



# **EPA Webinar: Plume Stability Analyses with GWSDAT**



# **GWSDAT**

## **GroundWater Spatiotemporal Data Analysis Tool**

**Wayne Jones, Principal Data Scientist, Shell Global Solutions (UK) Ltd.**

**[Wayne.W.Jones@shell.com](mailto:Wayne.W.Jones@shell.com)**

**Luc Rock, Soil and Groundwater Scientist, Shell Global Solutions International B.V.**

**[Luc.Rock@shell.com](mailto:Luc.Rock@shell.com)**

# Cautionary Note

The companies in which Royal Dutch Shell plc directly and indirectly owns investments are separate legal entities. In this presentation “Shell”, “Shell group” and “Royal Dutch Shell” are sometimes used for convenience where references are made to Royal Dutch Shell plc and its subsidiaries in general. Likewise, the words “we”, “us” and “our” are also used to refer to Royal Dutch Shell plc and subsidiaries in general or to those who work for them. These terms are also used where no useful purpose is served by identifying the particular entity or entities. “Subsidiaries”, “Shell subsidiaries” and “Shell companies” as used in this presentation refer to entities over which Royal Dutch Shell plc either directly or indirectly has control. Entities and unincorporated arrangements over which Shell has joint control are generally referred to as “joint ventures” and “joint operations”, respectively. Entities over which Shell has significant influence but neither control nor joint control are referred to as “associates”. The term “Shell interest” is used for convenience to indicate the direct and/or indirect ownership interest held by Shell in an entity or unincorporated joint arrangement, after exclusion of all third-party interest.

This presentation contains forward-looking statements (within the meaning of the U.S. Private Securities Litigation Reform Act of 1995) concerning the financial condition, results of operations and businesses of Royal Dutch Shell. All statements other than statements of historical fact are, or may be deemed to be, forward-looking statements. Forward-looking statements are statements of future expectations that are based on management’s current expectations and assumptions and involve known and unknown risks and uncertainties that could cause actual results, performance or events to differ materially from those expressed or implied in these statements. Forward-looking statements include, among other things, statements concerning the potential exposure of Royal Dutch Shell to market risks and statements expressing management’s expectations, beliefs, estimates, forecasts, projections and assumptions. These forward-looking statements are identified by their use of terms and phrases such as “aim”, “ambition”, “anticipate”, “believe”, “could”, “estimate”, “expect”, “goals”, “intend”, “may”, “objectives”, “outlook”, “plan”, “probably”, “project”, “risks”, “schedule”, “seek”, “should”, “target”, “will” and similar terms and phrases. There are a number of factors that could affect the future operations of Royal Dutch Shell and could cause those results to differ materially from those expressed in the forward-looking statements included in this [report], including (without limitation): (a) price fluctuations in crude oil and natural gas; (b) changes in demand for Shell’s products; (c) currency fluctuations; (d) drilling and production results; (e) reserves estimates; (f) loss of market share and industry competition; (g) environmental and physical risks; (h) risks associated with the identification of suitable potential acquisition properties and targets, and successful negotiation and completion of such transactions; (i) the risk of doing business in developing countries and countries subject to international sanctions; (j) legislative, fiscal and regulatory developments including regulatory measures addressing climate change; (k) economic and financial market conditions in various countries and regions; (l) political risks, including the risks of expropriation and renegotiation of the terms of contracts with governmental entities, delays or advancements in the approval of projects and delays in the reimbursement for shared costs; and (m) changes in trading conditions. No assurance is provided that future dividend payments will match or exceed previous dividend payments. All forward-looking statements contained in this [report] are expressly qualified in their entirety by the cautionary statements contained or referred to in this section. Readers should not place undue reliance on forward-looking statements. Additional risk factors that may affect future results are contained in Royal Dutch Shell’s 20-F for the year ended December 31, 2020 (available at [www.shell.com/investor](http://www.shell.com/investor) and [www.sec.gov](http://www.sec.gov)). These risk factors also expressly qualify all forward looking statements contained in this presentation and should be considered by the reader. Each forward-looking statement speaks only as of the date of this presentation, Sep 22<sup>nd</sup>, 2021. Neither Royal Dutch Shell plc nor any of its subsidiaries undertake any obligation to publicly update or revise any forward-looking statement as a result of new information, future events or other information. In light of these risks, results could differ materially from those stated, implied or inferred from the forward-looking statements contained in this presentation.

We may have used certain terms, such as resources, in this presentation that United States Securities and Exchange Commission (SEC) strictly prohibits us from including in our filings with the SEC. U.S. Investors are urged to consider closely the disclosure in our Form 20-F, File No 1-32575, available on the SEC website [www.sec.gov](http://www.sec.gov).

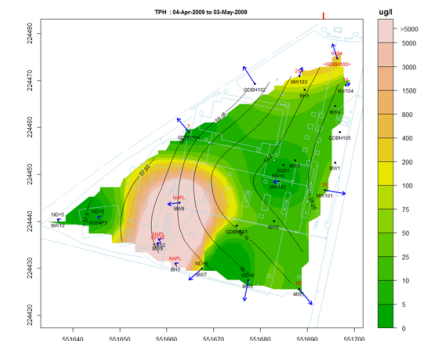
# GWSDAT – what is it?

- User-friendly, open source, **decision support software tool** for analysis & reporting of **monitoring data**.
- Robust, easy to install, intuitive to use, **requires only standard monitoring data input** (e.g. well coordinates, time series solute concentration data)
- Dataset **upload in variety of formats**, analysis at the **click of a button**, **export of output** (e.g. PowerPoint), no special expertise or software required.
- **Run locally** on a user's PC / laptop **or online** via web app.
- Works equally well for both **small** (e.g. retail) **or large** (e.g. refinery) **sites**.

GWSDAT (GroundWater Spatiotemporal Data Analysis Tool)

Author: Wayne W. Jones@shell.com Version: 3.10

WellName	Constituent	SampleDate	Result	Units	Flags
MW-01	BEZENEH	14/10/2002	78	ug/l	
MW-01	OPV	14/10/2002	92.43	ug/l	
MW-01	TOLLENE	14/10/2002	430	ug/l	
MW-01	XYLENE	14/10/2002	440	ug/l	
MW-02	BEZENEH	14/10/2002	48000	ug/l	
MW-02	OPV	14/10/2002	95.3	ug/l	
MW-02	TOLLENE	14/10/2002	1200	ug/l	
MW-02	XYLENE	14/10/2002	1300	ug/l	
MW-03	BEZENEH	14/10/2002	ND=10	ug/l	
MW-03	OPV	14/10/2002	94.43	ug/l	
MW-03	TOLLENE	14/10/2002	5.5	ug/l	
MW-03	XYLENE	14/10/2002	ND=50	ug/l	
MW-04	BEZENEH	14/10/2002	250	ug/l	
MW-04	OPV	14/10/2002	95.77	ug/l	
MW-04	TOLLENE	14/10/2002	630	ug/l	
MW-04	XYLENE	14/10/2002	5.5	ug/l	
MW-05	BEZENEH	04/03/2003	940	ug/l	



