

Instructions for Running the Analytical Code PAT (Purge Analyzer Tool) for Computation of In-Well Time of Travel of Groundwater under Pumping Conditions

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By P.T. Harte, B.J. Huffman, Tomas Perina, Herb Levine, and Daewon Rojas-Mickelson

Prepared in cooperation with the U.S. Environmental Protection Agency

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U.S. Department of the Interior
U.S. Geological Survey

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DAVID BERNHARDT, Secretary

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James F. Reilly II, Director

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Conversion Factors

U.S. customary units to International System of Units

Multiply	By	To obtain
Length		
inch (in)	2.54	centimeter (cm)
inch (in)	25,400	micrometer (μm)
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
Volume		
ounce, fluid (fl. oz)	29.57	milliliter (mL)
Flow rate		
gallon per minute (gal/min)	3.785	liter per minute (L/min)
cubic inch per minute (in^3/min)	16.39	milliliter per minute (mL/min)
cubic feet per minute (ft^3/min)	28.3168	liter per minute (L/min)
Velocity		
feet per minute (ft/min)	0.3048	meter per minute (m/min)
Hydraulic conductivity		
feet per day (ft/d)	0.3048	meter per day (m/d)

Glossary and Abbreviations

A_{well}	area of well
$A_{\text{rad-2ft}}$	area of mixing zone
b	thickness or length of well opening, ft
dt	time interval for solution to compute aquifer fractional capture, min
DTW	depth to water from land surface datum, ft
DTS	depth to top of screen from land surface datum, ft
D_{well}	diameter of well, in inches
HF	heterogeneity factor, a multiple between high and low hydraulic conductivity (K) of a modeled layer, dimensionless
K_{avg}	average hydraulic conductivity across the screen or well opening, ft/d
K_{High}	highest hydraulic conductivity per layer of the screen or well opening, ft/d
K_{layer}	hydraulic conductivity per layer, ft/d
K_{Low}	lowest hydraulic conductivity per layer, ft/d
K_{medium}	medium hydraulic conductivity per layer of the screen or well opening as determined from the average of the K_{High} and K_{Low} , ft/d
L_{cw}	Length (height) of casing water under pumping conditions above top of well opening, ft
L_{T}	cell thickness or layering used to calculate radial inflow and in-well flow, ft

L_s	length of screen or open interval, ft
M_z	mixing zone of pump, ft
PAT	Purge Analyzer Tool
P_L	pump location relative to top of screen or open interval, ft
Q_H	horizontal radial flow within the M_z ; ft ³ /min
Q_{h1-n}	individual layered radial flow from discretized layers (denoted as 1-N); the summation of Q_{h1-n} constitutes the Q_v term
Q_p	average pumping rate, L/min in input field
Q_p'	adjusted average pumping rate that accounts for wellbore storage (Q_w), ft ³ /min
Q_v	vertical flow entering the mixing zone (M_z) from the summation of layered radial flow; ft ³ /min
Q_w	flow from wellbore storage, ft ³ /min
Re	Reynolds number, a dimensionless number used to compare the ratio of inertia force to viscous force. In hydraulics it is used to assess flow turbulence.
R_o	radius of influence, ft
s	drawdown at the well, ft
S	storage coefficient, dimensionless
T	transmissivity
t_{purge}	actual (reverse mode) or anticipated (forward mode) purge time, min
t_{min}	potential minimum purge time, computed from the in-well travel time based on the V and the length of the well screen, min
V	unidirectional maximum vertical velocity (ft/min)
Volumetric purge time	amount of purge time required to evacuate the equivalent of three-saturated well volumes

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By P.T. Harte,¹ B.J. Huffman,¹ Tomas Perina,² Herb Levine,³ and Daewon Rojas-Mickelson³

Introduction

Understanding the optimal time needed to purge a well while pumping to collect a representative groundwater sample requires an understanding of groundwater flow in wells (in-well flow). Parameters that affect in-well flow include the hydraulic properties of the aquifer, well construction, drawdown from pumping, and pump rate. The time of travel relative to in-well flow is affected by the pump's intake location. The Purge Analyzer Tool (PAT) incorporates hydraulic calculations to help assess the optimal purge times required to vertically transport groundwater in the well to the pump intake (Harte, 2017). Harte (2017) includes a discussion on the rationale for determining in-well groundwater flow and time of travel and also discusses the limitations inherent in the PAT; an understanding of the limitations is important to ensure proper use.

The PAT calculates flow by use of the Dupuit-Theim equation (Lohman, 1979) that assumes steady-state radial flow and a total inflow from the well opening or screen equal to the pumping rate (eq. 1). A bulk average hydraulic conductivity (K_{avg}) is derived from this relationship. Once K_{avg} is calculated, the program calculates incremental (layered) horizontal radial inflow into the well over user defined increments (layers). These defined increments represent the screen or well opening as a fraction of the total inflow. The amount of inflow per layer is proportional to the user-defined layered distribution of hydraulic conductivity (K_{layer}) because drawdown is assumed to be uniformly distributed in the well. The water budget equation that guides the solution of the PAT (eq. 1) is specified as:

$$Q_p = Q_v + Q_H + Q_w \quad (1)$$

where

- Q_p is pumping rate,
- Q_v is vertical flow entering the boundary of the mixing zone (M_z) from the summation of layered radial flow ($\sum Q_{hl-n}$) where 1-n denotes number of layers,
- Q_H is horizontal radial flow into the mixing zone (M_z), and
- Q_w is flow from wellbore storage effects.

The in-well flow is computed from the convergence of incremental (layered) radial inflows (Q_{hl-n}) summed to the total vertical flow (Q_v) entering the adjacent zone to the pump intake (called mixing zone [M_z]) as shown in figure 1. The Q_v is transported as one-dimensional piston flow. Within the M_z , it's assumed that flow to the pump is dominated by horizontal radial flow (Q_H) when the pump is in the open interval of the well. Flow from the wellbore storage (Q_w) is computed from the volume of water pumped from the well at the time of the drawdown (s) measurement(s). Aquifer storage effects are unaccounted for but are likely to be problematic when (1) dewatering within the well opening occurs or (2) when the water table is close to the top of the well screen or open interval where additional flow into the upper portion of the well opening may occur. For fully saturated wells tens of feet below the water table, storage effects are likely to be more uniformly distributed across the well screen or open interval (regardless of confined or unconfined conditions). Therefore, radial inflow from storage will be less prominent under pump rates commonly used in groundwater sampling either for volumetric sampling (<3 gallons per minute) or low-flow sampling (<0.5 liters per minute).

A major benefit of the use of the PAT is the understanding of time-varying, vertical integration of captured pump water. The analytical model computes aquifer (formation) capture intervals relative to the open interval of the well. This information is displayed graphically (called aquifer fraction graphs) and can be used to assess the likely formation intervals contributing water to the sample at any time.

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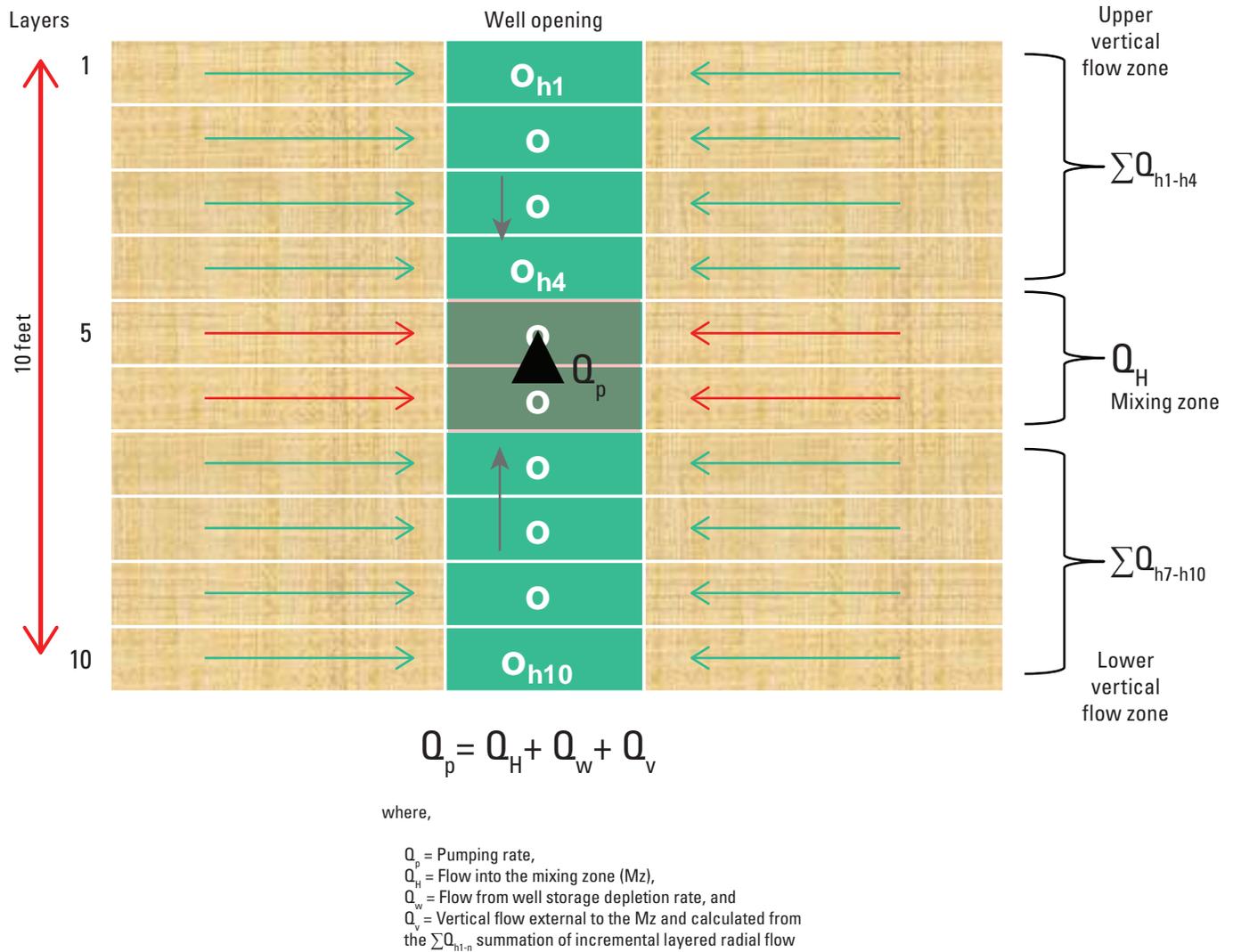


Figure 1. Schematic of the allocation of flow in the well while pumping for the Purge Analyzer Tool.

