



A Bayesian risk assessment framework for microcystin violations of drinking water and recreational standards in the Bay of Quinte, Lake Ontario, Canada

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ARTICLE INFO

Article history:

Received 12 November 2018

Received in revised form

31 May 2019

Accepted 2 June 2019

Available online 10 June 2019

Keywords:

Cyanobacteria
Harmful algal blooms
Bayesian inference
Microcystin
Eutrophication
Bay of Quinte

ABSTRACT

Freshwater ecosystems can experience harmful algal blooms, which negatively impact recreational uses, aesthetics, taste, and odor in drinking water. Cyanobacterial toxins can have dire repercussions on aquatic wildlife and human health, and the most ubiquitous worldwide are the hepatotoxic compounds known as microcystins. The factors that influence the occurrence and magnitude of cyanobacteria blooms and toxin production vary in space and time and remain poorly understood. It is within this context that we present a suite of statistical models, parameterized with Bayesian inference techniques, to link the retrospective analysis of important environmental factors with the probability of exceedance of threshold microcystin levels. Our modelling framework is applied to the Bay of Quinte, Lake Ontario, Canada; a system with a long history of eutrophication problems. Collectively, 16.1% of the samples of the system collected during the study period (2003–2016) exceeded the drinking water guideline of $1.5 \mu\text{g L}^{-1}$, while approximately 3% of recorded values exceeded the recommended recreational threshold of $20 \mu\text{g L}^{-1}$. Using a segmented regression model with a stochastic breakpoint of microcystin concentrations estimated at $0.54 \mu\text{g L}^{-1}$, we demonstrate that the environmental conditions associated with increased probability of exceedance of the drinking water standard are chlorophyll *a* concentration $\geq 7 \mu\text{g L}^{-1}$, water temperature $\geq 20^\circ\text{C}$, ammonium concentration $\leq 40 \mu\text{g L}^{-1}$, total phosphorus concentration $\geq 25 \mu\text{g L}^{-1}$, and wind speed $\leq 37 \text{ km h}^{-1}$. Considering the multitude of factors that can influence the ambient levels of toxins, our study argues that the adoption of probabilistic water quality criteria offers a pragmatic approach to accommodate the associated uncertainty by permitting a realistic frequency of violations. In this context, we present a framework to evaluate the confidence of compliance with probabilistic standards that stipulate less than 10% violations of microcystin threshold ambient levels.

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1. Introduction

Cyanobacteria-dominated harmful algal blooms (cHABs) are a growing concern in freshwater ecosystems globally (Scholz et al., 2017). Often manifested as dense surface scums, cHABs may be

responsible for significant environmental and socioeconomic impacts (Dodds et al., 2009; Watson et al., 2015), particularly due to the production of cyanotoxins which can have adverse health effects on those utilizing surface waters for drinking water and recreational activities (Carmichael and Boyer, 2016). The most ubiquitous cyanotoxins in freshwater ecosystems worldwide are the family of hepatotoxic compounds known as microcystins (MCs) (WHO, 2003). Several cyanobacterial taxa can synthesize MCs, particularly the major bloom-forming genera, *Microcystis*, *Dolichospermum*, formerly called *Anabaena*, and *Planktothrix* (Pick,

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2016). Grouped according to their amino-acid composition and methylation, MCs comprise ~90 variants with varying levels of toxicity; the most toxic of which are MC-LR and MC-LA (Sivonen and Jones, 1999). MCs are highly resistant to degradation and can persist in the water column several weeks after a visible cyanobacterial bloom (Zastepa et al., 2014). Conventional drinking water treatment methods (i.e., chlorination, coagulation, boil-water advisories) are often ineffective in eliminating MCs, and therefore costs for additional water purification measures can be significantly increased (Zamyadi et al., 2012). MCs pose human and animal health risks, through ingestion of contaminated drinking water or consumption of contaminated fish/shellfish (Watson et al., 2015). Many regulatory bodies have implemented water quality guidelines for MC concentrations (mostly based on the specific variant MC-LR) to protect human and animal health, ranging from 0.3 to 1.6 $\mu\text{g L}^{-1}$ for drinking water (WHO, 2011; U.S. EPA, 2015; HC, 2017), and $\leq 20 \mu\text{g L}^{-1}$ for recreational uses (HC, 2017).

Research into the environmental factors that influence cyanotoxin production has intensified over the past decade (Heisler et al., 2008; Pick, 2016). Similar to the ambient conditions influencing cyanobacterial blooms (i.e., nutrients, light, temperature, water column stability, grazing pressure), frequently identified environmental factors co-varying with ambient toxin levels have included, alone or in combination, elevated cyanobacterial (particularly *Microcystis*) biomass, chlorophyll *a* and nutrient concentrations, surface water temperature, wind speed and/or direction (Francy et al., 2016; Harris and Graham, 2017; Jacoby et al., 2000; Kotak et al., 2000; Wood et al., 2017). Likewise, total nitrogen to total phosphorus (TN:TP) ratio has been hypothesized to be a significant regulatory factor (Orihel et al., 2012; Scott et al., 2013; Jacoby et al., 2015), and so has the relative abundance of different nitrogen (N) species that may also modulate the toxicity of MC variants produced (Monchamp et al., 2014; Scott et al., 2014). Nonetheless, despite all the active research, the causal relationships and mechanisms leading to high MC events still remain elusive (Scholz et al., 2017; Harris and Graham, 2017). The dynamic response of cyanobacteria to changes in environmental conditions results in blooms that are highly variable in space and time (Stumpf et al., 2012). It has also been reported that the genetic capacity of cyanobacteria to produce toxins varies among taxa or even within strains of the same species (Rinta-Kanto et al., 2009), while both toxic and non-toxic genotypes can coexist within the same population and actively compete for the same natural resources (Kardinaal et al., 2007).

Understanding the site-specific mechanisms that drive the variability of MC concentrations is important to the water quality assessment process and ultimately to the development of effective water management policies. In this context, a major challenge is to interpret the data from a limited amount of samples and determine whether an apparent violation of toxin threshold levels warrants classifying a system as impaired or actions taken to address water quality degradation have brought about the desired improvements (Smith et al., 2001; Zhang and Arhonditsis, 2008). Considering the multitude of factors that can modulate the ambient levels of toxins, the adoption of probabilistic criteria offers a pragmatic approach to accommodate the associated uncertainty by permitting a realistic frequency of violations; that is, a system in question will be classified as impaired only if more than 10% of the samples collected exceed a critical toxin concentration. Another important step to establish an operational procedure is the coupling of predictive models with uncertainty analysis that will allow a shift in the focus from the mean model predictions to the tails of the derived error distributions. In doing so, we can draw predictive statements about the fraction of MC events that exceed a pre-specified critical risk level (Borsuk et al., 2002; Zhang and Arhonditsis, 2008; Ramin

et al., 2011). To date, less than a handful of studies have attempted to connect the prevailing environmental conditions with the likelihood of violations of water quality guidelines for MC threshold concentrations (Yuan et al., 2014; Hollister and Kreakie, 2016; Taranu et al., 2017).

It is within this context that we present a Bayesian modelling framework to identify thresholds of environmental factors influencing high MC events, while providing a probabilistic assessment of the risk of encountering violations. Our analysis aims to shed light on the nature of the relationships between MCs and several potentially important predictor variables, accounting for the nutrient concentrations, temperature, and meteorological conditions. Special emphasis is given to the chlorophyll *a* concentration, which is a frequently used surrogate variable of total phytoplankton biomass and is considered one of the most reliable predictors of toxin concentrations. We also illustrate a methodological framework to evaluate the confidence of compliance with candidate probabilistic standards that stipulate less than 10% violations of potential MC thresholds with different sample sizes and prior beliefs based on our empirical knowledge (Fig. 1). To showcase this modelling framework, we used data collected from the Bay of Quinte (Lake Ontario, Ontario, Canada), a system that has been experiencing water quality issues, and where the elimination of *CHABS* represents one of the major challenges of eutrophication management (Arhonditsis et al., 2016).

2. Materials and methods

Study site and probabilistic standards: The Bay of Quinte is a Z-shaped embayment located on the northeastern shore of Lake Ontario, Ontario, Canada (Fig. 1). Surrounded by a >18000 km² watershed, the Bay of Quinte has a total surface area of 254 km² that is divided into three segments: the upper bay is large and shallow (136 km², mean and maximum depth of 3.5 m and 8 m, respectively); the middle bay is smaller but deeper (49 km², mean depth 5.2 m, maximum depth 17 m) and represents an intermediate zone between the upper and lower bay, which is a deep and fjord-like system (72 km², mean depth 24.4 m, maximum depth 66 m) directly connected with Lake Ontario. As a result of decades of cultural eutrophication, the Bay of Quinte has been experiencing significant water quality problems, including the frequent occurrence of spatially extensive algal blooms and predominance of toxic cyanobacteria; most notably, the emergence of the MC-producing

Logic of our Model

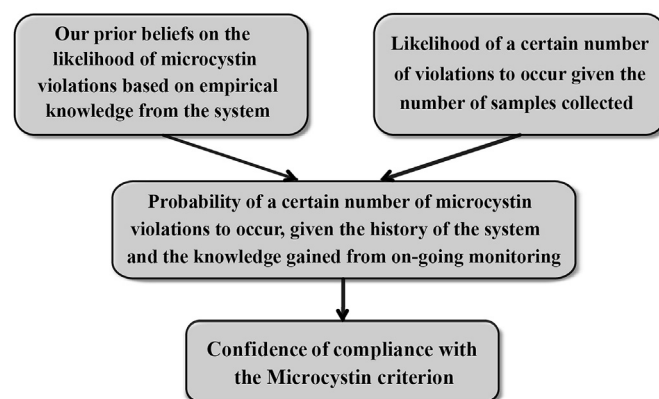


Fig. 1. The logic of the modelling framework used to evaluate the degree of impairment of the Bay of Quinte, regarding the frequency of violations of MC drinking water and recreational guidelines.

Microcystis aeruginosa after the invasion of zebra (*Dreissena polymorpha*) and quagga (*D. bugensis*) mussels in the mid-1990s (Nicholls et al., 2002). Consequently, eutrophication management in the area has primarily focused on the eradication of harmful algal blooms and restoration of optimal water quality conditions through reduction of external nutrient loading. Nonetheless, recent empirical and modelling evidence highlighted internal recycling as another key factor that shapes phosphorus dynamics in the Bay of Quinte (Kim et al., 2013; Doan et al., 2018). While the flow from Trent River is the predominant driver of water quality in the innermost area of the system (Fig. 2), the sediments in the upper and middle bay release a significant amount of phosphorus and the corresponding fluxes are modulated by the macrophyte and dreissenid activity (Kim et al., 2013). From a management perspective, the presence of an active nutrient regeneration mechanism suggests that the benefits of additional reductions of the external point and non-point loading may not be realized within a reasonable time frame (i.e., 5–10 years). In fact, Arhonditsis et al. (2016) showed that the restoration pace of the system could be slow, with no clear evidence of an establishment of an alternative stable state (Janse et al., 2010), even if the riverine total phosphorus concentrations reach levels significantly lower than their contemporary values, $<25 \mu\text{g TP L}^{-1}$.

