

# Water Resources Research<sup>®</sup>

## **METHOD**

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## **Key Points:**

- Temperature-depth profiles disturbed by climate change can be analyzed to quantify groundwater fluxes across aquitards
- Temperature-derived groundwater fluxes are analyzed in conjunction with hydraulic head data to estimate aquitard hydraulic conductivity
- Estimates of aquitard hydraulic conductivity agree with independent assessments based upon conventional methods

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# Inferring Aquitard Hydraulic Conductivity Using Transient Temperature-Depth Profiles Impacted by Ground Surface Warming

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**Abstract** Aquitard hydraulic properties are notoriously difficult to assess, yet accurate aquitard hydraulic conductivity estimates are critical to quantify recharge and discharge to and from semi-confined aquifer systems via hydraulic head gradients. Such flux quantification is required to evaluate the risks of aquifer exploitation by groundwater abstraction and aquifer vulnerability to surface contamination. In this study, we consider a regionally important aquitard and compare existing hydraulic head monitoring and thermally derived through traditional methods to those inferred from long-term hydraulic head monitoring and thermally derived vertical groundwater fluxes (0.04–0.25 m/y). We estimate the fluxes using numerical modeling to analyze the propagation of decadal climate signals into temperature-depth profiles and fitting the simulated and observed inflection point depths (location of minimum temperature). Results suggest that climate-disturbed temperature-depth profiles paired with multi-level head data can yield accurate vertical fluxes and aquitard hydraulic conductivities. This approach for characterizing groundwater systems and quantifying flows to and from sedimentary aquifers is more efficient but yields results that are comparable to conventional methods.

**Plain Language Summary** In sedimentary aquifer systems the in and outflow toward deeper groundwater is strongly controlled by the hydraulic conductivity of clay and silt layers and the quantification of these fluxes is crucial for the sustainable management of water resources. However, the low permeability of such units is difficult to establish from in-situ or laboratory measurements. Alternatively, environmental isotopes have been widely used to estimate travel times of groundwater across such units. In this paper we present a novel technique to estimate vertical groundwater flow rates, based upon heat as a tracer, that opportunistically exploits the impacts of accelerated surface warming on subsurface thermal regimes. We show how a parsimonious analysis of temperature-depth profiles that are disturbed by surface warming, in combination with hydraulic head data, lead to accurate and reliable estimates of aquitard hydraulic conductivity. This approach for characterizing groundwater systems and quantifying flows to and from sedimentary aquifers is more efficient and may be more accurate than conventional methods.

## 1. Introduction

Sustainable groundwater resource management for semi-confined aquifers relies on accurate estimations of vertical groundwater fluxes (Bierkens & Wada, 2019; Döll & Fiedler, 2008). However, groundwater recharge to shallow aquifers and subsequent flow across aquitards and toward deeper, pumped aquifers is notoriously difficult to measure or estimate (Scanlon et al., 2006). These flows can be quantified as the product of the aquitard vertical hydraulic conductivity ( $K_z$ ) and hydraulic gradients imposed by geological, climatological, and anthropogenic processes. Where available, piezometers in boreholes can readily provide direct multi-level measurements of hydraulic head and resultant vertical hydraulic gradients (Post & van Asmuth, 2013). In contrast, K and storage properties are challenging to evaluate, particularly for low-K units (Van der Kamp, 2001). The observed range of K values spans over 10 orders of magnitude (Sanchez-Vila et al., 2005). Low K values (~10<sup>-6</sup>-10<sup>-1</sup> m/day) in unconsolidated sedimentary aquifer systems are associated with clays and silty sediments that form aquitards, whereas more sand-rich to gravel units form aquifers (Freeze & Cherry, 1979). Aquitards limit the vertical exchange of groundwater and dissolved solutes between aquifers above and below aquitards. Hence, reliable quantification of aquitard  $K_z$  is fundamental to evaluate vertical groundwater fluxes, the impact of groundwater abstraction from deep aquifers on near-surface groundwater tables, and the risk of deep groundwater pollution by the ingress of shallow, low quality groundwater across aquitards (Filippini et al., 2020; Hart et al., 2005). Although aquifer hydraulic properties are classically obtained via pumping tests and other forms of in-situ hydraulic testing (Kruseman & De Ridder, 1994), such direct assessment of aquitard hydraulic conductivity is problematic because of the practical challenges of inducing significant groundwater flow rates in low-K field settings (Van der Kamp, 2001; Zhao & Illman, 2018). Under laboratory conditions, a variety of hydraulic methods are available to infer aquitard K (e.g., Ferris et al., 2020; Hiscock & Najafi, 2010; Smerdon et al., 2014; Timms et al., 2014). However, important questions remain as to whether aquitard K values yielded from laboratory testing under very high hydraulic gradients that exceed natural gradients are representative of aquitard field properties (Neuzil, 2019). Furthermore, the high spatial K variability in sedimentary aquifer-aquitard systems makes finding representative K values at scales relevant for regional groundwater flow models a significant challenge that persists after decades of focused research (Sanchez-Vila et al., 2005). Analysis of natural fluctuations of hydraulic head above and below aquitards can potentially yield accurate estimates of aquitard K (Jiang et al., 2013; Zhuang et al., 2015), but these approaches are restricted to settings with pronounced temporal hydraulic head fluctuations. Also in some cases, hydraulic test data from an aquifer directly below an aquitard can also be interpreted to yield aquitard properties (Van der Kamp, 2001).

