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A software tool for the spatiotemporal analysis and reporting of groundwater monitoring data☆

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ABSTRACT

The GroundWater Spatiotemporal Data Analysis Tool (GWSDAT) is a user friendly, open source, decision support tool for the analysis and reporting of groundwater monitoring data. Uniquely, GWSDAT applies a spatiotemporal model smoother for a more coherent and smooth interpretation of the interaction in spatial and time-series components of groundwater solute concentrations. Data entry is via a standardised Microsoft Excel input template whilst the underlying statistical modelling and graphical output are generated using the open source statistical program R. This paper describes in detail the various plotting options available and how the graphical user interface can be used for rapid, rigorous and interactive trend analysis with facilitated report generation. GWSDAT has been used extensively in the assessment of soil and groundwater conditions at Shell's downstream assets and the discussion section describes the benefits of its applied use. Finally, some consideration is given to possible future developments.

Software availability

Software name: GWSDAT (GroundWater Spatiotemporal Data Analysis Tool)
Developer: Wayne R. Jones
Contact address: Shell Global Solutions (UK) (wayne.w.jones@shell.com)
Year first official release: 2013
Hardware requirements: Standard PC
System requirements: Microsoft Windows (XP or later)
Software requirements: Microsoft Office (Excel, Word and PowerPoint) and R (www.r-project.org)
Program Size: 13 MB
Availability: www.claire.co.uk/GWSDAT
License: Free under a GNU General Public License (www.gnu.org) agreement.
Documentation and support for users: User manual, example data sets, FAQ document, presentations and posters.

1. Introduction

1.1. Background

Groundwater is water located beneath the Earth's surface in soil pore spaces and in the fractures of rock formations. Environmental monitoring of groundwater is routinely conducted in areas where the risk of contamination is high and for protecting human health and the environment following an accidental release of hazardous constituents. Groundwater monitoring strategies are designed to establish the current status and assess trends in environmental parameters, and to enable an estimate of the risks to human health and the environment. It involves installing a network of monitoring wells to enable access to the water table across the site (Barcelona et al., 1985). Samples of groundwater are periodically collected from these wells and sent to an accredited laboratory for chemical analysis. The resulting spatiotemporal data set has to be reviewed,

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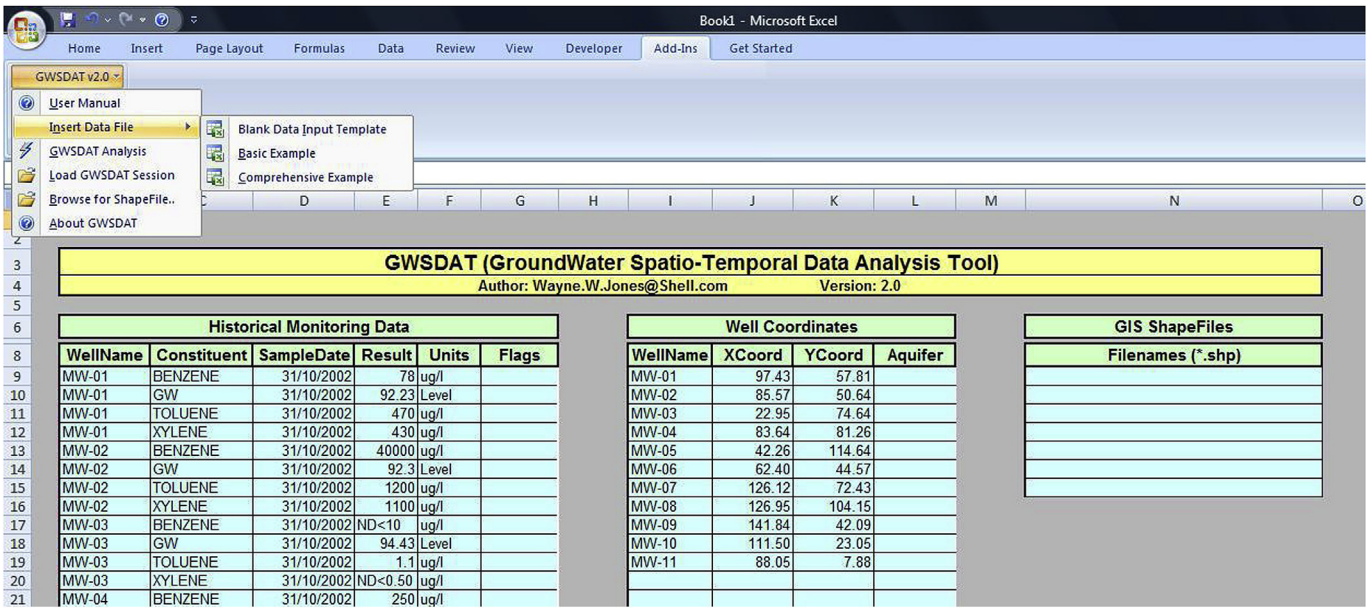