Water quality targets are based on an aggregated spatiotemporal (i.e., seasonal and system-wide) scale and are currently set at $30 \mu\text{g L}^{-1}$ and $10\text{--}12 \mu\text{g L}^{-1}$ for total phosphorus (TP) and chlorophyll *a* (hereafter chl *a*) concentrations, respectively (Arhonditsis et al., 2016). However, the adequacy of the coarse scale selected to establish water quality standards has been challenged, since it neither captures the intra-annual variability in the upper bay, nor does it represent the dynamics in nearshore areas of high public exposure, e.g., beaches (Kim et al., 2013, 2018; Arhonditsis et al., 2016). A single-valued water quality standard, monitored in a few offshore sampling stations, is unlikely to reflect the entire range of conditions experienced in time and space, including episodic events, such as excessively high end-of-summer ambient TP levels or *CHABs* (Kim et al., 2013). Instead, it has been advocated that the

water quality targets should revolve around extreme (and not average) values of variables of management interest and must explicitly accommodate all the sources of uncertainty by permitting a realistic frequency of standard violations. Namely, Arhonditsis et al. (2016) have proposed the critical threshold TP level should be set at a value of $40 \mu\text{g L}^{-1}$, which cannot be exceeded in more than 10–15% of the samples collected from selected monitoring sites during the growing (May–October) season. Based on empirical evidence that the TP concentrations in the Bay of Quinte follow a log-normal distribution and that TP values $<15 \mu\text{g L}^{-1}$ are typically registered in only 10% of the collected samples, 10–15% exceedances of the $40 \mu\text{g TP L}^{-1}$ level are approximately equivalent to a targeted seasonal average of $25\text{--}28 \mu\text{g TP L}^{-1}$. Similar probabilistic criteria to more comprehensively monitor the progress of the prevailing conditions with *CHABs* in the bay have not been proposed.

Dataset description: We compiled concurrent MC, water quality, and meteorological data from several monitoring programs. The Bay of Quinte Harmful Algal Blooms (*BQHABs*) initiative and Environment and Climate Change Canada (*ECCC*) have monitored water quality since 2003 (Watson et al., 2011). The Bay of Quinte Algae Watch (*BQAW*) program intensively sampled MCs and selected chemical and physical parameters over the course of a 4-year period (2010–2013). Under these programs, water samples, water column profiles, total MCs, and related site data were collected from various locations throughout the Bay of Quinte (i.e., beaches, embayments, offshore waters, downstream sites of wastewater treatment plant discharges, macrophyte beds, and river mouths). For all programs, total MCs were analyzed using an enzyme-linked immunosorbent assay (*ELISA*) and protein phosphatase inhibition assay (*PPIA*) (Watson et al., 2007). A suite of water quality parameters were measured from selected water samples and analyzed following standard methods at the National Laboratory for Environmental Testing in Burlington, Ontario (Watson et al., 2007, 2011).

Data collected from the *BQHABs*, *BQAW*, and *ECCC* surveys were combined with information from the Drinking Water Surveillance

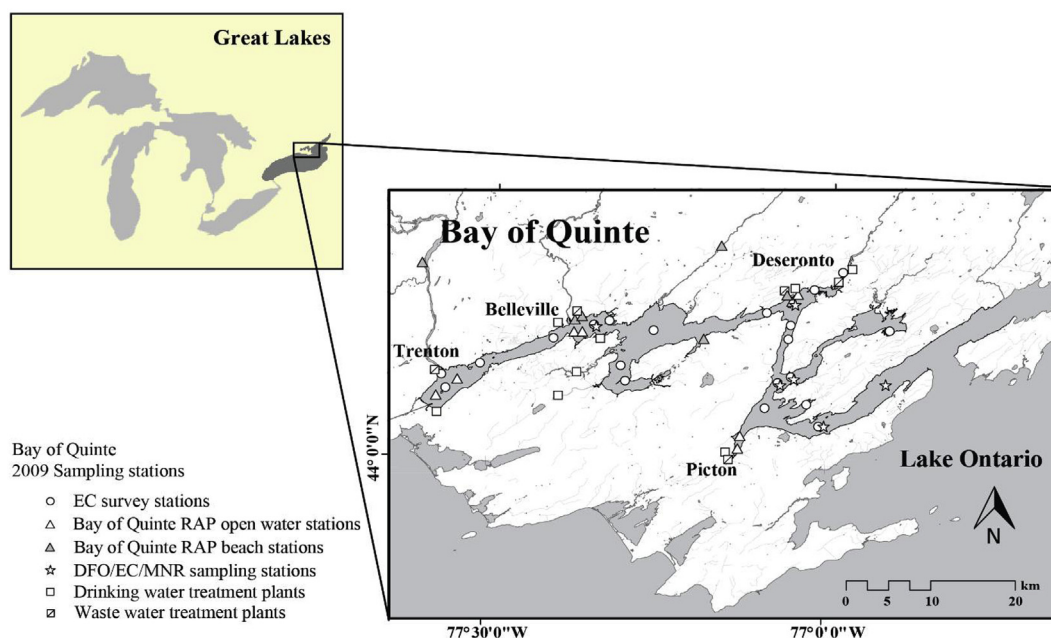


Fig. 2. Map of the Bay of Quinte, Lake Ontario (Ontario, Canada), and sampling stations collected by various agencies. Abbreviations in the legend stand for: Environment Canada (EC), Remedial Action Plan (RAP), Department of Fisheries and Oceans (DFO), Ministry of Natural Resources (MNR).

Program (DWSP) (<https://www.ontario.ca/data/drinking-water-surveillance-program>) for the Belleville Drinking Water System plant. Operated by the Province of Ontario's Ministry of the Environment and Climate Change (MOECC), in partnership with municipalities, the DWSP is a voluntary program that monitors water quality at selected municipal drinking water systems in order to gather information on drinking water quality in Ontario. Raw water samples were collected on a weekly basis from June to November (2011–2013) from inside the water treatment plant prior to addition of treatment chemicals, and thus the samples represent the water at the source. A series of microbiological, inorganic and organic chemical parameters, water temperature, emerging complex contaminants were monitored by drinking water systems staff and analyzed with standard methods at the MOECC Laboratory Services Branch (MOE, 2010). Additional data for chl *a* for the Belleville Drinking Water System plant were reported under the Great Lakes Intake Program (<https://www.ontario.ca/data/lake-water-quality-drinking-water-intakes>).

We compiled meteorological data from the ECCC digital archive of Canadian climatological data (<http://climate.weather.gc.ca/>). We accessed publicly available data from Trenton A weather station (Climate ID 6158875), which is the closest (<25 km) to the majority of the monitoring sites shown in Fig. 2, with consistent records throughout our study period. The first hypothesis examined was the presence of a lagged relationship between meteorological forcing and dominance of *Microcystis* in the summer algal assemblage or microcystin production. We examined a number of expressions that connected the microcystin ambient levels with the antecedent meteorological conditions (e.g., wind speed, wind direction, precipitation, air temperature, and evapotranspiration), such as moving time windows that averaged each of the weather-related variables for up to ten days prior to the measured microcystin concentrations. None of the tested permutations outperformed the models that considered contemporaneous values of the meteorological predictors. Given the large number of environmental (water quality and meteorological) predictors available, we chose to retain a subset based on three criteria: (i) those that had been found to influence MC concentrations in previous studies on freshwater systems; (ii) those that are used as primary indicators of local ecosystem conditions (Munawar et al., 2012); and (iii) data availability. Thus, our MC statistical models are based on the following predictors: TP and ammonium (NH₄⁺) concentrations, wind speed, water temperature, and chl *a* concentrations. In the absence of water column stratification records, we used wind speed (measured as the maximum instantaneous gust recorded over an elapsed time of 3–5 s during the day, km h⁻¹) as a proxy measure of water column stability, assuming that gustier days correspond to greater water column mixing and lower water column stability (Kann and Welch, 2005). It is also important to note that the consideration of multiple predictors for our statistical models reduced the total sample size (i.e., N = 186 across all the locations monitored over the course of our study), and the data used were mainly based on offshore waters and less so on beaches, embayments, macrophyte beds, and river mouths.

Bayesian modelling framework: Our first statistical model (Bernoulli model) examines the likelihood exceedance of an established drinking water standard for MC, equal to 1.5 µg L⁻¹, given different combinations of environmental conditions (HC, 2017). This model postulates that the violation of a MC standard resembles a Bernoulli process, such that the collected samples represent a sequence of independent identically distributed Bernoulli trials (Mahmood et al., 2014; Shimoda et al., 2016). For every sample collected, the model calculates the likelihood of violating the MC threshold level independently from the previous or subsequent samples, while the probability *p* of a certain MC violation is

determined by a series of potentially important causal factors, such as nutrient concentrations, water temperature, or meteorological conditions. The causal relationship between the probability of violation occurrence of the 1.5 µg MC L⁻¹ threshold and environmental conditions was modeled using logistic regression:

$$MC_{exceedance(i)} | p_i(\beta_0, \beta_x, x_i) \sim \text{Bernoulli}(p_i)$$

$$\text{logit}(p_i) = \beta_0 + \sum \beta_x \cdot \ln(x_i)$$

$$\beta_0, \beta_x \sim N(0, 10000)$$

$$i = 1 \dots M, \quad x = NH_4^+, WT, Wind, TP, Chl a$$

where $MC_{exceedance(i)}$ denotes the violation (or not) of the MC threshold (1 or 0) in the i^{th} sample; x_i corresponds to the value of each of the predictors in the same sample; and β_0 and β_x are the regression coefficients which were assigned flat (or diffuse) normal prior distributions with mean 0 and variance 10000; and $M (=186)$ is the size of our dataset.

Our second model aimed to examine the strength and monotonicity of the relationship between total MC and chl *a* concentrations within the domain delineated by our dataset. In particular, we use segmented (or piecewise) simple regression to identify a breakpoint in which the independent variable is partitioned into two intervals and then fit separate linear equations within each interval. Thus, the model can be summarized as follows:

$$\ln(MC_{modi}) = \beta_0 + \beta_{1j} \left(\ln(chl a_i) - \ln(chl a_{breakpoint}) \right) + \epsilon_i$$

$$j = 1 \text{ if } chl a_i < chl a_{breakpoint}$$

$$j = 2 \text{ if } chl a_i \geq chl a_{breakpoint}$$

$$\ln(chl a_{breakpoint}) \sim U(1.6, 2.3)$$

$$\beta_0, \beta_{1j} \sim N(0, 10000)$$

$$\epsilon_i \sim N(0, \sigma_\epsilon^2)$$

$$\sigma_\epsilon^{-2} \sim G(0.001, 0.001)$$

$$i = 1 \dots M$$

where $\ln(MC_{modi})$ represents the natural log-transformed predicted MC concentration in sample *i*; β_0 is the intercept term; β_{1j} denotes the slope terms for the two segments determined by the chl *a* concentration breakpoint or $chl a_{breakpoint}$; $U(1.6, 2.3)$ is the log-uniform prior distribution assigned to $chl a_{breakpoint}$ with lower and upper bounds of 1.6 and 2.3 $\ln(\mu\text{g chl } a \text{ L}^{-1})$ or 5 and 10 $\mu\text{g chl } a \text{ L}^{-1}$, respectively; ϵ_i represents the model error term which is a draw from a normal distribution with a mean equal to zero and error variance σ_ϵ^2 ; $N(0, 10000)$ is the normal distribution with mean 0 and variance 10000, and $G(0.001, 0.001)$ is the gamma distribution with shape and scale parameters of 0.001. These prior distributions are considered “non-informative” or vague.