Calibrating numerical models for groundwater management requires matching model output to observations of both hydraulic heads and groundwater fluxes to limit equifinality challenges, that is, hydraulic heads depend on both fluxes and the K distribution (Hill & Østerby, 2003). Therefore, groundwater management tools often require paired hydraulic head values and flux estimates. Methods to quantify downwelling fluxes across aquitards to deeper aquifers are commonly based on environmental tracers (e.g., Wilske et al., 2020), in particular the depth distribution of groundwater age (e.g., Visser et al., 2013). Heat can also serve as an environmental tracer to yield estimates of groundwater fluxes, with most methods focused on quantifying the vertical flux component (Anderson, 2005), or inferring hydraulic conductive fields at a range of scales (Saar, 2010). Heat has several advantages over geochemical tracers because groundwater temperature is ubiquitous and can be relatively easily measured, making this approach generally applicable across a range of spatial and temporal scales (Kurylyk et al., 2019). Also, because heat diffuses efficiently across piezometer casing, the temperature inside small-diameter piezometers represents the ambient ground temperature at the same depth outside the casing, enabling a depth-dependent profile from a single piezometer. In contrast, other environmental tracers often require multi-level piezometers to get depth-dependent profiles. Temperature depth profiles (TDPs) recorded in boreholes can display deviations from conduction-dominated conditions, with the effects of non-conductive heat transfer attributed to heat advection from groundwater movement (Bredehoeft & Papadopulos, 1965). Traditional steady-state approaches and associated assumptions are often now violated because global surface warming has resulted in transient heat flow in the upper tens to hundred meters of the subsurface (Ferguson & Woodbury, 2005; Kooi, 2008; Taniguchi et al., 1999). New methodologies for analyzing climate-disturbed TDPs (Bense et al., 2017, 2020; Kurylyk et al., 2019) have focused on estimating groundwater fluxes by tracking the depth of the TDP inflection point, where the minimum temperature is recorded and where the thermal gradient reverses.

In this study, we advance beyond past research by showing how transient TDPs paired with hydraulic head time series can yield reliable estimates of both vertical groundwater fluxes and aquitard K, which are critical combined data for numerical model calibration and groundwater management. To this end, we exploit the position of the inflection point in TDPs disturbed by recent climate change to infer vertical groundwater flow rates in aquifer-aquitard systems. We show that these estimates of vertical flow rates, when combined with hydraulic head data, yield aquitard K estimates over the thickness of the aquitard that are in the same order of magnitude as independent estimates obtained from upscaled aquitard K values based upon laboratory determinations of coreplug samples and in-situ hydraulic testing. Our methodology is a relatively simple and cost-effective approach with the potential to provide reliable aquitard K estimates that are comparable to more conventional field and laboratory techniques.

## 2. Data

The Renkum Brook catchment in the Netherlands (Figure 1) is underlain by an aquifer system consisting of loosely consolidated Quaternary sediments of sand, silt, and clay, which are primarily of riverine origin. Past glaciations have resulted in the development of moraine complexes on top of the otherwise predominantly layer-cake stratigraphy of the river sediments (Figure 1a). The sedimentary aquifer (lower aquifer) is undisturbed by glacio-tectonics and forms the preferred site of groundwater abstraction for domestic, and industrial water use. This aquifer







**Figure 1.** Map of the area of the Renkum Brook Valley in the Netherlands, as a digital elevation model with hill-shading. The locations of the 9 boreholes from which we analyze hydrogeological and thermal data are indicated and labeled with their site-ID. The upper panel illustrates the hydrogeological make-up of the area. This schematic cross-section (A-A') shows the position of the 'Waalre' aquitard of sity sand and clay, separating a phreatic upper aquifer, that consists mostly of coarse grained glacial moraine material and post-glacial outwash sediments commonly referred to as 'sandr' deposits, from a semi-confined lower aquifer made up of coarse-grained riverine deposits.