Contents of Program

The PAT is contained within a macro-enabled Microsoft Excel file with a *.xlsm extension. Contained in the Excel file are multiple worksheets. There are three worksheets for the case of homogeneous hydraulic conductivity (K_{layer} is uniform) and an additional worksheet if a heterogeneous condition (K_{layer} is nonuniform) is simulated. The operation of the analytical model is discussed in the “Operation” section.

Requirements

The PAT (Purge Analyzer Tool) is a Microsoft Excel VBA macro code for computation of in-well travel times of groundwater under pumping from wells. Excel versions dated 2016, 2013, or 2010 are required. For Excel 2007, certain

functions to display charts will not work. Many commands that do not work in Excel 2007 are associated with the charts aesthetic nature and can be commented out by adding a single quote (‘) to the beginning of the command line in the embedded VBA macro called “HV_Pump_Flow.” Most users (permission dependent) will be able to open the VBA macro by going to the Developer tab, selecting macro, and then selecting the VBA macro called “HV_Pump_Flow” under the module where macros are stored.

Excel files must be saved as a macro enabled .xlsm workbook. On certain computer systems, the user will need to open the file and then resave the macro-enabled Excel file under a new name to meet security requirements.

The Data Solver Add-ins in Excel must be enabled for VBA code operation. For many computer systems, the default configuration is likely to be disabled. There are several methods to check if Solver is enabled including on the “Data” tab

of an Excel workbook (if it is visible on the ribbon); under “Add-Ins” of the options menu under the “File” tab; and on the “Developer” tab under the “Excel Add-ins” menu. It may also be necessary to ensure that the “Developer” tab is shown on the command toolbar along with the “Add-ins” ribbon. This is done by selecting “Options” under “File” drop-down tab. Under options select “Customize Ribbon” and check “Developer” and “Add-ins” to make them viewable in the “Main Tabs” ribbon. In the new window, click the “Tools” tab and click on “References.” The box next to “Solver Add-ins” must be checked. Go back to the “Developer” tab and click on “Excel-Add-ins.” The “Data Solver Add-ins” should now be checked. After ensuring the “Data Solver Add-ins” is invoked, save the workbook using the macro-enabled .xlsm suffix.

Instructions

This and the following sections explain the general operational steps of the program for reverse and forward mode in the instructional worksheet. Normally, the PAT is used in reverse mode where field data were collected and the K_{avg} is unknown but can be calculated. In this case, some vertical flow is assumed to occur based on the relations specified in equation 1 because of the division of flow between Q_H in the M_z and the flow in the rest of the screen or open interval outside of the M_z where (Q_v) is computed and tracked. However, if K_{avg} is known from prior information then the PAT can be used in forward mode to assess the likelihood of Q_v occurring in the well. In other words, for a given drawdown, the programs checks if there is sufficient Q_H in the M_z to satisfy the adjusted pump rate (Q_p); under this case Q_v approaches zero. The macro (RUN MODEL button) is not invoked in this case because K_{avg} is already known.

Input Worksheet

Data are entered under the worksheet labeled “Input” of the *.xlsm Excel file. Input parameters that describe well purging, well construction, and water levels are specified in the gray shaded cells B4:B13 (fig. 2). The depth to water (DTW; cell B6) is the static water level in feet (ft) below land surface. The depth to screen or open interval (DTS; cell B7) is the top of the well opening in ft below land surface. The length of the screen (L_s) is the difference in ft between the top and bottom of the well opening. The diameter of the well (D_{well}) is for the well opening. If the well casing diameter differs from the opening, then a correction factor can be applied to the drawdown (s) cell B12. Values in cells B10:B12 should represent data that were collected contemporaneously. The anticipated purge time (t_{purge} ; cell B10) and drawdown (s; in cell B12) are used in the Q_w calculation for wellbore storage depletion rate. The assumption is that the drawdown has stabilized.

The heterogeneity factor (HF) is an important parameter to simulate homogeneous (HF = 1) or heterogeneous

PAT=PURGE ANALYZER TOOL		
Initial Inputs & Calculations		
Input Parameters	Inputs	Units
Well Name	test	
Date (mm/dd/yyyy)		
Depth to Water below reference, DTW	9.00	ft
Depth to Top of Screen below reference, DTS	30.00	ft
Length of Screen, L_s	10.00	ft
Well Diameter, D_{well}	1.5	inches
Actual or Anticipated purging time, t_{purge}	70.0	min
Averaged Purge Rate, Q_p	0.300	L/min
Drawdown, s	10.00	ft
Heterogeneity Factor, HF (1=Homogeneous)	1.00	Dimensi onless

Figure 2. Reproduction of user-specified input parameters (cells B4:B14) on the “Input” worksheet for the Purge Analyzer Tool. [ft, feet; min, minutes; L/min, liters per minute]

conditions (HF greater than 1). HF (cell B13) is specified as a multiple between the lowest and highest hydraulic conductivity of an individual layer (K_{layer}) encountered along the well opening. For example, if a multiple of 10 is specified as a value of HF, the highest K_{layer} would be 10 times the lowest K_{layer} . The thickness in which K_{layer} can vary is set depending on the layer thickness (L_T). For homogeneous conditions, the K_{layer} of individual layers will be uniform and equal to K_{avg} . For heterogeneous conditions, specifying a multiplier greater than 1 allows for layered variability in K_{layer} that is constrained by the multiple factor specified in cell B13. An initial estimate of K_{avg} can be entered in cell B14, however once the program is run in reverse mode the field will be updated to the calibrated value. See the “Operation” section of this report for additional details.

Additional input parameters to run the PAT (fig. 3; cells B29:B32) are the pump intake position (P_L) relative to the top of the screen or well open interval; the length of the M_z above or below the pump intake (specified as $\frac{1}{2} M_z$ in the PAT); a layering thickness (L_T) to compute Q_H into the well; and time discretization (dt) for the determination of aquifer capture (fig. 3).

The depth of the P_L within the well screen or open interval is specified by positive distances from the top of the well screen or open interval. For P_L within the casing, negative distances are specified. The middle point of the pump intake should be used for its pump position.

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Program Variables	Inputs	Units
Pump Location relative to top of screen (Above screen specify negative number for absolute distance), P_L	5	ft
1/2 Mixing Zone Buffer length above/below pump intake, $1/2 M_z$	0.5	ft
Cell Thickness of layers to compute horizontal radial flow, L_T	0.5	ft
Time interval (dt) for computation of flow and Aquifer Fraction graph	0.5	min

Figure 3. Reproduction of user-specified program variables (cells B29:B32) on the “Input” worksheet for the Purge Analyzer Tool. [ft, feet; min, minutes]

The M_z is the vertical length of the saturated water column surrounding the pump intake. In M_z , inflow into the well is proportioned to the Q_H term (eq. 1). As the vertical flow crosses into the M_z boundary (or boundaries), no computation of vertical travel time occurs, and flow is assumed as instantaneously evacuated. Therefore, vertical transport is computed to the edge of the M_z . The computation of Q_H is set to zero when the pump intake is located in the well casing as no radial flow can contribute in M_z . At a minimum, the M_z corresponds to the length of the pump intake. For a pump intake length of approximately 1 ft or less, a value of 0.5 ft for the $1/2 M_z$ length (distance above and below the midpoint of the pump intake) can be specified in the PAT. For high pump rates, an M_z extended beyond the length of the intake is likely desirable because of turbulence. A $1/2 M_z$ value of 0.5 ft is recommended for most pump intakes that are less than 0.8-ft long. The M_z affects the vertical time of travel computations and the time of aquifer fraction captured because vertical transport is only calculated up to the M_z boundary (or boundaries). This is regardless if the P_L is in the casing or well opening (appendix 1).

L_T is used to vertically discretize the saturated water column to compute horizontal flow and corresponding vertical flow over the user-defined distances. The L_T should be equal to or less than the M_z length and the M_z should be a divisible by L_T with no remainder, although a nondivisible L_T specification will still work. For example, if there is a M_z of 0.5, a L_T of 0.1 or 0.25 would be acceptable.

Specification of the dt allows for higher or lower resolution of the vertical time of travel computation. This allows for a higher resolution discretization of the aquifer fraction graph. The smaller the dt, the smoother the aquifer fraction graph will appear. Specification of a dt that is too small will result in a longer solution runtime. The user can initially specify a relatively large dt (2 minutes) and reduce in subsequent simulations if the aquifer fraction graph appears irregular or nonsmooth.

There are other cells in the “Input” worksheet that are not related to input parameters but are cells reserved for calculation and description of parameters. The cells B15:C16 (fig. 4) are reserved for forward mode only when manual specification of K_{avg} is input into cell B14 and the reverse mode is not invoked (“RUN MODEL” Button on “Input” worksheet is not used). In forward mode, whether Q_v occurs in the well for any given Q_p is dependent on whether Q_H for the assigned M_z is sufficient to satisfy the Q_p pump rate. Forward mode is further discussed in the “Operation” section.

