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Title: Modelling of Escherichia coli concentrations in bathing water at  
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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  $10.6 \pm 1.5$  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.

# 1 Modelling of *Escherichia coli* concentrations in bathing water at microtidal coasts

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10

## 11 **ABSTRACT**

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

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

## 26 **1. Introduction**

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

33 Monitoring the quality of coastal waters is carried out mainly in accordance with the European  
34 Directive on bathing waters (Directive 2006/7 / EC), measuring the concentration of *Escherichia coli*  
35 and intestinal Enterococci. These bacteria, present in the microbiota of humans and warm-blooded  
36 animals (Callahan *et al.*, 1995; Gantzer *et al.*, 1998), are used as an index of faecal contamination  
37 because they can cause gastrointestinal and respiratory tract infections, as well as ears, eyes, nasal

38 cavity or skin illness (W.H.O., 2003). Depending on the risk of infection, Directive 2006/7/EC classifies  
39 coastal waters as: excellent, good, sufficient and insufficient. The established limit values may, in  
40 rare circumstances, be adapted by the local authorities to each space, depending on the social,  
41 cultural, environmental and economic conditions.

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

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

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

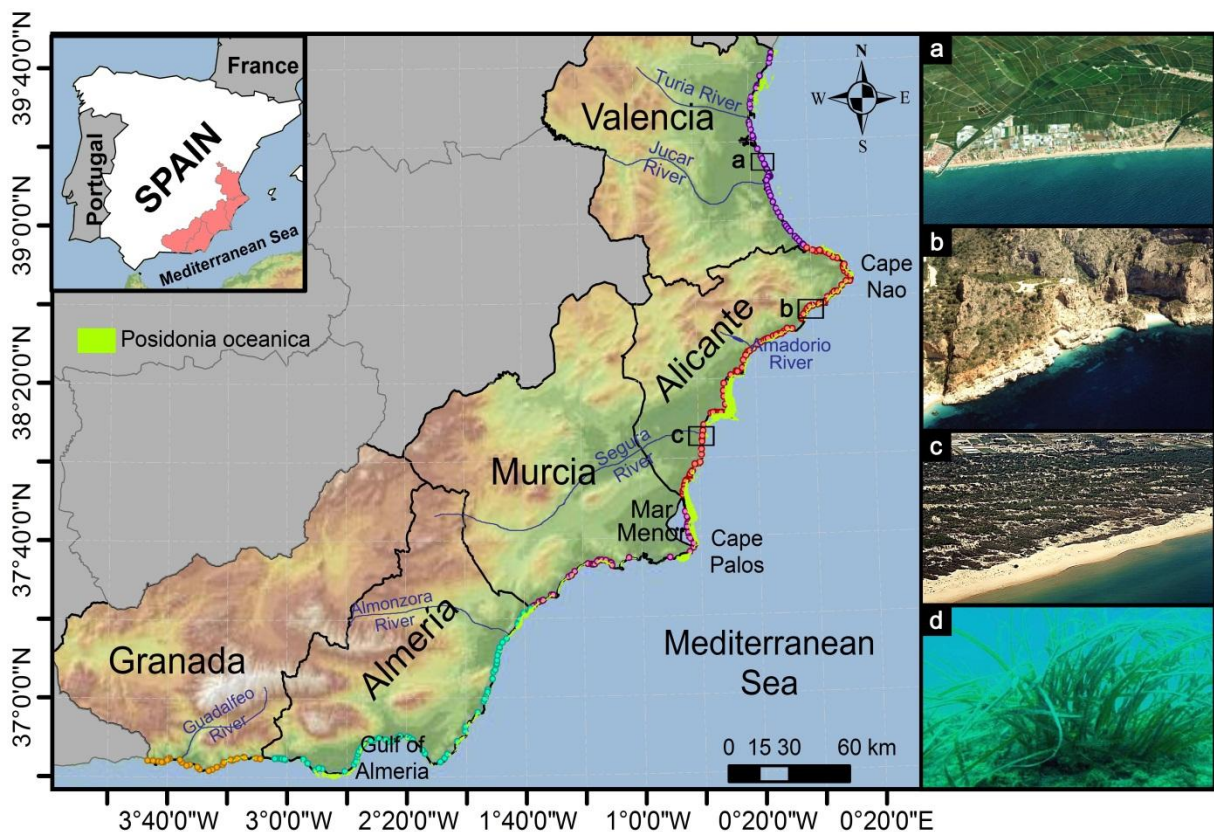
74 The objective of this study is to obtain a model that allows us to determine the concentration of *E.*  
75 *coli* in coastal bathing waters, in order to reduce the number of microbiological analyses. First, the  
76 correlations between *E. coli* concentration in 299 beaches and 33 variables related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

