

Transient or steady-state? Using vertical temperature profiles to quantify groundwater–surface water exchange

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Abstract:

Heat is recognized as a natural tracer to identify the exchange of water between the groundwater and surface water compartment. One-dimensional (1D) heat transport models have the ability to obtain quantitative estimates of vertical fluxes through the sediment matrix. Input to these models can come from temperatures observed in the surface water and in the bed material of rivers and lakes. The upper thermal boundary condition at the groundwater–surface water interface is affected by seasonal and diurnal temperature variations. We hypothesize that effects of these transient influences are negligible at certain times of the year, such that the vertical temperature distribution can be approximated to be at steady state. Temperature time series observed over a year in the surface water and at several depths below a river in Belgium and in sediments of an acid mine lake in Eastern Germany were simulated with a heat balance model implemented in FEMME and the water and energy model VS2DH to obtain seepage fluxes. Temperature variations throughout the year at all depths could be adequately reproduced with the transient models. Vertical temperature profiles at several measuring times during the year were also fitted with an analytical, steady-state solution for 1D heat transport and the obtained fluxes compared to the results from transient simulations. Fluxes obtained from the much simpler steady-state solution were compared well with the flux rates from transient simulations for moments between mid and late summer, as well as during the winter. During transitional seasons (fall and spring), the fluxes from the steady-state solution deviated significantly from the transient estimates with a tendency to underestimate at the beginning and to overestimate towards the end of those seasons. We conclude that fitting a simple analytical solution for 1D vertical heat transport to temperature data observed at particular well-selected times of the year can provide an inexpensive, simple method to obtain accurate point estimates of groundwater–surface water exchange in rivers and lakes. Copyright © 2009 John Wiley & Sons, Ltd.

KEY WORDS hyporheic zone; groundwater–surface water interaction; heat transport modelling; temperature; FEMME; VS2DH

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INTRODUCTION

Quantification of the exchange fluxes between groundwater and surface water is an important prerequisite for understanding and preserving groundwater–surface water ecosystems. Despite increased research efforts directed at near-channel and in-channel exchange of water, matter and energy (Sophocleous, 2002), quantifying water exchange remains difficult.

The hyporheic zone, the area of saturated sediments directly beneath and beside streams, rivers and lakes where groundwater and surface water is actively mixed and exchanged (Grimm and Fisher, 1984; Duff and Triska, 1990; Triska *et al.*, 1993a,b; Boulton *et al.*, 1998; Edwards, 1998; and Henry, 1999), is often characterized by high biogeochemical process rates and a

large variability of matter exchange in time and space. Hyporheic exchange of water and its constituents thus plays an important role in fundamental hydrologic and ecologic processes both in rivers and lakes such as discharge, moderation of water-level fluctuations, thermal buffering, biogeochemical reactions, transformation and retention of nutrients, pollutants and other matter with important implications for lake, stream and riparian ecology (Lowrance, 1984; Thibodeaux and Boyle, 1987; Stanford *et al.*, 1993; Brunke and Gonser, 1997; Boulton *et al.*, 1998; Fisher *et al.*, 1998; Woessner, 2000; Hayashi *et al.*, 2002; McClain *et al.*, 2003; Loheide and Gorlick, 2006; Kalbus *et al.*, 2006). The hyporheic zone also provides habitat for specialized microbial and invertebrate assemblages (Marshall and Hall, 2004). National and international regulations like the European Water Framework Directive (EU, 2000/60/EC; EU, 2006/118/EC) mandate the protection of linked groundwater–surface water systems. This requires the ability to assess mass

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fluxes across the groundwater–surface water interface and related biochemical attenuation processes leading to the development of reliable and transferable conceptual models of these processes (Smith, 2005).

Proper quantification of exchange fluxes remains difficult as there is limited possibility to measure the groundwater–surface water flux directly. Seepage meters (Lee, 1977; Krupa *et al.*, 1998; Isiorho and Meyer, 1999; Paulsen *et al.*, 2001; Murdoch and Kelly, 2003; Rosenberry and Morin, 2004), despite their relative technical simplicity, are difficult to use in the field and are unreliable in flowing waters (e.g. rivers and streams) (Murdoch and Kelly, 2003). Indirect methods based on Darcy's law using standpipes, piezometer nests and boreholes placed in the river bed itself or on the adjacent riparian zone require a reliable estimate of the soil hydraulic conductivity, which can vary over orders of magnitude (Chen, 2000) and are difficult to determine *in situ* (Cardenas and Zlotnik, 2003). Differential discharge gauging and the use of numerical models to estimate groundwater–surface water exchanges (Becker *et al.*, 2004; Fleckenstein *et al.*, 2004) yield fluxes averaged over longer river reaches. The same holds true for stream tracer tests using dye or other conservative tracers (Runkel *et al.*, 2003; Carey and Quinton, 2005). Local fluxes, however, can be highly variable (Conant, 2004; Keery *et al.*, 2007) with significant implications for biogeochemical processes. The use of remote sensing and airborne methods to sense temperature to evaluate groundwater–surface water exchange is relatively new (Becker, 2006); but to date only offers a qualitative assessment (Tcherepanov *et al.*, 2005) unless additional calculations of the energy balance are made (Loheide and Gorlick, 2006). Selker *et al.* (2006) introduce fiber-optics to sense the interaction of groundwater and surface water along a river channel from temperature signals.

An indirect method to estimate the groundwater–surface water interaction is the thermal method, sometimes referred to as heat flow method or temperature method (Anderson, 2005). It is based on the fact that the temperature distribution in the subsurface is not only the result of heat conduction, but also of advection by moving water through the porous medium (Stonestrom and Constantz, 2003; Kalbus *et al.*, 2006). Exchange patterns can be inferred qualitatively from temperature variations at the groundwater–surface water interface (Lowry *et al.*, 2007) or the magnitude of water fluxes can be quantified by inverse simulation of temperature distributions (Stonestrom and Constantz, 2003; Schmidt *et al.*, 2006). Temperature can be measured easily and rapidly, especially since cheap robust sensors and data loggers have become readily available (Stonestrom and Blasch, 2003; Anderson, 2005).

Van Orstrand (1934) was the first to recognize the influence of moving groundwater on heat fluxes in the subsurface. Stallman (1965) and Bredehoeft and Papadopoulos (1965) published the basic equations and a quantitative analysis, Kunii and Smith (1961) and Cartwright (1979) performed corresponding laboratory tests. Cartwright

(1970) and Sorey (1971) both successfully applied Bredehoeft and Papadopoulos (1965) analytical solution for heat flow with a steady-state boundary condition. Suzuki (1960) and Stallman (1965) published analytical transient solutions assuming a sinusoidal variation of temperature on the land surface, Lapham (1989) was the first to use vertical temperature profiles to estimate groundwater–stream exchange. He developed a methodology to calculate both groundwater flux and the vertical hydraulic conductivity of the sediment. Silliman *et al.* (1995) used surface water time series as an upper boundary condition for a one-dimensional (1D) analytical heat transport model to quantify recharge through the sediments of a creek. They concluded that their model, fitted to temperature time series measured in the stream and at shallow depth in the streambed sediments, allowed for inexpensive point estimates of water flux across the groundwater–surface water interface. Hatch *et al.* (2006); Hoehn and Cirpka (2006) and Keery *et al.* (2007) analysed phase shifts and differences in amplitude of stream and sediment temperature time series to determine streambed seepage rates.

