Groundwater

Educational Webtool Illustrating Groundwater Age Effects on Contaminant Trends in Wells

J.K. Böhlke[1], Bryant C. Jurgens[2], David J. Uselmann[3], and Sandra M. Eberts[4]

Trends in concentrations of nonpoint-source contaminants in wells, springs, and streams are related to the history of contamination in groundwater recharge and the age distribution in the groundwater discharge. The age distribution in discharge depends on the groundwater age distribution in the aquifer and the subset of flowpaths that are sampled by the discharge. Groundwater travel times from recharge to discharge are variable; consequently, responses at discharge locations to changing contaminant loading in recharge can include delayed initial responses, dilution of peak concentrations, and prolonged flushing times. These effects are well understood in principle and have important consequences for water resource management (Eberts et al. 2013), but their implications may not be easy to visualize or communicate.

Here we introduce GAMACTT: Groundwater Age Mixtures and Contaminant Trends Tool (Version 1)—an interactive webtool that can be used to explore the effects of basic aquifer properties (saturated thickness, porosity, and recharge rate) and well configurations (tops and bottoms of screened intervals) on groundwater age mixtures in groundwater discharge and on contaminant trends from varying nonpoint-source contaminant input scenarios. The webtool is based on the concept of groundwater stratigraphy whereby changes in contaminant concentrations in recharge may be recorded as a vertical concentration gradient in the aquifer that is related to groundwater age (Cook and Böhlke 2000). The webtool provides a groundwater stratigraphy model that derives age distributions for wells from well construction data by using a partial exponential model (PEM) (Jurgens et al. 2012). By varying the webtool input data (basic aquifer properties, well configuration, contaminant input scenario, and contaminant decay), users can explore concepts such as delays (lag times), dilution factors, and flushing times in hypothetical wells responding to changing contamination of surficial aquifers. In some configurations, results may be applicable to contaminant trends in discharge to surface water bodies like springs and streams. The webtool also illustrates spatial relations between wells and their contributing recharge areas, which are important considerations for point-source and nonpoint-source contaminants.

Important limitations of this webtool include: (1) groundwater model does not include transport through the unsaturated zone; (2) basic aquifer properties do not account for aquifer heterogeneity, flow discontinuities, or dispersion; (3) steady-state model by definition does not provide for transient flow conditions; (4) PEM assumes that the groundwater flow system is not perturbed by pumping or wellbore flow; (5) first-order contaminant degradation model may not be appropriate for some biogeochemical reactions. The webtool is not intended to be used as a prediction tool for real-world applications. Rather, it is presented as an illustrative (educational) tool that enables scientists, hydrogeology professionals, educators, and other interested persons to explore, understand, visualize, and explain various processes affecting how public-supply wells respond to groundwater contamination. The webtool is freely available and can be accessed at ~~http://cida.usgs.gov/gamactt/.~~

http://ca.water.usgs.gov/projects/gamactt/

Acknowledgments

The authors are grateful for useful comments from USGS colleague Bruce Lindsey and three anonymous reviewers. Support for this project was provided by the USGS National Water Quality Assessment Program,

[1]Corresponding author: U.S. Geological Survey, National Research Program, 431 National Center, Reston, VA 20192; 703-648-6325; jkbohlke@usgs.gov
[2]U.S. Geological Survey, California Water Science Center, Sacramento, CA 95819.
[3]U.S. Geological Survey, Center for Integrated Data Analytics, Middleton, WI 53562.
[4]U.S. Geological Survey, Ohio Water Science Center, Columbus, OH 43229.

doi: 10.1111/gwat.12261

the USGS Center for Integrated Data Analytics, and the USGS National Research Program.

Disclaimer

Although this software program has been used by the U.S. Geological Survey (USGS), no warranty, expressed or implied, is made by the USGS or the U.S. Government as to the accuracy and functioning of the program and related program material nor shall the fact of distribution constitute any such warranty, and no responsibility is assumed by the USGS in connection therewith. Any use of trade, product, or firm names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

Supporting Information

Additional Supporting Information may be found in the online version of this article:

Figure S1. Screen capture of webtool showing input data, output data, and graphic panels.
Figure S2. Model responses of various well configurations to a simple rectangular contaminant input record, illustrating differences in initial response time (delay), flushing time, and peak concentration.
Figure S3. Model responses of whole aquifer discharge (e.g., fully penetrating well, spring, or stream discharge) to various contaminant input scenarios, with and without degradation.
Appendix S1. Description of webtool including example applications (with figures).

References

Cook, P.G., and J.K. Böhlke. 2000. Determining timescales for groundwater flow and solute transport. In *Environmental Tracers in Subsurface Hydrology*, ed. P.G. Cook and A.L. Herczeg, 1–30. Boston, Massachusetts: Kluwer Academic Publishers.

Eberts, S.M., M.A. Thomas, and M.L. Jagucki. 2013. The quality of our Nation's waters: Factors affecting public-supply-well vulnerability to contamination: Understanding observed water quality and anticipating future water quality. Reston, Virginia: U.S. Geological Survey Circular 1385.

Jurgens, B.C., J.K. Böhlke, and S.M. Eberts. 2012. TracerLPM (Version 1): An Excel® workbook for interpreting groundwater age distributions from environmental tracer data. U.S. Geological Survey Techniques and Methods Report 4-F3.

Supporting information for
"Educational webtool illustrating groundwater age effects on contaminant trends in wells"

by J.K. Böhlke[1], B.C. Jurgens[2], D.J. Uselmann[3], and S.M. Eberts[4]

[1] Corresponding author: U.S. Geological Survey, National Research Program, 431 National Center, Reston, VA 20192; 703-648-6325; jkbohlke@usgs.gov

[2] U.S. Geological Survey, California Water Science Center, Sacramento, CA 95819

[3] U.S. Geological Survey, Center for Integrated Data Analytics, Middleton, WI 53562

[4] U.S. Geological Survey, Ohio Water Science Center, Columbus, OH 43229

Groundwater (2014)

Appendix S1. Description of webtool including example applications (with figures).

[plus minor formatting corrections, 20140926]

Appendix S1. Description of webtool including example applications (with figures)

Abstract

Trends in concentrations of nonpoint-source contaminants in wells, springs, and streams are related to the history of contamination in groundwater recharge and the age distribution in the groundwater discharge. The age distribution in discharge depends on the groundwater age distribution in the aquifer and the subset of flowpaths that are sampled by the discharge. Groundwater travel times from recharge to discharge are variable; consequently, responses at discharge locations to changing contaminant loading in recharge can include delayed initial responses, dilution of peak concentrations, and prolonged flushing times. These effects are well understood in principle and have important consequences for water resource management, but their implications may not be easy to visualize or communicate. Here we describe GAMACTT: Groundwater Age Mixtures and Contaminant Trends Tool (Version 1), a new web-based interactive tool with which users can specify basic aquifer properties, well configurations, and nonpoint-source contamination input records, to explore their effects on contamination trends in groundwater discharge. Age distributions in wells are derived from well construction data using a "partial exponential model". The webtool includes a drag-and-drop feature for adjusting the vertical dimensions of a well, accompanied by real-time graphic outputs showing the groundwater age distribution and contaminant history (or future) of the well. Another drag-and-drop feature can be used to illustrate contaminant concentrations in the aquifer and well at various selected times. Though operation of the webtool involves simplistic assumptions that are likely to be violated to varying degrees in the real world, it should assist scientists, hydrogeology professionals, educators and other interested persons in exploring, understanding, visualizing, and explaining processes affecting how water-supply wells and other aquifer discharges respond to groundwater contamination.

Introduction

Water supplies and aquatic ecosystems commonly are maintained by groundwater, which can be subjected to wide-spread (nonpoint-source) contamination. Nonpoint-source contaminant concentrations in recharging groundwater can change over a range of time scales including inter-annual, decadal, and longer. Groundwater travel times can range over similar time scales and commonly are related to depth. Because groundwater discharge is a mixture of water that entered the aquifer at different times and places, the concentration of a contaminant is a function of the aquifer hydrology, the placement of the well within the aquifer, the record of contaminant input over time, and the date of sampling. Therefore, contaminant concentrations in groundwater discharging to wells, springs, and streams commonly are different from contemporaneous concentrations in recharging groundwater, and contaminant trends in recharge and discharge can appear to be poorly related, even in the absence of natural attenuation (Gelhar and Wilson 1974; Zuber 1986; Duffy and Lee 1992; Böhlke and Denver 1995; Zoellmann et al. 2001; Kauffman et al. 2001; Böhlke 2002; Burt et al. 2008; Sanford and Pope 2013).

