Introduction

In order to validate the modified Ogata-Banks semi-analytical model and assess its applicability a numerical modelling exercise was undertaken. This involved conceptualising and constructing a numerically based model using the data available from various installations at the SWITCH test site. This approach would be used to examine selected periods to serve as a validation for the flux estimates obtained for the same period using the modified Ogata-Banks solution. The software chosen for numerical modelling was the United States Geological Survey (USGS) variably saturated two-dimensional water and heat flow program VS2DH (Healy & Ronan, 1996) which is combined with the graphical user interface VS2DI[*] (Hsieh *et al.*, 1999). This software package (herein referred to as VS2DI) can be used to simulate flow, solute transport and heat transport in porous media with variable saturation. The software setup involves: a graphical based pre-processor to construct the model domain and input various required parameters; two numerical models available to solve for water, solute and heat transport; and a postprocessor which provides visualisation of the results via a simple animation using outputs at selected time steps (Healy, 2008). The model solves the Richards equation (Richards, 1931) for flow and the advection-dispersion equation for solute or heat transport using the finite-difference method. There are many software packages which can be used for temperature time series analysis and thermal propagation through saturated sediments. The VS2DI model was chosen for this study because it offered an easy to use interface for model construction and did not demand extraneous volumes of information on thermal and hydraulic properties. This package has been used in numerous studies looking at

[*] The VS2DI package which includes all the software described in Section 5.1 is publically available and can be downloaded for free from the USGS website (http://www.usgs.gov)

heat flow in riverbed sediments and unconfined aquifers over the last two decades (see Constantz & Stonestrom, 2003; Constantz, 2008; Healy, 2008) and as a tool for evaluating analytical methods of calculating groundwater flux (Schmidt *et al.*, 2008), adding weight to its applicability here.

5.2 Conceptualisation and Construction

The conceptualised system which was used to construct the numerical model was simplified to great extents in order to maintain the assumptions which govern the semi-analytical modified Ogata-Banks solution. The system was assumed to be one-dimensional, homogeneous and isotropic with constant and uniform thermal and hydraulic properties during each model run. In order to validate the Ogata-Banks model the calibrated thermal parameters used for the numerical model were kept the same as the calibrated values obtained from the Ogata-Banks model for each given period. A range of hydraulic conductivity values were used for the purposes of numerical modelling as there is large uncertainty in the hydraulic conductivity of the sediments under investigation. The range used, 0.24 md^{-1} to 3.23 md^{-1} was given by Shepherd (2009) based on constant head permeameter tests conducted on repacked sediments samples from the HZ test site (discussed further in Chapter 6). Other parameters which were required were taken from inbuilt generic values given as an option by VS2DI when defining textural class and transport parameters. As the numerical model was to calculate flux based on input head data and other input hydraulic parameters, one of the main assumptions of the semi-analytical model, constant flux, could not hold. However, the maximum and minimum flux values calculated by the numerical model over the simulated time periods were acquired from the model output file and are given.

The dimensions of the model domain were defined based on the available data hydraulic data from the SWITCH test site. The domain was constructed to simulate a one

dimensional vertical column through the subsurface. Time varying head and temperature data was available for the river via the U/S and D/S divers, which were imported to form the top boundary of the model. The VS2DI package allows the import of a time series of data for head and/or temperature which allocates each imported value(s) to a user defined number of recharge periods. This allowed the creation of a topmost boundary with variable head and temperature. The bottom boundary was defined based on data which had been collected from the borehole diver, which showed a near constant head and temperature throughout the year. This boundary was set at 12m below the top boundary, using the diver position within the borehole as an approximate guide, and the temperature and head data from the borehole diver was imported in a similar fashion to the top boundary. No flow boundary conditions were applied to each side of the model domain to maintain the one-dimensionality of the model.

The initial temperature conditions at each investigated depth were input in accordance to those used in the modified Ogata-Banks model. Observation points were placed to match the four depths of the observed riverbed temperature. The observation points facilitated the output of temperature values for each time step at the designated depth, which could be plotted against observed data for that depth after each model run using a simple spreadsheet. Each recharge period was set at five minutes to match the frequency of the observed data, except the first recharge period which was set to last 4 hours. This allowed the model to reach a steady state of initial conditions before to reduce transient effects during the simulation.