Our third statistical formulation employs a segmented multiple regression model with a stochastic breakpoint set on the response variable. Specifically, this formulation dissects the multivariate data into two subsets on the basis of their MC concentrations within which two linear equations are being estimated. In doing so, we can

examine to what extent the nature of the relationship of the individual predictors changes against low or high *MC* values and subsequently examine if there are approximate thresholds for each predictor variable that increases the likelihood of violations of the drinking water guidelines. The third statistical model can be summarized as follows:

$$\ln(MC_{modi}) = \beta_{0j} + \sum \beta_{xj} \cdot \ln(x_i) + \varepsilon_i$$

$$j = 1 \text{ if } MC_i < MC_{breakpoint}$$

$$j = 2 \text{ if } MC_i \geq MC_{breakpoint}$$

$$\ln(MC_{breakpoint}) \sim U(-1.6, 0)$$

$$\beta_{0j}, \beta_{xj} \sim N(0, 10000)$$

$$\varepsilon_i \sim N(0, \sigma_\varepsilon^2)$$

$$\sigma_\varepsilon^{-2} \sim G(0.001, 0.001)$$

$$i = 1 \dots N, x = NH_4^+, WT, Wind, TP, Chl a$$

where β_{0j} and β_{1j} denotes the intercept and slope terms for the two segments determined by the *MC* concentration breakpoint or $MC_{breakpoint}$: $U(-1.6, 0)$ is the log-uniform prior distribution assigned to $MC_{breakpoint}$ with lower and upper bounds of -1.6 and $0 \ln(\mu\text{g L}^{-1})$ or 0.2 and $1 \mu\text{g L}^{-1}$, respectively. We also used a Tobit configuration to address the potential for bias due to the fact that $\sim 20\%$ of *MC* measured concentrations were below the detection limit ($<0.15 \mu\text{g L}^{-1}$). *MC* values falling below the detection limit were treated as random draws from a normal distribution parameterized such that its values were lying between the actual zero and the detection limit. This approach used a bounded distribution for the measurements, with an upper bound equal to either the detection limit or a very large (arbitrary) number, depending on whether or not the measurement fell below the detection limit. Model codes and computational aspects of our Bayesian modelling framework are provided in the Supporting Information section.

Confidence of compliance with probabilistic standards: Probabilistic standards stipulate that no more than a *stated frequency of exceedances* of a *targeted environmental threshold* should occur within a *given number of samples* collected over a compliance assessment domain. Simply put, a probabilistic standard requires that a targeted numerical value of a water quality variable should not be exceeded more frequently than a selected percentage (e.g., 10–15%) of all the samples collected from a pre-specified number of monitoring sites representative of the system dynamics over a time span of management interest. Hence, the evaluation of compliance with a water quality standard is subjected to sampling error associated with the total number of samples collected, as well as the decisions made regarding the locations and time frequency of the monitoring programs (McBride and Ellis, 2001). This uncertainty not only influences the potential for an error in the inference drawn regarding the compliance or breach of the probabilistic standard, but also the nature of the error – Type I (falsely inferring a breach of standard) or II (falsely inferring compliance) – that might occur. In a Bayesian context, compliance assessment has the potential to address such issues directly, without the need to consider significance levels, Type I and Type II error risks (McBride and Ellis, 2001; Zhang and Arhonditsis, 2008). In this study, similar to the modelling framework originally presented by McBride and Ellis (2001), we use beta-distributed prior information and a binomial likelihood to

produce “confidence-of-compliance” graphs (See Supporting Information section). For illustration purposes, we evaluated the confidence of compliance with probabilistic standards that stipulate less than 10% violations of two *MC* thresholds (1.5 and $5 \mu\text{g L}^{-1}$), when we consider different sample sizes and prior beliefs.

3. Results

The distribution of *MC* concentrations recorded from 2003 to 2016 was highly skewed (Fig. 3a). Collectively, 16.1% of *MC* values exceeded the drinking water guideline of $1.5 \mu\text{g L}^{-1}$, while 3.1% of observed values exceeded the recommended recreational threshold of $20 \mu\text{g L}^{-1}$. The maximum *MC* concentration measured was close to 3 mg L^{-1} in August 2015. Interestingly, a higher proportion of violations of water quality guidelines (both drinking water and recreational) was observed from 2009 to 2015 than in other periods (Fig. 3b). There were no *MC* violations of the drinking water quality guidelines registered in 2006, 2008, nor in 2016, but it should also be noted that sample sizes were low ($n < 25$) in those years (Fig. 3b). Records of *MC* violations of drinking water guidelines regularly occur from May through October, but the frequency is more pronounced from mid-summer to early fall (Fig. 3c). Violations of recreational guidelines mainly occur from July to August, although frequent violations have also been registered in September or even in October (Fig. 3c).

The Bernoulli model correctly classified 157 instances, where the drinking water threshold ($1.5 \mu\text{g L}^{-1}$) was not violated and the predicted probability of occurrence was similarly low ($p < 0.5$). There were no cases of non-violation that were assigned a high probability of occurrence ($p \geq 0.5$), i.e., no false alarms (Table 1). However, the model underestimated the number of *MC* violations experienced in the system, predicting only 5 cases with high probability of occurrence ($p \geq 0.5$), out of 29 recorded violations ($\sim 17\%$ accuracy). We thus infer that the Bernoulli model is prone to predicting false negatives (i.e., failure to predict the frequency of *MC* violations that actually occurred) and cannot offer a reliable tool from a public health perspective in the Bay of Quinte (Table 1). NH_4^+ displayed a negative (-0.33 ± 0.21) relationship with the probability of *MC* violations. In a Bayesian context, the significance of this result can be assessed with the odds ratio² for the corresponding regression coefficient to be negative, which was 16.2:1 in this particular case. In a similar manner, chl *a* displayed a strongly positive (0.89 ± 0.29) association with *MC* violations, characterized by an OR of 930:1 (Table 2). We can also infer that the relationships between the likelihood of *MC* violations and water temperature (-0.32 ± 0.71) or *TP* concentrations (-0.22 ± 0.47) were negative but the ORs ($\approx 2.1:1$) suggest that the corresponding coefficients were marginally discernible from zero. The same pattern held true with our model intercept (1.59 ± 4.66), i.e., the likelihood of *MC* violations when all four predictor variables tend to low values. Moreover, the simple piecewise regression model suggests a breakpoint at the level of $1.97 \ln(\mu\text{g chl } a \text{ L}^{-1})$ or $7.1 \mu\text{g chl } a \text{ L}^{-1}$, where the nature of the relationship between *MC* and chl *a* concentrations changes from weakly (0.21 ± 0.23) to strongly (0.96 ± 0.15) positive (Fig. 4). Importantly, the latter segment of this relationship comprises nearly all the daily snapshots from the system, when *MC* violations of the drinking water standard occurred.

The segmented multiple regression model identified a significant *MC* breakpoint at the level of $0.54 \mu\text{g L}^{-1}$ (or -0.62 ± 0.08 in the logarithmic scale), separating the relationship between environmental variables and *MC* concentrations into two regions

² The odds ratio (OR) of a regression coefficient being negative/positive is the ratio of the probability to be below/above zero to the probability above/below zero.

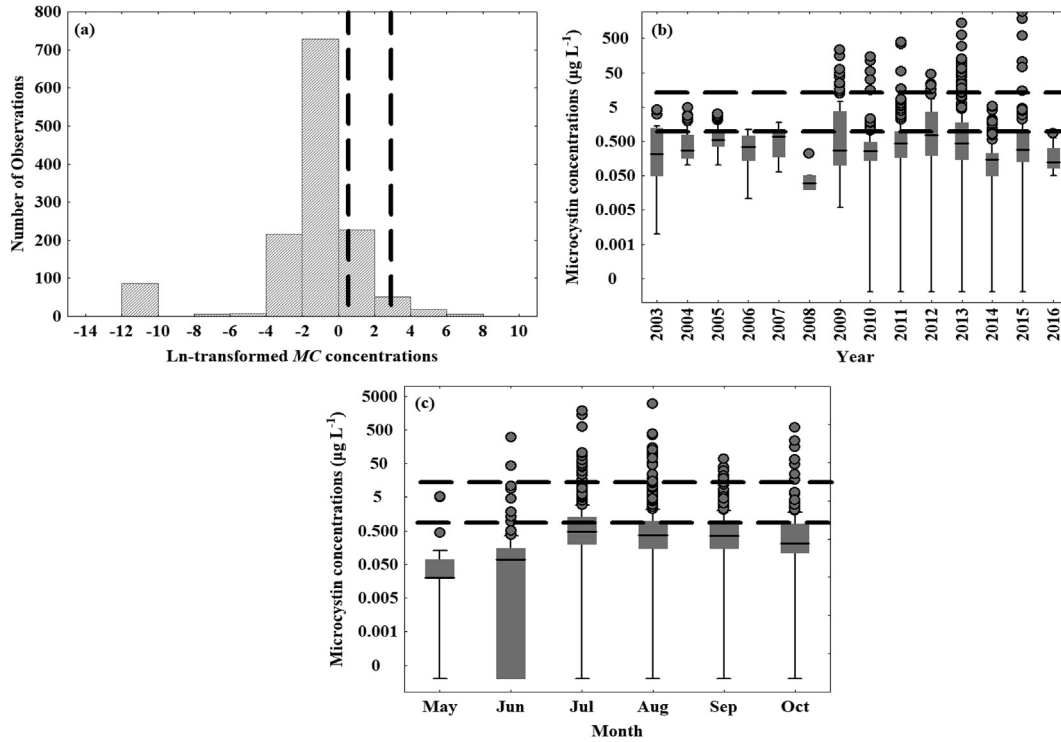


Fig. 3. (a) Frequency histogram of measured MC concentrations, (b) MC frequency distributions per year, and (c) MC frequency distributions per month (May–October), from all sampling events ($N = 1347$) conducted on the Bay of Quinte from 2003 to 2016. Dashed lines represent Health Canada drinking water ($1.5 \mu\text{g L}^{-1}$) and recreational ($20 \mu\text{g L}^{-1}$) water quality guidelines, respectively. In (a), 16.1% and 3.1% of all MC observations fell above the drinking water and recreational guidelines, respectively.

Table 1
Contingency table analysis classifying probability results from the Bernoulli model into binary occurrences of violations of microcystin drinking water guidelines ($1.5 \mu\text{g L}^{-1}$). p represents the predicted probability of a microcystin violation.

