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ORIGINAL ARTICLE

In-well time-of-travel approach to evaluate optimal purge duration during low-flow sampling of monitoring wells

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Abstract A common assumption with groundwater sampling is that low (<0.5 L/min) pumping rates during well purging and sampling captures primarily lateral flow from the formation through the well-screened interval at a depth coincident with the pump intake. However, if the intake is adjacent to a low hydraulic conductivity part of the screened formation, this scenario will induce vertical groundwater flow to the pump intake from parts of the screened interval with high hydraulic conductivity. Because less formation water will initially be captured during pumping, a substantial volume of water already in the well (preexisting screen water or screen storage) will be captured during this initial time until inflow from the high hydraulic conductivity part of the screened formation can travel vertically in the well to the pump intake. Therefore, the length of the time needed for adequate purging prior to sample collection (called optimal purge duration) is controlled by the in-well, vertical travel times. A preliminary, simple analytical model was used to provide information on the relation between purge duration and capture of formation water for different gross levels of heterogeneity (contrast between low and high hydraulic conductivity layers). The model was then used to compare these time–volume relations to purge data (pumping rates and drawdown) collected at several representative monitoring wells from multiple sites. Results showed that computation of time-dependent capture of formation water (as opposed to capture of preexisting screen water), which were based on vertical travel times in the well, compares favorably with the time required to achieve field parameter stabilization. If field parameter stabilization is an indicator of arrival time of formation water, which has been postulated, then in-well, vertical flow may be an important factor at wells where low-flow sampling is the sample method of choice.

Keywords In-well flow · Transport · Analytical model · Time of travel · Low-flow sampling · Groundwater

Introduction

A primary goal of low-flow sampling of groundwater [pumping at low rates (0.1–0.5 L/min)] is to minimize the amount of water pumped from in-well storage by avoiding drawdown in the well; consequently, in-well vertical flow from the stagnant water column above the screened part of the well (well casing) is minimized (Puls and Barcelona 1989, 1996; Pohlmann et al. 1994; Shanklin et al. 1995). Unlike water in the casing, water within the screened interval has traditionally been viewed as representative of formation water (Kearl et al. 1992). However, low-flow sampling does not minimize, by default, the capture of preexisting water in the screened interval (called screen storage) or mixing of water from screen storage with recent inflow of formation water induced from pumping.

Some benefits of low-flow sampling include a small purge volume, which minimizes the volume of investigation-derived waste, and collection of groundwater samples with low turbidity, which decreases the need for filtration in some cases. However, there are associated hydraulic and chemical concerns when purging and sampling using low

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rates of flow. According to the state of New Jersey sampling guidance (http://www.state.nj.us/dep/srp/news/1997/9711_04.htm):

The zone sampled within the well by low-flow methods is conceptually limited. If the contaminant distribution in the screened section of the aquifer is heterogeneous, which may be the case in most wells, the sample results obtained by low-flow sampling may be significantly biased low if the sampling device intake is not placed at the same depth as that of the highest contaminant concentration entering the well.

A common assumption inherent to low-flow groundwater sampling is that low-pump rates capture primarily lateral inflow (horizontal laminar flow) through the screened interval from the formation at depths coincident with the pump intake (Stone 1997; Britt 2005). However, because even low-flow methods result in some drawdown in the well, convergent, in-well, vertical flow is induced toward the pump intake from inflow across the entire well screen. Varljen et al. (2006) showed that the entire well screen is sampled during low flow with preferential sampling of high hydraulic conductivity layers under steady-state transport. However, once vertical in-well flow occurs, wellbore or in-well vertical travel times of groundwater (transient transport) will affect the temporal capture of water from different parts of the screen and likely affect the composition of the pump water until steady-state transport is achieved. Temporal variability in chemistry during purging has been at least partly attributed to in-well vertical flow and transport for several studies (Church and Granato 1996; Reilly and LeBlanc 1998). Flow convergence will promote the capture of flux-averaged concentrations—biased toward the capture of formation water from the highest head and transmissivity zones that intersect the well screen (Divine et al. 2005).

For monitoring wells characterized by little ambient flow through the screened interval, pump position, rates, and pump duration are important factors in capturing formation water (McMillan et al. 2014). Captured water during initial purging can consist of large volumes of screen storage and consequently a small volume of contemporaneous (induced flow from the formation that is initiated during purging) inflow from the formation (Martin-Hayden 2000). Degassing (Roy and Ryan 2010) and mixing (Britt 2005) in the well can affect the quality of the preexisting screen water and alter the chemistry from the formation water. Because of these and related concerns, hydraulic analysis of in-well travel times offers clues into likely sample capture locations in the well environment and a metric to assess sample chemistry.

This paper presents a preliminary, simple analytical model to evaluate in-well vertical travel times, purge duration, and likely screen capture intervals during purging with low-flow sampling methods. The simple analytical model is contained within an[1] Excel spreadsheet program and Visual Basic for Applications (VBA) program. The code for the preliminary analytical model is available for download at https://github.com/gmen16/IN-WELL-TRAVEL-TIME.git.

The model assumes constant rates of pumping for purge and sample-collection periods, negligible storage changes, and steady state, horizontal flow in the formation but vertical flow in the well-screened interval. Computation of in-well vertical time-of-travel (TOT), as determined from vertical flow, provides the framework metric to assess the optimum purge duration (OPD) to capture formation water. The metric is then used to evaluate its usefulness in assessing OPD for purge data (pumping rates and drawdown) from several monitoring wells located in diverse hydrogeologic settings with various magnitudes (differences between low and high hydraulic conductivity layers) of formation heterogeneity. The effects of gross variations of heterogeneity (at a 1-ft scale) on in-well, vertical travel times are examined.

This preliminary analytical model is a tool that provides insight into vertical transport times in wells during low rates (<0.5 L/min) of pumping. Further enhancements to the model of more complex wellbore flow processes as identified during field testing would provide additional simulation capabilities.

Conceptualization of in-well flow during low-flow sampling

Ideally, low-flow sampling causes negligible dewatering of the water column in the well and minimal depletion of in-well storage (Puls and Barcelona 1989, Barcelona et al. 1994). Even if these conditions are achieved, the sample collected during pumping (purged sample) can originate from anywhere across the screened section of the formation because the vertical transmissivity of the wellbore exceeds the transmissivity in the formation and the hydraulic response from pumping propagates vertically faster in the wellbore than laterally in the formation. Given a screened interval of no more than a few tens of feet, the source of this water during purging can vary significantly. This has a direct consequence on the OPD needed to capture formation water before a sample can be collected.

Because drawdown is minimal, a quasi-steady-state flow field near the well is quickly established. While a steady-state flow field may form quickly, the vertical TOT to the pump intake within the well screen is likely to take longer than the hydraulic response and drawdown stabilization

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[1] Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

because of the low rates of purging. This relation between flow and transport during low-flow sampling is shown in Fig. 1. For this conceptualized case, the pump intake is set at the midpoint, a common practice under low-flow sampling protocol, of a 10-ft screen and the maximum vertical travel distance of water in the screened interval is 5 ft. Three temporal flow and transport stages occur during low-flow sampling based on drawdown in the well and vertical TOT to the pump intake. In the early stage of purging, drawdown has not stabilized and flow and transport is transient; typically this condition is relatively quick (Fig. 1). In the middle stage, drawdown has stabilized and flow is essentially at a quasi-steady state. However, vertical transport has not travelled (arrival time) from all parts of the screen to the pump intake and time-varying water contributions occur (transient transport). Finally in the last stage, drawdown and transport have stabilized as denoted by the relatively stable drawdown and the arrival time of transport from the entire screened interval. Therefore, after steady-state transport is achieved, the water contribution from the entire screened interval to the pump intake is stable and does not change over time.

