Title: Modelling of Escherichia coli concentrations in bathing water at microtidal coasts

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Modelling of Escherichia coli concentrations in bathing water at microtidal coasts

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ABSTRACT

Monitoring of the quality of bathing water in line with the European Commission bathing water directive (Directive 2006/7/EC) is a significant economic expense for those countries with great lengths of coastline. In this study a numerical model based on finite elements is generated whose objective is partially substituting the microbiological analysis of the quality of coastal bathing waters. According to a study of the concentration of Escherichia coli in 299 Spanish Mediterranean beaches, it was established that the most important variables that influence the concentration are: monthly sunshine hours, mean monthly precipitation, number of goat cattle heads, population density, presence of Posidonia oceanica, UV, urbanization level, type of sediment, wastewater treatment ratio, salinity, distance to the nearest discharge, and wave height perpendicular to the coast. Using these variables, a model with an absolute error of 10.6 ± 1.5 CFU/100 ml is achieved. With this model, if there are no significant changes in the beach environment and the variables remain more or less stable, the concentration of E. coli in bathing water can be determined, performing only specific microbiological analyses to verify the water quality.

Keywords: numerical modelling; E. coli; beaches; water quality

1. Introduction

In the last fifty years enjoying leisure time on the coast throughout the year has increased in popularity. This requires minimum standards of quality in the coastal areas and its bathing waters to ensure the health of the users (Sardá et al., 2005). For this reason, the European health administration has been monitoring the quality of bathing water for more than 20 years. Bathing waters are the surface waters where a significant number of people are expected to bathe or there is an activity directly related to water sports.

Monitoring the quality of coastal waters is carried out mainly in accordance with the European Directive on bathing waters (Directive 2006/7 / EC), measuring the concentration of Escherichia coli and intestinal Enterococci. These bacteria, present in the microbiota of humans and warm-blooded animals (Callahan et al., 1995; Gantzer et al., 1998), are used as an index of faecal contamination because they can cause gastrointestinal and respiratory tract infections, as well as ears, eyes, nasal
cavity or skin illness (W.H.O., 2003). Depending on the risk of infection, Directive 2006/7/EC classifies coastal waters as: excellent, good, sufficient and insufficient. The established limit values may, in rare circumstances, be adapted by the local authorities to each space, depending on the social, cultural, environmental and economic conditions.

The variation in the concentration of these bacteria depends on many factors. On the one hand, physical characteristics such as beach environment, sediment type, radiation, or salinity are important variables. For example, urban beaches (with greater urban development and greater number of users) present lower quality than natural or semi-urban beaches (Ariza et al., 2010; May et al., 1999; McLellan, 2004; Winter and Duthie, 1998). The type of sediment (gravel or sand) is also important, since *E. coli* can reproduce in sand, because it is a humid environment, rich in organic matter (Alm et al., 2006; Yamahara et al., 2007). Furthermore, the type of sediment is directly related to the disinfection capacity of ultraviolet light (UV), which inactivates the microorganisms in the water (Salcedo et al., 2002), the greater the number of suspended solids in the water the lower disinfection capacity (Abdelzaher et al., 2010; Haugland et al., 2005; Salcedo et al., 2002). This is one of the reasons why sandy beaches have higher concentrations of bacteria than gravel beaches (Aragonés et al., 2016a).

On the other hand, beach users, pets (dogs) and birds, especially seagulls, are sources of this type of bacteria in the sand and therefore in the water (Abdelzaher et al., 2010; Haugland et al., 2005; Whitman et al., 2004). Likewise, livestock and agricultural developments near the beaches have adverse effects on the microbial quality of bathing water, with the negative effects mainly due to rainfall (Ackerman and Weisberg, 2003). Several authors have also related the concentration of *E. coli* to the presence of some species of marine vegetation. For example, *Cladophora* favours the survival of *E. coli* (Beckinghausen et al., 2014; Englebert et al., 2008; Vanden Heuvel et al., 2010), while other algae like *Ulva rigida*, *Codium bursa*, *Cystoseira barbata*, *Ceramium diaphanum* *Acanthophora sp.*, *Bryothamnion triquetrum*, *Gracilaria sp.*, *Gelidium sp.*, *Caulerpa mexicana*, *Caulerpa sp.*, *Halimeda incrassata*, *Ulva sp.*, *Codium decorticatum*, *Sargassum sp.* or *Posidonia oceanica* have an antibacterial activity against *E. coli* (Frikha et al., 2011; Hammami et al., 2013; Luzi et al., 2016; Ríos et al., 2009).

