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Simulating the effects of geologic heterogeneity and transient boundary conditions on streambed temperatures — Implications for temperature-based water flux calculations

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ABSTRACT

Analytical solutions to the one-dimensional heat transport equation for steady-state conditions can provide simple means to quantify groundwater surface water exchange. The errors in exchange flux calculations that are introduced when the underlying assumptions of homogeneous sediments and constant temperature boundary conditions are violated were systematically evaluated in a simulation study. Temperatures in heterogeneous sediments were simulated using a numerical model. Heterogeneity in the sediments was represented by discrete, binary geologic units. High contrasts between the hydraulic conductivities (K) of the geologic units were found to lead to large errors, while the influence of the structural arrangement of the units was smaller. The effects of transient temperature boundary conditions were investigated using an analytical equation. Errors introduced by transient boundary conditions were small for Darcy-velocities >0.1 m d^{-1} in the period near maximum and minimum annual surface water temperatures. For smaller fluxes, however, errors can be large. Assuming steady-state conditions and vertical flow in homogeneous sediments is acceptable at certain times of the year and for medium to high exchange fluxes, but pronounced geologic heterogeneity can lead to large errors.

1. Introduction

Understanding and quantifying groundwater–surface water interactions has become an important topic in hydrogeological and river ecological investigations [36]. The exchange and mixing of chemically different groundwater (GW) and surface water (SW) can enhance biogeochemical activity in the transition zone between ground- and surface water and may therefore govern the transport and attenuation of contaminants, nutrients and other solutes [7,18,27]. As groundwater fluxes to lakes and streams can be highly variable on small spatial scales [7,29] measurement methods are needed that are able to detect and quantify this variability. Identifying patterns of water flow in the streambed may be the key to identify hot spots of biogeochemical activity.

Using heat as a tracer to characterize the spatial patterns of GW–SW exchange is a promising approach and has increasingly been used to quantify stream–aquifer exchange [8]. Stream and streambed temperatures can easily and cost-efficiently be measured at many locations, and can hence be a valuable supplement to traditional measurement methods for GW–SW exchange (e.g. seepage meters, incremental gauging etc.). Comprehensive overviews of theory and application of heat as a tracer for GW–SW exchange are given by Stonestrom and Constantz [31], Anderson [2] and Constantz [8].

Thermal signals occur naturally as seasonal and diurnal temperature variations in the surface water. Groundwater temperatures on the other hand are quasi constant at sufficient depth with values about 1 °C to 2 °C higher than the mean annual surface temperature [2]. The temperature distribution in the subsurface is the result of heat being transported by conduction and advection with the flowing water [30] and hence indirectly reflects the magnitude of water fluxes.

Analytical solutions to the one-dimensional heat transport equation have been developed for sinusoidal surface water temperature boundary conditions [30] and for constant temperature boundaries [4,33]. Based on these equations, methods to estimate the vertical flow velocity from temperature time-series in the stream and streambed were presented and applied by Hatch et al. [16] and Keery et al. [21]. Streambed temperatures measured at many locations at a single point in time were used by Conant [7], Schmidt et al. [28] and Anibas et al. [3] to characterize spatial patterns of groundwater discharge to a stream. This snapshot or mapping approach has some appeal due to its simplicity in data collection and analysis. Uncertainties in parameter estimation are comparably small in steady-state approaches, as the only parameter required is the thermal conductivity of the solid–fluid system, which varies over a much narrower range for typical sediment textures than hydraulic conductivity [31]. Schmidt et al. [28] conducted a sensitivity

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analysis for the steady-state analytical solution of Turcotte and Schubert [33] and found that the error of the discharge estimate is proportional to the error in the thermal conductivity.

The underlying assumptions of the analytical equations namely vertical and steady flow of water and heat, homogeneous, isotropic, fully saturated sediments and either a sinusoidal surface water temperature boundary [30] or a constant temperature boundary [4] will often be violated under field conditions. The effects of non-ideal conditions on the performance of methods based on analytical heat flow equations to estimate water fluxes still need further investigation.

Lautz [23] generated synthetic time-series data using a numerical model to assess the influence of non-vertical flow, thermal gradients in the streambed and non-sinusoidal stream temperature signals. Non-vertical flow conditions in the model were identified as the greatest source of error in the estimation of downward water fluxes from the temperature time-series [23]. Despite high errors at points where the horizontal flow component was greater than the vertical, vertical flow velocities within the model could be adequately matched [23]. Therefore it was concluded that the time-series method still provides a valuable tool for mapping the spatial variability of fluxes within sites even under these conditions [23].

