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Predicting water quality at Santa Monica Beach: Evaluation of five different models for public notification of unsafe swimming conditions

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ABSTRACT

Bathing beaches are monitored for fecal indicator bacteria (FIB) to protect swimmers from unsafe conditions. However, FIB assays take ~24 h and water quality conditions can change dramatically in that time, so unsafe conditions cannot presently be identified in a timely manner. Statistical, data-driven predictive models use information on environmental conditions (i.e., rainfall, turbidity) to provide nowcasts of FIB concentrations. Their ability to predict real time FIB concentrations can make them more accurate at identifying unsafe conditions than the current method of using day or older FIB measurements. Predictive models are used in the Great Lakes, Hong Kong, and Scotland for beach management, but they are presently not used in California – the location of some of the world's most popular beaches. California beaches are unique as point source pollution has generally been mitigated, the summer bathing season receives little to no rainfall, and in situ measurements of turbidity and salinity are not readily available. These characteristics may make modeling FIB difficult, as many current FIB models rely heavily on rainfall or salinity. The current study investigates the potential for FIB models to predict water quality at a quintessential California Beach: Santa Monica Beach. This study compares the performance of five predictive models, multiple linear regression model, binary logistic regression model, partial least square regression model, artificial neural network, and classification tree, to predict concentrations of summertime fecal coliform and enterococci concentrations. Past measurements of bacterial concentration, storm drain condition, and tide level are found to be critical factors in the predictive models. The models perform better than the current beach management method. The classification tree models perform the best; for example they correctly predict 42% of beach postings due to fecal coliform exceedances during model validation, as compared to 28% by the current method. Artificial neural network is the second best model which minimizes the number of incorrect beach postings. The binary logistic regression model

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also gives promising results, comparable to classification tree, by adjusting the posting decision thresholds to maximize correct beach postings. This study indicates that predictive models hold promise as a beach management tool at Santa Monica Beach. However, there are opportunities to further refine predictive models.

1. Introduction

Epidemiological studies show that swimming in fecal contaminated waters may result in gastrointestinal and respiratory diseases (Prüss, 1998; Haile et al., 1999). To protect bathers from swimming in polluted waters, bathing beaches are typically monitored for fecal indicator bacteria (FIB), such as enterococci and *Escherichia coli*. Traditional methods to detect FIB take 18–24 h; even if rapid detection methods, such as qPCR (Noble et al., 2010), are used, there is still at least a 6-hour lag time between exposures of swimmers and public notification of beach water quality. Ample evidence has shown that waterborne FIB concentrations change in a matter of days or even hours (Boehm et al., 2002). Beach management based on out-dated sampling results can lead to contaminated beaches left open and clean beaches being posted or closed (Kim and Grant, 2004; Whitman and Nevers, 2004). A recent epidemiology study by Colford et al. (2012) showed that swimmer illness is associated with FIB concentrations measured on the same day but not the day before, further substantiating the need for better beach water quality warning systems.

Beach water quality prediction via a modeling approach for beach management was first introduced by the World Health Organization (WHO) (WHO, 2003). The approach has been incorporated by the European Union in the Bathing Water Directive (European Parliament, 2006) to advise the public against bathing during short term pollution. In 2012, The U.S. Environmental Protection Agency (USEPA) introduced new recreational water quality criteria and endorsed beach water quality predictive modeling as a rapid and inexpensive tool to reduce beach management errors due to the time lag in FIB measurement (USEPA, 2011). Exploratory studies on beach water quality modeling have been carried out worldwide since the early 2000s. These studies typically adopt statistical, data-driven models with hydro-meteorological factors (i.e., rainfall, solar radiation, tide level) as input variables. Multiple linear regression (MLR) is the most widely used model type; it has been tested at beaches in lacustrine (Olyphant and Whitman, 2004; Frick et al., 2008; Nevers and Whitman, 2008; Francy, 2009) and marine (Crowther et al., 2001; Boehm et al., 2007; Gonzalez et al., 2012; Thoe et al., 2012) coastal environments. Other common modeling methods include partial least square regression (Hou et al., 2006; Brooks et al., 2013) and artificial neural networks (Lin et al., 2003; He and He, 2008; Zhang et al., 2012). Categorical models such as decision trees have also been used in some studies (Parkhurst et al., 2005; Boehm et al., 2007; Bae et al., 2010; Stidson et al., 2012).

Predictive models have been successfully applied as management tools in the US Great Lakes (Francy, 2009; Francy et al., 2013), and in Scotland (McPhail and Stidson, 2009; Stidson et al., 2012). A pilot beach water quality model has also been developed in Hong Kong (Thoe and Lee, 2013). In general, predictive models are found to out-perform traditional beach monitoring to capture beach pollution primarily as the latter relies only on outdated FIB measurements. Past studies usually considered only one specific modeling tool, or compared two types of models (e.g., MLR versus ANN) (Mas and Ahlfeld, 2007; Thoe et al., 2012). The strengths and weaknesses of different models at different types of beaches have not been fully addressed. Additionally, there have not been general guidelines to choose the most appropriate type of model, limiting extensive application of predictive tools.

California has some of the most famous beaches in the world. Every year, over 150 million visits are made to Californian beaches, generating over 14 billion USD (Pendleton and Kildow, 2006). In 1997, the California State Legislature passed Assembly Bill 411 (AB411) (CDHS, 1997) which requires monitoring of bathing water at frequently visited beaches adjacent to flowing storm drains and creeks for enterococci (ENT), fecal coliform (FC) and total coliform (TC) during the bathing summer season (April–October). Predictive models are not used for beach management in California, except where the Scripps Institute of Oceanography uses CODAR to provide Tijuana River plume fate and transport information to the City of Imperial Beach in San Diego County (http://www.sccoos.org/data/tracking/IB/). Californian beaches are unique among other coastal beaches. Point pollution sources like wastewater treatment plant discharges have been identified and mitigated at many California beaches, and the bathing season (April–October) corresponds to the dry season. Additionally, in situ measurements of salinity and turbidity, which have been found important in other locations for model development (Nevers and Whitman, 2008; Gonzalez et al., 2012; Thoe et al., 2012) are not typically available for California beaches. Therefore, modeling experiences elsewhere cannot be directly applied to California. A few independent studies have been carried out at specific California beaches using a particular type of predictive model (Hou et al., 2006; Boehm et al., 2007; He and He, 2008; Bae et al., 2010), but it is still unknown if there exists one particular type of model that performs the best at California beaches with different pollution characteristics.