Historically, monitoring programs have led to geospatial analysis models (Grayson et al., 2008; Kelsey et al., 2004; Knothe, 2012), tracking microbial source (McQuaig et al., 2012), and evaluating microbial networks (Brooks et al., 2008; Faust and Raes, 2012) to more accurately predict human health risks after exposure to contamination. However, there are still difficulties in establishing predictive models, since microbial contamination can come from multiple point and non-point sources (Stewart et al., 2008), but having a large database can facilitate modelling (Mill et al., 2006). For example, Partyka et al. (2017), through 1740 samples, established data collection sites, and generated a model to predict changes in concentration in areas subject to large seasonal variations.

The objective of this study is to obtain a model that allows us to determine the concentration of *E. coli* in coastal bathing waters, in order to reduce the number of microbiological analyses. First, the correlations between *E. coli* concentration in 299 beaches and 33 variables related to climate, maritime climate, physical characteristics, environment, fauna and flora were studied. Next, different mathematical models were generated, and the optimum model was validated using data from later years.
2. STUDY AREA

The study area comprises 299 beaches along 983 km of the Spanish Mediterranean coast (Fig. 1), specifically the beaches located in the provinces of Valencia (47 beaches), Alicante (94 beaches), Murcia (37 beaches), Almeria (65 beaches) and Granada (27 beaches). It is a microtidal area where astronomical tides range from between 20 cm and 40 cm, and when affected by meteorological factors, the tide surges can be up to 75 cm (EcoMAG, 2009).

The zone to the North of the Cape of the Nao is bordered by marshes intensely transformed by the agricultural activity (Fig. 1a), while to the south to the Amadorio River the coast is characterized by a landscape of small coves and cliffs (Fig. 1b). Towards south there are dune ridges, beaches and lagoons such as Torrevieja or Guardamar (Fig. 1c). On the coast of Murcia, there is an important dune strip that forms the Mar Menor, which presents a higher temperature and salinity than the Mediterranean Sea. From Cape Palos to the border of the province of Granada, the coastal plains are very narrow and the coast is formed by cliffs and small beaches, except for the valleys of some rivers. The rivers throughout the study area are generally short and the flows have an important seasonal character.

An important feature of the study area is the extensive presence of *Posidonia oceanica* meadows on the seabed (Fig. 1d). *Posidonia oceanica* is a marine plant endemic to the Mediterranean and forms large meadows on sandy bottoms near the coast. To develop, Posidonia meadows need good quality, uncontaminated, transparent and well oxygenated waters, that is, their presence is representative of the good quality of the waters in which are located.

**Fig. 1.** Location of the study area, the *Posidonia oceanica* meadows, as well as the 299 beaches studied. **a)** Agricultural area. **b)** Cliffs and coves. **c)** Dune strips. **d)** *Posidonia oceanica*.
3. **Methodology**

The work was carried out in four phases: data collection and organization, analysis of variables, generation of models, and finally, validation.

3.1. **Data collection**

In this study, 33 variables have been analysed and can be grouped according to their relationship with: climatology (water temperature, hours of sun, ultraviolet radiation, rainfall or wind); maritime climate (wave height and salinity); physical characteristics (sediment, environment, density and population, morphology, orientation); livestock (goats, sheep or cow); sources of discharges and purification; and the existence of *Posidonia oceanica* (existence, depth, width of the meadow, etc.).

