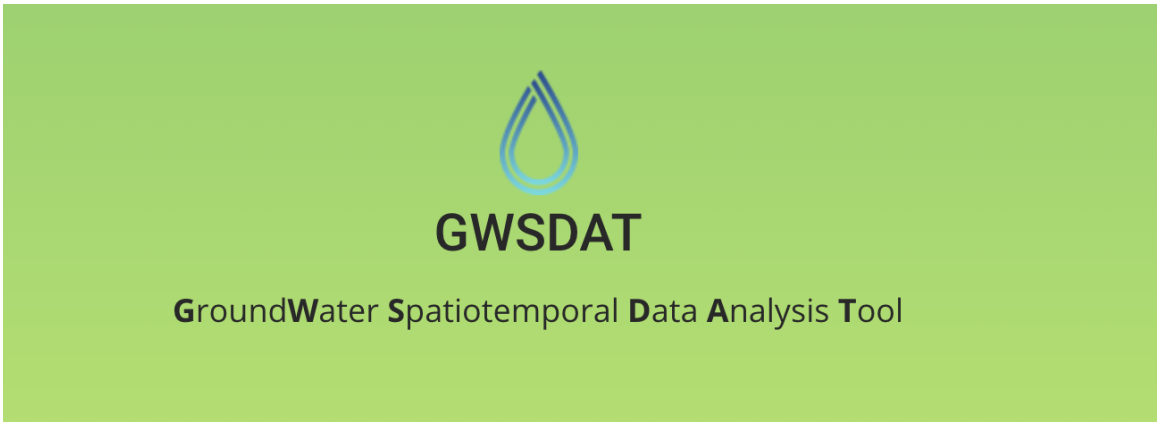

Version 3.1 User Manual

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1 Acknowledgements

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The original idea of GWSDAT was inspired by Marco Giannitrapani.

2 Introduction

The GroundWater Spatiotemporal Data Analysis Tool (GWSDAT[1]) has been developed by Shell Global Solutions and the University of Glasgow to help visualise trends in groundwater monitoring data. It is designed to work with simple time-series data for solute concentration and ground water elevation, but can also plot non-aqueous phase liquid (NAPL) thickness if required. Spatial data is input in the form of well coordinates, and wells can be grouped to separate data from different aquifer units. The software also allows the import of a site basemap in GIS shapefile format. Trend and contour plots generated using GWSDAT can be easily exported directly to a range of different formats, including Microsoft PowerPoint.

The underlying geostatistical calculations are generated using the open source statistical program R (R Development Core Team (2008)). Since version 3.0 the graphical user interface is the open source web framework R Shiny package (`https://shiny.rstudio.com`) which enables both local and online deployment. More details on the statistical methods can be found in the Appendices.

Potential applications where GWSDAT can add value (cost savings and reduction in environmental liabilities) through improved risk-based decision making and response include:

- Early identification of increasing trends or off-site migration.
- Evaluation of groundwater monitoring trends over time and space (i.e., holistic plume evaluation).
- Nonparametric statistical and uncertainty analyses to assess highly variable groundwater data.
- Reduction in the number of sites in long-term monitoring or active remediation through simple, visual demonstrations of groundwater data and trends.
- More efficient evaluation and reporting of groundwater monitoring trends via simple, standardised plots and tables created at the 'click of a mouse'.

[1] **Disclaimer**: There is no warranty for the Program (GWSDAT), to the extent permitted by applicable law. SHELL, Affiliates of SHELL, the copyright holders and/or any other party provide the Program 'as is' without warranty of any kind, either expressed or implied, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose. The entire risk as to the quality and performance of the Program is with the LICENSEE. Should the Program prove defective, the LICENSEE assumes the cost of all necessary servicing, repair or correction.

3 Accessing GWSDAT

There are several different ways for users to gain access to GWSDAT:

3.1 Online Version

With no software installation required, the easiest way is to use the online version, available at `www.gwsdat.net`. This web site also has general information about the software tool, including help files, videos and case studies (`www.gwsdat.net/case-studies`). The underlying architecture is the GWSDAT `R package` deployed as an app on a `Shiny server` hosted by the University of Glasgow's School of Mathematics and Statistics. See the GWSDAT GitHub development page `www.github.com/WayneGitShell/GWSDAT` for more details on how to deploy on a Shiny server.

3.2 Excel Add-in Interface

The most traditional and widely used method to access GWSDAT is to use the Excel Add-in interface. The latest version together with installation instructions and supporting information can can be found on the industry websites:

- American Petroleum Institute (API): `www.api.org/GWSDAT`
- Contaminated Land: Applications in Real Environments (CL:AIRE): `www.claire.co.uk/GWSDAT`

This method of deployment involves installing the open source statistical program R (R Development Core Team (2008)) and Excel Add-in locally on a user's computer. All data sets are retained and analysed locally with no information being sent over the internet. Please note that administrator rights may be required for successful installation.

3.3 GWSDAT R Package

GWSDAT uses the widely available, open source, statistical computing environment `R` (R Development Core Team 2008). This should be downloaded from `www.r-project.org` where versions for all major computing platforms are available. Installation is a very simple process. You may also find it convenient to install the *RStudio* 'Integrated Development Environment' for `R`, freely available from `www.rstudio.com`. This manages some aspects of the `R` environment in a helpful way.

When `R` or `RStudio` is launched, one of the visible windows is a 'console'. GWSDAT is available as a package in `R` and this can be installed by typing the instruction

```
install.packages("GWSDAT")
```

in the console window. Note the capital letters, as `R` is case-sensitive. The package is retrieved from the `R` archive (`CRAN`), so an internet connection is required for this step. The package will then be installed locally. GWSDAT uses several other `R` packages and these will be installed at the same time. There may be a warning message about a mismatch between the version of `R` used to build the package and the version of `R` installed on your computer if this is not the most recent one, but this is unlikely to cause any difficulty. The installation step is required only once. GWSDAT will now be available on your computer at any time, with or without an internet connection.

To launch GWSDAT, issue the following two instructions in the console window:

```
library(GWSDAT)
launchApp()
```

The first instruction loads the package so that it can be used in the current session of `R`. The second instruction launches GWSDAT.

See `www.github.com/WayneGitShell/GWSDAT` for the latest development version together with more advanced information and details on how to use the GWSDAT R package.

4 Input Data Format

There are a few different ways to enter user data into GWSDAT and the available choices will depend upon the way the user is accessing GWSDAT. However, no matter, which way you are `Accessing GWSDAT` the formatting standard and conventions of the raw data input tables are identical. Hence, this section is dedicated to describing the standardised data table input structure and formatting conventions. Later sections will discuss the data input details with respect to the mode of access. See Section 5 for data input via Excel Add-in and Section 6.1 for data input directly via the Graphical User Interface.

There are only two input tables that must be completed, namely, the *Historical Monitoring Data* table and the *Well Coordinates* table. Please note that there should be no empty rows in either table. Optionally, users can also specify links to the location of GIS shapefiles for use as basemaps or site plans.

4.1 Historical Monitoring Data Input Table

Contaminant Data | Well Coordinates

+ Add Row

	WellName	Constituent	SampleDate	Result	Units	Flags
1	SGS5 P1	Nitrate	11/05/2009	54.59	mg/l	E-acc
2	SGS5 P2	Nitrate	11/05/2009	67.93	mg/l	
3	SGS5 P1	Sulphate	11/05/2009	99	mg/l	E-acc
4	SGS5 P2	Sulphate	11/05/2009	61	mg/l	
5	GDBH102	Ethylbenzene	11/03/2009	ND<1	ug/l	
6	GDBH104	Ethylbenzene	11/03/2009	ND<1	ug/l	
7	GDBH104	Toluene	11/03/2009	ND<1	ug/l	
8	GDBH104	TPH	11/03/2009	36	ug/l	
9	MW10	Ethylbenzene	11/03/2009	ND<1	ug/l	
10	MW10	Toluene	11/03/2009	ND<1	ug/l	

Figure 1: Example Historical Monitoring Data.