For the case of steady-state flow and transient transport, several hydraulic scenarios are illustrated in Fig. 2. As before, scenarios assume the pump intake at the midpoint of the well screen. To help define scenarios, a simple water mass balance equation can be used (Eq. 1). The instantaneous rate of flow to the pump (q_p) can be defined as the rate of horizontal inflow from the formation to the pump (q_h) coincident with the zone around the pump intake (specified as a 2-ft thickness (1 ft in either direction) around the pump intake), the rate of storage depletion from the well (q_w), and the rate of vertical flow (q_v) in the well that is a summation of lateral inflow from the formation outside of the zone contributing horizontal inflow near the pump intake:

$$q_p = q_h + q_w + q_v \quad (1)$$

where $q_v = \sum q_{h'}$ is the summation of horizontal flow from zones not near the pump intake ($q_{h'}$). In cases where the horizontal inflow to the well by the pump intake (q_h) is equivalent to the pump rate (q_p) (2a, orange color), no vertical flow occurs in the well and all pumped water is derived laterally from the formation. This scenario is likely in very high horizontal hydraulic conductivity (HHK) formations. For a scenario where horizontal ambient (pre-pumped conditions prior to purging) groundwater flow is high relative to q_p, purging will capture just a component of ambient flow from the formation and no vertical flow in the well is required to meet q_p demands (2b, red color grade). When q_p rates exceed q_h, vertical flow is induced (2c, blue color grade). Lastly, parts of the formation and corresponding screen sections may have ambient flow unaffected during purging (2d, red color grade), whereas other parts of the screen respond to pumping (2d, blue, yellow, and orange color grade). The latter is likely to occur in scenarios where there is ambient vertical flow in the well. The work presented in this paper focuses on conditions where vertical flow in the well is likely to occur (2c, $q_p > q_h$).

Methods

Based on the scenarios identified in Fig. 2a, c, an analytical model was developed to compute potential vertical-flow patterns, flow rates, and TOT in the screen section of the well. The rate of vertical flow and TOT is determined by the relation presented in Eq. 1 and governed by the vertical distribution (over 1-ft thicknesses) of horizontal inflow from the formation into the well screen. The vertical flow and TOT were computed for different gross levels (difference between low and high hydraulic conductivity layers) of formation heterogeneity (at a 1-ft scale). The model was used to determine the likelihood of vertical flow in the well screen, compute vertical TOT, and determine the OPD to capture flow from the entire well screen for several monitoring wells using existing well purge records. Wells selected for examination reflect generic conditions from two waste sites with contrasting hydrogeologic settings in the USA and from two wells that are part of the U.S. Geological Survey, National Water Quality Assessment (NAWQA) Project, also in the USA. The comparison of temporal changes in formation water captured as determined from the analytical model to field records of water-quality monitoring and stabilization of parameters was made to assess whether the later data sets can be used as a proxy to constrain in-well vertical TOT and associated HHK. The implications on the timing of field parameter stabilization and vertical TOT are discussed.

The preliminary analytical model is contained within an Excel spreadsheet program and VBA program. The analytical model solution was compared to a numerical model of well flow from a simulation presented in McMillan et al. (2014). Limitations and inaccuracies associated with the analytical model are discussed. It is expected that further model enhancements and field verification of wellbore processes will benefit model development.

Analytical model

The analytical model assumes in-well drawdown is small (<0.3 ft) during low-flow sampling, the screen remains fully saturated, and the formation behaves similarly to confined conditions with storage also relatively small ($S < 0.001$). On the basis of a small drawdown and rapid equilibration, steady-state flow is achieved rather quickly

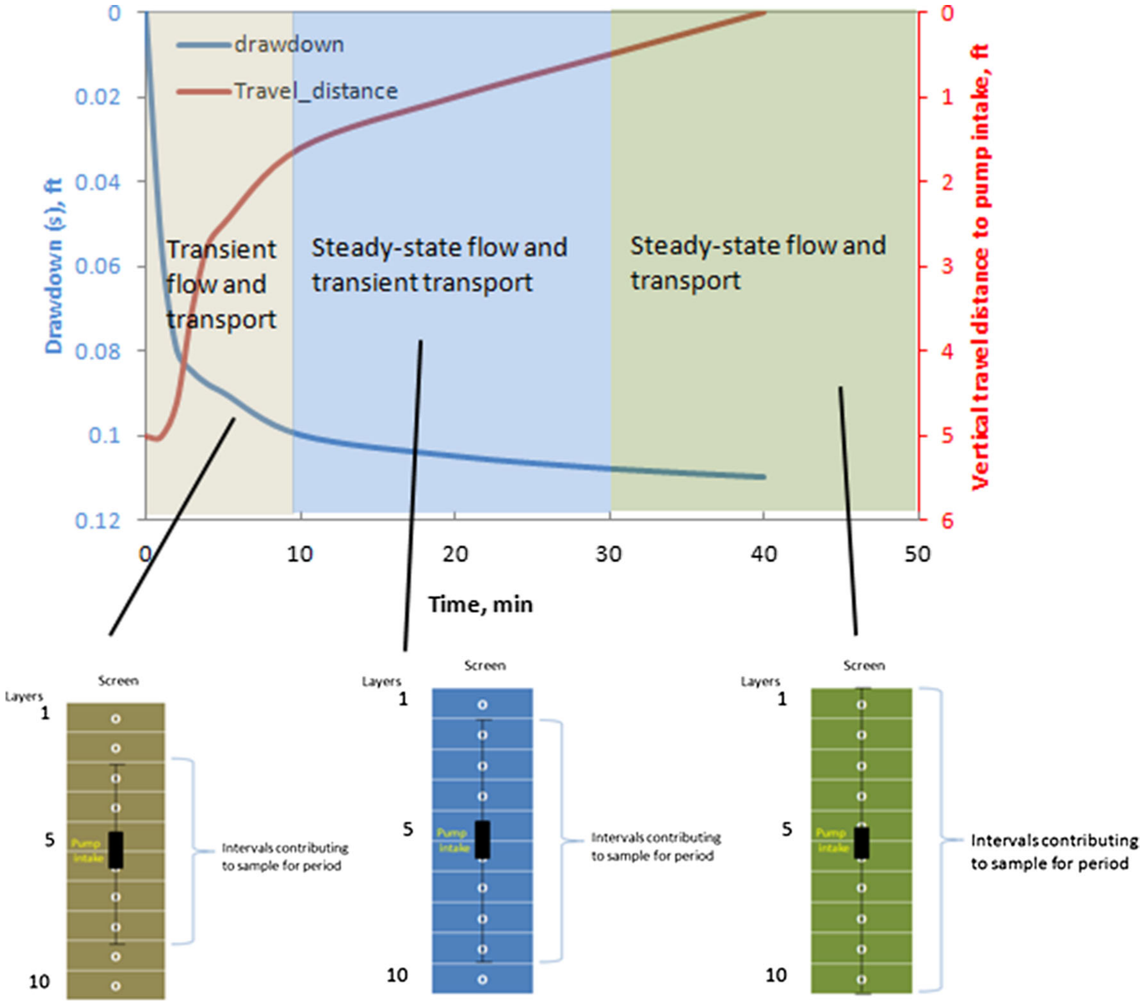

Fig. 1 Conceptualized relation between drawdown, time-of-travel, and corresponding temporal flow and transport conditions during low-flow sampling for a 10-foot screened well with the pump intake at the midpoint of the screen

(Fig. 1). Horizontal flow in the formation is assumed and computed from a series of horizontal radial flow equations; radial flow calculations are solved over 1-ft thicknesses along the well screen using the Thiem equation:

$$s_w = H - h_w = \frac{Q}{2\pi T} \ln\left(\frac{R_o}{rw}\right) \tag{2}$$

where s_w = drawdown in the well; Q = pump rate; T = transmissivity of the aquifer; R_o = radius of influence where H (head in aquifer) = 0; r_w = radius of well; and h_w = head in the well.

