

# **A web-based interface to visualize and model spatio-temporal variability of stream water quality**

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## **Key Points**

- We developed a web-based interface to visualize spatio-temporal variability of stream water quality in Victoria.
- The underlying models can identify key drivers of spatio-temporal variability following a Bayesian hierarchical modelling framework.
- This interface has been designed to support the decision-making processes of catchment managers.

## **Abstract**

Understanding the spatio-temporal variability in stream water quality is critical for designing effective water quality management strategies. To facilitate this, we developed a web-based interface to visualize and model the spatio-temporal variability of stream water quality in Victoria. We used a dataset of long-term monthly water quality measurements from 102 monitoring sites in Victoria, focusing on six water quality constituents: total suspended solids (TSS), total phosphorus (TP), filterable reactive phosphorus (FRP), total Kjeldahl nitrogen (TKN), nitrate-nitrite (NO<sub>x</sub>), and electrical conductivity (EC). The interface models spatio-temporal variability in water quality via a Bayesian hierarchical modelling framework, and produces summaries of (1) the key driving factors of spatio-temporal variability and (2) model performance assessed by multiple metrics. Additional features include predicting the time-averaged mean concentration at an un-sampled site, and testing the impact of land-use changes on the mean concentration at existing sites. This tool can be very useful in supporting the decision-making processes of catchment managers in (1) understanding the key drivers of changes in water quality and (2) designing water quality mitigation and restoration strategies.

## **Keywords**

Water quality, spatio-temporal variability, web-based interface, nutrients and sediments, statistical modelling, Bayesian hierarchical model

## **Introduction**

Stream water quality can vary significantly both in space and time (Vega et al. 1998; Bengraïne and Marhaba 2003; Chang 2008; Ai et al. 2015). At different locations, time-averaged water quality conditions can differ significantly (e.g. Meybeck and Helmer 1989); across time, water quality conditions can vary at event, daily, seasonal and inter-annual scales (Arheimer and Lidén 2000; Kirchner et al. 2004; Larned et al. 2004; Saraceno et al. 2009; Pellerin et al. 2012). These stream water quality variations are driven by three key processes, namely: (1) the source of constituents, which defines the total amount of constituents within the catchment; (2) the mobilization of these constituents due to weathering, erosion or biogeochemical processing; and (3) the delivery of mobilized constituents from the catchment to receiving waters (Granger et al. 2010).

Spatially, water quality can vary with human activities in the catchment (e.g., land use, vegetation cover and land management) and natural catchment characteristics (e.g., climate, geology, soil type, topography and hydrology), all of which influence the three key processes described above (Lintern et al. 2018). At the same time, temporal shifts in water quality can be influenced by factors including weather and hydrological conditions. Streamflow (Sharpley et al. 2002; Ahearn et al. 2004; Mellander et al. 2015) can affect the delivery of the constituent to receiving waters. Rainfall (Fraser et al. 1999) and air temperature (Lecce et al. 2006; Robson 2014) affect mobilization and transport in the catchment. Water temperature can control biogeochemical processing in the catchment and stream (Roberts and Mulholland 2007). Constituent sources can vary seasonally with antecedent conditions (Arheimer and Lidén 2000; Lecce et al. 2006), vegetation cover (Ouyang et al. 2010; Kaushal et al. 2014) and human activities (Stutter et al. 2008).