Each row of this table corresponds to a unique combination of well, sampling date and solute type. Groundwater and NAPL (Non-Aqueous Phase Liquids) gauging data may also be entered in this table. Figure 1 displays an example GWSDAT input data set for illustrative purposes. The columns (fields) in the *Historical Monitoring Data* input table are as follows:

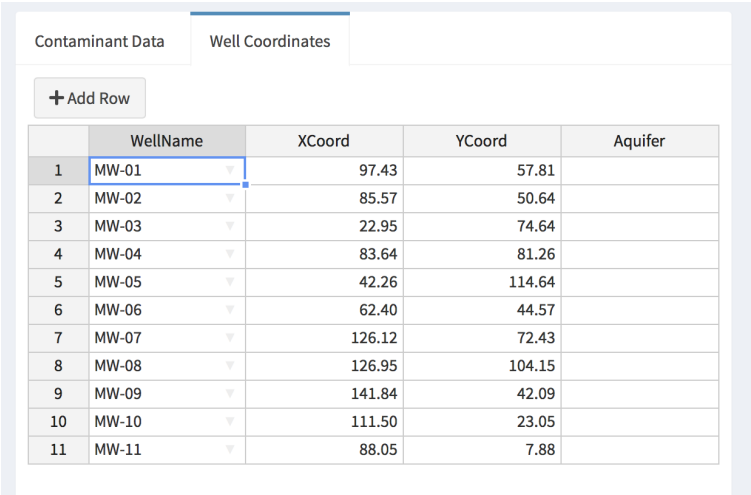
- **WellName**: the name or identifier of the well (or soil boring) from which the sample was collected. Well names must be consistent and unique. For example, 'MW-1' and 'MW1' will be treated as different wells.
- **Constituent**: Here enter the name of the solute type, e.g. Benzene, Toluene. Again in the same manner as WellName please ensure that the name of a solute is consistent and unique for all entries. The identifiers 'GW' and 'NAPL' are reserved for Groundwater elevation measurements and NAPL thickness data respectively, see further details below.
- **SampleDate**: the date at which the well was sampled (not the date the results were returned from laboratory analysis). Please use a calendar date format, the preferred format is 'dd/mm/yyyy'. Do not include a time of day.
- **Result**: the value of the measurement made. This will be a solute concentration, a groundwater level or a NAPL thickness, as specified in the *Constituent* column.
  - **Solute Concentrations**: The concentration of the constituent is entered here. Non-detect values should be entered as either '<X' or 'ND<X', where 'X' is the detection limit specified by the laboratory. For example, if the detection limit is 100ug/l then either '<100' or 'ND<100' is acceptable. The non-detect threshold value must be specified so 'ND' on its own is not permissible.

In the absence of known detection limits, a sensible value must be substituted. This could be the lowest measured value for the solute in the dataset.

  - **Groundwater** level data is entered as an elevation above a common datum, such as metres or feet above sea level or some other common reference height. All groundwater measurement entries should have the same units, such as metres or feet, and the 'Constituent' field should be set to 'GW'. In the presence of NAPL, please ensure that the groundwater level has been corrected for NAPL density.
  - **NAPL** thickness data is also entered here. Please ensure that all NAPL thickness entries have the same units, e.g. feet or metres and that the Constituent field is set to 'NAPL'. If no NAPL is present, do not add a NAPL entry with zero thickness; simply omit from the table. Where NAPL is recorded in soil borings that do not reach the water table the NAPL thickness should be entered as zero. Well location markers for soil borings or wells where NAPL has been recorded are highlighted in red.

- **Units**: Solute concentration data can either be 'mg/l' or 'ug/l'. For groundwater elevation and NAPL thickness data please set to one of 'mm', 'cm', 'metres', 'inches', 'feet' or 'level'. Units must be specified for each entry. All entered groundwater elevation measurements must have the same units. Likewise for NAPL thickness.
- **Flags**: Four different flags are available to modify the way in which certain types of data are handled by the software. The 'E-Acc' (Electron Acceptor), 'NotInNAPL' and 'Redox' flags are used to identify input data types which are to be omitted in the event that the user activates the NAPL substitution function (see Section 5.3). Note, that it is only necessary to flag one data row in this way for all rows containing that constituent to be excluded from NAPL substitution. The fourth flag ('Omit') can be used to exclude individual data entry rows from the GWSDAT analysis.

4.2 Well Coordinates Table



	WellName	XCoord	YCoord	Aquifer
1	MW-01	97.43	57.81	
2	MW-02	85.57	50.64	
3	MW-03	22.95	74.64	
4	MW-04	83.64	81.26	
5	MW-05	42.26	114.64	
6	MW-06	62.40	44.57	
7	MW-07	126.12	72.43	
8	MW-08	126.95	104.15	
9	MW-09	141.84	42.09	
10	MW-10	111.50	23.05	
11	MW-11	88.05	7.88	

Figure 2: Example Well Coordinates Table.

The *Well Coordinates* table is used to store the coordinates of groundwater monitoring wells or soil borings. For most of the purposes of GWSDAT modelling, it is only the relative distances between wells which are important. This means any arbitrary cartesian coordinate system can be used as long as well coordinate values have an aspect ratio very close to 1, i.e. a unit in the x-coordinate is the same distance as a unit in the y-coordinate. Hence, well coordinates can be measured directly from a map, or given in easting and northing, etc.

- **WellName**: the name or identifier of the well or soil boring. Well names must be identical to those specified in the *Historical Monitoring Data* table. On a point of detail, it is better to name wells using the convention of 'MW-01' rather than 'MW1' so that plots in GWSDAT are correctly ordered.
- **XCoord**: the x-coordinate of the well.
- **YCoord**: the y-coordinate of the well.
- **Aquifer**: The (optional) aquifer field allows the user to associate wells or soil borings with particular subsurface features (e.g. aquifers, sub-strata), in the event that data from these needs to be modelled separately. The user can enter the name (maximum of 8 characters) of the aquifer or sub-stratum, or select a letter A-G from the drop-down listbox. The aquifer field can also be used to partition the dataset from a large site, in the event that mutiple unrelated plumes are present or if wells are clustered with large gaps in between. On initiation of a GWSDAT analysis the user is asked to select an aquifer (subsurface feature) to analyse. **Note**: Plots generated using data associated with particular subsurface features have the feature name appended to the title, e.g. Shallow aquifer. If the user leaves the aquifer flag as blank, no such appending will occur.
- **CoordUnits**: Either leave this field blank or select 'metres' or 'feet'. The units specified in this field are used in the calculation of plume mass balance parameters (e.g. plume area and solute mass), for further details see Section **??** on plume diagnostics.

4.3 GIS ShapeFiles

A site plan can be superposed over plots of concentration distribution, NAPL thickness and groundwater elevation (see example in Figure 5). Site plans are imported into GWSDAT in the form of shapefiles (see `http://en.wikipedia.org/wiki/Shapefile` for more information). A shapefile is actually a collection of several files, typically created using ARC-GIS. See the section `Converting a CAD drawing to a Shapefile` for more details on how to generate a shapefile from a CAD drawing using ARC-GIS.

If using the GWSDAT Excel Add-in interface (Section 5.1) then only the location of the main shapefile (file ending with a '.shp' extension) needs to be specified in the GIS Shapefile table. The associated data files (e.g. .dbf, .sbn, .sbx, .shx) will be picked up automatically,provided they are in the same folder (see example in Figure 3).It is possible to overlay multiple shapefiles up to a maximum of seven.

Alternatively, if using the GWSDAT Graphical User Interface interface (Section 6.1) to input data then all the associated Shapefiles (e.g. .shp, .dbf, .sbn, .sbx, .shx) need to be selected and uploaded.

5 GWSDAT Excel Add-in

5.1 Add-in Menu

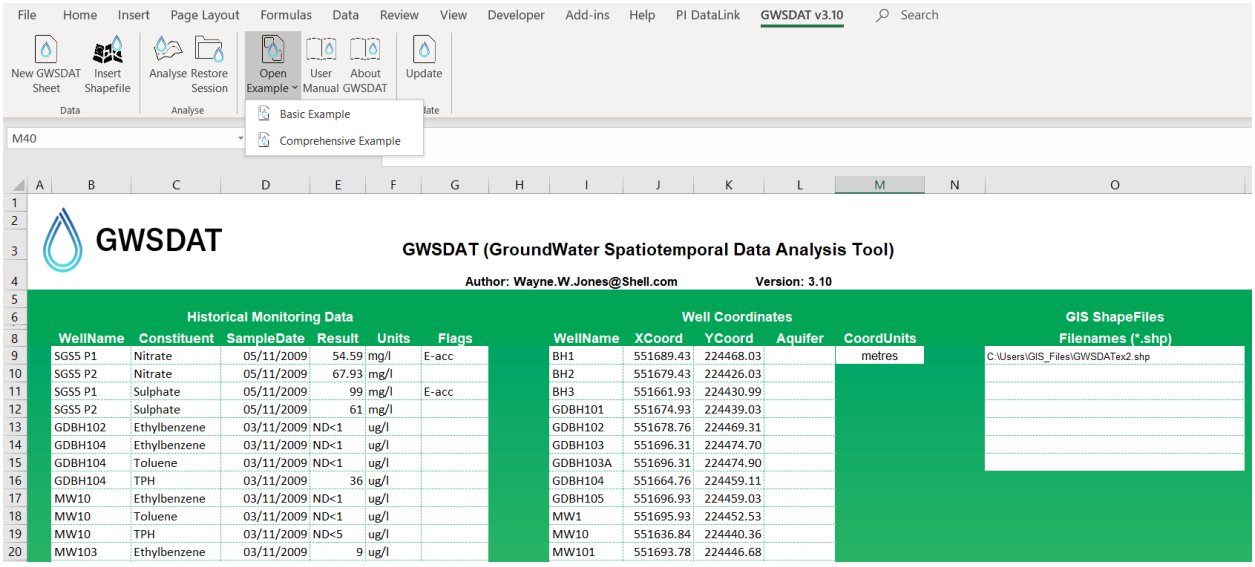


Figure 3: GWSDAT Excel Add-in menu and example data file.