## 80 2. STUDY AREA

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

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

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



100  
101  
102

**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*.

103 **3. Methodology**

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

106 **3.1. Data collection**

107 In this study, 33 variables have been analysed and can be grouped according to their relationship  
108 with: climatology (water temperature, hours of sun, ultraviolet radiation, rainfall or wind); maritime  
109 climate (wave height and salinity); physical characteristics (sediment, environment, density and  
110 population, morphology, orientation); livestock (goats, sheep or cow); sources of discharges and  
111 purification; and the existence of *Posidonia oceanica* (existence, depth, width of the meadow, etc.).  
112 Table 1 shows a summary of the studied variables and their origin.

113 **Table 1.** Summary of the studied variables and their origin.

Parameters	Variables	Origin
<b>Faecal bacteria</b>	<i>E. coli</i> (CFU/100 ml)	Treatment according to Directive 2006/7/EC of data from the Nayade (2016) database
<b>Physical characteristics</b>	Sediment (sand, sand with scattered rocks, sand and gravel, gravel and with scattered rocks, and rocks)	Visual corroboration of data from the MAGRAMA (2016b) database
	Level of urbanization (urban, semi-urban, natural)	
	Orientation (North, North-Northeast, Northeast, East-Northeast, East, East-South, etc.) Morphology (open, supported, Bi-supported, enclosed)	Measurement through a GIS system of data from Ecolevante (2006) and EcoMAG (2009)
<b>Population</b>	Population per town Population density (pop/km <sup>2</sup> )	INE (2016)database
<b>Climatology</b>	Ultraviolet (UV) rays	AEMET (2016) database
	Average monthly precipitation (mm/month)	
	Average hours of sunshine per month (h/month)	
<b>Maritime climate</b>	Average salinity (PSU)	Puertos del Estado (2016) database
	Average water temperature (°C)	
	Wind velocity perpendicular to the coast (m/s)	Treatment using AMEVA v.1.4.3 software of data from Puertos del Estado (2016) database
	Wave height perpendicular to the coast (m)	
	Period associated with wave height (s)	
<b>Livestock</b>	Heads of cattle (total number of cattle head/town)	MAGRAMA (2016a)
	Goat cattle (number of cattle head/town)	
	Sheep cattle (number of cattle head/town)	
	Pig cattle (number of cattle head/town)	
	Other cattle (number of cattle head/town)	
<b>Purification rate and source discharges</b>	Purification rate (percentage of purified wastewater)	MAGRAMA (2016c) database
	Ravines or rivers	Measurement through a GIS system of data from Ecolevante (2006) and EcoMAG (2009)
	Distance to ravines or river (m)	
	Residual discharges	
	Distance to residual discharges (m)	
	All discharges (rivers, gullies and waste)	
Distance to any type of discharge (m)		
<b>Posidonia oceanica</b>	Presence of <i>Posidonia oceanica</i>	Measurement through a GIS system of data from Ecolevante (2006) and EcoMAG (2009)
	Meadow final depth (m)	
	Meadow medium depth (m)	
	Meadow initial depth (m)	
	Meadow width (m)	
	Stem height (cm)	Ecolevante (2006) and EcoMAG (2009) databases
Plant density (stems/m <sup>2</sup> )		

114

115 *Escherichia coli* concentrations in each of the beaches were obtained from the database published  
116 by Nayade (2016) for the surveys conducted between 2012 and 2016. The data for 2012-2015 were  
117 used for the model adjustment, while the data from 2015-2016 were used for validation. These data  
118 were processed according to Directive 2006/7/EC to obtain P95 values of *E. coli* in each of the  
119 studied beaches. For more information on sampling, cadence of data collection, detection methods,  
120 etc., see <http://nayade.msc.es/Splayas/home.html>.