The domain grid was defined to allow only vertical movement of water. Horizontally, the mesh design allowed only one cell to cover the width of the domain. In the vertical direction the grid design formed the finest mesh at the top of the model domain, which became progressively coarser towards the bottom. The grid size for the zone under investigation was set at 0.02m, to a depth 0.46m, which then coarsened downwards to 1m for the lowermost 10m of the domain. The grid mesh size and time steps used for each recharge

period were well within the limits set by the Peclet and Courant numbers calculated for this model. Furthermore, VS2DI allows the user to select from four options to specify the relationship between pressure head and relative hydraulic conductivity (Healy & Ronan, 1996). In this study the preselected van Genuchten function was used to represent hydraulic characteristic functions. Outputs selected for each model run included velocity, fluid balance and energy balance.

5.3 Results

Output from the VS2DI model is provided at each time step, resulting in modelled values for flux being output every five minutes. In order to provide a comparison to the modified Ogata-Banks model, the range of vertical flux is given from the numerical model output for each run. These flux estimates shown in Table 7, along with mass balances errors for fluid and energy (heat). No head or temperature borehole data was available prior to 08/01/09 and as a result the numerical modelling focussed on periods where there was enough data to define the lower boundary condition over time.

Period	***Ogata-Banks Vertical Flux positive in downward direction x10^{-6} (ms^{-1})***	***VS2DI Vertical Flux positive in upward direction x10^{-6} (ms^{-1})***		***Total Mass Balance Error from VS2DI Simulation***	
		For K = 0.24md^{-1}	***For K = 3.23md^{-1}***	***Average Fluid Error (%)***	***Average Energy Error (%)***
09/01/09 – 11/01/09	-1.2	0.31 – 0.39	4.22 – 5.30	0.00	6.55
21/02/09 – 28/02/09	-0.4	0.22 – 0.56	2.34 – 7.60	0.00	1.88
21/05/09 – 28/05/09	-0.26 to -0.5	0.26 – 0.42	3.37 - 5.75	0.00	0.48

Table 7: Vertical flux estimates from numerical modelling using VS2DI. Hydraulic conductivity values based on estimates provided in Shepherd (2009)

6 HYDRAULIC DATA

6.1 Data Collection

Several hydraulic tests have been carried out at the site as part previous studies and the ongoing SWITCH research. Data from manual head tests carried out between October 2007 and July 2008 were made available as a caparison tool for the flux measurements derived from the models created during this study. The collection of this data is documented in Cuthbert *et al.* (In Press). The closest available hydraulic data was taken from piezometer installation P+005-1m, located approximately 0.5m upstream of the multilevel temperature probe. This piezometer is installed to a depth of 49 cm into the riverbed. As the multilevel temperature probe only monitors to a depth of 0.395m, the hydraulic calculations from piezometer P+005-1m includes a 0.105m region not monitored by the temperature probe but allowed a vertical gradient to be calculated over the entire depth interval it covers.

6.2 Freeze Coring

6.2.1 Introduction

In order to calculate flux manually based on Darcy's Law using head data, hydraulic conductivity values for the location around the temperature probe were required. As part of this and other studies at the SWITCH HZ test site (Shepherd, 2009; Cuthbert *et al.*, In Press) a campaign of sediment coring was undertaken with the aim of achieving intact samples of the upper region of the riverbed for analysis. During this sampling campaign, a core was purposefully extracted from close to the multilevel temperature probe to gain an accurate description of the sediment in that region of the riverbed. Through simple sediment analysis

these would allow estimates of hydraulic conductivity to be calculated. Field work was carried out by Mark Cuthbert, Richard Johnson, Simon Shepherd and the author.