Please see the section `Excel Add-in Interface` for details on how to install the GWSDAT Excel Add-in. The menu options, as shown in Figure 3, are as follows:

- **New GWSDAT Sheet**: Inserts a blank GWSDAT data input template worksheet into the active Excel workbook.
- **Insert Shapefile**: Interactively browse for a shapefile and add location to GIS Shapefiles table, see Section 4.3 for more information.
- **Analyse**: Begin GWSDAT analysis on the Excel active worksheet data.
- **Restore Session**: Load a previously saved GWSDAT session, see Section ?? for more information.
- **Open Example -> Basic Example**: Inserts an example GWSDAT worksheet data set into the active Excel workbook.
- **Open Example -> Comprehensive Example**: Inserts a more detailed example GWSDAT worksheet data set which includes a site plan, NAPL thickness data, 'Electron Acceptor' flagged solutes and multiple aquifers into the active Excel workbook.
- **User Manual**: Opens the online GWSDAT user manual via user's web browser. You must be connected to the internet for this to work.
- **About GWSDAT**: Displays version information and Terms & Conditions for GWSDAT.
- **Update GWSDAT**: Check if a newer version of the underlying GWSDAT R package exists at `https://cran.r-project.org/package=GWSDAT`. If a more recent version is detetced then it will be automatically installed. You must be connected to the internet for this to work.

5.2 Add-in Data Processing Options

On initiation of a GWSDAT analysis via the Excel Add-in, data processing options are displayed, as shown in Figure 4. The data processing options influence how the data is displayed and how non-detects are handled.

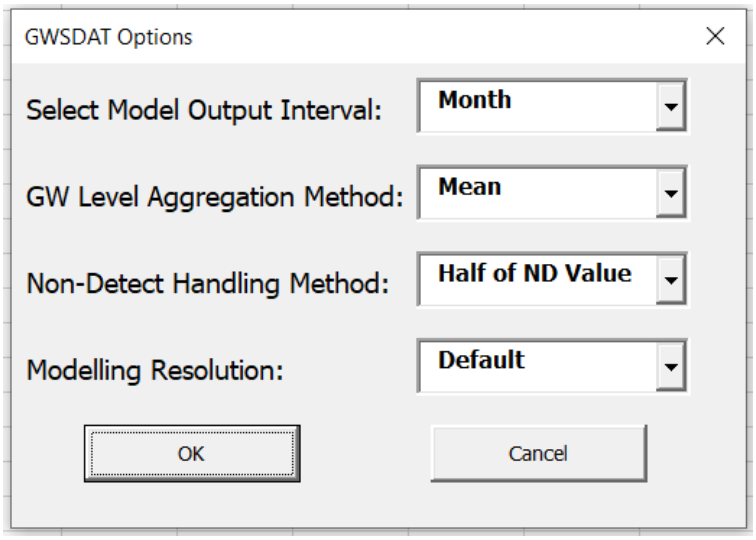


Figure 4: GWSDAT Excel Add-in Processing Options

- **Model Output Interval**: The spatiotemporal model can generate predictions at a user specified interval. The three different options are as follows:
  - **Day**: Concentration and groundwater elevation contour plots are generated for every date represented in the input dataset. This is a good option to choose if each monitoring event comprises samples/ measurements collected within one 24-hour period.
  - **Month**: Concentration and groundwater elevation contours are generated at monthly intervals, working backwards in time from the latest date in the input dataset. Choosing this option aggregates groundwater elevation data within each monthly interval so that a larger dataset is available for the plotting of elevation contours (by local linear regression).
  - **Quarter**: Concentration and groundwater elevation contours are generated at quarterly (3 month) intervals, working backwards in time from the latest date in the input dataset. Choosing this option aggregates groundwater elevation data within each 3-month interval so that a larger dataset is available for the plotting of elevation contours (by local linear regression).

  Note that both the monthly and quarterly model output options only aggregate the dataset used to plot groundwater elevation contours. The solute concentration dataset is not aggregated in time because the spatiotemporal model from which concentration contours are generated does not require this, i.e. the underlying spatiotemporal model used to generate the solute concentration smoother plots does not vary with the data aggregation interval.

  Note that if no monitoring data is present within a particular monthly or quarterly interval, then GWSDAT will not generate a groundwater elevation contour or spatio-temporal solute concentration smoother plot. This is to avoid producing potentially misleading spatial plots far away in time from any actual data.
- **GW Level Aggregation Method**: In the event that there are multiple groundwater elevation measurements from the same well within a given output interval, the user can select how to use this data. The user can select to calculate either the 'Mean', 'Median', 'Min', or 'Max' groundwater elevation. Again, this choice does not affect the spatiotemporal model used to generate the solute concentration smoother plots.
- **Non-Detect Handling Method**: GWSDAT handles non-detect data by a method of substitution. In accordance with general convention, the default option is to substitute the non-detect data with half its detection limit, e.g. ND<50ug/l is substituted with 25ug/l. For a more conservative choice, select

the alternative of non-detect data to be substituted with its full detection limit, e.g. ND<50ug/l is substituted with 50ug/l.

- **Model Resolution**: This option controls the resolution of the spatiotemporal solute concentration smoother (see Appendix 7.1). The user can select between either a default resolution or a higher resolution model fit. In most instances there will be little difference in the modelling results between the two settings. However, in some rare circumstances with complex data sets, it may well be necessary to use the higher resolution setting. Please note it takes approximately 3-4 times longer to fit a higher resolution model.

5.3 NAPL Handling Method

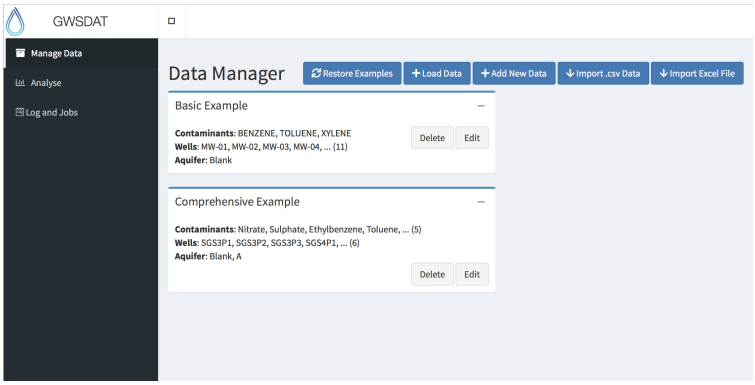
An additional pop-up box will be displayed after the GWSDAT options box if the input contains NAPL data (i.e. 'NAPL' is entered in the constituent field). Selecting 'Yes' to the question 'Do you wish to substitute NAPL values with maximum observed solute concentrations?' forces GWSDAT to recognise NAPL data in the input dataset as indicative of high dissolved solute concentrations. This option has been added to provide the user with a more realistic picture of the area of impacted groundwater in the event that NAPL in wells prevents direct measurement of CoC concentrations. *Before using this function the user should, however, be confident that dissolved solutes are derived from the observed NAPL and not from a different source.* Solutes flagged as 'Electron Acceptors' (see Section 4.1) are omitted from the NAPL substitution process.

6 GWSDAT Graphical User Interface (GUI)

The GWSDAT user interface is a web-based graphical user interface (GUI) which the user can interact with in many ways. The following sections will explain the interface in more detail.

6.1 Data Input via Graphical User Interface

GWSDAT comes supplied with examples of groundwater monitoring data and these can be used to experiment with the tools for analysis and visualisation. If you would like to do this you can move immediately to Section~X of this manual. However, the aim of GWSDAT is of course to provide means of analysing user-supplied data and various options are supplied to allow this. These options are all available from the *Manage Data* page which is the point of entry when GWSDAT is launched but can also be accessed at any time from the *Manage Data* item on the menu bar on the left hand side of the window.



A *Basic Example* and a *Comprehensive Example* are supplied but the buttons at the top of the page allow other data to be entered, in different forms.