## GWSDAT - business benefits

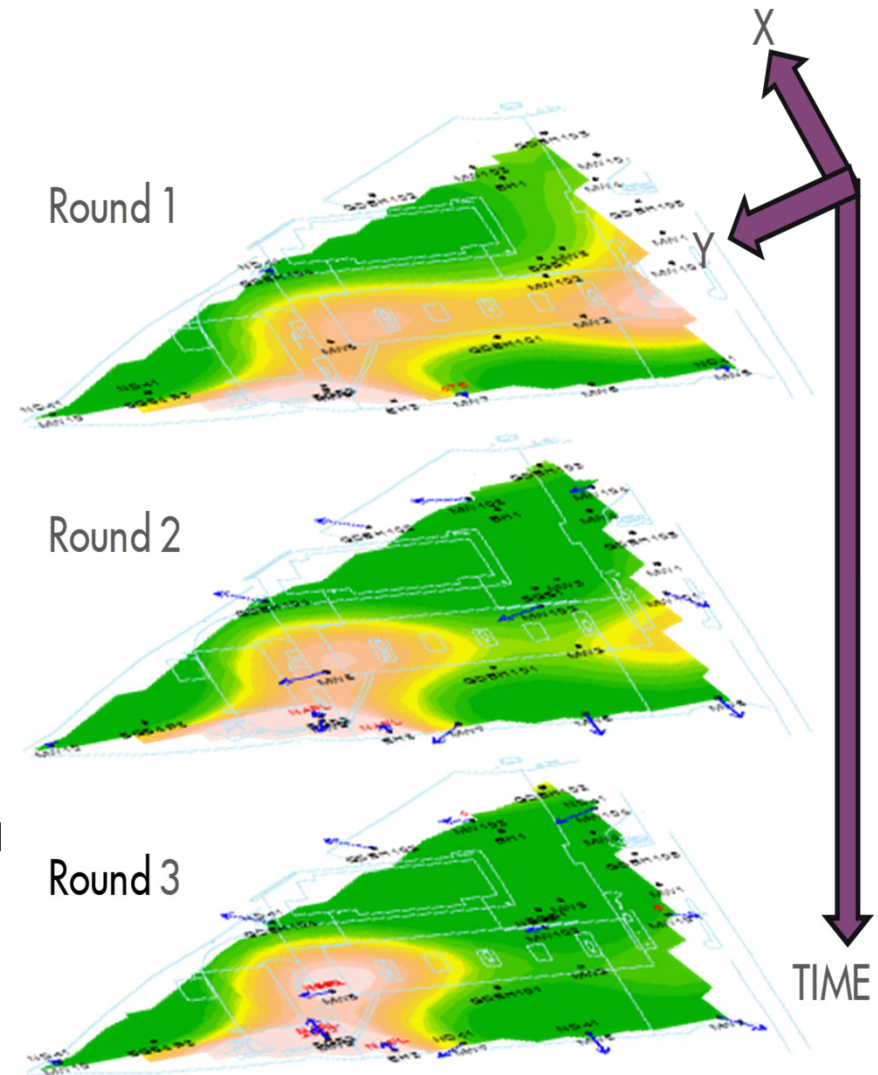
- **Tool used operationally in monitoring & assessment** of Shell's global downstream assets (e.g. refineries, terminals, fuel stations) for a period of **over 10 years** → achieved **significant efficiencies & savings**, e.g.:
  - Support **design and optimization** of monitoring and/or remediation programs (i.e., avoid collection of redundant data).
  - **Early identification** of potentially new releases, migration pathways, need for corrective action, stable / declining trends that may aid in assessing project closure.
  - **Rapid interpretation** of complex datasets from large monitoring networks (e.g. refineries, terminals).
  - **Efficient evaluation and reporting** of monitoring trends via simple, standardised plots and tables created at the 'click of a mouse'.

## **GWSDAT – evidence of increased global adoption.**

- More than 10 use-cases including Shell, US EPA, Exxon and training videos in Indonesian. <http://gwmdat.net/case-studies/>
- GWSDAT accepted by regulatory agencies, e.g. UK Env. Agency refers to tool as part of guidance document on contaminated land risk management. <https://www.gov.uk/government/publications/land-contamination-risk-management-lcrm/lcrm-stage-1-risk-assessment#GWSDAT>
- GWSDAT LinkedIn user group. <https://www.linkedin.com/groups/8715423/>
- ITRC. 2013. GW Statistics and Monitoring Compliance, Statistical Tools for the Project Life Cycle. GSMC-1. Washington. <https://projects.itrcweb.org/gsmc-1/>

## GWSDAT trend analysis

- **Smoothing Statistics** to capture the important patterns and trends in the data.
- **Time Series (Temporal) Statistics** to detect trend components.
- **Spatial Statistics:** for modelling geographic relationships.
- **Spatiotemporal Statistics** providing a clear interpretation of contamination plumes



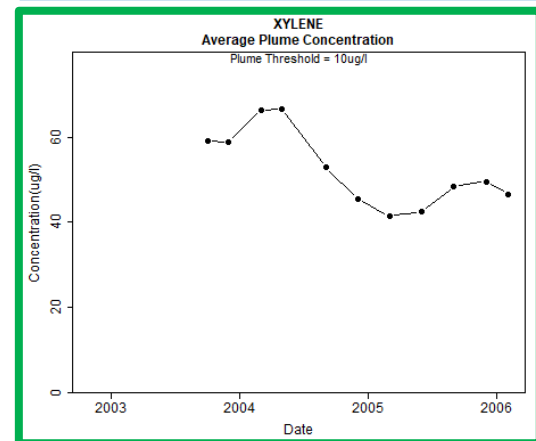
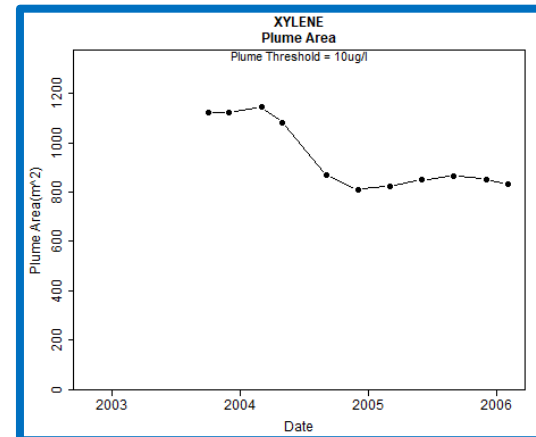
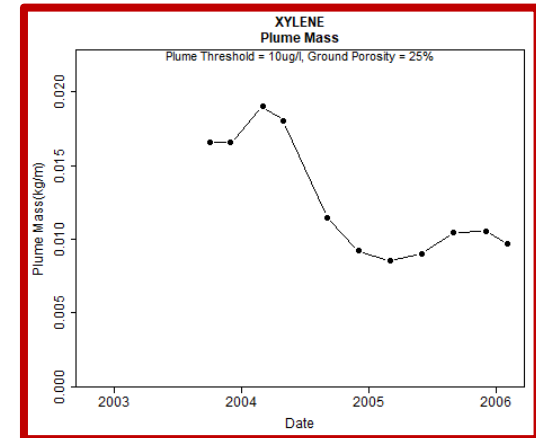
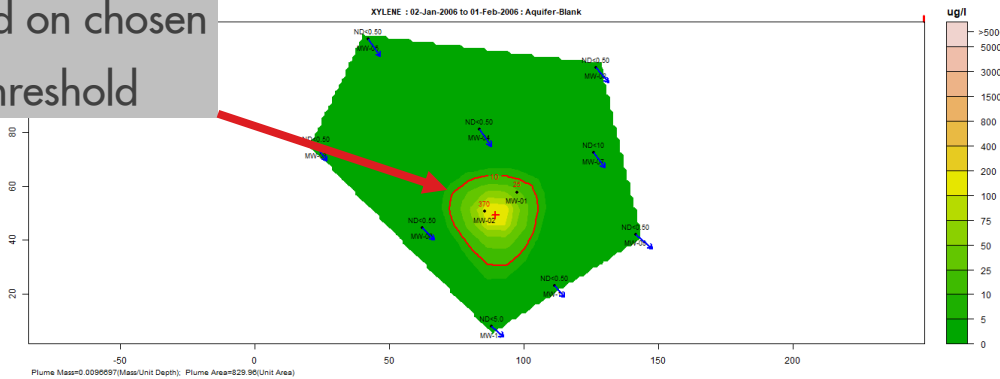
# GWSDAT plume diagnostics

■ for a specific analyte:

- plume mass
- plume area
- average plume concentration

→ Evaluation of plume stability

Plume boundary  
based on chosen  
threshold



# Network Optimisation

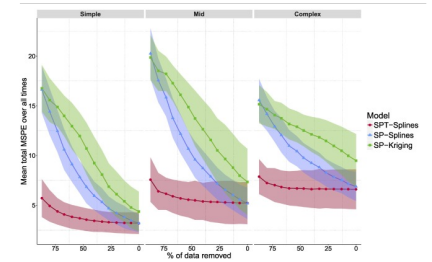
## ■ Recent Publication:

*“Statistical modelling of groundwater contamination monitoring data: A comparison of spatial and spatiotemporal methods” Science of the Total Environment:*

<https://doi.org/10.1016/j.scitotenv.2018.10.231> & PhD Thesis: <http://theses.gla.ac.uk/38975/>

## ■ Conclusions:

- **More** information using **fewer** observations with a spatiotemporal model
- Spatiotemporal methods can achieve same level of performance but with fewer data points. GWSDAT users are already enjoying this benefit.
- New PhD student started at University of Glasgow, Oct 2021: Implementation of cost-effective spatiotemporal approaches to optimize groundwater monitoring network design and data analysis.
- **Version 3.1 is the beginning of the journey in incorporating Network Optimisation tools into GWSDAT.**





## GWSDAT V3.1 – New Features and Enhancements

- **Well Redundancy Analysis:** allows user to very conveniently drop a well or a combination of wells from analysis and investigate resultant impact.
- **Updated user manual:** [http://gwmdat.net/gwmdat\\_manual/](http://gwmdat.net/gwmdat_manual/). Completely overhauled and updated.
- **Excel Add-in:** Updated technology to avoid frequently reported issue of the GWSDAT Excel Add-in menu not being displayed.
- **Updated branding:** Excel data input templates updated with more contemporary colour schemes which align with branding here: [www.gwmdat.net](http://www.gwmdat.net).
- **Custom Colour Key:** In response to user feedback added functionality to customise colour key in main GWSDAT spatial plot.
- **Export Contours to ArcGIS:** Export of GWSDAT solute concentrations contours via “tiff” output format.
- Other minor bug fixes and enhancements.