Radius of influence (R_o) can be determined from the equation:

$$R_o = \sqrt{\left(2.25 * T * \frac{t}{S}\right)} \tag{3}$$

where R_o = radius of influence (same as R in Eq. 1); t = time of purging; S = storage coefficient. As part of this study, the sensitivity of R_o for likely purge times for low-flow sampling was assessed based on likely transmissivity (T) and storage coefficient (S) values for porous media formations. Results in estimated R_o ranged from 3.5 to 15 ft. *The model currently uses a* R_o *of 10.* Transmissivity can be substituted in Eqs. 2 and 3 by

$$T = \text{HHK} * b \tag{4}$$

where HHK = horizontal hydraulic conductivity of the formation coincident with the well screen, and b = screen length.

Equations 1 and 2 are combined to iteratively solve for HHK using a smooth nonlinear solution of Excel called GPR nonlinear. A forward derivative option was used with a convergence of 0.0001 and a maximum iteration of 100. Solution errors were checked by comparing the summation of computed flows from Eq. 1 to the pump rate. Lateral flow (q_h) is computed from

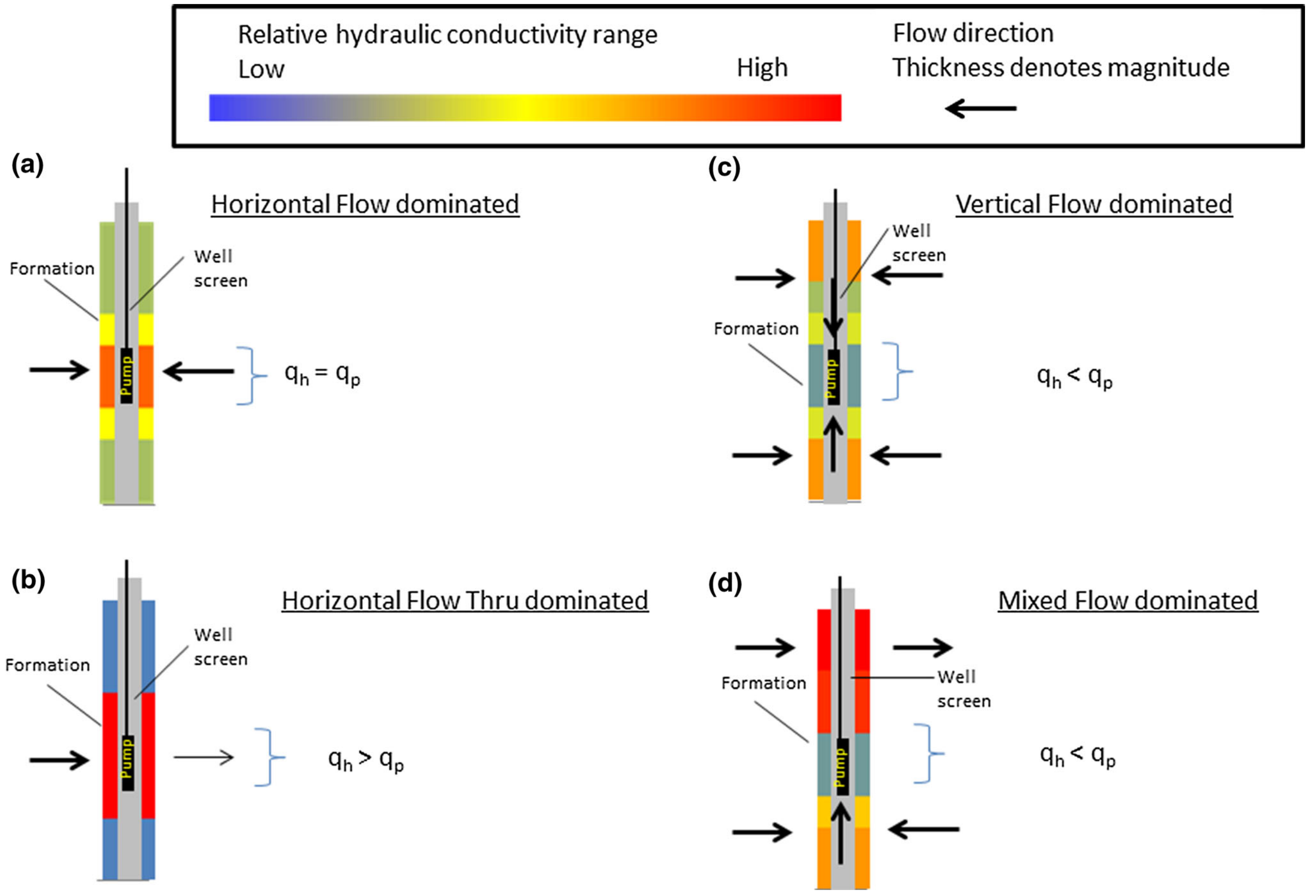

Fig. 2 Conceptualized groundwater flow patterns and flow in the well screen during low-flow sampling (pump rate q_p can be satisfied from a horizontal hydraulic conductivity equivalent to the symbol 🟧; q_h = horizontal flow rate near pump; *gray* denotes well screen)

$$q_h = (4\pi * \text{HHK} * s_w / (2.3026 - \ln r_w)) \tag{5}$$

Well storage (q_w) is computed from

$$q_w = \left(s_w * \pi r w^2\right) / t \tag{6}$$

Vertical flow (q_v) is computed from the interval outside the lateral flow zone

$$q_v = ((b - 2) * 2\pi * \text{HHK} * s_w / (2.3026 - \ln r_w)) \tag{7}$$

Vertical in-well time-of-travel (TOT) is determined assuming piston (plug) flow (Eq. 8). This provides an approximation to the variation of vertical velocities across the well diameter (Sevee et al. 2000; Martin-Hayden et al. 2014). The amount of induced vertical flow during purging (q_v) is determined from the relation in Eq. 1. Vertical TOT is controlled by the summation of horizontal inflow (Eq. 1) over 1-ft increments outside of the zone near the pump intake to derive a depth-dependent velocity.

$$t = D * \frac{(\pi r w^2)}{qv} \tag{8}$$

where D = distance.

The amount of time needed for well inflow at different depths of the screen to reach the pump (the OPD parameter) is a critical parameter in the analysis of purge times for various well dimensions, pump rates, and values of HHK. In particular, it is important to understand the relative proportions of pumped water (q_p) that captures recent well inflow from the formation and the capture of preexisting screen water (screen storage) that was already emplaced prior to purging.