Restore Examples	This allows the two in-built examples to be restored at any point, should this be needed.
Load Data	Use the *Browse* button to loaded from a previous GWSDAT session.
Add New Data	This allows data to be entered manually into a spreadsheet (and saved for later use).
Import .csv Data	Use the *Browse* buttons to load separate 'Contaminant Data' and 'Well Coordinates' files, each in '.csv' form. One or more shapefiles may also be loaded.
Import Excel File	Use the *Browse* button to load an Excel spreadsheet containing both 'Contaminant Data' and 'Well Coordinates'. One or more shapefiles may also be loaded.

Import Excel File	The file to be loaded should contain two spreadsheets labelled ‘Contaminant Data‘ and ‘Well Coordinates‘ and have the structure described above. An example spreadsheet is available at *web address at gwsdat.net*.
Import .csv Data	The data can be exported from *Excel() into ‘.csv‘ format. In this case there should be separate ‘.csv‘ files for the *Contaminant Data* and *Well Coordinates*. Click on the *Browse* button to select these files. For convenience, GWSDAT gives options for the *Column separator* and the *Quote for Character Strings* at the foot of this page. Click on the *Import|* button to read the data.
Add New Data	This creates blank spreadsheets with the required structure. Entries can by typed in directly or copied and pasted from another source. There is an *+Add Row* button and right clicking gives further options for adding and removing rows.
Load Data	This allows data which has previously been saved from GWSDAT to be loaded again.

The details of data entry are described below but it is helpful first to describe the format of the data which is required. The essential information is in are two spreadsheets - one which contains the contaminant data, and a second one which gives the co-ordinates of the wells. There is also an option to use shape files to superimpose map information on spatial plots.

An example of the first spreadsheet is shown for the *Basic Example* in the screenshot below. The full spreadsheet can be viewed by clicking the *Edit* button for the *Basic Example* in the *Manage Data* page of GWSDAT. (When you wish to return to the *Manage Data* page, click the ‘back-arrow’ button in the top left hand corner of the *Edit Data* page.) The columns of the spreadsheet are explained in detail below.

Wayne advises against the use of the term ’contaminant’ but this is the terminology used in the software.

GWSDAT is designed to produce informative visualisations of groundwater monitoring over space and time. To illustrate this, we will use the *Basic Example*. If you are still in the detailed pages of the *Manage Data* section, click on the ‘back-arrow’ in the top left hand corner to return to the main *manage Data* page and then click on *Analyse* on the left had sidebar. You will then be asked to specify which dataset you would like to analyse. In addition to the standard examples, any other datasets you have created will be listed here too. For the moment, click on the *Select* button for the *Basic Example’*. You should now see a screen similar to the image below.

The tabs at the top of this page give access to several different forms of analysis. These are described in detail below.

6.2 Spatial plot

The GWSDAT spatial plot (see Figure 5) is for the analysis of spatial trends in solute concentrations, groundwater flow and, if present, NAPL thickness. It displays the locations of the monitoring wells (black solid dots) together with the well names and actual measured solute concentration values (detect data is displayed in a red font; non-detect in a black font). The date interval for the displayed data is indicated above the spatial plot. If a GIS shapefile has been supplied then the major site features (roads, tanks, etc) are overlaid on the spatial plot as light blue lines.

A key feature of GWSDAT is the ability to produce estimates of contaminant concentrations over space and time simultaneously. This gives a more effective method of analysis than the examination of concentration maps at isolated time points, or of time trends at isolated locations. The simultaneous use of information over space and time allows estimates at particular locations and times to ‘borrow strength’ from neighbouring data. Use the slider at the foot of the page to explore how the estimates of Benzene concentration change across the month of October. Note that the slider box at the foot of the page can be moved to any convenient position by clicking and dragging with the mouse. The ‘Play’ symbol (forward-arrow) in the bottom right hand corner of the slider activates a ‘movie’, which can be paused by pressing the button again.

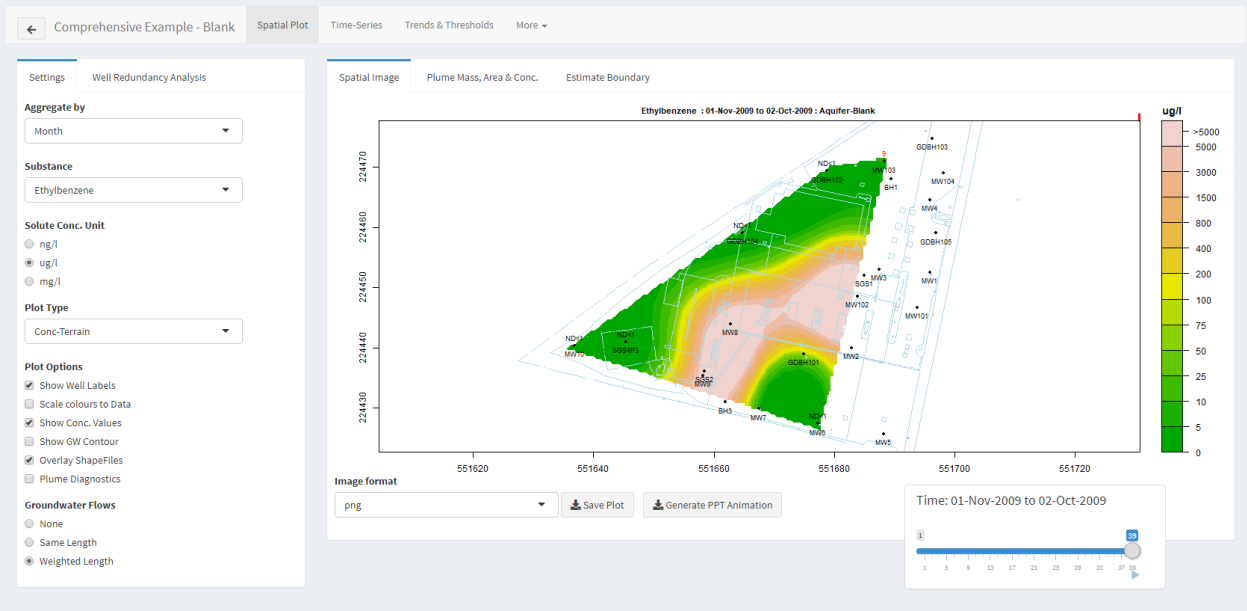


Figure 5: GWSDAT Spatial Plot

6.2.1 Settings

The *Settings* tab located to the left hand side of the spatial plot gives control over many aspects of the display:

- **Aggregate by**: provides a drop-down menu which allows the temporal plotting resolution to be altered (Day, Month, Quarter, Year). In the example in Figure 5, a monthly model output interval has been selected and the displayed actual solute concentration values were sampled between the 2nd Oct 2009 and the 1st Nov 2009. This functionality is identical to the 'Model Output Interval' detailed in Section 5.2.
- **Substance**: Drop-down listbox to select the different solutes to be inspected.
- **Solute Conc. Unit**: allows the units to be changed between one of 'ng/l', 'ug/l' or 'mg/l'.
- **Plot Type**: Drop-down listbox with the following choices:
  - **Conc-Terrain**: This option overlays the predictions of the spatiotemporal solute concentration smoother for a particular model output interval using a 'terrain' colour scheme - see example in Figure 5. Please note that the output of the spatiotemporal trend smoother is always given for the latest date in the displayed output interval. The dark green colours indicate low solute concentration and the colours are gradated through yellow and brown to almost white, to illustrate increasing estimated solute concentrations.The concentration values can be read off from the key on the right hand side of the plot. As the user iterates through time steps, it may be noticed that the area covered by the spatiotemporal solute concentration smoother changes. This is due to the fact that spatiotemporal predictions are only generated between interpolated data and are not extrapolated to regions where no data exists, which could potentially lead to erroneous results. For each time step, the area of the contour is calculated only from the collection of wells for which the monitoring period spans the current model output interval. GWSDAT generates predictions in the convex hull region dictated by these wells. The convex hull (see `http://en.wikipedia.org/wiki/Convex_hull`) may be visualised as the expected boundary if an elastic band was placed around the locations of these wells.
  - **Conc-Topo**: This function is identical to Conc-Terrain but uses a topograghic colour scheme which gradates increasing solute concentrations through blue, green, yellow and beige.