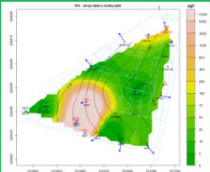


# **GWSDAT V3.1**


## **Demonstration**

## GWSDAT

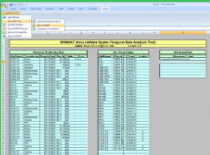
An open source, user-friendly, software application for the visualisation and interpretation of groundwater monitoring data.



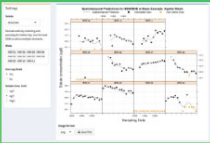
**A spatiotemporal model** provides a more powerful analysis than spatial modelling at isolated time points or temporal modelling at isolated locations.



**Visualisation** of site-wide trends in solute concentrations, with interactive control. Trend and threshold matrices can be constructed as summary indicators.



**Ease of data entry** through a MS Excel spreadsheet containing well co ordinates and solute concentrations at specific times. Wells can be grouped into separate aquifers. Site maps can be added as GIS shapefiles.




**Automatic report generation tools**, including site reports and spatial plots at user specified times with groundwater and NAPL data overlaid. Plots can be exported directly to MS PowerPoint.

The simplest form of access to GWSDAT is through the on-line tool.

[GWSDAT on-line](#)

Guidance on use of the tool is available in the [Getting Started](#) page.

A version of the tool which can be installed locally is available either as an [R package](#) from CRAN or as an Excel interface from the [API](#) and [Claire](#).



### GWSDAT

GroundWater Spatiotemporal Data Analysis Tool

# GWSDAT V3.1 – Updated Add-in menu and branding.

**GWSDAT (GroundWater Spatiotemporal Data Analysis Tool)**  
 Author: Wayne.W.Jones@Shell.com Version: 3.10

Historical Monitoring Data							Well Coordinates				GIS ShapeFiles	
WellName	Constituent	SampleDate	Result	Units	Flags		WellName	XCoord	YCoord	Aquifer	CoordUnits	FileNames (*.shp)
MW-01	BENZENE	31/10/2002	78	ug/l			MW-01	97.43	57.81		metres	
MW-01	GW	31/10/2002	92.23	Level			MW-02	85.57	50.64			
MW-01	TOLUENE	31/10/2002	470	ug/l			MW-03	22.95	74.64			
MW-01	XYLENE	31/10/2002	430	ug/l			MW-04	83.64	81.26			
MW-02	BENZENE	31/10/2002	40000	ug/l			MW-05	42.26	114.64			
MW-02	GW	31/10/2002	92.3	Level			MW-06	62.40	44.57			
MW-02	TOLUENE	31/10/2002	1200	ug/l			MW-07	126.12	72.43			
MW-02	XYLENE	31/10/2002	1100	ug/l			MW-08	126.95	104.15			
MW-03	BENZENE	31/10/2002	ND<10	ug/l			MW-09	141.84	42.09			
MW-03	GW	31/10/2002	94.43	Level			MW-10	111.50	23.05			
MW-03	TOLUENE	31/10/2002	1.1	ug/l			MW-11	88.05	7.88			
MW-03	XYLENE	31/10/2002	ND<0.50	ug/l								
MW-04	BENZENE	31/10/2002	250	ug/l								
MW-04	GW	31/10/2002	93.77	Level								
MW-04	TOLUENE	31/10/2002	410	ug/l								
MW-04	XYLENE	31/10/2002	5.5	ug/l								
MW-01	BENZENE	04/02/2003	900	ug/l								
MW-01	TOLUENE	04/02/2003	72	ug/l								
MW-01	XYLENE	04/02/2003	7.6	ug/l								

# GWSDAT V3.1 – Screenshot - Data Management Page (online version)

GWSDAT Beta

This is a temporary session. [LOG IN](#) [SIGN UP](#)

## Data Manager

[Restore Examples](#) [Load Data](#) [Add New Data](#) [Import .csv Data](#) [Import Excel File](#)

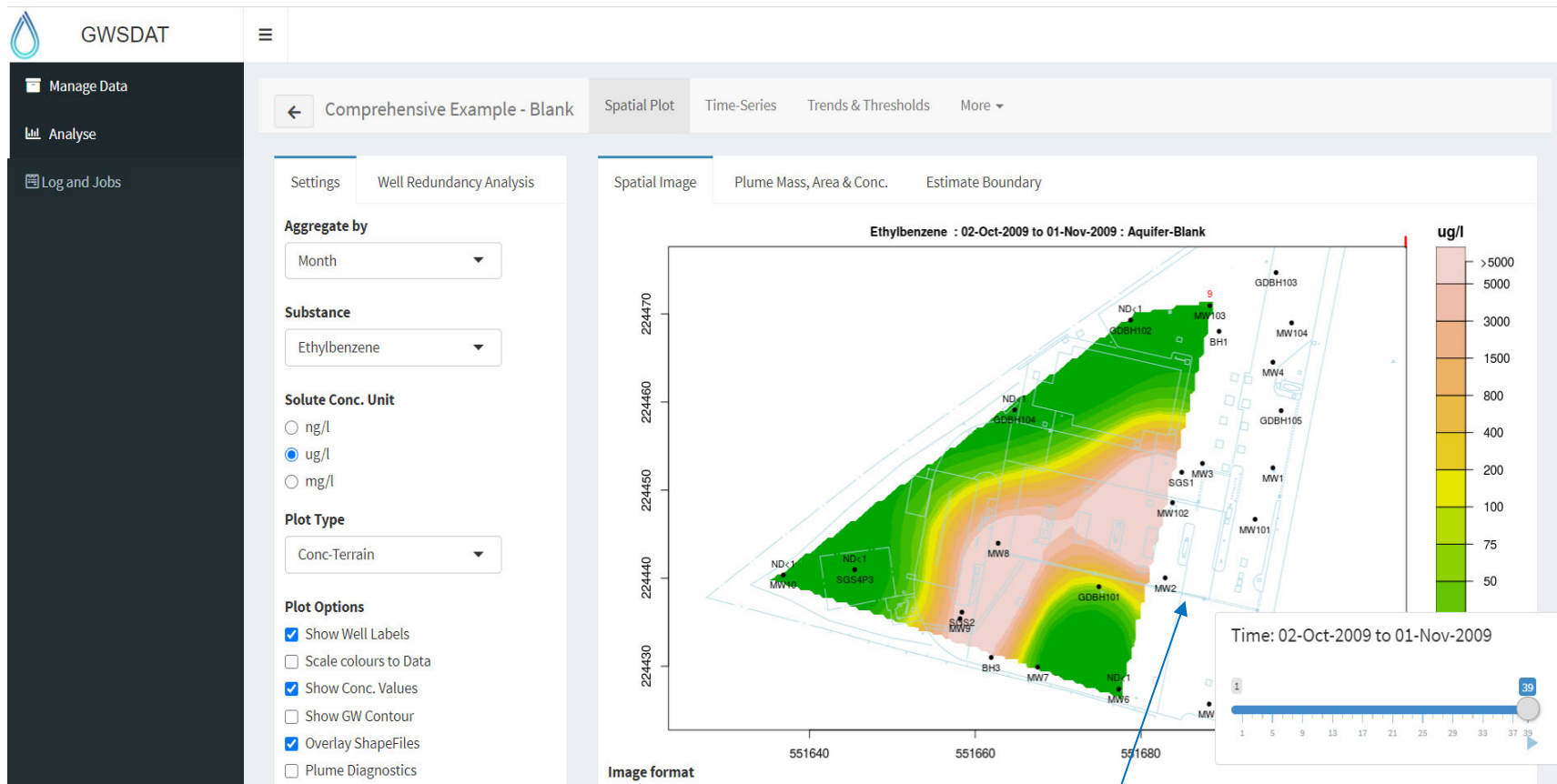
**Basic Example**

**Contaminants:** BENZENE, TOLUENE, XYLENE  
**Wells:** MW-01, MW-02, MW-03, MW-04, ... (11)  
**Aquifer:** Blank

**Comprehensive Example**

**Contaminants:** Nitrate, Sulphate, Ethylbenzene, Toluene, ... (5)  
**Wells:** SGS3P1, SGS3P2, SGS3P3, SGS4P1, ... (6)  
**Aquifer:** Blank, A

