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Theory, tools, and multidisciplinary applications for tracing groundwater fluxes from temperature profiles

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Quantifying groundwater fluxes to and from deep aquifers or shallow sediment is a critical task faced by researchers and practitioners from many environmental science disciplines including hydrology, hydrogeology, ecology, climatology, and oceanography. Groundwater discharge to inland and coastal water bodies influences their water budgets, thermal regimes, and biogeochemistry. Conversely, downward water flow from the land surface or from surface water bodies to underlying aquifers represents an important water flux that must be quantified for sustainable groundwater management. Because these vertical subsurface flows are slow and typically diffuse, they cannot be measured directly and must rather be estimated using groundwater tracers. Heat is a naturally occurring groundwater tracer that is ubiquitous in the subsurface and readily measured. Most of the academic literature has focused on groundwater temperature tracing methods capitalizing on the propagation of diel temperature sine waves into sediment beneath surface water bodies. Such methods rely on *temperature–time* series to infer groundwater fluxes and are typically only viable in the shallow subsurface and in locations with focused groundwater fluxes. Alternative methods that utilize *temperature–depth* profiles are applicable across a broader range of hydrologic environments, and point-in-time measurements can be quickly taken to cover larger spatial scales. Applications of these methods have been impeded due in part to the lack of understanding regarding their potential applications and limitations. Herein, we highlight relevant theory, thermal data collection techniques, and recent diverse field applications to stimulate further multidisciplinary uptake of thermal groundwater tracing methods that rely on temperature–depth profiles.

This article is categorized under:
Water and Life > Methods
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1 | INTRODUCTION

Characterizing and quantifying groundwater processes is increasingly recognized as an integral component of many environmental science disciplines. Groundwater–surface water exchanges impact the temperatures and biogeochemistry of surface

water bodies (Boulton, Datry, Kasahara, Mutz, & Stanford, 2010; Hayashi & Rosenberry, 2002; Kurylyk, Linnansaari, Mac-Quarrie, Cunjak, & Curry, 2015; Sophocleous, 2002), and influence the functioning, productivity, and diversity of aquatic ecosystems (Kløve et al., 2011; Power, Brown, & Imhof, 1999; Webb, Hannah, Moore, Brown, & Nobilis, 2008). Historically, most research addressing groundwater–surface water exchanges focused on inland settings. However, due to the increased awareness of groundwater discharge dynamics within the land–ocean continuum and the impacts on ocean and estuarine water quality, studies on submarine groundwater discharge have increased at an exponential rate (Moore, 2010; Sawyer, Michael, & Schroth, 2016). Also, monitoring and managing groundwater flows is emerging as a grand societal challenge (Castilla-Rho, Rojas, Andersen, Holley, & Mariethoz, 2017) to ensure future water security in the face of global environmental change (Vörösmarty et al., 2010). Although groundwater is acknowledged as a critical present and future water resource for ecosystems and society, many aquifers are presently being depleted as a consequence of unsustainable extraction (Famiglietti, 2014; Gleeson, Wada, Bierkens, & van Beek, 2012; Konikow & Kendy, 2005; Wada et al., 2010). Global aquifer depletion is expected to be exacerbated by further climate warming (Green et al., 2011; Taylor et al., 2012) and population redistribution to coastal and urban centers (Shah, 2005). Over-abstraction of groundwater can be avoided through effective planning, yet sustainable management is often precluded by the challenge of measuring groundwater fluxes to and from aquifers (Healy, 2010). The increasing interdisciplinary nature of groundwater science and the growing societal importance of sustainable groundwater management provide the impetus for this review outlining how temperature–depth (TD) profiles can be used to trace groundwater flow in a variety of hydrologic settings.

Groundwater flow induces heat advection and thereby affects subsurface temperature distributions. Due to this thermal signature imparted by mobile groundwater, an analysis of subsurface temperature distributions can yield quantitative insight into groundwater flow systems (Saar, 2011). The use of heat has several advantages over other groundwater tracers (Clark, 2015; Scanlon, Healy, & Cook, 2002) because it is present everywhere, it can be continuously monitored, it can be used to quantify multidirectional flow, and its measurement does not require specialized expertise. Seminal techniques for using heat as a groundwater tracer proposed in the 1960s (Bredehoeft & Papadopulos, 1965; Stallman, 1965) were adopted in a few hydrogeological studies (e.g., Cartwright, 1970; Sorey, 1971), but were not widely incorporated in the broader hydrologic sciences until an influential review paper revealed their wide applicability (M. P. Anderson, 2005). Methods based on Stallman's (1965) approach that use streambed periodic temperature signals to trace groundwater–surface water exchanges have been widely applied in aquatic sciences and have been thoroughly reviewed elsewhere (Constantz, 2008; Irvine, Briggs, et al., 2017; Rau, Andersen, McCallum, Roshan, & Acworth, 2014). As detailed in Section 2, methods relying on diel periodic temperature signals measured at point locations are limited to shallow zones (<1 m) with relatively high vertical flow rates. These approaches can also be applied to infer vertical groundwater fluxes from periodic seasonal temperature signals in shallow aquifers (e.g., Taniguchi, 1993), but typical basin average recharge rates are too low to be detectable with this method. Alternative techniques to trace vertical groundwater fluxes from TD profiles are potentially useful across a much wider range of hydrologic environments, often only require point-in-time measurements, and are sufficiently simple to be employed by nonspecialists. The objective of this study is to highlight classic and recently developed mathematical (analytical) models for estimating groundwater fluxes using TD profiles and to illustrate their potential multidisciplinary utility. Section 2 will review the importance of quantifying vertical groundwater fluxes in several environmental science disciplines and present past applications of TD methods. Sections 3 and 4 detail steady-state and transient TD mathematical models for estimating groundwater flows, explain how to choose an appropriate solution for a given application, and list open access computer programs for automating data analysis. Section 5 provides practical advice for TD data collection, and Section 6 highlights present method limitations and future research directions.

2 | INTERDISCIPLINARY NATURE OF THERMAL GROUNDWATER TRACING

The increasing interdisciplinary nature of academic science (Bridle, Vrieling, Cardillo, Araya, & Hinojosa, 2013; Porter & Rafols, 2009) is particularly apparent in groundwater hydrology, since groundwater processes influence surface and subsurface environments and many research questions lie at the interface between these domains. Estimating vertical groundwater fluxes is, of course, an important consideration in hydrogeology and groundwater engineering as the mass balance of an aquifer and sustainable yields of abstraction depend on the groundwater fluxes in (recharge) and out (natural groundwater discharge and well discharge). Past TD tracing applications in hydrogeology are listed in Sections 3 and 4 following the presentation of the different analytical solutions. In Sections 2.1–2.3, we highlight three other environmental science disciplines for which vertical groundwater flows are an important consideration and for which TD methods have been applied. In Figure 1, which illustrates these applications, the vertical spatial scale increases by two orders of magnitude from left to right and the time scales range from daily (a) to multidecadal (c), indicating that TD profile methods are applicable across diverse environments and spatiotemporal scales.
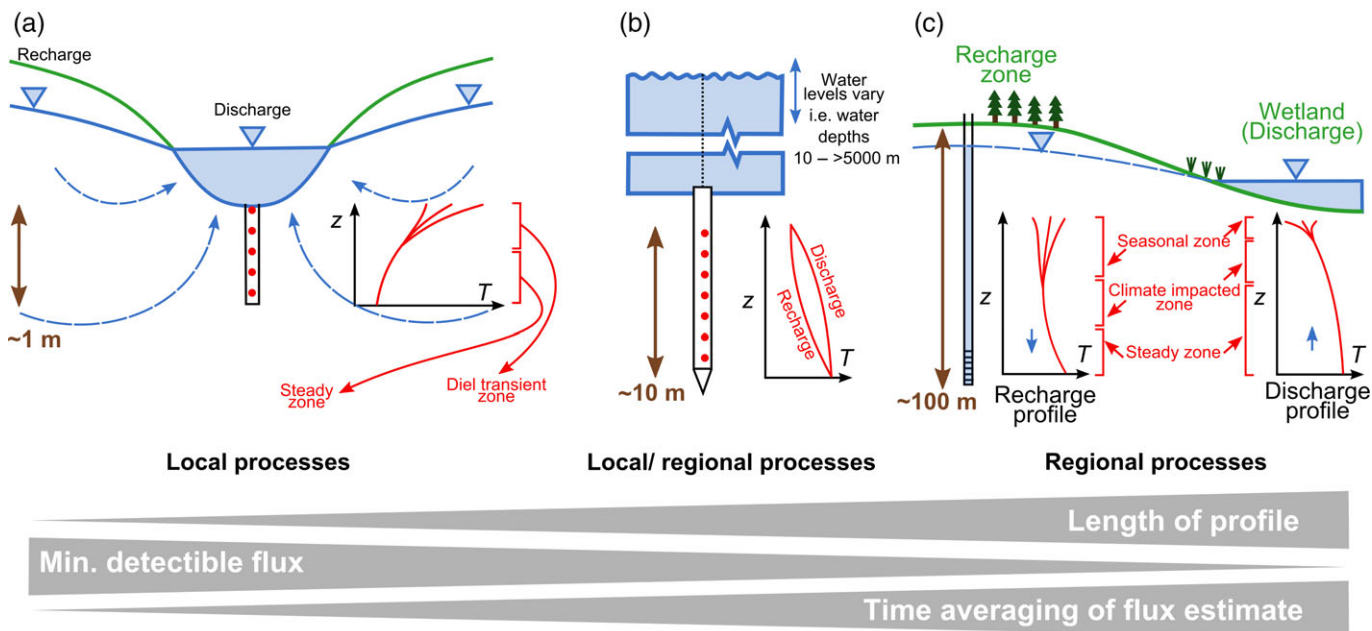
FIGURE 1 Diverse environments for using temperature–depth (TD) profiles to trace groundwater fluxes with the scale of the vertical TD profiles increasing and the minimum detectable groundwater flux decreasing from left to right. Potential environments include (a) streambeds separated into transient and steady-state zones, (b) offshore submarine applications (deep or shallow) for thermal groundwater tracing with concave-upward profiles indicating recharge zones and convex-upward profiles indicating discharge zones (note this implies the thermal profiles are at steady-state, but this is often not the case in very shallow coastal zones), and (c) deeper aquifer-scale applications in recharge and discharge zones with seasonal and climate impacts