Table 1 shows a summary of the studied variables and their origin.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Variables</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Faecal bacteria</td>
<td><em>E. coli</em> (CFU/100 ml)</td>
<td>Treatment according to Directive 2006/7/EC of data from the Nayade (2016) database</td>
</tr>
<tr>
<td>Physical</td>
<td>Sediment (sand, sand with scattered rocks, sand and gravel, and rocks)</td>
<td>Visual corroboration of data from the MAGRAMA (2016b) database</td>
</tr>
<tr>
<td>characteristics</td>
<td>Level of urbanization (urban, semi-urban, natural)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Orientation (North, North-Northeast, Northeast, East-Northeast, East, and South, etc.)</td>
<td>Measurement through a GIS system of data from Ecolevante (2006) and EcoMAG (2009)</td>
</tr>
<tr>
<td></td>
<td>Morphology (open, supported, Bi-supported, enclosed)</td>
<td></td>
</tr>
<tr>
<td>Population</td>
<td>Population per town</td>
<td>INE (2016) database</td>
</tr>
<tr>
<td></td>
<td>Population density (pop/km$^2$)</td>
<td></td>
</tr>
<tr>
<td>Climatology</td>
<td>Ultraviolet (UV) rays</td>
<td>AEMET (2016) database</td>
</tr>
<tr>
<td></td>
<td>Average monthly precipitation (mm/month)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average hours of sunshine per month (h/month)</td>
<td></td>
</tr>
<tr>
<td>Maritime climate</td>
<td>Average salinity (PSU)</td>
<td>Puertos del Estado (2016) database</td>
</tr>
<tr>
<td></td>
<td>Average water temperature (°C)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Wind velocity perpendicular to the coast (m/s)</td>
<td>Treatment using AMEVA v.1.4.3 software of data from Puertos del Estado (2016) database</td>
</tr>
<tr>
<td></td>
<td>Wave height perpendicular to the coast (m)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Period associated with wave height (s)</td>
<td></td>
</tr>
<tr>
<td>Livestock</td>
<td>Heads of cattle (total number of cattle head/town)</td>
<td>MAGRAMA (2016a)</td>
</tr>
<tr>
<td></td>
<td>Goat cattle (number of cattle head/town)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Sheep cattle (number of cattle head/town)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pig cattle (number of cattle head/town)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Other cattle (number of cattle head/town)</td>
<td></td>
</tr>
<tr>
<td>Purification rate</td>
<td>Purification rate (percentage of purified wastewater)</td>
<td>MAGRAMA (2016c) database</td>
</tr>
<tr>
<td>and source</td>
<td>Ravines or rivers</td>
<td></td>
</tr>
<tr>
<td>discharges</td>
<td>Distance to ravines or river (m)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Residual discharges</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Distance to residual discharges (m)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>All discharges (rivers, gullies and waste)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Distance to any type of discharge (m)</td>
<td></td>
</tr>
<tr>
<td>Posidonia</td>
<td>Presence of <em>Posidonia oceanica</em></td>
<td>Measurement through a GIS system of data from Ecolevante (2006) and EcoMAG (2009)</td>
</tr>
<tr>
<td>oceanica</td>
<td>Meadow final depth (m)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Meadow medium depth (m)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Meadow initial depth (m)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Meadow width (m)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Stem height (cm)</td>
<td>Ecolevante (2006) and EcoMAG (2009) databases</td>
</tr>
<tr>
<td></td>
<td>Plant density (stems/m$^2$)</td>
<td></td>
</tr>
</tbody>
</table>
Escherichia coli concentrations in each of the beaches were obtained from the database published by Nayade (2016) for the surveys conducted between 2012 and 2016. The data for 2012-2015 were used for the model adjustment, while the data from 2015-2016 were used for validation. These data were processed according to Directive 2006/7/EC to obtain P95 values of E. coli in each of the studied beaches. For more information on sampling, cadence of data collection, detection methods, etc., see http://nayade.msc.es/Splayas/home.html.

All data on climatology, population and maritime climate refer to the average of the period studied during the bathing season (May-September). The wave height $H_{s,12}$ (wave height exceeded 12 hours per year or with a probability of being exceeded of 0.137%), its associated mean period ($T$) and the median wind speed were calculated using the software AMEVA v1.4.3 (IHCantabria, 2013).

Regarding the physical characteristics, beach morphology was divided into four groups (open, supported, bi-supported and enclosed) as were proposed by López et al. (2015). The beaches were classified into 16 groups according to their orientation as follows: A perpendicular line was drawn from the coastline of each beach, thereby enabling us to read its orientation as given by the wind rose. A visual inspection of the sediment resulted in a classification into five groups: sand, sand with scattered rocks, sand and gravel, gravel with scattered rocks, and rocks. The level of urbanization was obtained from the MAGRAMA (2016b) classification, which follows the guidelines established by Ariza et al. (2010), distinguishing between urban, semi-urban and natural beaches.

