Groundwater Spatiotemporal Data Analysis Tool: Case Studies, New Features and Future Developments

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Abstract

Groundwater Spatiotemporal Data Analysis Tool (GWSDAT) is an open-source, user-friendly, software application for the visualization and interpretation of groundwater monitoring data. Since its first release, over 8 years ago, it has become increasingly well established and is now a globally adopted tool. Despite its widespread use, there is little published material considering the application of GWSDAT. The primary purpose of this article is to demonstrate the different benefits of using GWSDAT by considering a cross-section of real case studies. The first case study is an example of using GWSDAT to provide evidence to support a proposal to reduce sampling frequency. The next case study discusses the use of GWSDAT to support the recommendation for site closure. The third case study considers how GWSDAT can be used to identify gaps in a monitoring network. The final case study reports on the application of the, newly introduced, well redundancy analysis feature in GWSDAT. Finally, the road map for future developments in the optimization of monitoring network and the motivation for doing this in a spatiotemporal framework is discussed

Introduction

The GroundWater Spatiotemporal Data Analysis Tool (GWSDAT) is a user-friendly, open-source software tool used to analyze and report trends in standard groundwater quality monitoring data sets. It includes functionality to identify dissolved concentration trends and groundwater elevation fluctuations in individual wells together with the estimation of groundwater flow direction and strength. GWSDAT can also display light nonaqueous phase liquid (LNAPL) thickness trends. The most unique aspect of GWSDAT is the application of a spatiotemporal smoothing model where the spatial and temporal components of the solute concentration data are modeled jointly in a single modeling framework (Jones et al. 2014). This challenges industry convention where the most common practice is to apply a statistical model to separate monitoring events (e.g., Ricker 2008; Gong et al. 2014; Belkhiri et al. 2020) or apply a single spatial model to a data set consisting of multiple time steps within a certain time period (binning) (e.g., Aziz et al. 2003). McLean et al. (2019) demonstrated that the simultaneous statistical smoothing of both spatial and temporal components provides a clearer and more insightful interpretation of the groundwater monitoring site solute characteristics than would otherwise be gleaned from analyzing these two components separately. To the best of our knowledge, there is no other open-source “off-the-shelf” tool that use a spatiotemporal model for concentration data. The application of spatiotemporal modeling in recent literature is mostly applied to groundwater elevation rather than solute concentrations (e.g., Ruybal and Hogue 2019).

It has now been over 8 years since the first version of GWSDAT was made publicly available through the American Petroleum Institute (www.api.org/GWSDAT) and Contaminated Land Applications in Real Environments (www.claire.co.uk/GWSDAT) websites. Since then, it has continued to be maintained and developed as an open-source collaborative project between Shell plc and the University of Glasgow. The second major release included diagnostic tools to estimate plume mass, area, and average concentration through time (Ricker 2008; Jones et al. 2015). The third major release replaced the old graphical user interface with a web-based architecture which paved the way for the development of an online version (www.gwsdat.net). Users, most commonly for computational performance or data security reasons, can still opt for local installation. As well as a host of other updates, the most recent release (version 3.1) includes well redundancy analysis (http://gwsdat.net/gwsdat_manual/). This allows the user to conveniently

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drop a well or a combination of wells from the analysis and investigate the resultant impact on the estimated site plume dynamics. The primary intent of this tool is to understand which wells may have the most influence and provide supporting evidence that the conclusions of the analysis would not be significantly different with the omission of certain wells.

Due to its open-source design, GWSDAT has now become a standard, globally adopted software application in the groundwater monitoring industry. GWSDAT has already been downloaded over 10,000 times and is used by many engineers, environmental regulators, and students around the world. While literature is available on the underlying GWSDAT methodology (Jones et al. 2014; Molinari 2014; Evers et al. 2015; Jones et al. 2015; McLean 2018), little is available on real examples where GWSDAT has been applied. A common feedback from new and more experienced users has been the lack of case studies illustrating the use/applicability of GWSDAT. The main purpose of this article is to address this imbalance and give details on several case studies. The concluding section of this article is dedicated to the future direction of GWSDAT.

Case Studies

GWSDAT provides a variety of options to assess spatial and temporal trends within a groundwater monitoring dataset. It allows to display groundwater flow direction and relative magnitude, generate spatial maps of concentration data at specified time intervals from day, to month, to quarter, to year. Plume diagnostics is another functionality offered, which shows the temporal evolution of plume mass, area, and average concentration over time. The newest functionality added in version 3.10 is well redundancy analysis, which allows the user to take out one or more than one well from the dataset and re-evaluate spatial and temporal trends based on the reduced dataset and compare it to the original complete dataset. Based on a review of 76 sites covering 10 different countries covering the continents of Asia, Africa, and Europe (data not included), it was determined that for the majority (>80%) of the sites GWSDAT is used for concentration trend and plume stability analysis, as expected based on the design of the software. For about 20% of the sites included in the review, GWSDAT was primarily used to assess groundwater flow direction. GWSDAT was also specifically used to support (1) optimization of sampling frequency in about 20% of the cases, (2) site characterization and sampling gap assessment in about 30% of the cases, and (3) optimization of the analytical suite in about 5% of the cases. This snapshot of GWSDAT usage across almost 80 sites from around the world highlights the versatility and applicability of GWSDAT to support groundwater investigations.