2.1 | Aquatic ecology and thermal regimes of surface water bodies

Through its impact on the thermal and biogeochemical states of surface water bodies, groundwater discharge exerts critical control on the health, diversity, and complexity of aquatic ecosystems in several ways. Perhaps most importantly, groundwater discharge to lotic surface water bodies generates baseflow and enables stream and river flows to persist during dry periods (Boulton & Hancock, 2006; Hayashi & Rosenberry, 2002). Groundwater discharge also provides water for lentic water bodies such as lakes, ponds, and wetlands during dry periods (Winter, 1999). Hence, aquifers provide a source of water that sustains aquatic and riparian biota, and species that depend on these biota (Boulton & Hancock, 2006; Kløve et al., 2011). Also, groundwater discharge is cooler than surface water in the summer (Bilby, 1984; Briggs, Voytek, Day-Lewis, Rosenberry, & Lane, 2013) and warmer in the winter (Cunjak & Power, 1986; Power et al., 1999). The negative thermal offset between groundwater and surface water in summer enhances the spatial variability of water temperatures in surface water bodies by creating cold-water plumes at points of *focused* groundwater discharge. These are used by salmonids and other cold-water species for thermal refuge during high-temperature events (Ebersole, Liss, & Frissell, 2003; Power et al., 1999; Torgersen, Price, Li, & McIntosh, 1999), enabling ectotherms to persist across wider altitudinal or latitudinal ranges. On the other hand, *diffuse* groundwater discharge reduces the temporal (diel or seasonal) variability of temperature fluctuations in surface water bodies (Caissie, 2006; Kurylyk, Moore, & MacQuarrie, 2016) and thereby creates temporally modulated thermal environments. Subsurface water fluxes across the sediment underlying surface water bodies are not unidirectional as there is a constant cycling of water, heat, and solutes within the shallow hyporheic zone (Boano et al., 2014; Boulton et al., 2010; Cardenas, 2015; Findlay, 1995). This constant mixing has impact on dissolved oxygen levels, nutrient levels, pH, and other water quality parameters (Sophocleous, 2002).

Methods for estimating reach-scale contributions of groundwater discharge to streamflow using *surface water temperatures* include (a) surface water energy budgets (Loheide & Gorelick, 2006; Loinaz, Davidsen, Butts, & Bauer-Gottwein, 2013; Westhoff et al., 2007), (b) seasonal surface water temperature signal analysis (Briggs et al., 2018), and (c) regressions between mean daily air and surface water temperatures (Kelleher et al., 2012; Snyder, Hitt, & Young, 2015). These reach-based techniques are powerful for management decisions due to their potential large-scale applications, yet they are characterized by uncertainty because solar radiation and other interconnected surface heat fluxes complicate the relationship between groundwater inflows and surface water temperatures (Xie, Cook, Simmons, & Zheng, 2015). Alternatively, studies have been conducted at point locations using *subsurface temperature* beneath lentic (e.g., Stonestrom & Constantz, 2003) and lotic (e.g., Bravo, Jiang, & Hunt, 2002; Hunt, Krabbenhoft, & Anderson, 1996) surface water bodies as a groundwater tracer because subsurface heat transfer processes are better constrained and not directly impacted by solar radiation. The majority of these studies used methods relying on the downward propagation of periodic diel temperature signals into sediment to trace groundwater–surface water interactions (Hatch, Fisher, Revenaugh, Constantz, & Ruehl, 2006; Keery, Binley, Crook, &

Smith, 2007; Luce, Tonina, Gariglio, & Applebee, 2013; McCallum, Andersen, Rau, & Acworth, 2012). These methods require temperature–time series and are only applicable where periodic signals are present due to atmospheric variations or other forcing. Diel temperature signals tend to be fully damped within the upper ~0.5 m of the subsurface (Bense & Kooi, 2004; Irvine, Briggs, et al., 2017), and seasonal temperature signals are normally damped at depths of 15–20 m (Kurylyk, MacQuarrie, Caissie, & McKenzie, 2015; Taniguchi, 1993; Taylor & Stefan, 2009). Also, these temperature–time series methods are only useful when the groundwater flux and concomitant advection discernibly impact the periodic signal propagation. Analytical solutions suggest that, given the resolution of temperature loggers (Soto-López, Meixner, & Ferré, 2011) and the uncertainty in thermal property estimation, this requires a vertical groundwater flux at least 1 m/year (e.g., Stallman, 1965) for seasonal temperature signals. Fluxes on this order are common for locations of focused groundwater recharge or discharge such as in streambeds, but they are not typical of basin-average conditions.

Analytical methods using TD profiles, rather than temperature–time series, have also been applied to trace groundwater–surface water exchanges (Anibas, Buis, Verhoeven, Meire, & Batelaan, 2011; Anibas et al., 2009; Caissie, Kurylyk, St-Hilaire, El-Jabi, & MacQuarrie, 2014; Jensen & Engesgaard, 2011; C. Schmidt, Bayer-Raich, & Schirmer, 2006; C. Schmidt, Conant, Bayer-Raich, & Schirmer, 2007) because point-in-time TD profiles can be quickly measured at multiple locations along a river reach. As described in more detail in Section 3 and Figure 1, steady-state TD profiles exhibit a concave-upward shape for downwelling (groundwater recharge) conditions and a convex-upward shape for upwelling (groundwater discharge). Steady-state TD methods are especially powerful in the winter when ice-covered streams and underlying streambeds are at a constant temperature and cannot be analyzed with temperature–time series methods (Caissie et al., 2014). Section 5 explains how temperatures can be recorded at appropriate depths in sediment beneath surface water bodies to characterize fluxes using TD methods (Figure 1a) and how diel temperature changes in shallow streambed sediment can potentially be accounted for within steady-state methods.

2.2 | Coastal geography and oceanography

Groundwater discharging from terrestrial aquifers can transport land-based contaminants and nutrients to the sea and pollute marine or tidal waters (Beusen, Slomp, & Bouwman, 2013; Moore, 2010; Sawyer et al., 2016; Slomp & van Cappellen, 2004). The combination of rising sea levels and increased anthropogenic contamination of coastal aquifers gives rise to a "coastal groundwater squeeze" in which coastal zones of fresh, potable groundwater are under increasing pressure from both directions (Michael, Post, Wilson, & Werner, 2017). Near-shore water cycling between the ocean and underlying or adjacent aquifers impacts the ecosystem and biogeochemistry of marine water and the subsurface coastal mixing zone (Moore, 1999). Also, offshore groundwater discharge in deep-ocean settings occurs over large spatial scales and is a fundamental driver for biogeochemical cycles and processes (Kuhn et al., 2017; Wilson, 2003; Zektser & Dzhamalov, 2007).

Several different tracers (e.g., Ra and Rn isotope series) have been used to characterize submarine groundwater fluxes (Burnett et al., 2006), but these can be difficult to apply in deep-ocean settings. Seabed or coastal zone sediment that exhibits pronounced temperature variations can be suitable for adaptations of the classic heat tracing techniques that rely on temperature–time series and are used in aquifer–stream interaction studies (Goto, Yamano, & Kinoshita, 2005; Wilson, Woodward, & Savidge, 2016). However, such pronounced thermal variations are rare in deep-ocean settings, which are often considered to be at thermal steady-state. Ocean scientists began measuring deep-ocean seabed TD profiles in the 1950s (Bullard, 1954) to determine thermal gradients and conductive heat fluxes and to provide insight into lithosphere ages and plate tectonic processes. The instruments and techniques used in oceanography to collect TD profiles (Figure 1b) have been thoroughly reviewed in past studies (e.g., Wright & Louden, 1989). Seabed TD profiles in these settings are often curved and thus not linear as expected under conduction-dominated, homogeneous, and steady-state conditions. Several studies have attributed this curvature to the impacts of groundwater flow (Figure 1b) and have quantified submarine groundwater fluxes or geothermal circulation based on steady-state thermal groundwater tracing methods described in Section 3 (Abbott & Menke, 1981, 1983; R. N. Anderson, Hobart, & Langseth, 1979; Fisher & Becker, 1991; Geller, Weissel, & Anderson, 1983; Kurylyk et al., 2018; Wheat et al., 2004). However, such analyses can yield highly uncertain vertical groundwater fluxes because TD curvature may also be attributed to other factors such as vertical variations in seabed thermal conductivity and low-frequency bottom water temperature changes (Noel, 1984). Recent thermal tracing techniques (Sections 3 and 4) can be used to determine in which cases these compounding factors have to be accounted for in the mathematical model when studying groundwater fluxes in seabed sediment (Kurylyk et al., 2018).

2.3 | Climatology

Land surface schemes in global climate models usually represent groundwater processes with parsimonious approaches (Niu, Zong-Liang, Dickinson, Gulden, & Hua, 2007) that may not capture the complexity of groundwater flow systems. However,

large-scale groundwater flow systems influence the global cycling of water, energy, and carbon (e.g., Kessler & Harvey, 2001). Accurately representing deep groundwater flow and related processes in a manner that is scalable for these global models is an ongoing challenge in climatology (Krakauer, Li, & Fan, 2014). Also, the performances of global climate models are assessed through their ability to reconstruct historic climate change (Miao et al., 2014), preferably for periods extending before the observational record. Borehole climatology is a climate reconstruction technique in which pre-observational surface air temperatures are reconstructed from deep (e.g., 300 m) borehole TD profiles based on an understanding that low frequency air temperature changes propagate deeply into the subsurface and cause deviations in TD profiles (Smerdon & Pollack, 2016). Global borehole climatology studies (Huang, Pollack, & Shen, 2000; Pollack, Huang, & Shen, 1998) produced smooth global climate histories that differed substantially from the sharp warming reconstructions obtained from other proxies underlying the "hockey stick" reconstruction (Mann, Bradley, & Hughes, 1998). These borehole climate reconstructions were the subject of intense debate in the paleoclimate community for many years (Smerdon & Pollack, 2016).