WellName	Constituent	SampleDate	Result	Units	Flags
MW-01	BENZENE	31/10/2002	78	ug/l	
MW-01	GW	31/10/2002	92.23	Level	
MW-01	TOLUENE	31/10/2002	470	ug/l	
MW-01	XYLENE	31/10/2002	430	ug/l	
MW-02	BENZENE	31/10/2002	40000	ug/l	
MW-02	GW	31/10/2002	92.3	Level	
MW-02	TOLUENE	31/10/2002	1200	ug/l	
MW-02	XYLENE	31/10/2002	1100	ug/l	
MW-03	BENZENE	31/10/2002	ND<10	ug/l	
MW-03	GW	31/10/2002	94.43	Level	
MW-03	TOLUENE	31/10/2002	1.1	ug/l	
MW-03	XYLENE	31/10/2002	ND<0.50	ug/l	
MW-04	BENZENE	31/10/2002	250	ug/l	

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

Fig. 1. GWSDAT example data input template. The *Historical Monitoring Data* table captures the concentration data, groundwater levels and, if present, NAPL thickness. The *Well Coordinates Table* stores the location of the monitoring well. The GWSDAT add-in menu is displayed at the top left.

analysed statistically, interpreted, and the results presented to environmental regulators in a clear and understandable manner.

The most basic method of level and trend evaluation involves investigating the time-series of groundwater constituent concentrations independently on a well by well basis. The more sophisticated spatial methods, typically, involve fitting a concentration trend surface (i.e. Kriging) to evaluate spatial pattern and trend (Cameron and Hunter, 2002; Gaus et al., 2003). However, although spatiotemporal data lies at the heart of current research in statistical methods (see Cressie and Wikle (2011)), the most common practice is to independently apply spatial modelling techniques to separate monitoring events (e.g. Ricker (2008)) or apply a single spatial model to a data set which has been consolidated over a time period (e.g. Aziz et al. (2003)). The joint modelling of both spatial and time elements in a single spatiotemporal modelling framework leads to a more coherent interpretation of site groundwater characteristics (Evers et al., in press).

Whilst there is a range of freely available groundwater data analysis applications, the most sophisticated tend to be designed for large scale long term groundwater monitoring networks (Aziz et al., 2003; Cameron, 2004). These have a relatively large initial data warehousing setup burden, which may be viewed as a barrier to the more widespread use of advanced groundwater monitoring techniques to smaller more short term monitoring programmes. Similarly, whilst GIS applications (e.g. ArcGIS) have excellent visualisation tools for geographical interpretation they also have a high initial data setup cost, operator competence requirements, and perhaps surprisingly, only a limited number of geostatistical modelling techniques available.

2. Software design and aims

2.1. Development aims

To a large extent, GWSDAT has been developed to address the barriers discussed in Section 1.1. However, its most important aim is to provide a simple to use, but statistically powerful decision support tool to environmental engineers and practitioners who routinely report on the status of numerous groundwater monitoring sites. Such an application needs to be easy to setup yet powerful in its ability to objectively analyse and rapidly report on a groundwater monitoring site's characteristics.

In common with many other environmental applications, it was recognised that there would be a benefit in providing the software in an open and transparent manner because policy makers and environmental regulators generally prefer code and techniques which are fully transparent and supported by sound science (Carslaw and Ropkins, 2012).

2.2. Software architecture

GWSDAT has been designed to integrate with Microsoft Excel, a software routinely used by environmental engineers for storing and analysing environmental (e.g. soil and groundwater) data. The user entry point to GWSDAT is a custom built Excel Add-in menu (see top left of Fig. 1).

The statistical engine used to perform geostatistical modelling and display graphical output is the open source statistical programming language R (R Development Core Team, 2012). The R project is used across a wide range of disciplines and has been adopted with eagerness by the environmental sciences community (Carslaw and Ropkins, 2012). Members of the R community contribute statistical routines and functionality to this collaborative project by means of an open standardised package structure, which can be downloaded and installed from http://cran.r-project.org/web/packages/. GWSDAT makes use of several of these packages, which are all individually referenced in this article. A Graphical User Interface (GUI) is provided via the R packages *rpanel* (Bowman et al., 2007) and *tkrplot* (Tierney, 2011) which obviates the need for training GWSDAT users in the R programming language.

3. Data input

3.1. Background

Before describing the application of GWSDAT in more detail it is necessary to give a brief explanation of the nature of groundwater monitoring data. In general, routine sampling of a monitoring well involves measuring the groundwater elevation and taking a sample of the groundwater which is subsequently sent for laboratory