Cells in B18:B26 are calculated by the program and listed under the column heading “Outputs” (fig. 4). The minimum potential equilibrium pump rate, in cell B18, is the summed flow from Q_H and Q_v in cubic feet per minute. The minimized residual as determined by Excel’s solver when running the PAT in reverse mode can be seen in cell B19. This minimized residual is the difference between the minimum potential equilibrium pump rate (cell B18) and the Q_p (Q_p minus Q_w). The minimized residual should be close to zero. Additional discussion on Excel solver use is included in the “Solver” section of the report. The observed Q_w (cell B20) represents the volume of water in the well removed by the drawdown (s). The maximum vertical wellbore velocity (V ; cell B21) assumes unidirectional flow and is computed from Q_p , divided by the wellbore cross-sectional area. An external check on flow can be done using the value from cell B21 in the Reynolds equation (Streeter and Wylie, 1985) to check against the potential for turbulent flow, by calculating the Reynolds number (Re), where the laminar flow regime holds for cases of $Re < 2,000$. The adjusted maximum vertical wellbore velocity, in cell B22,

	A	B	C
15	Is vertical flow in well likely induced from purging, based on estimated radial flow in M_z ? (Forward mode)	YES	
16			
17	Calculated Parameters	Outputs	Units
18	Minimum potential equilibrium purge rate	0.0085	ft ³ /min
19	Difference between Radial flow - Purge Rate	0.0000	ft ³ /min
20	Observed wellbore storage volume	0.1227	ft ³
21	Maximum potential vertical wellbore velocity with no well storage	0.8613	ft/min
22	Adjusted maximum potential vertical wellbore velocity including well storage and horizontal flow into the M_z	0.6947	ft/min
23	Potential minimum purge time	28.8	min
24	Volumetric purge time	107.7	min
25	Transmissivity of well screen or open interval, T	1.0044	ft ² /day
26	Average K of well screen or open interval, K_{avg}	0.1004	ft/day

Figure 4. Reproduction of output fields (cells B15:B26) from the “Input” worksheet for the Purge Analyzer Tool. [ft³/min, cubic feet per minute; ft, feet; min, minute; ft²/day, square feet per day]

includes the Q_w that occurs during t_{purge} . The potential minimum purge time (t_{min} ; cell B23) is computed from the in-well travel time based on V and the L_s . The purge time required to remove three well casing volumes of water (volumetric purge time) is provided in cell B24 for comparison. The transmissivity (T) for the well opening (cell B25) is $K_{avg} * L_s$. Both K_{avg} and T are representative of the well opening length (L_s) and not the aquifer thickness.

Output Worksheet

The “Output” worksheet lists the results of the PAT in reverse mode (fig. 5). Columns A through J list tabular data related to radial flow, vertical velocity, and travel time to the P_L bounded by the M_z . Column A lists the index number for each discretized layer whereas columns B and C list the centroid position and radial inflow corresponding to the index number. Column D lists the index number for each vertical face between the discretized layers. Column E lists the vertical face position, and column F lists the vertical velocity calculated corresponding to the index number in column D. Column G lists the linear travel time, and column H lists the travel time accounting for acceleration. Column I lists the time since the start of pumping, and column J lists the fraction of inflow from recharge (aquifer) captured by the pump divided by the total inflow into the well from the formation.

There are four graphs displayed on the “Output” worksheet. They include the horizontal radial flow graph

(fig. 6), the vertical velocity graph (fig. 7), the in-well travel time to the M_z (fig. 8), and the aquifer fraction graph (fig. 9). For graphs in figures 6–8, the ordinate tick marks and labels correlate to the L_T specified on the “Input” worksheet; in this case, an L_T of 0.25 ft was specified. All output figures displayed in this report are for conditions specified in the input fields shown in figures 2 and 3.

In the example provided (fig. 6), the well inflow is uniform for a homogeneous condition. The pump intake is set at the middle of the well screen as delineated by M_z (fig. 6; green lines). No inflow occurs in the well casing as noted by zero inflow (fig. 6; red dotted line) above the top of the opening (fig. 6; black dashed line). Figures 7 and 8 also show the location of M_z and the top of the well opening.

Figures 7 and 9 show the vertical velocity and in-well travel times, respectively, under a homogeneous case. For a homogeneous condition where the pump is set at the middle of the well opening, radial flow, vertical velocity, and in-well travel time are symmetric. Both the linear velocity and acceleration velocity schemes are provided in figure 8; the acceleration velocity is used in the calculation of capture.

Figure 9 compares the fraction of inflow from the aquifer during pumping (red line) to the actual (reverse mode) or anticipated (forward mode) purge time (gray line) and the purging time required to remove three-casing volumes of water from the well (orange line). The purge time associated with the aquifer fraction needed to collect a representative sample is defined by the travel time to vertically

A	B	C	D	E	F	G	H	I	J
Index Number	Centroid Position (ft from top of opening)	Radial Flow (ft ³ /min)	Index Number	Vertical Face Position (ft from top of opening)	Vertical Velocity (ft/min)	Travel Time (min)	Travel Time (accel) (min)	Purge Time (min)	Aquifer Fraction (ratio)
0	-11.00	0.0000	0	-11.00	0.00	---	---	0.0	0.00
1	-10.88	0.0000	1	-10.75	0.00	---	---	0.5	0.10
2	-10.63	0.0000	2	-10.50	0.00	---	---	1.0	0.15
3	-10.38	0.0000	3	-10.25	0.00	---	---	1.5	0.15
4	-10.13	0.0000	4	-10.00	0.00	---	---	2.0	0.20
5	-9.88	0.0000	5	-9.75	0.00	---	---	2.5	0.20
6	-9.63	0.0000	6	-9.50	0.00	---	---	3.0	0.25
7	-9.38	0.0000	7	-9.25	0.00	---	---	3.5	0.25
8	-9.13	0.0000	8	-9.00	0.00	---	---	4.0	0.30
9	-8.88	0.0000	9	-8.75	0.00	---	---	4.5	0.30
10	-8.63	0.0000	10	-8.50	0.00	---	---	5.0	0.35
11	-8.38	0.0000	11	-8.25	0.00	---	---	5.5	0.35
12	-8.13	0.0000	12	-8.00	0.00	---	---	6.0	0.40

Figure 5. Reproduction of tabular data outputted on the “Output” worksheet for the Purge Analyzer Tool. [ft, foot; ft³/min, cubic foot per minute; ft²/min, square foot per minute]

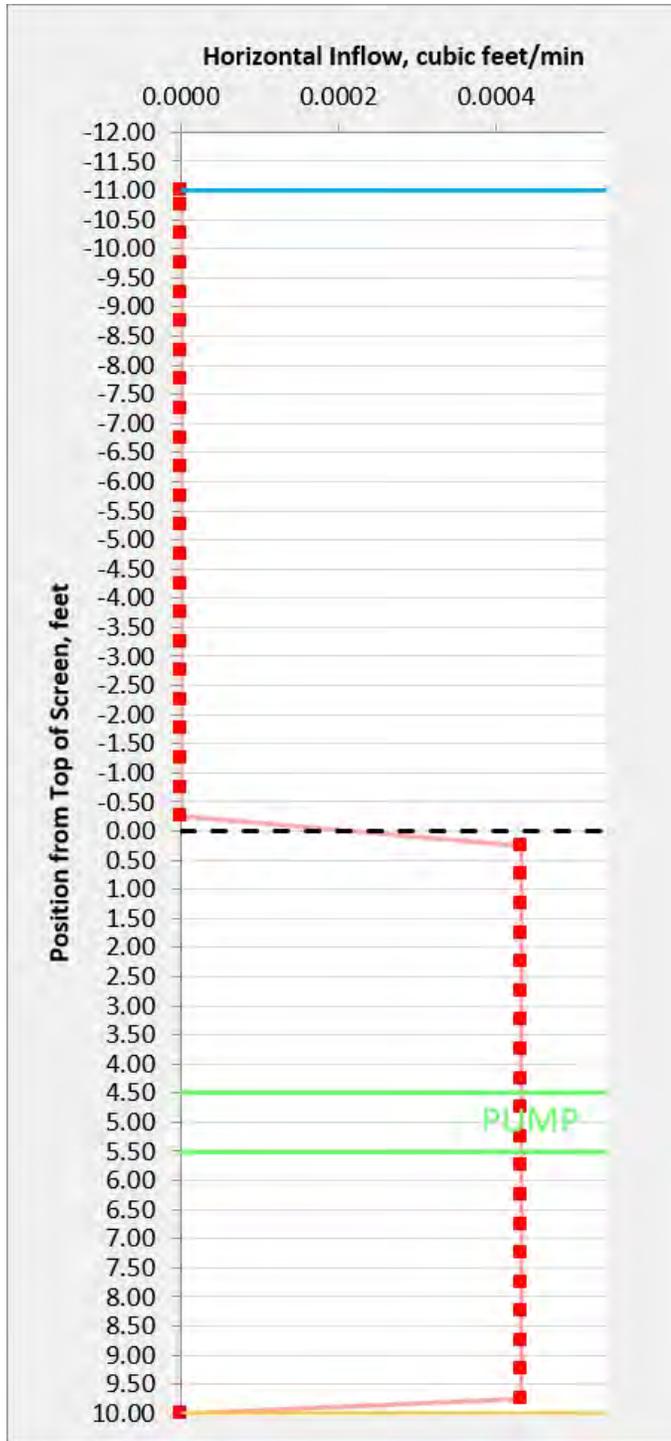


Figure 6. Reproduction of the horizontal radial inflow graph provided on the "Output" worksheet of the Purge Analyzer Tool. Example from a homogeneous condition. Simulated horizontal flow is uniform as denoted by the red dots and line. [cubic feet/min, cubic feet per minute]