Groundwater contamination is more likely to be near steady state (i.e., input = output) if contamination in recharge has been constant for a long time or if travel times through the aquifer are short. Groundwater contamination is more likely to be changing (input and output not the same) if contamination in recharge has changed recently or if travel times are comparatively long. Non-steady state situations can exhibit various trends, such as discharge concentrations rising while recharge concentrations are falling and vice versa. This is an important consideration for resource management because changes in contaminant sources may not produce immediate proportional effects at discharge locations.

In a simple hypothetical system, a nonpoint-source contaminant enters the groundwater system evenly across the water table in recharge and can be traced as it moves downward within the aquifer. Changes in contaminant concentrations in recharge may be recorded in surficial (water-table) aquifers as vertical concentration gradients that are related to groundwater age, giving rise to "groundwater stratigraphy" (Cook and Böhlke 2000). A common example of this is nitrate (NO_3^-), whose concentration in recharge in many areas of the world has changed on decadal time scales because of land use change and changes in agricultural practices such as nitrogen fertilizer application rates. Studies have shown many aquifers underlying agricultural land contain transient groundwater records of nitrate contamination spanning years to decades (Böhlke and Denver 1995; Böhlke et al. 2002; Dubrovsky et al. 2010; Liao et al. 2012).

The Groundwater Age Mixtures and Contaminant Trends Tool (GAMACTT, Version 1), is a new interactive web-based educational tool (webtool) designed to illustrate how contaminant trends in groundwater discharge can be affected by transient inputs and groundwater age mixtures. The webtool is based on the concept of groundwater stratigraphy, in which recharge to the groundwater system forms layers across the water table that push preceding layers downward into the aquifer and laterally through the aquifer in the downgradient direction toward a discharge area such as a stream. In the simplest case, a well placed in such a flow system can exhibit various contaminant concentration trends that depend on at least 4 major factors: (1) properties of the aquifer affecting groundwater flow and residence time, such as volume and recharge rate; (2) position of the well screen (open interval) within the aquifer; (3) contaminant concentration history in recharge; and (4) degradation rate of the contaminant.

Overview of the webtool

The webtool aims to demonstrate how the history of contamination in groundwater recharge, combined with the age distribution of groundwater entering a well, can affect the history (and future) of contamination in the well. The webtool provides a groundwater stratigraphy model, a well with a variable open (screened) interval, adjustable contaminant input scenarios, and an option for contaminant decay. The webtool workspace includes a set of input/output data boxes and 6 graphic panels illustrating results (Figure S1). The output data and graphic panels are linked and respond simultaneously to changes in input data made by the user. To facilitate user interaction, there are two sets of drag-and-drop features with which the user can manipulate selected parameters. Graphical output shows the groundwater flow system and vertical age profile in the aquifer, incremental and cumulative age distributions in the well, contaminant trends in recharge and discharge, and spatial relations between contaminant concentrations in the aquifer and well at any given time. Input parameters and figure panels are organized to emphasize progressive stages in the application of the webtool focusing on properties of the aquifer, the well, and the contaminant, respectively.

Groundwater model and aquifer properties

The groundwater stratigraphy model used for this webtool yields an exponential distribution of groundwater ages in the aquifer (Vogel 1967; Strack 1984; Cook and Böhlke 2000). This is a consequence of several assumptions, including: (1) The top and bottom of the water-filled portion of the aquifer are parallel (i.e., the aquifer has constant thickness within the saturated zone); (2) recharge is uniform across the top of the saturated zone; (3) discharge occurs from the whole thickness of the aquifer at the downgradient end (e.g., could be a stream or spring); (4) aquifer properties such as porosity and permeability are uniform; (5) groundwater does not mix vertically within the aquifer but remains stratified, with the more recently recharged layers on top. Normally, for groundwater flow to occur in a surficial (water-table) aquifer, there must be some difference in the elevation of the water table across the flow system, but that difference may be small in comparison to the thickness of the aquifer. Likewise, there must be some width to the area of discharge, but that may be small in comparison to the horizontal dimension of the aquifer. There are many aquifers for which this model would be inappropriate (see Limitations), and none of these assumptions is ever perfectly justified; nevertheless, many aquifers in unconsolidated sedimentary geologic units in humid to semi-arid climate regions can be described approximately by the exponential model. More information about the groundwater stratigraphy model is given in an Addendum (Equations).

To explore implications of the groundwater stratigraphy model, parameter values for vertical and horizontal aquifer dimensions, porosity, and recharge rate are entered by the user in aquifer property boxes in the upper left area of the webtool workspace (Figure S1). Thickness, porosity, and recharge rate define the mean age of water in the modeled aquifer, which is given in an output data list. There is flexibility in the scale of the model; the current version has a minimum resolution of the order of months to years and maximum age span of the order of 10^5 years.

The aquifer cross-section graphic (Figure S1A) shows idealized groundwater flow paths in a 2-dimensional vertical section of the aquifer (blue lines with arrow heads showing direction of flow). The top of the figure panel represents the water table (top of the saturated zone) where recharge occurs at a constant rate. The bottom of the panel is the bottom of the aquifer, representing a confining unit that does not permit vertical flow. On the left is a groundwater divide in the recharge area, which is considered to be a no-flow boundary. On the right is a groundwater discharge area, where all flow paths converge and turn upward toward a spring, stream, or other surface-water body. To accommodate recharge across the top of the aquifer and discharge from the right side of the aquifer in Figure S1A, the vertical component of groundwater velocity decreases downward and the horizontal component of groundwater velocity increases to the right. The configuration of flow paths shows that shallow groundwater at any observation point in the aquifer is likely to have infiltrated and recharged nearby, whereas deep groundwater may have recharged far away (large horizontal distance) from the observation point.

The age profile graphic (Figure S1B) shows the vertical variation of groundwater age in the model aquifer (blue curve). Given the assumptions and approximations listed above, the vertical age profile does not depend on the horizontal position in the aquifer; water of a given age will occur approximately at the same depth everywhere; that is, groundwater age contours (isochrons) are essentially horizontal. Because the vertical component of velocity decreases downward, isochrons deeper in the aquifer are closer together.

Varying the aquifer parameter values (thickness, porosity, and recharge rate) will not change the overall patterns in the orientation of groundwater flow lines or the vertical age profile, but it will change the magnitudes of groundwater ages in the profile. Switching from metric to English distance units will have no effect on the calculations, but this option is provided for users with different preferences. Varying the horizontal dimension of the aquifer will have no effect on the vertical profile or the calculations, but it can be done to illustrate flow paths and distances from contributing recharge areas to various observation points within a surficial aquifer.

Well configuration

The well configuration determines what portions of the groundwater flow system will be represented in water collected from the well. Wells can be open to flow (perforated or screened) over small or large intervals of the aquifer, depending on local conditions and requirements. In the simple model used here, it is assumed that pumping does not disturb the groundwater flow system, and that groundwater flows evenly into the well over the length of the open interval, where it mixes to form a representative sample of the part of the aquifer intersected by the open interval of the well. Shallower open intervals will sample younger groundwater and deeper open intervals will sample older groundwater. Groundwater entering a well with a small open interval will tend to have relatively uniform age, whereas groundwater entering a well with a long open interval will have a large range of ages (age span). Also, because isochrons are more closely spaced deeper in the aquifer, samples from a deeper well with a specific open interval length will have a larger age span than samples from a shallower well with a similar open interval length.

To explore these principles, the position of the top and bottom of the open interval of the well in the model can be changed by entering depth values in the well configuration boxes (Note: These are depths below the water table, not depths below land surface). Alternatively, the open interval of the well can be changed manually by clicking on the ends of the well indicator bar in the aquifer cross section graphic (Figure S1A) and dragging them up and down. Changes in the position of the well screen by either method are represented in the aquifer cross section graphic (Figure S1A) by a vertical gold bar representing the well screen and by a shaded region highlighting the collection of groundwater flow paths that connect the well screen to its contributing area at the water table. Changes in the position of the well are transferred to Figure S1B, which shows the portion of the groundwater age profile that is intersected by the open interval of the well (gold curve). Selected age-related output data for the user-defined groundwater model and well configuration are summarized in a table (Figure S1). There, calculated values are given for the mean age of groundwater in the aquifer (depending on aquifer properties), the mean age of groundwater entering the well (depending on aquifer properties and well configuration), the youngest and oldest groundwater intersected by the well, and the age span of groundwater intersected by the well. These parameters highlight the potential variability of age distributions that can be sampled in a well. The age span is important because the relation between the age span and the duration of contaminant input affects the peak contaminant concentration in the well (see Applications).

