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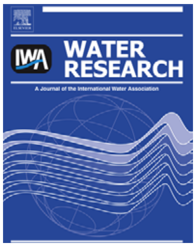

Calibrating and validating bacterial water quality models: A Bayesian approach

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ABSTRACT

Water resource management decisions often depend on mechanistic or empirical models to predict water quality conditions under future pollutant loading scenarios. These decisions, such as whether or not to restrict public access to a water resource area, may therefore vary depending on how models reflect process, observation, and analytical uncertainty and variability. Nonetheless, few probabilistic modeling tools have been developed which explicitly propagate fecal indicator bacteria (FIB) analysis uncertainty into predictive bacterial water quality model parameters and response variables. Here, we compare three approaches to modeling variability in two different FIB water quality models. We first calibrate a well-known first-order bacterial decay model using approaches ranging from ordinary least squares (OLS) linear regression to Bayesian Markov chain Monte Carlo (MCMC) procedures. We then calibrate a less frequently used empirical bacterial die-off model using the same range of procedures (and the same data). Finally, we propose an innovative approach to evaluating the predictive performance of each calibrated model using a leave-one-out cross-validation procedure and assessing the probability distributions of the resulting Bayesian posterior predictive *p*-values. Our results suggest that different approaches to acknowledging uncertainty can lead to discrepancies between parameter mean and variance estimates and predictive performance for the same FIB water quality model. Our results also suggest that models without a bacterial kinetics parameter related to the rate of decay may more appropriately reflect FIB fate and transport processes, regardless of how variability and uncertainty are acknowledged.

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1. Introduction

Effective water quality modeling involves two critical components (see National Research Council (2001, Section 4); Novotny (2003, Chapter 13) as well as DiToro (1984) and Chapra (2003)). First, a mathematical function f is identified which relates the expected value (or rather, an unobservable *in situ* value) of a pollutant concentration c_t at time t (in mass or counts per unit volume) to model parameters β and variables X. Second, discrepancies between f and measured values for c_t (represented as c_t') are characterized, often through an additive residual error term ϵ (following Borsuk et al., 2002):

$$c_t' = f(X, \beta) + \epsilon \tag{1}$$

or, less frequently, through a mathematical or probabilistic function (or combination thereof) g representing an

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Nomenclature

LN	lognormal distribution
N	number of samples in an experiment
No	normal distribution
Po	Poisson distribution
V	sample aliquot volume (ml)
X	set of model variables
c_t	*in situ* fecal indicator bacteria concentration at time t (organisms per ml)
c_0	*in situ* fecal indicator bacteria concentration at time $t=0$ (organisms per ml)
c'_t	fecal indicator bacteria concentration measurement at time t (organisms per ml)
f	mathematical function
g	probability function
i	index of sample number in experiment j
j	index of experiment number
k	first-order bacteria loss rate (1/day)
ln, $\log_{10}$	natural and base-10 logarithm
p	unitless model parameter
t	time (days)
t_e	duration of FIB maintenance phase (days)
y	number of colonies counted on a growth plate

Greek letters

β	set of model parameters
δ	dilution factor
ϵ	ordinary least squares (OLS) model residual error term
λ	expected number of bacterial colonies on a growth plate
σ	standard deviation of ϵ in ln(organisms per ml)

explicit (and perhaps hierarchical) relationship between c_t and c'_t:

$$\begin{aligned} c_t &= f(X,\beta) \\ c'_t &= g(c_t) \end{aligned} \tag{2}$$

Water resource management programs, exemplified in part by recent Total Maximum Daily Load (TMDL) assessments and similar studies (for more on the TMDL program, see Houck, 2002; Reckhow, 2003; Shirmohammadi et al., 2006), often rely on models resembling equation (1) which are calibrated using ordinary least squares (OLS) regression (as described in Weisberg, 2005, pp. 21–32). This approach implies that all sources of variability, including intrinsic variability in water quality measurements (such as those associated with the number and volume of sample aliquots, as described in McBride, 2005, Chapter 10) and natural variability in the pollutant fate and transport process (such as the variability associated with different environmental conditions, as described in Noble and Fuhrman, 1997; Noble et al., 2003), can collectively be acknowledged by an independent residual error term ϵ drawn from a normal $No(0,\sigma)$ or lognormal $LN(0,\sigma)$ probability distribution with standard deviation σ. While the validity of this assumption varies from one pollutant to the next (in part, due to the range of common assumed probability distributions, as discussed in Ott, 1995; McBride, 2005, Chapters 9 and Chapter 2, respectively), it may be particularly inappropriate for use in fecal indicator bacteria (FIB) water quality modeling studies because of how FIB concentrations are measured.

FIB concentrations are commonly reported as either colony-forming unit (CFU) or most probable number (MPN) values (in organisms per ml). Both measures have probability distributions which are not normal (for a range of historical and recent perspectives, see Greenwood and Yule, 1917; Eisenhart and Wilson, 1943; Gronewold and Wolpert, 2008), and are related to the true FIB concentration c by mathematical functions which include design elements of the laboratory procedure from which they are derived (such as the dilution ratio, or the number and volume of sample aliquots). It is commonly assumed, for example, that the number of colonies counted on a growth plate y in a membrane filtration (MF) procedure (see Dufour et al., 1981, for a description of membrane filtration procedures) has a Poisson $Po(\lambda)$ probability distribution with mean and variance λ (see Haas and Heller, 1988; Haas, 1989, for statistical assumptions related to CFU procedures). Some authors argue that a negative binomial model may more accurately represent the distribution of colonies on a filter plate when dispersion is greater than Poisson (see Pipes et al. (1977); El-Shaarawi et al. (1981); Christian and Pipes (1983) as well as McBride (2005, pp. 211)). Analysis of the negative binomial probability distribution model (and its effects on model calibration and predictive performance) is an area for additional research; here we discuss only the Poisson probability model (for more on Poisson and negative binomial probability models see McBride, 2005, Chapters 2 and 6):

$$\lambda = cV/\delta \tag{3}$$

$$y|\lambda \sim Po(\lambda) = \lambda^y e^{-\lambda}/y\,! \tag{4}$$

$$\mathrm{CFU} = y\delta/V \tag{5}$$

where $\delta=$ dilution factor; $y=$ number of identifiable colony-forming unit; $V=$ sample aliquot volume.

Because sample aliquot volume V, dilution factor δ, and similar features of a water quality analysis procedure might (if explicitly represented in a model) explain some of the variability observed in water quality samples (see, for example, Gronewold et al., 2008), it seems logical that they can be regarded as data during model calibration (as demonstrated in Qian et al., 2005) in a model of the form in equation (2) (for similar applications in epidimiology studies, see Frome et al., 1973; Frome and Checkoway, 1985). Nonetheless, we find that common approaches to representing uncertainty and variability in FIB water quality modeling studies (as suggested in Benham et al., 2006; Muñoz-Carpena et al., 2006; Manache et al., 2007) assume pollutant concentration measurements are best represented by models of the form in equation (1) and, furthermore, that those models are best calibrated using OLS regression procedures.