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

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

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

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

### 147 **3.2. Mathematical modelling**

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

156 After the study of correlations, the selection of variables to be included in the different models was a  
157 function of:

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

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

168 The methodologies of Navarro-González and Villacampa (2012, 2013) are numerical methodologies  
169 that allow the generation of models to represent the relationship between independent variables  
170 and a dependent variable(s), from the interpolation defined in n-dimensional finite element model,  
171 which is generated from the experimental data. The interpolation function implies the use of some  
172 initial conditions, which in the defined methodology implies the coincidence between the values of  
173 the function in a finite number of points. As normally occurs when applying the finite element  
174 method, the model function is obtained in a finite set of points called nodes (Zienkiewicz *et al.*,  
175 1977). In the applied methodologies, an optimization problem based on the determination of the  
176 minimum of an error function, generically defined in a finite element model, was solved. To improve  
177 the speed of resolution when the number of variables used is high (as in the case of some of the  
178 models generated in this paper), the methodology developed by Navarro-González and Villacampa  
179 (2016) was used.

180 In both methodologies, the experimental data are normalized to the n-dimensional hyper-cube,  
181 given by  $\Omega = [0,1]^n$ . Each interval  $[0, 1]$  is divided into  $c$  subintervals ( $c$  is called the complexity of  
182 the model). A set of  $c^n$  elements and  $(c + 1)^n$  nodes is generated, where the relationship between  
183 the independent variables and the dependent variable(s) is calculated. For example, if we consider a  
184 3-dimensional geometric model with a complexity  $c = 4$ , the total number of elements is  $4^3 = 64$ . To  
185 determine the output data, the model uses an interpolation function. The minimized error depends  
186 on the methodology used. Thus, in Navarro-González and Villacampa (2012, 2013) the sum of the  
187 squared error (Equation 1) of the values obtained by the interpolation function at each point ( $z_j$ ) and  
188 the initial conditions ( $P_j$ ) is minimized. While in the methodology based on the Galerkin method  
189 (Navarro-González and Villacampa, 2016), the error ( $e(x)$ -the difference between the solution and  
190 its approximation) is minimized by zeroing the integral defined in Equation 2, where NP is the  
191 number of variables in the model,  $\vec{N}(P_j)$  is the interpolation function used to determine the value of  
192 the model at any point and  $W_j(x)$  is the selected weight function (collocation method, sub-domain  
193 method, Least Square Method, Galerkin method, method of moments). In order to select the  
194 complexity, the generation and validation data of the model are used. Thus, the lower complexity  
195 that offers better results is selected, in order not to overfit the model.

$$196 \text{ Error} = \sum_{j=1}^{NP} (\vec{N}(P_j)\vec{u} - z_j)^2 \quad (1)$$

$$197 \quad \int D^{e(x) \cdot W_j(x)} dx = 0 \quad (2)$$

198 The criterion for selecting the optimal model was, first, the  $R^2$  value. The coefficient of  
 199 determination ( $R^2$ ) allows us to measure the goodness of fit and decide whether the linear  
 200 adjustment performed is sufficient or should alternative models be sought. However, for nonlinear  
 201 numerical models (as in our case), the value of  $R^2$ , is a guideline, since a model with a low value of  $R^2$   
 202 can offer good results. Therefore, to determine the performance of the models and select the  
 203 optimal model, the following errors were used: absolute error (Equation 3); mean magnitude of the  
 204 relative error (Equation 4); and relative percentage error (Equation 5), which have been previously  
 205 used by other authors (Aragónés *et al.*, 2016b; Hashemi *et al.*, 2010; Liu *et al.*, 2012).

$$206 \quad e = |r_i - o_i| \quad (3)$$

$$207 \quad MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{r_i - o_i}{r_i} \right| \quad (4)$$

$$208 \quad \delta = \sqrt{\frac{\sum_{i=1}^n (r_i - o_i)^2}{(n-p) \frac{1}{n} \sum_{i=1}^n (r_i)^2}} \quad (5)$$

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

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

#### 215 4. Results

216 Results obtained from linear correlations between the analysed variables and *E. coli* concentrations  
 217 are shown in Table 2. From the table it can be seen that the sun hours, rainfall and goat cattle have a  
 218 greater direct influence on *E. coli*. However, correlation values were generally low, always lower  
 219 than 0.35. Furthermore, nine main components, which explain 81.6% of the variance, were obtained  
 220 from the PCA (see supplementary material 2). Among these components, the first three explain  
 221 more than 52% of the variance. The variables that are more related to the first component are  
 222 representative of the livestock, and it is observed that the temperature of the water and UV have  
 223 also significant weight. The second component are related to the *Posidonia oceanica* (stem height (-  
 224 0.705) and plant density (-0.791)). And in the main variables of the third component are the hours of  
 225 sun (-0.814) and the purification rate (0.877), which by their definition have no relation between  
 226 them.

227 **Table 2.** Study of correlations (r) between studied variables and *E. coli*.