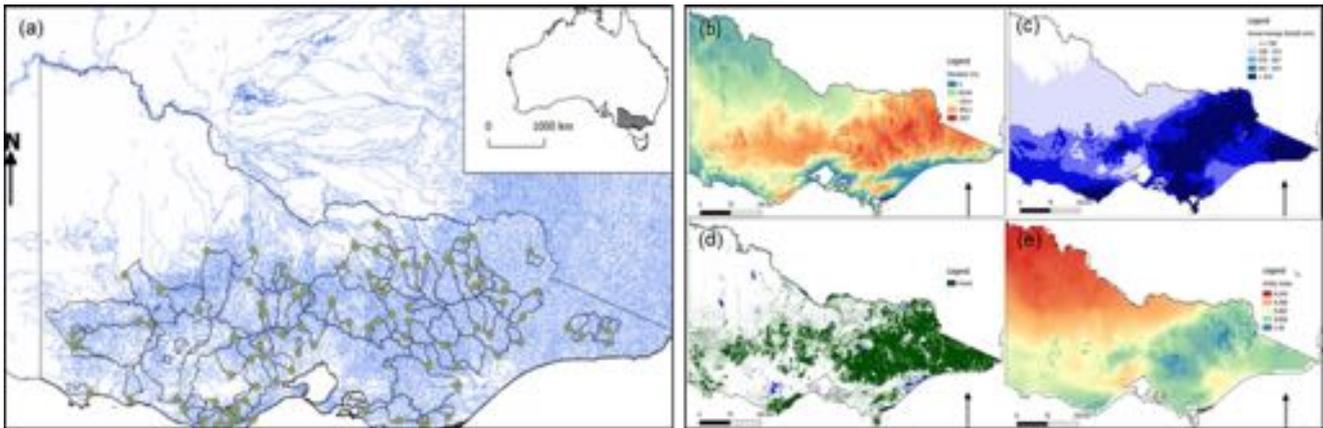
Understanding and modelling the spatio-temporal variability in water quality is critical for designing effective water quality management strategies. Conceptual or physically-based distributed models (Argent et al., 2009; Arnold and Fohrer, 2005) often require extensive datasets for their implementation. On the other hand, most statistical water quality models focus only on the temporal variability in water quality at a specific site (Kisi & Parmar, 2016; Kurunç, Yürekli, & Çevik, 2005; Parmar & Bhardwaj, 2015), instead of analyzing the spatio-temporal patterns over a wide region. This lack of modelling of spatio-temporal variability can not only limit our understanding of the key factors affecting water quality dynamics, but also hinder our ability to predict future water quality changes and/or predicting for unmonitored locations.

To facilitate the understanding and modelling of spatio-temporal variability in stream water quality, we developed a web-based interface with long-term stream water quality observations at 102 monitoring sites in Victoria. The interface has three components, namely: 1) data explorer; 2) modelling of spatial variability and 3) modelling of temporal variability. We introduce the data used in developing this interface, followed by the analyses and modelling background. We then illustrate the key features of each component with examples and discuss potential extensions. By facilitating quick and easy exploration of stream water quality data and linking with statistical water quality models, this interface can help support the decision-making processes of catchment managers in designing water quality mitigation and restoration strategies.

## **Method**

### *Data*

Stream water quality data were extracted from the Victorian to Water Measurement Information System (Department of Environment Land Water and Planning Victoria, 2016b). This database contains monthly ambient water quality data measured at approximately 400 sites across the state of Victoria, with some monitoring sites dating back to 1990. We used water quality data sampled between 1994 and 2014 at 102 sites (Figure 1) providing continuous monthly measurements over an extended and consistent period. The water quality constituents considered were: total suspended solids (TSS), total phosphorus (TP), filterable reactive phosphorus (FRP), total Kjeldahl nitrogen (TKN), nitrate-nitrite (NO<sub>x</sub>), and electrical conductivity (EC). The boundaries of the catchments corresponding to the water quality monitoring sites were delineated using the Geofabric tool (Bureau of Meteorology, 2012), with areas ranging from 5 to 16,000 km<sup>2</sup>.



**Figure 1. (a) Map of the 102 water quality monitoring sites and their catchment boundaries. Insert shows location of the state of Victoria in Australia; and the spatial distribution of (b) topographic, (c) rainfall, (d) vegetation and (e) aridity across the state of Victoria (Lintern et al., in revision).**

Potential spatial explanatory variables – catchment average land use, land cover, topographic, climatic, geological, lithological and hydrological catchment characteristics were derived using datasets obtained from Geoscience Australia (Geoscience Australia, 2004, 2011), the Bureau of Meteorology (BoM) (Bureau of Meteorology, 2012), the Bureau of Rural Sciences (BRS) (Bureau of Rural Sciences, 2010), the Victorian Department of Environment Land Water and Planning (DELWP) (Department of Environment Land Water and Planning Victoria, 2014, 2016a, 2016b), and the Terrestrial Ecosystem Research Network (Terrestrial Ecosystem Research Network, 2016). Fifty potential explanatory catchment characteristics were selected based on a literature review and conceptual understanding of the key factors affecting spatial variability in water quality (Lintern et al., 2018). A preliminary analysis of the land use data suggests less than 1% changes in the key land uses in these catchments (agricultural, grazing, conservation) between 1996 and 2011, allowing us to assume constant land use over the study period.