Age distribution graphics (Figure S1C, S1D) show the relative proportions of groundwater of various ages that are intersected by the well screen. The graph on the left presents this information in incremental form similar to a histogram (fraction of total sample representing each age interval intersected by the well, in percent per year) and the graph on the right gives similar information in cumulative form (fraction of total sample with age less than each age interval). Age distributions are determined from the well configuration input data (relative position of the top and bottom of the well screen within the aquifer) using the "partial exponential model" (Jurgens et al. 2012) (see Addendum. Equations). Incremental age fractions add up to 100 percent and are used subsequently to calculate contaminant concentrations in water from the well.

Changing the horizontal position of the well within the aquifer will have no effect on the age distributions of the well, thus illustrating the fact that the calculations are based entirely on vertical profiles. However, the horizontal position of the well can be used to explore connections between the well and various recharge areas contributing to flow paths that intersect the well. The horizontal distance between a well and its contributing recharge area is more likely to be smaller if the well screen is shallower and if the well is near a groundwater divide (left side of the aquifer flow path graphic) and the distance is likely to be larger if the well screen is deeper or if the well is near a discharge area (right side of flow path graphic). To illustrate these relations, Figure S1A includes a shaded region that highlights the groundwater flow paths connecting the well screen with its contributing area at the water table.

Contaminant transport and trends

Changes in concentration of a nonpoint-source contaminant introduced across the recharge area over time will be propagated into the saturated zone with groundwater flow. In an unmixed unconfined groundwater flow system like the one modeled here, a vertical profile of the aquifer will contain a record of past contaminant concentrations in recharge. For example, a single short contaminant pulse would move downward as a horizontal zone of high contaminant concentration with low concentrations above and below, whereas gradually increasing contamination in recharge would be preserved as a gradient in which concentration decreases downward with increasing groundwater age. The response of a well to changing contamination in recharge will depend on the groundwater flow system, well configuration, and contaminant history. Because the flow system is in steady state, the groundwater age at any location will be constant, but the corresponding date of recharge of water occupying the location will change with time. Because the contaminant concentration in recharge may have changed over time, the contaminant concentration in any water sample will depend not only on the distribution of ages within the sample, but also on the date the sample was collected.

The contaminant input parameter set has four dates that can be varied to describe temporal variation of contaminant concentration at the water table. The date parameters can be used to generate a variety of contaminant scenarios such as input pulses, rectangular time series, or gradual changes up or down that could mimic historical variations and future scenarios. In its current form, the model requires the contaminant to begin and end with zero concentration, so contaminant input functions are limited to relatively simple shapes.

The contaminant trends graphic (Figure S1E) shows the user-defined record of contaminant concentrations in recharge, along with the modeled record of contaminant concentrations in the well. For a stable (non-degrading) contaminant, the concentration in the well at any given time is calculated by combining the groundwater age distribution in the well and the contaminant recharge history at the water table. The fraction of water in the well representing each time interval of recharge (Figure S1C) is multiplied by the contaminant concentration in recharge for that time interval (Figure S1E), and these products are summed to give the total contaminant concentration in the mixture discharging from the well (see Addendum. Equations). This sum of products is done for each time point in the series to give the contaminant concentration in a sample from the well at each time point, thus yielding a record of contamination in the well over time (Figure S1E).

The contaminant concentration graphic (Figure S1F) shows the vertical distribution of contaminant concentrations in the aquifer at a single point in time, the position of the well screen with respect to the contaminant concentrations in the aquifer at that time, and the resulting contaminant concentration in groundwater discharge from the well at that time. For a stable contaminant, the concentration depth profile is equivalent to a groundwater record of contaminant history at the water table. This profile is generated for a specified date from the contaminant recharge curve (Figure S1E) by determining the depth to which each recharge date has moved, based on the age profile of the aquifer (Figure S1B). Recharge dates corresponding to the water table, beginning of contamination, and end of contamination, are indicated at appropriate depths on the right side of the contaminant concentration graphic (Figure S1F). As a contaminant pulse moves down into the aquifer, its vertical dimension decreases as groundwater age contours move closer together. The contaminant concentration graphic shows what parts of the contaminant profile are intersected by the well, thus illustrating how the contaminant concentration in the well represents a mixture of more of less contaminated groundwater. In the example shown (Figure S1F), the position of the contaminant in the aquifer in 2014 is such that the well screen intersects some uncontaminated groundwater below the contaminant pulse and most of the groundwater profile containing the contaminant pulse, which had varying concentration in recharge over time. Thus, the groundwater mixture entering the well has a contaminant concentration around 50 percent of the maximum concentration in recharge and it is projected to decrease in the future. The contaminant concentration in the well at the selected time is represented in both the time series and the profile graphic. By varying the date of the contaminant profile, users can explore how vertical distributions of contaminant concentrations in the aquifer (Figure S1F) are related to temporal variations in contaminant concentrations in the well (Figure S1E). The time point to be plotted in Figure S1F can be selected in three different ways: (1) enter a value in the date box, (2) click the left and right arrows (annual time steps), or (3) click on the drag-and-drop feature in the contaminant trend graphic (Figure S1E). Moving the drag-and-drop feature across Figure S1E gives a dynamic view in Figure S1F of a transient nonpoint-source contaminant pulse moving downward in the aquifer and being sampled by a well over time. Figure S1F includes a “zoom” option that switches the vertical axis dimension between the full saturated thickness of the aquifer (to match Figures S1A and S1B) and a smaller depth range focused on the portion of the aquifer near the well screen.

Contaminant degradation is included as an option in the model parameter set. Degradation along each groundwater flow path is treated as first-order decay and the input parameter is the decay constant (in units of 1/year), which is inversely related to the half-life of the contaminant in the aquifer (see Addendum. Equations). For a degrading contaminant, the decay equation is applied to each of the age fractions in the well before the fractions are summed to generate the modeled contaminant concentration in the well. Setting the decay parameter value to zero means the contaminant is stable (non-degrading). Setting it to 0.069/year would correspond to a half-life of 10 years, in which case the contaminant concentration along a flow path would decrease to 50 percent of its recharge value after 10 years of transport in the aquifer and to 25 percent of its initial concentration after 20 years of transport.

Webtool implementation

All model calculations and graphics for this webtool are done within the browser using live user input. The webtool uses HTML5 and two Javascript libraries, JQuery with Flot, to render the various graphs. HTML5 is the current specification for web development that allows for creating a rich user experience. Javascript is a computer programming language available within all browsers and recent developments provide run speeds sufficient for responsive dynamic content. JQuery and Flot are tools written in Javascript that reduce the development required to create rich content and graphs. These capabilities permit the webtool to run directly on a web page, rather than by installing an application on the local computer. Javascript is used to calculate output data from user input values and then passes the results to Flot, the primary graphing tool. For further customization, the application uses JQuery to enhance the user experience. For instance, JQuery is used to merge several plots into one panel for more coherent display, as in the contaminant concentration graphic (Figure S1F). JQuery is also used to customize legends and labels and to link corresponding graphs. To permit flexibility in the ranges of aquifer parameter values and time scales being modeled, the webtool automatically adjusts the scales of data integration and graphic output.

The webtool is designed primarily to explore trends on inter-annual and longer time scales. The model is based on a steady state groundwater flow system with transient (inter-annual or longer) contaminant input variations. Having the groundwater age distribution for the well (Figure S1C) and the contaminant history at the water table (Figure S1E), contaminant concentrations in the well are determined by convolution (i.e., taking the sum-product) of the age fractions and contaminant concentrations of all age fractions intersected by the well screen (Jurgens et al., 2012). In the webtool, these calculations are done numerically with integration time steps that vary depending on the time scale of the model. The optimal size of time steps used for numerical integration is adapted to each change of model parameter values to maximize temporal resolution while minimizing calculation time. This optimization is based on the age span of groundwater intersected by the well because the most time-consuming webtool operation is the convolution of contaminant concentrations and age intervals in the well. In the current version, the integration time step is 1 month for age spans < 200 years, 1 year for age spans of 200-2400 years, 10 years for age spans of 2400-24000 years, and 100 years for age spans > 24000 years.