One criticism of borehole climate reconstruction techniques is that they are based on heat conduction theory and do not accommodate heat advection due to groundwater flow (Lewis & Wang, 1992). In many regions of the world, the majority of boreholes are thermally influenced by groundwater flow (Wang, Lewis, Belton, & Shen, 1994), and thus accounting for groundwater flow remains a persistent challenge for borehole climate reconstruction (Bodri & Cermak, 2007). Past studies have demonstrated that concave-upward TD profile curvature induced by downward groundwater flow is similar to the effects of past land surface warming, while convex-upward TD profile curvature from upward groundwater flow is difficult to distinguish from the effects of prior surface cooling (Ferguson & Woodbury, 2005; Kukkonen, Cermák, & Safanda, 1994; Reiter, 2005; Taniguchi, Shimada, et al., 1999). Thus, climate reconstructions inferred from boreholes thermally influenced by horizontal or vertical groundwater flow can be highly inaccurate (Bense & Beltrami, 2007). Conversely, steady-state groundwater tracing TD methods (Section 3) applied by hydrogeologists in boreholes impacted by climate change can yield errors in the estimated water flux if the transient effects of climate change are not considered (Irvine, Cartwright, Post, Simmons, & Banks, 2016; Verdoya, Pasquale, & Chiozzi, 2008). Section 4 details analytical solutions for investigating subsurface thermal interactions between climate change and vertical groundwater flow. These can be applied to investigate the potential hydrogeologic "thermal contamination" of a borehole used for reconstructing climate. Figure 1c presents borehole TD profiles in recharge and discharge areas and illustrates the impacts of recent climate change.

3 | STEADY-STATE APPROACHES FOR ANALYZING TD PROFILES

In essence, groundwater fluxes are estimated from TD profiles by adjusting the groundwater flux in a thermal model until the modeled TD profile is fitted to the measured profile (Figure 2). Analytical solutions to heat transfer equations are well-suited for this purpose as their parsimony facilitates the solution to the inverse problem (Figure 2e). Most analyses of TD profiles to estimate vertical groundwater fluxes have used steady-state analytical solutions. Applying a steady-state equation offers key advantages because constant boundary conditions (BCs) can be applied and an initial condition (IC) for the TD profile is not required, and thus point-in-time measurements suffice. In this review, steady-state refers to the thermal regime as all analytical solutions assume a steady-state groundwater flow regime. Each analytical solution used for thermal tracing of groundwater solves a partial or ordinary differential equation describing subsurface heat transfer. The standard governing equation is based on the assumptions that subsurface heat transfer is restricted to the vertical dimension, limited to conduction and advection,
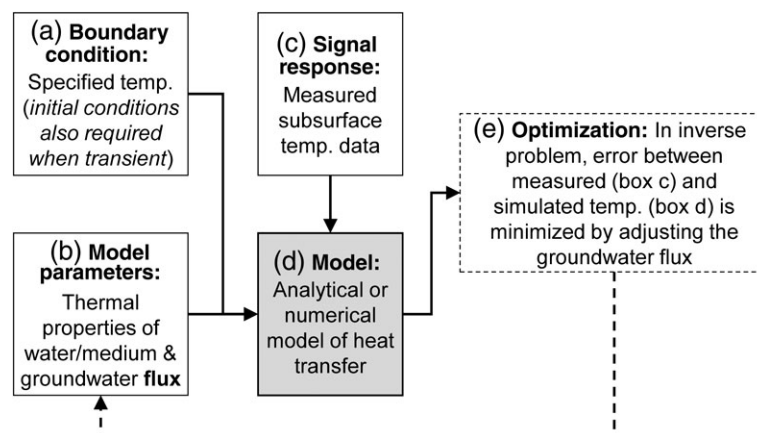

FIGURE 2 General approach for using heat as a groundwater tracer

and without any internal sources or sinks of heat. The governing partial differential equation is derived by equating the negative divergences of the conductive and advective heat fluxes to the rate of change of thermal storage (Suzuki, 1960):

$$\lambda \frac{\partial^2 T}{\partial z^2} - q c_w \rho_w \frac{\partial T}{\partial z} = c \rho \frac{\partial T}{\partial t},$$ (1)

where λ is the medium thermal conductivity (W/(m °C)), T is the temperature (°C), z is the depth below the surface (m), q is the steady-state vertical groundwater flux that is positive downwards (m/s), t is the time (s), c_w and c represent the specific heats of the water and the saturated medium, respectively (J/(kg °C)), and ρ_w and ρ are, respectively, the water and saturated medium densities (kg/m^3). Table 1 presents the symbols, definitions, and units for all parameters listed herein. The groundwater flux q (flow per unit area) is not equivalent to the groundwater velocity (v, m/s), since the entire porous medium contributes to the area used to calculate the flux, but the water is only mobile in the pore space. For saturated medium, these can be converted back and forth via the effective porosity n_e, the ratio of pore volume that contributes to flow divided by the total medium volume:

$$q = v n_e.$$ (2)

Effective porosity can range widely in geologic medium (e.g., 0.00005–0.5, Domenico & Schwartz, 1990, p. 26), and thus groundwater velocity may be orders of magnitude higher than Darcy flux.

Thermal dispersion is an advection-related subsurface heat transfer mechanism that arises because groundwater follows tortuous flow paths through porous media, and this tortuosity disperses thermal plumes (Bear, 1972). Sometimes the thermal conductivity term in Equation (1) includes the effects of both heat conduction and thermal dispersion with an "effective thermal conductivity" parameter (Molina-Giraldo, Bayer, & Blum, 2011; Sauty et al., 1982). However, there is still considerable disagreement in the hydrogeology community on the relative effects of conduction and thermal dispersion

TABLE 1 List of symbols and definitions

| Symbol	Definition	Units
α	Parameter for exponential surface warming (Figure 3d)	°C
b	Linear rate of top boundary warming	°C/s
β	Thermal Peclet number	–
c	Specific heat of medium	J/(kg °C)
c_w	Specific heat of water	J/(kg °C)
Δ_{max}	Maximum deviation from linear profile	°C
ΔT	Shift in the surface boundary temperature (Figure 3c)	°C
erfc	Complementary error function	–
G	Geothermal gradient (IC in Figure 3b,c)	°C/m
γ	Constant horizontal thermal gradient	°C/m
H	Heaviside function (=1 or 0)	–
κ	Parameter for exponential surface warming (Figure 3d)	1/s
L	Vertical distance between boundaries	m
λ	Thermal conductivity of medium	W/(m °C)
n_e	Effective porosity	–
q	Vertical groundwater flux	m/s
q_x	Horizontal groundwater flux	m/s
ρ	Density of medium	kg/m^3
ρ_w	Density of water	kg/m^3
t	Time	s
T	Temperature	°C
T_0	Top boundary temperature in several methods (Figure 3)	°C
T_i	Nonlinear initial condition parameter, $T_0 - \delta$	°C
T_L	Lower boundary temperature in BP method	°C
T_r	Constant thermal reservoir (lower) boundary temperature	°C
U	Thermal plume velocity due to advection	m/s
v	Vertical groundwater velocity	m/s
z	Depth below top boundary	m
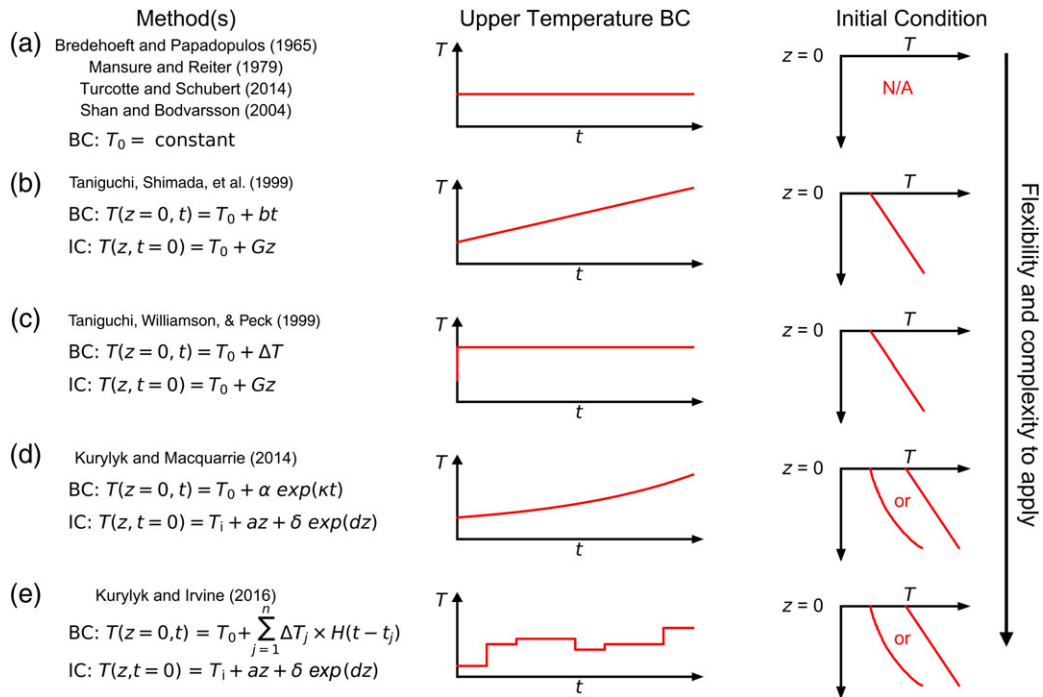
FIGURE 3 Different boundary conditions (BCs) and initial conditions (ICs) for the steady-state (a) and transient (b–e) solutions described in Sections 3 and 4, respectively. Citations and equations for each BC and IC are presented in the left column. Parameters are defined in Table 1

(M. P. Anderson, 2005; Rau et al., 2014). Thermal dispersion will not be further addressed in this review, since most of the applications are for low groundwater velocity scenarios for which thermal dispersion is not important (Bear, 1972; de Marsily, 1986).

If heat transfer is at steady-state, the right-hand side of Equation (1) equals 0, and the equation is reduced to an ordinary differential equation:

$$\lambda \frac{d^2 T}{dz^2} - q c_w \rho_w \frac{dT}{dz} = 0. \tag{3}$$

BCs are required to derive analytical solutions to Equations (1) and (3). Additionally, the transient systems (Section 4) for which Equation (1) needs to be solved require ICs (i.e., the TD profile at time = 0) that are not required for steady-state solutions. The range of possible BCs and ICs distinguish the alternate equations described below and their appropriate applications (Figure 3). The resultant analytical solutions are only presented below for the more parsimonious and/or commonly applied formulations. In other cases, readers are referred to the original studies.