system is semi-confined and overlain by the 'Waalre' aquitard consisting of silt and clay, which can be interlocked with sandy layers. In turn, on top of the aquitard is a phreatic aquifer formed by the glacially disturbed sediments in the western part of the study area, as well as by post-glacial river deposits (often referred to as 'sandr') in the Renkum Brook valley toward the center of the area (Figure 1). Groundwater abstraction for water supply and industrial purposes from the lower aquifer in the area is concentrated in the south (Bense et al., 2020). This, in combination with water table gradients mediated by the topography of the area (Figure 1), results in a regional tendency for phreatic water tables to be higher than the deeper aquifer potentiometric surface, causing groundwater downwelling through the Waalre aquitard.

For our analysis, we compiled readily available geological (borehole descriptions) and hydrogeological data (hydraulic heads observed in piezometers) from eight locations in the Renkum Brook catchment area (Figure 2) to assess the decadal average hydraulic gradient across the regionally significant Waalre aquitard. Detailed descriptions of the lithology encountered during drilling were available for all boreholes from the Dutch Geological Survey. During backfilling of each borehole, several multi-depth piezometers were installed using PVC pipes (diameter  $2.6-5 \cdot 10^{-2}$  m) slotted along the lowest 2 m of the tube. Aquitard intervals where significant clay/silt was encountered during drilling were backfilled with clay, and aquifer intervals were filled with coarse sand. These piezometer 'nests' have enabled the monitoring of hydraulic heads in the deeper semi-confined aquifers as well as the phreatic water table elevation since the mid 1980s for most boreholes.

Within the framework of hydrogeological investigations in the Netherlands, borehole cores are often taken during drilling, with care to not disturb the original packing and cohesion of the sediments. Smaller core plugs are then sampled to perform laboratory measurements of hydraulic conductivity. This has resulted in a database of laboratory-derived *K* values for the main hydrogeological units in the country. These form the basis of the REGIS hydrogeological schematization of the Netherlands (dinoloket.nl). In REGIS, effective aquitard  $K_z$  values are available that are based upon on a geostatistical upscaling (harmonic averaging of horizontal *K* from core-plug to obtain  $K_z$ ), and spatial interpolation to generate maps for use in regional groundwater flow models (Hummelman et al., 2019). The uncertainty in the effective aquitard  $K_z$  estimates obtained from this procedure is reflected in REGIS by listing a plausible range of values.

In the deepest piezometer at each site, the TDP was measured with either an autonomously logging RBR soloT instrument (RBR technologies, Inc., Canada), or by using a conventional PT100 thermistor probe attached via a data cable to a logging device at the surface. For both instruments, data were collected following the stop-go methodology (Harris & Chapman, 2007) at 1 m depth intervals. Figure 2 shows the TDPs (black dots) at the eight locations we considered, the depth and thickness of the Waalre aquitard (shading, Figure 2), and the piezometers from which decadal hydraulic head time series were available. The hydraulic head time series is variable (Figure 3), with some boreholes having a near continuous data set since 1985 (boreholes 549, 321, and 550). For other locations, data have only been collected since the late 1990s (580, 575), or instead have been discontinued since roughly that time either for all (224) or just one of the piezometers of interest (552, 541). Moreover, at locations where records do not end in the 1990s, the frequency



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**Figure 2.** The eight boreholes in which TDPs were measured for this study (a–h). In each panel (a–h) the TDP (black symbols) is shown together with the depth and thickness of the Waalre aquitard (blue shading), as well as the position of the piezometers above and below the aquitard from which hydraulic head were available (Figure 3) to assess the hydraulic head difference across the 'Waalre' aquitard at each location. The red circle in each TDP indicates the position of the inflection point used to estimate the vertical groundwater flow ( $q_z$ ) across the aquitard. Solid lines are model TDPs that are used to asses a value for  $q_z$  for the 'high' (blue line) and 'low' (green line) values for thermal diffusivity (see Section 3). The fluxes were obtained by specifically matching the depth and temperature of the modeled and measured inflection point, rather than the entire profile.

of observations has been increased since the early 2000s when bi-weekly or monthly manual measurements were replaced by daily records using automated pressure transducers.