Several types of discharges to the beaches can be found such as: rivers, ravines and residual discharges. Residual discharges, in turn, can be grouped in five types, according to their origin and end point: 1) outfall (discharge directly in the beach or nearby); 2) submarine outfall (discharges more than 500 m from the shoreline); 3) agricultural; 4) diffuse: generic, industrial and storm water; and 5) WWTP (Wastewater Treatment Plant). A GIS (Geographic Information System) system was used to measure the distance between each point of discharge and the midpoint of the beach in the direction of the main wave flow in each zone. The littoral discharge closest to the shoreline was selected, provided that the distance from the shoreline was less than 2 km. If the distance to the discharge point was greater than 2 km, it was considered that no discharge existed on the beach.

The characteristics of the Posidonia oceanica meadows (width and depth) were obtained by measuring the GIS data from Ecolevante (2006) and EcoMAG (2009). The remaining data (plant density and stem height) were obtained from the files of each of the Posidonia meadows found in the databases of the previous studies (Ecolevante, 2006; EcoMAG, 2009). For more information about the variables used see supplementary material 1.

### 3.2. Mathematical modelling

For the study and modelling of E. coli bacteria in the coastal waters, first the principal component analysis (PCA) and bivariate correlations were analysed. The bivariate Pearson Correlation produces a sample correlation coefficient ($r$) which measures the strength and direction of linear relationships between pairs of continuous variables. By extension, the Pearson Correlation evaluates whether there is statistical evidence for a linear relationship among the same pairs of variables in the population. This methodology is advantageous because it is less sensitive to atypical values and biased distributions, and works well even when there is strong interaction between input variables (Liao et al., 2016).
After the study of correlations, the selection of variables to be included in the different models was a function of:

- Degree of correlation
- The ease of obtaining the data of the variable
- The relative importance of these variables according to other research

For the generation of mathematical models, several methodologies were used. First, linear models (S-Plus2000, 1999) and (SPSS12.0., 2003), were determined. From the study of linear models, the results indicate that the existing relationship is not linear since the estimated regression coefficient is 0.23. For this reason, numerical models were used. Different numerical models (using data from the period 2012-2015) were generated using the methodologies based on the finite element method (Navarro-González and Villacampa, 2013; Navarro-González and Villacampa, 2012) and the formulation of the Galerkin method (Navarro-González and Villacampa, 2016).

The methodologies of Navarro-González and Villacampa (2012, 2013) are numerical methodologies that allow the generation of models to represent the relationship between independent variables and a dependent variable(s), from the interpolation defined in n-dimensional finite element model, which is generated from the experimental data. The interpolation function implies the use of some initial conditions, which in the defined methodology implies the coincidence between the values of the function in a finite number of points. As normally occurs when applying the finite element method, the model function is obtained in a finite set of points called nodes (Zienkiewicz et al., 1977). In the applied methodologies, an optimization problem based on the determination of the minimum of an error function, generically defined in a finite element model, was solved. To improve the speed of resolution when the number of variables used is high (as in the case of some of the models generated in this paper), the methodology developed by Navarro-González and Villacampa (2016) was used.

In both methodologies, the experimental data are normalized to the n-dimensional hyper-cube, given by \( \Omega = [0,1]^n \). Each interval [0, 1] is divided into c subintervals \( c \) is called the complexity of the model). A set of \( c^n \) elements and \( (c + 1)^n \) nodes is generated, where the relationship between the independent variables and the dependent variable(s) is calculated. For example, if we consider a 3-dimensional geometric model with a complexity \( c = 4 \), the total number of elements is \( 4^3 = 64 \). To determine the output data, the model uses an interpolation function. The minimized error depends on the methodology used. Thus, in Navarro-González and Villacampa (2012, 2013) the sum of the squared error (Equation 1) of the values obtained by the interpolation function at each point \( z_j \) and the initial conditions \( P_j \) is minimized. While in the methodology based on the Galerkin method (Navarro-González and Villacampa, 2016), the error \( e(x) \)-the difference between the solution and its approximation) is minimized by zeroing the integral defined in Equation 2, where \( NP \) is the number of variables in the model, \( N_j(P_j) \) is the interpolation function used to determine the value of the model at any point and \( W_j(x) \) is the selected weight function (collocation method, sub-domain method, Least Square Method, Galerkin method, method of moments). In order to select the complexity, the generation and validation data of the model are used. Thus, the lower complexity that offers better results is selected, in order not to overfit the model.