3.1 | The Bredehoeft and Papadopulos (1965) method

Bredehoeft and Papadopulos (1965) proposed what is now a classic analytical solution (hereafter the BP method) for estimating q from TD profiles. The solution employs specified-temperature BCs at the top ($z = 0$, Equation (4)) and bottom ($z = L$, Equation (5)) of a domain (Figure 3a):

$$T(z = 0) = T_0, \tag{4}$$

$$T(z = L) = T_L. \tag{5}$$

The thermal Peclet number β is a dimensionless number equivalent to the ratio of the advective heat flux to the conductive heat flux. For the BCs above, the average β across the domain is:

$$\beta = \frac{q c_w \rho_w L}{\lambda}. \tag{6}$$

The analytical solution to Equation (3) subject to the BCs in Equations (4) and (5) is:

$$T(z) = T_0 + (T_L - T_0) \frac{\exp(\beta z/L) - 1}{\exp(\beta) - 1}. \tag{7}$$

This solution provides the theoretical background for the previously noted phenomenon of homogeneous, steady-state TD profiles being concave-upward in recharge areas and convex-upward in discharge areas (Figure 1b,c). The BP method can be used to quantify q by matching a measured profile to a type curve or by using a computer program to solve the inverse problem (Figure 2e). Both spreadsheet (Arriaga & Leap, 2006; Kurylyk et al., 2017) and MATLAB-based (Swanson & Cardenas, 2011) programs have been developed for estimating q using the BP method.

The estimation of q using Equation (7) relies on the deviation of a TD profile from a linear relationship. The maximum deviation (Δ_{max}) is (Kurylyk et al., 2018):

$$\Delta_{max} = (T_L - T_0)\left\{\frac{\exp(\beta) - 1 - \beta}{\beta\exp(\beta) - \beta} - \ln\left[\frac{\exp(\beta) - 1}{\beta}\right]\frac{1}{\beta}\right\}. \quad (8)$$

Equation (8) can be applied to show that higher values of β result in larger deviations. Given that the volumetric heat capacity of water $c_w\rho_w$ is a constant and the thermal conductivity of saturated porous medium λ does not change substantially, higher β (Equation (6)) can be achieved with higher fluxes (q) or greater lengths (L). Thus, two core advantages of the BP method over any of the sine-based techniques are (a) that much smaller fluxes (e.g., $q = \pm 0.05$ m/year) can be estimated if the profile length, L, is sufficient and (b) the thermal perturbations of interest penetrate far more deeply than diel or seasonal periodic thermal signals, enabling these techniques to be applied in deeper zones. The influence of the spatial scale on the minimum detectable flux is shown conceptually in the bottom of Figure 1.

Equation (3), which underlies Equation (7), is based on the assumption that heat transfer is restricted to a single dimension that is almost universally taken as vertical. In the original BP conceptual model, the solution domain extended across a low hydraulic conductivity unit, in which groundwater fluxes tend to be predominantly vertical (Freeze & Cherry, 1979). However, the BP method is applicable across diverse hydrologic environments including streambeds (Caissie et al., 2014; Jensen & Engesgaard, 2011), submarine sediment (Taniguchi, Turner, & Smith, 2003), glacial drift (Boyle & Saleem, 1979), interlobate moraines (Ferguson, Woodbury, & Matile, 2003), and large groundwater basins (Cartwright, 1970; Irvine, Kurylyk, et al., 2017; Sorey, 1971). Figure 4a presents a BP application for two deep TD profiles in South Australia.

In general, the invoked steady-state assumption of the BP method can be violated in many of the environments in which the method is applied. Streambeds can exhibit time-varying temperatures throughout the day due to periodic surface temperature cycles, shallow aquifer thermal regimes are often transient due to seasonal cycles, and even deep TD profiles may evolve over time due to the propagation of low frequency climate change signals (Bense & Kurylyk, 2017; Lesperance, Smerdon, & Beltrami, 2010). In the case of upwelling, upward heat advection counteracts the downward conduction of surface temperature signals, causing steady-state conditions to be achieved at shallower depths than under downwelling conditions. Thus, streambeds underlying surface water bodies receiving groundwater discharge are more suitable for steady-state techniques than streambeds recharging aquifers. This general principle of steady-state approaches being more applicable in discharge areas also extends to deeper settings. For example, Irvine, Kurylyk, et al. (2017) used TD profiles across the Willunga Basin in South Australia to quantify q and found that transient approaches (Section 4) were required in groundwater recharge areas, but the BP method could be reasonably applied in groundwater discharge areas provided the top boundary was below the zones
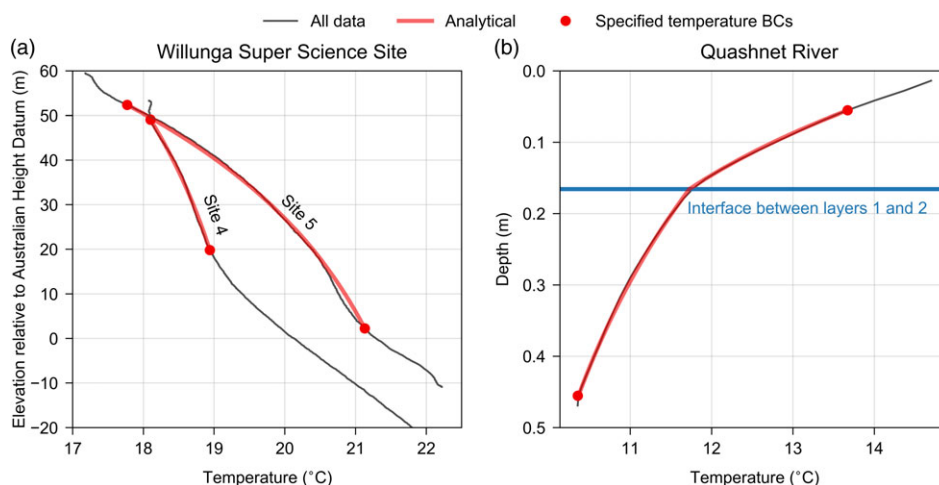

FIGURE 4   (a) Measured deep temperature–depth (TD) profiles (gray) at the Willunga Super Science Site, South Australia (data from Irvine, Kurylyk, et al., 2017) and the optimal Bredehoeft and Papadopulos fits (red series), that yielded q values of 366 and 352 mm/year upward flow for Sites 4 and 5, respectively. (b) A measured, daily average, streambed TD profile in the Quashnet River, Massachusetts, USA (gray) and the optimal fit using the two-layer Shan and Bodvarsson (2004) algorithm (red). In this example (data from Kurylyk et al., 2017), a low-λ organic mud layer overlies a high-λ sand layer. The blue line in (b) denotes the interface between the two layers. Vertical ranges for the analyses in (a) and (b) are explained in the original papers

impacted by climate change and seasonal variations (Figure 4a). Also, as noted, streambeds tend to be at steady-state in the winter in colder regions, as ice-covered water bodies remain close to 0°C (Caissie et al., 2014). Finally, streambed transient thermal effects may potentially be accounted for by using the daily average of a transient TD profile when conducting a BP analysis (Kurylyk et al., 2017), although this remains a subject of ongoing research. In summary, the steady-state assumption is a limiting factor for the BP method; however, in some cases, there are ways to circumvent or correct for transient disturbances.

3.2 | Variations of the Bredehoeft and Papadopulos (1965) method

Alternate forms of the BP method have been proposed to enable the approach to be applied in even more diverse settings. These other steady-state techniques (Figure 3a) are presented below in general order of their proximity to the BP conceptual model. Solutions have been derived with a specified thermal gradient BC at the bottom boundary (Harris & Chapman, 1995) or at both boundaries (Deming, 2001, section 11.4). These solutions can be difficult to apply for tracing groundwater as the gradient continuously changes for a curved TD profile, whereas a bottom specified temperature is easy to obtain directly from the measured profile. Also, the inferred q is very sensitive to even minor variations in the lower heat flux (Kurylyk et al., 2018). In general, solutions with specified heat flux (Neumann) BCs have seldom been used for estimating q.

Others have modified the BP approach to account for horizontal groundwater flow. Mansure and Reiter (1979) developed graphical TD analysis methods similar to the BP approach. However, they addressed the problem from the field of geothermics rather than hydrogeology, as they were particularly interested in accurately determining near-surface conductive heat fluxes in zones impacted by groundwater flow. Their approach quantifies the effects of horizontal and vertical heat advection on TD profiles and near-surface conductive fluxes by plotting the temperature gradient versus temperature. One example hydrogeological application is a multiwell study in Japan (Dapaah-Siakwan & Kayane, 1995). Reiter (2001) later enhanced this method and demonstrated how the horizontal and vertical components of groundwater flow could be extracted from a steady-state TD profile by plotting the vertical temperature gradient as a function of both depth and temperature. This approach has been applied in a few hydrogeological studies (e.g., Ferguson et al., 2003) but has not been widely implemented. Lu and Ge (1996) modified the governing equation (Equation (3)) to include a constant, horizontal flow of heat and fluid via a source/sink term:

$$\lambda \frac{d^2T}{dz^2} - qc_w\rho_w \frac{dT}{dz} - q_x c_w\rho_w\gamma = 0,$$ (9)

where q_x is the horizontal groundwater flux (m/s) and γ is the horizontal thermal gradient (°C/m). They derived the corresponding analytical solution subject to the same BCs (Equations (4) and (5)) and provided type curves to assess q from TD profiles. Reiter (2001) pointed out that the coupling between vertical and horizontal groundwater flows can lead to equifinality in the solution to the inverse problem. In general, there exists some disagreement in the hydrogeological community on the impacts of horizontal water fluxes on TD profiles. Lu and Ge (1996) suggest horizontal groundwater fluxes should be accounted for in the thermal analysis if their magnitudes exceed 10% of the vertical flux. In contrast, Irvine et al. (2016) used two-dimensional numerical models and proposed that TD profiles could be analyzed with one-dimensional approaches when horizontal groundwater fluxes were up to 1,000% of the vertical flux. These disparate conclusions stem from differences in the underlying conceptual models, especially with respect to the horizontal thermal gradients.