To illustrate the functionalities of GWSDAT, four case studies, based on anonymized data, are presented below covering small (e.g., retail) as well as large (e.g., depot) sites (Table 1). All sites used for the case studies are within a non-fractured siliciclastic geological setting. GWSDAT's applicability in fractured geological setting is limited. The tool does not consider preferential flow-pathways, which are critical to understand in a fractured setting. Nevertheless, in a fractured geological setting, GWSDAT can still provide an efficient tool (1) to assess temporal changes and threshold exceedances within individual wells and (2) to generate spatial maps using the scaled circle plot functionality to display observed solute concentrations at the various sampling locations, at the click of a button.

Case Study #1

The objective of using GWSDAT for case study #1 was to demonstrate plume stability with the aim to optimize the sampling frequency interval. Case study #1 is surrounded by residential and commercial land use and is located nearby surface water bodies. In the mid-1990's during a site investigation, an impact with primarily BTEX was observed, which was only partially remediated via soil excavation and replacement. In the early 2000's, groundwater monitoring was implemented, and additional field investigations for further site characterization and adjustments to the groundwater monitoring network were completed in following years. BTEX concentration in groundwater at this site are impacted by fluctuations in the groundwater level, and the source of the contamination is residual contamination in the unsaturated and saturated zones. Data have shown that the plume has migrated beyond the site boundary along the groundwater flow direction (Figure 1).

Groundwater sampling at this site ranged from quarterly to bi-annual in the past. After recent completion of bi-annual sampling at 17 locations, a change in sampling frequency to annual was proposed to the regulator based on observations related to the decrease in the BTEX plume over time. The recommendation of changing the sampling frequency, which was approved by the regulator, was supported through the

Table 1

Summary of case studies

Site #	Small (e.g., retail) or large (e.g., depot) site	Objective of using GWSDAT	Site setting	Geological setting
1	Small	Plume stability—optimization in sampling interval	Residential commercial	
2	Small	Plume reduction—close-out of groundwater monitoring	Residential commercial	*Siliciclastics * non-fractured
3	Small	Plume stability—gap in monitoring network, earlier adoption of tool	Residential commercial recreational	
4	Large	Well redundancy analysis	Industrial	