Applications

Selected observations that are important for characterizing contaminant trends in a well for regulatory requirements and management scenarios include initial response time (delay), flushing time, and maximum relative concentration (peak concentration) (Eberts et al. 2012; Eberts et al. 2013). A delayed initial response occurs when a change in contaminant concentration in recharge does not cause an immediate response in the well because the well does not intersect young groundwater; the initial response to a change in recharge concentration will be delayed by an amount of time equal to the age of the youngest groundwater intersected by the well. In Figure S1E, the contaminant does not arrive at the well until 9 years after it begins at the water table because the well does not intersect groundwater less than 9 years old. Flushing time is more complicated, as it depends on the total mixture of groundwater ages sampled by the well. The more old groundwater in the mixture, the longer the time required to reach steady state with a new contaminant concentration in recharge; that is, the longer it will take for the well either to feel the full effect of the contaminant after it begins at the water table or to recover fully from the effect of the contaminant after it ends at the water table. Wells can have long or short flushing times regardless of whether they have long or short initial response times. The maximum relative concentration (peak concentration) in the well is related to the shape of the contaminant input history in recharge and the shape of the age distribution sampled by the well. If all groundwater entering a well has a single age, then there will be some time when the contaminant concentration in the well is equal to the maximum concentration in recharge, assuming the contaminant is not degraded. In contrast, a well sampling groundwater with a large age span is more likely to discharge a mixture of variably contaminated groundwater. The peak concentration in discharge may be substantially less than the maximum concentration in recharge if the flushing time is long in comparison to the duration of the contaminant maximum in recharge. Such a well may be protected from high contaminant concentrations by mixing and dilution within the well. In Figure S1E, the peak concentration in the well is only about 50 % of the maximum concentration in recharge because there is no time when all groundwater contributing to the well has the maximum concentration in recharge.

It follows from the description of Figure S1 that the mean age of groundwater discharging from a well is insufficient information for estimating age-related effects on contaminant concentration in the discharge. By using the webtool, users can demonstrate that two wells discharging groundwater with identical mean age may have different contaminant responses if the well screens have different lengths.

For example, in contrast to the long-screen well illustrated in Figure S1A with mean age of 24 years, age span of 35 years, and maximum relative contaminant concentration of 50 %, a short-screen well with the same mean age of 24 years, but age span of only 3 years, would have maximum relative contaminant concentration of 100 %, all else being equal. This illustrates the general principle that, although mean age can be a useful parameter for calibrating some types of aquifer flow models, the mean age of a sample cannot be uniquely related to concentration of a contaminant or other environmental tracer unless accompanied by additional information about the age distribution in the sample (e.g., Figure S1C, S1D).

Contaminant degradation in the aquifer can alter substantially the peak concentration in the well, but will not necessarily change the initial response time or flushing time. Degradation can protect a deep well from contamination if the contaminant half-life is short and the travel time to the top of the well screen is long. Effects of degradation largely depend on the nature of the contaminant and corresponding reactivity of aqueous or solid phases in the aquifer. These factors may be difficult to model accurately (see Limitations).

The webtool model and graphics can be used to explore simple 2-dimensional (vertical) spatial relations between wells and their contributing areas. For example, a user could envision a dissolved point-source contaminant introduced at any point along the water table would move along a particular flow path as a cloud or plume that would reach a certain depth depending on its age and relative distance from the discharge end of the aquifer (Solomon et al. 1995). In Figure S1A, the area at the water table contributing to flow paths intersected by the well is approximately 250-750 m upgradient from the well. Thus, in this idealized model, the well is unaffected by contamination in recharge in the immediate vicinity of the well; whereas a different well with a shallower open interval would be more affected by nearby contamination and possibly less affected by distant contamination. Changing the horizontal position of the well also affects the distance to its contributing area.

The webtool also can be used to illustrate effects of groundwater storage on base-flow contaminant discharge from a watershed. A sample from a well that is open to the total aquifer thickness will have the same age distribution as the total discharge from the aquifer on the right side of the aquifer flow graphic. This full exponential age distribution may, therefore, represent groundwater discharge to surface water, such as a stream or spring, under steady-state flow conditions (Böhlke and Denver 1995).

Additional examples of webtool input and output illustrating some of the general principles of nonpoint-source contaminant movement to wells are given in Figures S2 and S3. Figure S2 contains webtool results for different well configurations in a common aquifer with a common contamination history. These examples use a rectangular contaminant input pulse to emphasize concepts related to initial response time, peak concentration, and flushing time (Eberts et al. 2013). Figure S3 contains webtool results for examples derived from previous studies of groundwater nitrate in agricultural areas to emphasize implications of groundwater age, input history, and degradation to understanding and management of this important contaminant (Böhlke 2002).

Limitations

The groundwater stratigraphy model used by the webtool has a number of important limitations, including:

(1) It represents movement of groundwater between recharge and discharge, but it does not include transport or residence time above the water table in soil or unsaturated subsoil. Depending on the location (geology, climate, land use), those other parts of the hydrologic cycle may be important components of contaminant travel times. For example, unsaturated-zone travel times can be decades to millennia in arid and semi-arid regions (Phillips 1994; McMahon et al. 2006; Scanlon et al. 2006).

(2) Results could be different if the saturated zone in the aquifer has a different shape or if its properties are not homogeneous. For example, a different vertical groundwater age distribution could result if the aquifer had a wedge-shaped profile or systematic downward trend in hydraulic conductivity or porosity (Zuber 1986; Cook and Böhlke 2000). Small-scale heterogeneities may not affect overall age distributions greatly in long-screen wells or springs, but can cause large differences in local age

distributions and contaminant concentrations entering wells with short screens (Weissmann et al. 2002; Green et al. 2010).

(3) The model is based on the assumption that groundwater flow is steady, so it has no provision for hydrologic variability such as inter-annual, seasonal, or event-based changes in water storage and movement. In some deep wells, short-term variability may not be an important limitation, but pumping and irrigation recharge could alter the age profile significantly. When applied to total discharge to springs and streams, the model will not account for runoff or rapid shallow subsurface flow, but it might be viewed as a simplistic representation of longer term base flow characteristics (Strack 1984; Michel 1992; Sanford and Pope 2013).

(4) The model is based on the assumption that groundwater flow is not perturbed by the well, whereas water-supply wells can alter groundwater flow paths and age gradients substantially. For example, intensive pumping from wells with deep open intervals can draw down and discharge larger fractions of young groundwater than indicated by the groundwater stratigraphy model, and those fractions can vary with pumping rate (Masterson et al. 2004; Eberts et al. 2013). Intensive pumping and (or) unpumped wellbore flow also can homogenize the flow system locally, thus reducing vertical gradients of age and contaminant concentration (Reilly et al. 1989; McMahon et al. 2004).

(5) For simplicity, contaminant degradation in the webtool is assumed to begin at the water table and it is modeled as a first-order process, whereas real contaminants in real aquifers may not follow these patterns. Biodegradation of contaminants in aquifers can occur by various mechanisms and the rates of reaction may change along groundwater flow paths. For example, because microbial reduction of nitrate to nitrogen gas (denitrification) is inhibited by dissolved oxygen and largely controlled by the distribution of reactive aquifer phases, the degradation rate of nitrate commonly is low near the water table and it can increase abruptly at depth within the aquifer (Postma et al. 1991; Böhlke et al. 2002; Liao et al. 2012). Degradation rate can be set to zero for applications of the webtool focusing on groundwater age mixing effects.

Future versions of the webtool could present increasingly complex scenarios to address some of the limitations listed above. Such scenarios would require additional model parameters and user insight, and might also be addressed by using other existing simulation software. Alternative groundwater age distribution models and more complex (realistic) contaminant input scenarios can be explored by using the TracerLPM program (Jurgens et al. 2012). This lumped-parameter program includes provision for incorporating multiple environmental tracer data and inverse modeling to derive age distributions for water samples from wells, springs, or streams. Many other programs are available for more sophisticated groundwater and contaminant transport modeling with spatially distributed parameters (see, for example http://water.usgs.gov/software/).