Potential temporal explanatory variables including instantaneous flows (ML/d) and water temperature ( $^{\circ}\text{C}$ ) were also extracted for each of the 102 sites over the study period (DELWP, 2016b). In addition to the instantaneous flow, the average flow over 1, 3, 7, 14 and 30 days preceding the water quality sampling dates were calculated. In addition, we used gridded climate data (Jones, Wang, & Fawcett, 2009) and the normalized difference vegetation index (NDVI) data (DAAC, 2017; Eidenshink, 1992) to calculate the catchment average daily rainfall (mm), daily evapotranspiration (ET) (mm), daily average temperature ( $^{\circ}\text{C}$ ), daily root zone (less than 1-m depth) and deep (more than 1-m depth) soil moisture, as well as monthly NDVI.

For the purpose of developing statistical water quality models, the raw input data were filtered and transformed to increase our modelling capacity. We first removed all water quality records with flags of quality issues and values below the limits of reporting (LOR). This is because values below the LOR are likely associated with higher proportional uncertainty in the transformed data set, and thus affect accurate modelling of the full variability of water quality. In addition, these below-LOR values had been recorded as equaling to the LOR, which effectively create a single ‘category’ of constituent concentration at the LOR and violate assumptions of continuous statistical models. Removal of these values also focuses our analysis more on higher concentrations, which are generally more concerning in water quality management. All observed constituent concentrations, catchment characteristics, and temporal explanatory variables were Box-Cox transformed to ensure greater normality in their distributions which will. For each variable, the optimal Box-Cox parameter  $\lambda$ , was identified at each site; and then the average  $\lambda$  across all sites was used for the final transformation. This ensures that all sites were being transformed using consistent transformation parameters.

### *Modelling spatio-temporal variability*

We used a Bayesian hierarchical approach to model the spatio-temporal variability in stream water quality. The Bayesian approach enables the inherent stochasticity in water quality to be incorporated into the model

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(Clark, 2005), while the hierarchical model structure enables the inclusion of temporal and spatial influences on water quality at multiple scales (e.g., Webb and King, 2009).

The transformed concentration of a constituent (TSS, TP, FRP, TKN, NO<sub>x</sub> and EC) at time  $i$  and site  $j$  ( $C_{ij}$ ) is assumed to be normally distributed with a mean  $\mu_{ij}$  and standard deviation  $\sigma$  representing inherent randomness (Eq. 1). To represent spatio-temporal variability,  $\mu_{ij}$  is modelled as sum of the site-level mean constituent concentration ( $\bar{C}_j$ ) and the deviation from that mean at time  $i$  ( $\Delta_{ij}$ ) (Eq. 2). To describe spatial variability, the site-level mean ( $\bar{C}_j$ ) is related to multiple catchment characteristics that vary spatially. Specifically,  $\bar{C}_j$  is modelled as a function of a global intercept ( $int$ ), and the sum of the effects of  $m$  catchment characteristics ( $eff.S_1$  to  $eff.S_m$ ) multiplied by the value of the catchment characteristics ( $S_1$  to  $S_m$ ) (Eq. 3). Temporal variability describes the deviation from the mean ( $\Delta_{ij}$ ) as a linear effect of  $n$  temporal variables,  $T_1$  to  $T_n$  (e.g., climate condition, streamflow, vegetation cover), scaled up by the observed standard deviation of the constituent at the site ( $\sigma_{j,obs}$ ) (Eq. 4). The use of  $\sigma_{j,obs}$  effectively standardizes the temporal variations across sites to make them comparable, and thus the coefficients ( $eff.T_{1,j}$ , ...,  $eff.T_{n,j}$ ) would also be comparable between sites. Currently, we use the observed site-level mean as  $\bar{C}_j$  in Eq. 4, so that temporal variability can be isolated from spatial variability and modelled specifically. However, in the future we plan to combine them in an integrated spatio-temporal model. The equations used for this study are:

$$C_{ij} \sim N(\mu_{ij}, \sigma) \quad \text{Equation 1}$$

$$\mu_{ij} = \bar{C}_j + \Delta_{ij} \quad \text{Equation 2}$$

$$\bar{C}_j = int + eff.S_1 \times S_1 + eff.S_2 \times S_2 + \dots + eff.S_m \times S_m \quad \text{Equation 3}$$

$$\Delta_{ij} = \mu_{ij} - \bar{C}_j = \sigma_{j,obs}(eff.T_{1,j} \times T_{1,ij} + \dots + eff.T_{n,j} \times T_{n,ij}) \quad \text{Equation 4}$$