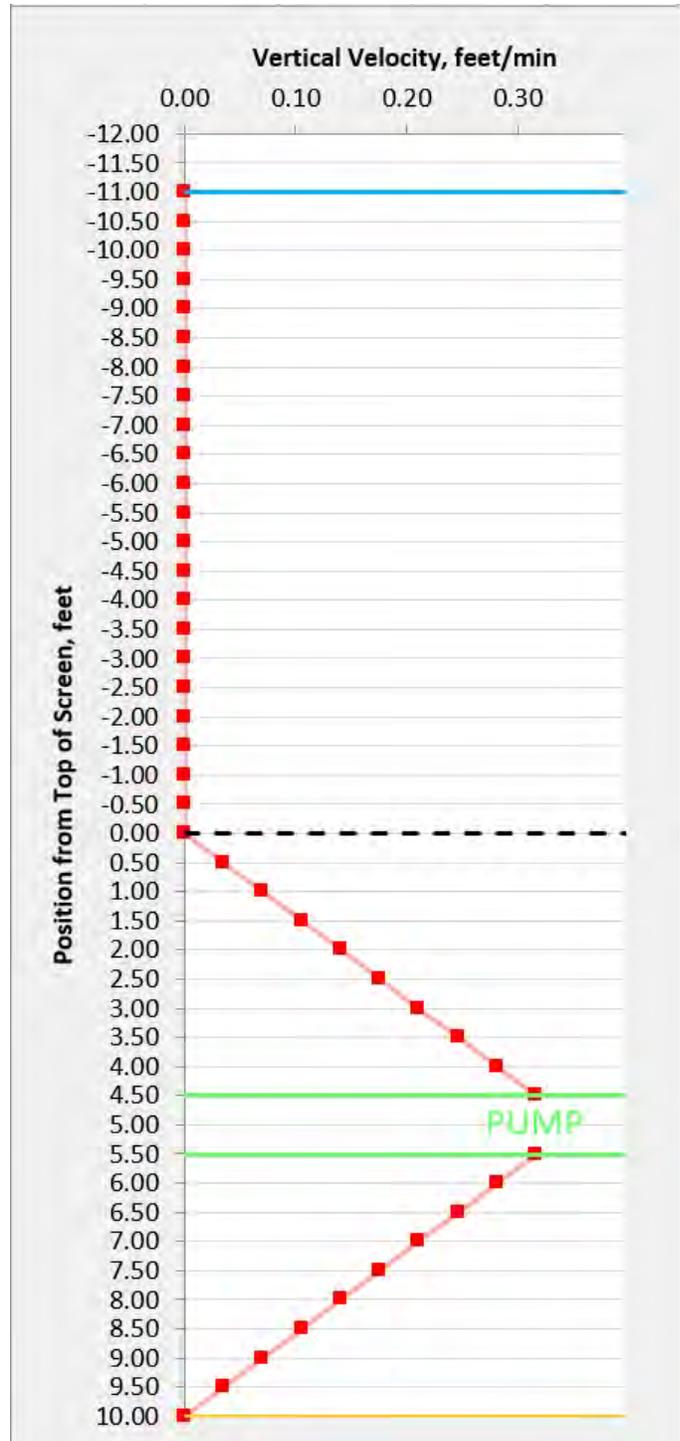


Figure 7. Reproduction of the vertical velocity graph from the "Output" worksheet for the Purge Analyzer Tool. Example from a homogeneous condition where uniform well inflow occurs. Vertical flow (red line) to the mixing zone (parameter M_z ; green line) is symmetric if the pump intake (parameter P_L) is set at the middle of the well opening. [feet/min, feet per minute]

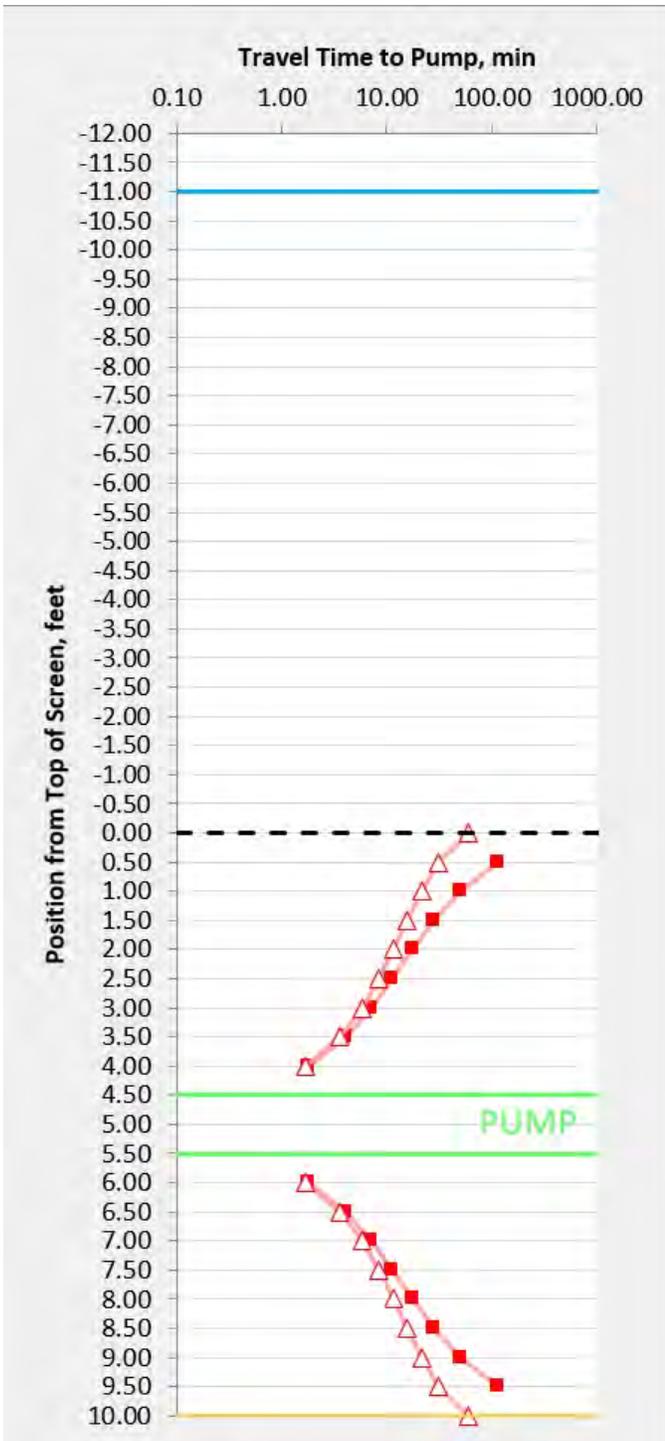


Figure 8. Reproduction of the in-well travel time graph from the "Output" worksheet for the Purge Analyzer Tool. Example from a homogeneous condition and pump intake at the middle of the well opening showing linear velocity and corrected for acceleration. For in-well travel time, the regular linear velocity (solid red square) and velocity corrected for acceleration (open red triangle) are shown for reference. Travel times computed when accounting for acceleration are significantly faster further from the mixing zone (M_z , green line). [min, minute]

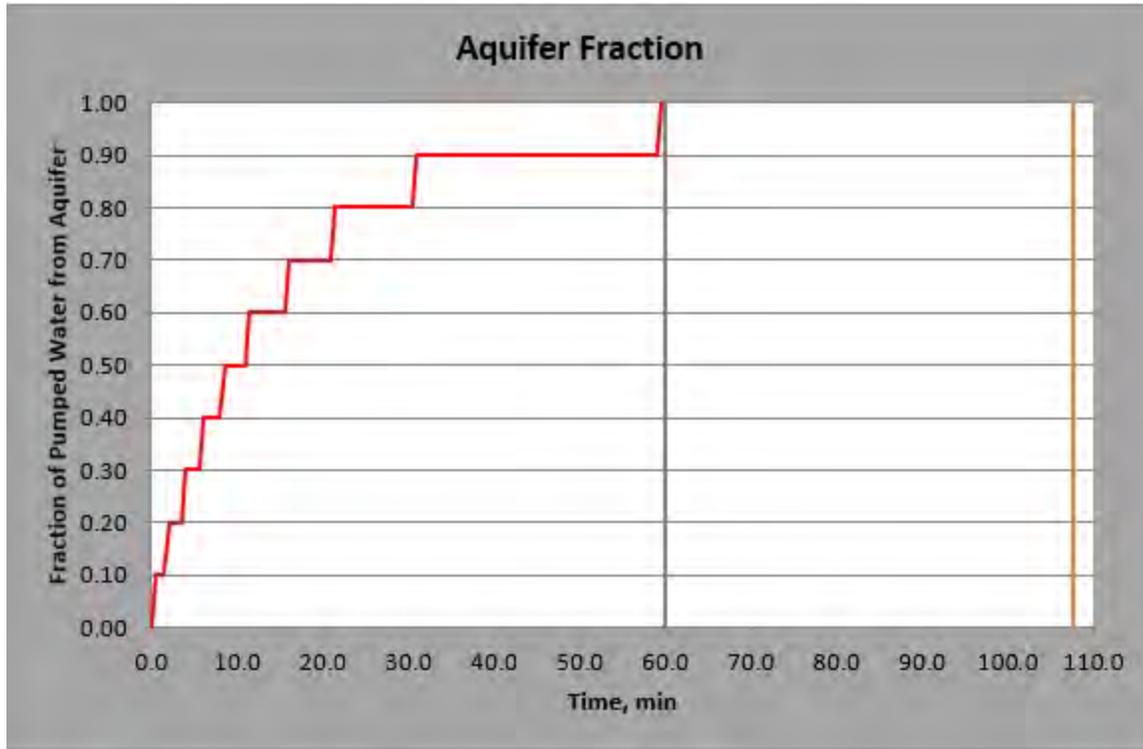


Figure 9. Reproduction of the aquifer fraction graph from the “Output” worksheet for the Purge Analyzer Tool. Example from a homogeneous condition and pump intake at the middle of the well opening. The red line is travel time to pump capture as calculated from the Purge Analyzer Tool, the gray line is the specified purge time, and the solid vertical orange line is the volumetric sample time from the extraction of the equivalent pumped volume of three well casings. [min, minutes]

transport inflow along the entire well opening; in this case at 60 mins (fig. 9). In contrast, the purge time needed to extract three-casing volumes of water is 107 mins (fig. 9). For sample collection purposes, if field parameters stabilize after 60 mins, the PAT indicates a representative sample can be collected anytime afterwards.