Conclusions

A new online interactive webtool, GAMACTT (Version 1), was designed to illustrate important concepts relating groundwater contamination, groundwater flow, and contaminant trends in water-supply wells. Drag-and-drop features with real-time model output allow users to see graphics in motion, thus clarifying spatial and temporal relations among these factors. The operation of the webtool involves simplistic assumptions that are likely to be violated to varying degrees in the real world. Important limitations of the model include (1) Groundwater-only model does not include transport through the unsaturated zone; (2) basic aquifer properties do not account for heterogeneity, flow discontinuities, dispersion, etc.; (3) steady-state model by definition does not provide for transient flow conditions; (4) partial exponential groundwater stratigraphy model assumes groundwater flow system is not perturbed by pumping or wellbore flow; (5) first-order degradation model may not be appropriate for some biogeochemical reactions. For these reasons, among others, the webtool is presented mainly as an illustrative (educational) tool, rather than a prediction tool. Despite these limitations, manipulation of model parameter values can be used to visually explore and understand various processes affecting how public-supply wells respond to groundwater contamination. For some model scenarios, results may be applicable to contaminant trends in discharge to surface water bodies like springs and streams. The webtool also can be used to explore spatial relations between wells and their contributing recharge areas, which are important considerations for point-source and nonpoint-source contaminants. Improved understanding of these concepts should be useful for setting management expectations, designing monitoring protocols, and performing management assessments. The webtool is freely available and can be accessed at ~~http://cida.usgs.gov/gamactt/~~. http://ca.water.usgs.gov/projects/gamactt/

Acknowledgments

Support for this project was provided by the USGS National Water Quality Assessment Program, the USGS Center for Integrated Data Analytics, and the USGS National Research Program. Bruce Lindsey and anonymous reviewers provided useful comments on earlier versions of the manuscript.

Disclaimer

Although this software program has been used by the U.S. Geological Survey (USGS), no warranty, expressed or implied, is made by the USGS or the U.S. Government as to the accuracy and functioning of the program and related program material nor shall the fact of distribution constitute any such warranty, and no responsibility is assumed by the USGS in connection therewith. Any use of trade, product, or firm names is for descriptive purposes only and does not imply endorsement by the U.S. Government. Note: Wiley-Blackwell is not responsible for the content or functionality of any supporting information supplied by the authors. Any queries (other than missing materials) should be directed to the corresponding author.

References

Böhlke, J.K. 2002. Groundwater recharge and agricultural contamination. *Hydrogeology Journal* 10: 153-179 (Erratum, 2002, *Hydrogeology Journal* 10: 438-439).

Böhlke, J.K., and J.M. Denver. 1995. Combined use of groundwater dating, chemical, and isotopic analyses to resolve the history and fate of nitrate contamination in two agricultural watersheds, Atlantic coastal plain, Maryland. *Water Resources Research* 31: 2319-2339.

Böhlke, J.K., R. Wanty, M. Tuttle, G. Delin, and M. Landon. 2002. Denitrification in the recharge area and discharge area of a transient agricultural nitrate plume in a glacial outwash sand aquifer, Minnesota. *Water Resources Research* 38(7), doi:10.1029/2001WR000663: 1-26.

Burt, T.P., N.J.K. Howden, F. Worrall, and M.J. Whelan. 2008. Importance of long-term monitoring for detecting environmental change: Lessons from a lowland river in south east England. *Biogeosciences* 5: 1529-1535.

Cook, P.G., and J.K. Böhlke. 2000. Determining timescales for groundwater flow and solute transport. In *Environmental Tracers in Subsurface Hydrology*, ed. P. G. Cook and A. L. Herczeg. Boston: Kluwer Academic Publishers: 1-30.

Dubrovsky, N.M., K.R. Burow, G.M. Clark, J.A.M. Gronberg, P.A. Hamilton, K.J. Hitt, D.K. Mueller, M.D. Munn, B.T. Nolan, L.J. Puckett, M.G. Rupert, T.M. Short, N.E. Spahr, L.A. Sprague, and W.G. Wilber. 2010. Nutrients in the Nation’s Streams and Groundwater, 1992–2004. Reston: *U.S. Geological Survey Circular* 1350: 174 p.

Duffy, C.J., and D.H. Lee. 1992. Base flow response from nonpoint source contamination: simulated spatial variability in source, structure, and initial condition. *Water Resources Research* 28: 905-914.

Eberts, S.M., J.K. Böhlke, L.J. Kauffman, and B.C. Jurgens. 2012. Comparison of particle-tracking and lumped-parameter age-distribution models for evaluating vulnerability of production wells to contamination. *Hydrogeology Journal* 20: 263-282.

Eberts, S.M., M.A. Thomas, and M.L. Jagucki. 2013. The quality of our Nation's waters: factors affecting public-supply-well vulnerability to contamination: understanding observed water quality and anticipating future water quality. Reston: *U.S. Geological Survey Circular* 1385: 132 p.

Gelhar, L.W., and J.L. Wilson. 1974. Ground-water quality modeling. *Ground Water* 22: 399-408.

Green, C.T., J.K. Böhlke, B. Bekins, and S. Phillips. 2010. Mixing effects on apparent reaction rates and isotope fractionation during denitrification in a heterogeneous aquifer. *Water Resources Research* 46(8), W08525, doi:10.1029/2009WR008903: 1-19.

Jurgens, B.C., J.K. Böhlke, and S.M. Eberts. 2012. TracerLPM (Version 1): An Excel® workbook for interpreting groundwater age distributions from environmental tracer data. *U.S. Geological Survey Techniques and Methods Report 4-F3*: 60 p.

Kauffman, L.J., A.L. Baehr, M.A. Ayers, and P.E. Stackleberg. 2001. Effects of land use and travel time on the distribution of nitrate in the Kirkwood-Cohansey aquifer system in southern New Jersey. West Trenton, NJ: *U.S. Geological Survey Water-Resources Investigations Report* 01-4117: 49 p.

Liao, L., C.T. Green, B.A. Bekins, and J.K. Böhlke. 2012. Factors controlling nitrate fluxes in groundwater in agricultural areas. *Water Resources Research* 48(2), W00L09, doi:10.1029/2011WR011008: 1-18.

Masterson, J.P., D.A. Walter, and D.R. LeBlanc. 2004. Transient analysis of the source of water to wells: Cape Cod, Massachusetts. *Ground Water* 42: 126-134.

McMahon, P.B., J.K. Böhlke, and S.C. Christenson. 2004. Geochemistry, radiocarbon ages, and paleorecharge conditions along a transect in the central High Plains aquifer, southwestern Kansas, USA. *Applied Geochemistry* 19: 1655-1686.

McMahon, P.B., K.F. Dennehy, B.W. Bruce, J.K. Böhlke, R.L. Michel, J.J. Gurdak, and D.B. Hurlbut. 2006. Storage and transit time of chemicals in thick unsaturated zones under rangeland and irrigated cropland, High Plains, United States. *Water Resources Research* 42(3), W03413, doi:10.1029/2005WR004417: 1-18.

Michel, R.L. 1992. Residence times in river basins as determined by analysis of long-term tritium records. *Journal of Hydrology* 130: 367-378.

Phillips, F.M. 1994. Environmental tracers for water movement in desert soils of the American southwest. *Soil Science Society of America Journal* 58: 15-24.

Postma, D., C. Boesen, H. Kristiansen, and F. Larsen. 1991. Nitrate reduction in an unconfined sandy aquifer: water chemistry, reduction processes, and geochemical modeling. *Water Resources Research* 27: 2027-2045.

Reilly, T.E., O.L. Franke, and G.D. Bennett. 1989. Bias in groundwater samples caused by wellbore flow. *Journal of Hydraulic Engineering* 115: 270-276.

Sanford, W.E., and J.P. Pope. 2013. Quantifying groundwater's role in delaying improvements to Chesapeake Bay water quality. *Environmental Science and Technology* 47: 13330-13338.

Scanlon, B.R., K.E. Keese, A.L. Flint, L.E. Flint, C.B. Gaye, W.M. Edmunds, and I. Simmers. 2006. Global synthesis of groundwater recharge in semiarid and arid regions. *Hydrological Processes* 20: 3335-3370.

Solomon, D.K., R.J. Poreda, P.G. Cook, and A. Hunt. 1995. Site characterization using $^{3}H/^{3}He$ ground-water ages, Cape Cod, MA. *Ground Water* 33: 988-996.