This study provides a comprehensive performance evaluation of five different statistical, data-driven predictive models to predict ENT and FC concentrations at Santa Monica Beach in the summer bathing season. Santa Monica Beach is one of the most visited beaches in California (Morton and Pendleton, 2001). The beach was reported to have the highest excess gastrointestinal illnesses among 28 beaches in Los

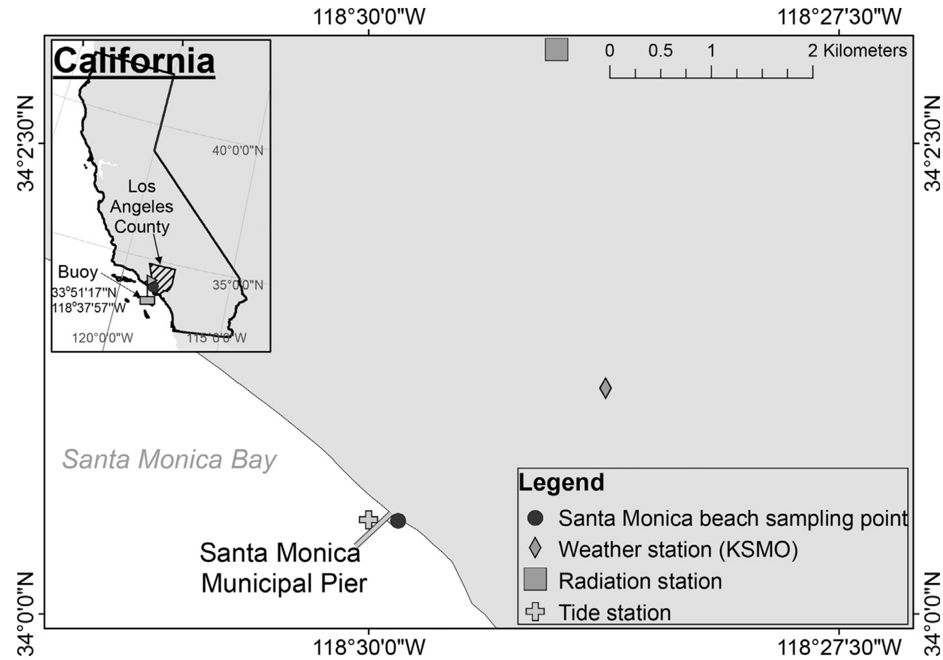

Fig. 1 – Location of Santa Monica Beach and the corresponding hydro-meteorological stations.

Angeles and Orange Counties in year 2000 (Given et al., 2006). This makes the beach an ideal site to test if predictive models are useful in providing early warnings of beach pollution. The five types of models considered in the study include multiple linear regression model, binary logistic regression model, partial least square regression model, artificial neural network, and classification tree. Subjective criteria are used to compare the predictive models with the current beach management procedure of using past measurements to determine whether the beach should be open or posted as unfit for swimming. Critical factors affecting beach water quality are also identified. This study represents a starting point of a feasibility study on water quality prediction at beaches along the California coast. The final goal is to develop a recommendation regarding the effectiveness of different types of predictive models for coastal beaches in California. Study results can also be used as model development and evaluation guidelines for other coastal beaches in California and around the world.

2. Methods and materials

2.1. Study beach

Santa Monica Beach (34°0′30″N, 118°29′50″W) is located in Los Angeles County of Southern California, facing Santa Monica Bay (Fig. 1). A municipal pier with amusement facilities is adjacent to the beach. According to land use data obtained from United States Department of Agriculture (http://datagateway.nrcs.usda.gov/), land cover adjacent to the beach is primarily urban. A storm drain is located at the south side of the pier. During dry weather, nuisance runoff in the storm drain is diverted to a nearby treatment plant. The only other potential flowing, land-based, FIB sources within 3 km of the study site are the Santa Monica Canyon (which receives flow from Santa Monica Canyon Creek and Rustic Creek) and Pico Kenter storm drain; as these have no flow during the summer and are not believed to affect water quality at Santa Monica Beach (City of Santa Monica (1999)), their discharge is not considered in the present study. The region has a Mediterranean climate, with hot and dry summers, and cool and relatively wet winters; annual rainfall is approximately 300 mm (with reference to the weather station at Santa Monica Municipal Airport, obtained from http://www.ncdc.noaa.gov/). Most of the rain is received between November and March.

2.2. Data

Concentrations of ENT and FC as well as the exact sampling time at the single sampling point at Santa Monica Beach were obtained from The City of Los Angeles for April 2006 to July 2012. The location where the samples were collected is seaward of the storm drain in ankle deep water. Water samples are collected every Tuesday through Saturday typically between 0900 and 1000 h. There are 1002 data points for each FIB collected in the summer (April–October). ENT are measured using Enterolert (IDEXX, Westbrook, ME). For FC, *E. coli* are measured using Colilert-18, and a 1:1 relationship of FC to *E. coli* is assumed for determining compliance with State standard. Upper and lower detection limits for FC are 13,000 and 67 most probable number MPN/100 mL respectively, and 2000 and 10 respectively for ENT. The numbers of data with concentration at or higher than the maximum detection limit for FC and ENT are 6 and 10 (of 1002 data), respectively, corresponding to ~ 1% of all data. The numbers of data with concentration at or lower than the minimum detection limit for FC and ENT are 375 and 262 (of 1002 data), respectively, corresponding to 37% and 26% of all data, respectively. The FIB

Table 1 – Independent variables used in this study with abbreviations and their respective sources.

Abbreviation	Independent variable	Source
logFIB1[a]	FIB concentration of the last sample – log-transformed	The City of Los Angeles, Department of Public Works, Bureau of Sanitation, Environmental Monitoring Division
1ogFIB30	Rolling geometric mean of FIB concentration in the past 30 days – log-transformed	
logFIB60	Rolling geometric mean of FIB concentration in the past 60 days – log-transformed	
logRainH	First 8-hour rainfall on the sampling day (in)	Airport weather station (KSMO)
logRain1-logRain7[b]	Daily rainfall in the past 7 days (in)	
logRain2T-logRain7T[c]	Cumulative rainfall for the past 2–7 days (in)	
logRain30T	Past 30 days cumulative rainfall (in)	
dday	binary variable of presence (1) or absence (0) of rain on the day of sampling × number of antecedent dry days since the last rain event	Derived
Tide	Tide level during the sampling time (m above chart datum)	Predicted by Extended Harmonic Analysis, tidal constituents obtained from National Oceanic and Atmospheric Administration
Tider	Tidal range on the sampling day (m)	
TideMax	Maximum tide level on the sampling day (m above chart datum)	
TideMin	Minimum tide level on the sampling day (m above chart datum)	
dTide	Relative change in tide level since 1 h before sampling time (m)	
TideH	Number of hours since last high tide	
WVHT	Offshore wave height during sampling hour (m)	National Data Buoy Center
DPD	Dominant wave period during sampling hour (s)	
APD	Average wave period during sampling hour (s)	
q_l	Alongshore current velocity (m/s)	Derived
Atemp	On-site measured air temperature	Santa Monica Bay Beaches Bacterial TMDLs Coordinated Shoreline Monitoring Plan report
Wtemp	On-site measured water temperature	
Storm	On-site observed storm drain condition (ordinal variable)	
upwell1	Previous day's upwelling index (m^3/s/100 m)	Pacific Fisheries Environmental Laboratory
rad1	Previous day's radiation (Langleys)	Integrated Pest Management Program – U.C. Davis
cc1	Previous day's cloud cover (Category 0–8)	Airport weather station (KSMO)
pres1	Previous day's air pressure (inch of mercury)	
wspd1	Previous day's wind speed (mph)	
owind1	Previous day's onshore wind speed (mph)	
awind1	Previous day's alongshore wind speed (mph)	