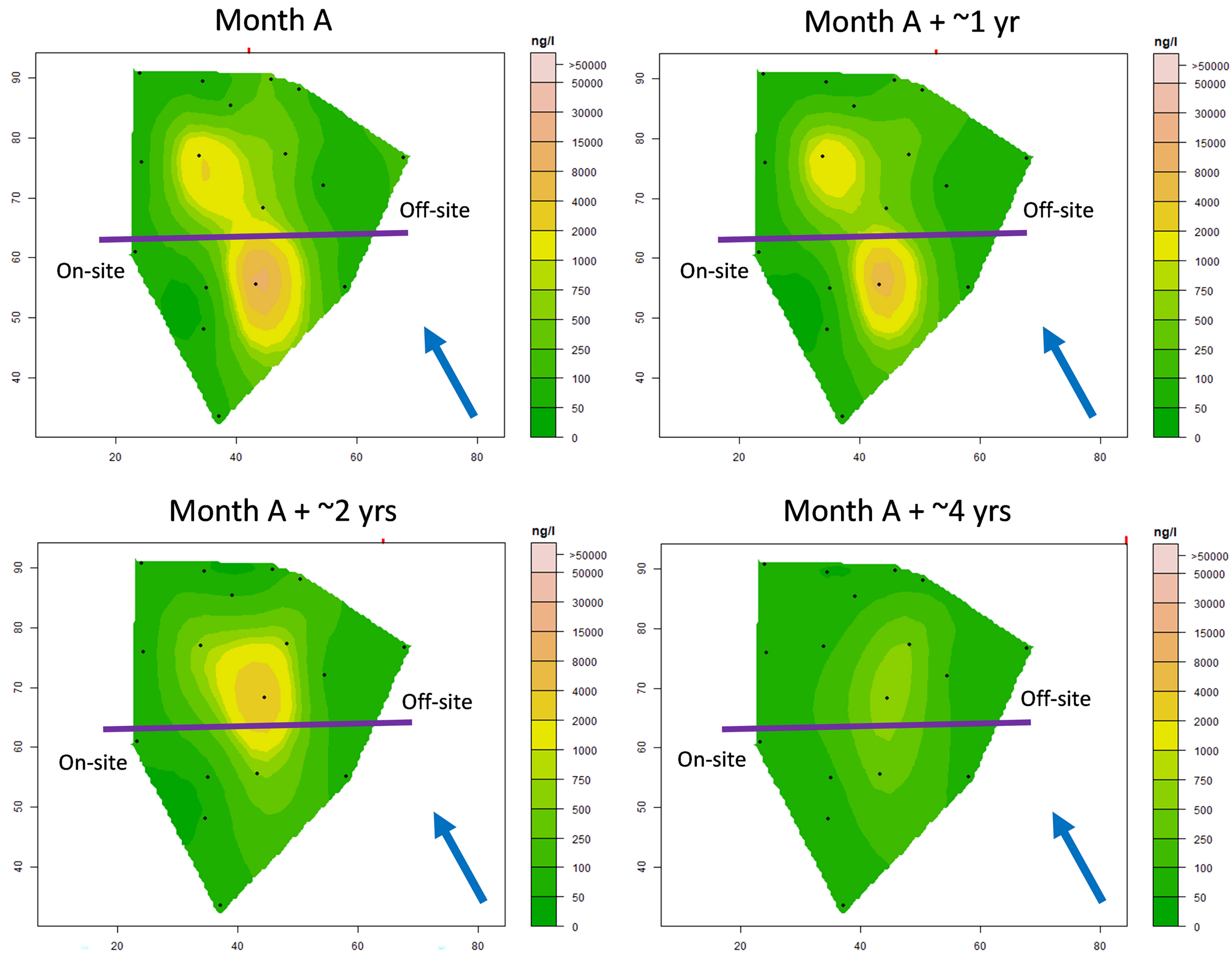

Figure 1. Time slices of the spatiotemporal plots showing historical BTEX plume evolution at case study site #1 over a four-year period. *Notes*: black dots refer to well sampling locations; site boundary shown by purple line; general groundwater flow direction at the site indicated by blue arrow.

use of GWSDAT to showcase the spatial–temporal evolution of the BTEX plume over time (Figure 1). A reduction in BTEX concentrations within the area of investigation can be observed over time. In addition, an assessment of the plume diagnostics functionality offered by GWSDAT also clearly indicated a decreasing benzene plume for a threshold value of 1 µg/L over time (Figure 2).

Case Study #2

Case study #2 falls within the category of a small site. It is in an area with residential and commercial land use, and near a drinking water protection zone. This site has been in operation for over 50 years. In the late 1990's, a site investigation determined an impact at this site by BTEX and TPH. Groundwater sampling was conducted for further site characterization, additionally, soil excavation and replacement were completed at the site. Residual BTEX contamination, however, remained at this site due to safety consideration during the remedial activities. This was documented based on verification samples taken along the excavated surfaces. Consequently, a hydraulic groundwater remediation technology was implemented for a few years. During a site investigation in the 2000's, elevated BTEX concentrations in soil and groundwater were detected, and the regulator requested further groundwater monitoring.

After completion of bi-annual sampling of groundwater at five locations over a 5-year period, it was recommended to stop the groundwater monitoring activities. Note that investigations and monitoring activities at this site go back more than 20 years. GWSDAT (Figure 3) was included in the data analysis and reporting to the regulator to demonstrate that there is no spread of the residual contamination, and that the pathway 'soil to groundwater' is not active. Within GWSDAT, it is possible to graphically represent the spatio-temporal plots using various plot types. In this case, the plot type "conc-terrain circles" was used to represent measured concentrations at each sampled well using scaled circles (Figure 3). This visual representation, obtained at the "click-of-a button" facilitated the communication to the regulator of the decreasing concentrations to below detection limit over time across the study area. After evaluation of the monitoring report, which included data over the last 5 years prior to stoppage in monitoring activities, the regulator approved of the recommendation.

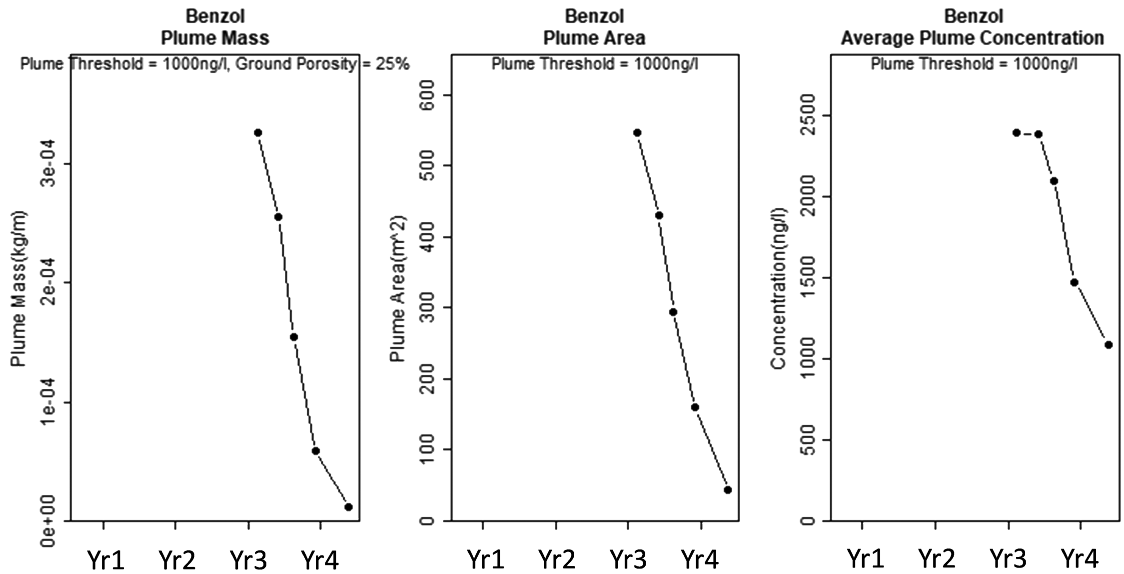

Figure 2. Plume diagnostics for benzene with a chosen threshold value of 1 μg/L at case study #1. Nb: Yr refers to year.