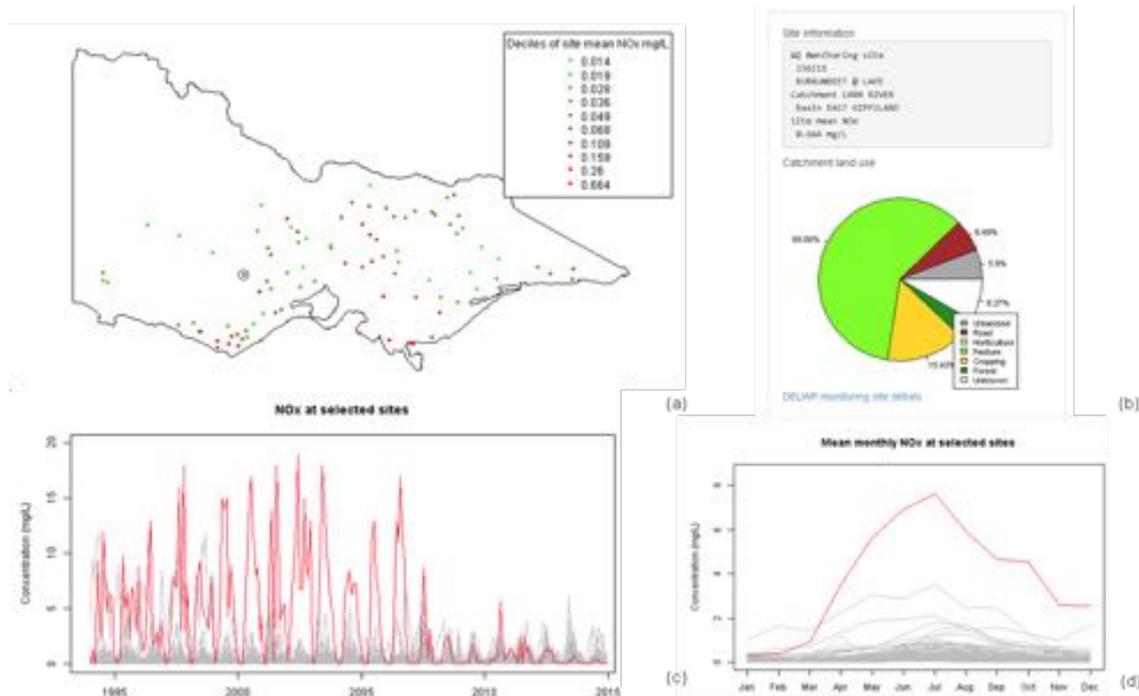
Statistical models of spatial variability in site mean concentrations were developed using an exhaustive search approach (Saft, Peel, Western, & Zhang, 2016). Spatial variation in different constituents is likely driven by different combinations of spatial variables ( $S_1$  to  $S_m$  in Eq. 3). Therefore, we considered several potential spatial predictors for each constituent, and then compared the fit of the spatial variability to all possible combinations of spatial predictors to identify a best set of predictors. The comparisons are based on the Akaike Information Criteria (AIC) (Akaike, 1974) of each fitted regression. The temporal variability in different constituents are also likely drive by different temporal variables. Therefore, for each constituent, the best combination of temporal predictors ( $T_1$  to  $T_n$  in Eq. 4) were selected in a similar way to the spatial predictors.

The Bayesian hierarchical model assumes that the value of each spatial parameter,  $eff.S_m$ , is drawn from a prior distribution defined by parameters referred to as the 'hyper-parameters'. Similarly, the 102 site-specific values of each temporal parameter  $eff.T_{n,j}$  are drawn from a common prior distribution defined by the corresponding hyper-parameters. In practice, this hierarchical structure effectively uses data at multiple sites to strengthen the site-specific models, and reduces unexplained variation in fitted parameters.

## Key Features of the Interface

### Data Explorer

The data explorer tool presents long-term observations of stream water quality, providing an overall summary of the spatio-temporal variability in each of the six user-selectable water quality constituents. For illustration purpose we focus on NO<sub>x</sub> here and for the rest of the paper. Spatial variability is summarized by a map of the 20-year time-averaged constituent concentration at each site, with dots colored by decile (Figure 2a). An optional selection of monitoring sites is allowed via two slider bars which define the range of longitudes and latitudes to focus on. Within the map, users can select an individual site to see the site mean concentration, as well as basic information about the monitoring site, including site name and ID, the corresponding catchment and basin, and major land uses within the catchment (Figure 2b).