[a] FIB = ENT (enterococci) or FC (fecal coliform).
[b] 7 different independent variables.
[c] 6 different independent variables.

concentrations were log-transformed to reduce skewness and variance, making them more stable estimators than the non-transformed concentrations. Further discussions on the choice of log-transformed concentrations can be found in Wymer and Wade (2007).

Table 1 shows the independent variables used in this study and their corresponding data sources. The locations of different weather and hydro-meteorological stations are shown in Fig. 1. These data were readily available for model development from data archives. No new measurements were collected. The variables were classified into the following six categories.

2.2.1. *Past FIB concentrations*

Three forms of log-transformed past FIB concentrations were considered in this study: FIB concentration of the last sample (logFIB1), rolling geometric mean of FIB concentration during the past 30 days (logFIB30) and 60 days (logFIB60). Only past FIB concentrations of the same type were used in the model (i.e., 'logFIB1' in a summer model for ENT refers to 'logENT1').

2.2.2. *Rainfall*

Rainfall data at the nearby airport weather station, Santa Monica Municipal Airport (KSMO), were obtained from National Climate Data Center (http://www.ncdc.noaa.gov/). Daily rainfall during each of the past seven days (logRain1, logRain2, logRain3, logRain4, logRain5, logRain6, and logRain7) and the cumulative values in the past two to seven days (logRain2T, logRain3T, logRain4T, logRain5T, logRain6T, and logRain7T) were considered. Cumulative rainfall in the past 30 days (logRain30) captures the rainfall condition over a longer period. In addition, a variable representing rainfall in the first

8 h on the sampling day (logRainH) was included. All rainfall variables were log-transformed to reduce both data skewness and outliners. Values of 0 were replaced with 1/2 of the reported minimum value (0.01 inch). Additionally, an interaction term representing the product of the binary variable of the presence (rainfall >0.1 inch/day) or absence of rain on the day of sampling and the number of antecedent dry days since the last rain event was developed (dday). This variable is used to represent the time for pollutants accumulation and the corresponding 'first-flush' effect of pollution.

2.2.3. *Tide*

Tide level (Tide) at the hour nearest the sampling time, tidal range (Tider), and maximum (TideMax) and minimum (TideMin) tide level on the sampling day were calculated using extended harmonic analysis (Lee, 1986). Tidal constituents at Santa Monica Beach were obtained from National Oceanic and Atmospheric Administration (NOAA) (http://tidesandcurrents.noaa.gov/). Relative change in tide level (dTide) and number of hours since the last high tide (TideH) were also computed (see supplementary materials (SM) for details).

2.2.4. *Wave*

Wave height (WVHT), and dominant (DPD) and average (APD) wave period during the sampling hour, measured by the nearest offshore buoy as available at National Data Buoy Center (http://www.ndbc.noaa.gov/). The buoy is 21 km from the beach. Wave height recorded at the buoy is significantly, positively correlated to observed wave height in the bay (data not shown); observed wave height was not used in this study owing to its imprecision (recorded to the nearest 0.5 foot). Alongshore current velocity (q_l) induced by incoming waves was computed. See SM for details.

2.2.5. *On-site observations/measurements*

On-site observations of storm drain condition, and measurements of air and water temperature reported daily by lifeguards were obtained from Santa Monica Bay Beaches Bacterial Total Maximum Daily Loads (TMDL) Coordinated Shoreline Monitoring Plan reports (Table 1). Storm drain condition is an ordinal variable reported as 'no flow', 'low flow', 'medium flow' and 'high flow'; it was changed to 0, 1, 2 and 3, respectively, for modeling purposes, by assuming a linear relationship between this variable and logFIB.

2.2.6. *Other hydro-meteorological variables*

Upwelling index, solar radiation, cloud cover, air pressure and wind speed (further decomposed to onshore and alongshore wind speed based on beach orientation and wind direction) were obtained from various sources (Table 1).

2.3. *Predictive models*

Individual models were developed for ENT and FC as dependent variables in summer (April to October), using data from a calibration period (years 2006–2010) and then tested using data from the validation period (years 2011–2012). A five-year calibration period was chosen to ensure sufficient data covered different hydro-meteorological conditions during model development. Five types of predictive models were developed for both FIB: multiple linear regression (MLR), binary logistic regression (BLR), partial least square regression (PLS), artificial neural networks (ANN), and classification tree (CT).

The MLR models were developed using SPSS Statistics (version 20, IBM, Chicago, IL). The stepwise regression algorithm was adopted for variable selection with entry and removal probability of 0.05 and 0.1, respectively. Adjusted R^2 values for the MLR models, and standardized coefficients for input variables are reported. A two-step process was used to minimize the impact of variable multi-collinearity on the estimation of variable coefficients. First, correlation coefficients among all independent variables were calculated; confounding independent variable pairs with a correlation coefficient greater than 0.5 were identified; the one with lower linear correlation with logFIB under study was removed from model development. A relatively high correlation of 0.5 was used to avoid the exclusion of too many potentially useful variables. Next, the variance inflation factor (VIF) was calculated. Variables with VIF greater than 5 were removed from the model (Mason et al., 1989). These two screening methods together ensured that multi-collinearity was not problematic.

The BLR models were also developed using SPSS. 'Forward: conditional algorithm' was adopted for variable selection. The dependent variable is a binary variable representing whether or not the beach was posted based on the single sample standard (SSS) for the modeled indicator (104 and 400 MPN/100 mL for ENT and FC, respectively). The output of the BLR model is an odds ratio (OR). Probability of exceedance is defined as:

$$\%\text{ of exceedance} = \frac{\text{OR}}{\text{OR}+1} \times 100 \quad (1)$$

The default interpretation of the BLR models is: if % exceedance >50%, the beach is predicted to be posted. In this study, the % exceedance threshold above which a beach was posted was varied between 0 and 100% to investigate how 'tuning' the BLR model (BLR-T) might improve its performance. Cox & Snell R^2 and Nagelkerke R^2 values of the BLR models and OR for the input variables were reported. Confounding independent variable pairs with correlation greater than 0.5 were identified, and the one with lower linear correlation with logFIB was removed from model development.