The lateral extent of capture of formation water (L_x) is computed from the q_h term, radius (r), time of purging (t), thickness of the lateral zone (2 ft), and the effective porosity (n) of the formation (Eq. 9). Although maximum extent of lateral capture may not be restricted to the designated lateral zone by the pump, this method provides an approximation that can be used to assess the amount of the formation that is laterally captured during purging.

$$L_x = t * (q_h / 4\pi r n) \tag{9}$$

In addition to an assessment of vertical flow, the program calculates an average HHK over the screen interval, and potential ranges of HHK based on a specified level of heterogeneity likely to be encountered in the field, such as an order of magnitude variation (10×). An automatic solver option in Excel is used that solves for the best-fit high HHK and low HHK values that satisfy q_p. This is called a reverse assessment of flow because HHK is calculated.

Model assumptions and limitations

Although drawdown and pump discharge data from low-flow sampling have been used by previous studies to estimate hydraulic properties (Robbins et al. 2009), there are many accompanying assumptions and limitations that are important to recognize. Simulation of more complex wellbore flow processes could consider the use of numerical models of wellbore flow such as the Multi-Node Well (MNW) Package of MODFLOW (Halford and Hanson 2002).

Important assumptions of the model include:

1. Confined, steady-state conditions approximate flow (Thiem equation).
2. Vertical velocity in the well-screened interval is an average velocity and calculated assuming piston flow (no friction effects).
3. The pump intake is set at the middle or upper part of the screened interval.
4. Flow in the formation is horizontal.
5. Flow into the well (well inflow) is horizontal and calculated over 1-ft increments.
6. Flow in the well is vertical toward the pump intake outside of a zone coincident with the pump intake (lateral flow zone), where flow in the lateral flow zone is assumed to be horizontal.
7. Drawdown (s_w) in the well is uniform over the screened interval.
8. Vertical flow (q_v) is calculated from the differences in horizontal well inflow $q_{h'}$ over 1-ft increments.
9. Radius of influence (R_o) is set at 10 ft.
10. Storage (S) other than from inside the well (q_w) is assumed negligible.
11. The initial uppermost position of the high HHK layer is assumed ½ the distance of the well screen to identify maximum potential TOT (OPD); however, because the thickness of the layer can vary, the distance (D) to the pump intake will vary accordingly.
12. The effect of the sand pack on the horizontal or vertical flow is not accounted for.
13. Full penetration screen or negligible vertical flow in the formation relative to horizontal flow is assumed, which may not be the case for many shallow monitoring wells.
14. Travel time from the pump intake to the surface is not accounted for.

There are several limitations that are important to consider when evaluating in-well TOT with this approach. First, significant partial penetration effects may result in underestimation of well inflow at the top and bottom parts of the screened interval. Consequently, because the method assumes a mass balance between the q_p and well inflow, flow from the middle parts of the screen will be overestimated. The combined effect will likely cause an overestimate of the q_h term, an underestimate of the q_v term, and an overestimate of the TOT. Second, ambient vertical flow will affect vertical capture intervals and TOT estimates. Wells with ambient vertical flow will preferentially intercept flow from the zone with ambient flow and capture less flow from zones with no ambient flow (Fig. 2d). In other words, ambient vertical flow (before purging) would need to be negligible relative to the q_p for the application of this model. Third, transient storage effects may be significant in cases where drawdown takes a long time to stabilize, in which case the analysis will overestimate values of HHK. The impact of formation storage (S) on HHK was evaluated by comparing HHK calculated from the Theis equation, which accounts for storage, to HHK calculated from the Thiem equation as used by the analytical model. For a 1-ft drawdown or less, the effect of S for values <0.001 results in a small error (factor of 2) in the average HHK calculated with this model. As long as the distribution of well inflow remains the same along the screen (S is uniform), impacts to vertical flow and TOT calculated with the analytical model should be small. Lastly, wells with a sand pack filter may have vertical flow in the sand pack contributing to q_p, and therefore the model will overestimate the effects of q_v within the well screen. In this case, TOT to the pump could be longer than what is computed from this analysis.

Model evaluation

The preliminary, simple analytical model presented in this paper was compared to simulations from a numerical model of wellbore flow as presented in McMillan et al. (2014). A q_p of 0.3 L/min, a s_w of 0.03 ft, and a well with a 10-ft screen and a 2-in. diameter screen was simulated. The principal differences between the numerical and analytical model are that the numerical model accounts for partial penetration, vertical flow in the aquifer, and casing storage (flow from the casing to the pump). The graphical output in McMillan et al. (2014) is reproduced in Fig. 3a and the partial results (fraction of formation water) from the numerical model and the analytical model in Fig. 3b. The numerical model computes the amount of casing water, screen water, and water contributing to the pumped water from the formation as shown in Fig. 3a. The analytical model computes only the amount of screen water and conversely the amount of formation water; the fraction of formation water to the pumped water is shown in Fig. 3b.

McMillan et al. (2014) shows that it takes about 60 min to evacuate all in-well storage including a small amount of casing water that arrives at the pump intake after 30 min (Fig. 3a). At 30 min, about 80% of the pumped water is from the aquifer as computed by the numerical model (Fig. 3a, b). In contrast, the analytical model computes 100% capture of aquifer water at 30 min (Fig. 3b). The slope of the fractional contribution of formation water to the pumped water is relatively similar between the two models. The comparison suggests the analytical model presented in this paper provides a reasonable approximation to more complex wellbore flow dynamics that may occur during purging.

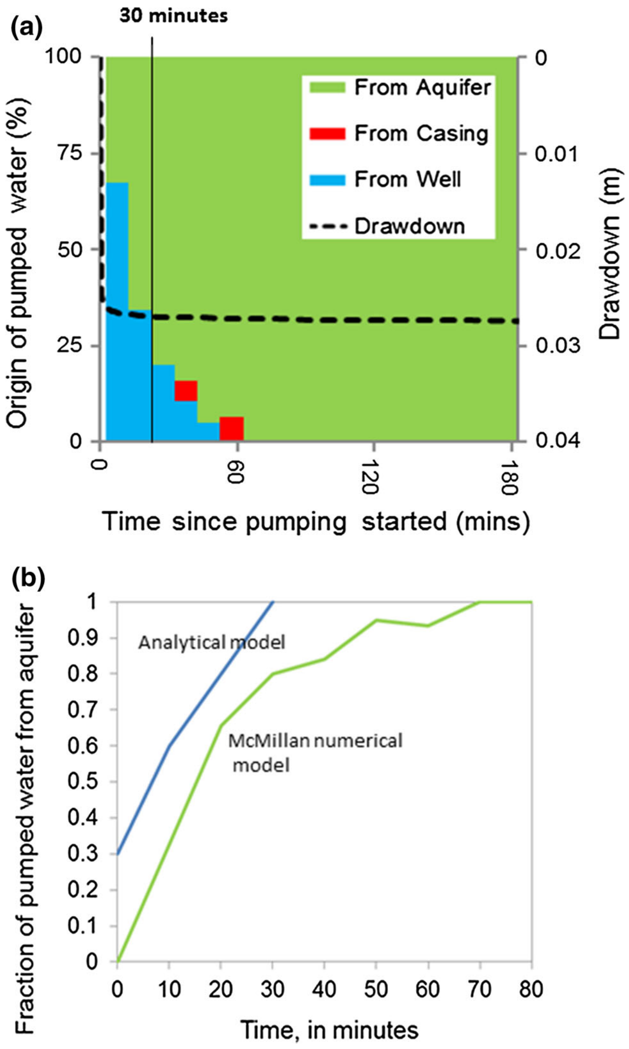

Fig. 3 Comparison of **a** solution from McMillan et al. (2014) and **b** the analytical model presented in this paper