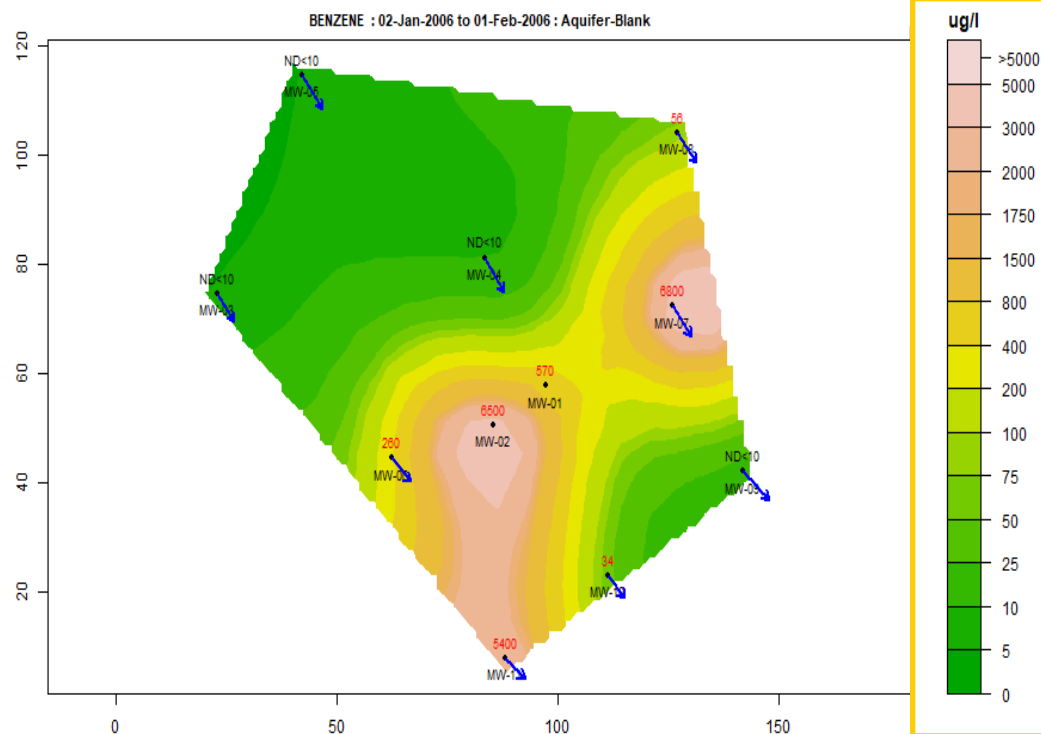
# GWSDAT V3.1 – Screenshot - Spatial Plot



➤ Option to add map of site infrastructure



# Ability to customise Spatial plot Colour Key.



## Customise the Spatial Plot Colour Key

Specify the contouring intervals for each solute in ug/l.

BENZENE	TOLUENE	XYLENE
0.00	0.00	0.00
5.00	5.00	5.00
10.00	10.00	10.00
25.00	25.00	25.00
50.00	50.00	50.00
75.00	75.00	75.00
100.00	100.00	100.00
200.00	200.00	200.00
400.00	400.00	400.00
800.00	800.00	800.00
1500.00	1500.00	1500.00
1750.00		
2000.00		
3000.00	3000.00	3000.00
5000.00	5000.00	5000.00

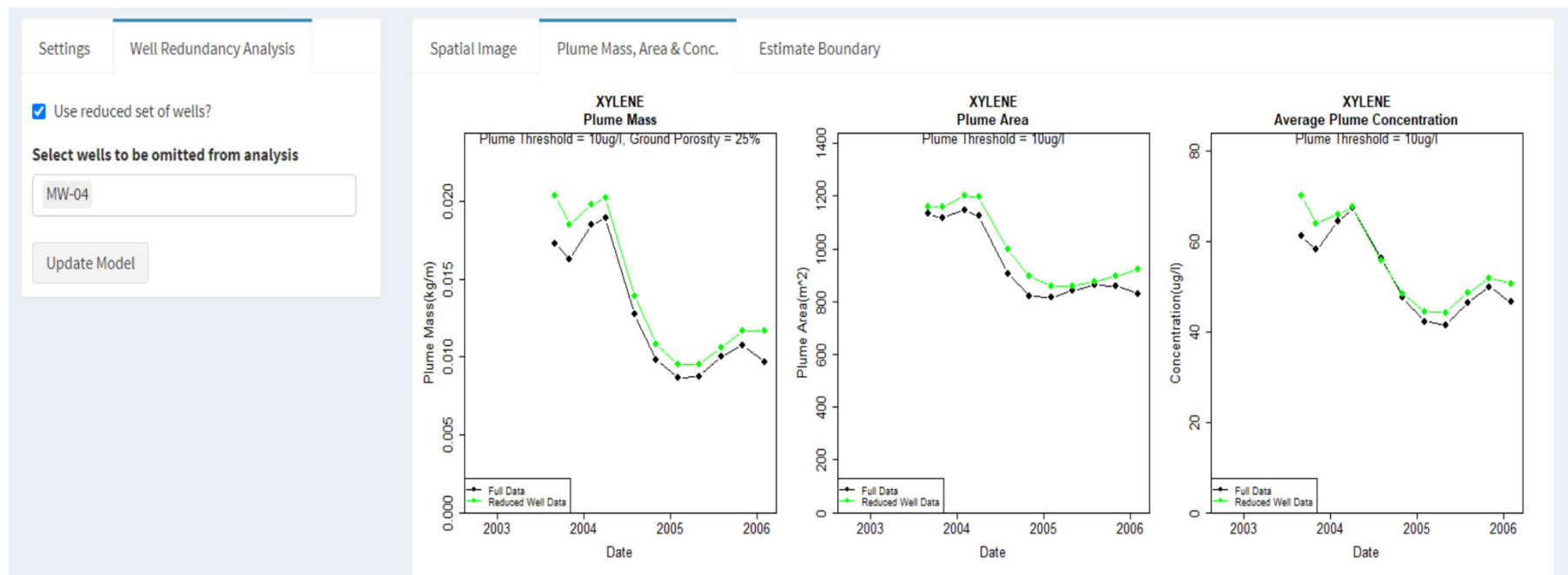
(Double-click on cells to edit)

(Right-click on cells to add or delete rows)