The PLS models were developed using MATLAB (version R2012b, Natick, MA). 39 principle components were computed from the same number of independent variables, and a regression was performed between the principle components and the dependent variable. A stepwise regression algorithm was adopted for variable selection with entry and removal probability of 0.05 and 0.1 respectively. Adjusted R^2 values were reported. As the principle components are linearly independent, multi-collinearity is not an issue for the PLS models.

The ANN models were developed using the MATLAB 'Neural Network' Toolbox. A feed-forward back-propagation ANN structure was adopted. The ANN consists of three consecutive layers (input, hidden and output layers) connected by nodes. Signals are transmitted from input to hidden and then output layers according to the weights of different

Table 2 – Independent variables in the MLR models for ENT and FC and their corresponding standardized coefficients and variance inflation factor (VIF), calibrated against data of years 2006–2010. Adjusted R^2 that can be explained by the MLR and PLS models (bracketed value) are also given.

Order	ENT			FC		
	Variable	Standardized coefficient	VIF	Variable	Standardized coefficient	VIF
1	logENT1	0.190	1.215	logFC60	0.312	1.457
2	Storm	0.193	1.301	dTide	0.186	1.616
3	TideMax	0.157	1.144	logFC1	0.148	1.357
4	logRain2T	0.118	1.257	Storm	0.175	1.209
5	Tide	0.128	1.125	Wtemp	−0.158	1.454
6	APD	−0.117	1.04	APD	−0.063	1.223
7	Wtemp	−0.132	1.334	owind1	−0.087	1.120
8	logRain30	−0.124	1.564	TideMin	−0.112	1.529
9	logENT30	0.105	1.464	WVHT	−0.150	1.571
10				q_l	−0.130	1.734
11				cc1	−0.074	1.204
12				logRain30	−0.078	1.456
Adjusted R^2		0.221 (0.240)			0.307 (0.337)	

nodes. In the input layer, only variables included in the MLR model for that particular indicator were included in the ANN model. The inputs then go through a five-node hidden layer to the output layer predicting the logFIB concentration. A sigmoidal transfer function was used between the input and hidden layers. A linear transfer function was used between the hidden and output layers (Thoe et al., 2012).

The CT models were developed using the MATLAB ‘Classification Tree’ Toolbox. The model output is a binary variable representing whether the beach is posted or open based on the SSS of the modeled indicator. A parent node is branched into two leaf nodes based on an if/then type independent variable criterion; branching continues until the lowest node impurity is achieved, where node impurity is represented by the Gini's Diversity Index (Jost, 2006). All independent variables were used to develop the CT models.

An acronym table for model related terms is given in Table S1 and specific model calibration details for the ANN and CT models are given in the SM.

2.4. Assessment of model performance

Predictive model performance was compared with the ‘current method’ that is presently used by beach managers. This method assumes that the water quality at the present time is well predicted by water quality obtained during the last measurement - which is usually the previous day for Santa Monica Beach, or in some instances, several days ago. The models were compared in their ability to predict SSS exceedance or compliance for ENT and FC (104 and 400 MPN/100 mL, respectively), in which a SSS exceedance will result in beach being posted as unfit for swimming (hereafter refer to as ‘beach posting’). The following assessment criteria were used:

1. Sensitivity (%): percentage of SSS exceedance days that can be predicted by the model;
2. Specificity (%): percentage of SSS compliance days that can be predicted by the model;
3. Total correct prediction (%): overall correct prediction of SSS exceedance and compliance days.

Further discussion of these metrics can be found in the SM. Correlation coefficients and root mean square errors (RMSEs) between observed and predicted logFIB were also calculated for the current method and continuous models (MLR, PLS, and ANN). Correlation coefficients and RMSEs are commonly used indicators to quantify the linear dependence and the difference in magnitude between observed and predicted data, respectively (Berthouex and Brown, 2002).

3. Results

3.1. Water quality trends

At Santa Monica Beach, FC exceeded SSS frequently at about 50% from 2006 to 2009, and was reduced to about 20% since 2010. The reduction in FC exceedance was likely a result of the installation of bird exclusion nets and new storm drain infrastructure (HtB, 2011). The exceedance rate for ENT was relatively stable throughout the study period at about 10%.

3.2. Prediction results

Table 2 provides lists of independent variables retained in the MLR models (all $p < 0.05$) for ENT and FC and their corresponding standardized coefficients and VIF. There are 9 and 12 variables for ENT and FC models, with adjusted R^2 of 0.22 and 0.31, respectively. Variables include past FIB concentrations, storm drain condition, tide, and rainfall. Correlations between observed and MLR predicted FIB (0.48/0.57 in calibration and 0.33/0.35 in validation for ENT/FC, Table 3) are higher than the current method (0.29/0.35 in calibration and 0.23/0.20 in validation). RMSE obtained by MLR is 0.4–0.5 log MPN/100 mL in both the calibration and validation period, as compared to 0.5–0.7 log MPN/100 mL for the current method.

Four and seven independent variables are retained in the BLR models for ENT and FC (Table 4), with Cox & Snell R^2 of 0.09 and 0.21, and Nagelkerke R^2 of 0.19 and 0.29, respectively. Important BLR variables include storm drain condition, past FIB concentrations, and tide.

The PLS models retained 4 and 7 of the principle components for the final fit for ENT and FC, with adjusted R^2 of 0.24 and 0.34 respectively (Table 2). Correlations obtained by PLS models for ENT/FC are 0.49/0.59 in calibration, and 0.34/0.33 in validation (Table 3). RMSE is 0.43–0.50 log MPN/100 mL for both periods.

The ANN models were developed using only input variables included in the MLR models (Table 2). Correlations obtained by ANN models for ENT/FC are 0.55/0.58 in calibration and 0.38/0.38 in validation (Table 3). RMSE is 0.41–0.48 log MPN/100 mL for both periods.

The number of end-nodes in the CT models for ENT and FC are 6 and 22 respectively (Fig. 2). ENT and FC models each use 3 and 13 variables, some of the variables show up repeatedly in the CT; for example, Tide and dTide both appear twice in the ENT model. Important variables that appear in high levels of the CT include past FIB concentrations, tide and solar radiation.

Fig. 3 (a) and (b) show the scatter plots between observed and predicted logENT using the current method and MLR in the calibration period, respectively, while Fig. 3 (c) and (d) show the corresponding scatter plots in the validation period. Scatter plots for other models (PLS, BLS and ANN) and for FC are provided in Figs. S2–S5. The model-predicted FIB concentrations are in closer agreement with observed concentrations (closer to 1:1 line in plots) than previous FIB concentrations (the current method). However, correlation between the data-driven model outputs and observed FIB is reduced by 0.15–0.2 from calibration to validation (Table 3). In particular, high observed ENT concentrations (i.e., >100 MPN/100 mL) in the validation period are usually under-predicted by the models.