Shan and Bodvarsson (2004) derived an algorithm for a multilayered version of the BP method with each layer characterized by a different thermal conductivity. They demonstrated its application using TD profiles in the vadose zone. Kurylyk et al. (2017) extended the application to multilayered streambeds (Figure 4b) and multilayered aquifer systems and presented Flux-LM (Flux in Layered Media), a spreadsheet-based tool for automating the solution to the inverse problem for the BP method and the Shan and Bodvarsson (2004) solution. They also demonstrated that layering can introduce TD profile curvature that can be falsely attributed to groundwater flow and that not accounting for layering may yield errors in both the direction and magnitude of the inferred q.

Turcotte and Schubert (2014, p. 444, and in earlier versions of this text) present an analytical solution to Equation (3) for a semi-infinite domain. Their conceptual model has a large, constant temperature thermal reservoir at great depths. Their lower BC at an infinite depth is thus an insulating (no conductive flux) thermal boundary. The analytical solution, which is somewhat similar in form to the BP solution but extended to a semi-infinite domain, is a function of the reservoir temperature T_r (°C) and parameters previously defined:

$$T(z) = T_r - (T_r - T_0)\exp\left(\frac{c_w\rho_w qz}{\lambda}\right).$$ (10)

This solution has been employed to estimate q from TD profiles above geothermal reservoirs (e.g., Hanano & Kajiwara, 1999) and to estimate groundwater discharge to streams (C. Schmidt et al., 2007). Ferguson and Bense (2011) suggested that this approach yields similar flux estimates to the BP method.

4 | TRANSIENT APPROACHES FOR ANALYZING TD PROFILES

4.1 | The Taniguchi, Shimada, et al. (1999) method

BCs and ICs for the transient analytical solutions discussed below are shown schematically in Figure 3b-e. As discussed above, curvature in TD profiles can arise due to transient effects from changes in ground surface temperatures caused by deforestation, urbanization, or climate change. Taniguchi, Shimada, et al. (1999) recognized that these transient effects could induce curvature and thereby invalidate q estimates inferred from disturbed TD profiles using steady-state approaches. They simplified a solution previously presented by Carslaw and Jaeger (1959, p. 388) and adopted it to study the combined subsurface thermal impacts of surface temperature changes and vertical groundwater flow. The IC and top BC are expressed as linear functions (Figure 3b) to represent a linear climate warming rate and a linear initial geothermal gradient. The analytical solution to the transient form of the governing equation (Equation (1)) subject to the linear BC and IC is:

$$T(z,t) = T_0 + G(z - Ut) + \frac{1}{2U}(b + UG) \times$$
$$\left[(UT - z)\, \mathrm{erfc}\left(\frac{z - Ut}{2\sqrt{\lambda t/(c\rho)}} \right) + (UT + z)\exp\left(\frac{Uzc\rho}{\lambda} \right) \mathrm{erfc}\left(\frac{z + Ut}{2\sqrt{\lambda t/(c\rho)}} \right) \right],$$
(11)

where G is the geothermal gradient (°C/m), b is the rate of surface warming (°C/s), erfc is the complementary error function, and U is the thermal plume velocity due to advection ($U = qc_w\rho_w/(c\rho)$, m/s). This solution is hereafter referred to as the CJT method (Carslaw & Jaeger (1959); Taniguchi, Shimada, et al., 1999). The CJT method demonstrates that vertical groundwater flow and surface temperature change signals interact in the subsurface, creating offsetting or superimposed disturbances (Figure 5).

One challenge with the CJT method is that both an initial TD profile (Figure 3b) and a later TD profile are required for first initializing the problem and then using the later profile to solve the inverse problem and estimate q. The IC represents the TD profile at some point in the past prior to the impacts of recent climate warming. The initial profile is typically just assumed, and then the measured, present-day TD profile is used for solving the inverse problem (Taniguchi, Shimada, et al., 1999). A common approach (e.g., Gunawardhana & Kazama, 2011) for estimating the IC is to extrapolate the lower (presumably linear) portion of the TD profile that has not yet been impacted by climate change to the land surface. This is similar to what is done in borehole climatology when generating an IC (Bodri & Cermak, 2007). However, over time, the CJT method creates shifts between the initial and final TD profiles even at great depths (Bense, Kurylyk, van Daal, van der Ploeg, & Carey, 2017) due to a lack of agreement in the implicit q of the IC (a linear profile implies no groundwater flow) and the explicit q of the forward modeling. Depending on the direction and magnitude of groundwater flow, these shifts can be positive (Figure 5a), negligible (Figure 5b), or negative (Figure 5c). Practically speaking, the CJT method usually requires that the initial TD profile be offset (shifted to the right or left) from the extrapolated linear portion of the measured TD profile to enable matching between the present-day measured and calculated profiles. The CJT approach has been applied in hydrogeology studies, particularly in Asia, to estimate q from TD profiles impacted by climate change or urbanization (e.g., Gunawardhana & Kazama, 2011; Gunawardhana, Kazama, & Kawagoe, 2011; Miyakoshi, Uchida, Sakura, & Hayashi, 2003; Taniguchi, Shimada, et al., 1999, 2003; Uchida & Hayashi, 2005).

4.2 | Variations of the Taniguchi, Shimada, et al. (1999) method

Other transient equations for estimating q from TD profiles have been proposed, although to date these have been less frequently applied than the CJT method. In the same year, Taniguchi, Williamson, and Peck (1999) modified the identical Carslaw and Jaeger (1959, p. 388) solution to incorporate a BC with a single step change in temperature (Figure 3c) to represent the sudden and persistent thermal impact of land cover change. The IC remains the same as the standard CJT method. The modified analytical solution was applied to study groundwater fluxes in a region of Western Australia that experienced surface and subsurface warming following forest clearing (Taniguchi, Williamson, et al., 1999).

Kurylyk and MacQuarrie (2014) questioned the use of a linear IC to represent steady-state TD profiles, noting that according to the BP approach, steady-state TD profiles in hydrogeologically active areas are nonlinear. They suggested that an additional exponential term should be added to the IC to allow for curvature (Figure 3d). This IC was sufficiently flexible to
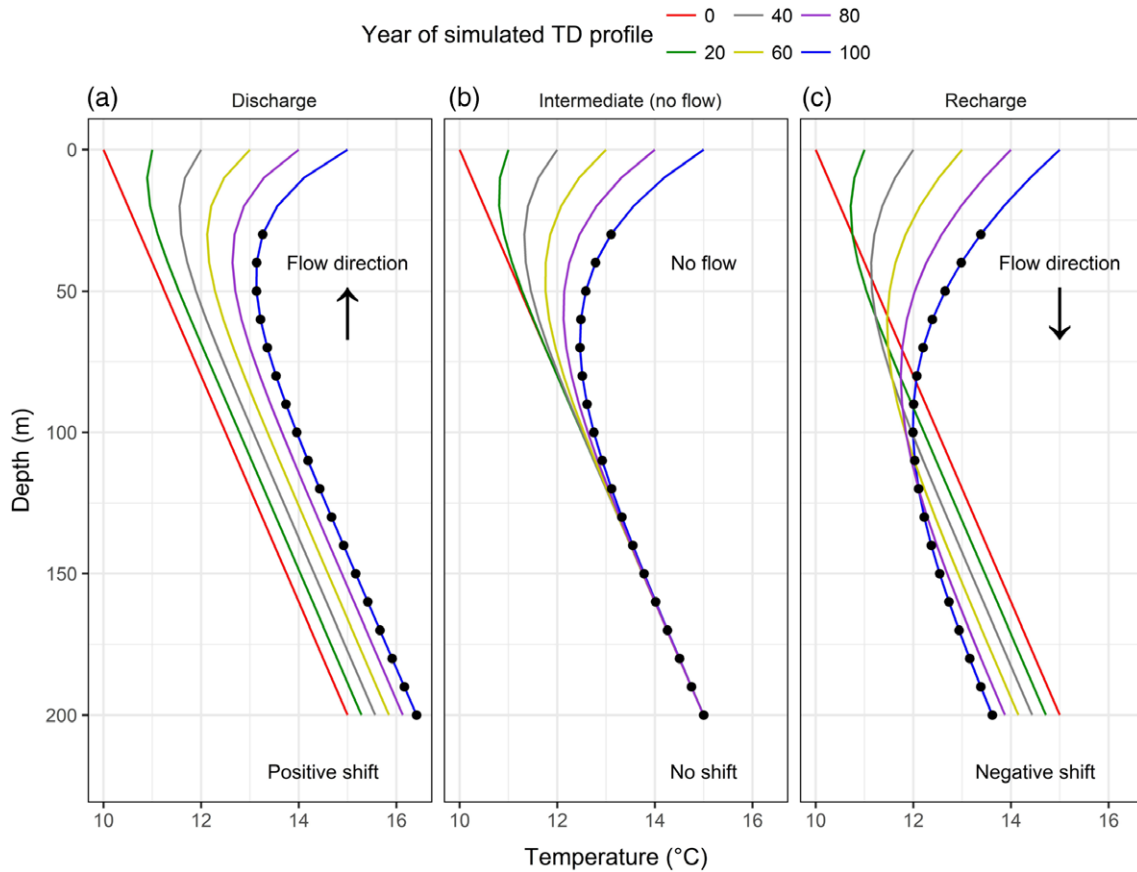
FIGURE 5 Temperature–depth (TD) profiles simulated over 100 years by the CJT method (Equation (11)) for (a) discharge, (b) intermediate, and (c) recharge conditions. In (a) and (c), q has a magnitude of 0.4 m/year. Thermal properties represent those for saturated sand. Black circles represent theoretical, present-day (i.e., 100 years from the IC) measured TD profiles that are the fitting objective for the CJT method

match present-day, observed TD profiles in Japan, and the resultant analytical solution was applied to simulate future groundwater warming for different climate scenarios (Kurylyk & MacQuarrie, 2014).

