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Sampling frequency for water quality variables in streams: Systems analysis to quantify minimum monitoring rates

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ABSTRACT

Insufficient temporal monitoring of water quality in streams or engineered drains alters the apparent shape of storm chemographs, resulting in shifted model parameterisations and changed interpretations of solute sources that have produced episodes of poor water quality. This so-called 'aliasing' phenomenon is poorly recognised in water research. Using advances in *in-situ* sensor technology it is now possible to monitor sufficiently frequently to avoid the onset of aliasing. A systems modelling procedure is presented allowing objective identification of sampling rates needed to avoid aliasing within strongly rainfall-driven chemical dynamics. In this study aliasing of storm chemograph shapes was quantified by changes in the time constant parameter (*TC*) of transfer functions. As a proportion of the original *TC*, the onset of aliasing varied between watersheds, ranging from 3.9–7.7 to 54–79 %*TC* (or 110–160 to 300–600 min). However, a minimum monitoring rate could be identified for all datasets if the modelling results were presented in the form of a new statistic, ΔTC. For the eight H^+, DOC and NO_3-N datasets examined from a range of watershed settings, an empirically-derived threshold of 1.3(ΔTC) could be used to quantify minimum monitoring rates within sampling protocols to avoid artefacts in subsequent data analysis.

1. Introduction

Storm-driven spikes in dissolved organic matter, nitrate, phosphorus, acidity, pharmaceutical residues and microorganisms in natural streams and engineered drainage systems pose significant risks to human health (Viviano et al., 2014; Carstea et al., 2016; Fauvel et al., 2016). Because stream water quality is typically highly variable through rain-storms (Rozemeijer et al., 2010; Viviano et al., 2014), *attribution of human-induced change* is difficult without continuous, rapid monitoring through sequences of storms (Kirchner et al., 2004; Wade et al., 2012). Furthermore, episodes of poor water quality in streams that induce human health issues or ecological damage may be short-lived during storms (Viviano et al., 2014; Fauvel et al., 2016). Continuous, rapid monitoring of water quality variables in streams (or engineered drainage systems such as sewers) is, therefore, needed to characterise these short-lived but environmentally–significant events (Kirchner et al., 2004; Wade et al., 2012; Viviano et al., 2014; Blaen et al., 2016; Fauvel et al., 2016).

In order to model observed dynamics of particular stream water quality variables through storms (so called 'storm chemographs'), studies have shown that models may need to comprise multiple solute pathways. This arises because:

(1) Different components of the chemograph recession may be associated with different hydrological pathways in the watershed (Barnes, 1939),
(2) Many watersheds exhibit more than one dominant hydrological pathway, and
(3) Over short time scales, stream water quality dynamics are often most strongly associated with hydrological dynamics (Petry et al., 2002; Rozemeijer et al., 2010; Jones and Chappell, 2014; Fauvel et al., 2016).

The fast hydrological pathways can be the ones responsible for producing the 'hot moments' of biogeochemical response in streams, and so must be monitored and modelled at a sufficiently high resolution to capture the salient dynamics during model calibration (and validation). If monitoring (and subsequent modelling) is not undertaken at a sufficiently high sampling rate,

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the *shape of each chemograph* through storms may be altered (in observations and simulated data). When the observations are modelled, changes to the shape of the chemograph are exhibited in changes to model parameters or their derived characteristics capturing features such as the 'flashiness' of the chemograph (seen in for example a Time Constant, *TC*, of a transfer function model of rainfall to solute response). This may cause the modeller to infer a different type of hydrological and/or solute pathway (cf. Barnes, 1939) or pathways with incorrect hydrological and/or chemical characteristics. This shift from the true dynamics by generating modelling artefacts is known as 'aliasing' within Signal Processing Theory. Aliasing is another term for the effects of signal spectrum distortion known as 'spectrum folding' where signals at frequencies higher than $f_N = 1/(2\Delta t)$ are misrepresented in the lower part of the spectrum. Here Δt is the time-step in the observations and f_N is known as Nyquist frequency. Aliasing phenomena are often illustrated with subsampled cyclical data displaying a completely different cycle after subsampling. However, it applies equally to episodic (also called transient or finite length record) time series data (Lathi, 2010), such as storm-induced water quality responses. The phenomenon is little acknowledged in hydrological modelling (Littlewood and Croke, 2013) or hydro-chemical modelling of storm dynamics (Kirchner et al., 2004).