Assessment of horizontal well inflow (q_h) near pump intake

Currently, the analytical model assumes a 2-ft zone around the pump intake contributes primarily horizontal flow (q_h) almost instantaneously. In some permeable formations, this is sufficient to satisfy pump rates (q_p) as shown in Fig. 2a. However, in many cases horizontal flow near the pump intake is not sufficient (Fig. 2c; $q_h < q_p$). Analytical model solutions based on a manual specification of HHK (forward assessment of q_h) are provided in Table 1 for a range of pump rates (0.1–0.3 L/min) and drawdowns (0.01–0.1 ft). The simulations assume either a homogeneous formation or that the highest HHK layer is coincident with the pump intake location. Results demonstrate that a minimum HHK of approximately 50 feet per day (ft/day) is required for q_h to satisfy q_p for pump rates (q_p) varying from 0.1 to 0.3 L/min. Conditions where $q_h \ll q_p$ require that the majority of pump water (q_p) is derived from vertical flow (q_v).

Model application

The analytical model allows for a quick assessment on the impact of vertical flow on OPD. For any given pump rate and time, the analytical model determines the vertical capture interval of the screened interval, which is useful for associating the capture intervals along the screen with corresponding formation layers at coincident depths. Potential variations in vertical chemistry can be inferred from this comparison.

Purge data from monitoring wells at a waste site in East Texas were evaluated for in-well TOT by solving for HHK and specifying different levels of heterogeneity that match formation heterogeneity based on lithologic logs. The geology of the site consists of a shallow, undifferentiated Quaternary alluvium aquifer of silts and sands overlying the Eocene Wilcox formation consisting of sandstones and shales. At the waste site, most wells have screened intervals that range from 5 to 30 ft lengths and are screened in the shallow Quaternary alluvium aquifer. Some well screens are partially saturated but those wells were not selected for analysis. Well diameter is typically 4 in. Pump intake is at the middle of the screened interval. Most wells examined had been pumped at low rates (approximately 0.1 L/min) for approximately 30–45 min and drawdown from pumping was minimal, at about 0.2 ft. Total volume pumped is about 4 L (0.14 cubic feet). With no well inflow, that volume is equivalent to well storage volume of 6 ft of water in a 2-in. well or 1.6 ft of water in a 4-in. well.

The results of the in-well TOT analysis of a typical purge data record from the East Texas waste site indicate that groundwater samples are being collected prior to flushing of the well screen and samples may reflect

Table 1 Forward assessment of horizontal hydraulic conductivity (HHK) required for lateral flow (q_h) by the pump intake to satisfy pump rate (q_p)

HHK (ft/day)	q_p (L/min)	Drawdown (s_w) ft	Lateral flow (q_h) dominated (Y = yes)
1000	0.1	0.01	Y
1000	0.3	0.01	Y
1000	0.1	0.1	Y
1000	0.3	0.1	Y
500	0.1	0.01	Y
500	0.3	0.01	N
500	0.1	0.1	Y
500	0.3	0.1	Y
100	0.1	0.01	N
100	0.3	0.01	N
100	0.1	0.1	Y
100	0.3	0.1	Y
50	0.1	0.01	N
50	0.3	0.01	N
50	0.1	0.1	Y
50	0.3	0.1	N
10	0.1	0.01	N
10	0.3	0.01	N
10	0.1	0.1	N
10	0.3	0.1	N

N requires the majority of q_p is derived from vertical flow (q_v); *Y* requires $q_h \approx q_p$

primarily water derived from screen storage. For a case of a 20-ft long screen and 4-in. diameter well, a 40-min purge of a well that is screened in a simulated homogeneous aquifer (Fig. 4a), <30% of the pumped water is from recent formation inflow and most water is from screen storage (Fig. 4c). It takes approximately 500 min for the entire screened interval to reach the pump intake (Fig. 4c). At 40 min purge time (t), only water from a 4-ft interval of the screen, from layers at 8–12 ft depth of the screened interval, contributes to the sample and arrives at the pump intake (Fig. 4b).

At a 10:1 variation in HHK (heterogeneous case), the flow to the well is dominated by the location of the high HHK layer. For this example, a thin, 1-ft-thick high HHK layer was specified at the top of the screen and a low HHK layer was specified for the remaining part of the screen. Specification of layers in this fashion will produce the largest variation of HHK between low and high HHK. The consequence of a well screen intersecting the high HHK layer is that water from the low HHK layers arrives at the pump intake much later and it takes over 1300 min for water across the entire screen to arrive at the pump intake (Fig. 5).

Purge data from monitoring wells located at a waste site in New England were evaluated for in-well TOT by solving for HHK and specifying different levels of heterogeneity that match formation heterogeneity based on lithologic logs. The geology of the site consists of a surficial sand and gravel aquifer from Pleistocene glacial deposition overlying a basal till deposit. The sand and gravel aquifer is highly permeable and 10–100 times more permeable than the basal till deposit. Screens vary from 5 to 10 ft length and are fully saturated. Well diameter is typically 2 in. Pump intake is at the middle of the screen. Most wells are pumped at rates of approximately 0.3 L/min, for approximately 30–45 min. Drawdown is minimal (about 0.1 ft).

The results of the in-well TOT analysis of a typical purge data set from the New England site indicate that groundwater samples are generally being collected after the entire screen is flushed and samples reflect primarily formation water. For a typical 40 min purge time (t) in a 2-in. well that is screened in a simulated homogeneous aquifer (Fig. 6a), the model shows that 100% of the pumped water is from the formation (Fig. 6c).

When heterogeneity is introduced into the simulation of the monitoring well from the New England site, TOT of formation water to the pump intake can be delayed from the low HHK layers. At a 10:1 variation of HHK in the formation (heterogeneous case), the flow is dominated by the location of the high HHK layer (Fig. 7a). For this example, a thin, 1-ft-thick high HHK layer was specified at the top of the screen and a low HHK layer was specified for the remaining part of the screen. Specification of layers in this fashion will produce largest variation of HHK between low and high HHK. The consequence of intersecting the high HHK layer is that the lower HHK layers arrive at the pump intake much later and it takes over 50 min (Fig. 7b) for the low HHK layers at the bottom of the screen to travel to the pump intake. The entire screen contributes to the sample after 60 min (Fig. 7c).

The variation in OPD due to TOT is more sensitive to simulated variations in heterogeneity for the East Texas site than the New England site. For the East Texas site, the difference in complete capture of formation water varied by 800 min (500–1300 min) between homogeneous and heterogeneous conditions. In contrast, for the New England site, the difference in complete capture of formation water varied by only 20 min (40 to 60 min) between homogeneous and heterogeneous conditions.