Menberg, Blum, Kurylyk, and Bayer (2014) capitalized on the linear form of the governing partial differential equation (Equation (3)) and proposed that superposition principles could be used to derive an analytical solution when the BC was represented as a series of n step changes (Figure 3e):

$$T(z=0,t) = T_0 + \sum_{j=1}^{n} \Delta T_j \times H(t-t_j), \tag{12}$$

where ΔT_j is the change in surface temperature for step change j (°C), t_j represents the time when step change j begins (s), and H is the Heaviside function that turns the steps on through time since $H(t - t_j) = 0$ before t_j and 1 after t_j. The advantage of Equation (12) over the more commonly applied CJT linear BC is that it is more capable of matching complex surface temperature evolution over time due to changes in climate or land cover. Menberg et al. (2014) derived an analytical solution to Equation (3) subject to a constant IC and a multistep BC (Equation (12)) and applied the solution to reconstruct multidecadal time series of observed groundwater warming in Germany. The ability to successfully reproduce historic groundwater warming using these parsimonious solutions parameterized with known recharge rates provides support for their utility to infer groundwater fluxes in regions with known recent climate history.

Kurylyk and Irvine (2016) built upon these prior foundations and derived a flexible solution with a nonlinear IC and a multistep BC (Figure 3e). To automate the data analysis, Kurylyk and Irvine (2016) created the Python-based model FAST (Flexible Analytical Solution using Temperature) to enable the user to quickly fit a series of boundary step changes to represent measured time series of past surface air temperatures and to forward model from an initial TD profile to the present-day measured TD profile (Figure 6). Surface air temperatures are used to generate the BC steps, but it is ground surface temperatures that actually drive the shallow subsurface thermal regime. Ground surface and air temperatures are offset on a mean annual basis, but changes in these temperatures are often thought to be coupled on a multidecadal basis (Bodri & Cermak, 2007). The FAST user must specify a thermal offset between mean annual air and ground surface temperatures (Figure 6a). The user can adjust q to achieve the optimal fit to the data by minimizing the root mean square error of the present-day
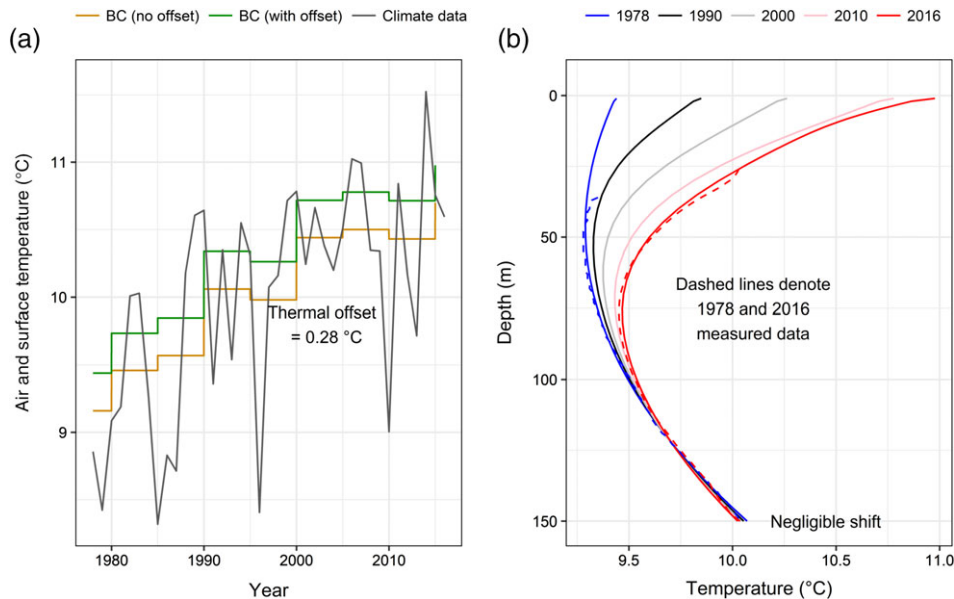
FIGURE 6 (a) Air temperatures from the Netherlands (gray) used to generate the Flexible Analytical Solution using Temperature (FAST) surface temperature boundary condition (BC). These air temperatures are represented using 5-year steps. The influence of the offset (Section 4.2), which was determined to be 0.28°C for this site, is apparent in the upward shift from the gold to the green BCs. (b) Measured temperature–depth (TD) profiles in Deelen, the Netherlands, in 1978 (blue dashed line) and 2016 (red dashed lines). The 1978 profile was used as the FAST initial condition (blue solid line), and the forward model (forced by the green BC) produced the optimal 2016 modeled TD profile (red solid line) with a downward q of 0.3 m/year. Data underlying this figure are from Bense et al. (2017)

observed and modeled TD profiles (Figure 6b). FAST has been applied to estimate groundwater fluxes in Japan (Kurylyk & Irvine, 2016), South Australia (Irvine, Kurylyk et al., 2017), and the Netherlands (Bense et al., 2017).

Like the CJT approach, one challenge with FAST is that the ICs are normally unknown, and the initial curvature is dependent on the unknown q value. Kurylyk and Irvine (2016) detail an iterative approach to circumvent this limitation and to generate a steady-state initial TD profile that has the same implied q as the value explicit in the forward modeling. This approach minimizes the thermal shifts obtained at depth (Figure 5). Bense et al. (2017) overcame this IC issue by using repeated TD profiles from the Netherlands (Figure 6b), with the earlier recorded profile forming the IC and the later profile becoming the fitting objective. Such repeated profiles are rare but are becoming more common (Benz et al., 2018; Davis, Harris, & Chapman, 2010; Dĕdeček, Šafanda, & Rajver, 2012; Ferguson & Woodbury, 2007; Kooi, 2008; Šafanda, Rajver, Correia, & Dĕdeček, 2007; Yamano et al., 2009) as several decades have passed since early TD logging was conducted through the 1970s and 1980s. Bense et al. (2017) also demonstrated that the CJT approach yielded drastically different vertical groundwater fluxes using TD profiles from the same wells but different years, and that FAST and a numerical model yielded consistent q values through time.

As a result of warming over the past century, the typical geothermal gradient near the Earth's surface is reversed in direction, and temperatures decrease with depth until they reach a minimum temperature (Figure 7b), known as the "inflection point" (Bense & Kurylyk, 2017). The CJT analytical method has often been used to infer q by matching simulated and measured TD profiles across a large depth range. However, Taniguchi, Shimada, et al. (1999) originally proposed an insightful approach for estimating q from the downward propagation of the inflection point. They showed that the derivative of the analytical solution (Equation (11)) could be set to 0 to solve for the inflection point depth (global minimum), and they demonstrated that the downward migration of this inflection point strongly depends on q. Although their analytical approach was self-contradictory due to the IC issues already noted, their inflection point concept is very powerful and innovative. Bense and Kurylyk (2017) used a numerical model to show that the q values obtained from the inflection point migration of repeated TD profiles logged in the Netherlands (Figure 7) agreed well with those estimated from Darcy's Law by combining measured hydraulic head gradients and hydraulic conductivity estimations. They proposed that such data could be used for estimating long term, average groundwater fluxes, which must be quantified to inform sustainable groundwater management. However, to date, no physically accurate analytical approach has been presented for conducting such analyses, forcing users to adopt numerical techniques to solve the inverse problem (Figure 2e). It is important to note that methods relying on repeated TD profiles are somewhat similar to temperature–time series methods used in streambeds. In the former, subsurface temperature is effectively continuous with depth but recorded at discrete points in time, whereas in the latter, temperature is effectively continuous in time but recorded at discrete depths.
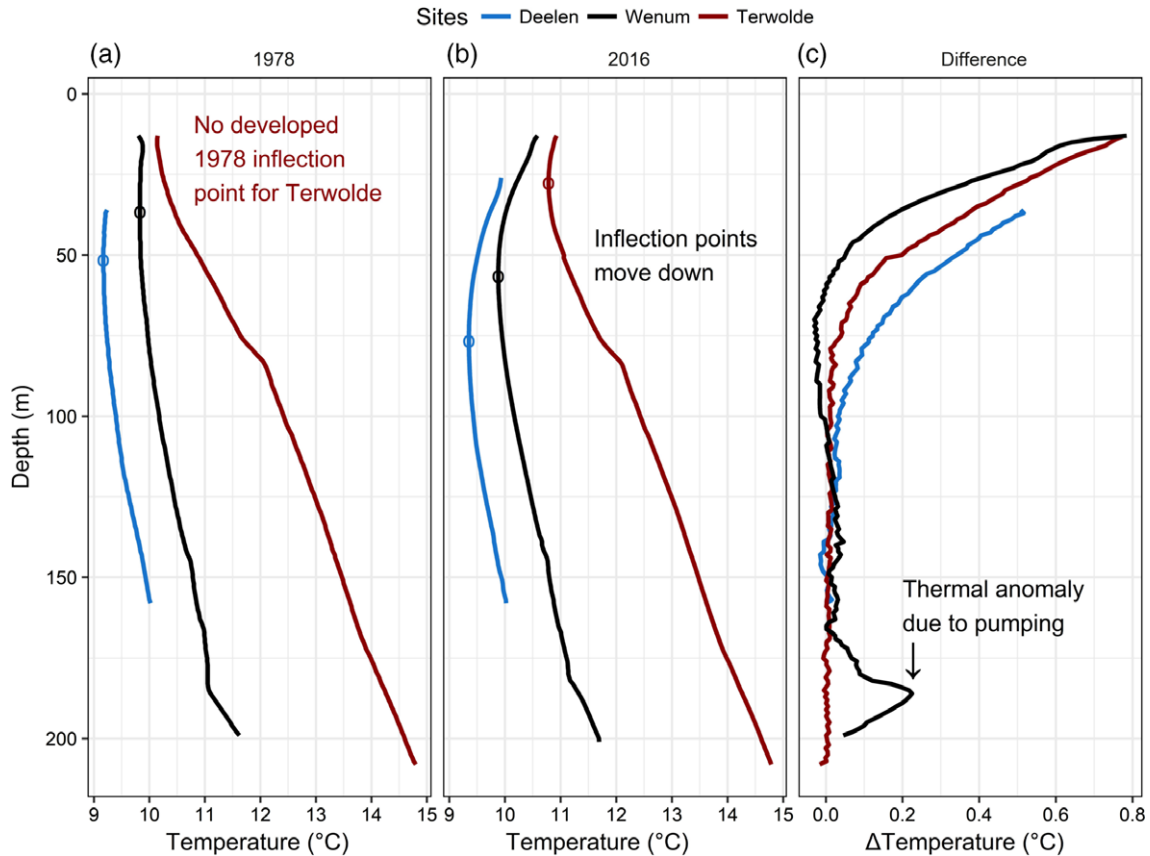
FIGURE 7 (a) Measured 1978 temperature–depth (TD) profiles for three sites in the Netherlands representing recharge (Deelen, blue), intermediate (Wenum, black) and discharge (Terwolde, red) conditions (data from Bense & Kurylyk, 2017). Symbols show inflection points in the TD profile (see text). (b) Data from the same boreholes reprofiled in 2016 with inflection points that have migrated downwards. Inflection points appear earlier and migrate more deeply in recharge zones (Deelen) than in discharge zones (Terwolde). (c) Thermal difference between (a) and (b). The Deelen profile was analyzed in FAST (see Figure 6) since this profile was characterized by homogeneous conditions