\[
Error = \sum_{j=1}^{NP} \left( N_j(P_j)\bar{u} - z_j \right)^2 \tag{1}
\]
The criterion for selecting the optimal model was, first, the $R^2$ value. The coefficient of determination ($R^2$) allows us to measure the goodness of fit and decide whether the linear adjustment performed is sufficient or whether alternative models should be sought. However, for nonlinear numerical models (as in our case), the value of $R^2$ is a guideline, since a model with a low value of $R^2$ can offer good results. Therefore, to determine the performance of the models and select the optimal model, the following errors were used: absolute error (Equation 3); mean magnitude of the relative error (Equation 4); and relative percentage error (Equation 5), which have been previously used by other authors (Aragonés et al., 2016b; Hashemi et al., 2010; Liu et al., 2012).

\[ e = |r_i - o_i| \]  
\[ MAPE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{r_i - o_i}{r_i} \right| \]  
\[ \delta = \frac{\sum_{i=1}^{n} (r_i - o_i)^2}{(n-p) \sum_{i=1}^{n} r_i^2} \]  

Where $r_i$ are the real measured data, $o_i$ are the data estimated by the model, $n$ is the number of data, and $p$ is the number of free parameters.

Numerical models were validated with the 10% of the studied beaches (30 beaches) using experimental data from subsequent years (2015-2016) to model adjustment data (2012-2015). Beaches were selected randomly, but taking into account that all the types of studied beaches (type of sediment, level of urbanization, etc.) were included.

### 4. Results

Results obtained from linear correlations between the analysed variables and *E. coli* concentrations are shown in Table 2. From the table it can be seen that the sun hours, rainfall and goat cattle have a greater direct influence on *E. coli*. However, correlation values were generally low, always lower than 0.35. Furthermore, nine main components, which explain 81.6% of the variance, were obtained from the PCA (see supplementary material 2). Among these components, the first three explain more than 52% of the variance. The variables that are more related to the first component are representative of the livestock, and it is observed that the temperature of the water and UV have also significant weight. The second component are related to the *Posidonia oceanica* (stem height (-0.705) and plant density (-0.791)). And in the main variables of the third component are the hours of sun (-0.814) and the purification rate (0.877), which by their definition have no relation between them.

<table>
<thead>
<tr>
<th>Variables</th>
<th>Correlation (r)</th>
<th>Variables</th>
<th>Correlation (r)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sun hours</td>
<td>-0.349</td>
<td>Distance to any type of discharge</td>
<td>-0.164</td>
</tr>
<tr>
<td>Rainfall</td>
<td>0.335</td>
<td>Width of meadow</td>
<td>-0.162</td>
</tr>
<tr>
<td>Goat cattle</td>
<td>0.308</td>
<td>Temperature</td>
<td>-0.148</td>
</tr>
<tr>
<td>Depth final meadow</td>
<td>-0.271</td>
<td>Density of beams</td>
<td>-0.139</td>
</tr>
<tr>
<td>Depth medium meadow</td>
<td>-0.268</td>
<td>Orientation</td>
<td>-0.134</td>
</tr>
<tr>
<td>Presence of <em>Posidonia oceanica</em></td>
<td>-0.267</td>
<td>All discharges (rivers, gullies and waste)</td>
<td>0.128</td>
</tr>
</tbody>
</table>
Following the criteria stated in section 3.2 for the selection of variables, more than 20 mathematical models, using different combinations of the 33 studied variables, were generated to express the relationship between the variables and the concentration of E. coli in bathing waters. Among the models there were 6 that provided significant results and they are reproduced in Table 3.