Another approach is to analyse vertical temperature profiles obtained at one instance in time. Schmidt *et al.* (2006) used a temperature probe that can be inserted into the streambed sediments and records vertical temperature distribution at this point. Assuming a quasi-constant groundwater temperature at depth and a limited penetration depth of diurnal temperature variations at the upper boundary, the profile can be adequately fitted with an analytical steady-state solution of the 1D heat transport equation. Schmidt *et al.* (2007) showed that streambed temperatures mapped at one depth in a gaining stream were in quasi-steady-state at moderate-to high-flux conditions and could be accurately simulated with an analytical solution. The advantage of a steady-state solution is its simple application and limited needs regarding temperature measurements, which can be relatively easily and accurately obtained. However, Schmidt *et al.* (2007) qualitatively reasoned that only during certain periods of the year conditions are met to justify the assumption of a quasi-steady-state temperature distribution.

In this work, the exchange fluxes between groundwater and surface water are estimated by inverse modelling of the vertical 1D transient and steady-state heat flow using the analytical solution by Bredehoeft and Papadopoulos (1965). The United States Geological Survey (USGS) water and heat model VS2DH (Healy and Ronan, 1996) was applied to a groundwater-fed lake in Eastern Germany and a heat balance model implemented in FEMME (Soetaert *et al.*, 2002) was applied to temperature data sets from a river-aquifer system in Belgium. Steady-state results at different times in the year are compared with results from the calibrated transient simulations to evaluate the validity of the steady-state assumption. It is hypothesized that the use of a steady-state approximation is justified at certain times of the year, when variations in heat flow resulting from seasonal temperature changes are

minimal and the penetration depth of diurnal variations is small compared to the depth of the temperature profile.

In the following paragraph, a short description of the thermal method including the main equations and the analytical solution by Bredehoeft and Papadopoulos (1965) will be presented, followed by a description of the numerical models, field sites and measurements.

METHODS

The thermal method is based on the principle that heat (energy) in the subsurface is transported by flowing water (advection), as well as by heat conduction via the fluid and solid parts of the soil matrix. The advective flow strongly influences the temperature distribution in the mixing zone between groundwater and surface water. Hence water fluxes between groundwater and surface water can be traced by measuring temperature distributions between the two systems (Stonestrom and Constantz, 2003; Anderson, 2005). Flux estimates are obtained by fitting solutions of the heat flow equation to observed temperature distributions in the soil.

Whereas deeper groundwater shows an almost constant temperature throughout the year of about 1–2 °C above the mean annual surface temperature (Anderson, 2005), surface water is influenced by seasonal and diurnal heating and cooling of the land surface. Consequently, groundwater temperatures are generally cooler than stream temperatures (especially in discharge areas) during the summer months and usually warmer in winter.

Suzuki (1960); Stallman (1965) and Lapham (1989) describe the 1D, vertical, anisothermal flow of heat through an incompressible fluid through a homogeneous, porous media as:

$$k \frac{\partial^2 T}{\partial z^2} - v_z c_w \rho_w \frac{\partial T}{\partial z} = c \rho \frac{\partial T}{\partial t} \tag{1}$$

where k is the thermal conductivity of the soil–water matrix in $J s^{-1} m^{-1} K^{-1}$, T the temperature at depth z in m and time t in the soil in K (°C), c_w the specific heat capacity of the fluid in $J kg^{-1} K^{-1}$, ρ_w the density of the fluid in $kg m^{-3}$, v_z the vertical component of the darcian fluid velocity in the soil in $m s^{-1}$, c the specific heat capacity of the rock–fluid matrix in $J kg^{-1} K^{-1}$, and ρ the wet-bulk density (density of the rock–fluid matrix) in $kg m^{-3}$. The terms $c_w \rho_w$ and $c \rho$ represent respectively the volumetric heat capacity of the fluid and the rock–fluid matrix in $J m^{-3} K^{-1}$. The first term of the left hand side of Equation 1 represents the conductive and the second term the advective part of heat transport.

Figure 1 presents the concept of typical fluid and heat transport between groundwater and surface water. The upper thermal boundary is usually given by the surface water temperature time series (e.g. the temperature at the interface surface water–river/lakebed), while for the lower boundary a quasi-constant groundwater temperature is assumed at a sufficient depth. Under a hydraulic

steady-state (constant exchange flux between groundwater and surface water), Equation 1 can be used to simulate the shape of the vertical temperature profile at any given time (denoted by the dashed line in Figure 1). Upward flow of water (i.e. gaining conditions, negative sign of v_z) is referred to as groundwater discharge, whereas groundwater recharge is defined as downward movement of surface water (i.e. a losing condition, positive sign of v_z).

Equation 1 can be solved numerically if the thermal boundary and initial conditions are known (Lapham, 1989; Silliman and Booth, 1993; Taniguchi, 1993; Silliman *et al.*, 1995; Constantz, 2002; Hoehn and Cirpka, 2006). Continuous temperature data at the boundaries can be obtained from direct measurements in the field. Groundwater temperature at the lower boundary is assumed to be quasi-constant (Arriaga and Leap, 2006; Schmidt *et al.*, 2006) and can usually be obtained from deep piezometers. The cost of instrumentation and installation of self-recording sensors often make it difficult to measure continuous data from more than just a few locations. Therefore, a method that allows for a flux estimate based on single measurements would provide significant benefits.

If the temperature distribution is at a steady-state, only the temperatures at the upper and lower boundaries, as

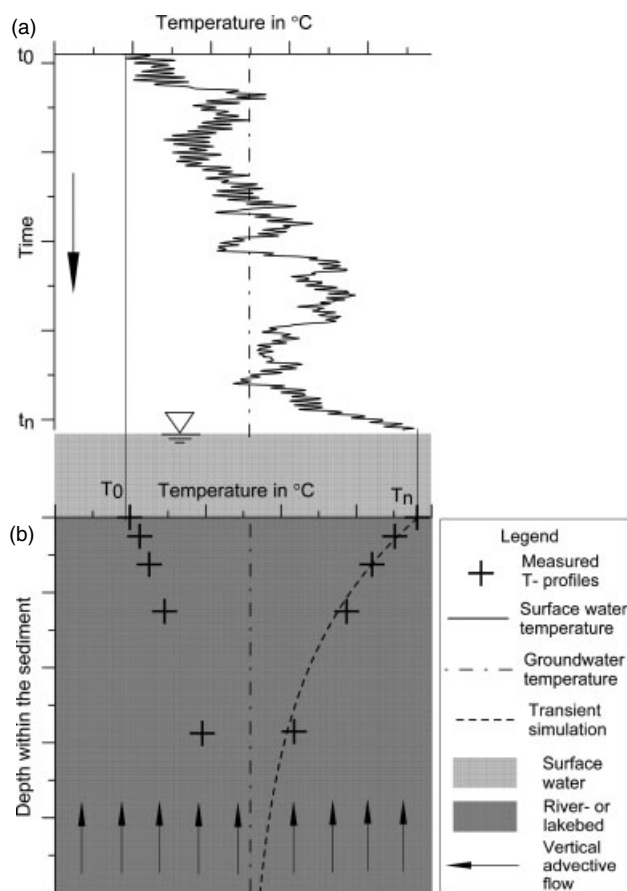


Figure 1. Concept of transient simulation of vertical 1D-fluid-heat transport in a river or lake bed; part a indicates the continuously measured surface water temperature used as upper boundary condition; part b indicates the soil column and its changing temperature distribution represented in the numerical models

well as the thermal conductivity of the porous medium need to be known to determine the exchange flux or velocity (v_z in Equation 1), reducing the necessary input data significantly.