Strack, O.D.L. 1984. Three-dimensional streamlines in Dupuit-Forchheimer models. *Water Resources Research* 20: 812-822.

Vogel, J.C. 1967. Investigation of groundwater flow with radiocarbon. In *Isotopes in Hydrology*. Vienna: International Atomic Energy Agency: 355-368.

Weissmann, G.S., Y. Zhang, E.M. LaBolle, and G.E. Fogg. 2002. Dispersion of groundwater age in an alluvial aquifer system. *Water Resources Research* 38(10), doi:10.1029/2001WR000907: 1-8.

Zoellmann, K., W. Kinzelbach, and C. Fulda. 2001. Environmental tracer transport (^{3}H and SF_6) in the saturated and unsaturated zones and its use in nitrate pollution management. *Journal of Hydrology* 240: 187-205.

Zuber, A. 1986. Mathematical models for the interpretation of environmental radioisotopes in groundwater systems. In *Handbook of Environmental Geochemistry, Volume 2, The Terrestrial Environment B*, ed. P. Fritz and J. C. Fontes, Elsevier: 1-59.

Addendum. Equations

The groundwater stratigraphy model is based on mass balance principles. For a transmissive homogeneous rectangular saturated groundwater flow system at steady state, with evenly distributed recharge across the water table, focused discharge from one end of the system, and no-flow boundaries elsewhere, the vertical and horizontal fluxes of water require that vertical velocity decreases downward and horizontal velocity increases toward the discharge end, with flow paths as illustrated in Figure S1A (Vogel 1967; Strack 1984; Cook and Böhlke 2000). If the system is unmixed, this idealized pattern of flow yields a vertical groundwater age profile that ranges from 0 at the water table to infinity at the bottom of the aquifer, as illustrated in Figure S1B. In the numerical model for groundwater discharge from a well, spring, or stream, a water sample is considered to be a mixture of parcels, each of which represents a discrete age interval and each of which has a tracer concentration appropriate for the time it entered the system, adjusted for first-order decay. The following definitions of time and age are used in the equations below:

t_i time (date) when a water parcel (i, a fraction of a water sample that is modeled as having a discrete age) entered the system; $t_i = t_s - \tau_i$, the date a sample was collected minus the age of a parcel within the sample

t_s time (date) when a water sample (s) was collected for analysis

τ_i age of a discrete water parcel ($\tau_i = t_s - t_i$, the date of a sample minus the date when the parcel entered the system in recharge)

τ_s mean age of all water parcels in a sample

τ_{aq} mean age of all water parcels in an aquifer

Where the exponential model can be used to describe groundwater stratification within a surficial aquifer, the variation of groundwater age with depth is given by:

[1] $$\tau_i = (n \bullet Z/r) \bullet ln[Z/(Z-z_i)],$$

which can be re-arranged to give the variation of depth with age:

[2] $$z_i = Z - Z \bullet exp[(-\tau_i \bullet r)/(n \bullet Z)],$$

where t_i = travel time of a groundwater parcel (i) from the water table to the point of interest; n = porosity (volume fraction); Z = total thickness of the saturated zone within the surficial aquifer; r = recharge rate; and z_i = depth below the water table at the point of interest. The mean age of groundwater in the aquifer (τ_{aq}) is given by:

[3] $$\tau_{aq} = n \bullet Z/r.$$

For the situation where the whole thickness of an unconfined aquifer is represented in discharge locally to a stream or well, the frequency distribution of groundwater ages in the discharge is exponential (younger water being relatively abundant), and the fraction of the total discharge comprised of water of a given age interval (τ_j-τ_k) is equal to the fraction of the aquifer thickness that is occupied by water in that age interval (F_i):

[4] $$F_i = q(\tau_j-\tau_k)/Q = (z_j-z_k)/Z = exp(-\tau_k/\tau_{aq}) - exp(-\tau_j/\tau_{aq}),$$

where q = the partial discharge flux of water, Q = the total discharge flux of water, and τ is related to z as in Equation 1. The horizontal distance from the point of recharge to any groundwater parcel within the aquifer can be determined by using similar geometric relations based on mass conservation (Solomon et al., 1995):

[5] $$z_i/(Z-z_i) = (x_i°-x_i) / (X-x_i°),$$

which can be rearranged to simplify calculation of flow paths from various recharge points (as in Figure S1A):

[6] $$z_i/Z = (x_i°-x_i) / (X-x_i),$$

where $x_i°$ = the distance between the stream and the recharge point, x_i = the distance between the stream and the sample point, and X = the distance from the stream to the groundwater divide. The horizontal groundwater velocity ($V_{h,i}$) at any distance (x_i) from the stream can be estimated from:

[7] $$V_{h,i} = V_v^o \bullet (X-x_i) / Z,$$

where V_v^o = the vertical velocity of groundwater at the water table, which is equal to r/n.

The concentration in discharge at any given time of sampling (t_s) of a conservative tracer with a varying input concentration is determined by numerical convolution; that is, by computing the sum over all age intervals of the fraction of discharge corresponding to each age interval in discharge (from Equation 4) multiplied by the contaminant concentration corresponding to each age interval (from the contaminant input record):

$$[8] \qquad C_{s,ts} = \Sigma[F_i \bullet C_{i,ti} \bullet \exp(-\lambda \bullet \tau_i)],$$

where $C_{s,ts}$ = the concentration in a discharge sample at the time (date) of interest, F_i is the fraction of the sample consisting of a parcel representing an age increment as defined by Equation 4, $C_{i,ti}$ = the contaminant concentration in recharge when the parcel entered the aquifer, and the last term accounts for contaminant degradation within the parcel modeled as first-order decay:

$$[9] \qquad C_{i,ts}/C_{i,ti} = \exp(-\lambda \bullet \tau_i), \text{ where}$$

$$[10] \qquad \lambda = \ln(2) / t_{1/2},$$

where λ is the contaminant decay constant, τ_i is elapsed time between recharge and sample date, and $t_{1/2}$ is the contaminant half-life.

In the partial exponential model (PEM) (Jurgens et al. 2012), equations above are rearranged to give the age fractions intersected by a well placed within an aquifer that conforms to the groundwater stratigraphy model. Well construction data (top and bottom of the open interval) are used to derive a normalized set of F_i values for groundwater intersected by the open interval of the well, and those values are used in the contaminant numerical convolution calculation.