**Table 3.** Variables used in each of the models.

<table>
<thead>
<tr>
<th>6 Variables</th>
<th>8 variables</th>
<th>11 variables</th>
<th>11 variables_2</th>
<th>12 variables</th>
<th>13 variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sun hours</td>
<td>Sun hours</td>
<td>Sun hours</td>
<td>Sun hours</td>
<td>Sun hours</td>
<td>Sun hours</td>
</tr>
<tr>
<td>Rainfall</td>
<td>Rainfall</td>
<td>Rainfall</td>
<td>Rainfall</td>
<td>Rainfall</td>
<td>Rainfall</td>
</tr>
<tr>
<td>Goat cattle</td>
<td>Goat cattle</td>
<td>Goat cattle</td>
<td>Goat cattle</td>
<td>Goat cattle</td>
<td>Goat cattle</td>
</tr>
<tr>
<td>UV</td>
<td>UV</td>
<td>UV</td>
<td>UV</td>
<td>UV</td>
<td>UV</td>
</tr>
<tr>
<td>-</td>
<td>Level of urbanization</td>
<td>-</td>
<td>Level of urbanization</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>-</td>
<td>Sediment</td>
<td>-</td>
<td>Sediment</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>-</td>
<td>Purification rate</td>
<td>-</td>
<td>Purification rate</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>-</td>
<td>Salinity</td>
<td>-</td>
<td>Salinity</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>-</td>
<td>Distance to ravines or rivers</td>
<td>-</td>
<td>Distance to any type of discharge</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Hs,12</td>
<td>-</td>
<td>Period (T)</td>
</tr>
</tbody>
</table>

Fig. 2 shows the $R^2$ values for each of the generated models, with significant results. The values of $R^2$ increase as the complexity of the model and the number of independent variables increase. However, for more than 11 variables, the value of $R^2$ decreases slightly (12 variables model, $R^2=0.775\pm0.019$). Thus, for example, the model with six variables has an $R^2$ value of $0.458\pm0.037$, and for the 11 variables_2 model is $0.780\pm0.057$, but when the number of variables is increased to 13, the $R^2$ decrease slightly ($0.752\pm0.035$).
However, when the errors are analysed, a big difference is observed. Thus, Fig. 3 shows that the model of eight variables improves by 29.8% the absolute error of the six variables model. When adding two new variables (models with 11 variables) the mean absolute error decreased (13.1±1.9 CFU/100 ml for 11 variables and 12.8±2.7 CFU/100 ml 11 variables_2). If variables continued to be added (12 variables) the error decreased to 11.3±1.1 CFU/100 ml. However, when the variables were increased (13 variables) so did the error 13.5±1.9 CFU/100 ml. As observed, the error of the 13 variables model is similar to 11 variables model but with a greater standard deviation for each of the studied complexities (2.02 versus 1.35 CFU/100 ml).

Regarding the MAPE (Fig. 4a) and the relative percentage error (Fig. 4b) something similar to what happens with absolute error occurs. As the number of variables and the complexity of the model increases, errors decrease, reaching the values indicated in the 12 variables model and the complexity 90 of 27.1±4.1% and 0.370±0.055 for MAPE and relative percentage error, respectively. However, when the number of variables increases to 13 variables, the mean error is very similar to
the 11 variables model but the standard deviation increases. For example, for complexity 90, the MAPE of 13 variables model is 38.3±5.7% and the relative percentage error is 0.372±0.056.

![Fig. 4. a) MAPE and b) relative percentage error, for each of the studied models.](image)

Once the model was chosen (12 variables), the results were validated. As can be seen, the errors committed during validation (Fig. 5) were very similar to those made during calibration. For the absolute error, errors increase by a mean of 9.2% (+1.04 CFU/100 ml), except for the model of complexity 80 where the increase is 17.4% (+1.9 CFU/100 ml). Something similar happens with MAPE, but with higher increase, reaching 22.1% (+11.4%) on average. Finally, the measured data were compared with the modelled data and the quality limits established by Directive 2006/7/EC (Fig. 6). The differences observed are small and the quality assigned to the modelled data is the same as that assigned to the measured data.

![Fig. 5. a) Absolute error and b) MAPE, for validation data.](image)
Fig. 6. Measured and modeled data during the model (12 variables and complexity 70) calibration and validation, for the 30 beaches used for validation.