5 | GUIDELINES FOR DATA COLLECTION

5.1 | Data collection in shallow environments

Practical resources are available that detail best practices for thermally monitoring shallow streambeds (e.g., Briggs, Lautz, Buckley, & Lane, 2014; Irvine, Briggs, et al., 2017; Stonestrom & Constantz, 2003). These sources provide guidelines on temperature data collection when applying temperature–time series (sine-based) methods. Herein, the focus is on measuring data in streambeds and shallow wells for analysis with TD methods. The simplest approach to collect multidepth stream-bed temperatures (Figure 8a) is to progressively pound a probe containing a single embedded temperature sensor into the streambed (Anibas et al., 2009). This approach yields point-in-time discrete TD data that can be converted into a continuous TD profile via interpolation. The primary advantage of this approach is that an inexpensive tool can be used to quickly obtain point-in-time TD profiles in many locations along a streambed. To our knowledge, no research has been conducted to examine potential impacts from frictional heat generated with this approach, although decades of work has revealed that frictional heating from the larger driven probes used in oceanography should be accounted for (e.g., Wright & Louden, 1989).

Alternatively, self-contained temperature loggers can be installed in the streambed at different depths (Figure 8a) to yield temperature–time series (Hatch et al., 2006). Such data can be analyzed using sine-based methods (Hatch et al., 2006; Keery et al., 2007; Luce et al., 2013; McCallum et al., 2012; Stallman, 1965). However, when periodic signals are absent, such as in the winter for ice-covered streams (Caissie et al., 2014), these data can still yield groundwater fluxes via steady-state TD methods (Section 3). It is important to note that if streambed temperature data are to be analyzed with TD methods, a sufficient number of loggers (usually ≥5) must be installed at different depths to accurately characterize the curvature of the TD profile. Also, the elevation difference between the top and bottom temperature sensors in the vertical array will influence the minimum detectable flux since deviations from a linear profile are more discernible with a longer profile. Equation (8) can be used to estimate an appropriate vertical range that will accommodate different flux magnitudes and directions. As a rule of thumb,
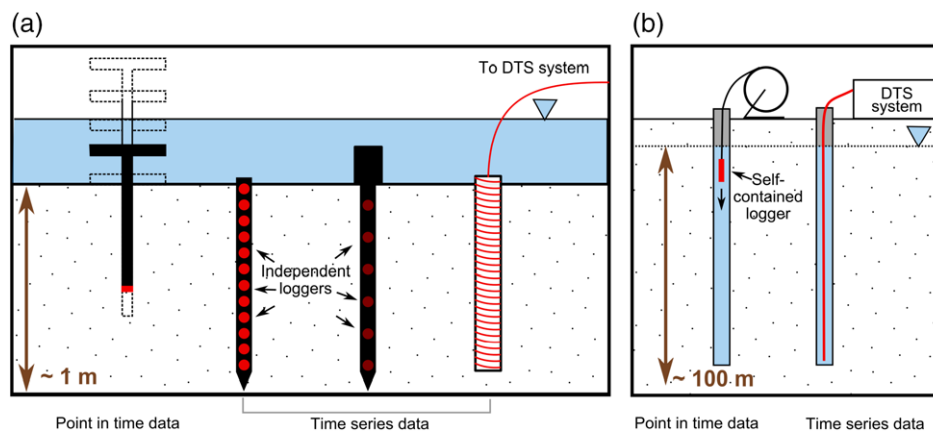
FIGURE 8 (a) Methods for temperature–depth (TD) profile recording in shallow sediment include (from left to right) progressively lowering a probe with a single temperature sensor, stakes with embedded, multidepth temperature loggers, self-contained thermal logging instruments, and high-resolution temperature sensors. (b) Methods for TD profile recording in wells include slowly lowering a temperature probe (including continuous logging and the stop–go method) or installing a fiber optic table cable to conduct distributed temperature surveys

0.5 m is typically a sufficient vertical length to characterize the TD profile curvature and quantify stream–aquifer exchanges. Different self-contained thermal loggers can be installed in wooden stakes or metal rods, and these stakes or rods can be manually driven into the streambed and left to collect data for durations of days to months. The iButton is a common, inexpensive choice for a self-contained thermal logger with many applications in environmental sciences (Hubbart, Link, Campbell, & Cobos, 2005; Johnson et al., 2005; Wolaver & Sharp, 2007). These are available with different specifications, and the high-resolution version (e.g., 0.0625°C, the "L" series) is often applied for heat-as-a-tracer applications (Briggs et al., 2014). They are not waterproof, and thus researchers normally cover the loggers with silicone or some other type of sealant (Roznik & Alford, 2012). These loggers can be embedded in stakes or dowels by drilling holes slightly larger than the iButtons and then making a tight seal with the waterproofing agent around the embedded iButton.

One disadvantage of using an array of self-contained loggers is that the loggers must be individually removed at the end of every deployment in order to download the data. This time-consuming process provided the motivation for recent integrated streambed thermal probes containing multiple sensors that can be concurrently programmed and queried using an external controller (Naranjo & Turcotte, 2015). Similar devices have existed in oceanography for decades as reviewed by Louden and Wright (1989). Thermal probes used to record seabed TD profiles are normally lowered from marine vessels and slowly driven into the seabed sediment with large weights (Wright & Louden, 1989). In this way, seabed thermal data can be recorded even with overlying ocean depths of several kilometers (Kurylyk et al., 2018). Instruments to thermally monitor shallow coastal zones are often similar to those applied in streambed applications (e.g., Wilson et al., 2016).

Temperatures sensors may also be installed at multiple depths in shallow wells to record TD profiles within the seasonal zone of the subsurface (depths <20 m). Only a few studies (e.g., Kikuchi & Ferré, 2017; Kurylyk, Bourque, & MacQuarrie, 2013; Lapham, 1989; Taniguchi, 1993; Taylor & Stefan, 2009) have reported these seasonally varying TD profiles. Thermal properties can be estimated from the lagging and damping of seasonal ground surface temperature signals (Kurylyk et al., 2013). Seasonal subsurface sine waves can also be used to infer vertical groundwater fluxes (Taniguchi, 1993) using a variant of the Stallman (1965) analytical solution or related numerical methods; however, this method can only be applied where the vertical flux is high, such as beneath a streambed (Lapham, 1989) or in heavily irrigated regions (Taniguchi, 1993).

One relatively recent development in streambed thermal monitoring is the application of high-resolution temperature sensors that rely on fiber-optic cables connected to a distributed temperature sensing (DTS) system (Briggs, Lautz, McKenzie, Gordon, & Hare, 2012; Vogt, Schneider, Hahn-Woernle, & Cirpka, 2010). The spatial resolution of the first-generation DTS systems used in hydrology is low (~1 m), but the vertical resolution can be improved by wrapping the fiber-optic cable around a piezometer (Figure 8a) producing a vertical resolution in the order of ~0.01 m (Briggs et al., 2014). High-resolution data obtained from such systems can be used to detect groundwater fluxes with the BP method or the Shan and Bodvarsson (2004) approach and even to discern variations in the thermal properties within a streambed (Kurylyk et al., 2017).

5.2 | Data collection in deep environments

Boreholes allow the measurement of TD profiles potentially to depths of kilometers (e.g., Yamano & Goto, 2005). The basic assumption underlying the use of boreholes for thermal profiling of the Earth's crust is that the temperature stratification

recorded in the water column inside the borehole is an accurate reflection of the ambient temperatures in the surrounding geologic medium. The validity of that assumption is controlled by the borehole diameter, the presence of casing, the geothermal conditions, and the TD measurement technique (Cermak, Safanda, & Kresl, 2008; Colombani, Giambastiani, & Mastrocicco, 2016; Eppelbaum & Kutasov, 2011). Density-driven convection of water within large-diameter boreholes is a particular concern, as this creates rapid vertical thermal mixing that is not reflective of the ambient geologic medium (Cermak et al., 2008; Eppelbaum & Kutasov, 2011). Equations proposed by Hales (1937) for estimating critical geothermal gradients can be rearranged to isolate for the critical borehole radius that would induce convection (see equation 6 in Ferguson et al., 2003). Uncased, large-diameter (e.g., 1,000 mm) boreholes are often located in areas of fractured rock as the purpose is to intersect as many water-bearing fractures as possible. Such boreholes are prone to vertical thermal convection as well as internal vertical flow where they mediate a "short-circuit" between horizontal fractures (Drury, Jessop, & Lewis, 1984; Read et al., 2013). This in-borehole flow can be quantified by analyzing TD profile characteristics (Klepikova, Le Borgne, Bour, & Davy, 2011). If thermal disturbances from vertical convection or fractures are not present, standard hydrogeological techniques to record groundwater quality variations with depths, such as long well screens or samples from multilevel piezometers, are not required for thermal logging due to efficient radial heat transfer into the borehole through the casing.

The simplest technique to record a TD profile is to lower a thermometer, or temperature sensor, attached to a cable or tape into a borehole to record temperatures at regular depth intervals (Figure 8b). This approach is known as wire-line logging. Logging is usually conducted from the top down so that the probe measures ahead of the disturbed water column. The temperature sensor can be embedded in a small datalogger to eliminate the need to transfer signals through the attached cable back to the surface. Using a datalogger simplifies the choice of the cable as a steel cable with >1 mm thickness is usually sufficient. The disadvantage of this design is that the temperatures sensed at depth cannot be directly inspected, and logging issues may not be apparent until data are later downloaded. Conversely, a disadvantage of using a data cable to interrogate the sensor is that readings from thermistor-based temperature sensors usually need to be corrected for the electrical resistance of the data cable. This electrical resistance is also temperature dependent and likely to vary over the duration of the measurement. The use of digital sensors might help to overcome this issue, but these do not currently have the required precision to be useable for TD logging.