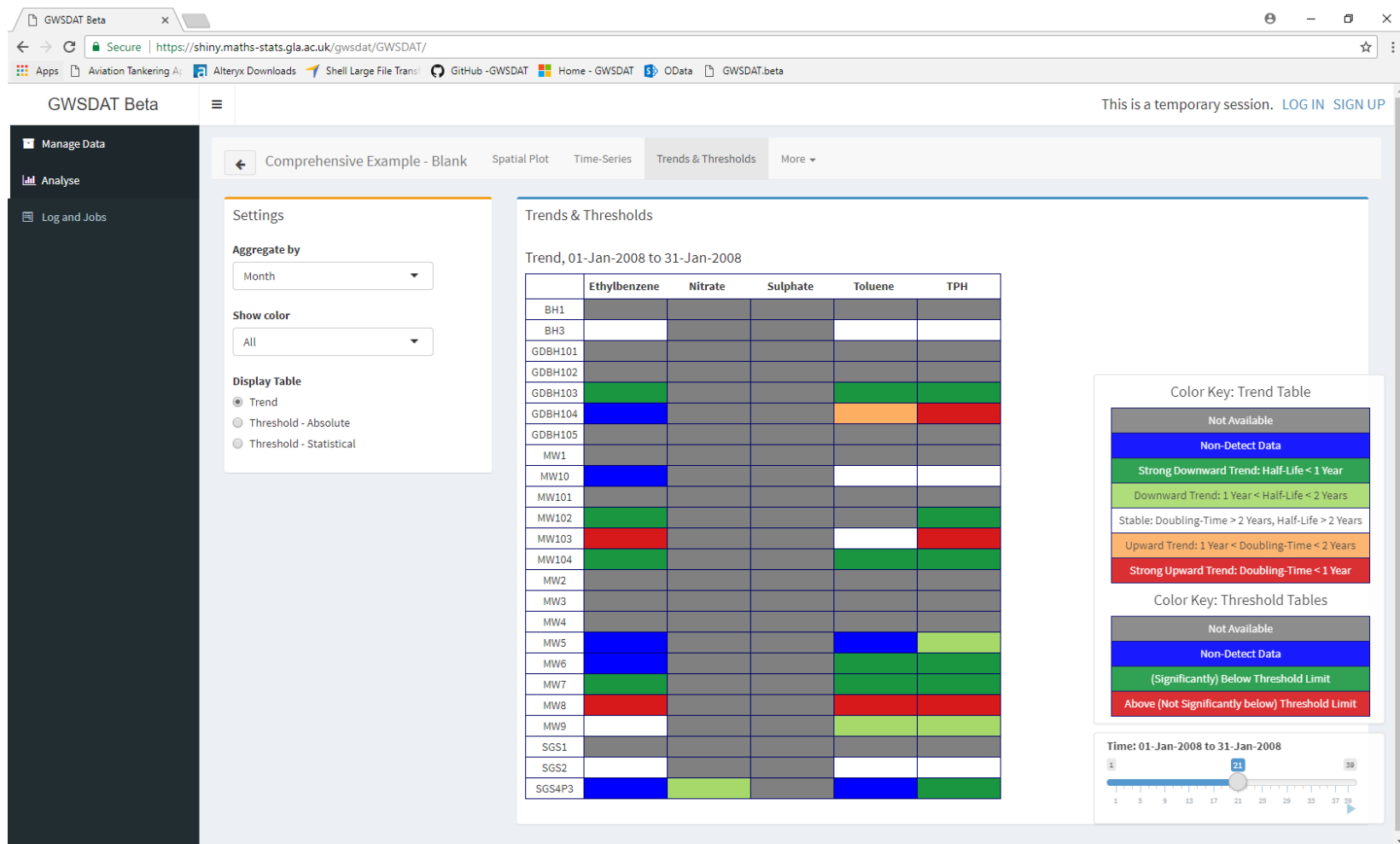
# Well Redundancy

(Comparing Plume metrics with well MW-04 removed)

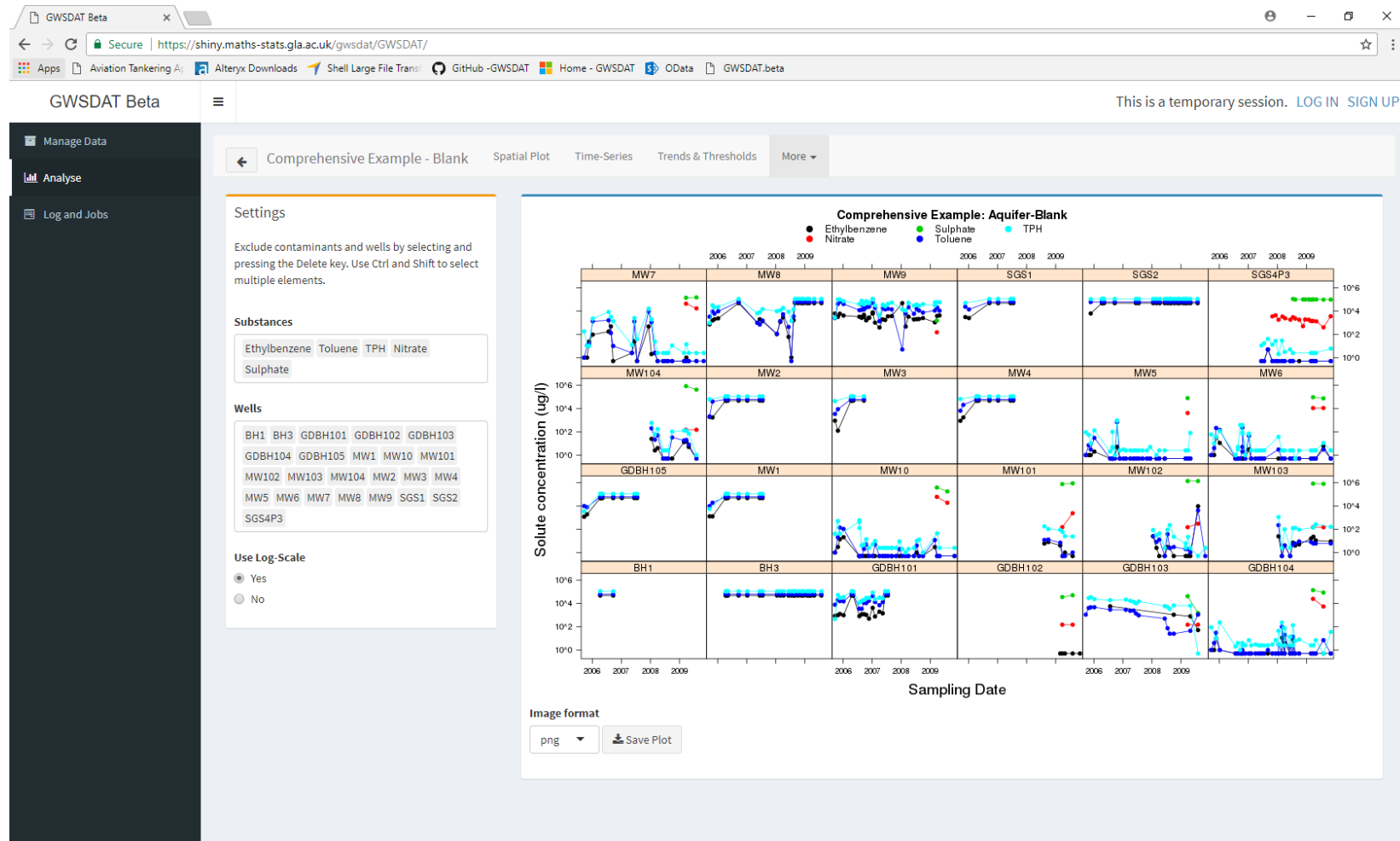


- Black line: original dataset
- Green line: reduced dataset

# GWSDAT V3.1 – Screenshot - Traffic Light Plot

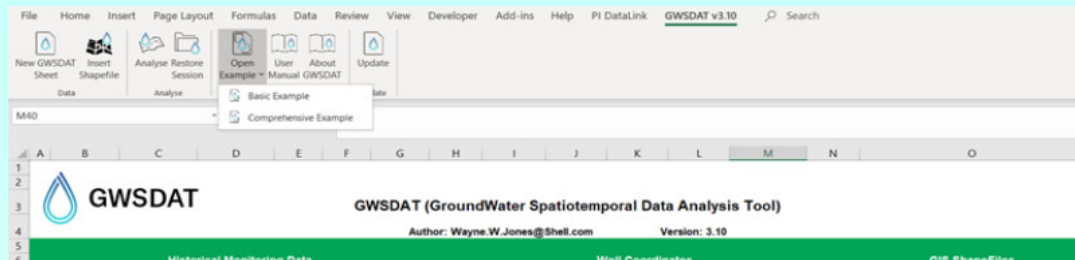


# GWSDAT V3.1 – Screenshot - Well Time Series Reporting



## GWSDAT Version 3.1 now released!

by Peter Radvanyi | Jun 14, 2021 | Updates



- GWSDAT V3.1 released in August.
- Available to download from: [www.api.org/GWSDAT](http://www.api.org/GWSDAT) , [www.claire.co.uk/GWSDAT](http://www.claire.co.uk/GWSDAT) and [www.gwsdat.net](http://www.gwsdat.net).
- On a longer term basis, we are interested to hear ideas about features related to Well Network Optimisation, e.g. New well placement, Well sampling schemes/strategies, etc.

# **GWSDAT - Case studies: “Plume stability”**

## Background on case studies

- **Data source:** real, anonymized from 2 sites
- **Geological setting:** non-fractured siliciclastic
- **Site general information:**

Site	Objective	Site setting
#1	Plume stability – optimization in sampling interval	residential commercial
#2	Plume stability – gap in monitoring network, earlier adoption of tool	residential commercial recreational

- **Support:** Gratefully acknowledge B. Kautsch (Shell); A. Wesch, E. Marzusch (Arcadis)

## Case study – Site #1

### ■ Objective:

Demonstrate plume stability with the aim to optimize sampling frequency interval

### ■ Site history:

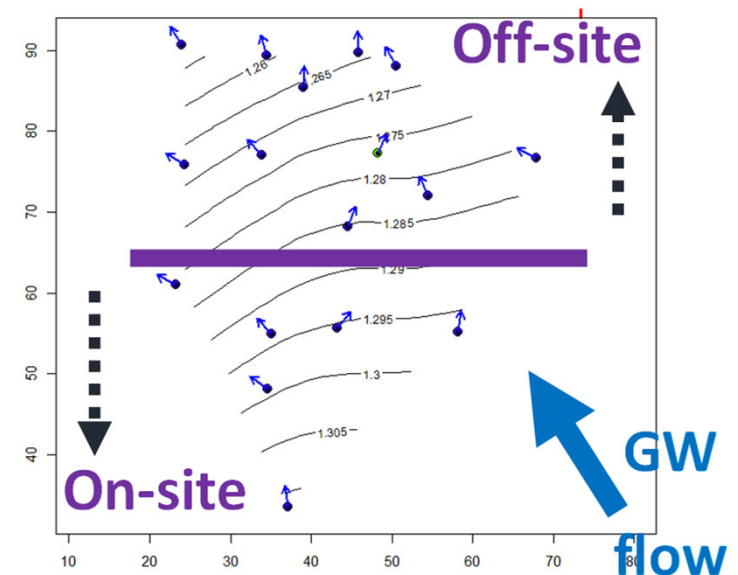
- Mid 1990's: impact observed, primarily BTEX, partial remediation soil excavation