6.2.2 Methodology

The method of sediment coring was taken from (Stocker & Dudley Williams, 1972). This method involved driving a hollow metal stake into the river bed and pouring liquid nitrogen into the hollow stake, freezing the sediment onto the stake. The depth to which core could be sampled were limited by the length of the metal stake and the water level in the river. Thus sampling was undertaken after at least three days of little or no rainfall to ensure the river level was low enough to work in safely and to retrieve adequate core lengths. Cores were taken from 9 separate locations within the HZ test zone as indicated in Figure 4. The cores were logged on site and samples taken for laboratory analysis. For the present study the information from only one core (Freeze Core FC8) was used to provide estimates of hydraulic conductivity and as a guide to the likely lithological properties in the substratum. Freeze core FC 8 was taken as close to the multilevel temperature probe as possible, without disturbing installation.

6.2.3 Results

The extracted core is shown in Figure 12. Sediment analysis by Shepherd (2009) provided values for hydraulic conductivity at different depths which were used for manual flux calculation and for numerical modelling, as stated in Section 5.2. A lithological description of core FC8 is given in Appendix A. Full details of the method used and results obtained from sediment analysis for all freeze cores extracted at the HZ test site can be found in Shepherd (2009) and Cuthbert *et al.* (In Press).

Figure 12: Image showing freeze core FC8, shortly after extraction, highlighting the sedimentary textures present in the riverbed near temperature probe P+005-1T

6.3 Vertical Flux Derived from Hydraulic Data

A differential head was calculated using the difference between the water level in piezometer P+005-1m and the water level of the river. A gradient was then calculated by dividing the differential head by the depth from riverbed surface to the middle of the piezometer (Durand *et al*., 2008). As the hydraulic gradient was measured at several times from October 2007 to July 2008 by Durand *et al.* (2008), the maximum (0.19) and minimum (0.09) gradients will be used for calculation. Hydraulic gradients were used to estimate vertical flux based on Darcy's Law. Hydraulic conductivity estimates for various depths (Shepherd, 2009) and calculated flux values are shown in Table 8. These estimates were based on constant head permeameter test on repacked sediment samples from various lithologically distinct layers in core FC8, giving a range of values for hydraulic conductivity. . It should be noted that the range given by Shepherd (2009) for this sediment core is in broad agreement with the values obtained by slug test for the HZ test site by Durand *et al*. (2008) during initial research in autumn 2007.

Depth (m)	*Hydraulic Conductivity (md-1)*	*Calculated Vertical Flux range (ms-1)*
0 - 0.15	Unknown	Unknown
0.15 – 0.17	1.47	1.53E-06 – 3.23E-06
0.17 – 0.25	1.47	1.53E-06 – 3.23E-06
0.25 – 0.39	0.24	2.5E-07 – 5.28E-07
0.39 – 0.46	1.51	1.57E-06 – 3.32E-06
0.46 – 0.51	2.41	2.51E-06 – 5.30E-06
0.51 - 0.56	2.35	2.45E-06 – 5.17E-06
0.56 – 0.61	3.23	3.36E-06 – 710E-06

Table 8: Estimated flux values derived from Darcy based calculations. Nb. hydraulic gradients were measured manually from 23/10/07 to 04/07/08 at piezometer P+005-1m. Range of measured vertical hydraulic gradient is 0.09 – 0.19.

7 DISCUSSION

7.1 Model Results

7.1.1 Comparison of derived vertical flux values

The present study aimed to provide estimates of water flux by applying temperature time series analysis using data from the HZ test site on the River Tame, Birmingham. The semi-analytical model created in this study was able to provide estimates of average flux over a given time period based on direct comparison of observed and simulated data. Vertical flux derived from the modified Ogata-Banks solution are within an order of magnitude range compared to numerically derived values for the same periods of time, i.e. using identical thermal parameters, initial conditions and surface temperature oscillations. For the period between 21/05/09 and 28/05/09 the Ogata-Banks derived flux is at the lower end of the numerically modelled range.

Estimates of vertical flux values from the modified Ogata-Banks solution also lie within the range calculated from hydraulic gradients measured at the site. The role of hydraulic conductivity is important when considering the results from the numerical model and Darcian based equations. At higher flow rates hydraulic conductivity has a larger impact on calculated flux than thermal parameters, with thermal properties becoming more important for simulating flux at period of lower flow (Constantz & Stonestrom, 2003). The uncertainty of hydraulic parameters for the SWITCH site has been discussed by several authors (Durand *et al*., 2008; Shepherd, 2009; Cuthbert *et al*., In Press) and it is for this reason that a range of hydraulic conductivity values were used in the numerical model and hydraulic calculations. Although not providing complete validation for the modified Ogata-Banks method, the

similarity in flux ranges developed from all three sources of flux estimation do provide encouragement for its use.