- **Conc-GreyScale**: This function is identical to Conc-Terrain but uses a grey scale colour scheme which gradates increasing solute concentrations through light grey to black. This is useful for printing on black and white printers!
- **Conc-Terrain-Circles**: This selection overlays (terrain) colour coded circles located at the wells which have been monitored within the current model output interval. The size of the circles scales with the log of the observed solute concentration values and the solute concentration range can be read off from the colour key to the right of the plot.
- **Conc-Topo-Circles**:This selection is identical to Conc-Terrain-Circles but uses a topographic colour scheme.
- **Conc-GreyScale-Circles**: This selection is identical to Conc-Terrain-Circles but uses a grey scale colour scheme.
- **NAPL-Circles**: This selection displays the observed NAPL thicknesses within the current model output interval as size scaled and colour coded circles. NAPL thickness ranges are read off from the colour key on the right hand side of the plot. Colours are gradated from dark red through yellow to almost pure white to illustrate increasing NAPL thickness. The location of wells which have recorded NAPL in any part of their monitoring history are coloured with red solid dots instead of the usual black solid dots.

Hint: In the presence of poor well location network design or limited data then it is recommended the user select either the 'Terrain-Circles' or 'Topo-Circles' plot type.

- **Plot Options**:
  - **Show Well Labels**: This controls whether to display well names/labels immediately below the well locations.
  - **Scale colours to Data**: By default the colour key of solute concentrations is subdivided as shown in Figure 5. By using the same subdivisions the spatiotemporal solute concentration smoother plots can be directly compared between different model output intervals. This control will produce a new colour key whose subdivisions span the concentration predictions for the current model output interval only.
  - **Show Conc. Values**: This controls whether to display actual sampled concentration values immediately above the well locations. If the data is identified as a NAPL measurement the value will be displayed as 'NAPL' in a red font.
  - **Show GW Contour**: To add contour lines of groundwater level data. This superposes isobars of smoothed groundwater elevation data on top of the solute concentration plot. This is achieved through a 2D extension of the local linear regerssion method described in Appendix 7.4.
  - **Overlay Shapefiles**: This controls whether to overlay a site plan.
  - **Plume Diagnostics**: This controls whether to calculate and display plume diagnostic quantities from the predictions of the spatiotemporal solute concentration smoother (see Figure **??**).The delineated plume is displayed with a solid red contour line which also includes a label displaying the plume boundary threshold value. The plume centre of mass is displayed with a red cross and the plume mass and area printed at the bottom left margin of the spatial plot. Note: in order for the correct plume diagnostics units to be used the *CoordUnits* field in the *Well Coordinates* table must be specified, see Section 4.2. More details about plume diagnostics can be found in Section **??** and Appendix 7.2.
- **Groundwater Flows**: The blue arrows in Figure **??** display the estimated direction and (relative) hydraulic gradient of groundwater flow at monitoring points across the a site. This is calculated from the combination of well coordinates and recorded groundwater elevations for this particular model output interval (see Appendix 7.3 for more details). This radiogroup allows the user to choose either

'not to display groundwater arrows' or 'direction only arrows' or 'both direction and relative strength arrows' (default).

The spatiotemporal solute concentration smoother is a function which simultaneously estimates both the spatial and time series trend in site solute concentrations. By smoothing the data in both space and time it provides a clearer interpretation of site solute concentration dynamics than would otherwise be gleaned from the raw data. However, it is important to note that it is a smoother function and as such, the predictions do not necessarily lie on the observed data points. In the event that a sampled concentration value is significantly larger than the predictions of the spatiotemporal smoother, the well label is coloured red and surrounded by braces, e.g. '<MW-1>'. This serves as a very useful method for outlier detection. In addition, the analysis may be skewed if data are input from monitoring wells with disparate construction or screened in different aquifer systems.
Another important point to consider is that the quality of the spatiotemporal smoother is directly influenced by quality of the underlying data. In general, data originating from sites with many evenly spatially distributed wells with a long time history leads to better quality smoother predictions. The converse of a small number of wells or poor well location network design (e.g. wells located in almost a straight line), or short monitoring history, will lead to less reliable smoother predictions, particularly at the edges.
In summary, the 'spatiotemporal solute concentration smoother' plot is provided to help the user visualise the distribution of solutes and as an aid to risk-based decision-making. However, for the reasons stated above, the predictions should be interpreted with care and a more detailed evaluation may be necessary to understand observed trends and outliers.
Further methods for assessing the goodness of fit of the spatiotemporal smoother can be found in Section **??**. For more details on the spatiotemporal smoothing algorithm, please see Appendix 7.1.

Output formats + PPT movie

6.3 Time Series

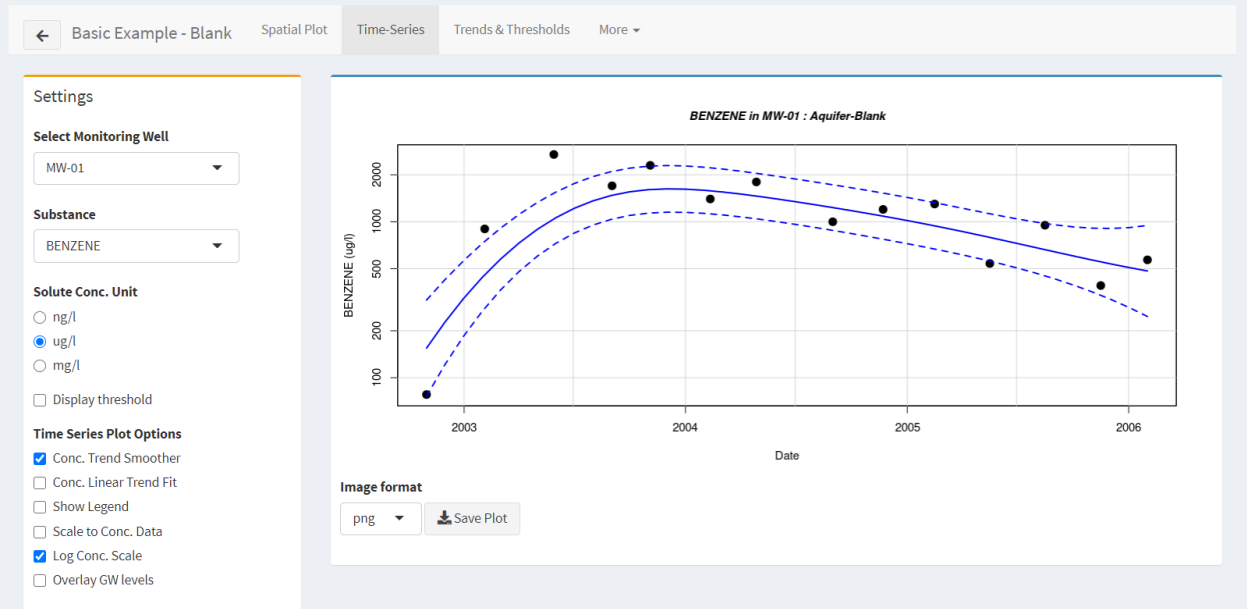


Figure 6: GWSDAT Time Series Plot

The Time Series plot enables the user to investigate time series historical trends of solute concentrations in individual wells. Figure 6 displays an example GWSDAT Time Series plot of' 'Benzene' in well 'MW-01' using an illustrative example dataset. The actual sampled concentration values are plotted against sampling date

and are represented as black solid points. Orange points represent the substituted non-detect values according to the selection chosen in Section 5.3. Red points represent the NAPL substitued solute concentration values.

To switch between different solutes and monitoring wells, simply select from the *Substance* and *Select Monitoring Well* listboxes. The *Solute Conc. Unit* radiogroup allows the units to be changed between one of 'ng/l', 'ug/l' or 'mg/l'. The *Display Threshold* checkbox allows the user to overlay threshold value used to colour code the Trend and Threshold Inidictor plot - see Section 6.4.

The *Time Series Plot Options* checkbox control includes:

- **Conc. Trend Smoother**: This displays the estimated time series trend in solute concentration using a nonparametric smoother (see Figure 6. The solid blue line displays the estimate of the mean trend level at a particular point in time. The upper and lower dashed blue lines depict a 95% confidence interval around this estimate. This is interpreted as *'one is 95% confident that the actual mean trend level lies within this region'*. The smaller the 95% confidence interval, the more confidence one has in the estimated time series trend. Areas of the trend smoother fit in which the 95% confidence intervals are very large (i.e. very low confidence in the trend smoother fit)are coloured grey instead of blue and are disregarded from the 'Trend' and 'Threshold - Statistical' matrix plot calculations, see Section 6.4. The advantage of this nonparametric method is that the trend estimate is not constrained to be monotonic, i.e. the trend can change direction. More details of this nonparametric smoothing algorithm are given in Appendix 7.4
- **Conc. Linear Trend**: This displays a traditional linear time series trend estimate (green solid line) together with 95% confidence intervals (green dashed lines) to the log of historical solute concentrations values. This is equivalent to fitting an exponential decay/growth model on a linear scale. The statistical significance of this trend is assessed by means of the well established Mann-Kendall trend test Mann (1945). The Mann-Kendall p-value and the estimated solute concentration half-life is displayed immediately below the main title of the *Time Series* plot. Users should be aware that individual well half-life values should not be used to estimate the plume half-life.