- Early 2000's: GW monitoring implemented
- Plume beyond site boundary

### ■ GW sampling:

- Frequency varied - quarterly to bi-annual
- Over 15 locations

→ Proposed change to annual after recent bi-annual sampling event

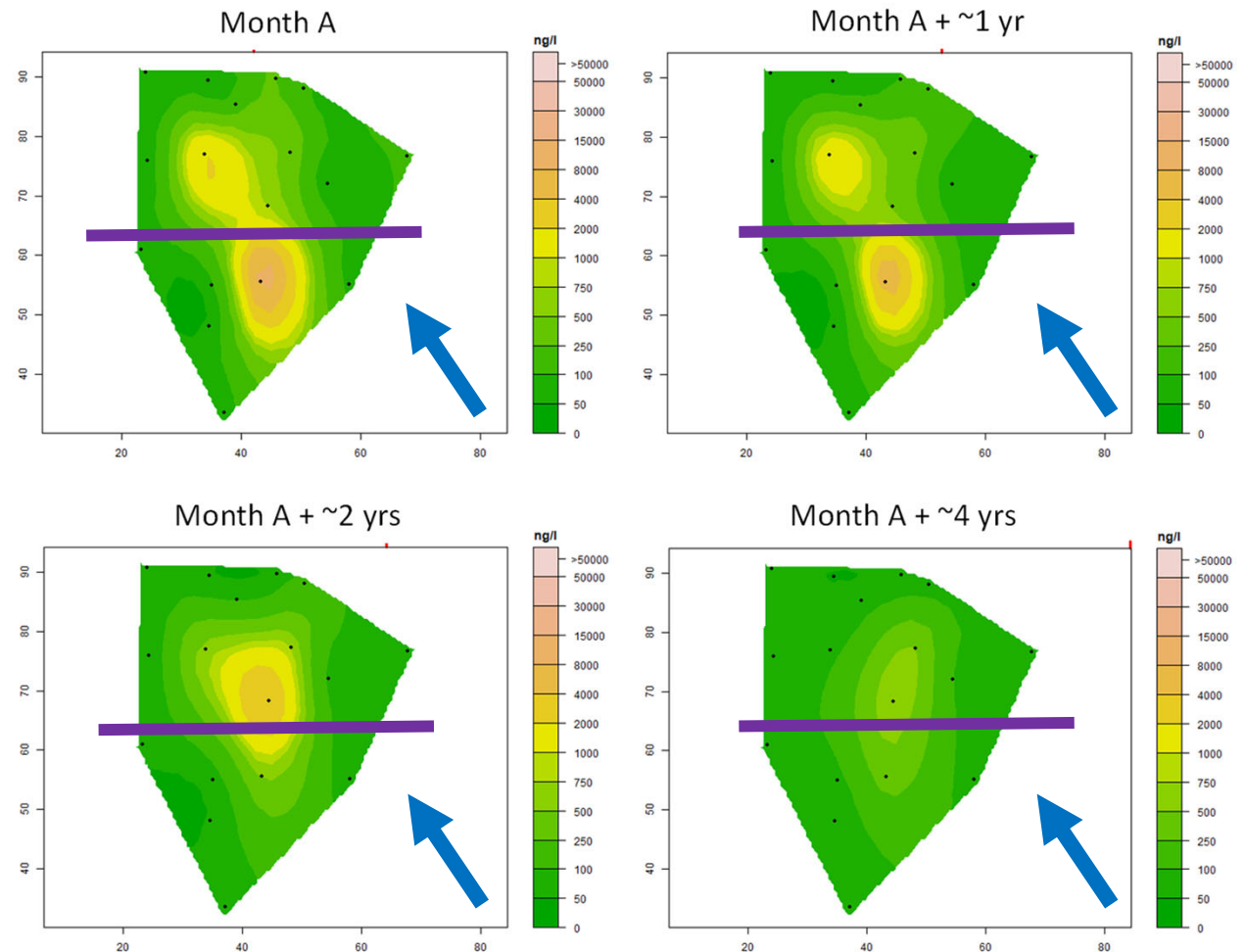
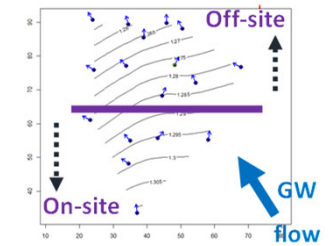


## Case study – Site #1

### ■ Observations:

- Time slices of spatiotemporal plots showing part of historical BTEX plume evolution
- **Plume:** stable and shrinking

*Data shown*  
  
*to most recent*





## Case study – Site #1

### ■ Observation:

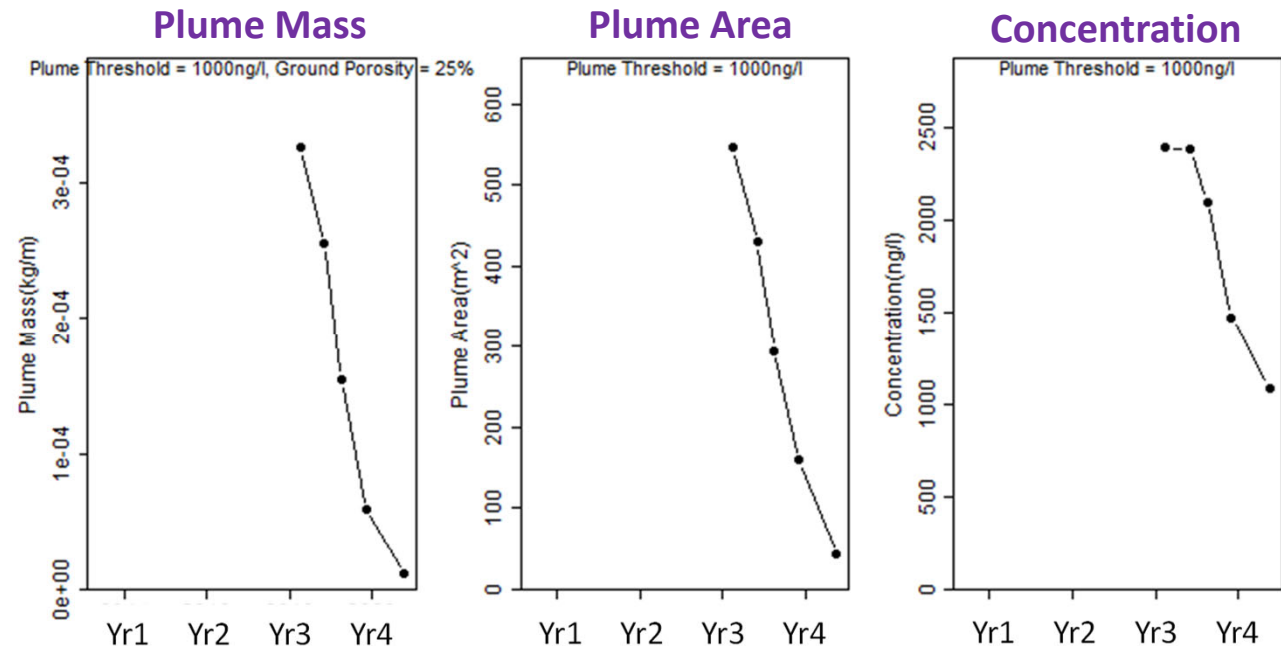
#### ■ Plume

diagnostics  
functionality  
output for  
benzene

#### ■ Plume trends:

decreasing mass,  
area, & average  
concentration

## Benzene



Benzene: threshold value of 1 ug/L

➤ **Outcome:** Regulator **approved** change in sampling frequency

## Case study – Site #2

### ■ Objective:

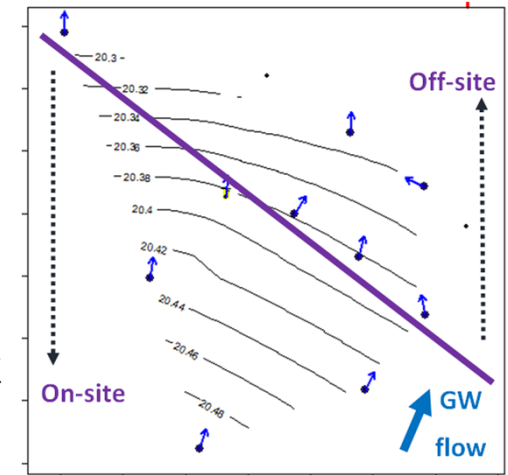
Assess plume stability and evaluation of monitoring network