5. Discussion

Several studies have shown that there is a relationship between gastrointestinal symptoms and the quality of recreational waters, which is determined by measuring the number of bacteria (Prüss, 1998). Therefore, given the popularity of the use of coastal waters for recreational purposes, quality minimums must be met (Sardá and Fluviá, 1999). In order to avoid endangering the health of users, regulators set limits on the maximum concentrations of faecal bacteria in the water. In Europe these values are described in Directive 2006/7/EC. To know the concentration of faecal bacteria during the bathing season, regulators carry out costly microbiological analyses once every 2 weeks. In this study, a model was generated to obtain the concentration of *E. coli* in coastal bathing waters, in order to reduce the number of microbiological analyses.

First, the bivariate correlations between the analysed variables and the concentration of *E. coli* were studied (Table 2). The variables with the highest direct correlation are: sun hours (-0.349), precipitation (0.335) and goat cattle (0.308), so these variables are in all models. To these three variables were added other variables following the criterion described in section 3.2. Thus, the first model that presented significant results was the 6 variables model (sun hours, rainfall, goat cattle, presence of *Posidonia oceanica*, population density and UV), with values of $R^2$ between 0.396-0.504 (Fig. 2), and average absolute error of 25.9 CFU/100 ml. From the PCA, it is extracted that there are no strong relationships between the explanatory variables that have been used later to generate the models. It is observed that there are no correlation between variables that a priori can be thought that are possibly correlated to each other, as can be the temperature, the hours of sun and the ultraviolet radiation. Although, it is true that there is a certain relationship between ultraviolet radiation and temperature, neither of the two variables has been used together in the generated models.
The results of this model (6 variables) confirm the relationship, established by other authors, between these six variables and the concentration of *E. coli*. For example, according to Abdelzaher *et al.* (2010); Whitman *et al.* (2004); Zagarese *et al.* (1998) the concentration of *E. coli* decreases with UV, and increases with the low temperatures which is directly related to the hours of sunlight (Bathingwatercommittee, 2009; Bogosian *et al.*, 1996; Brettar and Höfle, 1992; Sampson *et al.*, 2006; Smith *et al.*, 1994). Other authors, such as Rijal *et al.* (2009) indicate the importance of the volume of precipitation. Higher precipitation influences *E. coli* concentration in the following ways: i) allows an increase in bacteria dilution, which could reduce the concentrations (Cho *et al.*, 2010); ii) modifies salinity conditions of water; iii) runoff waters clean the land surface and drag the pathogens toward the coast, increasing the bacterial concentration in coastal waters; and iv) Increases the flows of rivers, ravines, rainwater, which flow out to sea with all kinds of contaminants, such as animal defecations (Gibbs, 2001). This last point, could explain the high correlation obtained between the goat cattle and the *E. coli*, since in the studied area, goats usually freely graze on pastures (Meseguer and Espín, 2001), while the other livestock (bovine, porcine, etc.) are characterized by intensive, farms, and their excreta accumulate in the barn and are used as manure in agriculture (Ferrer *et al.*, 2000). Meanwhile, Hammami *et al.* (2013) and Luzi *et al.* (2016) observed that *Posidonia oceanica* has an antibacterial function against *E. coli* bacteria.

Moreover, population density during the bathing season has a significant influence on bacterial concentration, due to the drastic increase in the number of users (Ariza *et al.*, 2010). Also, urban development in the beach environment generally worsens the water quality of the beach. Ariza *et al.* (2008) observed that urban sandy beaches are the most affected by bacterial contamination since they are more accessible and accommodate more bathers. In addition, several recent studies indicate that bacterial indices may be associated with sewer leakage (generally ubiquitous in urban areas) due to aging infrastructure (Sercu *et al.*, 2009). The type of sediment also influences the concentration of bacteria, because *E. coli* is able to reproduce in the sand if the necessary conditions of nutrients, predators and environmental conditions occur (Alm *et al.*, 2006; Yamahara *et al.*, 2007), where it can persist for longer and then be transferred to the sea. In addition, the smaller the sediment size, the greater the number of particles that can be suspended when the waves break, making it difficult to purify water by UV (Abdelzaher *et al.*, 2010; Haugland *et al.*, 2005; Salcedo *et al.*, 2002). The degree of urbanization and the sediment type has a significant influence on bacterial concentration, as confirmed by the results of the 8 variables model, which decreases the absolute error by 30%, although it is higher than 16 CFU/100 ml (Fig. 3).