If the Mann-Kendall p-value is below 0.05, then the estimated trend is deemed statistically significantly different from 0, i.e. there is indeed trend present in the data. A p-value above 0.05 should be interpreted as there is no evidence to suggest that trend is present.

- **Show Legend**: This controls whether to display a legend in the top right hand side of the plot giving a key of the plotting symbols.
- **Scale to Conc. Data**: By default the *Time Series* plot x-axis is scaled such that it spans the sampling dates of all data. The y-axis is scaled to span the current data concentrations and the user-specified trend threshold limit, see Section 6.4. By checking this control the x and y axes are scaled to the span the current combination of well and solute concentration data only.
- **Log Scale**: Controls whether to use a logarithmic or linear scale for the y-axis, i.e. solute concentration values.
- **Overlay GW levels**: Allows the user to overlay the corresponding groundwater level measurements on the well trend plot. The scale is read from the right hand axis. This function is useful for assessing correlations between groundwater levels and solute concentrations.
- **Overlay NAPL Thickness**: Allows the user to overlay the corresponding NAPL thickness level measurements on the well trend plot. The scale is read from the right hand axis. This function is useful for assessing correlations between NAPL thickness and groundwater levels.

Wayne: Check for 'Well trend plot' and replace with *Time Series* plot.

6.4 Trends & Thresholds

The Trends and Thresholds Indicator Matrix plot (a.k.a. Traffic Light Plot) is a summary of the level and time series trend in solute concentrations at a particular model output interval, see Figure 7. The rows

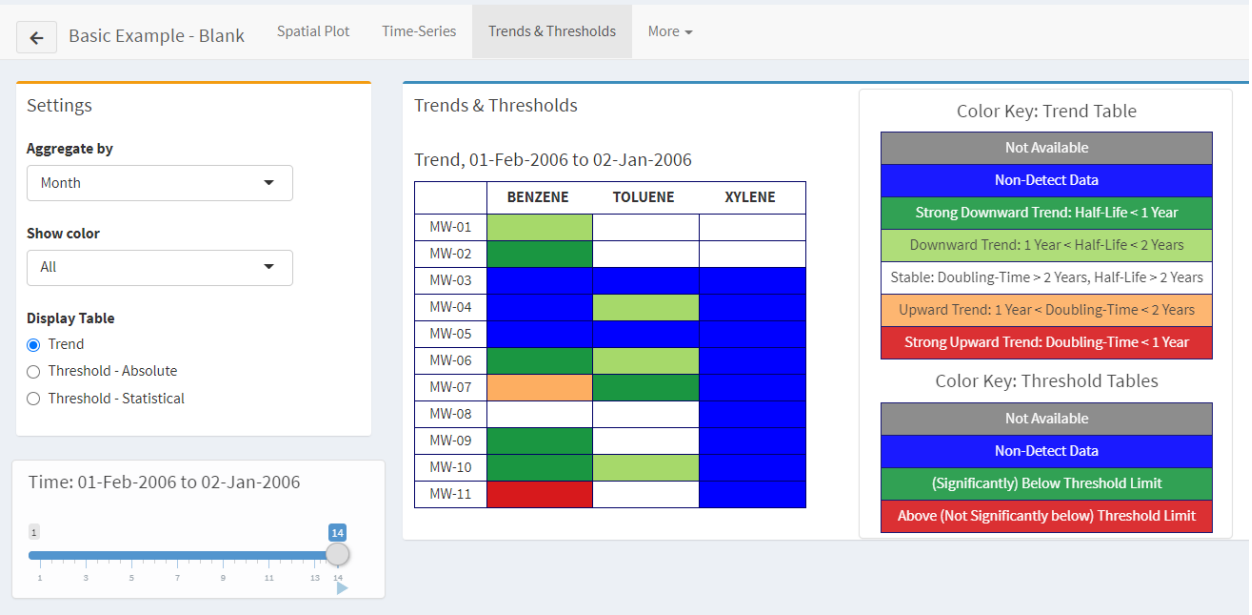


Figure 7: GWSDAT Trends and Thresholds Indicator Matrix Plot.

correspond to each well and the columns correspond to the different solutes. The options are as follows:

- **Display Table**: This drop-down listbox allows the user to select from the following options:
  - **Trend**: This reports the concentration trend for each solute in every well within the selected model output interval. The Trend Threshold Indicator Matrix looks at the instantaneous gradient of the trend smoother (solid blue line) where it crosses the end of the current model output interval in the *Time Series* Plot, see Figure 6. The cells of the Trend Threshold Indicator Matrix are coloured to indicate the strength and direction of the current trend. White cells indicate a generally flat trend where the solute concentration is estimated to no more than double or half in the next two years. Light red and light green indicate that solute concentrations will no more than double or half in the next year, respectively. Dark red and Dark green indicate stronger upward and downward trends, respectively. In the event that the trend cannot be calculated, e.g. no data or our confidence in the trend smoother estimate is poor then the corresponding cell is coloured grey. Blue cells represent non-detect data. As an example consider Figures 6 and 7. It can be seen that the trend at the end of the current model output interval (01-Feb-2006) for 'Benzene' at monitoring well 'MW-01' is decreasing. The corresponding cell in Figure 7 (top left) has been coloured light green to illustrate this.
  - **Threshold - Absolute**: This assesses if the **observed** solute concentration values for all well and solute combinations are below a user-specified threshold value (default value of 500 ug/l) within any given model output interval. The threshold value is displayed as a horizontal dashed red line in the *Time Series* Plot, see Figure 6 when the *Display Threshold* checkbox has been selected, see Section 6.3. The 'Threshold - Absolute' Indicator Matrix compares the observed concentration values with the threshold value. If any observed concentration values within a model output interval are above the threshold value then the corresponding cell is coloured dark red. If the concentration values within a model output interval are all below the threshold value then the corresponding cell is coloured dark green. In the event that no data exists then the cell is coloured grey. If the current concentration value is classified as non-detect, then the corresponding cell is coloured blue. See Section **??**) for details on how to edit the threshold values for each solute.
  - **Threshold - Statistical**: This assesses if current solute concentration levels for all well and solute combinations are below a user-specified threshold value **with a statistical degree of**

confidence. Again the threshold value is displayed as a horizontal dashed red line in the *Time Series* Plot, see Figure 6 when the *Display Threshold* checkbox has been selected, see Section 6.3.The 'Threshold - Statistical' Indicator Matrix looks at the intersection of the end of the current model output interval (vertical grey line) and the trend smoother (solid blue line). If the upper 95% confidence interval (upper dashed blue line) is below the user-specified threshold value, the cell is coloured dark green. If the upper 95% confidence interval is not below the threshold value, the corresponding cell is coloured dark red. In the event that this cannot be calculated, e.g. no data or our confidence in the trend smoother estimate is poor then the cell is coloured grey. If the current concentration value is classified as non-detect, then the corresponding cell is coloured blue.

See Section **??**) for details on how to edit the threshold values for each solute.

- **Show colour**: this drop-down listbox allows the user to filter the *Trends and Thresholds* plot according to the different colours. For example, if the user selects red then the plot will only display the corresponding rows and columns which contain a red entry. This function is particularly useful when there exists a large number of wells and/or solutes.
- **Aggregate by**:

A floating 'Colour Key' graphic displaying the colour key explained above for the Trend and Threshold Indicator Matrix plot. Use the slider at the foot of the page to explore how the estimates of Benzene concentration change across the month of October. Note that the slider box at the foot of the page can be moved to any convenient position by clicking and dragging with the mouse. The 'Play' symbol (forward-arrow) in the bottom right hand corner of the slider activates a 'movie', which can be paused by pressing the button again. The Settings box gives control over many aspects of the display. Aggregate by provides a drop-down menu which allows the temporal resolution to be altered (Day, Month, Quarter, Year). This gives different perspectives on the trends present in the data. Of course, the highest resolution (here, day) will be constrained by the frequency of data collection.

6.5 Reporting

In addition to providing visualisation of groundwater monitoring data, GWSDAT is also able to export displays in a variety of file formats, for inclusion in reports. The map displays in the *Spatial Plot* tab of the *Analyse* section are used to illustrate this. At the foot of the main map display there are three buttons.

- **Image format** provides a drop-down menu of the file type used when a spatial plot at a particular time point is created. The available file types `png`, `jpg`, `pdf`, `ps` and `pptx`.
- **Save Plot** creates and downloads a file in the specified format.
- **Generate PPT Animation** creates a downloads a sequence of plots which display concentration maps across the whole time course. Paging through these slides provides a very simple but effective means of animation.