Operation

The PAT can be run in reverse (calculation of K_{avg}) or forward mode (user-specified K_{avg}). For the reverse mode, the Excel solver is automated and executed from within the program. Additional information on the subject is discussed in the “Solver” section of the report.

Reverse Mode

Reverse-mode execution is invoked by clicking on the “RUN MODEL” button on the “Input” worksheet. If an HF of 1 is specified, then the program will terminate on the “Output” worksheet, otherwise an intermediate step is involved. In this

step, the PAT active worksheet is moved to the “K-Distribution” worksheet where the distribution of K_{layer} will be defined.

Option 1: Homogeneous (HF = 1)

The PAT brings the user directly to the “Output” worksheet when HF = 1. Each layer’s K_{layer} is set equal to K_{avg} . Regardless of whether homogeneous conditions are simulated, the PAT will display homogeneous conditions (red line) as a reference on the graphs plotted in the “Output” worksheet.

Option 2: Heterogeneous Conditions (HF > 1)

When HF > 1, the PAT takes the user to a worksheet called “K-Distribution.” This intermediate step requires the user to specify a distributional pattern for each K_{layer} assigned to each discretized cell. The range allowed for any K_{layer} is calculated based on the HF entered at the “Input” worksheet, and the calculated K_{avg} for the screen or open interval is also on the “Input” worksheet. The calculations for the allowable values, highest hydraulic conductivity (K_{high}), middle hydraulic conductivity (K_{medium}), and low hydraulic conductivity (K_{low})

are shown in equations 3 and 4. The K_{medium} is allowed to vary by ± 50 percent of the calculated K_{avg} . An example of the “K-Distribution” worksheet is shown in figures 10 and 11.

$$K_{\text{medium}} = \frac{K_{\text{high}} + K_{\text{low}}}{2}, \quad (3)$$

$$K_{\text{high}} = HF * K_{\text{low}} \quad (4)$$

Once at the “K-Distribution” worksheet, the user can select a distribution of K_{layer} from the drop-down menu in cells D2:E2 (fig. 10). Values of K_{layer} are specified in absolute hydraulic conductivity units. There are eight different K_{layer} patterns to select from (oscillating formation, rock fracture at top of well opening, rock fracture at middle of well opening, rock fracture at bottom of well opening, double rock fracture, bimodal formation, trimodal formation, and randomized formation). With a pattern selected, the user must hit the “Populate” button (cells D1:E1, to have K_{layer} pattern automatically designated within the worksheet. It also is possible to specify a user-defined pattern where each layer can be manually entered a value of “L” (K_{low}), “M” (K_{medium}) or “H” (K_{high}) in column A under the heading “K Type.” In this case, the “Populate” button is not invoked. Before continuing with the program, the “Residual” button (“Resolve Error” button) and then the “Done with the Script” button (cells H1:J1) must be invoked. After hitting the “Done with the Script” button, the program continues and ends on the “Output” worksheet.

An example of a populated K_{layer} distribution is shown in figure 11. After the K_{layer} values have been populated or manually entered, the user must click the “Resolve Error” button (cells D3:E3) to minimize the difference between the bulk average of the K_{layer} distribution and K_{avg} computed on the “Input” worksheet. Some variation (up to 10 percent) is allowed between the summation average of the specified K_{layer} and the K_{avg} . This is done to facilitate solution under heterogeneous conditions and from a practical standpoint to acknowledge an appropriate level of precision in the computed K_{layer} . To continue the PAT, the user then hits the “Done! Continue Script” button (cells H4:J5) to complete the task and move to the “Output” worksheet.

Forward Mode

For forward-mode processing, the user specifies the known K_{avg} in cell B14 of the “Input” worksheet. The Q_{H} from the Dupuit-Theim equation is calculated within the associated M_z using K_{avg} and compared against the Q_{p} , to assess if Q_{v} outside M_z can take place. A “NO” is shown in cells B15:C16 of the “Input” worksheet when it is unlikely that Q_{v} in the well is dominant, as discussed in Harte (2017). Note that if the P_{L} is in the casing, Q_{v} is assured. When the solver is invoked (reverse mode), the solver minimizes differences between the Q_{p} , and the combined flow from Q_{H} and Q_{v} . Therefore, for the

reverse mode, the default assumption is some Q_{v} contributes to satisfying Q_{p} .

Solver

The Excel data solver is embedded into the PAT macro and is invoked in reverse mode to reduce the residual (specified in cell B19 in the “Input” worksheet) between Q_{p} , and the summation of Q_{H} and Q_{v} by altering K_{avg} . The lowest K_{avg} value allowed is 0.01 ft per day. Values < 0.01 ft per day are primarily affected by aquifer storage during sampling and the PAT does not calculate aquifer storage.

The generalized reduced gradient nonlinear solver option with forward derivatives is used with a convergence criterion of 0.0001. This method looks at the gradient or slope of the objective function as the input values or decision variables change and determines if an optimum solution is reached when the partial derivatives equal zero. Of the two nonlinear solving methods, generalized reduced gradient nonlinear is the fastest. However, the solution derived from this algorithm is highly dependent on the initial conditions and may not be the global optimum solution. The solver may stop at the local optimum value nearest to the initial conditions, giving the user a solution that may or may not be optimized globally (Engineeringexcel.com, 2018). The user may want to perform repeated simulations of the same purge to evaluate if the same K_{avg} is being obtained for each solution. Calculation of the same K_{avg} would suggest a global solution is being obtained by the solver and not a localized solution.

Under certain cases, a solution may not be reached for cases of excessive drawdown (dewatering of the well screen), dewatering of the M_z , or in the solution of low hydraulic conductivity values of “tight” formations. Reducing the length of M_z may assist in achieving a solution in some cases.

Assumptions and Limitations

There are multiple assumptions and limitations associated with the use of the PAT. The most important limitation is that the PAT assumes steady-state conditions although depletion of well storage is accounted for by adjusting pump rates by the well volume depleted. Users who need simulations of more complex wellbore flow processes should consider the use of numerical models for wellbore flow such as the Multi-Node Well package of MODFLOW (Halford and Hanson, 2002).

Important assumptions of the model include:

1. Confined, steady-state conditions approximate radial flow (Dupuit-Theim equation).
2. The formation adjacent to the well opening is the controlling part of the aquifer contributing water to the well.

10 Running the Analytical Code PAT for Computation of In-Well Time of Travel of Groundwater under Pumping Conditions

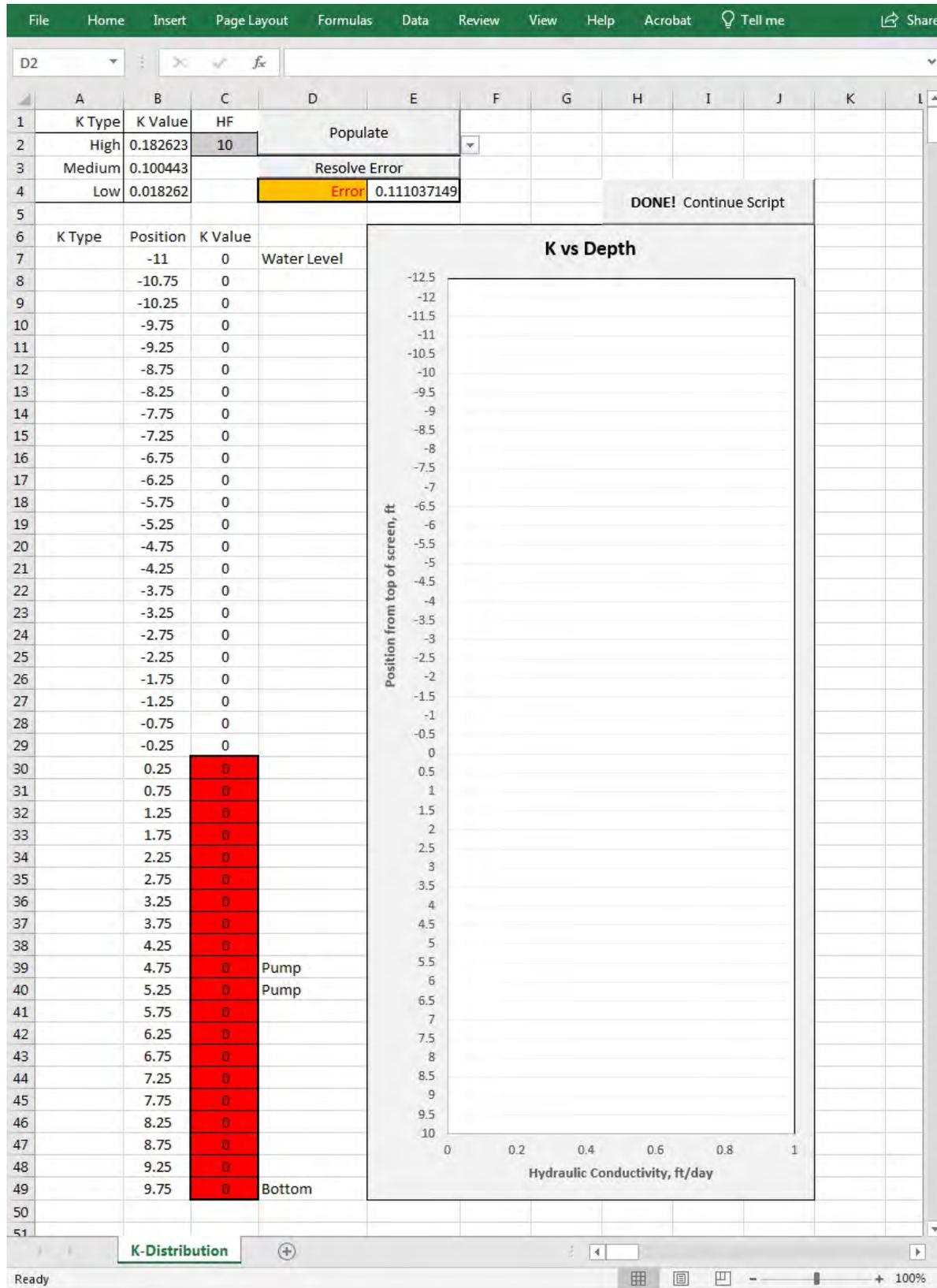


Figure 10. Reproduction of the “K-distribution” worksheet before layer entry for the Purge Analyzer Tool. [HF, heterogeneity factor; ft, feet; ft/day, feet per day]