For steady-state, Equation 1 reduces to:

$$k \frac{\partial^2 T}{\partial z^2} - v_z c_w \rho_w \frac{\partial T}{\partial z} = 0 \quad (2)$$

Bredehoeft and Papadopoulos (1965) presented for this equation the following analytical solution.

$$T_z = \frac{\exp\left(\frac{v_z \cdot \rho_w c_w}{k} \cdot z\right) - 1}{\exp\left(\frac{v_z \cdot \rho_w c_w}{k} \cdot z_L\right) - 1} \cdot (T_L - T_0) + T_0 \quad (3)$$

where T_z is the temperature at depth z ; z_L the depth of the lower boundary; and T_0 and T_L are the constant temperatures at the upper (surface water) and lower (groundwater) boundaries, respectively. As this solution assumes that the temperature distribution in the subsurface is not changing over time, no continuous input data is necessary to describe the boundary conditions (Figure 2). A temperature profile consisting of a few measurement points with depth and the temperatures at the upper and lower boundaries are sufficient to obtain a fit with Equation 3 (Schmidt *et al.*, 2007). In this equation, the thermal conductivity k remains as the single parameter determining the physical (and thermal) properties of the fluid–soil matrix. Values for c_w and ρ_w can easily be obtained from the literature. In contrast to hydraulic conductivity, the thermal conductivity k has a small range across different sediment textures (Stonestrom and Constantz, 2003). If the assumption of a thermal steady-state is valid then brief knowledge of the sediment texture is sufficient to obtain reasonable flux estimates. This strongly reduces uncertainties in parameter estimation and hence values of k are commonly taken from the literature.

For the case of no advective heat flow, the simulated temperature profile would be a straight line connecting

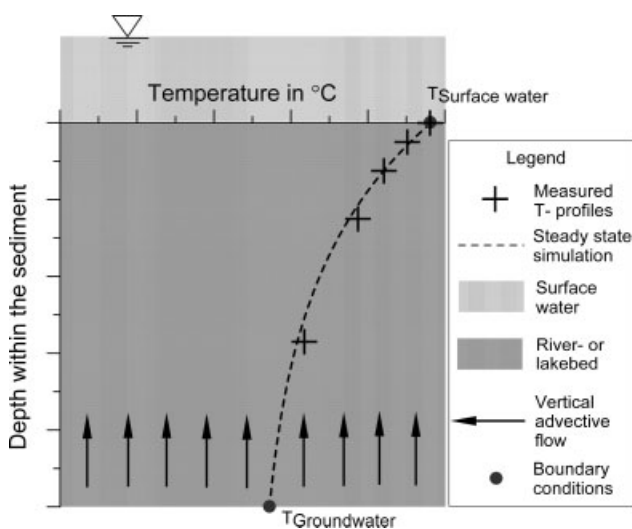


Figure 2. Concept of steady-state simulation of vertical 1D-fluid-heat transport in a river or lake bed. Just a singular value is required as boundary condition

the temperatures at the boundary conditions. Upward flow of water will bend the temperature profile 'upward' (e.g. in direction of the surface; Figure 2) and infiltration will bend the curve in the other direction (see also Stonestrom and Constantz, 2003; Arriaga and Leap, 2006; Schmidt *et al.*, 2006). According to Schmidt *et al.* (2007), the steady-state solution is limited to upward flow conditions.

Numerical codes

For the simulation of the vertical 1D heat transport two different numerical codes were used. A vertical 1D heat flow model was embedded in the FEMME ecosystem modelling platform (Soetaert *et al.*, 2002). Vertical temperature profiles at Lake 77 were simulated using the USGS code VS2DH. VS2DH (Healy and Ronan, 1996) is a two dimensional (2D) finite difference code for variably saturated flow and heat transport. Both codes have been used independently to analyse data from the two field sites and were therefore well adapted to the local conditions. The codes have been tested and verified (e.g. Healy and Ronan, 1996; Anibas *et al.*, 2008) and were found to yield almost identical results for a subset of the Lake 77 data.

FEMME (Flexible Environment for Mathematically Modelling the Environment) is a modular FORTRAN-based model platform developed for dynamic ecosystem modelling. FEMME is used to map different ecologically relevant 1D/2D exchange processes. STRIVE (Stream River Ecosystem model) is a package of subroutines for FEMME, which enables the simulation of different physical, biogeochemical and transport processes, and retention or exchange of matter. One part of the STRIVE module is a hyporheic zone module, HYPOGRID, which is based on the diagenetic model of Soetaert *et al.* (1996). This module can simulate vertical 1D heat transport, enabling the quantification of the groundwater–surface water interaction by numeric integration. FEMME–STRIVE in fact consist of several different modules, which can be linked together. In this work only the module HYPOGRID and its heat transport routines are used.

The heat transport models were calibrated to the measured temperature profiles by changing the value of the vertical flux velocity (v_z in Equation 1) to minimize the difference between measured and simulated temperatures at different depths. FEMME performs the minimization according to a user-defined internal integration routine (Soetaert *et al.*, 2002). In VS2DH, the inversion was performed in a trial and error mode. The final flux value obtained indicates the best estimate of the average vertical component of the advective darcian flow through the porous medium.

FIELD SITES AND MEASUREMENTS

Aa River

With an average inclination of about 0.48‰ the Aa River is a typical lowland river located in Flanders, Belgium (Figure 3), representing an alluvial river ecosystem.

The Aa River is a tributary of the Kleine Nete River and part of the Scheldt River catchment with a drainage area of 237 km². Field data were collected along the lower stretch of the river located 30-km east of Antwerp. The Aa River is a straightened and canalized river course; the catchment is dominated by agricultural landuse. At the field site the Aa has an average water depth of 1.1 m, a width of 14 m and an average discharge of 1.8 m³ s⁻¹. The riverbed is predominantly composed of fine sand with some organic matter resulting in an assumed thermal conductivity of 1.8 J s⁻¹ m⁻¹ K⁻¹ (see also Stonestrom and Blasch, 2003). The hydrologic regime is influenced by weirs, which lead to relatively constant water levels throughout the year, disrupted only by sharp peak discharges.

Beside the continuous measurement of the surface water temperature ‘roaming surveys’ have been conducted on a regular bases along the Aa River sampling T-profiles at the centre of the river bed with a purpose built device called ‘Temperature stick’ (Figure 4a). The

T-stick is a 2-m long rod holding a thermistor (Davis Instruments Model 7817, Hayward, CA, USA; accuracy 0.3 °C) at its tip. The instrument is driven into the river or lake sediments. The pipe has an opening at its lower end, through which the thermistor gets in contact with the sediment and can record the ambient temperature. Each temperature profile consists of five temperature measurements whose positions were fixed by using a graduation on the T-stick instrument relating the position of the sensor to the interface of surface water–air. The measurement was conducted first at the interface between surface water and groundwater (≈0.0 m), continuing at 0.1, 0.25, 0.5-m depth and the maximum depth possible to access with the Temperature stick, generally about 0.40–1.20 m (average 0.85 m). Around 15 min were necessary to measure a temperature profile with the T-stick instrument, as the sensor needs several minutes to accommodate to the ambient temperature at a certain measurement location. After a stable indication of 10 s or more on the multimeter a thermal equilibrium was assumed. Notice that results from a single measurement point are presented in this article.