Spatial variability of the exchange flux at the groundwater–surface water interface has been attributed to geologic heterogeneity of the connected aquifer [7,11,20,32,37]. Kalbus et al. [19] inferred the heterogeneity of the hydraulic conductivity of an aquifer from measured streambed temperatures and simulated streambed temperatures for different geostatistical models of aquifer heterogeneity. A large range of methods has been developed to characterize and simulate geologic heterogeneity [10,13,25,26]. Geostatistical models commonly rely on the Gaussian assumption with heterogeneity fields that do not always adequately account for the discrete structure and connectivity of geologic units [12,24]. Geostatistical indicator models based on Markov chain representations of transition probabilities [5] or genetic models that better allow to represent connected paths of high hydraulic conductivity and preferential flows [22,26,34] offer an alternative. Preferential flow has been shown to play a crucial role in the transport of contaminants [34], but also in creating distinct spatial patterns of GW–SW exchange [7,11,14]. Vertical temperature profiles which are relatively easy to obtain at high spatial resolution can be used to identify preferential GW discharge areas in a stream [3,7,28,29]. However, preferential flow induced by streambed and aquifer heterogeneity violates the assumption of homogeneous sediments and strictly vertical flow. Moreover, heat is a non-conservative tracer and lateral dissipation of heat might conceal preferential pathways or small zones of high exchange fluxes [9]. In numerous field studies, steady-state approaches to delineate and quantify water fluxes at the groundwater–surface water interface based on streambed temperatures have been applied [1,3,7,28,29]. Hence there is a need to systematically analyze the general applicability and accuracy of temperature-based water flux calculations in heterogeneous sediments.

Streambed or lake sediment temperatures may be in a quasi steady-state below the depth influenced by diurnal temperature fluctuations. However, it has been shown that during seasonal temperature transition in spring and autumn, steady-state approaches are erroneous since the assumption of a quasi steady-state is not valid at these times. For instance, Anibas et al. [3] observed temperature time-series in the course of a year in the surface water and at several depths in the sediments of a river and a lake. Seepage fluxes obtained from transient simulations were compared to fluxes from steady-state analysis. Results significantly differed during transitional seasons (fall and spring) but were comparable during and towards the end of summer and winter. They concluded that the steady-state assumption is valid at certain times of the year.

Goto et al. [15] examined the general characteristics of the thermal response of saturated sediments to a sinusoidally varying surface water temperature boundary. Their approach is applied here to systematically investigate the influence of varying surface temperature on the performance of the steady-state approach.

The objective of our study was to evaluate the error introduced when estimating seepage fluxes with a steady-state analytical solution of the heat flow equation under field conditions that violate the underlying assumption of homogeneous sediments and steady-state temperature boundaries. Our analysis is limited to gaining conditions because the application of Eq. (2) to mapped streambed temperatures provides only reasonable estimates of seepage fluxes, if the streambed is not influenced by diurnal temperature variations. This is typically not the case for losing streams where the diurnal temperature oscillation propagates with the water flow deep into the sediment. We conducted numerical experiments where streambed temperatures were simulated in a 2D domain. On the one hand water fluxes were obtained from the numerical model, and on the other hand they were estimated with a simple analytical expression for temperature profiles sampled from the numerical model. Subsurface heterogeneity was implemented as different realizations of binary discrete geological units to evaluate the effect of heterogeneity on the accuracy of water flux estimates. Streambed temperatures under transient temperature boundary conditions were simulated analytically and the resulting water fluxes were compared with water fluxes derived from the analytical equation with constant temperature boundaries developed by Bredehoeft and Papadopulos [4].

2. Methods

2.1. Water flux calculation

The governing equation for diffusive and advective heat transport in homogeneous, saturated porous media is:

$$\frac{K_{fs}}{\rho c}\nabla^2 T - \frac{\rho_f c_f}{\rho c}\nabla \cdot (Tq) = \frac{\partial T}{\partial t} \tag{1}$$

where T [°C] is temperature; K_{fs} [J s^{-1} m^{-1} K^{-1}] is thermal conductivity of the solid–fluid system; ρc [J m^{-3} K^{-1}] is volumetric heat capacity of the solid–fluid system ($\rho c = n\rho_f c_f + (1-n)\rho_s c_s$), t [s] is time; $\rho_f c_f$ [J m^{-3} K^{-1}] is volumetric heat capacity of the fluid; $\rho_s c_s$ [J m^{-3} K^{-1}] is heat capacity of the dry solid; n [–] is porosity; and q [m s^{-1}] is the seepage velocity or specific discharge vector.

The analytical equation that was used to estimate water fluxes in this study is a solution to Eq. (1) for constant temperature boundary conditions $T(z) = T_0$ at $z = 0$, $T(z) = T_L$ at $z = L$ and one-dimensional steady water and heat flow [4]:

$$T(z) = \frac{\exp\left(\frac{q_z \rho_f c_f}{K_{fs}} z\right) - 1}{\exp\left(\frac{q_z \rho_f c_f}{K_{fs}} L\right) - 1} \cdot (T_L - T_0) + T_0 \tag{2}$$

where z [m] is the depth below the surface water–groundwater interface ($z = 0$); and q_z [m s^{-1}] is the vertical Darcy-velocity ($q_z < 0$ for upward flow).

The discharge to the surface water q_z can be estimated from a single streambed or lake bed temperature profile by finding the value for q_z that minimizes the squared differences between the measured (or in our case simulated) temperatures and the temperatures calculated with Eq. (2). The seepage fluxes were calculated from the simulated temperatures at 5 depths (0.1 m, 0.15 m, 0.2 m, 0.3 m and 0.5 m).

In the following, seepage fluxes calculated with Eq. (2) will be referred to as 'calculated' (q_z^{cal}), whereas the reference seepage fluxes derived from both the numerical model and the transient analytical simulations will be referred to as 'simulated' (q_z^{sim}).