Using specific conductance to understand the fraction of formation water captured during purging

Purge data were modeled for two shallow wells [well station identifier (ID) 344747076352901 and 353037077502601] from the North Carolina Coastal Plain, a Quaternary Age,

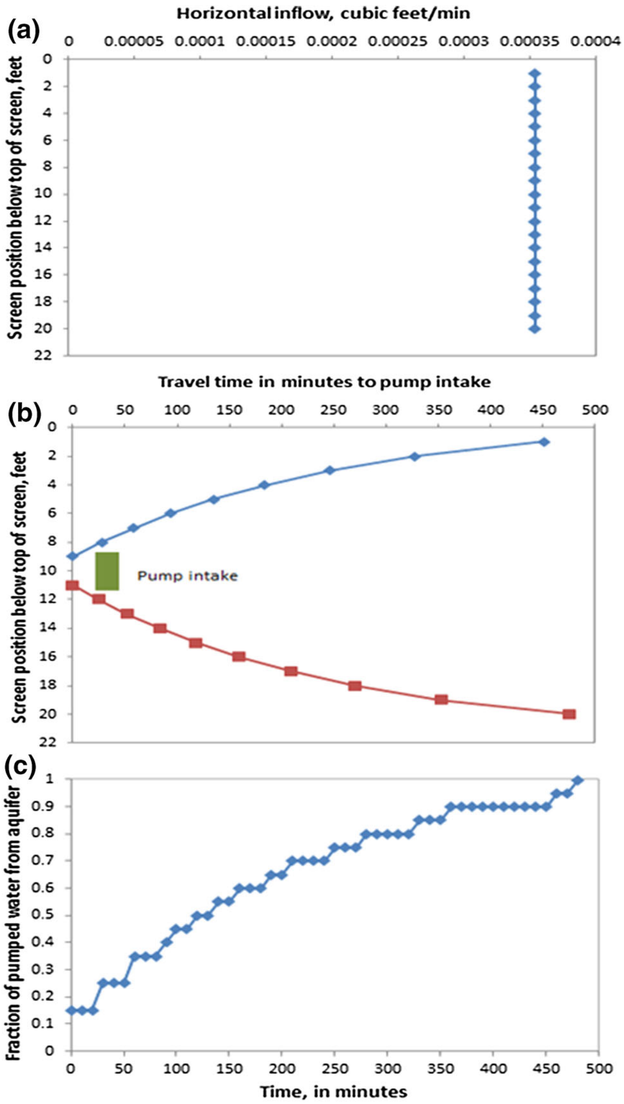

Fig. 4 In-well, vertical time-of-travel (TOT) for a monitoring well with a 20-ft screen and low purge rates (0.1 L/min) in a simulated homogeneous aquifer for purge conditions typical of a waste site in East Texas showing **a** horizontal flow, **b** TOT to pump intake from vertical flow, and **c** fraction of formation water captured

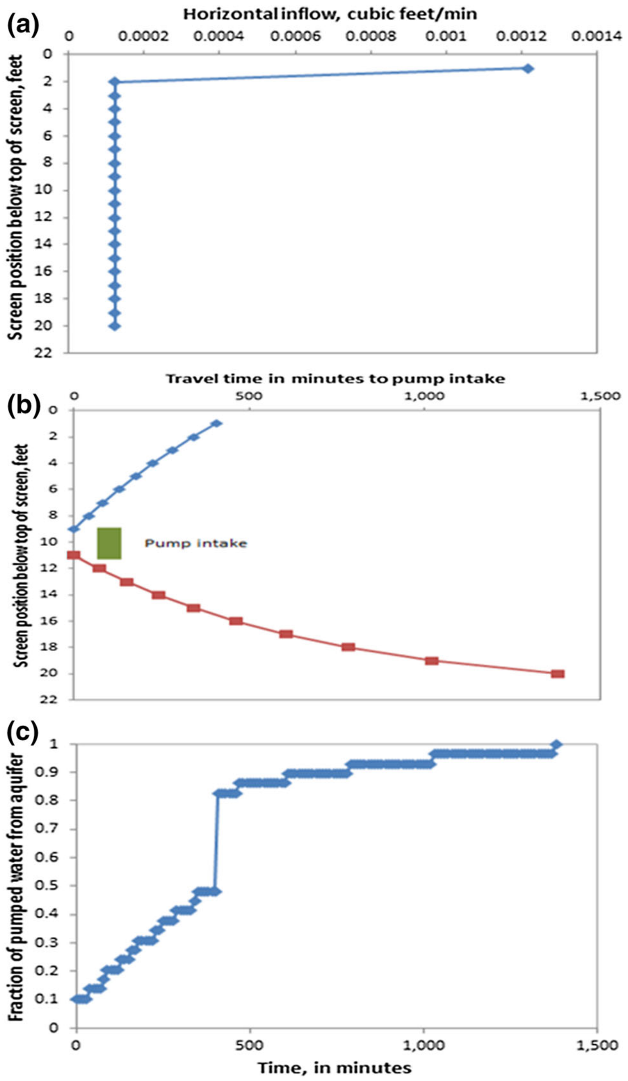

Fig. 5 In-well, vertical time-of-travel (TOT) for a monitoring well with a 20-ft screen and low purge rates (0.1 L/min) in a simulated heterogeneous aquifer for conditions typical of a waste site in East Texas showing **a** horizontal flow, **b** TOT to pump intake from vertical flow, and **c** fraction of formation water captured

unconsolidated formation. Specifically, modeled TOT and fraction of formation water captured were manually calibrated to trends in specific conductance (time to stabilize) measured during purging by adjusting the level of heterogeneity of the formation.

The two wells examined are part of a network sampled by the U.S. Geological Survey, NAWQA Project. Wells are purged with the pump intake at the top of the well screen following methods described by Lapham et al. (1995), and larger volumes of water (three equivalent casing volumes) are pumped than during typical low-flow sampling. Well 344747076352901 is a 2-in. diameter well, cased to 9 ft and screened from 9 to 14 ft below land surface. The screen was fully saturated, and no dewatering of the screen occurred during purging. The formation consists of a moderate HHK unit of sand and silt. Well 353037077502601 is also a 2-in. diameter well, cased to 5.2 ft and screened from 5.2 to 10.2 ft below land surface. The screen was initially fully saturated, but some dewatering of the screened interval occurred during purging due to excessive drawdown (5.46 ft of drawdown resulting in approximately 2.5 ft of the screen being dewatered). The formation consists of a low HHK unit of silt and clay.

In-well TOT compares favorably to specific conductance trends measured during purging. Quick stabilization of measured specific conductance during purging corresponds to quick simulated TOT. Slower stabilization of