We calculated the median hydraulic head differential across the Waalre aquitard for all locations, as well as the standard error around the median (Figure 3). To avoid any bias from the higher frequency of recent observations, we interpolated and re-mapped all observations for the data series onto the same regular time interval before calculating the statistical values of each data set. The hydraulic gradient (*i* [m/m]) across the Waalre aquitard, with a thickness D [m] from the borehole description, is then found by assuming that the head difference ( $\Delta h$  [m]) between the piezometers in aquifers above or below the Waalre aquitard is representative of the hydraulic head difference within the Waalre aquitard, that is,  $i = \frac{\Delta h}{D}$ . This assumes any vertical hydraulic head gradient inside the aquifer is negligible compared to that across the aquitard, which is a common assumption in the hydrogeological analysis of such layered aquifer-aquitard systems (Freeze, 1971). We note that with the exception of well 321, all piezometers are vertically within 10 m of the Waalre aquitard.

# 3. Analysis and Modeling

We inferred the vertical aquitard hydraulic conductivity  $(K_{z})$  by rearranging Darcy's law:

$$K_z = -\frac{q_z}{i} \tag{1}$$

in which  $q_z$  [m/s] is the vertical component of the steady-state groundwater flux across the aquitard estimated from the thermal analysis, and *i* [m/m] is the hydraulic gradient across the aquitard found from the aquitard head difference (Figure 3) and vertical thickness as previously described. Our focus was on steady-state hydraulic conditions, and therefore transient groundwater flow and potential water storage changes in the aquitard over





**Figure 3.** Time-series of hydraulic head as observed in boreholes (between 1985 and 2020) at the eight sites in the piezometer above (blue) and below (red) the Waalre aquitard (upper panel in each figure). Note that not all data have been collected for the same duration, and at the same measurement intervals. The lower panel in each figure shows the head difference between the upper and lower piezometer as well as the median hydraulic head difference ( $\overline{\Delta h}$ ; dashed line) and standard error ( $\sigma_e$ ; solid lines), listed in Table 1, derived after interpolation of time series to avoid observational bias. The position of the screen of the piezometers in relation to the depth and thickness of the Waalre aquitard is indicated in Figure 2.

time were not considered. Negative values of  $q_z$  denote groundwater upwelling toward the surface, while positive values indicate downwelling.

We based our analysis on the conceptual and numerical models used by Bense and Kurylyk (2017) who developed a 1D model of transient heat flow controlled by surface warming for the central part of the Netherlands. We used an updated version of this numerical model (FlexPDE, PDE Solutions Inc., 2006; http://www.pdesolutions. com) to simulate the evolving characteristics of the TDPs, including the inflection point (location of minimum temperature) propagation as a function of a range of groundwater fluxes. As described more later, our purpose in considering a range of groundwater fluxes was twofold: (a) to yield an estimate of the actual groundwater flux via agreement between the modeled and observed inflection point depths, and (b) to elucidate the control of the groundwater flux on the inflection point and thereby gain insight into the sensitivity of our approach. These 1D models solve the transient conduction-advection heat flow equation in the Cartesian *z*-direction (depth; Stallman, 1963):

$$c_b \frac{\partial^2 T}{\partial z^2} - q_z c_w \rho_w \frac{\partial T}{\partial z} = c_b \rho_b \frac{\partial T}{\partial t}$$
(2)

where  $T [^{\circ}C]$  is temperature, t [s] is time,  $\kappa_b [W \cdot m^{-1} \cdot {^{\circ}C^{-1}}]$  is the bulk thermal conductivity of the solid-fluid mixture,  $c_w$  and  $c_b [J \cdot kg^{-1} \cdot {^{\circ}C^{-1}}]$  are respectively the specific heats of the fluid and solid-fluid medium, and  $\rho_w$ and  $\rho_0 [kg \cdot m^{-3}]$  represent the densities of the water and medium, respectively. We assumed fully saturated conditions and uniform water density and viscosity. This equation does not include lateral heat transfer, but a previous analysis of lateral versus vertical hydraulic head gradients in the area (Bense & Kurylyk, 2017) indicated that lateral groundwater flow rates likely only have a negligible impact on the downward inflection point progression. Moreover, for the relatively low groundwater flow rates encountered at this site, the effects of thermal dispersion on heat transfer by groundwater movement can be assumed to be negligible (Rau et al., 2012).

We assumed that steady-state thermal conditions existed at the start of the 18<sup>th</sup> century (1706) and thus first calculated a steady-state TDP for 1706 that serves as the initial condition for our transient numerical model runs disturbed by climate change. Meteorological data for central Netherlands have enabled the reconstruction of monthly average temperatures since January 1706 (Van der Schrier et al., 2011). For the surface temperature boundary conditions, we use the long-term average temperature trend (red line, Figure 4a), derived from annual average temperatures (black dots, Figure 4a) to represent decadal changes in surface temperature. For the bottom model boundary, we used a heat flux condition  $(50 \cdot 10^{-3} [W \cdot m^{-2}])$ , representing diffuse background geothermal heat flow, as estimated from many TDPs across the study area (Bense & Kurylyk, 2017). The bottom boundary was placed at a depth of 150 m to represent the maximum depth of active groundwater circulation in the area (Bense & Kurylyk, 2017).