Boreholes are often thermally logged by stopping for a few seconds at predetermined intervals to allow the sensor to equilibrate to a new stable temperature reading. This process is known as the stop–go method (Costain, 1970). The stop–go method yields precise and accurate TD logs, but values are only available at discrete depths. The appropriate depth intervals depend on the amount of spatial detail required, which in turn is related to the precision of the temperature sensor and the expected vertical thermal gradients. Depth intervals of 1 m are often chosen for deep TD logging, and this interval seems to be appropriate for groundwater flux estimations for a range of hydrogeological conditions. These depth intervals can be manually recorded from a tape with marked incremental depths, automatically logged using an electric tape, or inferred from water pressure data if a coupled temperature–pressure sensor is used. An alternative logging technique is to lower the sensor at a constant rate to yield effectively continuous temperature data (Conaway & Beck, 1977). The probe movement must be sufficiently slow to avoid any artifact from the sensor not equilibrating to the changing temperatures. As this rate is difficult to achieve, data collected from continuous logging are often processed to deconvolve the probe response time effects from the measurements (Conaway, 1977). Harris and Chapman (2007) proposed a hybrid approach in which continuous logging is conducted as the probe moves progressively downward, but "stops" are also made at discrete depths to allow for thermal equilibration. Figure 7 presents illustrative TD data recorded in 50-mm diameter cased boreholes in the Netherlands using the Harris and Chapman (2007) approach. These measured profiles revealed that the temperature precision required to record very small changes in thermal gradients should be 0.002°C or higher (Bense & Kurylyk, 2017). This is especially the case in areas where surface warming and groundwater flow have led to a strong decrease or reversal of thermal gradients in the upper ~100 m of the subsurface.

The use of DTS with fiber-optic cables (Hurtig, Groβwig, & Kühn, 1996; J. S. Selker et al., 2006; F. Selker & Selker, 2018) to monitor borehole temperatures has been thoroughly discussed in a recent review (Bense et al., 2016). This technology has several potential advantages and disadvantages compared to thermal wireline logging. One advantage is that fiber-optic cables can be installed in a borehole, and at a later point in time, TD profiles can be obtained instantaneously over large depth ranges without disturbing the water column. Also, the spatial resolution (e.g., 0.12 m) of more recent DTS systems is superior to what is practical using a stop–go approach in wireline logging. Thus, DTS systems effectively allow for subsurface temperatures to be recorded continuously in space and time. On the other hand, the temperature precision of well-calibrated thermistor-based loggers is better than what can be obtained with DTS systems (e.g., 0.001°C vs. 0.01°C), and the cost of a wireline logging setup is presently at least an order of magnitude lower than the somewhat prohibitive costs of state-of-the-art DTS systems.

6 | LIMITATIONS AND FUTURE ADVANCES

6.1 | Limitations

Limitations of TD groundwater tracing methods have been noted briefly above but are listed together here. Applications of the analytical solutions discussed in Sections 3 and 4 can be complicated as field data and processes are never as idealized as the governing equations and solutions assume. The primary limitations of more recent, transient TD methods relate to the underlying assumptions of the governing equation rather than the form of the BC. First, in these methods, groundwater fluxes are assumed to be constant in space, yet hydrogeologists have long known that the vertical component of the groundwater flux in aquifer-scale systems tends to decrease with depth and in higher hydraulic conductivity zones (Freeze & Cherry, 1979). This trend of decaying vertical flux with depth is also apparent at smaller scales in streambeds (Stonestrom & Constantz, 2003). Irvine et al. (2016) demonstrated that one-dimensional heat tracing methods yield the average vertical groundwater flux when applied across a vertical domain with a changing vertical component of flux.

Second, groundwater fluxes are also assumed to be at steady-state, even for the transient thermal equation (Equation (3)). Groundwater fluxes vary seasonally in the vadose zone and in shallow aquifers and thereby limit heat tracing applications (Clutter & Ferré, 2018). Although these variations are damped with depth (Dickinson, Ferre, Bakker, & Crompton, 2014), long-term changes in groundwater recharge due to climate change (e.g., Kurylyk & MacQuarrie, 2013; Scibek & Allen, 2006; Taylor et al., 2012) or land cover change (Ranjan et al., 2006; Scanlon et al., 2006) impact deeper groundwater flow regimes and likely invalidate steady-state flow assumption in certain cases. Although, widely cited analytical solutions have been presented that accommodate time-varying groundwater fluxes (e.g., Kumar, Jaiswal, & Kumar, 2010), these have later been shown to be mathematically invalid (Deng & Qiu, 2012).

Third, with the exception of a few quasi-two-dimensional steady-state solutions (Section 3), heat transfer is assumed to be constrained to the vertical dimension. However, lateral heat advection due to horizontal diffuse groundwater flow or focused fracture flow can violate this assumption. Even in the absence of groundwater flow, horizontal conductive heat flow can be caused by surface topography (Blackwell, Steele, & Brott, 1980; Noel, 1984; Šafanda, 1994) or land cover heterogeneity (Ferguson & Beltrami, 2006). Fourth, the equation assumes homogeneous conditions for thermal properties, but vertical variations in subsurface thermal properties can impact TD profiles (Ferguson, 2007) and alter the solution to the inverse problem to estimate groundwater flux (Kurylyk et al., 2017). Finally, air temperature records or projections are often used to form the ground surface BC for these models since ground surface temperatures are usually not available. Decoupling of air and surface temperatures on multidecadal timescales may invalidate this approach (Beltrami & Kellman, 2003; Mann & Schmidt, 2003; Mellander, Löfvenius, Laudon, Lofvenius, & Laudon, 2007; W. L. Schmidt, Gosnold, & Enz, 2001; Smerdon et al., 2004).

Although not a limitation per se, it is also important to note that the explicit or implicit temporal and spatial scales of consideration when using heat as a groundwater tracer are influenced by the environment in question. As Figure 1 and the preceding sections detail, many of the same methods are applicable in a range of hydrologic environments, yet there are important differences between the use of temperature as a groundwater tracer in deep versus shallow environments. For example, groundwater fluxes yielded from TD profiles in shallow streambeds (e.g., upper 0.5 m) represent hydrogeological processes averaged over small spatial domains and for relatively short time periods (e.g., 1 day). In contrast, groundwater fluxes estimated from deep (e.g., 100 m) TD profiles represent decadal averages for groundwater fluxes averaged across much larger spatial domains. The former scales are useful for studying dynamic environments, such as stream–streambed interfaces, while the latter scales are useful for informing long-term sustainable groundwater resources management. Related to this, the timescales for the steady-state assumption invoked by the simpler TD methods (Section 3) are related to the TD profile length. For example, streambed thermal profiles can be considered to be in a quasi-steady-state condition if there is little thermal change on a daily basis (e.g., Kurylyk et al., 2017), whereas deeper TD borehole profiles should be temporally invariant on decadal timescales in order to apply steady-state approaches.

6.2 | Future research directions

The above-noted potential method limitations represent future research opportunities. Improved theoretical (numerical or analytical) approaches that can accommodate these complexities, while still being sufficiently simple to enable the solution to the inverse problem, would be welcomed by this research community. Also, numerical studies indicating when and where these assumption violations in the analytical methods are important for groundwater flux estimations are rare and only available for select hydrogeological environments (Irvine et al., 2016). In addition to these theoretical advancements, there are opportunities to develop improved thermal logging techniques to either increase the thermal precision or spatial resolution of existing techniques or to prevent fracture flow from thermally contaminating boreholes. For example,

Colombani et al. (2016) recently demonstrated that a packer system could be installed vertically between large fractures to prevent vertical flow and accurately record the ambient geologic temperatures. There are also many opportunities to collect deep TD data and enhance global datasets, particularly in boreholes that were thermally logged in past decades. Such repeat thermal profiles are not common in hydrogeologically active areas and can be used to overcome issues associated with unknown ICs (Section 4).

The theoretical development and application of equations to investigate interactions among groundwater flow, surface temperature change, and subsurface thermal regimes have traditionally been conducted in segregated academic disciplines. A more transdisciplinary approach that combines hydrogeologists, borehole climatologists, and thermal geophysicists for deep TD applications and hydrologists, stream ecologists, and oceanographers for shallow sediment applications is recommended. Also, few studies show multimethod comparisons of groundwater fluxes obtained from TD methods and other groundwater tracing techniques (Scanlon et al., 2002). It is imperative that more multitracer groundwater flux estimation studies be conducted to compare the accuracy of these techniques and to provide independent assessments of the methods. Finally, new, user-friendly models with intuitive graphical user interfaces could be developed to enable new researchers in this field to process data and assess the potential limitations and viability of applying heat as a groundwater tracer at their field site(s).

7 | SUMMARY AND CONCLUSIONS

In the past 15 years, there has been a resurgence of academic study related to the use of heat as a groundwater tracer. This revival has been spurred by intensified interest in quantifying groundwater fluxes in many environmental science disciplines. Prior to this time period, most hydrogeology studies using heat as a tracer applied the steady-state TD method (Bredehoeft & Papadopulos, 1965). However, since 2005, the vast majority of related publications have relied on streambed temperature–time series methods that are variations on the classic Stallman (1965) approach. New transient TD methods (Section 4) have recently been proposed to overcome some of the steady-state limitations of the Bredehoeft and Papadopulos (1965) solution. These transient methods will become more important as climate change is increasingly perturbing borehole thermal profiles and limiting the utility of steady-state methods. Since TD techniques can detect smaller fluxes than sine-based heat tracing approaches and can be applied in more diverse hydrologic environments, we call for more studies examining the applications and potential limitations of these approaches in hydrology, hydrogeology, oceanography, stream ecology, borehole climatology, thermal geophysics, and other relevant environmental science disciplines. Herein, we have provided fundamental theory, data analysis tools, and practical data collection tips to equip new researchers in this topic and enable them to progress beyond the present state-of-the-art in this field.

CONFLICT OF INTEREST

The authors have declared no conflicts of interest for this article.

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