**Figure 2. Elements within the data explorer tool, consisting of: a) map of time-averaged constituent concentration; b) information for a selected monitoring site from the map (circled); c) time-series of constituent concentrations at all monitoring sites, with the user-selected site shown in red; and d) mean monthly concentrations at all monitoring sites again with the user-selected site shown in red.**

Temporal variability in water quality is summarized first by a time-series plot of constituent concentrations at all monitoring sites (Figure 2c), and then by a plot of monthly average concentrations at all these sites (Figure 2d). Once the user selects a site on the mean concentration map (Figure 2a), the corresponding time-series and monthly mean pattern are highlighted in the two time-series plots for comparison with other sites.

Potential updates to the data explorer in future include: 1) improving multiple site selection, including selection by basin and ranges of annual rainfall and temperature; 2) incorporating additional layers among which users can select as the background of the site mean concentration map (e.g. land-use, topography, elevation); 3) allowing visualization of different quantiles of site concentrations on the map.

### Spatial Variability Modelling

The spatial variability modelling tool is based on the spatial model described in Eq. 3. For each constituent, users can choose among multiple possible structures, which have different sets of model predictors but similar predictive power (Lintern et al., in revision). The tool informs the user which spatial predictors are important (Figure 3a). The effects of these predictors are then summarized with a box-plot showing the median and the 95% confidence interval of each parameter estimated during model calibration (Figure 3b). Note that the absolute parameter values (on the y-axis) are affected by the transformation and standardization performed on both the model inputs and outputs. Instead, the parameters should be interpreted by their directions and relative magnitudes. The performance of the spatial model is summarized by 1) a plot of simulated against observed site mean concentration and for all sites (transformed), and the corresponding Nash-Sutcliffe Efficiency (NSE) (Nash & Sutcliffe, 1970) (Figure 3c) and 2) a map of site-specific residuals (Figure 3d).

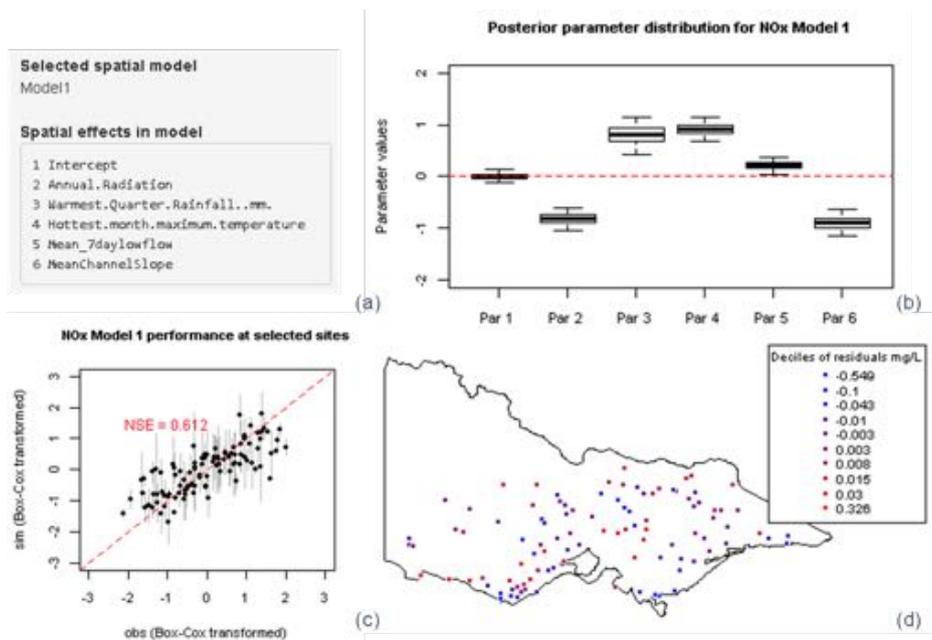
The tool enables prediction of mean concentration at a new site (i.e. un-sampled) with a selected model, from its key spatial predictors. Given the location of the new site, the prediction can be visualized on the map of site mean concentrations, with the associated uncertainty acknowledged. The tool can also support assessment of impacts of land-use changes on site mean water quality for a chosen model. This requires users to first specify the expected change in specific land-use type that is included as a model predictor (Figure 4a). The predicted change of site mean concentration is shown on a map (Figure 4b). The predicted change can