We ran these models for three uniform values for the bulk subsurface thermal properties, as represented by the thermal diffusivity  $\left(\alpha_T = \frac{\kappa_b}{\rho_b c_b}\right)$ , to cover the range of values expected in the region (Bense et al., 2020; Witte et al., 2002):  $\alpha_{T,\min} = 4.3 \cdot 10^{-7} \text{ m}^2/\text{s}$ ,  $\alpha_{T,\text{average}} = 7.8 \cdot 10^{-7} \text{ m}^2/\text{s}$ ,  $\alpha_{T,\max} = 9.6 \cdot 10^{-7} \text{ m}^2/\text{s}$ . By using single values for  $\alpha_T$ , we ignored the potential effects of vertical stratification of lithologies and associated heterogeneity in thermal properties and their impact on the propagation of the TDP inflection point. However, earlier studies showed these to be insignificant for this site (Bense & Kurylyk, 2017). We ran each of these three thermal property scenarios for 75  $q_z$  values ranging from -0.1 to +0.64 m/y at 0.01 m/y increments, and for the two different surface temperature representations, resulting in a total of 450 models. We then used the range of model outcomes to investigate the relationship between  $q_z$  and the inflection point depth in 2019 and subsequently inferred a  $q_z$  value by matching the observed and simulated inflection point depths (*IFD*s) in 2019 (Figure 2). This modeling approach allowed us to assess the robustness of the model estimates of  $q_z$  based on our parameter uncertainty.

We use the *IFD* as the sole observation to fit the model to rather than evaluating a goodness of fit between the entire observed and modeled TDP as was done in earlier studies (Bense et al., 2017). We chose to focus on the inflection point in the fitting process because the entirety of the observed TDP is strongly sensitive to lithological heterogeneities and associated depth-variability of thermal properties, and the absolute temperature in the TDP is strongly controlled by site-specific surface conditions (Bense et al., 2020). Conversely, the inflection point depth is primarily controlled by  $q_z$  as first demonstrated by Taniguchi et al. (1999), and shown more recently by Bense and Kurylyk (2017).



**Figure 4.** (a) Surface air temperature (SAT) across the central part of the Netherlands from 1706 to 2020 (data from knmi. nl), as annual average temperatures (black dots) and a trend line (red line) representing approximately decadal trends in SAT. (b) Inflection point depth (*IFD*) for 1706–2020 for a range of vertical groundwater flow rates ( $q_z$  [m/year]) as indicated by labels on curves. In this diagram, results are shown for models using average values for subsurface thermal diffusivity in the area. (c) The relationship between  $q_z$  and 2019 *IFD* when *IFD*s were collected in our study area, as derived from numerical models like that shown in (b) for a range of thermal diffusivity values. These curves are used to estimate  $q_z$  and the sensitivity and uncertainly therein at each site from observed inflection point depths in our study area (Table 1). In (b and c) the gray area indicates the maximum depth of the zone in which seasonal fluctuations would be visible in field-observed TDPs (e.g., Figure 2) and thus obscure the presence of thermal inflection points.

# 4. Results

Model outcomes describing the generic development of an *IFD* in the TDP (Figure 4b) suggest that decadal surface temperature fluctuations resulted in inflection point development several times since 1706 during periods when average surface temperatures were rising. Figure 4b shows the modeled development of the inflection point depth since 1706 using the average  $\alpha_T$  value and selected values of  $q_z$ . Modeling suggests that inflection points appear and disappear following relatively short periods of moderate warming and cooling respectively, as happened in the 18<sup>th</sup> and 19<sup>th</sup> century. The ability of surface cooling to remove inflection points from the TDP after a period of warming is dependent on the magnitude of  $q_z$ . For higher  $q_z$ , inflection points penetrate deeper during warming and then remain during cooling; in contrast, inflection points disappear more frequently during cooling for relatively low values of  $q_z$ . These model runs suggest that surface warming from the start of the 20<sup>th</sup> century until the mid 1960s is sufficient to trigger the development of inflection points for all  $q_z$  values considered here, but for lower fluxes, the appearance and penetration of inflection points is interrupted during periods of