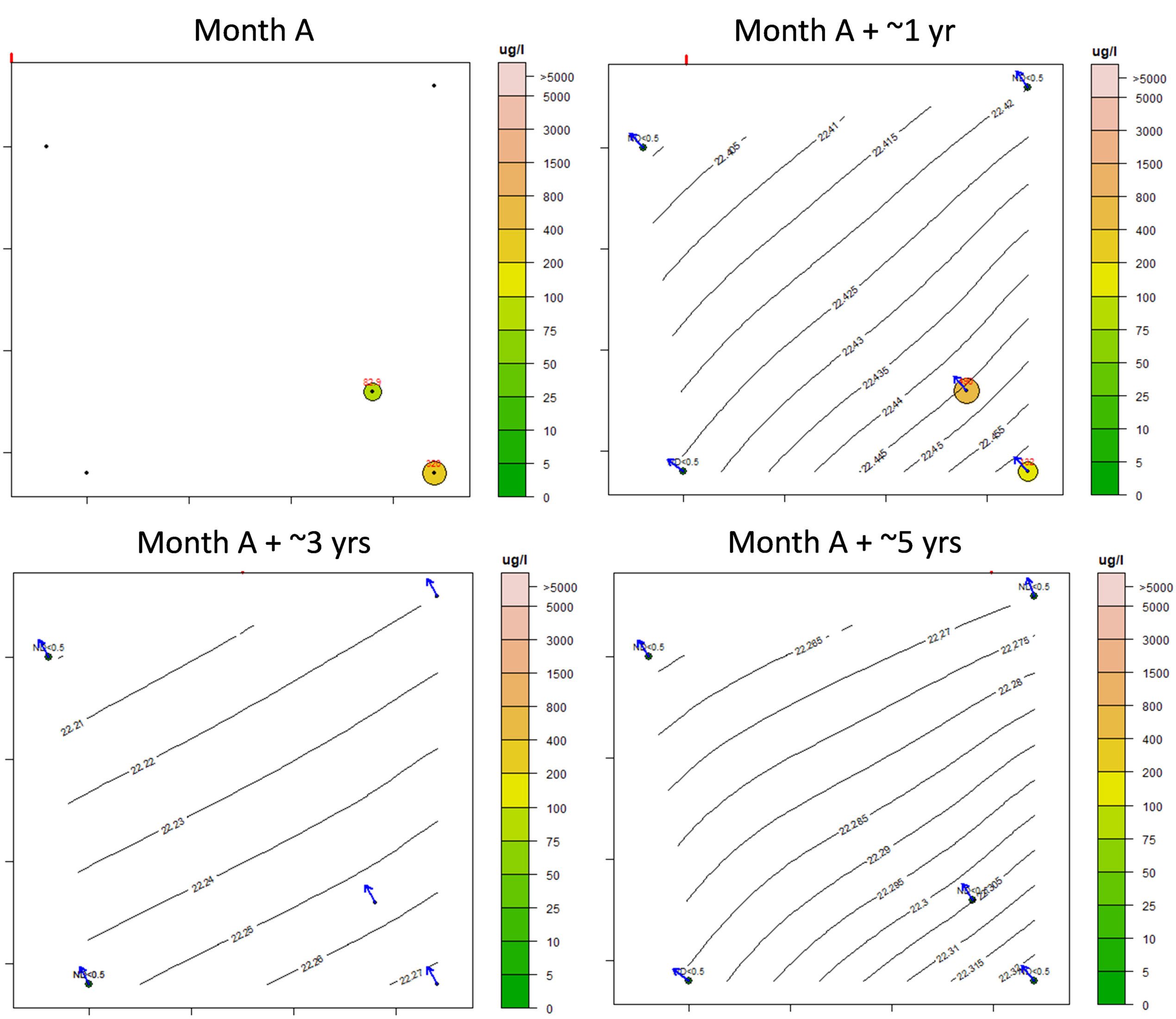

Figure 3. Time slices of the spatiotemporal plot (using plot type conc-terrain circles) showing historical BTEX concentration at case study site #2 over a five-year period. ***Notes*****: black dots represent well sampling locations; groundwater contours and groundwater flow direction at a specific well location also shown, no data on GW level were collected for data shown under "month A" plot. Size of circles scales with log of measured concentration with concentration range given in color key to right of graph.**

Case Study #3

Similar to case studies #1 and #2, case study #3 refers to a small site. This site is surrounded by residential, recreational, and commercial land use. In the 1990's, several soil and groundwater investigations including remedial activities (such as soil excavation and replacement, as well as hydraulic measures) were undertaken at this site. Some residual contamination, however, remained at this site due to safety consideration during the remedial activities, like case studies #1 and #2. In the 2000's, additional site characterization work was completed in addition to installing new groundwater monitoring wells. Since about 2012, a regular groundwater monitoring program continued at this site to assess the evolution of TPH, BTEX, and MTBE concentrations in the monitoring wells. While groundwater monitoring data were collected over several years, GWSDAT was not part of the data interpretation workflow process for many years.