Figure 3. Location of the Aa River study site

Lake 77

Lake 77 is located in Lower Lusatia, which is part of the state of Brandenburg in Eastern Germany (Figure 5). The area has been highly impacted by open-pit coal mining with severe consequences for water quantity and quality. For mining, groundwater levels had to be significantly lowered. After shut down of the mine pits, water tables rose again and in the abandoned pits post-mining lakes developed. Most lakes are characterized by very low pH values (<3) caused by weathered pyrite in the mine tailings and mineral transformations at the groundwater–lake interface. Lake 77 is at the southern edge of the former mining area. Hence, it

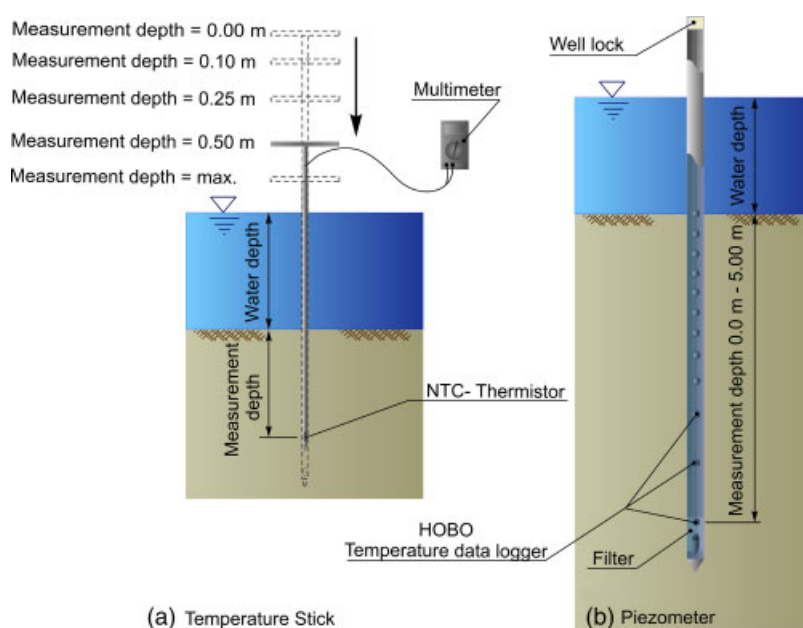


Figure 4. Measurement setup of temperature profiles in the Aa River with the temperature stick (a), and with a piezometer equipped with data loggers in Lake 77(b)

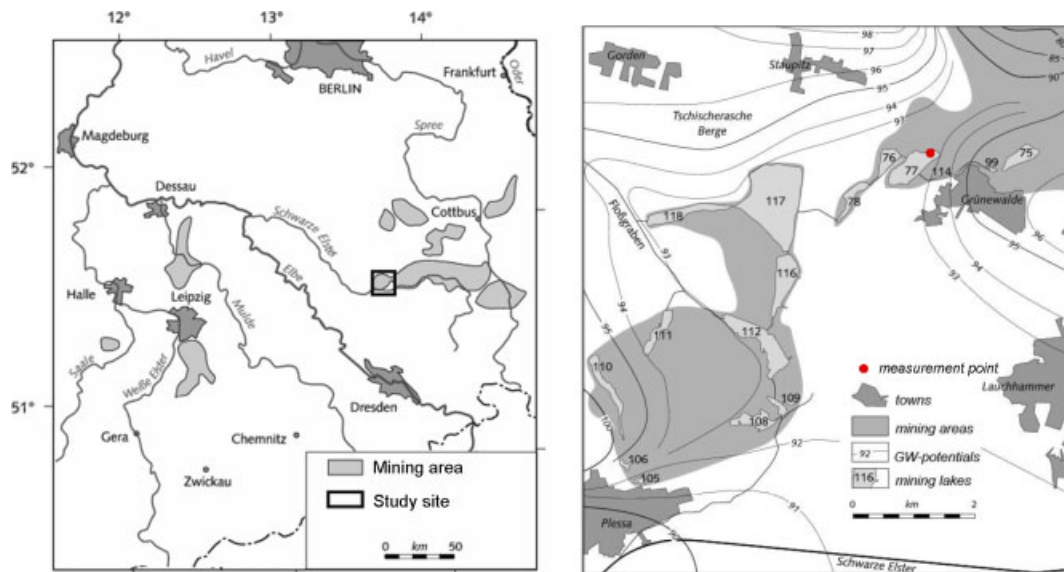


Figure 5. Location of Lake 77 and regional groundwater contours (after Peine *et al.*, 1998)

is surrounded by undisturbed tertiary and quaternary sediments in the south and east, whereas in the north and north-western parts tailings shape the shoreline. The tailings mainly consist of silty fine-to-coarse sand with little gravel and clay as well as coal remains. General direction of groundwater flow is from north and north-east to south-west (Figure 5) and annual groundwater recharge is about 180 mm (Knoll *et al.*, 1999). Lake 77 has a maximum depth of 8.5 m, a water volume of about 1.2910^6 m^3 and a surface of 24.4 ha. Groundwater discharge rates to the lake, which are spatially variable, were found to be an important control on acidity generation at the groundwater-surface water interface (Blodau and Knorr, 2006).

Temperature measurements were made in a stainless steel piezometer (inner diameter 37 mm, outer diameter 42 mm) installed to a depth of 5 m in the lake sediments (Figure 4b) about 7 m from the northern shore. Hobo Pendant temperature sensors (Onset Inc.) were installed in the piezometer at the water-sediment interface (0 cm) and at 10, 20, 30, 40, 60, 80, 100, 130, 160, 190, 220, 260, 300, 340, 380, 420 and 460-cm depth. Temperatures were recorded every 15 min. For the comparison between observed and simulated temperatures only hourly values were used. From the consistently steep temperature gradients in the upper 2–3 m it was concluded that the measurements were not affected by thermal convection in the piezometer pipe (convection would have homogenized the temperature profile resulting in less-pronounced gradients). It was further assumed that heat conduction along the steel pipe does not significantly affect the measured temperature profiles. This assumption is supported by Constantz *et al.* (2008), who showed, based on temperature measurements in the Santa Clara River, California at 30-cm depth in a steel piezometer and in the riverbed sediment at the same depth, that heat conduction along the steel pipe is negligible when heat is also transported advectively. Groundwater temperature was measured in a

nearly well (about 300 m away) over a depth range that corresponds to about 5–10 m below lake bottom at the piezometer and was found to be relatively constant at an average 11.5°C (deviations over the measurement period were less than 0.2°C).

Model setup, discretization and boundary conditions

The FEMME model for the Aa River is discretized as a vertical, 1D saturated and homogeneous soil column of 5-m length and composed of 100 layers. The spacing of the model layers follows a sinusoidal distribution, providing layer thicknesses of 0.1 cm at the upper and lower boundary, while the thickness of the layers is increasing towards the centre of the model domain. The upper boundary is the interface of the soil and the water column, whereas the lower boundary is defined as the subsurface depth where annual temperature changes are low enough to be assumed constant. The continuously measured surface water temperature (hourly values) serves as upper boundary condition of the domain. FEMME was setup with a variable-coefficient ordinary differential equation (VODE) numerical integration routine creating hourly output values.