## Table 1

Calculations of  $K_z$  for the Waalre Aquitard at Eight Locations (See Figure 2a) Which Are Based (This Study) Upon Estimates of  $q_z$  From an Analysis of the Inflection Point Depth (IFD) Observed in Temperature-Depth Profiles (TDPs; Figures 2b–2j) Combined With Measured Hydraulic Head Differences ( $\Delta h$ ; Figure 3)

Well ID	Date of TDP	$\overline{\Delta h} \pm \sigma_e[\mathrm{m}]$	D [m]	<i>IFD</i> <sub>2019</sub> [m]	q <sub>z,min</sub> —q <sub>z,max</sub> [m/year]	i <sub>min</sub> —i <sub>max</sub> [m/m]	$K_{z,\min}$ — $K_{z,\max}$ [· 10 <sup>-3</sup> m/d] (This study)	$K_{z,\min} - K_{z,\max}$ [· 10 <sup>-3</sup> m/d] (REGIS)
B39F0224	16/07/2019	$0.34\pm0.02$	8.4	41	0.040-0.050	0.037-0.043	2.6-3.6	1.0-5.0
B39F0575	23/09/2019	$0.42\pm0.28$	12.5	54	0.100-0.120	0.012-0.056	4.9–28	10–50
B39F0580	05/07/2019	$1.11 \pm 0.26$	21.0	57	0.120-0.140	0.040-0.065	5.0-9.5	5.0-10
B39F0321	16/07/2019	$1.20\pm0.12$	20.0	60	0.130-0.160	0.054-0.066	5.4-8.1	10–50
B39F0552	20/08/2019	$7.56 \pm 0.43$	24.5	63	0.150-0.180	0.291-0.326	1.3–1.7	1.0-5.0
B39F0549	17/07/2019	$2.42\pm0.10$	9.1	63	0.150-0.180	0.255-0.277	1.5–1.9	1.0-5.0
B40A0541	23/09/2019	$0.44 \pm 0.05$	11.5	65	0.160-0.190	0.034-0.043	10–16	1.0-5.0
B39F0550	11/02/2019	$10.17\pm0.45$	27.9	75	0.220-0.270	0.348-0.381	1.6–2.1	1.0-5.0

*Note.* The  $K_z$  values we obtain for the eight sites in our study area are listed alongside those that are reported for the Waalre aquitar within the Netherlands hydrological instrument (REGIS) which are based upon conventional field data analysis (see main text for details). A comparison between these results is visualized in Figure 5.

retarded or reversed surface warming (e.g., in the 1960s). However, surface warming accelerated after the early 1960s, resulting in the rapid development of inflection points until the present day for all  $q_z$  values. Figure 4c shows the modeled relationship between  $q_z$  and the *IFD* for 2019, when our TDP measurements were taken, for three thermal diffusivity values covering the plausible range for the area. TDPs for three sites (i.e., 224, 580, 321) illustrate the presence of thermal transience due to seasonality in surface temperature (Figure 2), reaching to a maximum depth of 15 to 18 m (shaded zone, Figures 4b and 4c). Any inflection point developing above this depth would be obscured in observed TDPs unless they were measured multiple times per year and then averaged.

We find that there is a range of 35 m (40–75 m; Figure 4c) in observed (2019) *IFDs* across our study area (Figure 2). Model TDPs are fitted, using the *IFD*, to the observed TDPs for the end of 2019 as shown in Figure 2, for the high and low limit of thermal properties. This process enabled us to infer a range of  $q_z$  values. For the purposes of evaluating the goodness of fit of the entire model TDP to the observed TDP (Figure 2), the modeled temperature at the inflection point was matched (Figure 2) with the observed temperature at the inflection point. However, this is not part of the methodology to infer a  $q_z$  value from the TDP. Such adjustments are needed to consider contrasts in average annual surface temperature due to differing land-surface conditions among sites.

The derived range of  $q_z$  values from our model analysis are summarized in Table 1 in concert with the median hydraulic head gradient  $(\overline{\Delta_h})$  and its standard error  $(\sigma_e)$ , as observed across the Waalre aquitard between 1985 and 2020 (Figure 3). Since there is a unique value for  $q_z$  associated with a particular *IFD* for a given set of thermal properties, and for a particular year (Figures 4b and 4c), this method allows us to directly translate an observed *IFD* to a  $q_z$  value. Hence, our modeling results suggest that the depth range of observed *IFD*s reflects a variation in groundwater flux conditions, with  $q_z$  varying between 40 and 265 mm/year. We then used Equation 1 with the maximum (minimum) value for  $q_z$  and the minimum (maximum) value of  $i_z$  to produce an upper (lower)  $K_z$ estimate (Table 1). Finally, we compared these  $K_z$  values from our analysis to commonly accepted  $K_z$  values for the Waalre aquitard as used in regional groundwater modeling that are reported in the Netherlands Hydrological Instrument (REGIS; *nhi. nu*; Figure 5).