To illustrate the use of GWSDAT at this site for plume stability assessment, data for BTEX are presented covering a period of 8 years of groundwater monitoring data. Note that GWSDAT was used the first time when compiling the annual reporting for the groundwater monitoring events related to years 6 and 7 of the data presented in this case study. During compilation and assessment of the monitoring data from years 6 and 7, which integrated data from previous sampling campaigns, the following observation was made. While existing downstream wells (A, B) had no concentrations above the defined threshold, and were for almost every sampling event below the detection limit (Figure 4), there is a gap in the monitoring network in the downstream direction of groundwater flow. No wells were present in the downstream direction of wells C and D, which had concentrations above the defined threshold, especially well C (Figure 4). Two new wells were drilled, indicated by the red circles on Figure 4, during year 8, about a year after the first integration of GWSDAT in the data evaluation. The regulator agreed with the recommendation for the installation of additional groundwater monitoring wells. A sampling event after the installation of the additional groundwater monitoring wells indicated that BTEX concentrations in these wells were below detection limit (Figure 5). An evaluation of the GWSDAT spatiotemporal plots from years prior to year 8 predicted that concentrations would likely be below detection limit at the two

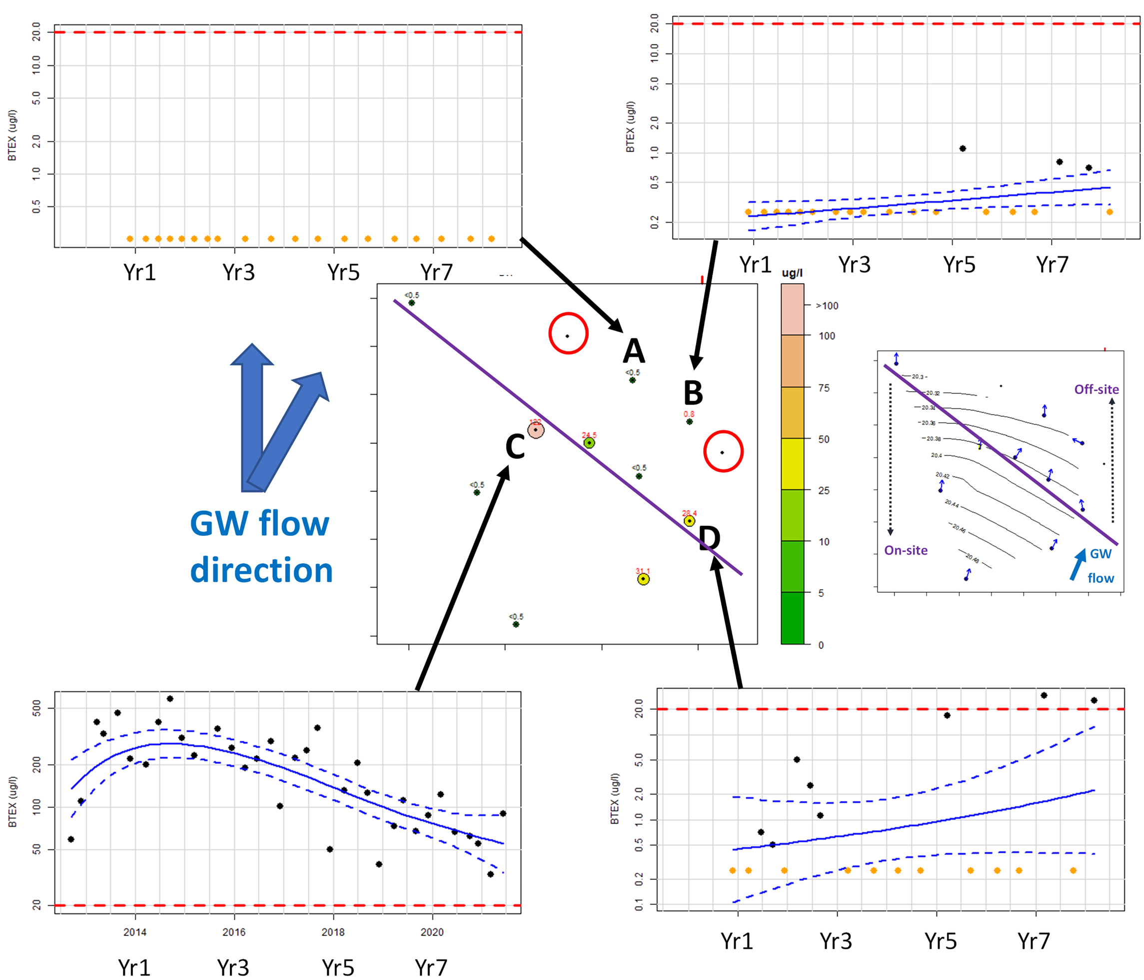

Figure 4. Time slice of spatiotemporal plot (using plot type conc-terrain circles, central plot) showing BTEX concentration including plots showing temporal evolution of concentrations at a select number of wells for case study site #2. Notes, temporal plots: red dashed line refers to user-defined value of threshold concentration value, black dots refer to actual measured concentration values, orange dots refer to non-detect data, blue solid line refers to concentration trend smoother values including upper and lower 95% confidence interval around the estimate (dashed blue line); spatial plot: purple solid line represents site boundary. Insert graph (middle right) shows groundwater contour and flow directions, including site boundary (purple solid line) and location of wells sampled (black dots).