The models that showed improvement —11, 12 and 13 variables models— included salinity which is inversely correlated to *E. coli* (Aragonés *et al.*, 2016a; Mallin *et al.*, 2000), the purification ratio and the distance to discharges. It was observed that the distance from the rivers or ravines to the beach is important (Fig. 3-5), since there is a great improvement in the results when this variable is added to the models (improvement of 28% against the 8 variables model). However, the distance to any type of discharge is more important, because to replace the variable "distance to rivers and ravines" by the variable "distance to any type of discharge" the improvement is 35%. This is logical considering that the purification ratio of wastewaters is usually not 100%, but they are treated to eliminate the highest possible percentage of pollution and then are discharged into the sea to continue the purification process (Yamahara *et al.*, 2007). In addition, other studies have observed that areas located near agricultural or similar discharges present a higher concentration of faecal bacteria than those located near other kind of discharges (Palazón *et al.*, 2017). This can be due to
the trapping of fertilizers and contaminants of the irrigation waters, as well as to the lack of regulation and control in the discharge of these waters into the sea.

The incident wave \((H_s, T_1)\) and its related period are intimately linked to the discharges and their distance to the beach, since currents may move the discharges onshore or offshore. It has also been observed that, generally, beaches whose coasts are parallel to the wave front have a higher concentration of bacteria (Palazón et al., 2017), perhaps because of the turbidity that is generated when the wave breaks. This explains the improvement that occurs in the modelling by including the wave height as input variable. Although the absolute error is similar to that of the 11 variables model \((11.4 \text{ vs. } 12.8 \text{ CFU/100 ml, Fig. 3})\), the MAPE is much lower \((29.3\% \text{ vs. } 43.8\%, \text{ Fig. 4a})\). However, including the period in the models does not improve the results, they are even slightly worse \((11.35 \text{ vs. } 13.09 \text{ CFU/100 ml, Fig. 3})\).

For validation, unlike conventional models that use a percentage of the set data to calibrate the model and the rest for validation, in this study, a set of data from the 2015-2016 bathing season was used whereas data from 2012-2015 was introduced into calibration model. The data used for validation come from 30 beaches, randomly selected, but taking into account that they include all the types and degrees of urbanization, sediment, etc. The errors during the validation are similar to the errors during calibration (Fig. 5), which means that the model is valid and not over-adjusted. If the model were over-adjusted, when different data are used for validation the results would be much worse than the results of the calibration.

Finally, the analysis of the models shows that there are two types of variables: i) variables directly related to humans or their activity (population density, livestock, level of urbanization and purification ratio); and ii) variables related to the environment (rainfall, UV, sunshine hours, \textit{Posidonia oceanica}, sediment and salinity). Therefore, we can affirm that except for important modifications in the analysed variables, the concentrations of \textit{E. coli} will remain more or less stable.

In that case, the model can replace microbiological analysis, which could be performed only once during each bathing season (rather than every two weeks) in order to corroborate the model results. This study also shows that in order to further improve the results of the models, the effect of currents, tides, or sediment transport should be included in future studies.

6. Conclusion

Quality control and monitoring of bathing water based on measuring the concentration of faecal bacteria, such as \textit{E. coli}, requires numerous microbiological analyses. The objective of this study to obtain a model that enables the measurement of \textit{E. coli} in coastal bathing waters in order to reduce the microbiological analyses has been achieved. From the analysis of the results and the models that were generated, the following conclusions can be made:

- The relationship between the studied variables and the concentration of \textit{E. coli} is not linear, which is confirmed by the study of correlations and the poor results of the linear models.
- The model with the best results is the 12 variables model and complexity 70, obtaining an mean absolute error of 10.6±1.5 CFU/100 ml and a MAPE of 29.9±4.5%.
- The most important variables are: sun hours, rainfall, goat cattle, UV, presence of \textit{Posidonia oceanica}, population density, level of urbanization, type of sediment, purification ratio, salinity, distance to the nearest discharge, and wave height perpendicular to the coast.
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