In VS2DH, a 1D domain extending from the lake bottom (lake water-sediment interface) was discretized to a depth of 15 m with a grid spacing ranging from 1 cm at the top (where vertical temperature gradients are greatest) to 10 cm at the bottom. Constant head boundary conditions were applied at the top and bottom of the domain. The head at the top was taken from the lake water depth at the piezometer where the temperatures were measured. The head at the lower boundary was varied to obtain an optimal fit with the observed temperature data. The upper thermal boundary condition was specified from the observed temperature time series (hourly values). At the lower boundary a constant groundwater temperature was assumed (see previous paragraph). Numerical convergence criteria in the model were set so

that mass balance errors for flow and energy were below 1% for all simulations at all times. The model was run with hourly stress periods and an adaptive time step. Time steps were constrained at a minimum and maximum of 1 and 60 min, respectively.

For the steady-state solutions (Equation 3), the depth of the lower boundary (z_L) was set to 5 m at both sites. The assumption of a quasi-constant groundwater temperature at that depth was supported by data from the piezometer at Lake 77, which showed relatively constant temperatures at depths below 3–4 m. For the Aa River it was assumed that groundwater temperature fluctuations at 5-m depth would be negligible, which is in-line with the recommendation by Schmidt *et al.* (2006) of a minimum depth for z_L of 1 m for a similar river-aquifer system in Germany. The stable groundwater temperature of 12.2 °C was assumed by interpolation of temperatures values from 640 temperature profiles measured with the T-stick in the Aa River over several years.

Table I is summarizing the most important input parameters and boundary conditions for both FEMME and VS2DH models.

RESULTS AND DISCUSSION

Figures 6 and 7 show the temperature time series at the water-sediment interface at the Aa River and Lake 77, respectively. Both temperature time series show similar diurnal as well as seasonal variations. For comparison, a sine curve with a period of 1 year is plotted indicating that seasonal temperature fluctuations can be approximated by a sine function. Lowest temperatures during the winter are around 4 °C; summer temperatures can be as high as 26 °C on the Aa River and 28 °C at Lake 77. Diurnal fluctuations tend to be higher in the summer (2–5 °C) and slightly lower in the winter (2–3 °C). At both sites the shape of the vertical temperature profiles indicates upward flow from groundwater to surface water.

For the transient simulations, both models (FEMME and VS2DH) yielded an acceptable fit with observed temperatures. The root mean square error (RMSE) between the measured and simulated temperatures was 0.41 °C for the Aa and 0.41 °C for Lake 77 (Table II). The temporal course of the temperatures at all depths in the sediment of Lake 77 was well reproduced by VS2DH.

Table I. Summary of parameters and boundary conditions used by FEMME and VS2DH models for the steady-state and transient simulations

Site	Thermal conductivity k ($\text{Js}^{-1} \text{m}^{-1}\text{K}^{-1}$)	Porosity n (–)	Volumetric heat capacity ^a $c\rho$ ($\text{Jm}^{-3}\text{K}^{-1}$)	Thickness of the model domain (m)	Stream/Lakebed T (°C)
Aa River ^b	1.8	0.42	$2.7 \cdot 10^6$	5.0	12.2 ^c
Lake 77 ^d	1.8	0.35	$2.5 \cdot 10^6$	15.0 ^e	11.1

^a Volumetric heat capacity of the saturated soil water matrix; $c_w\rho_w$ is for both sites $4.2 \cdot 10^6 \text{ Jm}^{-3} \text{ K}^{-1}$.

^b Parameters estimated based on Lapham 1989; Simulated with FEMME.

^c Estimated from 640 temperature profiles measured in the Aa River between August 2004 and February 2007.

^d Simulated with VS2DH.

^e 5.0 m for the steady-state analysis.

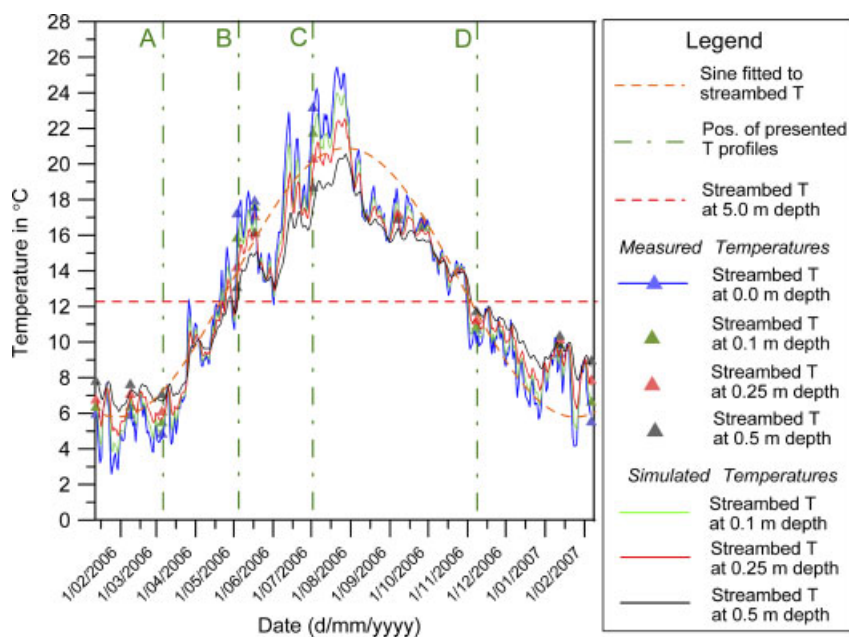


Figure 6. Continuously measured streambed temperature at the Aa between January 2006 and February 2007 (hourly values); the triangular symbols indicate temperature profiles measured with the T-stick instrument; the lines indicate simulated temperature time series derived with FEMME; the dash-point line indicates times where steady-state simulations were obtained

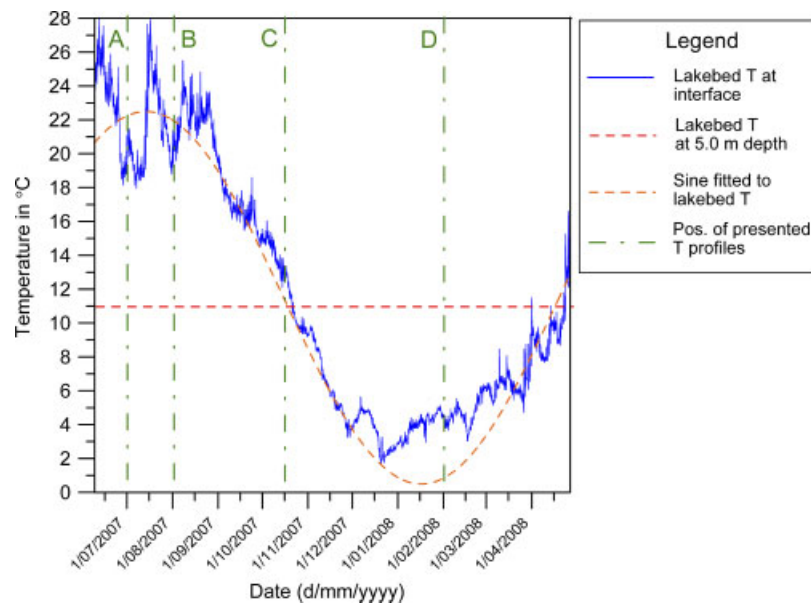


Figure 7. Measured temperatures at the water-sediment interface at the north shore of Lake 77 between June 2007 and April 2008 (hourly values), water depth is approximately 1 m, the dash-point line indicates points in time, for which a steady state model was fitted

Smaller deviations at some depths are attributed to heterogeneities in the sediment. At the Aa River, vertical temperatures profiles measured with the T-stick were also adequately represented by the FEMME model at all 11 measured times, indicated by triangular signatures in Figure 6. A mean outflow of groundwater to the river of -24 mm d^{-1} was obtained. For Lake 77, an average outflow of -51 mm d^{-1} was inverted from the temperature measurements.