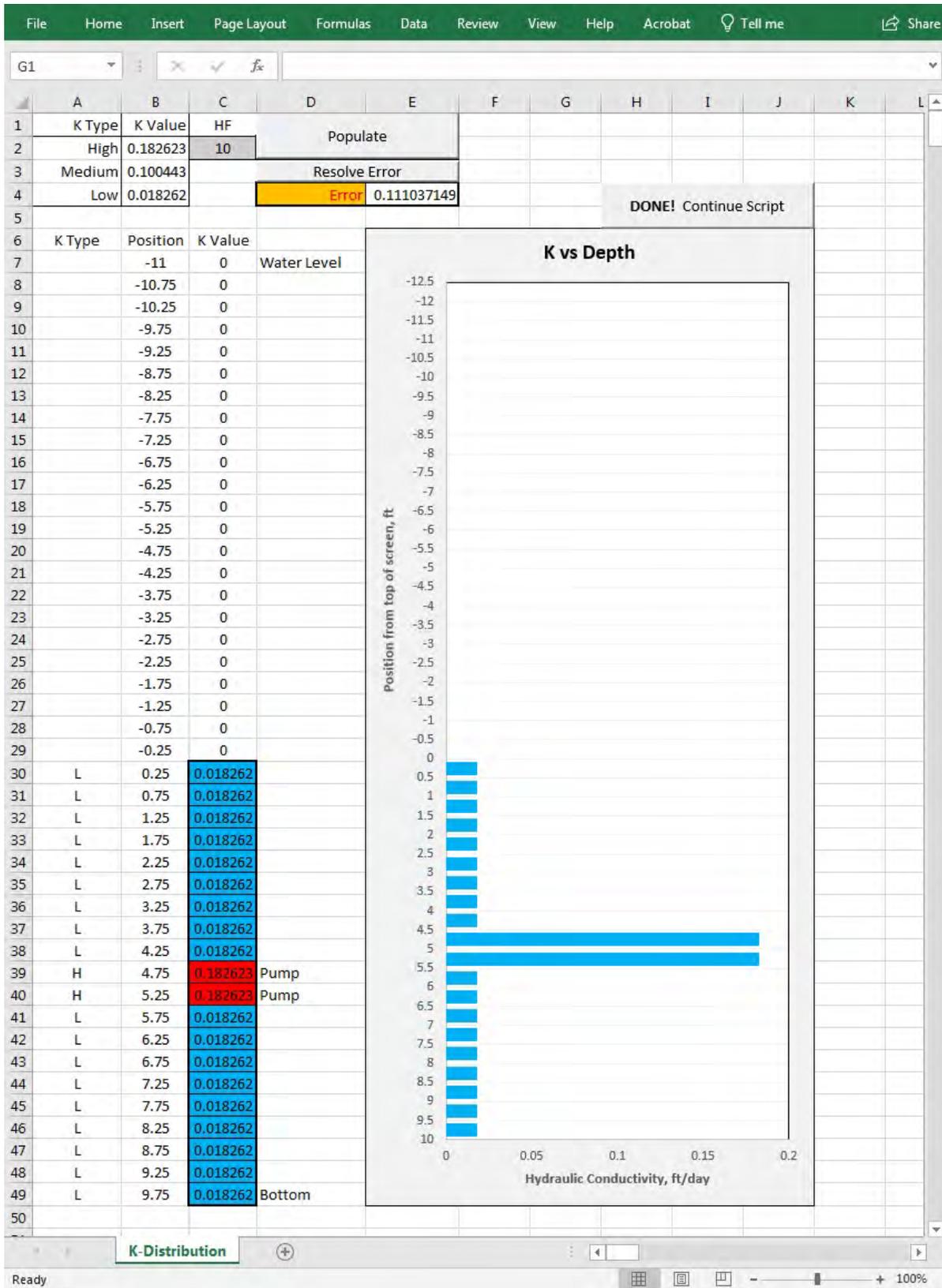


Figure 11. Reproduction of the “K-distribution” worksheet after layer entry using a rock fracture analogy where the fracture exists at the middle of the well opening for the Purge Analyzer Tool. Values are absolute and specified based on relation in equation 3 [HF, heterogeneity factor; ft, feet; ft/day, feet per day]

12 Running the Analytical Code PAT for Computation of In-Well Time of Travel of Groundwater under Pumping Conditions

3. Vertical velocity in the well-screened interval is an average velocity calculated by assuming piston flow (no frictional effects).
4. Horizontal flow into the well from the formation is assumed. Users should know that this may not be the case for many shallow monitoring wells or partially penetrating wells that are affected by converging vertical flow.
5. Flow in the well is vertical toward the pump intake outside M_z .
6. Drawdown (s) in the well is uniform over the well opening.
7. Q_v is calculated by a conservation of mass at each discretized interval.
8. The radius of influence (R_o) is set at 10 feet.
9. Storage (S) contributions from outside the well is assumed negligible.
10. The effects of the sand pack on the horizontal or vertical flow is not accounted for.
11. The well screen or well opening is assumed to be unclogged and not a limiting factor in well inflow.
12. Travel time from the M_z to the pump intake and to the surface via the discharge line is not accounted for but is assumed to be small.
13. In-well flow outside the M_z is laminar.
14. No ambient flow is present.
15. For the reverse mode, Q_v contributes to satisfying pump rate Q_p .

Transient storage effects may be significant in cases where the drawdown (s) takes significant time to stabilize, in which case the analysis will overestimate values of K_{avg} . The impact of formation S on K_{avg} was evaluated by comparing the calculated K_{avg} from the Theis equation, which accounts for aquifer storage, to the calculated K_{avg} from the Dupuit-Theim equation as used by this analytical model (Harte, 2017). For a 1-ft drawdown or less, the effect of S for values of < 0.001 results in a small error (approximately a factor-of-2 difference) in the K_{avg} calculated with this model. As long as the distribution of well inflow remains relatively the same along the screen and S is uniform, effects on the computation of travel time by the PAT should be relatively small.

Another important limitation is the effect of the M_z and pump tubing in extending travel time to the surface where samples are retrieved, as the PAT does not account for these. Travel times could be a factor for $M_z > 3$ ft and discharge lines > 100 ft. In most cases, an M_z of 1 ft will produce a delay of only a couple of minutes. However, a discharge line of 100 ft could delay travel times to the surface by more than 3 mins.

Therefore, as a rule of thumb, samples should be collected after 10 mins of reaching capture criteria indicated by the PAT.

A sand pack is not simulated in the model. For an open borehole, a sand pack is not applicable because it is not used. However, a sand pack for a well screen can affect the distribution of well inflow particularly if it extends beyond the well screen interval. In this case, it will increase radial flow in the adjacent upper or lower interval of the well screen.

Lastly, well clogging can prevent well inflow from layers that may or may not be productive. Where a sand pack is used, the sand pack will redistribute well inflow to other intervals of the well screen that are not clogged. Therefore, the interval receiving redistributed radial well inflow will have water from another layer and not be indicative of water chemistry from that layer. Simulations with PAT will not be able to replicate the redistributed well inflow.

Applications

With little information besides well construction, anticipated P_L , and pumping rates, the effect of various levels of heterogeneity can be assessed on in-well flow and time of travel during sampling. Table 1.1 and figure 1.1 illustrate differences between homogeneous and heterogeneous conditions for a hypothesized case of a single fracture in a rock well where the fracture is positioned at different locations (intersections) in the well opening. For the simulations shown, the P_L is located at 2 ft below the top of the casing and within a 10-ft well opening using the input parameters from figure 2 of this report. The homogeneous case shows a smoother transition of aquifer capture. For the heterogeneous cases that simulate a single fracture 100 times the hydraulic conductivity of the rock matrix (nonfractured part of rock), the distance between the P_L and fracture location dominates in-well flow and travel times. A one-order-of-magnitude difference (10 to 100 mins) in arrival time of flow from the fracture, as indicated by the first steep rise on the aquifer fracture graph, occurs when the fracture is located at opposing ends of the well opening (top or bottom of well opening). The tails are a product of the small inflow from the rock matrix, and the spikes represent the large inflow from the fracture. Placing the P_L in the well casing will exacerbate this difference and increase differences in capture times.

Based on fracture location, an elongated tail may occur between 90 to 100 percent capture or 0 to 10 percent capture depending on the P_L (appendix 1). When the fracture is located at the bottom of the well opening (appendix 1), the initial percent capture of water is small, increasing slowly until the water contributed by the fracture reaches the pump intake (approximately at 90 min) ramping the percent capture to 90 to 100 percent almost immediately; under this case there is no elongated tail at the end. This sequence of percent capture is flipped when the fracture is located at the top of the well opening (appendix 1). Following the start of capture of water

from the fracture (appendix 1; >10-min mark), an elongated tail ensues between 90–100 percent capture time from the contribution of flow from the rock matrix. For all practical purposes, stabilization of physicochemical characteristics of water quality would likely occur at the 90 percent capture mark. Other application examples are provided in appendixes 2 and 3. In appendix 2, an example showing the application of assigning heterogeneity in the simulation based on a lithologic log is included. In appendix 3, an example showing the effect of well construction on travel times and aquifer capture is provided.

Summary

The Purge Analyzer Tool (PAT) can be used to help guide sample considerations (pump location, rate, and time) needed to help collect representative groundwater samples from wells. The criteria used to assess sample representativeness is the time needed to complete flushing of the well opening by allowing sufficient piston transport time for groundwater originating from the well opening to reach the pump intake. Prior to that time, pumped water is a combination of well water in storage and recent inflow from the aquifer. In reality, sample representativeness is a subjective term dependent on study objectives. Therefore, the greatest utility of PAT may be the insight gained into the nature of time-varying capture of purged water and how that may relate to targeted sample volumes. The PAT can be used also to assess the sensitivity of aquifer capture of groundwater sampling networks to factors such as heterogeneity; providing a new variable in the assessment of water chemistry results. Users should be fully aware of the limitations and assumptions incorporated into the PAT including the assumption of steady-state flow although well storage depletion is accounted for by adjusting the pump rate.