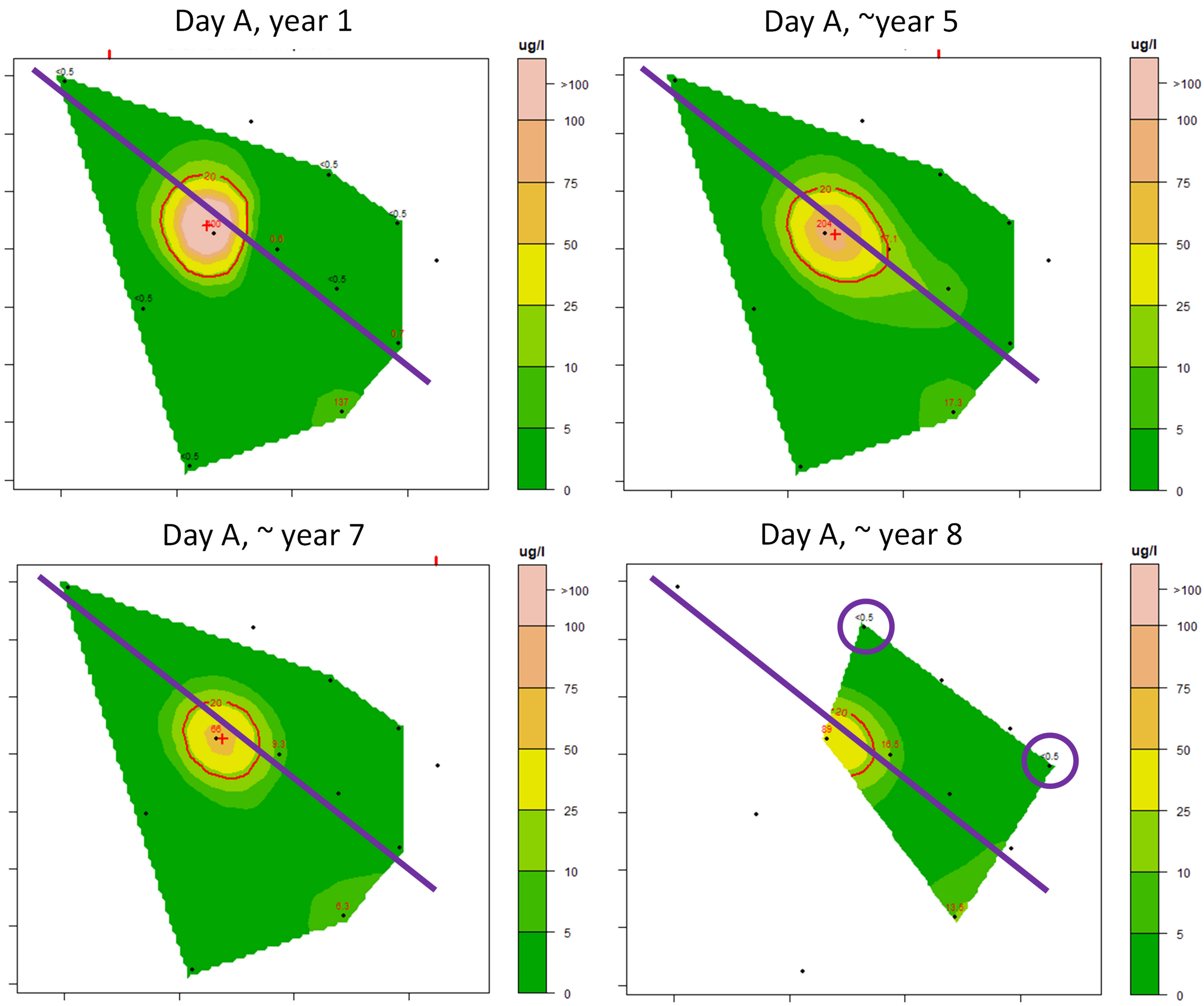

Figure 5. Time slices of the spatiotemporal plots showing historical BTEX plume evolution at case study site #3 over an eight-year period. Notes: red circle refers to predicted plume outline based on a threshold value of 20 µg/L; purple circles indicate location of two new monitoring wells installed in year 8 after evaluation of the monitoring results from years 6 and 7 with integration of monitoring results from previous years; Purple solid line represents site boundary (as per Figure 4 caption). GWSDAT predicted that concentrations in the two new wells will likely be below detection limit when looking at available historic data.

new locations chosen (Figure 5). Hence, this case study showcases that an earlier integration of GWSDAT could potentially have optimized site understanding and decision making around well sampling network and frequency earlier during the lifecycle of this project, which is still on-going. In future groundwater monitoring campaigns, GWSDAT will be an integral part of visualizing and assessing plume evolution/stability over time at this site. For instance, when using the plume diagnostic functionality, a clear trend of a decreasing BTEX plume at this site can be observed over time (Figure 6).

Case Study #4

The last case study presented in this paper relates to the application of the newly introduced well redundancy feature to a large monitoring site. This functionality allows the user to investigate the impact of omitting a well or a combination of wells and investigate the resultant impact on the estimated site plume dynamics. This is performed by independently applying the spatiotemporal smoothing model (Jones et al. 2014) to both the complete and the reduced solute concentration data sets and comparing the results. The site considered is in an industrial area and has been operational for several decades. Over the years, a few impacts to soil and groundwater have occurred, and a large network of groundwater monitoring wells exists at this site (several 10's of wells). To assess the effectiveness of the groundwater monitoring network, GWSDAT's new functionality of well redundancy analysis is being used. Three examples from this site will be presented below to cover the following two scenarios of groundwater well use:

- Scenario 1: Required wells for plume delineation
- Scenario 2: Redundant wells for plume delineation

At this site, groundwater is impacted by various CoPCs (constituents of potential concern). The examples provided here will be based on BTEX. Figure 7 provides an example