### ■ Site history:

- In 1990's: several SGW investigations including remedial activities
- Residual contamination remained
- Since ~2012: regular GW monitoring to assess TPH, **BTEX**, MTBE
- Plume at/beyond? site boundary
- GWSDAT not part of data interpretation workflow process for many years

### ■ GW data:

- BTEX data over 8-year period presented
- GWSDAT used 1<sup>st</sup> time for annual reporting of GW monitoring events related to years 6 and 7

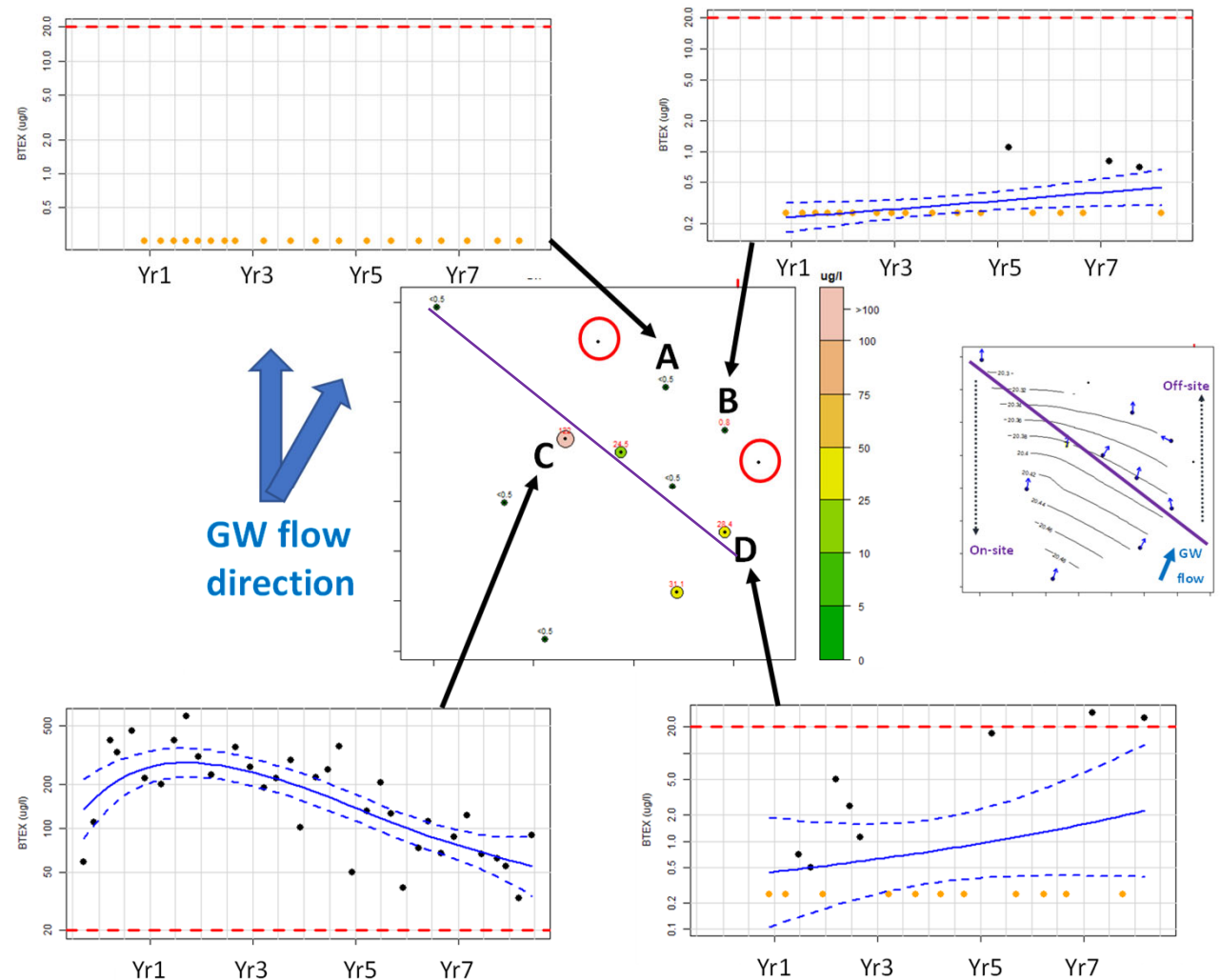


→ Proposed additional wells for gap closure

## Case study – Site #2

### ■ Observations:

- Existing downstream wells below threshold
- Gap in monitoring network in downstream direction of wells with exceedances



➤ **Outcome:** Regulator **approved** 2 new wells

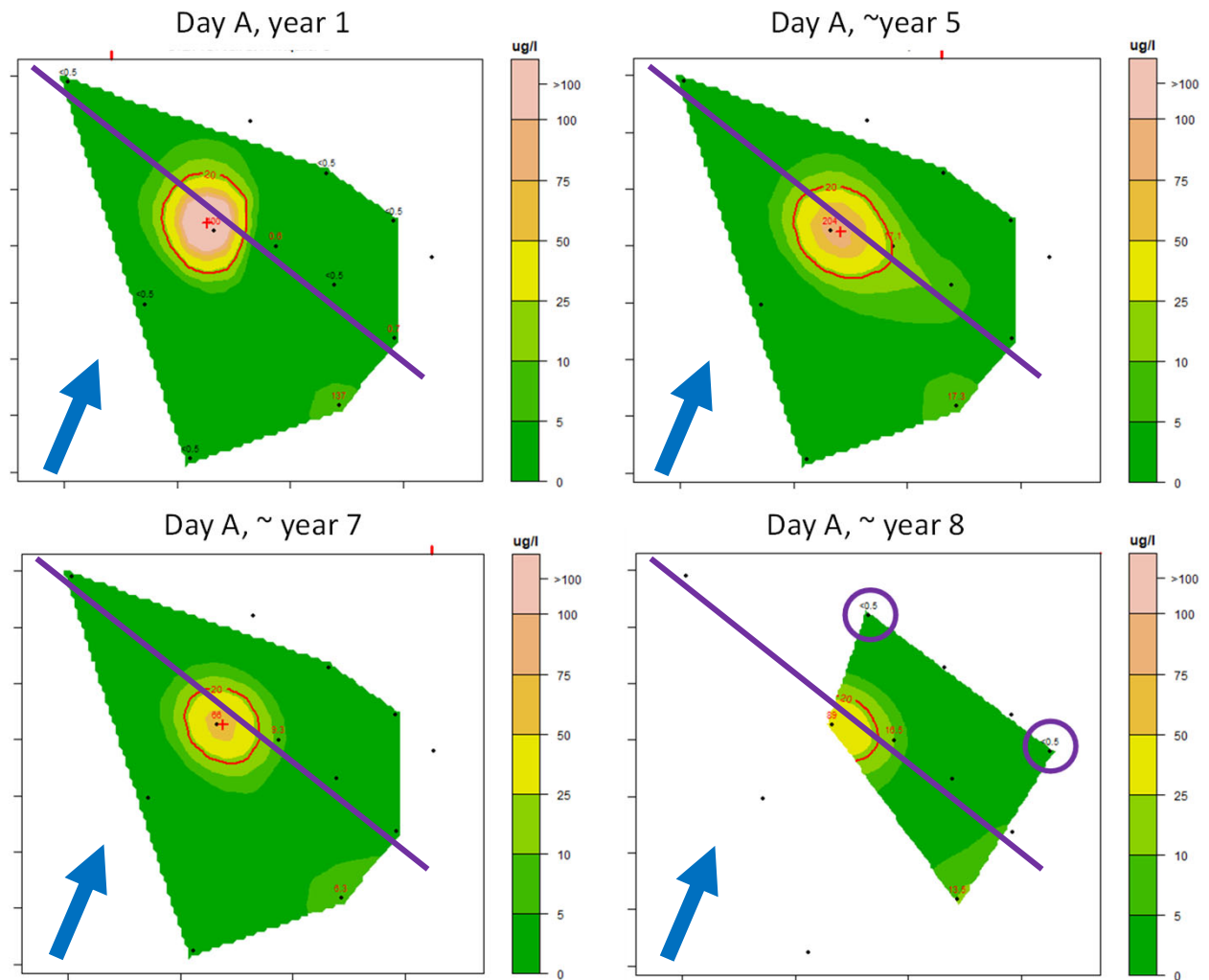
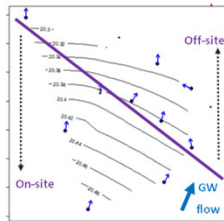
## Case study – Site #2

### ■ Observations:

- Time slices of spatiotemporal plots showing part of historical BTEX plume evolution