7 Appendices

7.1 Spatiotemporal Solute Concentration Smoother

The spatiotemporal solute concentration smoother is estimated using a non parametric regression technique known as Penalised Splines (P-Splines). It is beyond the scope of this document to give a full and detailed explanation of this technique here. However, the following outlines some of the most important aspects for the purposes of GWSDAT. For a more detailed explanation the reader is referred to Eilers and Marx (1992) and Eilers, Rijnmond, and Marx (1996).

Let y_i be the solute concentration at $\boldsymbol{x_i} = (x_{i1}, x_{i2}, x_{i3})$ where x_{i1} and x_{i2} stand for the spatial coordinates of the well and x_{i3} represents the corresponding time point for the *i-th* observation with $i = 1, \ldots, n$. We start by modelling the solute concentration as

$$y_i = \sum_{j=1}^{m} b_j(\boldsymbol{x_i})\alpha_j + \epsilon_i \tag{1}$$

where the b_j, $j = 1, \ldots, m$ are m functions (known as *basis functions*) conveniently chosen to achieve smoothness (generally a particular kind of polynomial of order 3). The first term in equation (1) is a linear combination of the basis functions b_j, each evaluated at $\boldsymbol{x_i}$, and aims at capturing the deterministic part of the *i-th* observation, generally known as 'signal'; the second term, ϵ_i, accounts for the variability in the measurement due to randomness and is usually termed as 'noise'. The behaviour of ϵ_i is described in terms of a convenient probabilistic model; such a model guarantees that the value of ϵ_i fluctuates around zero conveying the idea that we do not expect to make any systematic error in the measurement. This model also comprises the notion that the expected spread of ϵ_i is given by σ^2, %a non-negative parameter σ; its squared %value is known as the *variance* of the random component ϵ_i. By using the matrix notation

$$\boldsymbol{B}(\boldsymbol{x}) = \begin{pmatrix} b_1(x_1) & \cdots & b_j(x_1) & \cdots & b_m(x_1) \\ b_1(x_2) & \cdots & b_j(x_2) & \cdots & b_m(x_2) \\ \vdots & \cdots & \vdots & \cdots & \vdots \\ b_1(x_i) & \cdots & b_j(x_i) & \cdots & b_m(x_i) \\ \vdots & \cdots & \vdots & \cdots & \vdots \\ b_1(x_n) & \cdots & b_j(x_n) & \cdots & b_m(x_n) \end{pmatrix}$$

equation (1) can be written in a more compact fashion as $\boldsymbol{y} = \boldsymbol{B}(\boldsymbol{x})\boldsymbol{\alpha} + \boldsymbol{\epsilon}$. Because, as mentioned earlier, we expect the ϵ_i's to oscillate around zero, a sensible choice for the regression parameters $\boldsymbol{\alpha}$ is the one that minimises the norm of the vector $\boldsymbol{\epsilon}$ defined as $\mathrm{S}(\boldsymbol{\alpha}) = \|\boldsymbol{\epsilon}\|^2 = \|\boldsymbol{y} - \boldsymbol{B}(\boldsymbol{x})\boldsymbol{\alpha}\|^2$. A large value of basis functions is generally chosen to allow the model to capture most of the signal. The downside of this approach is that it tends also to overfit, that is to fit the noise in the observations, with the consequent loss of smoothness. To overcome this hurdle, the objective function %to be optimised $\mathrm{S}(\boldsymbol{\alpha})$ is modified with the addition of a term that penalises the lack of smoothness of the fit.

The objective function now takes the form $\mathrm{S}(\boldsymbol{\alpha}) = \|\boldsymbol{y} - \boldsymbol{B}(\boldsymbol{x})\boldsymbol{\alpha}\|^2 + \lambda\|D\alpha\|^2$ where λ is a non-negative smoothing parameter and D is the $(m-2) \times m$ matrix

$$\boldsymbol{D} = \begin{pmatrix} 1 & -2 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & & \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 \end{pmatrix}$$

The additional term in the objective function

$$\|D\alpha\|^2 = (\alpha_1 - 2\alpha_2 + \alpha_3)^2 + \ldots + (\alpha_{m-2} - 2\alpha_{m-1} + \alpha_m)^2$$

controls the smoothness of the fit by applying penalties over adjacent coefficients. By minimising the new objective function for a given value of λ, we obtain the least squares estimator of the parameters

$$\hat{\boldsymbol{\alpha}} = \left(\boldsymbol{B}'\boldsymbol{B} + \lambda \boldsymbol{D}'\boldsymbol{D}\right)^{-1} \boldsymbol{B}'\boldsymbol{y}.$$

Consequently, the fitted values are given by:

$$\hat{\boldsymbol{y}} = \boldsymbol{B}\hat{\boldsymbol{\alpha}} = \boldsymbol{B}\left(\boldsymbol{B}'\boldsymbol{B} + \lambda \boldsymbol{D}'\boldsymbol{D}\right)^{-1} \boldsymbol{B}'\boldsymbol{y} = \boldsymbol{H}\boldsymbol{y}$$

When $\lambda = 0$, the expression for the estimator of the parameters $\{\ \hat{\boldsymbol{\alpha}}\ \}$ boils down to the classical solution in linear models theory. As $\boldsymbol{\lambda} \to \boldsymbol{\infty}$, the fitted function tends to a linear function. The Figure below shows the effect of penalisation: it forces the coefficients to yield a smooth pattern. The fitting process of a function using B-Splines is pictured with and without penalisation, together with the basis functions (the columns of the $\boldsymbol{B}$ matrix). The left plot results from not penalising ($\boldsymbol{\lambda = 0}$) the term in the objective function that accounts for the smoothness; it can be noticed that it yields a rather wiggly regression function. In the right plot, a suitable choice for $\boldsymbol{\lambda}$ constrains the optimisation method to find values for the coefficients $\hat{\boldsymbol{\alpha}}$ which result in a smoother regression curve.

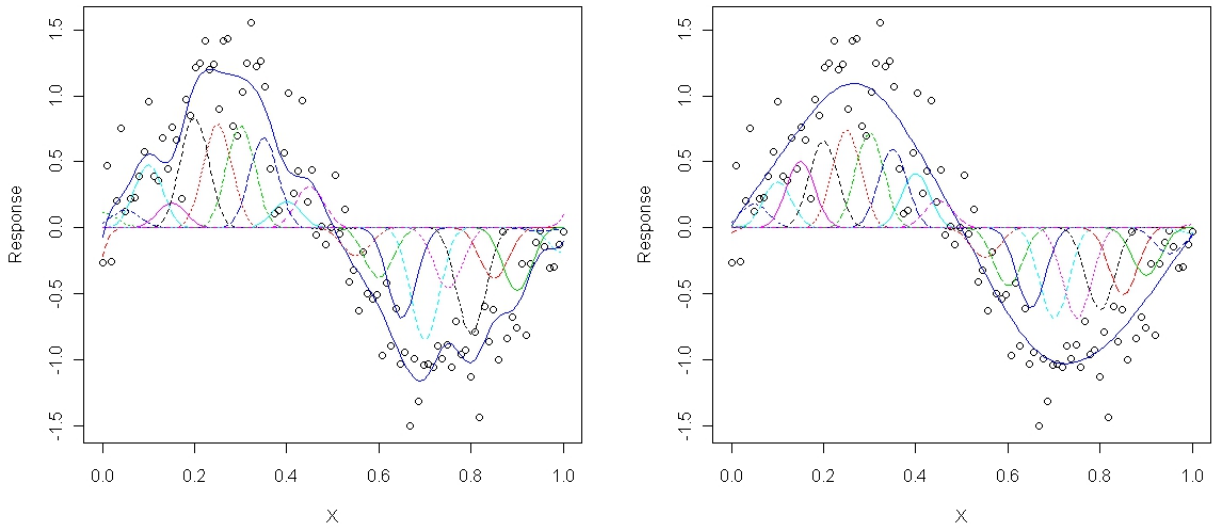


fig.cap: Curve based on 20 nodes in the basis, without penalisation (left), with penalisation (right).

Prior to fitting the regression coefficients $\boldsymbol{\alpha}$ the observed solute concentration values are natural log transformed. This avoids the possibility of predicting negative concentration values and also helps the model cope with data which often spans several orders of magnitude. Furthermore, the uncertainty in the measured concentrations can reasonably be expected to be proportional to the magnitude of the value, e.g. the uncertainty around a measured value of 10ug/l would be expected to be very much less than the uncertainty surrounding a measured value of 10000ug/l. The natural log transformation stabilises the variance.