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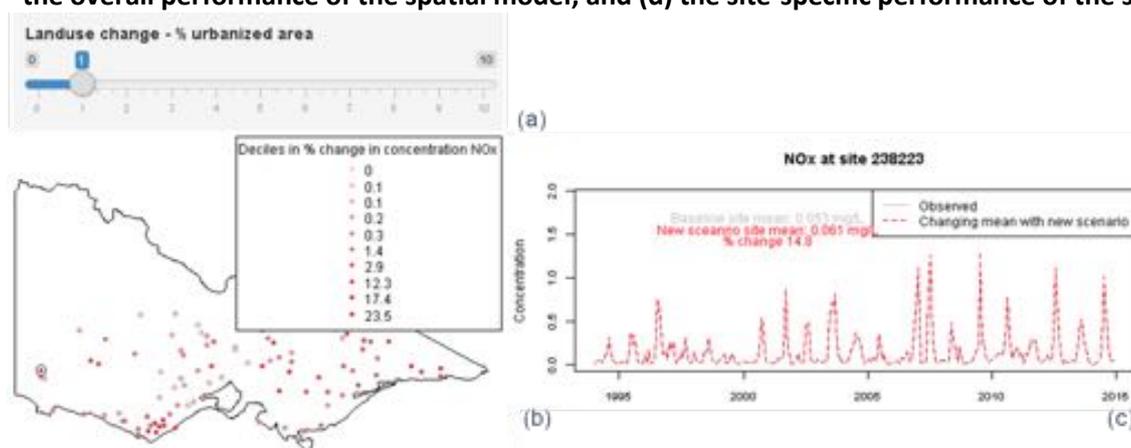
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also be visualized for individual sites as a scaled change to the corresponding time-series, which appears after clicking on a single site within the predicted change map (Figure 4c).

Currently, the tool focuses on only changes in land-use, with potential extensions to assessing the impacts of changes in long-term climate conditions. These climate change scenarios will be carefully designed to ensure that: 1) the allowable ranges of changes of climatic variables (e.g. temperature and rainfall) are physically plausible, which can be guided by recent climate change projections (e.g. CSIRO and Bureau of Meteorology, 2015; Stocker et al., 2013); and 2) the combination of changes in climate variables are internally consistent to maintain the observed cross-correlations among different variables (e.g. Richardson, 1981).



**Figure 3.** Elements within the spatial variability modelling tool, include: (a) key factors that the model uses to explain spatial variability in stream water quality; (b) the effects of these key driving factors; (c) the overall performance of the spatial model; and (d) the site-specific performance of the spatial model.



**Figure 4.** Predicting impacts of changes in land-use on the site-mean concentrations with the spatial variability modelling tool: (a) user input for land-use change; (b) map of the predicted changes in site-mean concentrations (selected site is circled); and (c) observed time-series of at a selected site, and the predicted time-series obtained by scaling with the predicted changes at the site.