Historically, confirmation of sample representativeness for low-flow sampling and volumetric extracted sampling (Barcelona and others, 1994) has depended on stabilization of drawdown and stabilization of physicochemical water quality characteristics such as specific conductance and water temperature. The PAT offers another method to assess capture by coupling arrival time of sample water to the pump intake to the stabilization of physicochemical water quality characteristics. In cases where contemporaneous stabilization and arrival times (as demonstrated in capture graphs) are noted, physicochemical stabilization can be confirmed, thereby avoiding premature sampling based on temporary periods of stabilization. In cases where they are not contemporaneous, the differences in time can be assessed to help evaluate whether further purging may be required given sampling objectives.

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Appendixes 1–3

Appendix 1. Solution Examples using Purge Analyzer Tool

The effect of P_L and M_z on simulated travel times is presented in this section. Both parameters affect hydraulic controls on flow and time of travel. Also, in this section, the effect of formation heterogeneity on travel times is illustrated for a simple case of a single fracture in competent rock intersecting the well at different depths.

Effect of the mixing zone (M_z)

Table 1.1 summarizes the range of travel times for well and hydraulic conditions noted in figure 1 while adjusting values for two parameters: (1) the placement of the pump intake (P_L) and (2) size of the mixing zone (M_z). Capture times are sensitive to both parameters as denoted by the time to achieve 100 percent capture. For example, a pump intake set in the casing ($P_L < 0$) will increase travel times by over 8 minutes. Additionally, a larger M_z will decrease computed travel times by 1.5 minutes because vertical travel is determined up to the boundary of M_z .

Effect of Heterogeneity

This section includes an example of the effect of fracture position relative to P_L on travel times and the amount of aquifer fraction captured during pumping. While steady-state flow is assumed for these simulations, transport is transient, and the amount of aquifer capture varies until equilibrium is reached as measured by the arrival time of the most distant intervals of formation water. The shape of the aquifer capture curves provides insight into the proximity of the fracture relative to the P_L (fig. 1.1).

Table 1.1. Effect of pump location (P_L), mixing zone (M_z), and horizontal flow (Q_H) on travel times. [ft³/min, cubic feet per minute; ft, feet]

Simulation number	Q_p^8 (ft ³ /min)	$Q_p'^9$ (ft ³ /min)	s^1 (ft)	L_s^4 (ft)	L_{cw}^2 (ft)	P_L^6 (ft)	Q_H^7 (ft ³ /min)	$1/2M_z^5$ (ft)	L_T^3 (ft)	100-percent capture time (minutes)
1	0.0106	0.0085	10	10	11	-3	0	1.5	0.25	83.5
2	0.0106	0.0085	10	10	11	-3	0	0.5	0.25	85
3	0.0106	0.0085	10	10	11	-1	0	0.5	0.25	82
4	0.0106	0.0085	10	10	11	2	0.0008	0.5	0.25	76.5
5	0.0106	0.0085	10	10	11	5	0.0008	0.5	0.25	69
6	0.0106	0.0085	10	10	11	5	0.0017	1.5	0.25	60.5
7	0.0106	0.0085	10	10	11	8	0.0008	0.5	0.25	76.5

- ¹s Drawdown
- ² L_{cw} Length (height) of casing water under pumping conditions above top of well opening, ft
- ³ L_T Cell thickness or layering used to calculate radial inflow and in-well flow, ft
- ⁴ L_s Length of screen or open interval, ft
- ⁵ M_z Mixing zone of pump, ft
- ⁶ P_L Pump location relative to top of screen or open interval, ft
- ⁷ Q_H Horizontal radial flow within the M_z , ft³/min
- ⁸ Q_p Average pumping rate, L/min
- ⁹ Q_p' Adjusted average pumping rate that accounts for well storage (Q_w), ft³/min

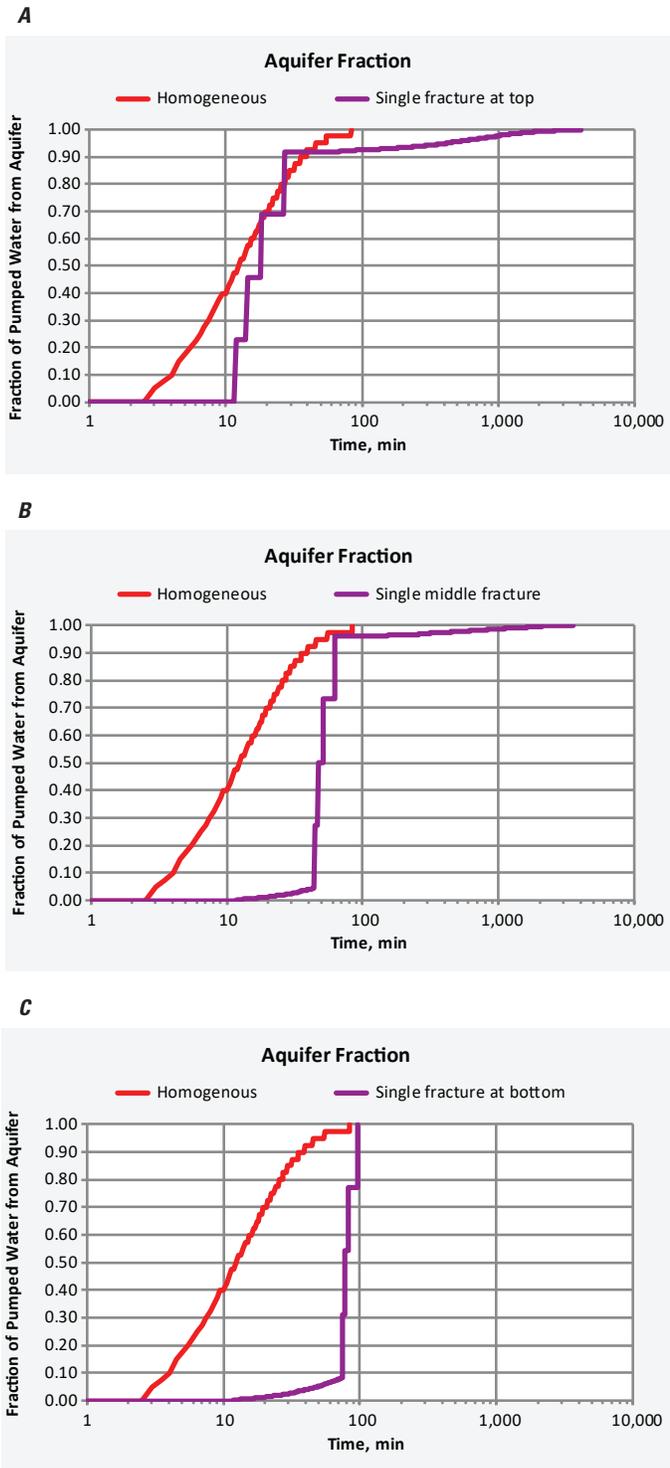


Figure 1.1. Graphs showing effect of heterogeneity on amount of pumped water captured from the aquifer (aquifer fraction capture) for *A*, fracture at top of well opening, *B*, fracture at middle of well opening, and *C*, fracture at bottom of well opening. [min, minutes; Pump position is at 2 feet below the top of the well opening]

Appendix 2. Incorporation of Stratigraphic Information in Simulation

While appendix 1 included simulation examples of hypothetical conditions, appendix 2 (and 3) include examples of actual field data from sites. Appendix 2 includes an example of a lithologic log from a monitoring well at the Longhorn Army Ammunition Plant in Karnack, Texas (AECOM Technical Services, Inc., 2015), and the simulated output from a bimodal hydraulic conductivity distribution that was informed by the log (figs. 2.1 and 2.2). The upper part of the well screen was simulated with a relatively low hydraulic conductivity and the underlying unit was simulated with a high hydraulic conductivity to match the stratigraphic pattern from the log.

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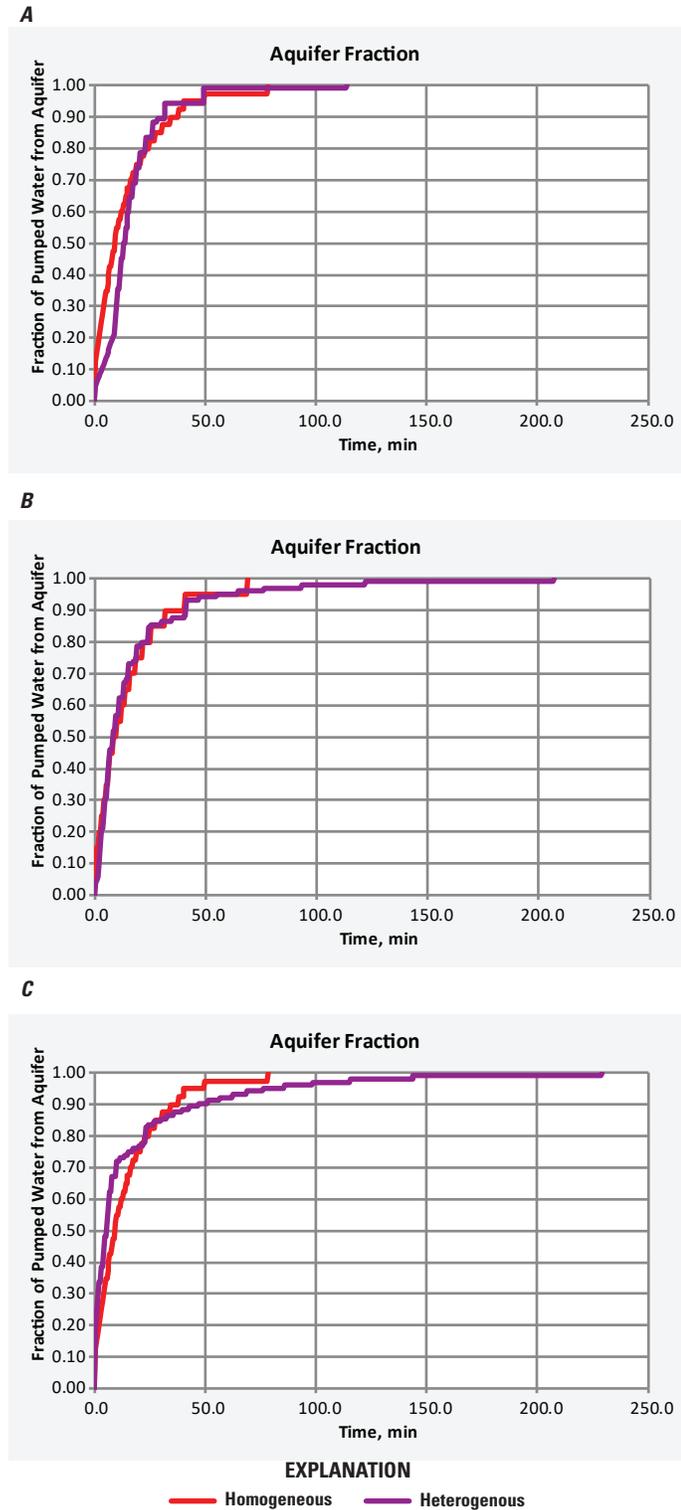