3.3. *Model sensitivity, specificity, and total correct prediction*

Fig. 4 shows the sensitivity, specificity, and total correct prediction of the models during calibration and validation periods. The current method achieves a sensitivity and specificity for ENT/FC of 27/54% and 92/70%, respectively, in the calibration period and 18/28% and 94/88%, respectively, in the validation period. The current method achieves typically the lowest total correct prediction (64–88%) when compared to other models (71–94%).

CT can predict the largest percentage of beach postings of all model types during the calibration period (38/78% sensitivity for ENT/FC). In the validation period, sensitivity is reduced, but still achieves the overall highest sensitivity among all types of models (24/42%). For example, a sensitivity of 42% for FC in the validation indicates that the CT model can capture 15 beach postings of 36, when compared to 10 beach postings captured by the current method (28% sensitivity). The model has slightly lower specificity for FC in the validation period (82%) than the current method (88%) and other models (>90%).

ANN has the second highest sensitivity after CT. In the validation period, ANN achieves 30% and 28% sensitivity for ENT and FC, respectively. Specificity is very high in both calibration and validation periods (85–99%), consistently higher than the current method (70–94%).

MLR, BLR, and PLS perform similarly. They have very high specificity in both calibration and validation periods (83–100%), on average 10% higher than the current method. However, the models usually achieve lower sensitivity than the current method. For the ENT model, both MLR and PLS cannot predict any beach posting in the validation period, when BLR predicts 1 (6% sensitivity). Accordingly, exceedance % threshold for the BLR model was 'tuned' (BLR-T) to increase sensitivity. For ENT, by decreasing the threshold from 50% to 30% (Fig. 5), model sensitivity increases from 16% to 27% in the calibration period, and from 6% to 24% in the validation period, while keeping excellent specificity (> 98%) and total correct prediction (~ 92%) nearly unchanged. For FC, 35% is found to be the best decision threshold, giving sensitivity = 73% and 39%, specificity = 65% and 86% in the calibration and validation periods, respectively.

Table 3 – Correlation coefficients and RMSE between observed and predicted logFIB obtained by current method, MLR, PLS and ANN models during calibration (cal, 2006–2010) and validation (val, 2011–2012) periods.

FIB	Current		MLR		PLS		ANN	
	Cal	Val	Cal	Val	Cal	Val	Cal	Val
	correlation coefficient							
ENT	0.29	0.23	0.48	0.33	0.49	0.34	0.55	0.38
FC	0.35	0.20	0.57	0.35	0.59	0.33	0.58	0.38
	RMSE							
ENT	0.67	0.62	0.50	0.48	0.50	0.48	0.48	0.47
FC	0.66	0.53	0.47	0.41	0.46	0.43	0.46	0.41

Table 4 – Independent variables in the BLR models and their corresponding odds ratios, calibrated against data of years 2006–2010. Cox & Snell R^2 and Nagelkerke R^2 that can be explained by the BLR models are also given.

Order	ENT		FC	
	Variable	Odds ratio	Variable	Odds ratio
1	Storm	4.564	logFC60	16.229
2	logENT1	2.173	dTide	27.797
3	Tide	3.189	pres1	51.884
4	APD	0.734	q_1	0.357
5			logFC1	1.592
6			WVHT	0.387
7			Storm	2.282
Cox & Snell R^2	0.087		0.214	
Nagelkerke R^2	0.186		0.291	

4. Discussion

4.1. *Critical factors affecting beach water quality in Santa Monica*

Beach water quality at Santa Monica Beach can be better predicted by the models than the current method using different environmental variables as inputs, as indicated by the consistently higher correlation and lower RMSE between observation and prediction obtained by the continuous models than the current method. The MLR models can explain