Variables	Correlation (r)	Variables	Correlation (r)
Sun hours	-0.349	Distance to any type of discharge	-0.164
Rainfall	0.335	Width of meadow	-0.162
Goat cattle	0.308	Temperature	-0.148
Depth final meadow	-0.271	Density of beams	-0.139
Depth medium meadow	-0.268	Orientation	-0.134
Presence of <i>Posidonia oceanica</i>	-0.267	All discharges (rivers, gullies and waste)	0.128



Others cattle	-0.224	Sediment	-0.127
Population density	0.220	Distance to residual discharges	-0.122
Depth beginning of meadow	-0.207	Purification rate	0.088
UV	0.202	Wave period	-0.060
Heads of cattle (total number)	-0.194	Level of urbanization	-0.059
Ravines or rivers	0.177	Morphology	-0.056
Salinity	0.176	Sheep cattle	-0.045
Residual discharges	-0.175	Distance to ravines or river	-0.029
Wind	0.175	Population	0.017
Stem height	-0.172	H <sub>5,12</sub>	-0.004
Pig cattle	-0.165		

228

229 Following the criteria stated in section 3.2 for the selection of variables, more than 20 mathematical  
 230 models, using different combinations of the 33 studied variables, were generated to express the  
 231 relationship between the variables and the concentration of *E. coli* in bathing waters. Among the  
 232 models there were 6 that provided significant results and they are reproduced in Table 3.

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

6 Variables	8 variables	11 variables	11 variables_2	12 variables	13 variables
Sun hours	Sun hours	Sun hours	Sun hours	Sun hours	Sun hours
Rainfall	Rainfall	Rainfall	Rainfall	Rainfall	Rainfall
Goat cattle	Goat cattle	Goat cattle	Goat cattle	Goat cattle	Goat cattle
UV	UV	UV	UV	UV	UV
Population density	Population density	Population density	Population density	Population density	Population density
Presence of <i>Posidonia oceanica</i>	Presence of <i>Posidonia oceanica</i>	Presence of <i>Posidonia oceanica</i>	Presence of <i>Posidonia oceanica</i>	Presence of <i>Posidonia oceanica</i>	Presence of <i>Posidonia oceanica</i>
-	Level of urbanization	Level of urbanization	Level of urbanization	Level of urbanization	Level of urbanization
-	Sediment	Sediment	Sediment	Sediment	Sediment
-	-	Purification rate	Purification rate	Purification rate	Purification rate
-	-	Salinity	Salinity	Salinity	Salinity
-	-	Distance to ravines or rivers	Distance to any type of discharge	Distance to any type of discharge	Distance to any type of discharge
-	-	-	-	H <sub>5,12</sub>	H <sub>5,12</sub>
-	-	-	-	-	Period (T)

234

235 Fig. 2 shows the R<sup>2</sup> values for each of the generated models, with significant results. The values of R<sup>2</sup>  
 236 increase as the complexity of the model and the number of independent variables increase.  
 237 However, for more than 11 variables, the value of R<sup>2</sup> decreases slightly (12 variables model, R<sup>2</sup>=  
 238 0.775±0.019). Thus, for example, the model with six variables has an R<sup>2</sup> value of 0.458±0.037, and for  
 239 the 11 variables\_2 model is 0.780±0.057, but when the number of variables is increased to 13, the R<sup>2</sup>  
 240 decrease slightly (0.752±0.035).