For most sites, the  $K_z$  values that we calculate for the Waalre aquitard are in close agreement with those independently reported in REGIS (Figure 5). These values range between  $10^{-3}$  and  $5 \cdot 10^{-2}$  m/day, which are in middle of the range of K values (~ $10^{-6}$ – $10^{-1}$  m/day m/d; Freeze & Cherry, 1979) for aquitards. Also, the range of  $K_z$  values that we calculate from the observed variation in the Waalre aquitard hydraulic gradient combined with the sensitivity of model-based  $q_z$  estimates is similar to the plausible  $K_z$  range reported in REGIS.





**Figure 5.** Values of the vertical hydraulic conductivity ( $K_z$ ) of the Waalre aquitard from this study (in blue) compared to independently derived estimates reported for the REGIS model that is part of the Netherlands Hydrological Instrument (in orange), for the eight sites in our study area. Data for this graph can be found in Table 1.

# 5. Discussion and Conclusion

Our analysis suggests that downwelling rates through the Waalre aquitard across our study area vary over an order of magnitude (Table 1). The highest aquitard fluxes are found in the topographically highest part of the area (well ID 550), while the lowest are found in the northern end of the Brooke valley furthest away from the pumping area to the south (well ID 224). Notably, the well closest to this abstraction area (well ID 575) has a relatively low inferred  $q_z$ . Hence, the analysis suggests that there is no clear pattern of vertical flux increase across the Waalre aquitard toward where abstraction occurs, and that topography exerts a primary control on groundwater downwelling rates in this catchment.

We note that the agreement between the entire profile of the modeled and observed TDPs (Figure 2) is generally reasonable even though the optimisation was solely based on the modeled and measured *IFD*. Obvious mismatches occur up to a depth of 20 m for which the observed TDP is still under the influence of seasonal surface temperature fluctuations not considered in our model. Elsewhere (e.g., at the depth of the Waalre aquitard), lithological heterogeneity is probably important as a control on the TDP, and such heterogeneities were also not taken into account in our model.

The single  $q_z$  values that we infer from our model-data comparison can be interpreted as mean values across the model depth domain (Bense & Kurylyk, 2017). However, in a 2D or 3D system, and under field conditions, the vertical component of the groundwater flow vector would likely decline with depth, and would be maximal near the surface where it equals groundwater recharge (i.e., the flux across the water table), and zero at the hydrogeological base of the system. Therefore, our  $q_z$  estimates are likely be an underestimate of groundwater recharge, but might be representative of vertical flow across

the Waalre aquitard which is halfway between the water table and the base of the system generally considered to be at a depth of approximately 150 m (Bense & Kurylyk, 2017). Also, we consider our  $q_z$  assessment in combination with the hydraulic gradient across the entire aquitard thickness to calculate  $K_z$ . Classic studies using combined hydraulic head differences and (thermally stable) TDPs across aquitards have previously argued that the spatial scale of the  $q_z$  estimate from the TDP comports with the scale of the hydraulic gradient measured across the aquitard (e.g., Bredehoeft & Papadopulos, 1965). Further analysis in future studies could investigate the alignment of scales for our approach of using the *IFD* in concert with the gradient across the entire aquitard. In general, our inferred  $K_z$  values should be comparable to regionally representative aquitard  $K_z$  values reported in REGIS given the scale of the multi-level head measurements and thermal profiles. Obtaining  $K_z$  estimates at this scale is critical for regional scale flow assessments (Saar, 2010) as preferential flow paths can occur in some sites as a result of geological heterogeneities (e.g., sedimentary structures and/or fractures), and the effect of these on effective hydraulic conductivity may not be represented in upscaled  $K_z$  estimates from core plug samples.

Our estimated vertical groundwater flow rates are assumed to be representative of long-term average values (Bense & Kurylyk, 2017). We do not consider any potential impacts of groundwater recharge fluctuations, seasonal pumping conditions, or longer term increases in annual volumes abstracted. Evaluation of such effects would require TDPs repeated over timescales of years to decades, which are not available at our site except in one borehole (321). A previous study (Bense et al., 2020) suggested that a relatively sudden increase in pumping rate in the mid 1980s, and a deepening of groundwater abstraction wells might have given rise to a two-to threefold increase in local downwelling rates across the Waalre aquitard. Since historic TDP data are not available for any other wells in the area, we cannot evaluate whether long-term transience had an impact on the  $K_z$  values estimated in this study. Further sensitivity analysis of our results for these effects would likely widen the uncertainty interval for  $K_z$ . We note, however, that for many wells the range of uncertainty that we calculate without such additional analysis is relatively small compared to the  $K_z$  range reported in REGIS (Table 1).