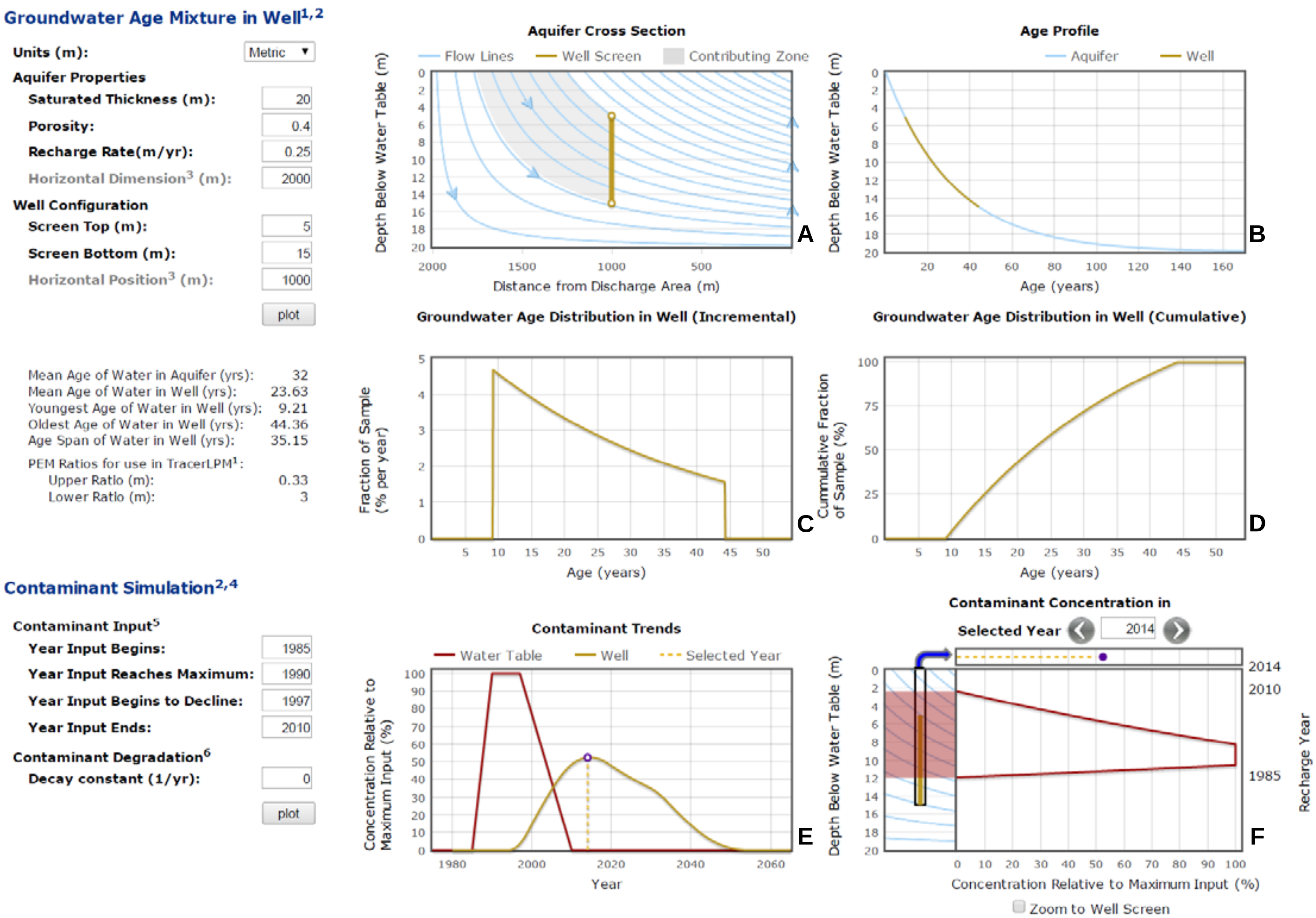

Figure S1. [caption on next page]

Figure S1. Screen capture of webtool showing input data, output data, and graphic panels.

Panel A shows the aquifer cross section based on the aquifer properties and well configuration defined by input data boxes to the left. Blue arrows indicate model groundwater flow paths. The gold bar indicates the vertical extent of the open interval of the well (well screen). The gray shaded area shows the collection of flowpaths leading from the contributing area of the well at the water table to the well screen. The top and bottom of the well screen can be changed manually by dragging the circles on the gold bar.

Panel B shows groundwater ages intersected by the well (gold curve) superimposed on the vertical groundwater age profile in the aquifer (blue curve).

Panel C shows the incremental age frequency distribution of groundwater intersected by the well as fractional contributions to a sample, in percent per year for any given age.

Panel D shows the corresponding cumulative age distribution of groundwater intersected by the well, in total percent less than a given age.

Panel E shows the record of relative contaminant concentration at the water table defined by input data boxes to the left (red curve) and the corresponding calculated record of contaminant concentration in the well (gold curve).

Panel F shows the vertical distribution of contaminant concentrations in the aquifer (red curve) and the corresponding concentration in the well (purple dot) at any given time (in this case 2014, when the concentration in the well is near its peak value). The “zoom” button changes the scale of the depth axis. The selected year for the vertical contaminant concentration plot in Panel F can be changed by entering a value in the data box, by activating the left and right arrows, or by dragging the circle on the gold curve in Panel E. Contaminant degradation should be set to zero for a stable contaminant.

Superscripts in the figure refer to footnotes in the webtool:
1- The partial exponential model (PEM) is used for all age distribution calculations (Jurgens et al. 2012).
2- Users may interact with the webtool input data boxes and the open circles on the graphs.
3- Horizontal dimensions do not affect calculations.
4- Simulates nonpoint-source contaminant input across the entire contributing area of well.
5- Contaminant years may be between 1850 and 2100. Each year must be equal to or greater than the previous value.
6- Degradation is modeled as first-order decay. The decay constant (1/yr) is equal to ln(2) divided by the half life in years.

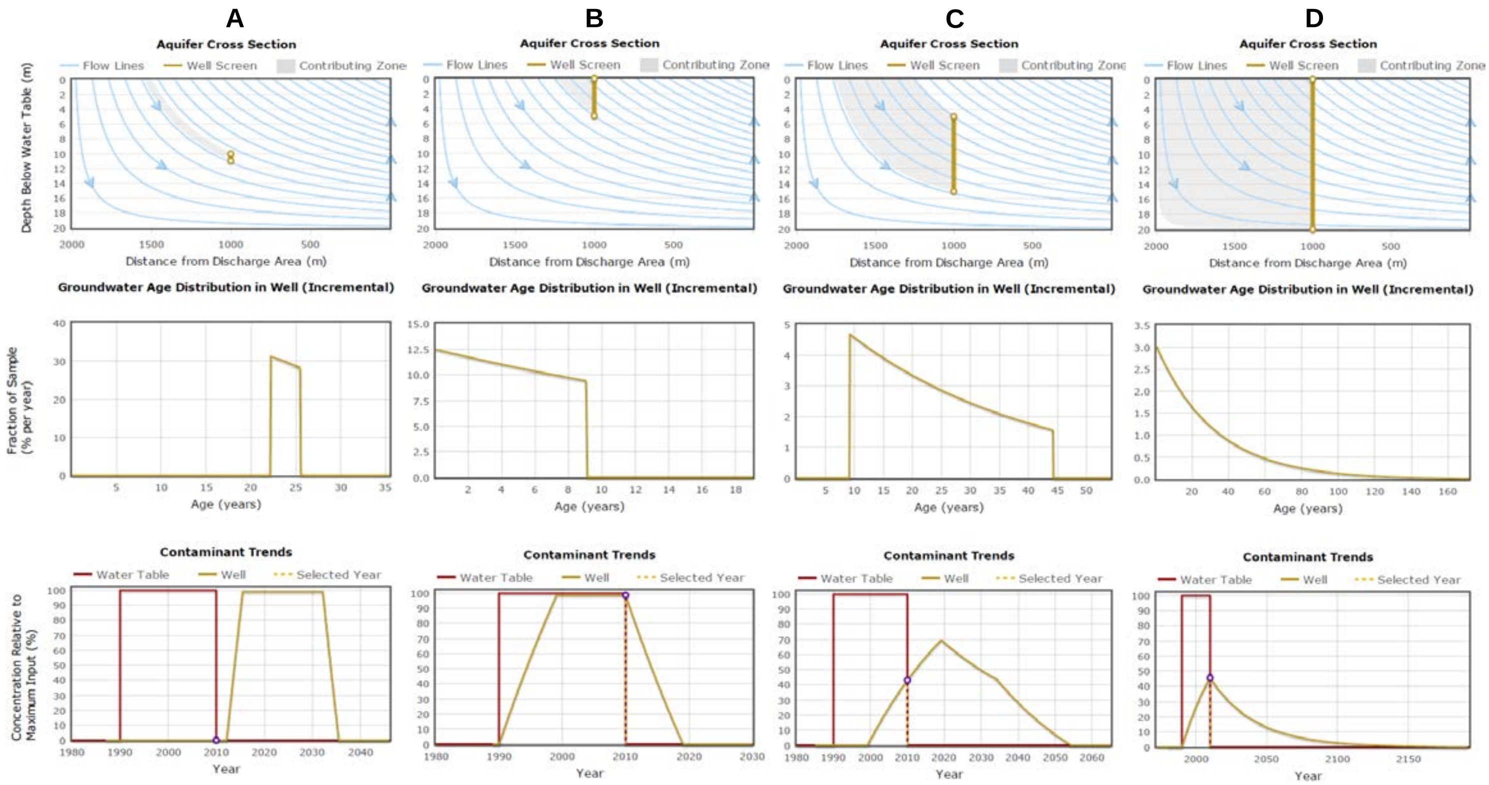

Figure S2. [caption on next page]

Figure S2. Model responses of various well configurations to a simple rectangular contaminant input record, illustrating differences in initial response time (delay), flushing time, and peak concentration.

Each figure column is a partial vertical screen capture of the webtool showing three lefthand graphic panels. The aquifer model for these scenarios is the same as the one shown in Figure S1 (thickness = 20 m, porosity = 0.4, recharge = 0.25 m/yr). The contaminant pulse in recharge begins in 1990 and ends in 2010. The contaminant concentration in the well in the year 2010 is highlighted for reference. *NOTE: Change of scale in age and date axes (optimized for individual models, rather than for comparison between models).*

Column A. In a well with a short open interval in the middle of the aquifer, discharge has a limited age span and a contaminant trend that is similar to that at the water table but delayed by time equal to the age of groundwater at the well depth. In this well, delay = moderate, flushing time = low, and peak concentration = high.