Figure 2.2. Aquifer fraction captured while pumping for monitoring well 18CPTMW18 with a simulated bimodal hydraulic conductivity distribution at a factor of 5 between low (top of screen) and high (bottom of screen) K_{Layer} where pump position was placed at *A*, 1 foot below top of opening, *B*, 5 feet below top of opening, and *C*, 9-ft below top of opening. [K_{Layer} , hydraulic conductivity of modeled layers; min, minutes]

Appendix 3. Additional Examples of Input and Output

Appendix 3 includes input and output example of a homogeneous condition for two monitoring wells located in New Mexico near the Homestake Superfund site (Harte and others, 2019). Whereas the formation at both wells have similar K_{avg} , the differences in well diameter and length of screen affects capture times (figs. 3.1 and 3.2). The time to achieve 90 percent aquifer capture is much quicker for well ND (fig. 3.1) than for well DD2 (fig. 3.2) because of the longer screen interval for well DD2.

References Cited

Harte, P.T., Blake, J.M., Thomas, J.V., and Becher, K.D., 2019, Identifying natural and anthropogenic variability of uranium at the well scale, Homestake Superfund site, near Milan, New Mexico, USA: *Environmental Earth Science*, v. 78, p. 95, <https://doi.org/10.1007/s12665-019-8049-y>.

Initial Inputs & Calculations		
Input Parameters	Inputs	Units
Well Name	ND	
Date (mm/dd/yyyy)	10/6/2016	
Depth to Water below reference, DTW	38.93	ft
Depth to Top of Screen below reference, DTS	52	ft
Length of Screen, L_s	20	ft
Well Diameter, D_{well}	4	inches
Actual or Anticipated purging time, t_{purge}	65	min
Averaged Purge Rate, Q_p	6.064	L/min
Drawdown, s	1.72	ft
Heterogeneity Factor, HF (1=Homogeneous)	1.00	Dimensionless
Hydraulic Conductivity, K_{avg}	5.7785	ft/day

Program Variables	Inputs	Units
Pump Location relative to top of screen (Above screen specify negative number for absolute distance), P_L	-2	ft
1/2 Mixing Zone Buffer length above/below pump intake, 1/2 M_z	0.5	ft
Cell Thickness of layers to compute horizontal radial flow, L_T	0.5	ft
Time interval (dt) for computation of flow and Aquifer Fraction graph	0.5	min

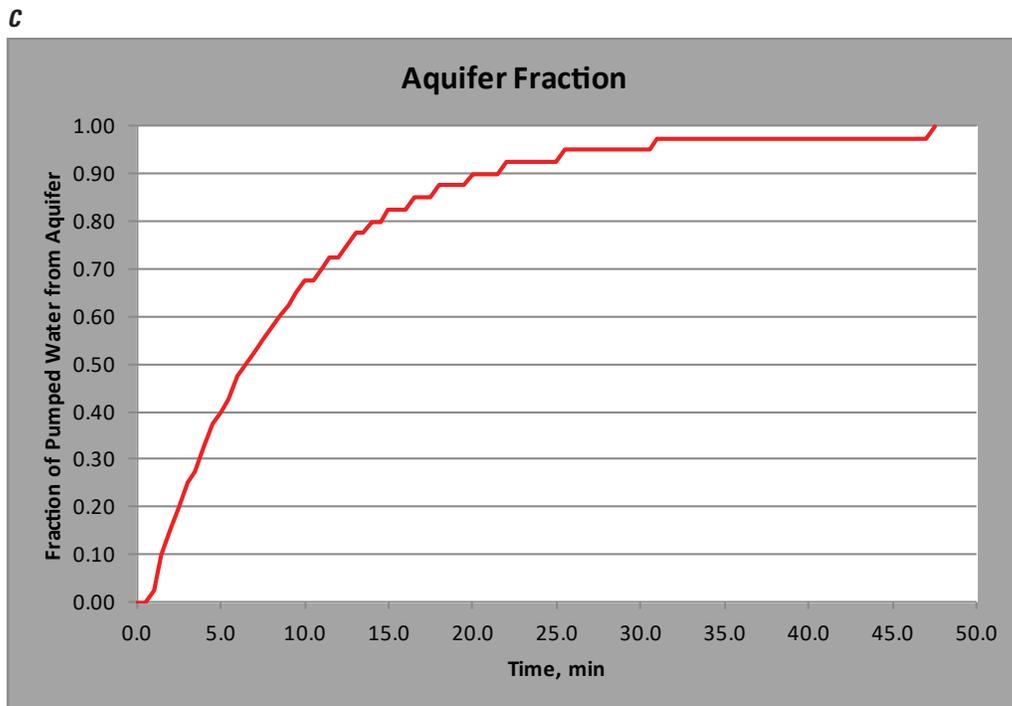


Figure 3.1. Reproduction of A, input parameters, B, model simulation parameters, and C, aquifer fraction captured while pumping for monitoring well ND in New Mexico under homogeneous conditions. [90 percent capture is at 21 minutes; ft, feet; min, minutes; L/min, liters per minute]

A

Initial Inputs & Calculations		
Input Parameters	Inputs	Units
Well Name	DD2	
Date (mm/dd/yyyy)	10/7/2016	Units
Depth to Water below reference, DTW	45.26	ft
Depth to Top of Screen below reference, DTS	50	ft
Length of Screen, L_s	40	ft
Well Diameter, D_{well}	5	inches
Actual or Anticipated purging time, t_{purge}	138	min
Averaged Purge Rate, Q_p	6.06	L/min
Drawdown, s	0.91	ft
Heterogeneity Factor, HF (1=Homogeneous)	1.00	Dimensi onless
Hydraulic Conductivity, K_{avg}	5.1943	ft/day

B

Program Variables	Inputs	Units
Pump Location relative to top of screen (Above screen specify negative number for absolute distance), P_L	-2	ft
1/2 Mixing Zone Buffer length above/below pump intake, 1/2 M_z	0.5	ft
Cell Thickness of layers to compute horizontal radial flow, L_r	0.5	ft
Time interval (dt) for computation of flow and Aquifer Fraction graph	0.5	min

C

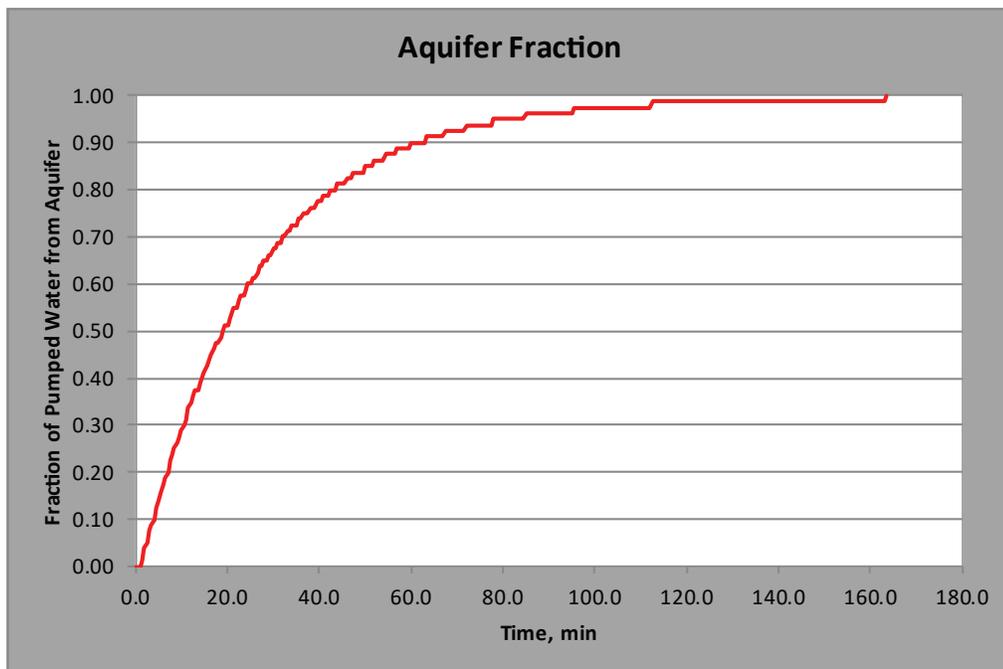


Figure 3.2. Reproduction of A, input parameters, B, model simulation parameters, and C, aquifer fraction captured while pumping for monitoring well DD2 in New Mexico under homogeneous conditions. [90 percent capture is at 63 minutes; feet, min, minutes; L/min, liters per minute]

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