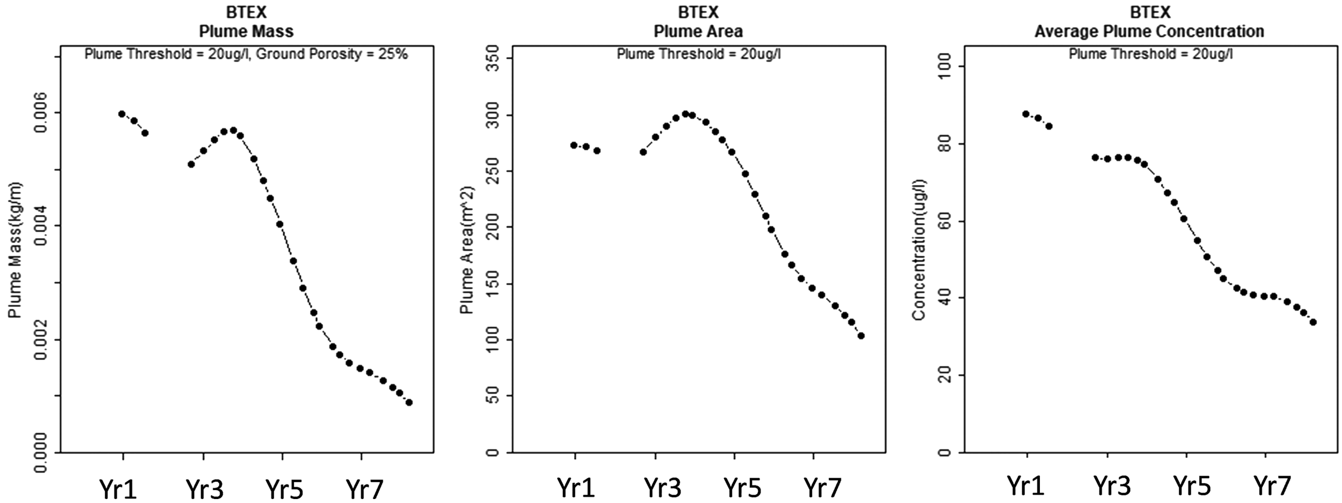

Figure 6. Plume diagnostics for BTEX with a chosen threshold value of 20 μg/L at case study #3. Nb: Yr refers to year.

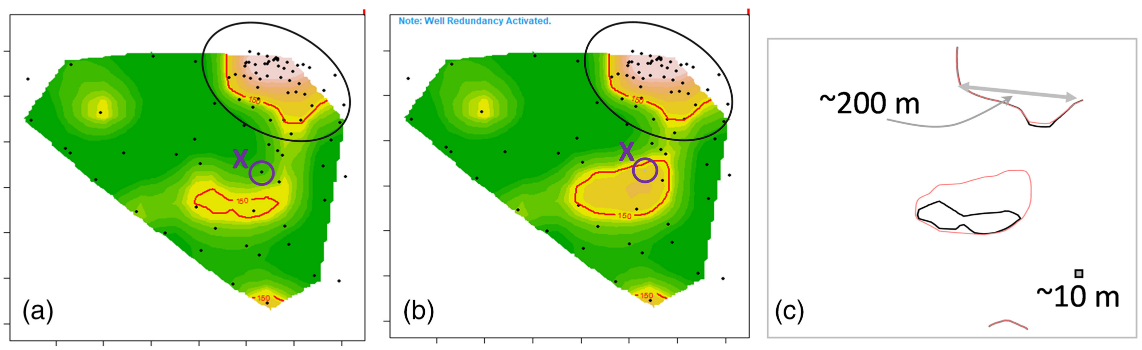

Figure 7. Time slices of a spatiotemporal plot for predicted BTEX plume delineation at case study site #4 with (a) all available data used in analysis and (b) with well redundancy functionality activated (well X removed from analysis). Red outlines show a user-chosen BTEX concentration contour to showcase. (c) Comparison of plume delineation outline (based on chosen concentration contour) for complete dataset (black line) versus reduced dataset (light red line). *Note*: black ellipsoid shows areal extent covered in Figure 8.

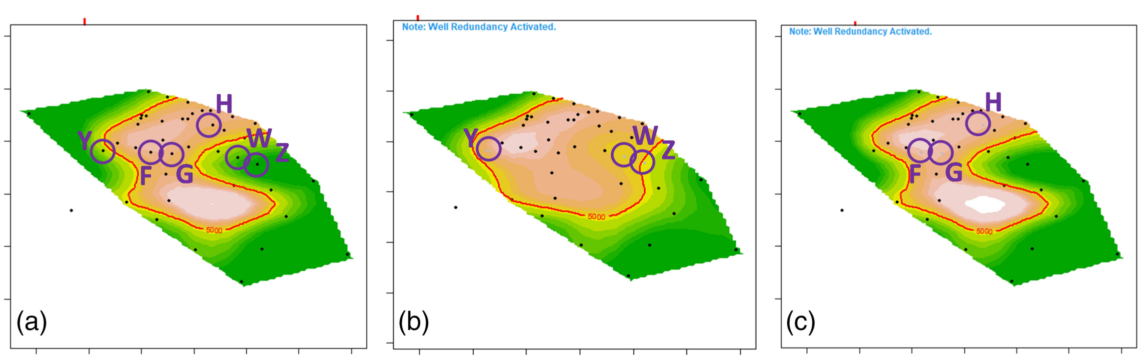

Figure 8. Time slices of a spatiotemporal plot for predicted BTEX plume delineation at case study site #4 with a) all available data used in analysis, and with well redundancy functionality activated for (b) wells Y, W, Z removed and (c) wells F, G, H removed from analysis). *Note*: red outline shows a user-chosen BTEX concentration contour to showcase the impact on plume delineation by removing wells from the data analysis; BTEX concentration below the user-chosen contour are shown in "yellow-green" colors, while concentration above are shown in orange to white colors.

of scenario 1. Figure 7a is a time-slice of the spatiotemporal model illustrating the modeled BTEX plume extent across a part of the site considering all wells available in the dataset. Figure 7b is a time-slice of the spatiotemporal model illustrating the modeled BTEX plume extent across a part of the site with the well redundancy functionality being active. As can be seen, removal of well X highlighted on the Figures 7a and b has a clear impact on the geometry of the plume.