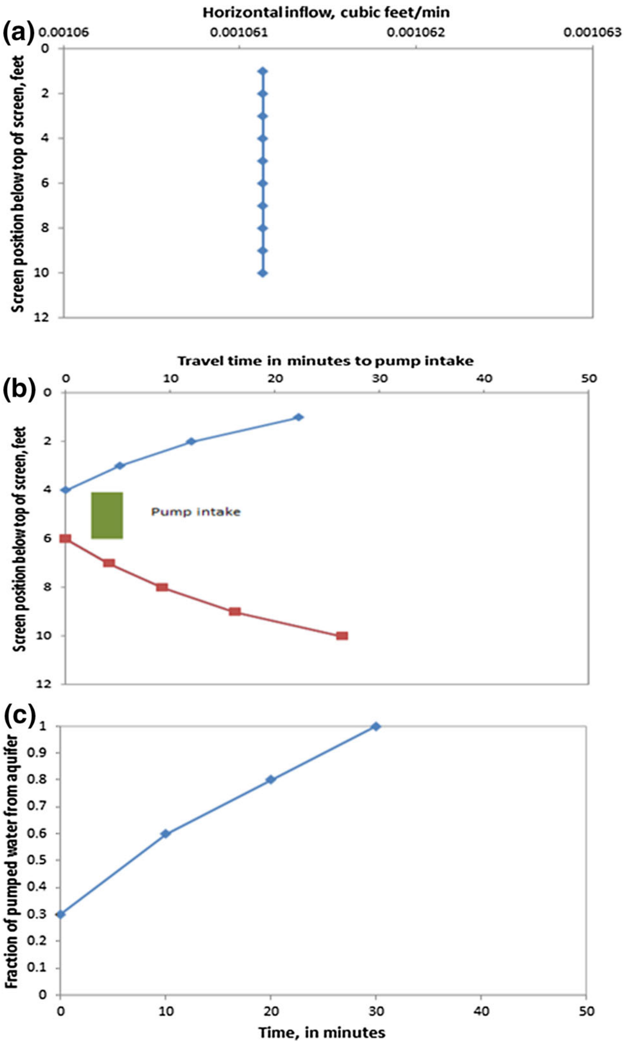

Fig. 6 In-well, vertical time-of-travel (TOT) for a monitoring well with a 10-ft screen and low purge rates (0.3 L/min) in a simulated homogeneous aquifer for conditions typical of a waste site in New England showing **a** horizontal flow, **b** TOT to pump intake from vertical flow, and **c** fraction of formation water captured

measured specific conductance during purging corresponds to slow simulated TOT. Purge data indicated a distinct difference in HHK between the two wells that are substantiated by the lithologic logs. Well 344747076352901 was simulated with a homogeneous, relatively high HHK, which resulted in a quick TOT, and a high amount of flushing of the screened interval (Fig. 8). The log from this well reported a sand and silt formation. The well was pumped for 57 min at a rate of 2.72 L/min although an adequate sample could have been taken after 30 min (equivalent to three well screen volumes flushed). Note that the specific conductance measured during purging stabilized almost immediately (Fig. 8a). At 57 min, the lateral capture radius for this well is approximately 8 ft. Well 353037077502601 was simulated with a heterogeneous 10× difference in lower and higher HHK (still relatively low) values, which resulted in a slow TOT, and a low amount of flushing of the screened interval (Fig. 9). The log from this well reported a silt and clay formation. Transport to the pump from the bottom parts of the screen takes about 40 min. Note that specific conductance measured during purging stabilized after 50 min and showed a bimodal distribution (Fig. 9a). The bimodal distribution could be the result of dewatering of the upper screened interval and preferential capture of deeper groundwater. Purge time for this well was 68 min at a rate of 0.26 L/min. At 68 min, the lateral capture radius for this well is approximately 1.5 ft.

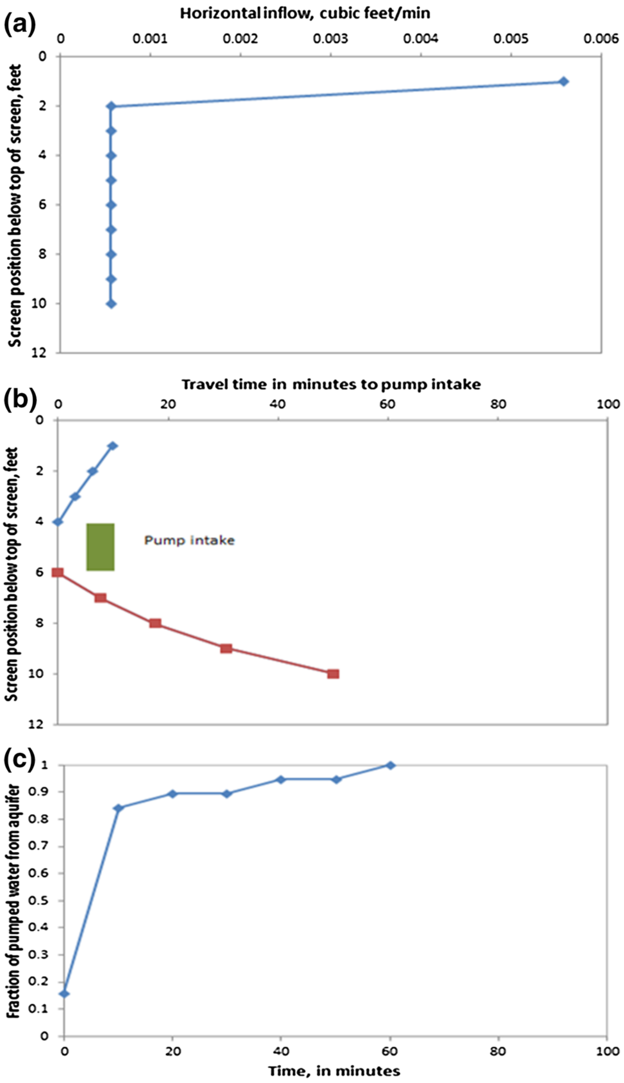

Fig. 7 In-well, vertical time-of-travel (TOT) for a monitoring well with a 10-ft screen and low purge rates (0.3 L/min) in a simulated heterogeneous aquifer for conditions typical of the New England site showing **a** horizontal flow, **b** TOT to pump intake from vertical flow, and **c** fraction of formation water captured

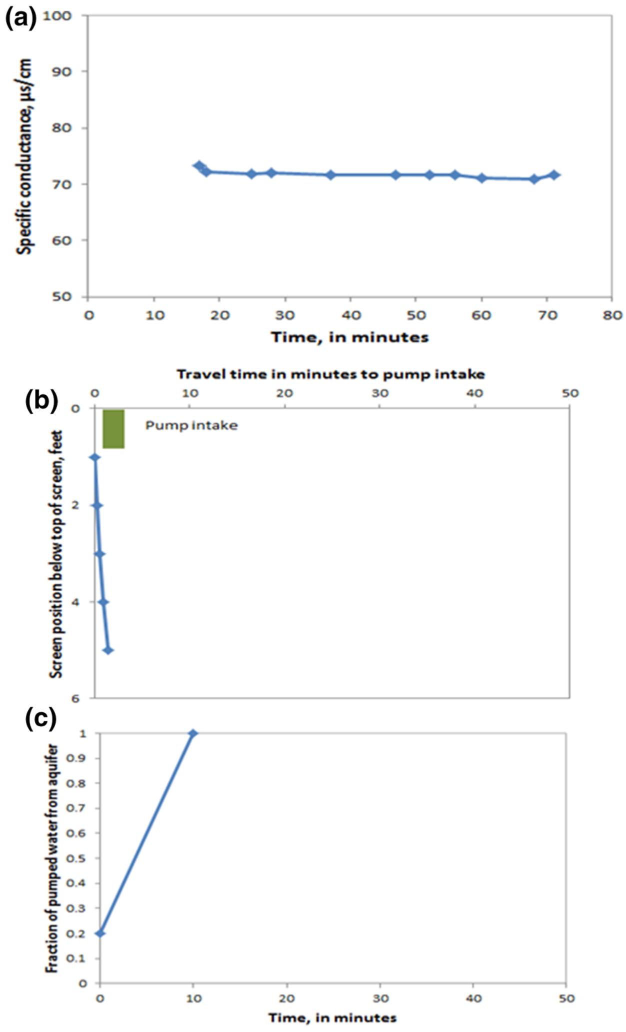

Fig. 8 Plots of **a** specific conductance measured in the field during purging from well 344747076352901, **b** time-of-travel (TOT) to pump intake from vertical flow, and **c** fraction of formation water captured