**Temporal Variability Modelling**

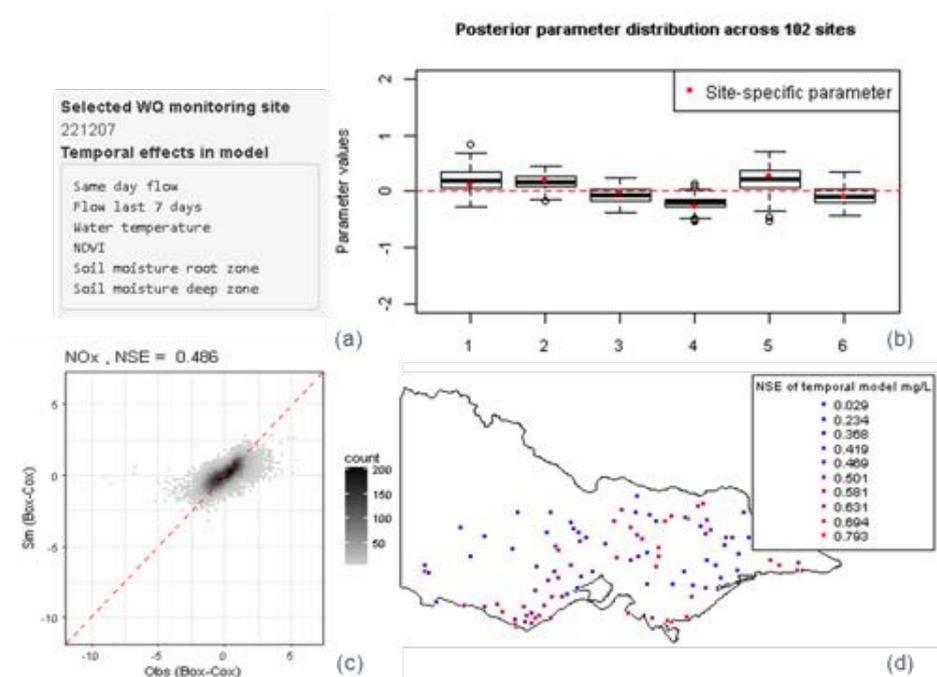
The temporal variability modelling tool is based on the temporal model described in Eq. 4. Similar to the spatial modelling tool, the tool identifies the key predictors affecting temporal variability in water quality

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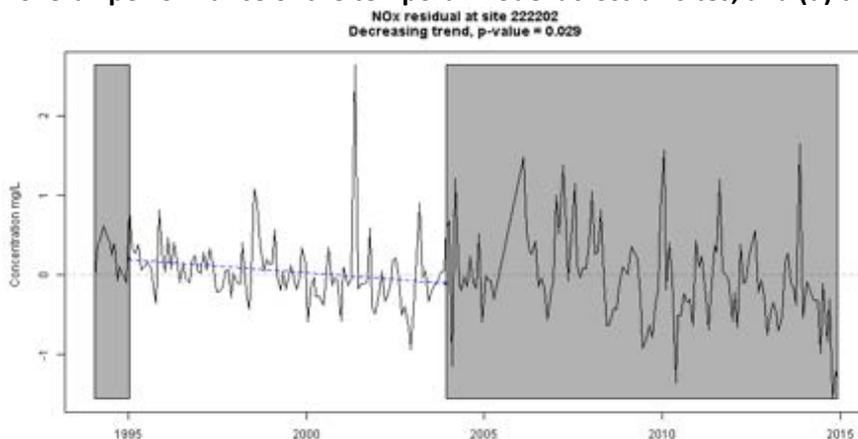
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(Figure 5a), and summarizes the effects of these temporal predictors using a box plot of parameter values across all 102 sites (Figure 5b). As with the spatial model, the transformation and standardization means that temporal parameters should be interpreted by their signs and relative magnitudes, instead of the absolute values. Users can also select a single monitoring site, which is highlighted in red within the box-plot. The temporal model performance is summarized by: 1) a plot of simulated against observed temporal variability at all sites concentration and for all sites (transformed), and the corresponding NSE (Figure 5c); and 2) a map showing the spatial distribution of NSEs at each site (Figure 5d).

The fit of the temporal variability model for an individual site (previously selected) can also be explored in more detail by comparing the simulated and observed concentration time-series. Note that the temporal model only simulates the temporal variation component of concentration (Eq. 4), so the time-series used for plotting are obtained by adding the observed site mean concentration to the simulated and observed temporal variation. Time-series of the model residuals are also presented, which allows interactive investigation of residuals for any user-specified periods within the study period (Figure 6).



**Figure 5. Elements within the temporal variability modelling tool, include: (a) the key factors that the model uses to explain water quality temporal variability; (b) the effects of these key factors; (c) the overall performance of the temporal model across all sites; and (d) the site-specific model performance.**



**Figure 6. Interactive investigation of model residuals within the temporal variability modelling tool.**

## **Conclusions**

The breadth and complexity of water quality data sets make it inherently difficult to present and interpret them. However, such interpretation is necessary if existing monitoring data are to be useful for informing water quality management programs. The interface presented here is an attempt to summarize both raw data and model outputs to support management decision-making. Thus far, user testing of the tool has been restricted to the industry collaborators of the project through which the tool was developed. These interactions have led to the proposed future improvements suggested in each of the three components as detailed previously. The next challenge is to widen this user base and to chart a way for the tool to start to inform management decision-making. This tool will be further developed with our project partners to make the leap from an academic output to a useful component of managers' decision-making armory.

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