Column B. In a well with a longer open interval that includes the water table, the contaminant concentration in discharge responds quickly to change and reaches steady state with that in recharge before changing again. In this well, delay = low, flushing time = low, and peak concentration = high.

Column C. In a well with a long and deep open interval, the discharge response to contamination at the water table is delayed and gradual, and the maximum concentration in discharge is less than that in recharge because steady state is not achieved. Because young groundwater is not intercepted by the well, the contaminant concentration continues to increase for a period of time after the input at the water table ends. In this well, delay = moderate, flushing time = high, and peak concentration = moderate.

Column D. In a well open to the total thickness of the aquifer, or in a spring or stream fed by groundwater discharge, the contaminant concentration in discharge responds quickly but only gradually to change and the maximum concentration in discharge is less than that in recharge because steady state is not achieved. In this well, spring, or stream, delay = low, flushing time = moderate, and peak concentration = moderate.

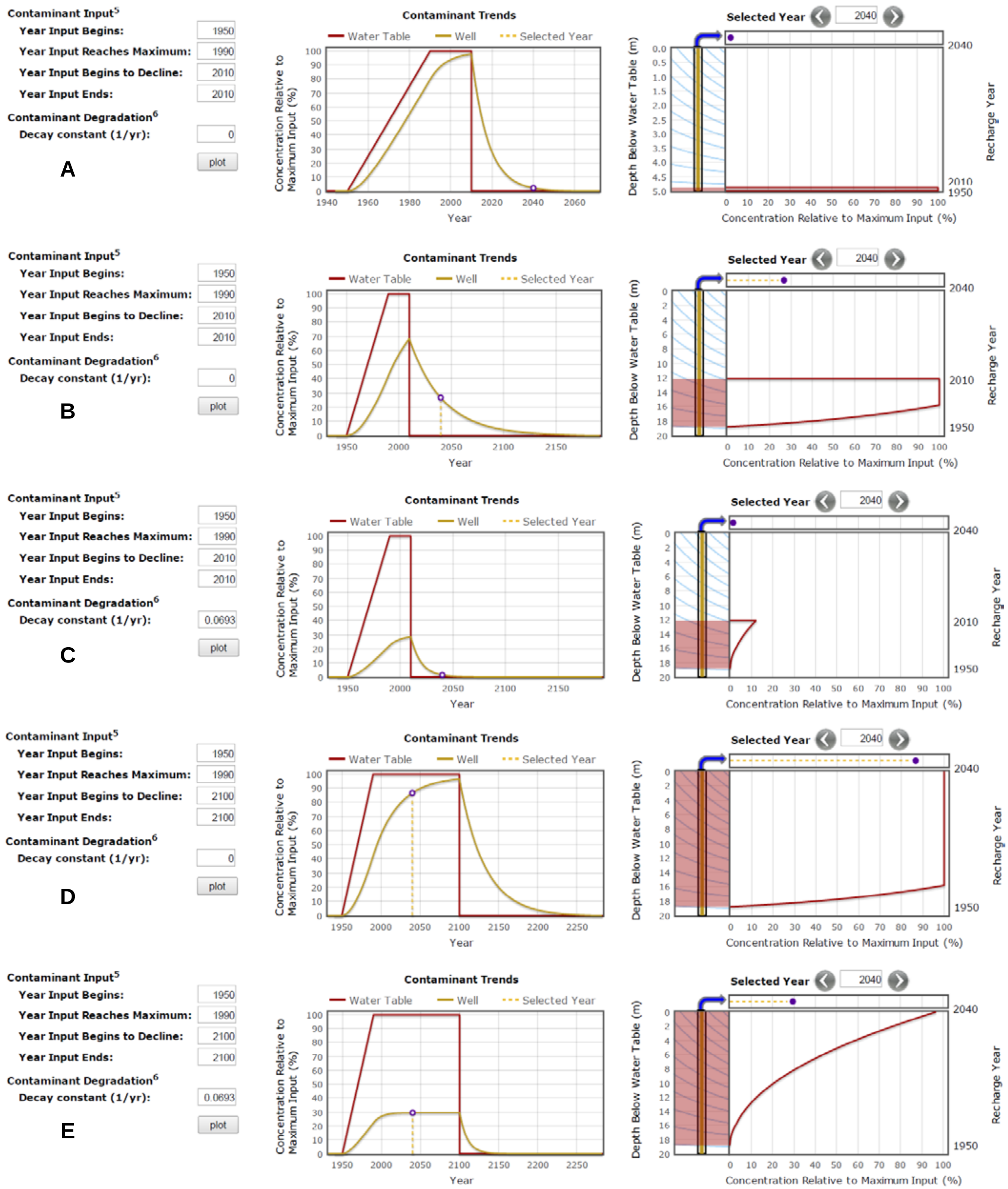

Figure S3. [caption on next page]

Figure S3. Model responses of whole aquifer discharge (e.g., fully penetrating well, spring, or stream discharge) to various contaminant input scenarios, with and without degradation.

Each figure row is a partial horizontal screen capture of the lower part of the webtool. The record of contaminant concentrations at the water table is an idealized representation of common patterns for nitrate in fertilized agricultural areas before 2010, followed by alternative scenarios after 2010. The aquifer model for these scenarios is the same as the one shown in Figure S1 and Figure S2, except for Panel A, which has a smaller aquifer thickness of 5 m. The date of the contaminant profile is held constant at 2040 for comparison.

Row A. In a 5-m thick aquifer (mean age = 8 years), contaminant concentration in the well follows behind the recharge concentration curve, is near steady state with constant contaminant input after 20 years, and flushes out within approximately 20-30 years after contaminant input ends. By 2040, the contaminant has been almost completely flushed from the aquifer.

Row B. In a 20-m thick aquifer (mean age = 32 years), contaminant concentration in the well increases at a lower rate than the recharge concentration and does not approach steady state after 20 years of constant contaminant recharge. Flushing time after cessation of contamination in recharge is more than 100 years. In 2040, the contaminant still occupies a substantial portion of the aquifer and the concentration in the well is almost 30 percent of the maximum input concentration.

Row C. For the same aquifer properties and contaminant input parameter values as B, but with degradation rate constant of 0.0693 (contaminant half-life = 10 years), the peak concentration in discharge is lower and the concentration in 2040 is much lower in the aquifer and in the well.

Row D. For the same aquifer properties as B, but longer period of constant high contaminant concentration in recharge, the concentration in the well approaches steady state after 100 years, and flushing time is more than 100 years.

Row E. For the same aquifer properties and contaminant input parameter values as D, but with degradation rate constant of 0.0693, the concentration in the well approaches steady state relatively quickly because concentrations in old groundwater are near 0. The contaminant concentration profile in the aquifer in 2040 (right panel) has a shape reflecting decay with age and depth.

Some general observations about Figure S3, with reference to nitrate (Böhlke 2002): (1) In a well open to the total aquifer thickness, or in a spring or stream fed by groundwater discharge, nitrate concentrations approach steady state relatively rapidly in a thinner aquifer and more gradually in a thicker aquifer. When not in steady state, nitrate concentration in discharge may continue to increase after recharge concentrations have stabilized. When recharge nitrate concentration decreases abruptly, full aquifer discharge exhibits rapid partial initial response (i.e., no delay), but full recovery can take much longer. (2) Degradation can alter the vertical distribution and temporal trend of a reactive contaminant in the aquifer and well, such that a deep well may be fully protected in some cases. Nitrate commonly is reduced to nitrogen gas by microbial activity in suboxic groundwater and such samples commonly are recovered in well discharge. The first-order decay model used in the webtool may not reproduce such biogeochemical processes accurately (see Limitations), but it can be used to illustrate qualitatively the importance of contaminant degradation with respect to groundwater ages and well configurations. (3) Because nitrate concentrations in recharge increase gradually in the model until 1990, various combinations of well configurations and degradation rate constants can yield roughly similar trends in the early part of the record. This ambiguity is a common issue in field situations; patterns may be more distinctive where input concentrations change abruptly and where they reverse (e.g., after 2010 in Rows A-C).