Deployment of high frequency (i.e., sub-hourly monitored) sensors of stream-water for certain water quality variables (e.g., electrical conductivity, pH, temperature, turbidity, dissolved oxygen, fluorescence) has been increasing in recent years (Carstea et al., 2016). Additionally, the number of variables that can be monitored accurately with *in situ* stream sensors has also increased, to include for example, dissolved organic carbon (DOC), dissolved organic matter (DOM), nitrate (NO_3-N) and chlorophyll-a (Blaen et al., 2016; Reynolds et al., 2016). Other technological advances now permit sampling and rapid chemical analysis by colorimetry on stream banks for determinands at trace concentrations, e.g., phosphorus. Consequently, there is now greater opportunity to obtain storm-related chemographs with shapes that are not compromised by under-sampling, and so avoiding sampling-related artefacts in model parameterisations (Jones et al., 2014). There has been much recent research examining the effects of monitoring frequency on the calculation of average solute concentrations (e.g., Reynolds et al., 2016). This research has demonstrated that seasonally-averaged concentrations are relatively insensitive to under-sampling. Littlewood and Croke (2013) have, however, demonstrated for hydrological data that within-storm dynamics and the resultant model parameterisation is very sensitive to the effects of degrading the temporal resolution of the input-output time-series. It is our belief that *no studies have examined systematically the impact of under-sampling stream chemical concentrations upon model parameters capturing chemical concentration changes through storms, and the consequent impact on interpretation of solute pathways.*

While the cost of gaining water quality values using stream sensors is relatively insensitive to the numbers of values collected, unlike water sampling followed by laboratory-based chemical analyses, there are practical/cost constraints on the use of these *in situ* sensor systems. Sensor systems without automated telemetry have a finite local data storage capacity. Greater monitoring rates also result in greater power requirements that may be limited if sufficient renewable energy or mains electricity is unavailable. Consequently, there is considerable value in knowing the *minimum monitoring rate* that does not distort the true shape of chemographs needed for hydro-chemical modelling without creating unnecessary logistical issues for monitoring.

In many headwaters, dynamics in stream water quality may be dominated by short-term changes in the hydrology (i.e., rainfall time-series) via one or more water pathways (Langan and Whitehead, 1987; Littlewood, 1987; Jones and Chappell, 2014). Some process-based models of hydro-chemistry show sensitivity of solute concentration responses to rainstorms, e.g., TNT2-P (Dupas et al., 2016). Rigorous uncertainty analyses applied to process-based models have, however, shown that many are attempting to capture too many processes and so have the downside of producing distributions of the most sensitive model parameters (and related Dynamic Response Characteristics, DRCs) that are too uncertain, i.e., poorly identifiable. This makes process interpretation or quantification of change in DRCs of water quality variables difficult to ascertain. There is, therefore, a compelling argument, for making sure that water quality models are no more complex than warranted by the dynamics observed in the stream water quality variables of interest. Indeed, Langan and Whitehead (1987), Littlewood (1987) and Jones and Chappell (2014) have presented examples systems models based on linear transfer functions where they achieve this using model structures based solely on information from hydrological dynamics.

The aim of this study was to quantify the point at which a reducing monitoring rate would result in a significant shift in model parameters of strongly hydrologically-driven water quality models based on transfer functions, where the identified model for fine monitoring intervals was very well-defined (i.e., high simulation efficiency). These points of change were then analysed to attempt to produce a new procedure for users of water quality sensors (and bank-side analysers) deployed on streams to help identify the minimum monitoring intervals necessary for later modelling (whether by systems analysis or process-based algorithms). Five specific objectives were defined to achieve this aim:

1/ To identify parsimonious transfer function models of example stream water quality variables (based solely on rainfall input) with data monitored at example sites at a high-frequency (i.e. 1, 5 and 15 min). These initial models need to have high simulation efficiency (and so be based upon only a short period of storm-related dynamics) and ideally the DRCs should be physically interpretable.

2/ To subsample the observed time-series of each water quality variable to mimic successively longer monitoring intervals. Parsimonious transfer function models of these data (combined with the rainfall input integrated at the same interval) will be identified using the same numerical tools.

3/ To identify the first significant drift in the key transfer function DRC of the Time Constant (i.e., residence time of response or *TC*) arising from successive models with increasing time-step length.

4/ To attempt to understand and generalise the point at which data and model time-step affects the parameters of systems models based on transfer functions, and by inference the parameterisation of process-based models, and

5/ To outline a recommended procedure for identifying the minimum monitoring intervals necessary for modelling storm-driven, water quality dynamics in streams.

2. Methods

2.1. Selection of illustrative stream water quality datasets

The data utilised consist of those collected continuously at 1-min or 5-min resolution specifically for this study, and existing data collected continuously at 15-min intervals. Hydrogen ion (H^+) concentration (derived from *in situ* pH measurements) is the key chemical variable examined in this study because it is widely