MC concentration threshold ($\mu\text{g L}^{-1}$)	$p < 0.5$	$p \geq 0.5$	Totals
< 1.5 (0)	157	0	157
≥ 1.5 (1)	24	5	29
Totals	181	5	186

(Table 2). The comparison of the posterior predicted median MC values against the measured ones was satisfactory ($R^2 = 0.73$; Fig. 5) with a mean standard error of the estimate equal to $0.77 \pm 0.04 \ln(\mu\text{g MC L}^{-1})$. Below the MC breakpoint of $0.54 \mu\text{g L}^{-1}$, our analysis suggests a fairly strong, positive relationship of chl a (0.14 ± 0.08), TP (0.22 ± 0.15), and water temperature (0.34 ± 0.25) with MC concentrations, where the ORs for the corresponding regression coefficients to be positive were 24.0:1, 13.0:1, and 10.5:1. In contrast, the signature of wind speed (-0.29 ± 0.39), and NH_4^+

(-0.08 ± 0.07) was weakly negative with ORs of a negative relationship equal to 3.4:1 and 6.9:1, respectively (Table 2). When MC concentrations exceed the breakpoint of $0.54 \mu\text{g L}^{-1}$, our analysis underscores the strongly positive association with chl a ($OR = 3.8 \cdot 10^5:1$), the negative relationship with the ambient TP ($OR = 19.1:1$) and NH_4^+ ($OR = 80.8:1$) levels, and the weakly negative (practically non discernible from zero) effects of wind speed ($OR = 1.4:1$) and water temperature ($OR = 1.1:1$) (Table 2). To identify approximate thresholds of environmental predictors that increased the probability of exceedance of the $1.5 \mu\text{g L}^{-1}$ MC drinking water guideline, we selected the values above (or below) which 80% of the daily snapshots recorded from the Bay of Quinte are characterized by a greater than 10% probability of exceedance of that threshold. Overall, our analysis suggests the environmental conditions that appear to increase the probability of exceedance of the MC drinking water standard are chl a concentrations $\geq 7 \mu\text{g L}^{-1}$, water temperatures $\geq 20^\circ\text{C}$, NH_4^+ concentrations $\leq 40 \mu\text{g L}^{-1}$, TP concentrations $\geq 25 \mu\text{g L}^{-1}$, and wind speeds $\leq 37 \text{ km h}^{-1}$ (Fig. 6).

Table 2
Posterior (mean \pm standard deviation) regression coefficients of the Bernoulli and two segmented regression models to predict MC concentrations ($\mu\text{g L}^{-1}$). Subscripts of the regression coefficients correspond to the predictor variables used for each model: NH_4^+ = total ammonium concentration ($\mu\text{g L}^{-1}$); WT = water temperature ($^\circ\text{C}$); $Wind$ = speed of maximum wind gust (km h^{-1}); TP = total phosphorus concentration ($\mu\text{g L}^{-1}$); $Chl a$ = chlorophyll a concentration ($\mu\text{g L}^{-1}$).

Model	Breakpoint	Standard error of the estimate (σ_ϵ)	Regression coefficients					
			β_0	$\beta_{NH_4^+}$	β_{WT}	β_{Wind}	β_{TP}	β_{Chla}
Stochastic segmented on $Chl a$	$< 1.97 \pm 0.12^a$	1.16 ± 0.07	-1.05 ± 0.13	-0.33 ± 0.21	-0.32 ± 0.71	-0.79 ± 1.22	-0.22 ± 0.47	0.21 ± 0.23
	$\geq 1.97 \pm 0.12$							0.96 ± 0.15
Bernoulli Stochastic segmented on MC	$< -0.62 \pm 0.08^b$	0.77 ± 0.04	1.59 ± 4.66	-0.08 ± 0.07	0.34 ± 0.25	-0.29 ± 0.39	0.22 ± 0.15	0.89 ± 0.29
	$\geq -0.62 \pm 0.08$		1.29 ± 1.92	-0.18 ± 0.08	-0.02 ± 0.35	-0.09 ± 0.46	-0.28 ± 0.17	0.41 ± 0.09

^a Represents a threshold level of $7.1 \mu\text{g chl } a \text{ L}^{-1}$, where the slope of the MC relationship with chlorophyll a changes.

^b Represents a threshold level of $0.54 \mu\text{g MC L}^{-1}$, where the nature of the MC relationship against NH_4^+ , WT , $Wind$, TP , and $Chl a$ changes.

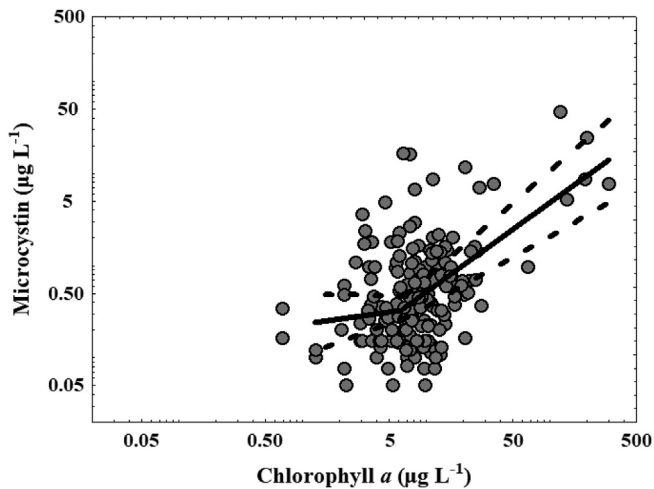


Fig. 4. Simple piecewise regression model for microcystin (MC) concentrations as a function of chlorophyll *a*. The relationship between MC and chl *a* concentrations changes at the breakpoint level of $1.97 \ln(\mu\text{g chl } a \text{ L}^{-1})$ or $7.1 \mu\text{g chl } a \text{ L}^{-1}$, from poorly identified (0.21 ± 0.23) to strongly positive (0.96 ± 0.15). The coefficient of determination (R^2) between the posterior predicted median MC values against the measured ones was 0.35 with a mean standard error of the estimate equal to $1.16 \pm 0.07 \ln(\mu\text{g MC L}^{-1})$

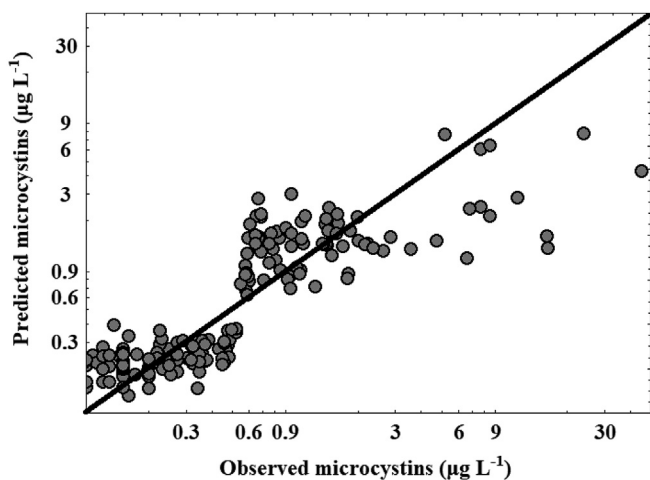


Fig. 5. Comparison between the measured and mean predicted MC values ($R^2 = 0.73$) from the segmented multiple regression model.

To demonstrate the applicability of our modelling exercise for risk management decisions, we examined the frequency histogram of the predicted probability values from the stochastic segmented model or “the probability of exceedance probabilities” (Fig. 7). In this histogram, we included a benchmark value of 10% representing the maximum acceptable probability to violate the $1.5 \mu\text{g MC L}^{-1}$ drinking water guideline for each sample collected from the Bay of Quinte. According to our analysis, only 56.6% of the mean predicted probabilities of MC violations were below this benchmark, and thus the probability of exceedances greater than 10% has been relatively high ($\approx 45\%$) over the course of the study period. By contrast, when we apply the same procedure for the likelihood of violations of the recreational ($20 \mu\text{g MC L}^{-1}$) water quality guidelines, we found that 98.9% of the mean predicted probabilities of MC violations were below the 10% benchmark. Employing an intermediate threshold between the two values established in the water resource management literature could serve as evidence of excessive risks when using the system for drinking water supply, as well as an early warning sign about its suitability for recreational purposes. For

example, if we opt for a $5 \mu\text{g L}^{-1}$ target, the distribution of probabilities for MC violations had more than 89% of the daily snapshots recorded from the Bay of Quinte below the 10% benchmark. It is also interesting to note that the same threshold was exceeded in 7.2% of the samples collected from all the sites during the study period.

From an operational standpoint, the number of samples required during the growing season (end of May–early October) in order to assess system compliance with targeted MC thresholds can vary from 30 to 216, depending on the number of locations monitored, sampling frequency used, and duration of the period examined (Table 3). For illustration purposes, we created “confidence-of-compliance” graphs to evaluate the likelihood of compliance against two probabilistic criteria that stipulate less than 10% violations of two MC threshold concentrations, i.e., 1.5 and $5 \mu\text{g L}^{-1}$, when we consider different sample sizes and prior beliefs (Fig. 8). Based on empirical evidence regarding the achievability of the two MC values in the Bay of Quinte, the former target was assigned a conservative prior, $\text{Be}(1, 7.2)$, whereby we accorded relatively high probabilities to exceedance rates up to 20% (Fig. 8a). The latter MC threshold was given a more optimistic prior, $\text{Be}(0.2, 9)$, with a high probability assigned to very low exceedance rates ($<5\%$) and practically negligible prior probabilities thereafter (Fig. 8a). According to the “confidence-of-compliance” graph (Fig. 8c), after collecting samples from four sites on a biweekly basis during two growing seasons ($n = 80$; see Table 3), 4 exceedances of the $1.5 \mu\text{g MC L}^{-1}$ threshold (point A) suggest our confidence of compliance that the standard will not be exceeded more than 10% is 87.0%. Similarly, if we register 6, 8, 10, or 12 violations of the same MC threshold (points B–E in Fig. 8c), then our confidence of compliance that the standard will not be violated by more than 10% will be 64.2%, 35.4%, 14.3%, and 4.2%, respectively. Intended to offer an early warning sign for the likelihood of impairment of the recreational guideline, the “confidence-of-compliance” graph for the $5 \mu\text{g MCL}^{-1}$ target paints a more favorable picture with respect to the frequency of MC violations in the Bay of Quinte. Even if there are 4 violations, after collecting samples from four sites on a biweekly basis over the course of two growing seasons, our confidence of compliance with the MC standard will be 97.1% (point A in Fig. 7d). Likewise, 6, 8, 10, and 12 violations of the $5 \mu\text{g MCL}^{-1}$ target would suggest our confidence of compliance with lower than 10% violations of the MC target will be 87.4%, 64.1%, 35.5%, and 15.2% (points B–E in Fig. 8d), respectively. As a final exercise, we attempted to eliminate any subjectivity with the formulation of our prior beliefs and instead used empirical knowledge about the frequency of MC violations in the Bay of Quinte, as depicted by the piecewise-regression model with sole predictor the recorded chl *a* concentrations (Fig. 3). In this case, we formulated beta prior distributions with shape parameters derived from the predicted mean exceedance rate and the associated model error variance (or residual variability). It is interesting to note the similarity between the empirically derived priors and those based solely on our prior perception without any consideration of the available data (Fig. 7a and b). According to the MC estimates derived by the chl *a* data, if there are again 4 exceedances of the drinking water guideline out of 80 samples collected during two growing seasons, then our confidence of compliance that the standard will not be exceeded by more than 10% will be 93.6% (Fig. 8e). In a similar manner, if we experience 6, 8, 10, or 12 violations of the same MC threshold (points B–E in Fig. 8e), it would suggest that our confidence of compliance is 76.0%, 47.9%, 22.2%, and 7.7%, respectively. When collecting the same sample size, our degree of confidence with 4 violations of the $5 \mu\text{g MCL}^{-1}$ target will be 96.4% (Fig. 8f). Interestingly, the inference drawn (degree of confidence of compliance) remains consistently higher, i.e., 82.5%, 56.2%, 28.6%, and 10.4%, if 6, 8, 10, or 12 violations of the same MC threshold (points B–E in Fig. 8f) are registered over the course of two growing seasons.