It has to be noted that the flux rates inverted from the transient simulations (Table II) represent an integration of fluxes over the entire simulation period. As such they reflect the long-term average exchange rate under the assumption that hydraulic gradients between surface water and groundwater are quasi-constant. Data of lake water levels and groundwater heads from Lake 77 support that assumption. For the river environment, however, it was observed that the flux varies over time, mainly as a result of short-term river stage fluctuations. Simulations conducted over shorter time periods yielded variable flux rates usually showing exfiltrating conditions, but also changing to infiltrating conditions ranging from -58 mm d^{-1} to $+57 \text{ mm d}^{-1}$. These fluctuations may be responsible for some deviation between the measured

and simulated temperatures at certain points in time. General hydraulic gradients, however, can be assumed to be relatively constant, as the river stage is controlled by weirs at both ends of the river reach. Hence, it is assumed that effects of short-term stage fluctuations can be neglected in this study.

The analytical solution by Bredehoeft and Papadopoulos (1965) for 1D steady-state heat transport (Equation 3) was used to match the observed vertical temperature profiles at several points in time by a least squares minimization. The deviations and fluxes between simulated and observed temperatures of the transient and steady-state analysis are compared in Figures 8 and 9. In general all simulations, transient as well as steady-state, show good agreement with observed temperature profiles. The fluxes inverted from the steady-state solution, however, are only in good agreement with transient results at certain times (Figure 8a and c, Figure 9a and d). At other times flux rates deviate significantly (Figure 8b and d, Figure 9b and c) even when the fit between the steady-state simulated profile and the measured temperature profile is very good.

Figures 10 and 11 depict the water temperature at the interface between groundwater and river or lakebed and the deviations between the estimated fluxes from the transient and steady-state solutions. At times when the seasonal sine function is reaching its maximum or minimum, the difference between the steady-state and the transient approaches a minimum. In contrast, at the inflection point of the sine curve deviations are at a maximum. Negative values of the deviation stand for a systematic underestimation of fluxes by the steady-state simulation, whereas positive deviation indicates an overestimation of this flux.

The temperature signal resulting from diurnal surface water temperature variations only propagates to shallow

Table II. Summary of results of the transient simulations

Site	Simulation period	Measure of fit (RMSE) ($^{\circ}\text{C}$)	Estimated mean flux v_z [mmd^{-1}]
Aa River	13/01/2006–08/02/2007	0.41 ^a	–24
Lake 77	16/07/2007–15/12/2007	0.41 ^b	–51

^a Root mean square error (RMSE) in $^{\circ}\text{C}$ between the measured T profile and the results from the transient simulation ($n = 50$; accuracy of the T sensor = 0.3°C).

^b RMSE in $^{\circ}\text{C}$ ($n = 251\,328$ every 15 min in each depth; accuracy of the T sensor = 0.3°C).

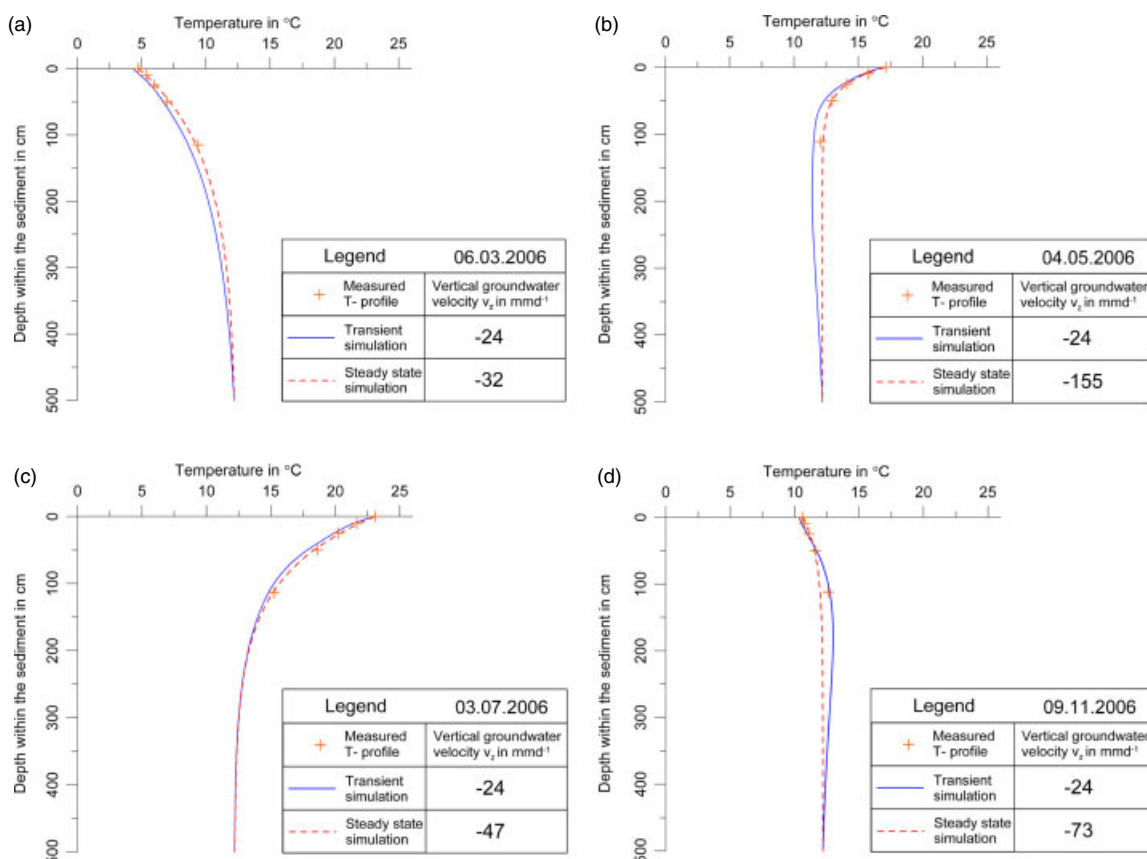


Figure 8. Measured and simulated (steady-state and transient) T-profiles of the Aa River; profile a was taken on the 6th of March 2006; b on the 4th of May 2006; c on the 3rd of July 2006 and d on the 9th of November 2006 respectively