7.1.2 Temporal variability of flux

Analysis of the derived flux estimates indicates a general lowering of flux during the winter months but this could a result of the relative stability of the river level during winter or may be due to the effects of the long term pumping test which began in December 2008. The latter suggestion is given support by the increase in flux values obtained from the days immediately after the pump was switched off, suggesting that the flux rate was dampened by the ongoing pumping at site, although this remains inconclusive. Modelled flux values from immediately after the test do suggest that the thermal profile within the subsurface was altered by the pumping test, although quantifying this effect would require a more complex analysis of the system, and would likely profit from temperature time series data from other areas within this reach.

7.1.3 Thermal properties and flux

Estimated values for heat capacity and thermal conductivity for the most part fall within the range given by Lal (2005) and shown in Table 9. In analysing the calibrated thermal values from the modified Ogata-Banks method a general decrease in volumetric heat capacity was seen except for an anomalous value during the period from 09/01/09 to 11/01/09. A less obvious decline in thermal diffusivity could be argued but given the uncertainties in the input parameters this remains unconvincing. This is not mirrored in any obvious way by the vertical flux values obtained from the modified Ogata-Banks solution with variable vertical flux estimates being calculated throughout the year. The temporal heterogeneity of river bed sediments is not as well documented as the spatial heterogeneity but studies have shown

significant variation in hydraulic conductivity (Chen *et al*., 2008; Genereux *et al*., 2008) and significant erosion and/or deposition over a period of months resulting in clogging of the stream bed via colmation (Brunke & Gonser, 1997; Rehg *et al*., 2005; Veličković, 2005,

Material	***Heat Capacity (MJ m^{-3} K^{-1})***	***Thermal Conductivity (W$m^{-1}$$K^{-1}$)***
Sandy soil	2.09	1.8
Silt loam soil	1.02	1.2
Peat soil	3.14	0.29
Quartz	2.13	8.8
Other soil minerals	2.39	2.9
Organic matter	2.50	0.25

Table 9: Thermal properties of common sediments from Lal (2005)

Collins & Walling, 2006) and depth filtration (Brunke, 1999). Differences in hydraulic conductivity and thermal propagation could result from such modification of the layered heterogeneity in HZ test site riverbed sediments over time as a result of particulates being released back into the water column during effluent flow and downwelling of fine sediment during flow reversals caused by storm events (Collins &Walling, 2006).

The sedimentary architecture beneath the River Tame is extremely complex as highlighted by the sediments cores taken from the site (Shepherd, 2009; Cuthbert *et al*., In Press) and as such it is impossible to use the method described here to accurately reflect the heterogeneity in the system. Comparable multilevel temperature time series data from other regions of the riverbed would provide a useful validation of the model to assess whether the various anomalous temperature signatures discussed in Section 4.5.1 are a result of more complex goings on in the subsurface or indeed a simple malfunction of equipment. The unusually high residuals observed for 0.185m depth over several stable periods described in Section 4.5.1 highlight the limited scope of this model for assessing and characterising a multidimensional saturated system such as that seen at the HZ test site. There are numerous reasons why this level may experience a unique temperature signature, but given the

lithological description given by Shepherd (2009) is possible that the clay content of this layer is exerting a noticeable effect on the average thermal properties of the sediment column. However, it could also be explained by a simple thermistor malfunction.

The average results presented here over the entire 0.395m of investigation seem to indicate certain influences at different depths which can ultimately not be accounted for by a simple change in flux magnitude or thermal properties. The role of gas storage within the sediments may also contribute to the variance in thermal parameters over time. Cuthbert *et al*. (In Press) report significant volumes of gas stored within the riverbed, which seem to be ubiquitous at the HZ Test site. Preliminary analysis suggests that the build up of gas within the sediments may be attributed to denitrification within the hyporheic sediments, but work on this began during the latter stages of this project and hence could not be incorporated into this study. Although the effect of gas on thermal parameters is not considered here, if the production of gas at the HZ test site is indeed significant and variable over time, then this may also influence the subsurface thermal properties and may also aid in the explanation of unusual thermal signature at different depths and different times.