For large sites, one needs to consider that at times there is a need to split the dataset into subsets. This is illustrated in Figure 8, which provides an example for scenario 1 (Figure 8b) and scenario 2 (Figure 8c). Figure 8 covers part of the area

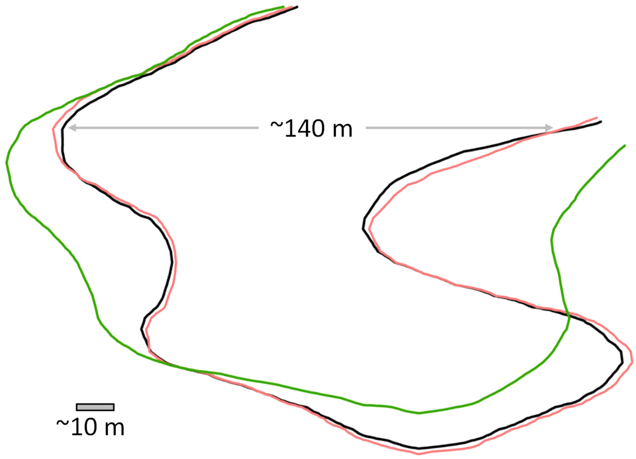

Figure 9. Comparison of plume delineation outline (based on user-chosen BTEX concentration contour) for complete dataset (black line) versus reduced datasets considered in Figure 8b (green line) and Figure 8c (light red line).

included in Figure 7 to get a more detailed understanding of the BTEX plume in that part of the site. A qualitative comparison between Figures 8a–c, highlights that wells Y, W, and Z are important for horizontal plume delineation at this site; while wells F, G, and H could potentially be removed from monitoring activities, as they have little impact on overall understanding of plume geometry (Figure 9).

Future Developments

The major area for future development is the addition of monitoring network optimization tools in GWSDAT. The aim is to support users to develop optimized groundwater monitoring strategies to create datasets that fully support site management decisions and requirements while minimizing exposure, time, and expense associated with collecting and interpreting data. Traditionally, within the environmental monitoring industry, network optimization decision support tools have predominantly been designed from either a spatial (e.g., kriging) or temporal perspective—see, for example, Aziz et al. (2003) and Cameron and Hunter (2002). These tools do not explicitly model the interaction effects across both spatial and temporal components. McLean et al. (2019) demonstrated that spatiotemporal modeling methods result in clearer more accurate plume estimations. This means that significantly smaller sample sizes can be used while retaining estimation accuracy. Hence, this observation together with the body of research in McLean (2018) provides a clear road map for additional integration of spatiotemporal network optimization tools into GWSDAT.

The well redundancy tool released in version 3.1 of GWSDAT, and illustrated in case study #4, is the first step on this journey of expanding GWSDAT's functionality for the application to network optimization. This functionality allows the user to conduct a "with and without" scenario analysis on a user-selected set of wells. Future versions will offer users more assistance by providing a list of wells ordered by an analytical assessment of which may be the most suitable for the omission. Going further forward, it is planned to complement well redundancy analysis with functionality to investigate the benefit of additional wells. This will involve optimally augmenting the existing network with new well locations such as to minimize the uncertainty in monitoring goals, for example, estimated plume extent, area, and mass.

The remaining piece of the road map to be implemented is decision support tools for efficient monitoring well sampling schemes which maximize information extraction while minimizing sampling effort. Once again, the literature in this area is primarily concerned with spatial design arguments, for example, Diggle and Lophaven (2006). The adoption of sampling design principles that accommodate the spatiotemporal nature of the data into GWSDAT will lead to even greater information extraction efficiency than that described in McLean et al. (2019). One such intuitive example of a spatiotemporal design is to sample, for instance, half of the wells spread out across the site for good spatial coverage in one sampling round and to sample the complement of these in the next sampling round. Such a design coupled with a spatiotemporal model would borrow and pool information from the combination of most recently sampled locations, both spatially and temporally, leading to good accuracy with reduced sampling effort.

Shell plc and the University of Glasgow continue to collaborate on developing new and innovative methodologies in the field of monitoring network optimization. Some aspects of this cutting-edge area of research are highly technical and consequently may not be immediately intuitive to understand as compared to, say, leave-well-out redundancy arguments. These techniques could therefore potentially be perceived as "black-box" in nature and lead to a lack of trust and consequently a lack of adoption by practitioners and regulators. To mitigate this risk the developers of GWSDAT plan to continue to work in an open manner and publish the underlying methodologies in peer-reviewed journals while always making the code open-source and completely transparent.

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Disclosure

The authors declare no competing interests.

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