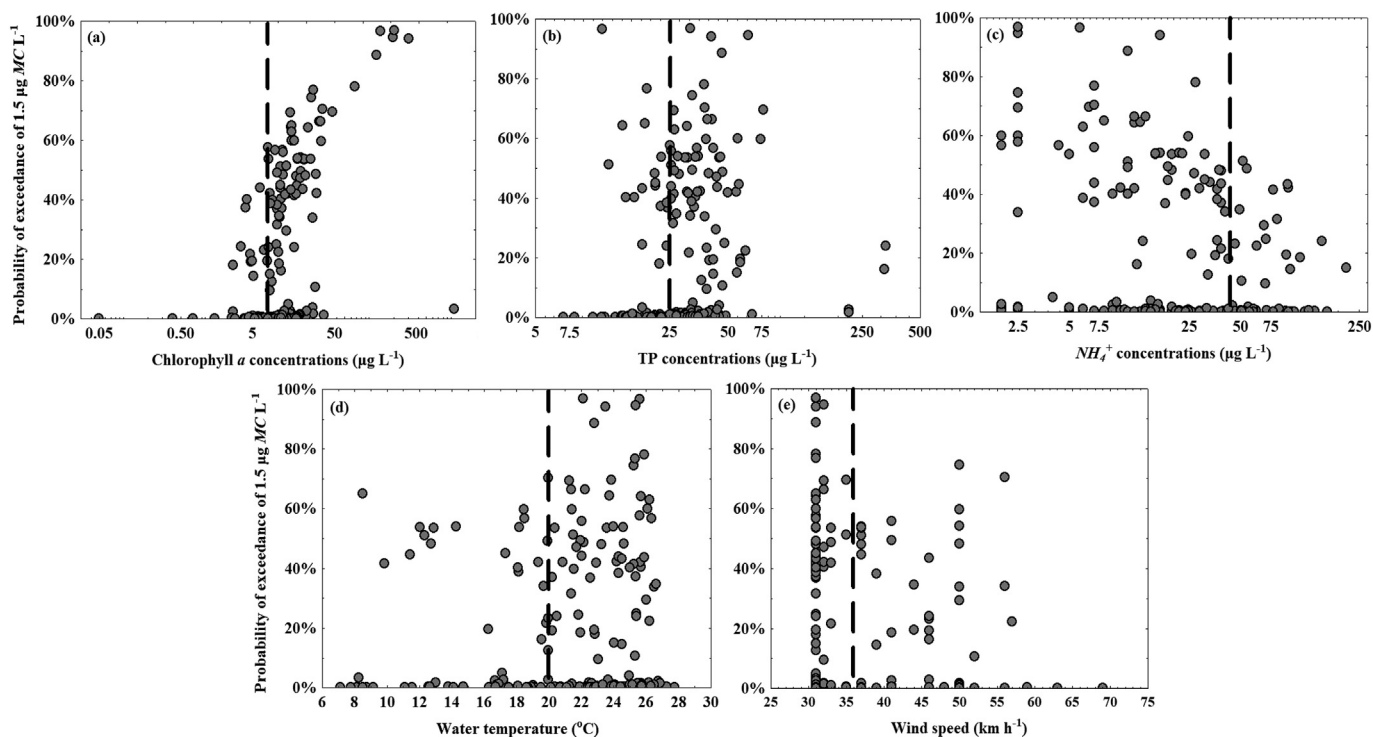


Fig. 6. Scatterplots depicting the relationship between the probability of exceedance of $1.5 \mu\text{g MC L}^{-1}$, as predicted from the segmented multiple regression model, against different chlorophyll *a* concentrations; water temperature; total phosphorus concentrations; speed of maximum daily wind gust; and ammonium concentrations. The vertical dashed lines identify approximate thresholds, above (or below) which 80% of the daily snapshots from the Bay of Quinte are characterized by a greater than 10% probability of exceedance of the $1.5 \mu\text{g MC L}^{-1}$ drinking water guideline.

4. Discussion

Owing to the increasing frequency of cyanobacteria-dominated harmful algal blooms (*CHABs*), as well as to their potential to inflict socioeconomic damages and ecological impairments, predicting their occurrence and magnitude has become an essential management exercise in many freshwater ecosystems around the world. In this study, we used different statistical models, parameterized with Bayesian inference techniques, to identify critical levels of key environmental factors that influence the exceedance risk of specific *MC* thresholds in the Bay of Quinte (Lake Ontario, Canada). Our results suggest that chl *a* concentrations $\geq 7 \mu\text{g L}^{-1}$, *TP* concentrations $\geq 25 \mu\text{g L}^{-1}$, NH_4^+ concentrations $\leq 40 \mu\text{g L}^{-1}$, water temperatures $\geq 20^\circ\text{C}$, and wind speed $\leq 37 \text{ km h}^{-1}$ significantly increase the likelihood of violation of the drinking water advisory level. For the Bay of Quinte, these threshold values collectively reflect meso-eutrophic conditions during periods of warm water and calm winds, which were observed on approximately 17% of the sampling dates (i.e., all sampling dates that met all five conditions) and typically occur between late July and early September. These environmental conditions are commonly experienced in the area, particularly in summer months, which suggests that high *MC* concentrations will continue to occur for the foreseeable future without any additional management interventions.

Identifying reliable predictors of microcystin production: Using a Bernoulli-logistic regression model, Shimoda et al. (2016) found that *TP* concentrations alone failed to predict exceedances of various levels of *MC* concentrations, and concluded that more comprehensive modelling was needed to reliably predict drinking water violations. Building upon the recommendations of Shimoda et al. (2016), our application of the Bernoulli-logistic model with additional environmental variables also failed to reliably predict

the occurrence of *MC* violations (i.e., false negative predictions). In contrast, the delineation of two subsets on the basis of *MC* concentrations ($0.54 \mu\text{g L}^{-1}$), as determined by our segmented multiple regression model, allowed us to effectively accommodate non-monotonic/non-linear relationships with environmental predictors and to quantify the uncertainty surrounding the risks of exceeding *MC* drinking water guidelines. Thus, even though our modelling analysis in its current form cannot be used for forecasting purposes (i.e., lack of predictors that reflect the antecedent conditions, breakpoint on the response rather than on the explanatory variables), it does allow to delineate critical values of explanatory variables associated with increased probability of exceedance of the drinking water standard. Moreover, the fact that it is founded upon explanatory variables that are readily available from nearly all the monitoring programs in the Great Lakes and elsewhere (see also the statistical models presented by Shimoda et al., 2016) provides a plausible framework upon which stronger causative foundation can be built by designing suitable lab/field experiments or monitoring programs with finer granularity.

Our modelling analysis identified chl *a* concentrations, as the predictor variable with the strongest relationship with *MC* concentrations. Often used as an indicator of phytoplankton standing biomass in freshwater systems, it includes all toxic and non-toxic cyanobacteria and other algal taxa. Despite this fact, chl *a* can be a significant predictor of *MC* violations (Harris and Graham, 2017), *MC* presence-absence (Taranu et al., 2017), or is positively correlated with *MCs* (Rinta-Kanto et al., 2009). Likewise, there are also several attempts to identify chl *a* thresholds that could be associated with a higher likelihood of exceedance of selected health advisory *MC* levels. For example, Taranu et al. (2017) found that a high probability of exceeding *MC* concentrations of $1.6\text{--}2.0 \mu\text{g L}^{-1}$ occurred at *TN* concentrations $>650 \mu\text{g L}^{-1}$ and cyanobacterial

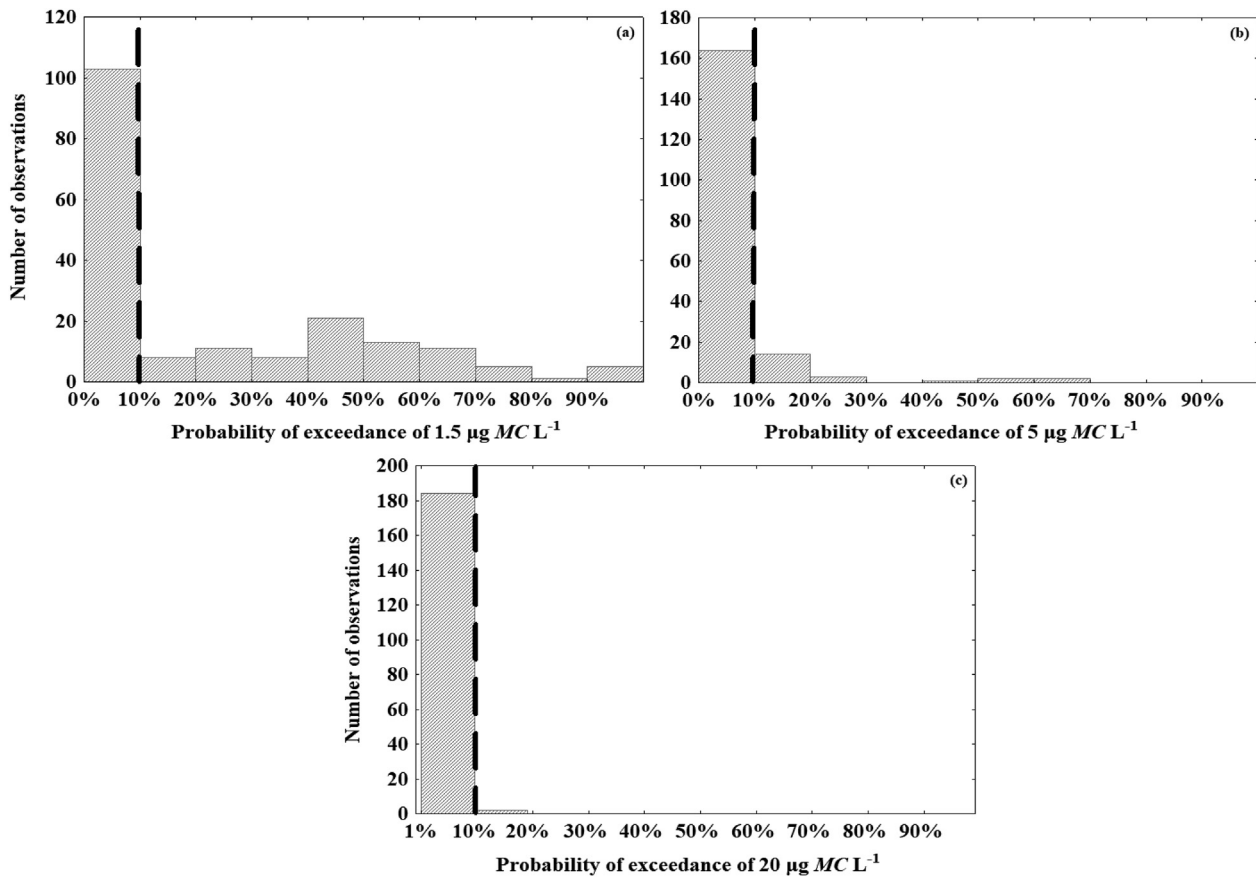


Fig. 7. Frequency histograms of mean probability values for MC concentrations to exceed the (a) $1.5 \mu\text{g L}^{-1}$, (b) $5 \mu\text{g L}^{-1}$, and (c) $20 \mu\text{g L}^{-1}$ threshold values, as predicted by the segmented multiple regression model. The vertical dashed lines represent a tentative benchmark of 10% probability of MC violations in the Bay of Quinte. In (a) 56.6%, (b) 89.8%, and (c) 98.9% of all MC observations fell below this tentative benchmark.