The choice of the penalisation parameter $\boldsymbol{\lambda}$ is a crucial matter as a too small value would result in 'overfitting' (tracking the noise) whereas an extremely large value would lead to 'underfitting' (producing a flat estimated function as a result of loss of signal). Several criterias have been proposed, such as those described by C. Hurvich and Simonoff (1998) and Wood (2006), but we tackled the issue by a *Bayesian* approach; see Denison et al. (2002), Raftery, Madigan, and Hoeting (1997) and Wood (2011).

Under this paradigm, $\boldsymbol{\lambda}$ is not considered to be a fixed unknown quantity to be estimated but rather a random variable whose value may vary within a given range. This behaviour is described in probabilistic terms which assign a measure of confidence or *probability* to each of the values $\boldsymbol{\lambda}$ may take on.

The Bayesian framework allows to compute the probability that the random variable $\boldsymbol{\lambda}$ may take a particular value, conditional on the fact that $\boldsymbol{y}$ has already been observed. This probability, indicated as $\boldsymbol{f(\lambda|y)}$, is known as the *posterior distribution* of $\boldsymbol{\lambda}$.

Bayes' rule states that $\boldsymbol{f(\lambda|y) \propto f(y|\lambda)f(\lambda)}$ where $\boldsymbol{\propto}$ stands for "proportional to". $\boldsymbol{f(y|\lambda)}$ is known as the *likelihood function* and expresses the conditional probability of observing data $\boldsymbol{y}$, given that the true value of the parameter is $\boldsymbol{\lambda}$; $\boldsymbol{f(\lambda)}$ is known as the *prior distribution* of the random variable $\boldsymbol{\lambda}$ and comprises our prior beliefs on its uncertainty.

The optimal value of $\boldsymbol{\lambda}$ is the one that maximises the posterior distribution and is computed using numerical methods.

7.2 Plume Diagnostics

GWSDAT calculates plume diagnostic quantities from the predictions of the `Spatiotemporal Solute Concentration Smoother`. In common to Aziz et al. (2003) and Ricker (2008), numerical methods are employed to integrate out the plume diagnostic quantities. For a given model time step a fine spatial mesh grid of predictions is generated. The plume boundary region $\boldsymbol{D}$, for a given plume threshold concentration value, is calculated using the R function *contourLines* which is included in the base distribution of the R programming language (R Development Core Team (2008)). The plume area, $\boldsymbol{A}$, is defined as

$$\boldsymbol{A = \iint_D dxdy} \tag{2}$$

where where $\boldsymbol{x}$ and $\boldsymbol{y}$ are the spatial coordinates and is calculated numerically using the *areapl* function from the R package splancs Rowlingson et al. (2021). The average plume concentration is defined as

$$\boldsymbol{\frac{1}{A} \iint_D \hat{s}_t\,(x, y)\,dxdy} \tag{3}$$

where $\boldsymbol{\hat{s}_t\,(x, y)}$ represents the predictions of the spatiotemporal solute concentration smoother evaluated at time $\boldsymbol{t}$. This integral (and all subsequent integrals in this section) is calculated numerically using a method described in Oloufa (1991). A Delaunay triangulation is performed using the R package 'deldir', Turner (2021), on the spatial mesh grid of predictions within the plume boundary, $\boldsymbol{D}$.
The integral is numerically approximated by summing up the individual volumes under each prism formed.

Plume mass is calculated from the scaled product of plume area and average concentration. The scaling factor encompasses the user specified value of ground porosity (see `Plume Diagnostics`) and appropriate scaling values for mapping together the volumetric concentration units (e.g. ug/l) with the length scale (see **CoordUnits** in `Well Coordinates Table`) of the Well coordinates (e.g. metres or feet). The plume mass is calculated on a mass per unit aquifer depth basis (e.g. kg/m). To calculate the total plume mass the user must multiply this value by the aquifer depth.

The plume center of mass $\boldsymbol{(x, y)}$ is defined as the mean location of the concentration distribution within the plume boundary region $\boldsymbol{D}$. The x-coordinate of the plume Centre of Mass is evaluated by numerical calculation of

$$\boldsymbol{X_c = \frac{\iint_D x\hat{s}_t\,(x, y)\,dxdy}{\iint_D \hat{s}_t\,(x, y)\,dxdy}} \tag{4}$$

where x and y are the spatial coordinates and $\hat{s_t}(x, y)$ represents the predictions of the spatiotemporal solute concentration smoother evaluated at time t. In a completely analogous manner the y-coordinate of the plume Centre of Mass is evaluated as follows:

$$Y_c = \frac{\iint\limits_D y\hat{s_t}(x, y)\, dxdy}{\iint\limits_D \hat{s_t}(x, y)\, dxdy} \tag{5}$$

In the event that multiple plumes are detected then the above quantities are calculated for each individual plume and aggregated together. The individual plume areas and masses are summed to calculate the total over all plumes. The aggregate average plume concentration and aggregate plume centre of mass is calculated by taking a weighted average of the individual quantities.

7.3 Groundwater Flow Calculation

For a given model output interval the Groundwater (GW) flow strength and direction are estimated using available GW level and well coordinates data. The model is based on the simple premise that local GW flow will follow the local direction of steepest descent (hydraulic gradient).

For a given well, a linear plane is fitted to the local GW level data:

$$L_i = a + bx_i + cy_i + \epsilon_i \tag{6}$$

where L_i represents the GW level at location (x_i, y_i). Local data is defined as the neighbouring wells as given by a Delauney triangulation (http://en.wikipedia.org/wiki/Delaunay_triangulation, Ahuja and Schacter (1983)) of the monitoring well locations. The gradient of this linear surface in both x and y directions is given by the coefficients b and c. Estimated direction of flow is given by:

$$\theta = \tan^{-1}\left(\frac{c}{b}\right) \tag{7}$$

and the relative hydraulic gradient (a measure of relative flow velocity) is given by

$$R = \sqrt{b^2 + c^2} \tag{8}$$

For any given model output interval this algorithm is applied to each and every well where a GW level has been recorded.

7.4 Well Trend Plot Smoother

The well trend plot smoother is fitted using a nonparametric method called local linear regression. This involves solving locally the least squares problem:

$$\min_{\alpha,\beta} \sum_{i}^{n} \{y_i - \alpha - \beta(x_i - x)\}^2 w(x_i - x; h) \tag{9}$$

where $w(x_i - x; h)$ is called the kernel function. A normally-distributed probability density function with standard deviation h is used as the kernel. h is also called smoothing parameter that controls the width of the kernel function, and hence the degree of smoothing applied to the data (the higher the value of h, the smoother the estimates). Within GWSDAT, local linear regression is deployed using the R package 'sm' (Bowman and Azzalini (1997)) and the bandwidth is selected using the method published in C. M. Hurvich, Simonoff, and Tsai (1998).

7.5 Converting a CAD drawing to a Shapefile

System requirements: ArcGIS comprising ArcMap, ArcEditor, ArcCatalog

1. Open ArcCatalog from the Start Menu ('Start' -> 'All Programs' -> 'ArcGIS' -> 'ArcCatalog').
2. In ArcCatalog navigate to ArcMap (globe with magnifying glass icon).
3. When ArcMap opens a screen will pop-up. Select 'A New Empty Map' then click 'OK'.
4. Go to 'File' -> 'Add Data' (positive sign with yellow triangle underneath) -> Select site CAD drawing saved as a '.dxf' file -> 'Add'.
5. Click on the '+' symbol to expand the sub-layers of the dxf file (e.g. 'Polyline', 'Polygon', 'Multipatch', 'Point').
6. Right click on required layer (e.g. Polyline or an edited & exported shapefile) to open the drop down menu.
7. On drop down menu select 'Data' -> 'Export Data'.
8. On 'Export Data' pop-up menu choose 'Select All Features' + 'This Layers Source Data' and select the folder you wish to save the shapefile into, then click 'OK'.
9. Click 'Yes' to add the exported data as a new layer.
10. Repeat steps 6-9 to convert all the layers required to produce the base-map in GWSDAT into shapefiles.
11. Add the shapefiles into GWSDAT (see `GIS ShapeFiles Table`) one by one to produce the complete base-map image.

The next section details how to edit layers in ArcMap after their conversion to shapefiles, prior to upload into GWSDAT (useful for removing gridlines etc)

1. Uncheck the CAD layer used to produce shapefile to remove image from view window.
2. Ensure exported Shapefile is selected and visible in view window.
3. Click 'Start Editing' on the 'Editor' toolbar above the map.
4. Use the arrow pointer to select lines and press delete on the keyboard to remove from drawing. (Select 'UnDo' from 'Edit' Toolbar in case of errors).
5. 'Editor' -> 'Stop Editing'. Click 'Yes' to save edits.
6. Repeat data export as detailed in steps 6-9 above and re-save as new shapefile.

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