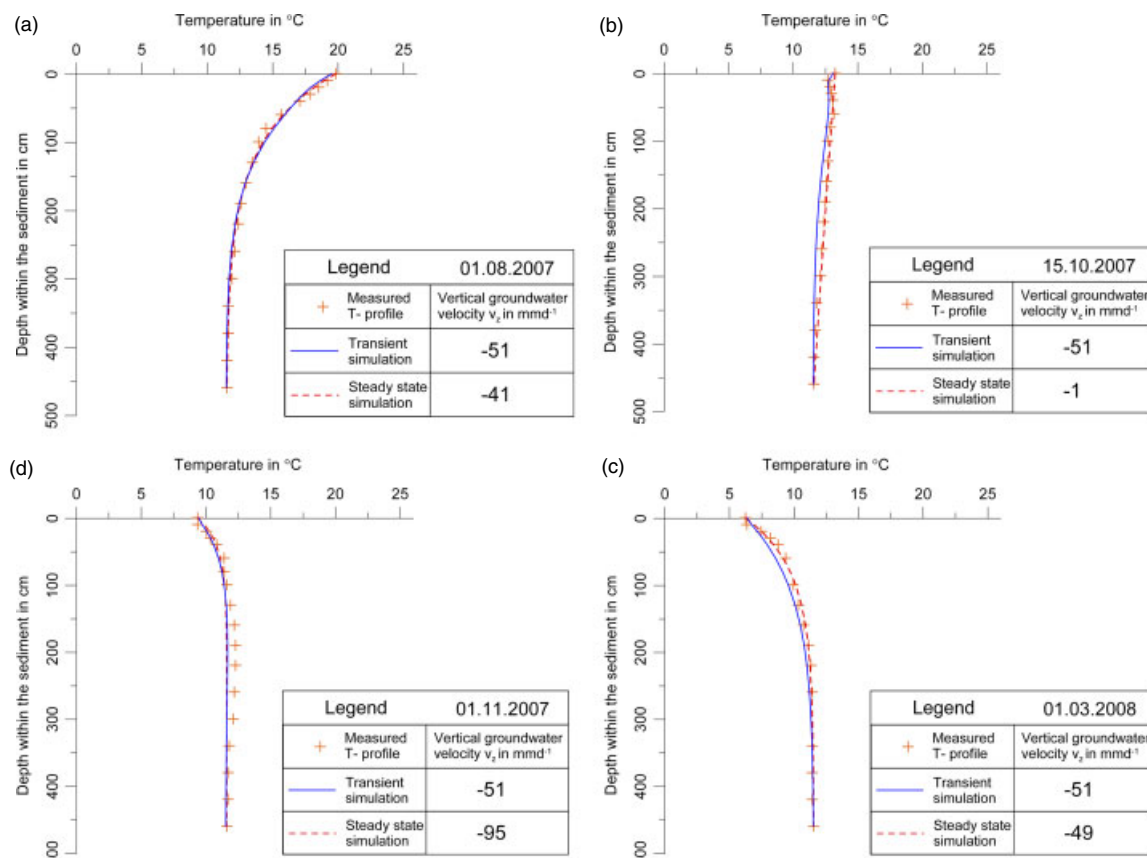


Figure 9. Measured and simulated (steady-state and transient) T-profiles of Lake 77; profile a was taken on the 1st of August 2007; b on the 15th of October 2007; c on the 1st of November 2007 and d on the 1st of March 2008 respectively

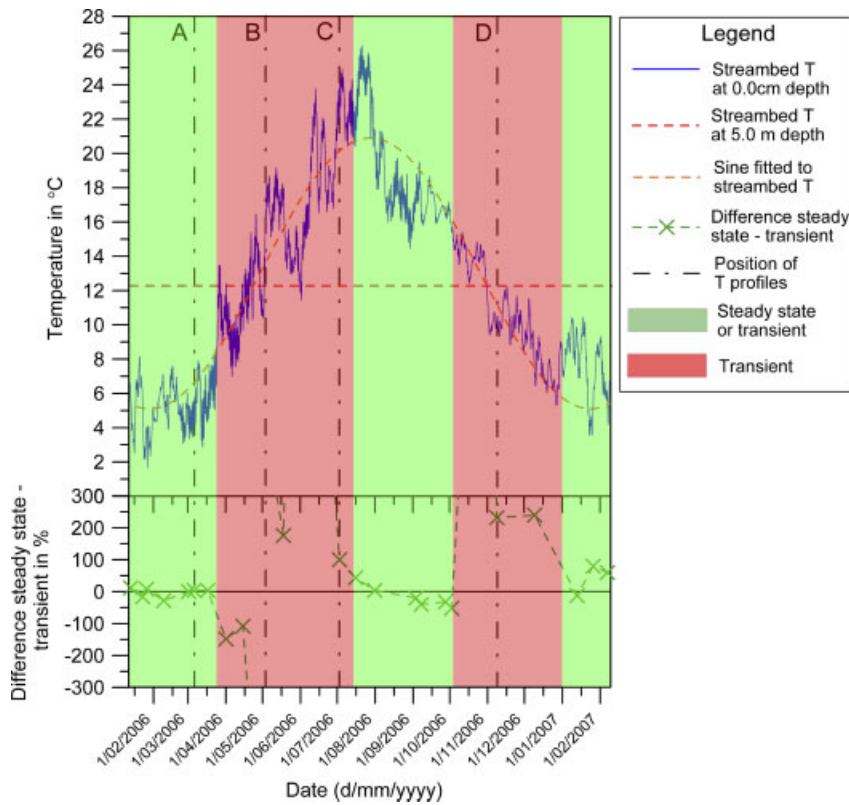


Figure 10. Comparison between steady-state and transient simulation results for the Aa River. The lower graph shows the relative deviation between the two approaches ('-' indicates steady-state yields results lower then transient result; '+' means steady-state result is higher than transient); the transparent green (light grey) areas indicate periods where a steady-state approach is acceptable; transparent red (darker grey) areas indicate periods where a flux estimate requires a transient simulation

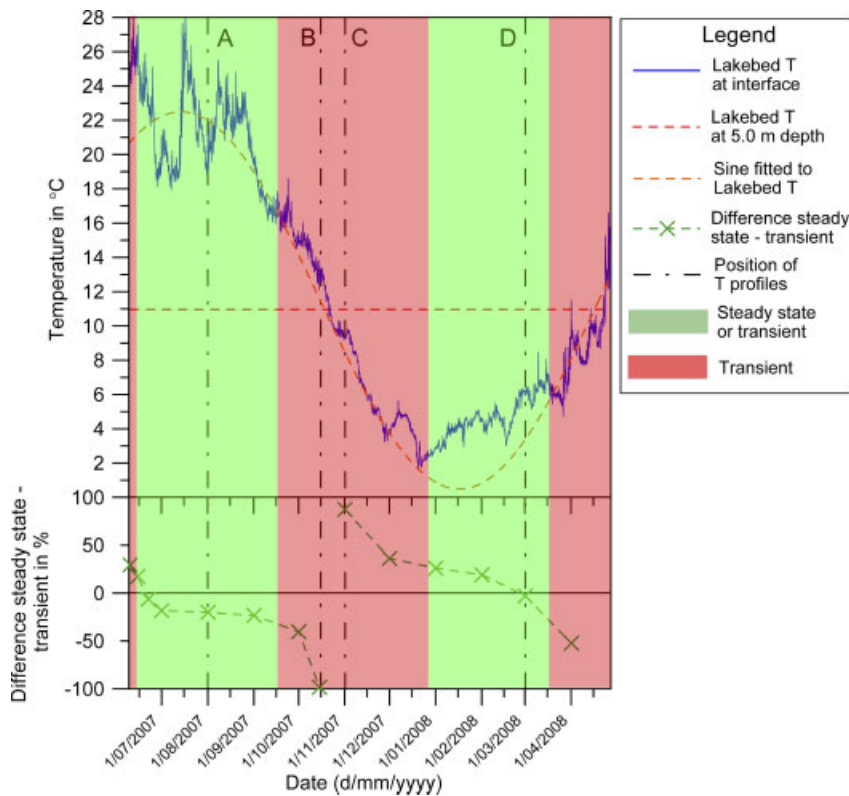


Figure 11. Comparison between steady-state and transient simulation results for Lake 77. The lower graph shows the relative deviation between the two approaches ('-' indicates steady-state yields results lower then transient result; '+' means steady-state result is higher than transient); the transparent green (light grey) areas indicate periods where a steady-state approach is acceptable; transparent red (darker grey) areas indicate periods where a flux estimate requires a transient simulation