### ■ GWSDAT model:

- concentrations in 2 new wells will likely be below detection limit



red circle: modelled BTEX plume outline based on threshold value of 20 ug/L; purple circles indicate location new wells

## Case study – Site #2

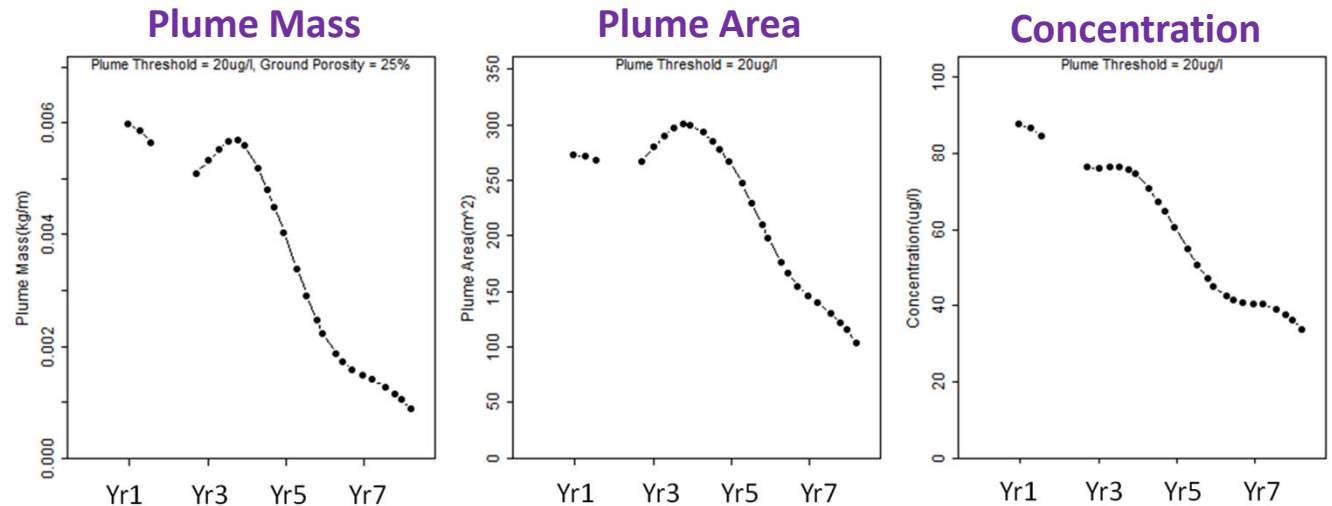
### ■ Observation:

■ Plume  
diagnostics  
functionality  
output for BTEX

### ■ Plume trends:

decreasing  
mass, area, &  
average  
concentration

## BTEX



BTEX: threshold value of 20 ug/L

➤ **Reflection:** earlier integration of GWSDAT  
could have optimized site understanding &  
decision making

---

## Q & A

# Q&A

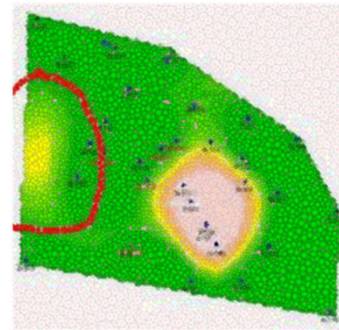


## Things to consider..

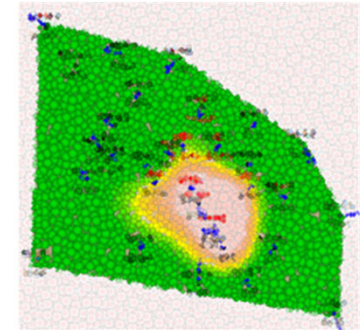
## Ballooning..

- Ballooning is a statistical anomaly where predictions can be high in areas where there are no data.

Modelling resolution:  
**Default & Higher Resolution**



Modelling resolution:  
**10**



Nb: data from actual site, figures anonymized

- The best way to improve the model is to up the model resolution...

### Model Settings

Select the resolution for the PSpline model fit. The resolution is defined by the number of segments, which can also be directly defined in the right input field below (min:2, max: 12).

#### PSplines Resolution

Default ▼  
Default  
High

or

#### Number of segments

6

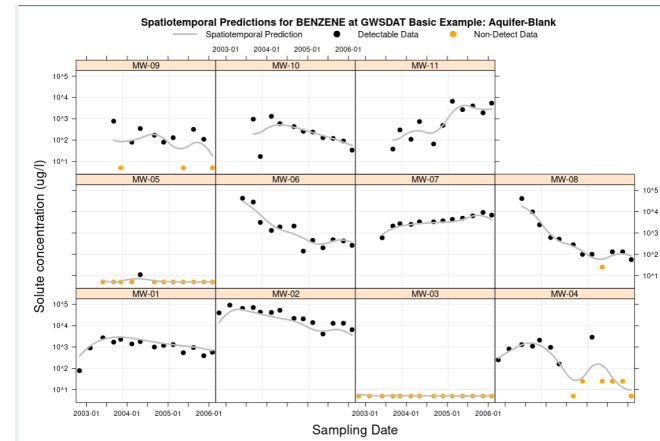
- See Evers, et al. , 2015. *Efficient and automatic methods for flexible regression on spatiotemporal data, with applications to groundwater monitoring*, Environmetrics.



# Major Assumptions + Useful pointers

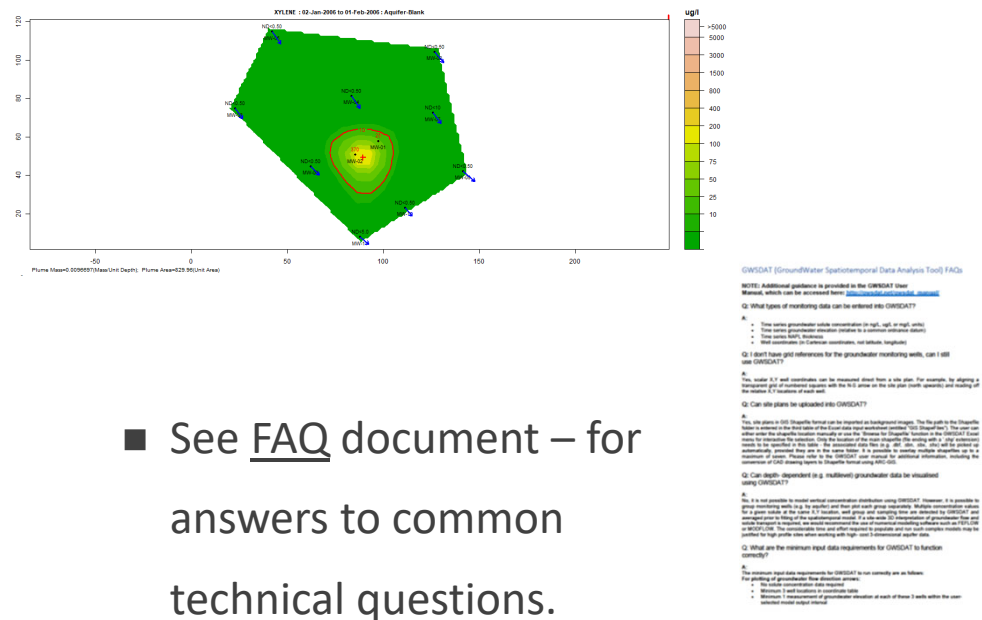
## ■ Model Checking:

- The Spatiotemporal prediction plot compares model output with lab results.



## ■ Plume Diagnostics:

- GWSDAT assumes a homogenous aquifer in depth and analyses the data on an aquifer-by-aquifer basis.
- Plume mass calculated per unit depth. Multiply by aquifer depth to yield plume mass.



- See FAQ document – for answers to common technical questions.

## References (open access articles)

- Molinari, D. A., 2014. Spatiotemporal modelling of groundwater contaminants, PhD Thesis (Glasgow).
- Jones, et al., 2014. A software tool for the spatiotemporal analysis and reporting of groundwater monitoring data. Environmental Modelling & Software.
- Evers, et al. , 2015. Efficient and automatic methods for flexible regression on spatiotemporal data, with applications to groundwater monitoring, Environmetrics.
- Jones, et al., 2015. Analyzing Groundwater Quality Data and Contamination Plumes with GWSDAT, Groundwater.
- Mclean, M. I., 2018. Spatiotemporal models for the analysis and optimisation of groundwater quality monitoring networks, PhD Thesis (Glasgow).
- Mclean et al., 2018 . Statistical modelling of groundwater contamination monitoring data: A comparison of spatial and spatiotemporal methods. Science of the Total Environment.
- User Manual: [http://gwsdat.net/gwsdat\\_manual/](http://gwsdat.net/gwsdat_manual/)