Table 3

The number of samples required during the growing season (end of May–early October) in order to assess compliance with the microcystin target of $1.5 \mu\text{g L}^{-1}$ at three or four locations in the Bay of Quinte, with a weekly or biweekly sampling frequency over the course of 1-, 2-, or 3-year periods. The last two rows represent the corresponding maximum allowable number of samples, in which the targeted criterion can be exceeded and the system will still be classified as non-impaired, i.e., if we permit a <10% violation frequency.

Sites in the Upper Bay	1-year period		2-year period		3-year period	
	Biweekly	Weekly	Biweekly	Weekly	Biweekly	Weekly
3	30	54	60	108	90	162
4	40	72	80	144	120	216
10%	3	5	6	11	9	16
10%	4	7	8	14	12	21

biomass $>160 \text{ mg L}^{-1}$. Using a conditional probability approach, Hollister and Kreakie (2016) estimated a 50% chance of exceeding health advisory MC thresholds of 1 and $2 \mu\text{g L}^{-1}$ when chl *a* concentrations reached 68 and $104 \mu\text{g L}^{-1}$, respectively. When paired with low TN concentrations ($570 \mu\text{g L}^{-1}$), Yuan et al. (2014) found a 10% chance of exceeding the $1 \mu\text{g MC L}^{-1}$ level when chl *a* concentrations were $37 \mu\text{g L}^{-1}$ (see their Fig. 3), although the same probability level was also associated with a much lower chl *a* threshold ($3 \mu\text{g L}^{-1}$) when TN concentrations were elevated ($1100 \mu\text{g L}^{-1}$). Our chl *a* threshold is apparently different from these estimates, but it should also be noted that our analysis is focused on the variability recorded within a particular system, as opposed to the cross-sectional (multi-site) character of the aforementioned modelling work that teased out information from broader regions. Chl *a* is used as an important indicator of the Bay of Quinte ecosystem state, and a remediation target for chl *a* concentrations

of $10\text{--}12 \mu\text{g L}^{-1}$ has been established for the restoration of water quality (Munawar et al., 2012). However, our analysis indicated that the average exceedance probability of the drinking water guideline ranges between 20 and 25% at these targeted concentrations (see also the scatter of the predicted probabilities once the black vertical line in Fig. 6a is exceeded).

The role of cultural eutrophication in promoting harmful algal blooms in freshwaters is well-established (Heisler et al., 2008; Pick, 2016), but the causal linkages between exogenous nutrient enrichment and MC production is an on-going debate (e.g., see Orihel et al., 2012; Scott et al., 2013). In a similar manner, the relationship between MCs and external nutrient loading remains unclear in the Bay of Quinte, as a greater risk of exceedance of the drinking water guidelines was associated with intermediate TP and low NH_4^+ concentrations. P availability is considered the primary limiting factor influencing cyanobacterial growth in freshwaters,

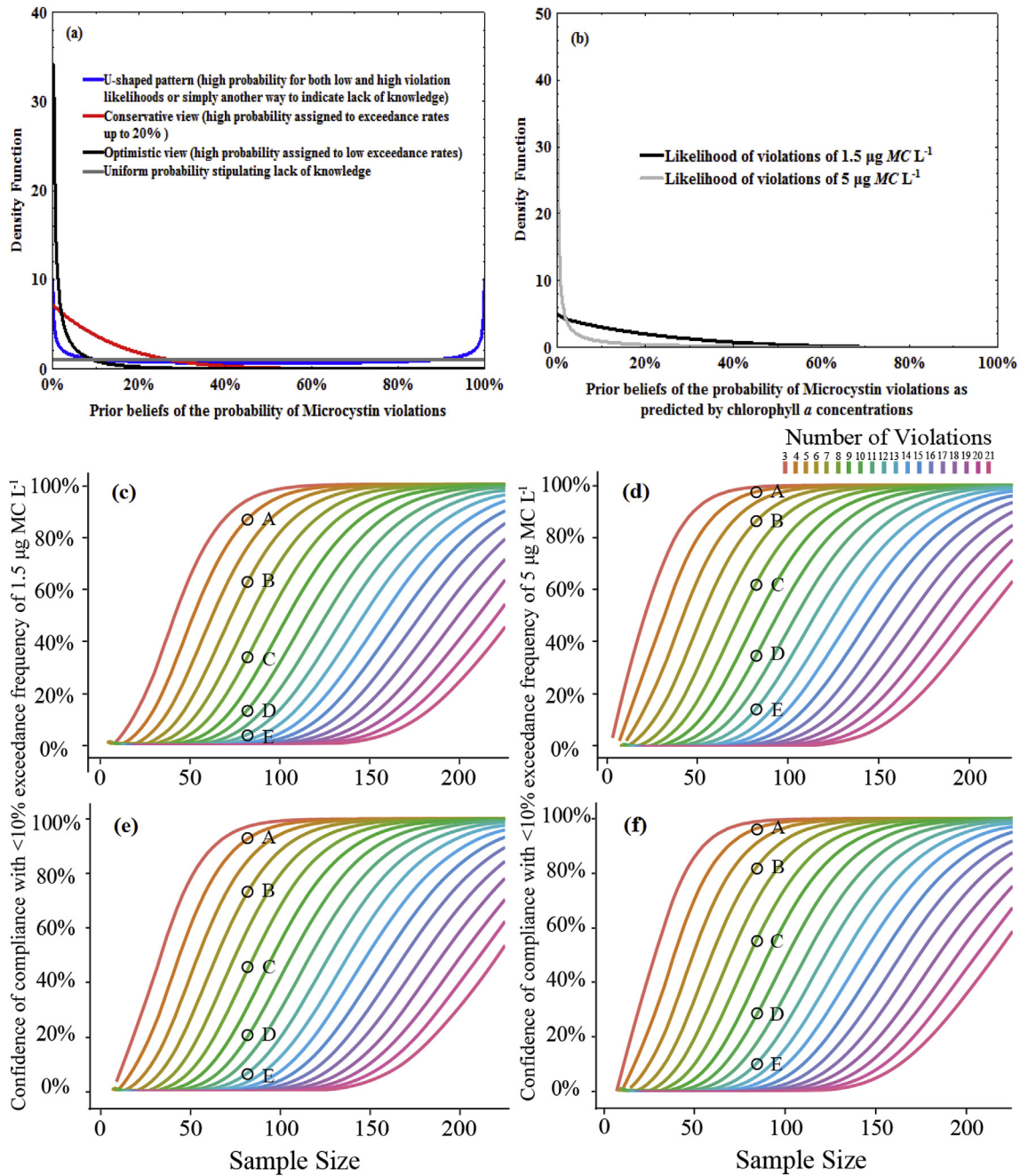


Fig. 8. (a) Our prior beliefs on the likelihood of MC violations expressing pessimistic, $Be(1, 7.2)$, and optimistic, $Be(0.2, 9)$, views regarding the likelihood of compliance with two probabilistic standards that stipulate less than 10% violations of two MC threshold concentrations, i.e., 1.5 and 5 $\mu\text{g MC L}^{-1}$, over time and space, respectively. For the sake of comparison, the uniform reference prior, $Be(1, 1)$, along with the U-shaped prior derived from “Jeffreys’ rule”, $Be(0.5, 0.5)$, are also illustrated. The latter prior implies that extreme probability values of exceedance (i.e., close to 0 or 1) are more likely than intermediate values. (b) Our prior beliefs on the likelihood of compliance with two probabilistic standards when the ambient MC levels are estimated by the corresponding chl *a* data through our simple piecewise regression model (See Supporting Information section). Panels (c) and (d) assess our confidence that the 1.5 and 5 $\mu\text{g MC L}^{-1}$ standards will not be exceeded by more than 10% for different sample sizes collected from the Bay of Quinte. Panels (e) and (f) present the same “confidence-of-compliance” graphs when the ambient MC levels are predicted by the recorded chl *a* concentrations. Points A-E represent 4, 6, 8, 10, and 12 violations of the two MC thresholds, after collecting samples from four sites on a biweekly basis during two growing seasons ($n = 80$).

but the availability of various forms of *N* could be another important factor for the production of *N*-rich MC and toxicity (Gobler et al., 2016, and references therein). Elevated *N* levels have been associated with higher cellular quotas of MCs in the non-diazotrophs *Microcystis* and *Planktothrix*, and thus *N* enrichment, particularly in *P*-replete environments, may increase MC production (Donald et al., 2011). Monchamp et al. (2014) observed elevated MC concentrations in NH_4^+ -depleted waters in Quebec

lakes, regardless of the total cyanobacterial biomass observed. Along the same line of evidence, *Microcystis* is known to have high affinity for NH_4^+ , and often displays superior uptake capacity for rapidly recycled, reduced *N* under nitrogen limiting conditions (McCarthy et al., 2009; Glibert et al., 2014). Given the presence of active nutrient cycling in the Bay of Quinte, mediated by sediment diagenesis, dreissenids excreta/egesta, and macrophyte decomposition (Arhonditsis et al., 2016; Doan et al., 2018), we hypothesize

that once the “internal nutrient pump” begins to replenish the overlying water, an interplay of increased *P* sequestration and rapid uptake of energetically favorable NH_4^+ may trigger *Microcystis* growth and *MC* production. Considering the low summer ambient levels of all inorganic nitrogen forms (NH_4^+ , NO_2^- , NO_3^-) in the Bay of Quinte, Shimoda et al. (2016) surmised that there are two additional factors that promote *Microcystis* dominance: (i) the selective dreissenid filtration that may be responsible for the reduced biovolume of N_2 -fixers *Aphanizomenon* spp. and *Anabaena* spp.; and (ii) the bioavailability of other nitrogen forms such as urea, which can enter cells either via light-independent transport or by diffusion, and which produce two NH_4^+ per molecule of urea transported inside the cells. In this case, the need for active uptake of HCO_3^- at high pH is minimized, and CO_2 can be released by intracellular urease (Valladares et al., 2002; Flores and Herrero, 2005; Donald et al., 2011).