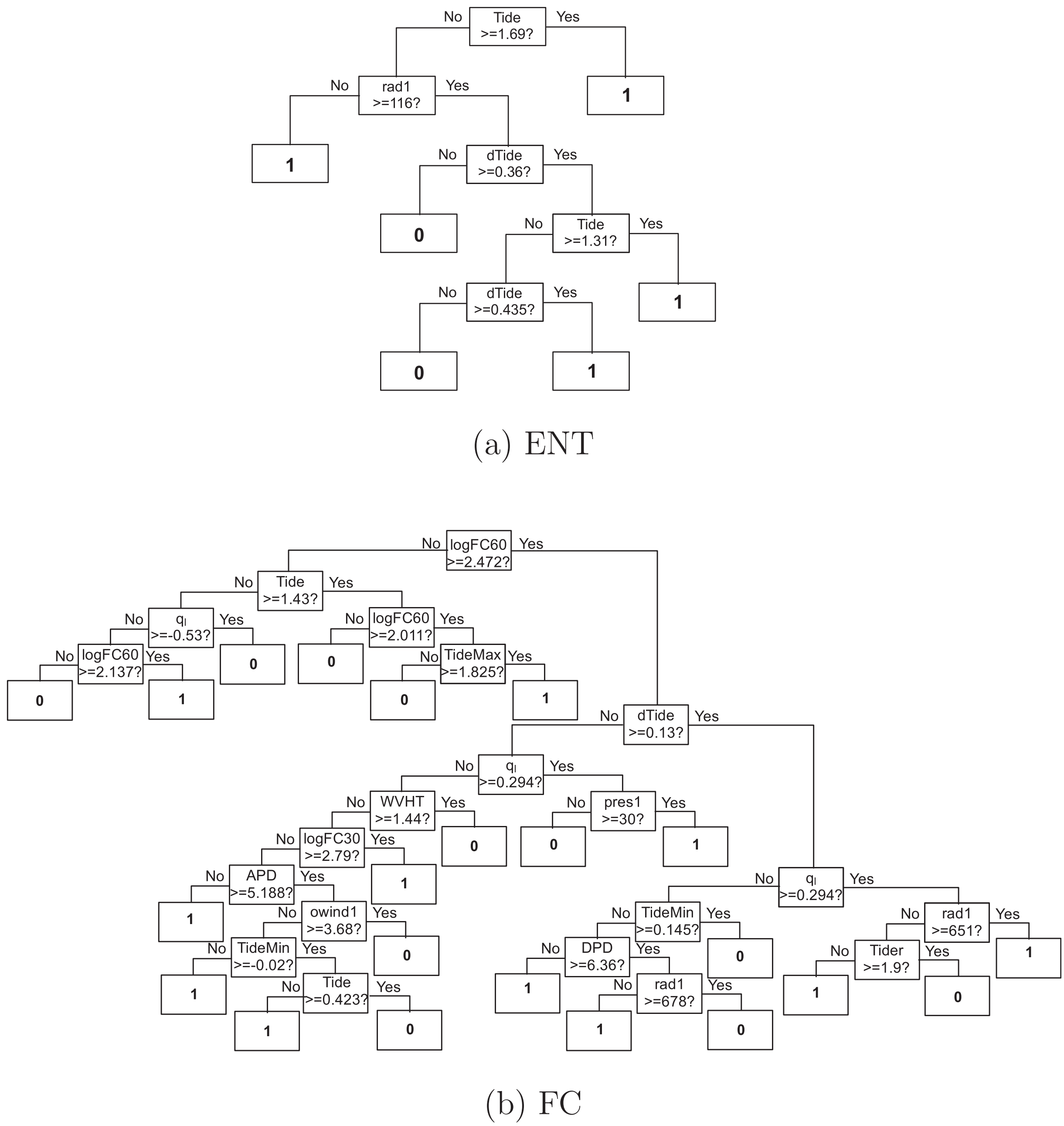

Fig. 2 – CT structure for (a) ENT and (b) FC, calibrated against data of years 2006–2010. '1' and '0' in the end-nodes represent 'SSS exceedance' and 'SSS compliance' respectively. Abbreviations of input variables are listed in. Table 1.

22% and 31% of ENT and FC variance respectively in the calibration data, comparable to other studies for marine, coastal beaches (e.g., Hou et al. (2006); Thoe et al. (2012)). Critical factors affecting beach water quality at Santa Monica Beach include: past FIB concentrations, storm drain condition, tides, rainfall, and solar radiation.

Past FIB concentrations, either the most recent sample (logENT1) or rolling geometric mean (logFC60), explains the most variance of logFIB, even when the current method does not perform satisfactorily in predicting beach posting. This suggests the past FIB concentrations provide 'static' background concentrations, which need to be further modified by other hydro-meteorological factors to reflect the 'dynamic' water quality conditions. Thoe et al. (2012) showed the importance of past *E. coli* concentrations to water quality prediction especially at beaches with relatively stable water quality.

Storm drain condition has the largest standardized coefficient in the MLR model for ENT, and the third largest in the FC model. This variable can be easily obtained through site observation, and can explain a large portion of logFIB variance. The positive standardized coefficients for both FIB show

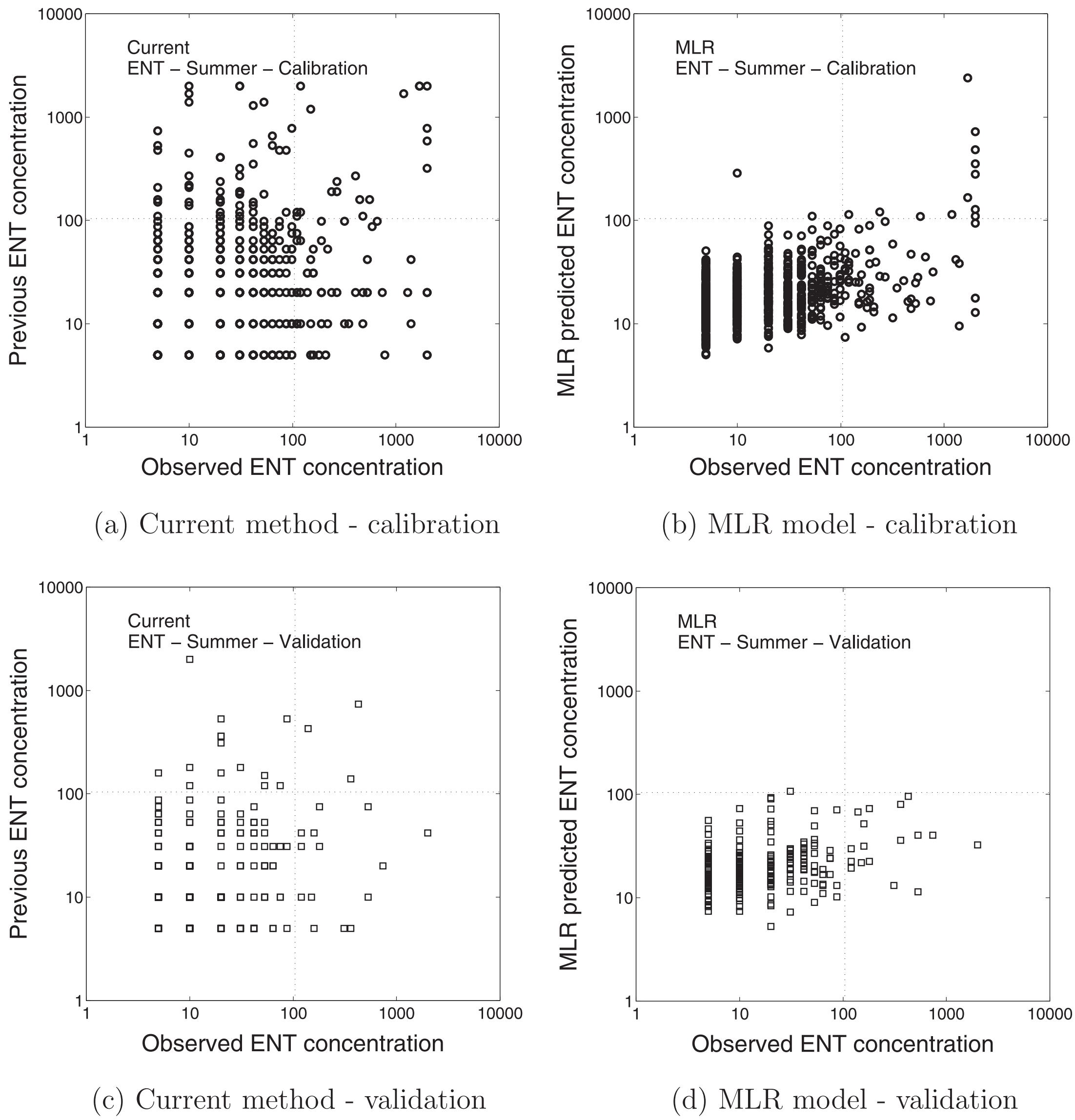

Fig. 3 – Scatter plots between observed and predicted logENT in summer using (a) current method and (b) MLR model in the calibration period (2006–2010), and (c) current method and (d) MLR model in the validation period (2011–2012).

that the higher the storm drain flow, the higher the FIB concentration.