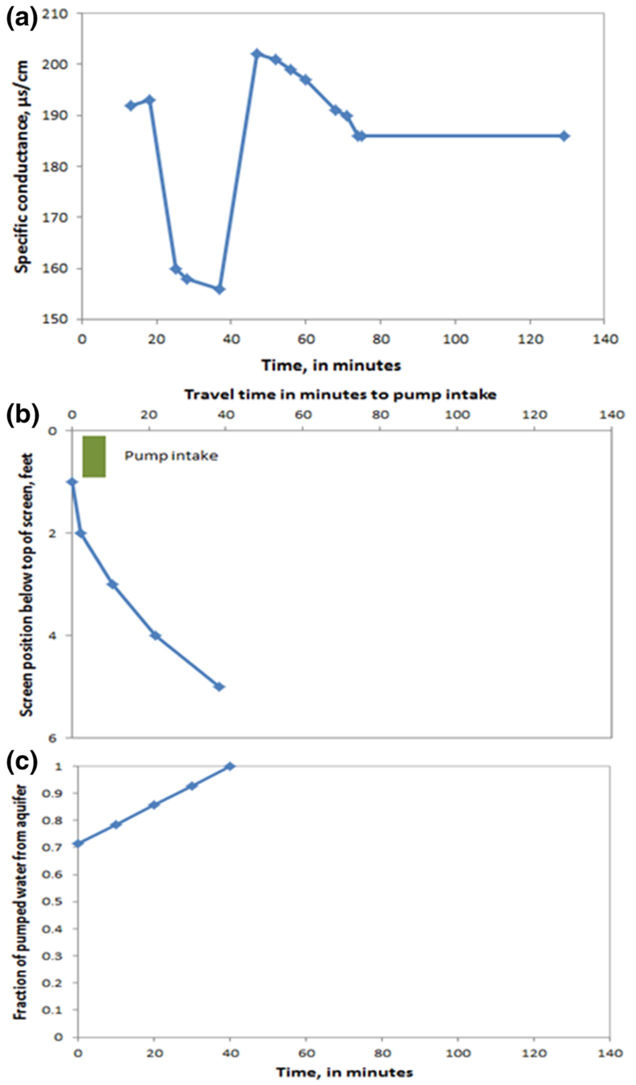

Fig. 9 Plots of **a** specific conductance record during purging from well 353037077502601, **b** time-of-travel (TOT) to pump intake from vertical flow, and **c** fraction of formation water captured

The well from the lower HHK formation was likely under purged with minor flushing of the well screen, while the well from the higher HHK formation was likely over purged. Drawdown at the well from the lower HHK formation was 5.46 ft, and it is likely that some water from casing storage is a component of the pumped water. The screen is partially dewatered, which is also problematic for analytical modeling purposes. The consequences of under purging include collection of a non-representative sample not reflective of formation water due to potential atmospheric interference in-well chemistry and mixing of water in the wellbore with water from casing storage. Over purging affects the volume of the formation sampled (size of the capture zone) and can have implications on the reproducibility of measurements in subsequent sampling events. For example, the lateral capture radius of well 344747076352901 increases by 1 foot every 18 min so variations in sample time in subsequent sampling events will integrate the water chemistry from potentially different volumes and parts of the formation.

Discussion

For low-flow rate purge methods that are widely used to collect groundwater samples, the emphasis is on collecting representative samples while minimizing drawdown to avoid capture of stagnant casing water. However, this concept does not eliminate the possibility of capturing preexisting (prior to purging) water from within the well screen. To facilitate the capture of representative formation water from outside the well, field parameters are monitored to ensure stability. This work has shown that calculated in-well TOT supports the collection of groundwater samples after field parameters have stabilized. The in-well TOT can be used to determine an OPD needed to collect a representative groundwater sample. Further, the time to achieve stabilization of field parameters can be used to understand gross levels of a formation hydraulic and chemical heterogeneity.

The removal of multiple casing volumes has been a metric to assess whether a groundwater sample is representative of formation water. However, evacuation of casing storage is not applicable with low rates of pumping because the total volume purged often is much less than the total volume of water storage in the well (casing and screen). For example, a pump rate of 0.1 L/min at 40 min purges a total volume of 0.14 cubic ft. For a 50-ft saturated column of water in a 2-in. diameter well, a volume of 0.14 cubic ft represents only 13% of the equivalent water volume in the well. However, when considering only the volume of water from the screened interval of a well, for a 10-ft saturated screened interval that same volume represents 64% of the equivalent water volume within the screen. Increasing the pump rate to 0.3 L/min equals 39% of the well volume but 194% of the screened interval volume. For permeable formations, simulated TOT to the pump intake from the entire 10-ft screened interval was often less than 40 min at a pump rate of 0.3 L/min in 2-in. diameter wells. Therefore, tracking of both the equivalent water volume evacuated from the screened interval and in-well TOT may be a useful gauge to ensure collection of formation water.

Although not part of this evaluation, chemical heterogeneity coupled with the hydraulic heterogeneity, as shown here, could result in large temporal variation in chemical concentrations during purging. However, time-series sampling of contaminants except for monitoring of field parameters during purging is rarely done. Time-series sampling during a period of steady-state flow and transient transport (Fig. 1) can be coupled with calculation of in-well TOT to understand levels of chemical and hydraulic heterogeneity affecting the well. For example, sampling of low HHK formations during remediation may be the most critical factor in evaluating performance metrics for achieving remediation targets. Yet results from this modeling exercise showed that collection of samples after purging for 30–40 min with low-flow sampling in low-permeability formations may selectively capture preexisting water from screen storage and may not reflect inflow from low HHK layers. Therefore, coupling of arrival times from vertical TOT with time-series sampling may prove beneficial in deciphering chemistry from low HHK layers.

While a useful tool, further testing of the analytical model is recommended. A proof of concept approach would help evaluate the utility of the analytical model to track sample capture intervals, vertical flow, and TOT to the pump intake during low-flow sampling. Further, field collection activities geared toward tracking vertical TOT would help guide model enhancements.

Conclusions

Simulations performed using a preliminary, simple analytical model incorporated into an Excel-based VBA model indicate that for pump rates typical of low-flow sampling, formations with a horizontal hydraulic conductivity less than 50 ft/day will capture a large volume of screen storage (preexisting well water) at the expense of lower volumes of formation water unless adequate purge times are reached. Pump intakes that are coincident with low hydraulic conductivity layers or formations will likely induce vertical flow in the well screen. In this case, substantial volumes of preexisting water from the well screen will be captured during purging until well inflow from the higher hydraulic conductivity layers or formations can travel to the pump. Therefore, in-well, vertical time-of-travel (TOT) from the relatively high hydraulic conductivity layers to the pump intake is a major driver in assessing the amount of recent inflow of formation water being sampled during pumping. Significant heterogeneity along the well screen can also delay travel times from the low HHK layers to the pump intake. The consequence of delayed travel times is a partial sampling of the screened interval and the optimal purge duration (OPD) to ensure a representative sample may be longer than for homogeneous formations.

Field monitoring of pumped water for specific conductance shows excellent comparison between stabilization of specific conductance readings and computation of in-well vertical TOT for the two cases evaluated. This demonstrates the utility of the model to help understand and describe in-well flowpaths and assess screen capture intervals. The similarity between vertical TOT and trends in specific conductance at monitoring wells likely indicates that vertical flow in the well screen predominates where low-flow sampling is the method of choice. Prior to stabilization, which essentially marks the achievement of in-well steady-state flow and transport, in-well transient transport contributes to fluctuations in field monitoring of specific conductance.

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