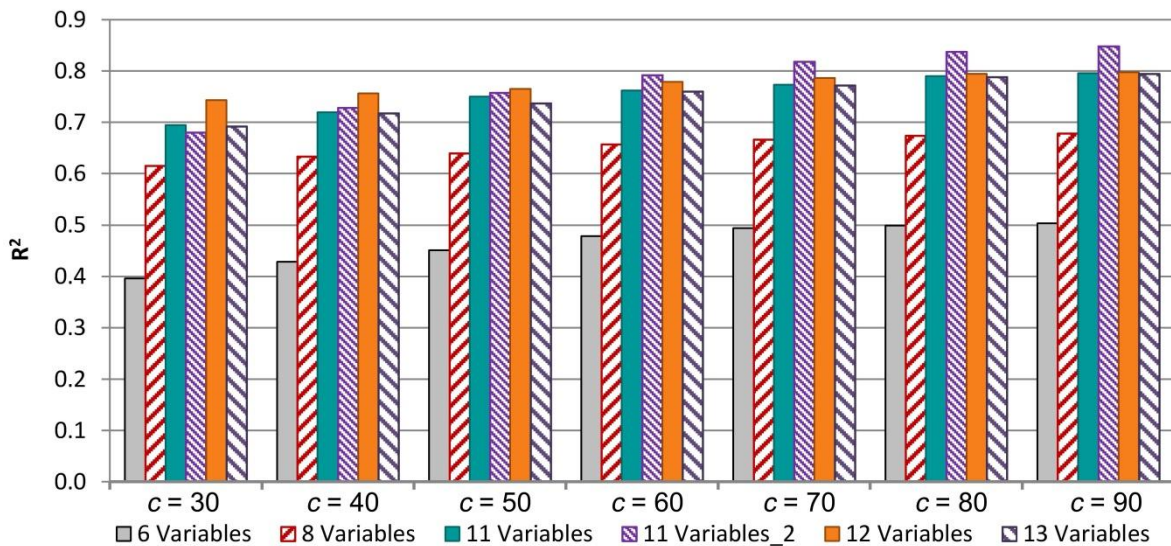


Fig. 2. R<sup>2</sup> values for each of the studied models.

241  
242

243 However, when the errors are analysed, a big difference is observed. Thus, Fig. 3 shows that the  
 244 model of eight variables improves by 29.8% the absolute error of the six variables model. When  
 245 adding two new variables (models with 11 variables) the mean absolute error decreased ( $13.1 \pm 1.9$   
 246 CFU/100 ml for 11 variables and  $12.8 \pm 2.7$  CFU/100 ml 11 variables\_2). If variables continued to be  
 247 added (12 variables) the error decreased to  $11.3 \pm 1.1$  CFU/100 ml. However, when the variables were  
 248 increased (13 variables) so did the error  $13.5 \pm 1.9$  CFU/100 ml. As observed, the error of the 13  
 249 variables model is similar to 11 variables model but with a greater standard deviation for each of the  
 250 studied complexities (2.02 versus 1.35 CFU/100 ml).