Tide related variables (Tide, dTide, TideMax) are consistently among the top three variables that explain the most variance of logFIB in MLR and BLR models based on the stepwise R^2, and also play a major role in CT (e.g. Tide and dTide are two of the three selected variables for ENT CT). Tide may modulate submarine groundwater discharge (Robinson et al., 2007), storm drain, or lagoon discharge (Grant et al., 2001). The consistent positive standardized coefficients associated with Tide and dTide variables suggesting beach water quality is worse during high and flood tides, when bacteria could be washed off from beach sands and wrack, potentially causing elevated bacterial levels (Russell et al., 2014).

Rainfall variables appear to be secondary in Santa Monica models for both FIB, although it is usually reported as the most critical variable in beach water quality prediction, as rainfall and the associated surface runoff bring pollutants accumulated on the land through a non-point source manner. One example is the Scotland system which predicts beach water quality based only on rainfall and river flow rate (Stidson et al., 2012). This suggests in Santa Monica storm drain condition may capture some of the important patterns that may have been captured by the rainfall variables. The summer dry weather in California also certainly contributes to the weaker dependence of FIB concentration on rainfall; there is rarely measurable rainfall in the summer season.

Solar radiation is not included in MLR or BLR models, but appears in CTs for both FIB. Solar radiation significantly increases the mortality rate of FIB in marine waters (Boehm et al., 2009), and is commonly used in predictive modeling studies (e.g. Hou et al. (2006); Frick et al. (2008); Thoe et al. (2012)). A study conducted in Avalon, California found that swimmers who swallowed water are more likely to experience

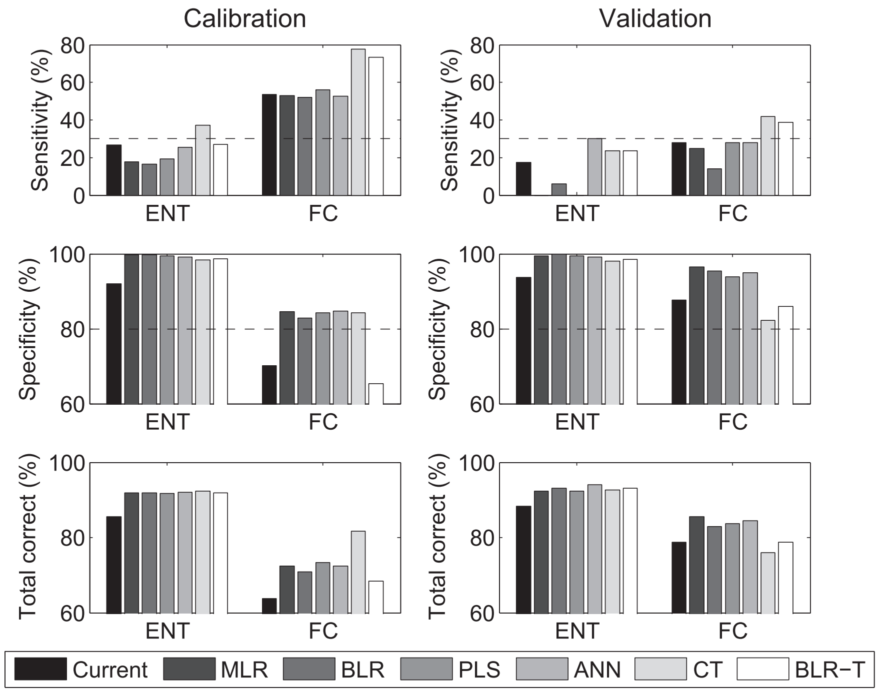

Fig. 4 – Sensitivity, specificity and total correct prediction obtained by different models in the calibration period (2006–2010) and validation period (2011–2012). Criteria for sensitivity (30%) and specificity (80%) are plotted for reference.

gastrointestinal illness when solar radiation is low (Yau et al., 2014). As reflected by the decision rules in CT, lower solar radiation is more likely to have a beach posting.

It is also interesting to note that the critical factors in the ENT and FC models are different. This suggests that there are different ENT and FC sources to Santa Monica Beach. For example, storm drain and rainfall variables are more important in ENT models than in FC models, implying rainfall-driven surface flow is a more important contributor of ENT than FC.

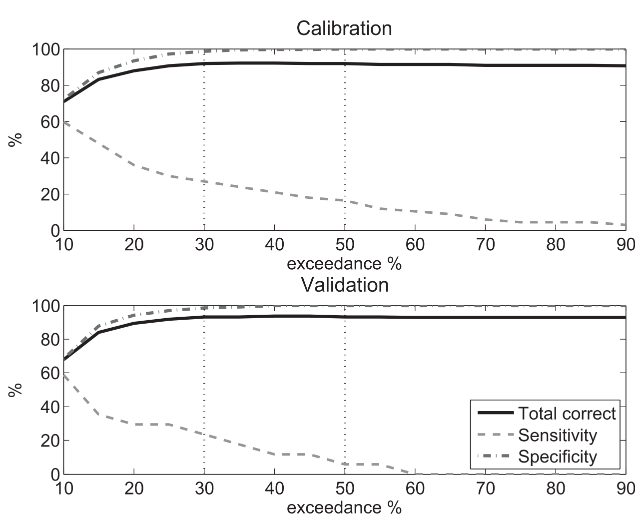

Fig. 5 – Changes in BLR model performances with exceedance probability for ENT-S in calibration (2006–2010) and validation (2011–2012) periods.

4.2. *Comparing model performances*

The current method generally achieves lower total correct prediction than the predictive models; it reveals that having near-daily sampling frequency does not necessarily indicate that beach management decisions are correct. Continuous models are scientifically feasible alternatives to assist beach management. However model performances in predicting beach posting status vary. Also, model sensitivity is generally reduced from calibration to validation. In particular, the reduction in sensitivity for FC in the validation period (and a corresponding increase in specificity) might be attributed to the decrease in FC exceedance rate from 50% in calibration period to 20% in validation period due to changes in beach infrastructure. In this study, we propose criteria that define a model ready for management applications in order to compare the performance of different types of model in both calibration and validation periods. From the public health protection perspective, a model ready for management applications should predict a greater percentage of beach postings than the current method, without an expense of excessive 'false alarms'. We propose the following criteria to determine whether a model is effective for beach management:

1. Model sensitivity is greater than 30%;
2. Model sensitivity is 10% greater than the current method;
3. Model specificity is greater than 80%.

These criteria were developed based on in-depth discussions with the Technical Advisory Committee for our project (see Table S2 in SM) in consideration of model performance at

25 different beaches in California. A similar set of criteria are used in the Great Lakes to evaluate the MLR or PLS models (D. Francy, person. commun.). Although these criteria are used in the present study, a future decision to change these criteria can be readily implemented. The sensitivity criterion of 30% was chosen because the current method usually achieves a sensitivity lower than 30% (considering results at a wide range of California beaches, data not shown); it represents a minimum sensitivity threshold for a model. The 10% criterion was chosen to ensure that the model produced better results than the current method. Finally, the 80% specificity criterion was chosen to ensure clean beaches were not incorrectly predicted to exceed the SSS. These thresholds may not be appropriate for every geographical location as they are set relative to the performance of the current method at Californian beaches.