Flux estimates using the modified Ogata-Banks method give confidence to identifying flow reversals during high water levels events using temperature time series. In all modelled storm scenarios the calibrated flux direction simulated influent conditions, contrasting to the dominantly effluent conditions of the calibrated stable periods. This reach of the River Tame is described as being generally effluent under ambient conditions (Durand *et al.,* 2008). The results from analytical modelling here support this description, at least for the section of the streambed around the installed multilevel temperature probe.

7.2 Model Evaluation

The modified Ogata-Banks program written for this study has a number of simple advantages in analysing temperature time series. Firstly, it is possible to gain an insight into the thermal properties of the media and derive estimates of vertical flux without requiring excessive information in regard to thermal and hydraulic properties. No hydraulic gradient or conductivity data is required to utilise this method. As discussed in Constantz & Stonestrom (2003) the greatest uncertainty when modelling seepage through sediments tends to come from hydraulic parameters, which can vary over several orders of magnitude for a single textural class. Thermal parameters however have a much smaller range when it comes to sediment class and are almost independent of texture (Constantz & Stonestrom, 2003).

This method provides an easy to use analysis of vertical flux and thermal properties using temperature time series data directly without the need for any pre-processing or complex numerical computation.

Disadvantages of the model are generally linked to the simplified assumptions of isotropy, homogeneous properties and average flux which govern the operation of the modified Ogata-Banks solution. In particular, yielding of an averaged constant flux value over a set time interval presents a distinct limit to the use of the modified Ogata-Banks method, making this approach unsuitable for high resolution flux estimation. Other semi-analytical methods are available which utilise the Stallman (1965) solution and can output a time series of flux.

Methods such as that developed by Keery *et al*. (2007), can provide more detailed information about flux change over time but these can require data to be processed before being analysed with the analytical solution. The stepwise, modified Ogata-Banks approach described here can be applied quickly to observed temperature time series and provide useful information regarding the averaged flux and thermal behaviour of a saturated medium.

Moreover, during periods of low flow e.g. 14/09/08 to 18/09/08, the model uncertainty increases considerably, resulting in questionable estimates for thermal parameters, flux direction and magnitude. Stallman (1965) estimated that his solution would be useful for calculating fluxes to a lower limit of around 2.3 $x10^{-7}$ ms^{-1} using standard thermal properties for porous sediments. Similarly, there is a lower threshold for calculating a flux value using the modified Ogata-Banks Solution which would be on a comparable scale to the limit suggested by Stallman (1965) based on sensitivity analysis (Section 4.6). In cases where derived flux values were in the region of $3x10^{-7}$ ms^{-1} or lower, the sensitivity of the model to incremental variation of thermal parameters and/or flux was relatively low, and as such the estimates are delivered within an increased uncertainty.

For the purposes of this project, trial and error seemed an appropriate method from which to calibrate the analytical model given the simplicity of the model setup. During early calibration efforts a best fit simulated thermal profile for each depth was attempted but proved excessively time consuming. In addition, the large dataset which was made available for analysis meant that calibration of every time period would be impossible given the time constraints of this project. In hindsight the development of an optimization code for use in calibration may have been beneficial. It is important to note, however, that optimisation based on residual error within the model may not have yielded the best simulated thermal profile and any optimisation routines implemented would have to be subjected to manual visual analysis to insure the best fit of observed and modelled thermal signatures.

The application of this model is best suited for broad spectrum analysis of average flux and thermal properties, providing a quick and easy to execute method of temperature time series analysis. More precise analysis would require the use of additional methods which are likely to involve more complex implementation.