The agreement between our calculated  $K_z$  values and those determined independently reinforces the notion that analysis of *IFDs* in temperature profiles can yield invaluable hydrogeological insight. While inflection point analysis was proposed in an earlier study (Bense & Kurylyk, 2017), previous inflection point research focused on inferring fluxes and did not consider the potential to quantify  $K_z$ . The combined  $q_z$  and  $K_z$  values obtained from the analysis of transient TDPs in conjunction with multi-level hydraulic head data appear quantitatively accurate and could help inform groundwater budget calculations for semi-confined aquifers. Such calculations would otherwise typically rely on groundwater flow model simulations calibrated on hydraulic head values and potentially groundwater age-based estimates of  $q_z$  derived from the analysis of environmental isotopes (McCallum et al., 2015). While the approach of analyzing paired multi-level hydraulic head data and subsurface temperature data is relatively common for estimating both vertical Darcy fluxes and sediment hydraulic conductivity in groundwater-surface water interactions studies (e.g., Hatch et al., 2010; Lapham, 1989), this approach has rarely been applied in deeper settings (e.g., Bredehoeft & Papadopulos, 1965), and, to our knowledge, never applied to climatically disturbed profiles.

The estimated range of  $q_z$  variability is representative of groundwater recharge conditions in a temperate climate zone. Modeling results (Figure 4) suggest that for lower recharge in more arid climates, inflection points would still be detectable, provided they are manifested below the zone of seasonal fluctuation. However, for climatically wetter conditions with more groundwater recharge, and therefore deeper inflection points (>100 m), our model results show that thermal dispersion makes the relationship between the inflection point and  $q_z$  more uncertain. Consequently, since inflection points will migrate more deeply in the coming decades (Figure 4), the precision of this method will diminish with sustained warming. Thus, present-day, shallow TDP inflection points resulting from relatively recent (decadal) acceleration of surface warming (Figure 4) provides a unique opportunity to characterize aquitard hydraulic conductivity and vertical fluxes to and from aquifers. The impacts of recent anthropogenic climate change on TDPs, and the present-day opportunity to exploit these disturbances for hydrogeological assessment, is somewhat analogous to the aftermath of a temporary increased fallout of radioactive isotopes (e.g., Tritium) from the atmosphere that is detectable in subsequent decades to millennia depending on the half-life of the particular isotope (McCallum et al., 2015). Likewise, shallow TDP inflection points that can yield precise flux estimates are a temporary phenomenon given projected, sustained climate warming rates.

The parsimonious model that we use to interpret TDPs for  $q_z$  yields a simple relationship between  $q_z$  and the *IFD* for a particular time (2019, Figure 4). We assess uncertainty for this relationship by varying thermal properties of the model domain between plausible limits. It is important to note that uncertainty in thermal property estimates is much lower than uncertainty in  $K_z$  estimates. For the sake of simplicity, we overlook a suite of conditions that might impart a thermal imprint on TDPs, including lateral groundwater flow, geological heterogeneity and transience in groundwater flow. Taking these and other aspects into account in a more complex numerical model would likely lead to a better understanding of TDP dynamics, but this would not necessarily significantly alter the relationship between  $q_z$  and the *IFD*. Likewise, the temporal variability of hydraulic head differences as observed across the Waalre aquitard is used here to obtain the long-term median hydraulic gradients driving  $q_z$ , and we do not consider transience in groundwater flow. Recent work shows that, where repeated TDPs separated by years or decades are available, they reveal the *IFD* progression directly, and such data can possibly be used to detect temporally changing groundwater flow conditions (Bense et al., 2020). A further evaluation on the uncertainty of aquitard *K* determinations using the methodology outlined in this paper, resulting from aspects such as the use of hydraulic head time series of variable durations, and ongoing changes in environmental conditions, will be the focus of future studies.

In summary, we demonstrate that aquitards can be hydraulically characterized by combining hydraulic head observations above and below an aquitard with a single observation of the thermal inflection point (minimum temperature) in a thermal profile disturbed by climate change. The derived aquitard vertical  $K_z$  values agree with independently established values at the same locations using more conventional approaches. This approach offers potential for aquitard characterization in many geological settings, which in turn may be transformative for measuring groundwater fluxes and managing semi-confined aquifer systems worldwide.

## **Data Availability Statement**

The data that support the findings of this study are openly available at the following URL/DOI: https://doi. org/10.17026/dans-24v-unnz (Bense, 2022).

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