In the calibration period, CTs for both FIB pass these criteria, whereas none of the MLR, BLR, PLS, ANN, and BLR-T models pass. In the validation period, CT and BLR-T models for FC and ANN model for ENT pass the criteria, whereas MLR, BLR and PLS models do not pass. Based on these criteria, as well as the fact that FC is the most exceeding FIB in Santa Monica, CT appears to be the best model type for Santa Monica Beach, while ANN and BLR-T the next best.

CT has not been commonly used in beach water quality prediction in practice and it has generally been excluded from previous research at California Beaches (Hou et al., 2006; He and He, 2008; Bae et al., 2010); the only study in California using CT was conducted at Huntington State beach (Boehm et al., 2007), and was mainly for an exploratory purpose, without comparing CT results with other types of predictive models. The one example where CT is used in practice, in parallel with a simple rainfall/flow triggering model, is in Scotland where beach pollution is mainly rainfall-driven (Stidson et al., 2012). Based on their performance in this study, the CT models appear to capture exceedances more successfully than the linear models. Relationships between independent variables and SSS exceedance/compliance can be easily understood through a CT model. For example, based on the ENT model, a beach posting is predicted when:

1. Tide level is higher than 1.69 m;
2. Tide level is lower than 1.69 m and radiation is lower than 116 Langleys;
3. Tide level is between 1.31 and 1.69 m, radiation is greater than 116 Langleys and change of tide level is greater than 0.36 m;
4. Tide level is lower than 1.31 m, radiation is higher than 116 Langleys and change in tide level is greater than 0.44 m.

In addition, the CT model (as well as the BLR model) has a binary dependent variable, its model performance is not affected as other continuous models by data censorship (the number of data above and below detection limit) and whether the FIB concentration is log-transformed (Segal, 1988); therefore it may be more suitable to be used at Santa Monica Beach because the beach has a considerable percentage of FIB data below the assay detection limit (37% for FC and 26% for ENT). At the same time, CT has the greatest reduction in sensitivity from calibration to validation period (on average 25% reduction when compared to 10–22% for other models). This implies the need of a careful model calibration, i.e., selecting model parameters including 'the minimum number of cases in a parent node which permits further branching' (MP) and 'the minimum number of cases that is permitted to be branched from a parent node into a leaf' (ML) (see SM). In this study, the overall best CT with the highest sensitivity and total correct prediction in both calibration and validation periods was selected among 72 CTs developed with different MP and ML. In addition, a 'bushy' CT model with many end nodes can be obtained at times, especially when the dependent variable has complicated relationships with the independent variables. There are 22 end-nodes in the CT for FC, 11 of which predict a beach posting. Despite the large number of nodes which might suggest over-fitting, the good performance of the CT model in validation indicates over-fitting is not a problem.

ANN is the second best model type for Santa Monica Beach. It achieves higher sensitivity for ENT and higher specificity for both FIB when compared to the current method in the validation period. ANN can capture the nonlinear relationship between dependent and independent variables, and also tends to be more successful in capturing exceedances than linear models. However, ANN has a disadvantage of being a 'black-box' model, the underlaying relationships between variables cannot be interpreted directly. The model can also be weak in extrapolation, i.e. it may predict unreasonably high/low FIB concentrations when the values of input variables are beyond the calibration range (Thoe et al., 2012).

BLR gives lower sensitivity than the current method for both FIB in the validation period. However, if the exceedance % thresholds for ENT and FC are lowered to 30% and 35%, respectively, sensitivity of the tuned BLR-T model is increased, and is comparable to that of the CT model. As the tuning decreases model specificity at the same time, i.e. increases the number of 'false positives', a balance between model sensitivity and specificity should be maintained when tuning a model. For example, if it is decided to maximize sensitivity and only maintain a 80% specificity, sensitivity can reach 41% for ENT (threshold = 13%) and 50% for FC (threshold = 30%) in the validation period. A similar approach has been suggested by Brooks et al. (2013) to use a 'decision threshold' as a tuning parameter to calibrate PLS models.

Other continuous models (MLR and PLS) obtain low sensitivity relative to ANN and CT, despite the fact that MLR is the most commonly used model in practice (Crowther et al., 2001; Frick et al., 2008; Francy, 2009; Thoe and Lee, 2013). This can be attributed to its under-prediction of high FIB concentrations. The observed under-prediction may be a result of data censorship. Despite the lower sensitivity of the MLR and PLS models, they consistently obtain lower RMSE, higher correlation, and higher specificity than the current method in both calibration and validation periods. Thus, an approach similar to the 'threshold tuning' used in the BLR models may also be useful for increasing the MLR and PLS model sensitivities. We plan to explore this in future studies.

It is important to note that predictive models were developed based on an assumption that the dependent variable, FIB concentration of a single sample collected at a particular time of a day, is a reliable indicator for health risk of that entire day. However, there exists diurnal variation of FIB concentrations (Boehm et al., 2002) and inherent uncertainties in FIB enumeration methods (Gronewold and Wolpert, 2008). While this study found that predictive models have better performance than the current method to predict concentrations of single samples, it may be possible to extend the model to predict the diurnal variation of beach water quality driven by tidal current, waves, and solar radiation as well as to quantify and incorporate the uncertainty of the FIB concentrations.

5. Concluding remarks

1. This study illustrates a framework to evaluate performances of five types of models (MLR, BLR, PLS, ANN, CT) to predict concentrations of ENT and FC at Santa Monica Beach in Southern California.
2. Despite a high sampling frequency of five times per week, the current method does not perform satisfactorily and gives consistently higher RMSE and lower correlation when compared to other continuous models.
3. Based on the three criteria suggested in this study (model sensitivity >30% and 10% greater than the current method, and model specificity >80%), CT appears to be the best model type.
4. ANN minimizes the number of incorrect beach postings, and is the second best model type.
5. The BLR model also performs well after lowering the exceedance % threshold, achieving sensitivity comparable to the CT model. MLR and PLS models, on the other hand, obtain relatively low model sensitivities.
6. Past FIB concentrations, on-site observed storm drain condition, and tide level are found to be critical environmental factors affecting beach water quality; rainfall and solar radiation also modulate FIB concentrations.
7. This effort represents a starting point to evaluate the efficacy of predictive models to assist beach management in California. However, continuous communication with the beach managers is needed to seek for the best method to implement predictive models and disseminate modeling results.
8. All the models considered in this study can be implemented in a simple spreadsheet and yield results in a timely fashion; input variables are also readily available and no additional data collection is necessary.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.watres.2014.09.001.

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