8 SUMMARY AND CONCLUSION

In recent times efforts to understand the interactions between rivers and groundwater have been increased substantially. The international SWITCH (Sustainable Water (management) Improves Tomorrows' Cities' Health) project is part of this global push to characterise the exchange of surface and subsurface waters along river corridors. In collaboration with the Environment Agency for England and Wales, the University of Birmingham has devised and implemented a dense monitoring network, termed the Hyporheic Zone (HZ) test site, on a reach of the River Tame, Birmingham, for the express purpose of achieving a greater understanding of the nature of the hyporheic zone. As part of the River Tame SWITCH project, high resolution temperature time series data has been collected from a multi-level temperature probe for a period between August 2008 and June 2009.

In this separate study, temperature time series analysis using data from the SWITCH site was used to derive estimates for flux and thermal properties of the hyporheic sediments at the SWITCH HZ test site. Conventional methods of flux calculation based on Darcy's Law can be difficult to implement in such environments and a method was developed to directly utilise the raw observed temperature time series data to provide estimate of thermal flux. The semi-analytical method is based on a thermal analogue of the step function solution developed by Ogata & Banks (1961) for the one dimensional advection-dispersion equation used in solute transport calculations. This method employs a modified version of the Ogata-Banks solution, with substitution of solute transport properties for equivalent thermal properties. The principle of superposition is used in conjunction with the modified Ogata-Banks step function to simulate the temperature profiles at depth within a column of saturated sediment. A program written in Visual Basic (VB) language was used to solve the modified Ogata-Banks equation. By varying the inputs for the program and calibrating using the

graphical output and residual error statistics it is possible to derive an estimate of vertical flux, and other thermal properties.

The application of this method to the HZ test site temperature time series data yielded flux estimates within an order of magnitude range of estimates derived from Darcian based flux calculations based on manual piezometer data gathered by the University of Birmingham during fieldwork at the HZ test site. To further test the validity of the modified Ogata-Banks solution for estimating vertical flux, a one dimensional numerical model was constructed using the USGS software package VS2DI which is capable of modelling flow solute and energy transport in variably saturated media. Estimated thermal parameters derived from the modified Ogata-Banks model were input into the numerical model along with data from borehole and river divers installed at the HZ test site and run over three identical periods which had been modelled using the semi-analytical method. The estimates of flux from the modified Ogata-Banks model fell within the range computed by the numerical model.

Results from the modified Ogata-Banks model indicate consistent upwards flux of varying magnitude during periods of stable river level. Flow reversals are also indicated by vertical flux estimates derived from periods of increased river head. It has also been shown that the influence of borehole testing can seen in the subsurface temperature profile, but the exact magnitude of this influence is inconclusive.

The method developed here can be easily and directly applied to temperature time series data and provides useful averaged estimates of vertical flux and thermal parameters. Although not suitable for complex and high resolution time series analysis, the application of this method can provide useful information regarding water movement and temperature propagation within a saturated medium without the need to define uncertain hydraulic parameters or perform complex pre-processing of data.

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APPENDIX A

Freeze Core FC8

Sample date: 26/06/09

Core collected by M. Cuthbert, M.B. Hendrie, S. Shepherd

Logged by S. Shepherd

Location: 35cm toward borehole side bank from piezometer P+005-1p (box1)

Depth (m)	***Description***	***Hydraulic Conductivity (md^{-1})***
0 - 0.15	sediment lost during extraction	unknown
0.15 – 0.17	Dark brown organic soil; angular and rounded pebbles (0.3 – 1cm)	1.47
0.17 – 0.25	Grey brown clayey sand; pebbles, sub-rounded (0.3 – 1cm)	1.47
0.25 – 0.39	Grey brown clayey sand; pebbles and cobbles, sub-rounded (0.3 –7cm)	0.24
0.39 – 0.61	Orange-brown sand, uniform, fine to medium grained, abundant quartz, some mica	1.51 - 3.23

Table 10: Log and data taken of freeze core FC8. Hydraulic conductivity values were derived from a constant head permeameter teat on repacked sediments samples. (Modified from Shepherd, 2009)

LIST OF ELECTRONIC APPENDICES

Electronic Appendix A (on CD-ROM)

A copy of the data collated for the purposes of this studied is provided

Electronic Appendix B (on CD-ROM)

A version of the modified Ogata-Banks model developed and used in this study is provided, with instructions for use.