depth and has no significant effect on the deeper vertical temperature profile (Schmidt *et al.*, 2007). As the accuracy of the used T sensors is $0.3\text{ }^{\circ}\text{C}$, a detectable diurnal signal of an amplitude of $5\text{ }^{\circ}\text{C}$ is not penetrating deeper than 0.3 m into the sediment at the average estimated flux of -24 mm d^{-1} for the Aa River and thus has no significant influence on this simulation. During winter and summer, surface water temperatures stay at a relatively constant level. Towards the end of the summer and winter, the heat distribution in the sediments approaches a 'quasi-steady-state'. A complete steady-state along the entire temperature profile can not be reached, because of diurnal temperature variations at the upper boundary and the propagation of long-term (seasonal and/or meteorological events) signals deeper into the sediment. Figure 8a and c represents such a situation for the Aa River, Figure 9a and 9d for Lake 77. Here a close agreement between the fluxes determined from the transient and the steady-state approaches can be observed. These times are indicated by transparent green rectangles in Figures 10 and 11. Red rectangles indicate times in the year where just a transient simulation will lead to reliable estimates of groundwater flux. In times where the deviation is less than 25% for Lake 77 and 50% for the Aa River (to address the higher variability in a river system) between transient and steady-state results, we concluded that a simulation in steady state is acceptable.

In contrast, at times when surface water temperatures are in transition from the warm season to the cold season or vice versa, i.e. spring and fall (around the inflection point of the sine function) both approaches yield deviating flux results (Figure 8b and d, 9b and c). During those times the temperature distribution in the sediments is dominated by seasonal surface water temperature variations propagating into the subsurface. The assumption of a quasi-steady-state is no longer valid. The temperature profile observed at Lake 77 at the inflection point of the surface water temperature time series in mid-October 2007 (Figure 9b) practically resembles a straight line. The steady-state approach fits a straight vertical temperature profile to the observed data implying no advective heat transport (flux = zero). However, this temperature profile is clearly not the result of a steady-state distribution of heat, but rather a snapshot in time of a system that is affected by seasonal temperature variations. During those times, fitting a steady-state solution will result in erroneous fluxes no matter how good the fit between the measured data and the model is (Figure 8b and d, 9b and c). On the other hand, periods with stable thermal conditions can occur outside of the summer and winter months resulting in steady-state heat distributions for which Equation 3 would yield reasonable flux estimates.

It is clear that the steady-state assumption is an approximation and its validity is sometimes difficult to test, in particular, when observed data are sparse. Hydraulic and thermal conditions in all groundwater–surface water systems are variable to some degree (e.g. river stages, diurnal temperature variations). Groundwater flow to surface

water is not always strictly vertical. But the comparison between transient and steady-state simulation of temperature distributions for the two groundwater–surface water systems presented here shows that in temperate climates the steady-state assumption is acceptable during and towards the end of the summer and winter. During the transitional seasons, spring and fall, steady-state fits will usually result in erroneous flux estimates with a consistent pattern to underestimate fluxes at the beginning and to overestimate them at the end of the transitional seasons (Figures 10 and 11).

A reliable temperature-based flux estimate can also be obtained in the transitional seasons, if a transient model is used and all parameters and boundary conditions are known and clearly defined. However, in practice, the latter is rarely the case and obtaining the appropriate data for a transient model can be cumbersome. Therefore the much simpler steady-state approach has great appeal. As demonstrated here it can, despite its simplifications, yield acceptable flux estimates during the appropriate times of the year.

CONCLUSIONS

Simulations of 1D transient heat flow between groundwater and surface water at a river in Belgium and a lake site in Germany were conducted over a period of several months. Observed temperatures at several depths in the sediment at the interface between groundwater and surface water could be adequately reproduced with the models. Comparison of the obtained fluxes between groundwater and surface water with fluxes inverted from fitting observed vertical temperature profiles to an analytical solution for 1D steady-state heat flow, showed good agreement of fluxes during and towards the end of the summer and winter. However, underestimation and overestimation of transient fluxes by the steady-state solution occurs in fall and spring respectively.

It is concluded that for a temperate climate like in Western and Central Europe during certain periods of the year, namely from mid-July, August up to mid-September in the summer season and January, February up to mid-March in the winter season, exchange fluxes between groundwater and surface water can be inverted from a steady-state heat flow model. In other words, during those times the assumption that vertical temperature distributions at the interface between groundwater and surface water are at a quasi-steady-state, is acceptable. Under certain meteorological conditions it might be possible to also get accurate flux estimates outside of those periods. The results presented here further suggests that the steady-state approach might work better in larger water bodies (e.g. lakes), which are usually less affected by hydraulic (e.g. stage changes) and thermal variations (e.g. temperature fluctuations). Analysis of the data from the Aa River shows that in winter, the agreement is better than in summer, as the thermal environment is generally more stable and diurnal influences are less pronounced.

However, it should be noted that a steady-state approach is an approximation and should therefore always be seen as providing a first quantitative estimate of groundwater–surface water flux rather than an exact absolute value. Its appeal lies in its simple and fast analysis. The method allows for a quick assessment of spatial patterns of groundwater–surface water exchange and can be used for ‘roaming’ surveys (Conant, 2004; Schmidt *et al.*, 2006). With the measurement setup as applied on the Aa River around 15–20 temperature profiles can be measured by a team of two persons in 7 h.

For scientific as well as engineering projects of a greater extent, we propose the steady-state solution to be used in the initial stages of an examination. ‘Hot spots’ of special interest could be detected with the method, thus the resources for further measurements could be allocated in a more economic way. Where intensive monitoring campaigns involving extensive field instrumentation and complex transient modelling are not feasible, a simple steady-state model as proposed by Bredehoeft and Papadopulos (1965) or Arriaga and Leap (2006) together with an instrument like the T-stick could provide an attractive alternative to get first estimates of local groundwater–surface water interactions.

We tested this approach for a river–groundwater and a lake–groundwater system in Western and Central Europe and concluded that it yields reasonable flux estimates if certain assumptions are not violated (e.g. flow is predominantly vertical) and measurements are conducted during favourable time periods (mid to end summer and winter at our sites). In principle, however, the steady-state method is applicable under all climatic conditions as long as there is a discernable difference between surface water and groundwater temperatures resulting in a detectable vertical temperature gradient (dependent on the accuracy of the T sensor, this should be around 1–2 °C within the first 1.0 m of the sediment). As the course of seasonal temperature variations in surface water and the amplitude of diurnal fluctuations will be different in different climates, the time windows within which vertical temperature profiles between surface water and groundwater can be adequately approximated with a steady-state model might change.

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