Although multiple studies have demonstrated the linkages between increasing water temperature and toxic cyanobacterial blooms (Jacoby et al., 2000; Wood et al., 2017), fewer have directly connected temperature to ambient *MC* levels (Francy et al., 2016). In our study, we were able to identify a threshold of $\sim 20^\circ C$, above which the exceedance likelihood of *MC* drinking water guidelines increases. The cyanobacterium *Microcystis* has been found to out-compete other phytoplankton species at or above $25^\circ C$ (Paerl and Paul, 2012), while the number of genes or transcripts associated with *MC* production increase with water temperature (Davis et al., 2009). Thus, there is growing concern that increases in temperature due to global climate change will increase the frequency and magnitude of *cHABs* and promote the growth of toxic strains of cyanobacteria (Kosten et al., 2012). These changes have important implications for future water quality trends, particularly in the Bay of Quinte. For example, Trumpickas et al. (2009) predicted future summer surface water temperatures in Lake Ontario to rise by $2.5^\circ C$ (above 1971–2000 norms) under the Intergovernmental Panel on Climate Change A2 emissions scenario, and by $2.25^\circ C$ under the B2 scenario, for the 2041–2070 period. Further, Nicholls (1999) predicted that an increase in average summer water temperature by $3\text{--}4^\circ C$ would double the summer average *TP* concentrations. In line with current warming trends, maximum summer surface waters in the Bay of Quinte have warmed by almost $1^\circ C$ from 1972 to 2008 (Minns et al., 2011). If we also consider that the mean summer (Jun–Aug) *TP* concentrations and surface water temperatures measured in the upper Bay were approximately $32\ \mu g\ L^{-1}$ and $23^\circ C$, respectively, then it is reasonable to assume that the likelihood of *MC* violations will continue to be relatively high; especially, since the internal nutrient feedback loop is projected to remain active in the near future (Arhonditsis et al., 2016; Doan et al., 2018).

To our knowledge, few studies to date have examined the influence of physical conditions (other than temperature) in predicting *MCs* in freshwater lakes. Cyanobacteria can regulate their buoyancy to take advantage of optimal nutrient and light conditions, and thus could gain a competitive advantage over other eukaryotic phytoplankton under these conditions (reviewed in Watson et al., 2015), leading to higher *MC* concentrations and increased risk of *MC* health advisory violations. Jacoby et al. (2000) found that higher water column stability and decreased lake flushing were associated with a pronounced and prolonged toxic bloom of *Microcystis aeruginosa* during summer 1994 in Steilacoom Lake (Washington, USA), although *MC* concentrations (per gram of phytoplankton) were found to be unrelated to the prevailing environmental conditions except from soluble reactive phosphorus. More recently, Wood et al. (2017) found that an extended drought in the shallow eutrophic Lake Rotorua (New Zealand) led to prolonged stratification, increased dissolved reactive phosphorus and

inorganic nitrogen concentrations, which interacted with temperature to influence cyanobacterial *MC* cell quotas. Because direct measurements of water column stability were unavailable for the Bay of Quinte, we used wind speed as a representative proxy of mixing conditions, assuming a negative relationship whereby higher wind speeds reduce water column stability (Kann and Welch, 2005). This relationship would be particularly pronounced for locations in the middle and lower bay, which are deep enough for stratification to occur throughout the year, and thus wind-driven mixing could interrupt water column stability to a greater extent at these locations. Nonetheless, because the hypothesized strong negative association between wind speed and the probability of *MC* violations did not manifest itself in our modelling analysis, future investigation of the direct role of physical lake dynamics, and in particular water column stability, and interactions with water temperature, is clearly warranted in order to gain a better understanding of *MC* production dynamics.

Setting probabilistic criteria for microcystin concentrations:

In the management of impaired waterbodies, the establishment of probabilistic water quality criteria is often considered an effective strategy to deal with the inherent uncertainty and/or our imperfect knowledge of natural systems (e.g., McBride and Ellis, 2001; Shabman and Smith, 2003; Zhang and Arhonditsis, 2008; Mahmood et al., 2014; Smith and Canale, 2015). It is within this context that our statistical framework can assist with the development of realistic water quality criteria to track the occurrence of high *MC* levels (or other cyanotoxins), as demonstrated by the derived “probability of exceedance probabilities”. In particular, the Bayesian nature of our work gives direct answers to questions of confidence of compliance with percentile standards (see panels (b)–(e) in Fig. 8), and as such can effectively guide management decisions and monitoring practices that consider both risks of reaching false conclusions, i.e., falsely inferring a breach of standard or falsely inferring compliance (McBride and Ellis, 2001). Instead of basing inference solely on the exceedance frequency level of a threshold *MC* concentration, the estimated probabilities are regarded as a continuous variable about which we make confidence statements. Simply put, we introduce an extra dimension of uncertainty by targeting the probability of an acceptable *MC* exceedance risk (or margin of safety) across all water samples taken (Zhang and Arhonditsis, 2008; Mahmood et al., 2014). The conceptual advantages of the proposed framework presumably come at the “cost” of having to state one’s prior belief as to likely exceedance rates. Namely, our first two illustrations were based on the formulation of prior distributions that reflected our subjective (pessimistic or optimistic) beliefs regarding the likelihood of compliance with two (1.5 and $5\ \mu g\ MC\ L^{-1}$) targeted thresholds. Nonetheless, this issue was rectified with our subsequent examples in which empirical knowledge from the system was used to characterize our prior beliefs; that is, the mean predictions about the achievability of the two targets along with the associated error of the simple piecewise regression model provided the basis for the specification of the shape parameters of our beta prior. Even more so, a well-known property of Bayesian analysis is that the results from classical and Bayesian statistics become more similar at larger numbers of samples, as the information in the data increasingly dominates over that in the chosen prior distributions (McBride and Ellis, 2001; Arhonditsis et al., 2008). Our “confidence-of-compliance” graphs can determine the optimal sample size that will allow to draw robust inference about the prevailing ambient conditions, and address any criticism about the potential subjectivity with methodological practices followed.

From a management viewpoint, our analysis suggests that the occurrence of *cHABs* could be a manifestation of the tight control exerted by the sediments, which act as a net source of phosphorus

and the corresponding fluxes are likely magnified by the macrophyte and dreissenid activity, e.g., nutrient pump effect and pseudofeces production (Kim et al., 2013). According to recent empirical and modelling evidence (Arhonditsis et al., 2016; Doan et al., 2018), the presence of significant nutrient regeneration mechanisms is primarily responsible for the elevated end-of-summer P ($>25\text{--}30\ \mu\text{g TP L}^{-1}$) in the upper Bay of Quinte, which in turn appears to be the first condition for structural shifts to occur in the algal assemblage (see also the positive linkage between MC and TP concentrations below the breakpoint of $0.54\ \mu\text{g L}^{-1}$). Once ambient P is no longer a limiting factor, the inter-specific competition for energetically favorable nitrogen forms coupled with the water temperature and/or water column stability are some of the factors that likely shape the development of $cHABs$ and production of toxins. Thus, while additional reductions of the external point and non-point nutrient loading are warranted, it is also important to note that the ability of the sediments to modulate the relative abundance of bioavailable nitrogen and phosphorus forms indicates that the anticipated benefits may not be realized immediately and $cHABs$ may still occur in the near future. In view of this prospect, our analysis reinforces the pragmatic standpoint that the compliance rules should explicitly accommodate all the sources of uncertainty, such as insufficient information, lack of knowledge, natural variability, unaccounted “ecological unknowns”, by adopting a probabilistic approach that permits a realistic frequency of violations (10%) and satisfactory level of confidence ($>75\text{--}80\%$). Recognizing that $cHABs$ are inherently episodic events, the compliance assessment should be based on multiple sites and over the course of two or three years, as their nonoccurrence in a particular year does not necessarily guarantee that the problem has been eradicated. We also recommend the introduction of an additional intermediate threshold value (e.g., $5\ \mu\text{g MC L}^{-1}$) between those used in the drinking ($1.5\ \mu\text{g MC L}^{-1}$) and recreational ($20\ \mu\text{g MC L}^{-1}$) guidelines that could serve as an early warning sign for an imminent highly toxic bloom; especially, since the water quality monitoring takes place in the open waters of the Bay of Quinte (see monitoring sites Fig. 2), where the initiation of $cHABs$ frequently takes place.

The question arising is whether the precautionary spirit of our approach with the introduction of several layers of uncertainty is constructive, or if it is overly conservative and runs the risk of perpetuating the management of impaired waterbodies with an overly alarmist mindset (Arhonditsis et al., 2019). With respect to the latter issue, the perspective of the public in the Bay of Quinte area has been positive that it does matter. Based on the responses of more than 1500 local residents and tourists, Ramin et al. (2018) indicated that the degree of public satisfaction changes between the beginning and end of summer season, following the gradual deterioration of the water quality conditions and the occurrence of harmful algal blooms. Importantly, the same study showed a distinctly higher degree of satisfaction of the public when chl a concentrations remain below the $10\ \mu\text{g L}^{-1}$ threshold or ambient TP levels are lower than $20\text{--}25\ \mu\text{g L}^{-1}$, which is remarkably close with the critical levels of the two water quality variables associated with elevated risk of MC violations. The fact that the sentiment of the public is clearly influenced by the prevailing environmental conditions offers ammunition to develop and implement an ambitious long-term management plan that protects the Bay of Quinte from excess nutrients associated with urban runoff, sewage treatment plants, and agricultural land uses (Arhonditsis et al., 2019). Thus, the presented probabilistic framework is intended to facilitate the policy-making process in the area, as the local water quality managers have long realized the expectation of a system that 100% satisfies the water quality standards is overly ambitious (if not unrealistic), given the currently prevailing conditions. It is

important though to communicate to the public that harmful algal blooms may still occur in the foreseeable future, and their reduced frequency within a pre-specified spatiotemporal domain is the most pragmatic way to evaluate the success of the local restoration efforts (Kim et al., 2018; Arhonditsis et al., 2019).

5. Conclusions

Using the Bay of Quinte as a model ecosystem, we demonstrated that the probability of violations of the MC drinking water guideline, deemed protective of human and animal health, increased significantly under specific thresholds of a suite of eutrophication indicators (i.e., chl a , nutrients) and physical environmental variables. Our analysis highlights that nutrient management remains the best option to reduce the frequency of high MC events, through their link in controlling chl a concentrations and undesirable shifts in the phytoplankton community composition. In the context of environmental policy, the uncertainty regarding the achievability of quality goals, stemming from (i) the (often unknown) important drivers of ecological degradation; (ii) the need to effectively balance environmental concerns with socioeconomic values; and (iii) our desire to have contingency plans to deal with the unexpected, should be a focal point when making management decisions and designing restoration/monitoring plans accordingly. The logic of our modelling framework is founded upon this concept and can be used to guide the decision-making process in systems that experience episodic outbreaks of toxic cyanobacteria.

Acknowledgment

Funding for this study was provided by the Krembil Foundation and National Sciences and Engineering Research Council of Canada (NSERC) through a Discovery Grant (George Arhonditsis). The authors are grateful to all the scientists and technical personnel, who have been involved with the development of the toxin dataset in the Bay of Quinte.

Appendix A. Supplementary data

Supplementary data related to this article can be found at <https://doi.org/10.1016/j.watres.2019.06.005>.

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A Bayesian Risk Assessment Framework for Microcystin Violations of Drinking Water and Recreational Standards in the Bay of Quinte, Lake Ontario, Canada

[SUPPORTING INFORMATION]

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Bayesian Modelling Framework

We used Bayesian inference to estimate model parameters because of its ability to include prior information (e.g., literature reviews, expert knowledge, metadata, past parameter estimates) in the modelling analysis and to explicitly deal with model structural/parametric uncertainty as well as missing data and measurement errors (Gelman et al., 2013). Bayesian inference treats each parameter θ as a random variable and uses the likelihood function to express the relative plausibility of different parameter values given the available data from the system:

$$P(\theta|data) = \frac{P(\theta)P(data|\theta)}{\int_{\theta} P(\theta)P(data|\theta)d\theta}$$

where $P(\theta)$ represents the prior distribution of the model parameter θ , $P(data|\theta)$ indicates the likelihood of the data observation given the different θ values, and $P(\theta|data)$ is the posterior probability representing our updated beliefs on the θ values, contingent upon empirical knowledge from the system. The denominator is often refer to as the marginal distribution of the available data and acts as a scaling constant that normalizes the integral of the area under the posterior probability distribution (Gelman et al., 2013).

Confidence of compliance with probabilistic standards: The calculations associated with the “confidence-of-compliance” graphs were based on the following posterior probability density function:

$$f(x|e, n) = \left[\frac{L(e|n, x)}{\int_0^1 L(e|n, x)g(x)dx} \right] g(x)$$

where e is the number of exceedances in n samples; $f(x|e, n)$ is the posterior probability density function of x for a given value of e and n ; $L(e|n, x)$ is the likelihood function for any n and x ; and $g(x)$ is the prior posterior probability density function of x . This equation shows that our

prior belief about the true exceedance rate x , described by $g(x)$, is updated by the standardized likelihood (the term in brackets) to derive the required posterior probability density f . For a sample size equal to n , the likelihood function L is the probability mass function for a particular value of e and is described as a binomial process, with x (instead of e) being regarded as a parameter:

$$L(e|x, n) = \binom{n}{e} x^e (1-x)^{n-e}$$

where $\binom{n}{e}$ is the binomial coefficient which is cancelled in the standardized likelihood function, and thus the posterior probability density is given by:

$$f(x|e, n) = \left[\frac{x^e (1-x)^{n-e}}{\int_0^1 x^e (1-x)^{n-e} g(x) dx} \right] g(x)$$

Our choice of the prior density $g(x)$ was based on a “conjugate distribution” that guarantees the prior and posterior probability densities belong to the same family of distributions, making the calculations much simpler. In particular, because the likelihood function follows a binomial distribution, we chose $g(x)$ to follow the beta distribution, $Be(a, b)$:

$$g(x; a, b) = \frac{1}{B(a, b)} x^{a-1} (1-x)^{b-1}, \text{ where } B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

where $a, b > 0$ are the shape parameters, Γ is the gamma function, and the beta term, B , is a normalization constant to ensure that the total probability is 1. The posterior probability density then becomes:

$$\begin{aligned} f(x|e, n) &= \frac{\frac{1}{B(a, b)} x^{e+a-1} (1-x)^{n-e+b-1}}{\int_0^1 \frac{1}{B(a, b)} x^{e+a-1} (1-x)^{n-e+b-1} dx} \\ &= \frac{x^{e+a-1} (1-x)^{n-e+b-1}}{B(e+a, n-e+b)} \end{aligned}$$

To formulate informative prior distributions, we can then calculate a and b from the known expressions for the mean and variance of the beta distribution, i.e., $\bar{x} = \frac{a}{a+b}$ and $s^2 =$

$\frac{ab}{[(a+b)^2(a+b+1)]}$, from which we obtain:

$$\alpha = \bar{x} \left[\frac{\bar{x}(1-\bar{x})}{s^2} - 1 \right] \text{ and } b = \alpha \left[\frac{1}{\bar{x}} - 1 \right]$$

In panels 7d and 7e, the “confidence-of-compliance” graphs for the 1.5 and 5 $\mu\text{g MC L}^{-1}$ standards were based on shape parameters a and b , derived from the predicted mean exceedance rates, $\bar{x}_{1.5} = 18.4\%$ and $\bar{x}_5 = 4.4\%$, and associated standard deviations, $s_{1.5} = 15.5\%$ and $s_5 = 10.5\%$, of the piecewise regression model with the chlorophyll a data as the sole predictor. Finally, the probability (or confidence) of compliance, denoted as CC , is calculated from the distribution function as follows:

$$CC = F(x \leq X|e, n) = \int_0^x f(x|e, n) dx$$

Given that f is a beta density, the cumulative distribution function F follows an incomplete beta function ratio (Lee, 2012), written as $I_X(a, b)$, and thus after incorporating the different informative priors, our CC estimates become:

$$CC = I_X(e + a_{prior}, n - e + b_{prior})$$

Model computations: Sequences of realizations from the model posterior distributions were achieved by using Markov Chain Monte Carlo (*MCMC*) simulations (Gilks et al., 1998). We used a general normal proposal Metropolis algorithm which is based upon a symmetric normal proposal distribution, whose standard deviation is adjusted over the first 4,000 iterations so that the acceptance rate ranges between 20% and 40%. For each analysis, we used three chain runs of 50,000 iterations, keeping every 20th iteration (thin of 20) to avoid serial correlation. We discarded the first 10,000 samples to eliminate the effect of the initial parameter values assigned

(*burn-in*), and took samples after the MCMC simulation converged to the true posterior distribution. We assessed convergence to the true posterior distribution: (i) qualitatively, through visual inspection of plots of the Markov chains for mixing and stationarity, as well as the corresponding density plots of the pooled posterior Markov chains for unimodality; (ii) quantitatively, using the modified Gelman-Rubin convergence statistic (Brooks and Gelman, 1998). The BGR factor is the ratio between *among-chain* and *within chain* variability. The chains have converged when the upper limits of the BGR factor are close to one. The accuracy of the posterior parameter values was inspected by assuring that the Monte Carlo error (an estimate of the difference between the mean of the sampled values and the true posterior mean) for all parameters was less than 5% of the sample standard deviation (Spiegelhalter et al., 2003).

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WinBUGS codes

Bernoulli model

```
model {  
  
  for (i in 1:N) {  
#Data transformations  
    lnChla[i]<-log(Chla[i])  
    lnTP[i]<-log(TP[i])  
    lnNH4[i]<-log(NH4[i])  
    lnWT[i]<-log(WT[i])  
    lnWind[i]<-log(Wind[i])  
#Model likelihood  
logit(p[i]) <-a[1]+a[2]*lnTP[i]+a[3]*lnNH4[i]+a[4]*lnChla[i]+a[5]*lnWT[i]+a[6]*lnWind[i]  
Tobs[i] ~ dbern(p[i])  
  }  
#Priors  
  for (i in 1:6) {a[i] ~ dnorm(0, 0.001)}  
}
```

Stochastic segmented model on Chl a

```
model {  
  
  for (j in 1:M) {  
#Data transformation  
    lnChla[j] <- log(Chla[j])  
    lnMicroCys[j] <- log(TotalMC[j])  
#Tobit model  
MicroCys_tobit[j] <- (-1.89)*is.detlim[j]+10000*(1 - is.detlim[j])  
is.detlim[j] <- step(0.1499-TotalMC[j])  
#Model likelihood  
J[j] <- 1 + step(lnChla[j]-Chla_change)  
MicroCys_mu[j]<- alpha + beta[J[j]]*(lnChla[j]-Chla_change)  
Microcys[j] ~ dnorm(MicroCys_mu[j],tau)I(,MicroCys_tobit[j])  
#Exceedance Frequency Calculations  
ExceedFreq_1.5[j]<- 1-phi((log(1.5)-MicroCys_mu[j])/sigma)  
ExceedFreq_5[j]<- 1-phi((log(5)-MicroCys_mu[j])/sigma)  
  }  
ExceedFreq_mean_1.5<-mean(ExceedFreq_1.5[])  
ExceedFreq_sd_1.5<-sd(ExceedFreq_1.5[])  
ExceedFreq_mean_5<-mean(ExceedFreq_5[])  
ExceedFreq_sd_5<-sd(ExceedFreq_5[])  
#Priors  
Chla_change~dunif(1.6, 2.3)  
alpha ~ dnorm(0, 0.001)  
for (j in 1 : 2) {beta[j] ~ dnorm(0, 0.001) }
```

```
tau ~ dgamma(0.01,0.01)
sigma<-sqrt(1/tau)
}
```

Stochastic segmented model on MC

```
model {

  for (j in 1:M) {
    #Data transformations
    lnNH4[j]<-log(NH4[j])
    lnWind[j] <- log(Wind[j])
    lnWaterTemp[j] <-log(WaterTemp[j])
    lnTP[j]<-log(TP[j])
    lnChla[j] <- log(Chla[j])
    lnMicroCys[j] <- log(TotalMC[j]+0.000001)
    #Tobit model
    MicroCys_tobit[j] <- (-1.89)*is.detlim[j]+10000*(1 - is.detlim[j])
    is.detlim[j] <- step(0.1499-TotalMC[j])
    #Model likelihood
    J[j] <- 1 + step(lnMicroCys[j]-MicroCys_change)
    Microcys[j] ~ dnorm(MicroCys_mu[j],tau)I(,MicroCys_tobit[j])
    MicroCys_mu[j]<- beta[1,J[j]] + beta[2,J[j]]*lnNH4[j] + beta[3,J[j]]*lnWaterTemp[j]
      + beta[4,J[j]]*lnWind[j] + beta[5,J[j]]*lnTP[j] + beta[6,J[j]]*lnChla[j]
    #Exceedance Frequency Calculations
    Prob_1[j]<-phi((MicroCys_mu[j]-0)/sigma)
    Prob_1.5[j]<-phi((MicroCys_mu[j]-0.4055)/sigma)
    Prob_5[j]<-phi((MicroCys_mu[j]-1.609)/sigma)
    MicroCys_pred[j]<-exp(MicroCys_mu[j])
  }

  #Priors
  MicroCys_change~dunif(-1.6,0)
  for (i in 1 : 6) {
    for (j in 1 : 2) {
      beta[i,j] ~ dnorm(0, 0.001)
    } }
  tau ~ dgamma(0.01,0.01)
  sigma<-sqrt(1/tau)
}
```

Confidence-of-Compliance Graphs

Pessimistic Prior

```
model {
  # Binomial-beta model
  for (i in 1:N) {
    Viol[i]<-i
    for (j in i:L) {
```

```

r[i,j] <-Viol[i]
p[i,j] ~ dbeta(1, 7.2)
r[i,j] ~ dbin(p[i,j], j)
CC[i,j]<-step(0.10-p[i,j]) } }
}

```

#Data

```
list(N=21, L=216)
```

Prior derived by the stochastic segmented model on Chl a

```
model {
```

Binomial-beta model

```

for (i in 1:N) {
  Viol[i]<-i
  for (j in i:L) {
    r[i,j] <-Viol[i]
    p[i,j] ~ dbeta(alpha, beta)
    r[i,j] ~ dbin(p[i,j], j)
    CC[i,j]<-step(0.10-p[i,j]) } }
}

```

```

alpha<-ExceedFreq_mean_1.5*(ExceedFreq_mean_1.5*(1-ExceedFreq_mean_1.5)/
  pow(ExceedFreq_sd_1.5,2) -1)
beta<- alpha*(1/ExceedFreq_mean_1.5-1)
}

```

#Data

```
list(N=21, L=216, ExceedFreq_mean_1.5= 0.1841, ExceedFreq_sd_1.5=0.1556)
```