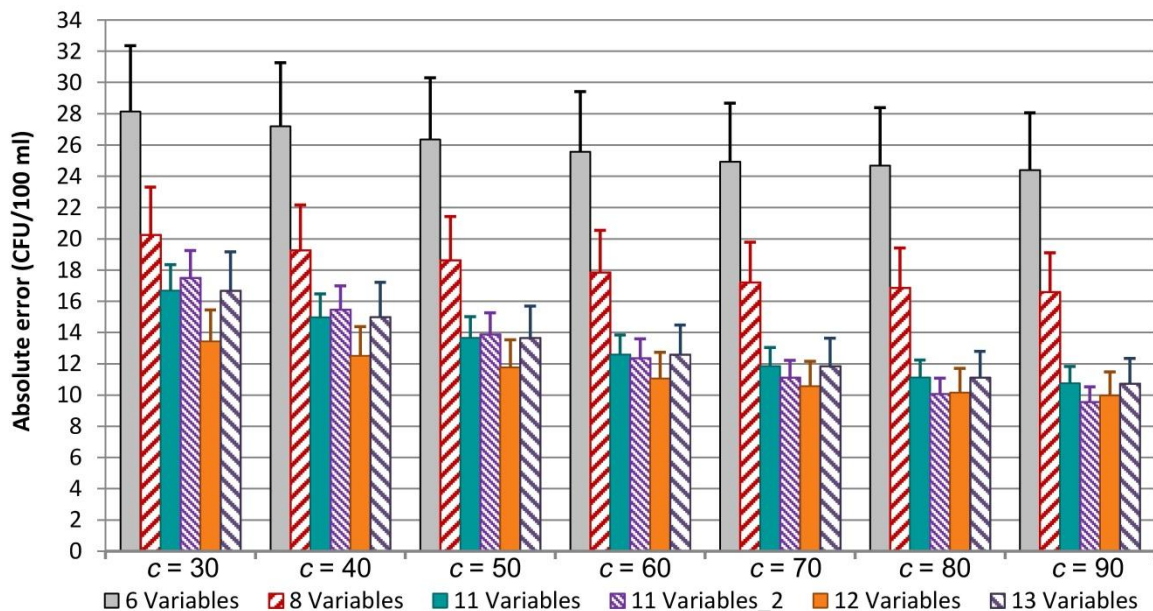
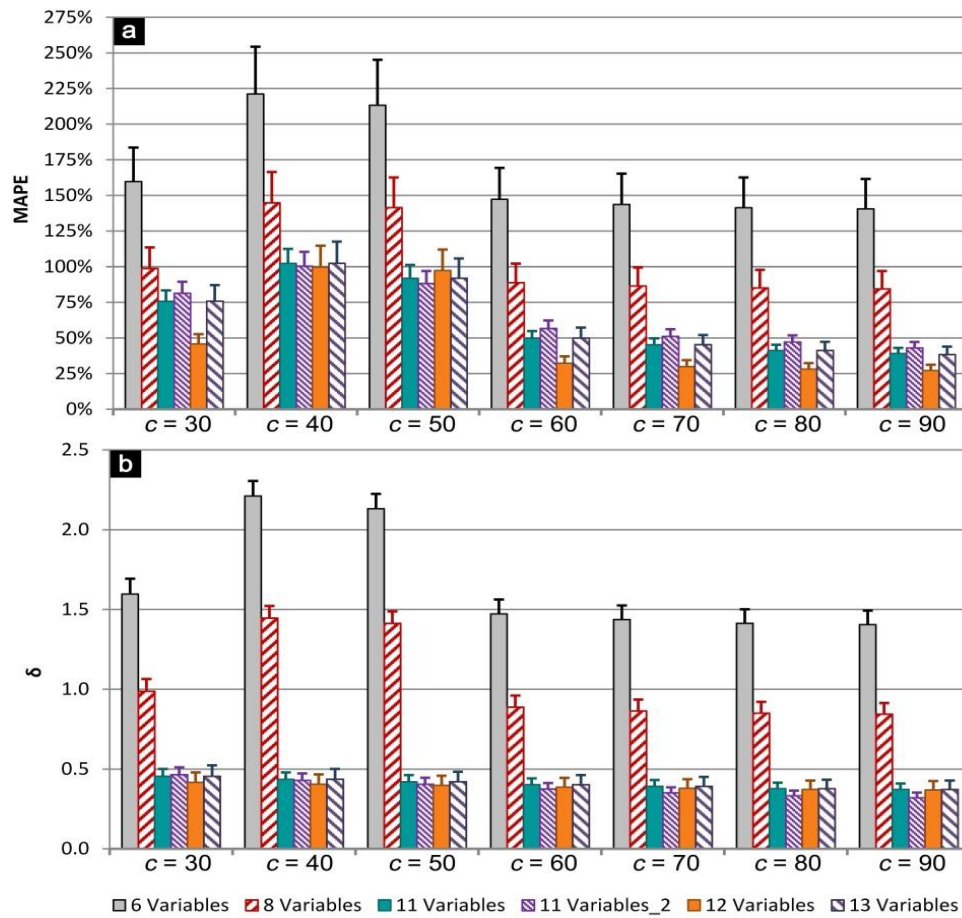


Fig. 3. Absolute error (CFU/100 ml) for each of the studied models.

251  
252

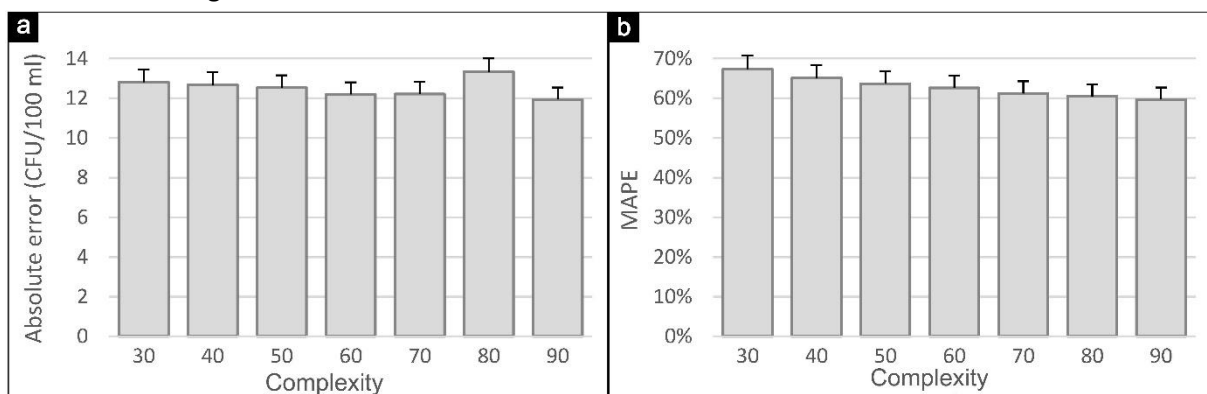
253 Regarding the MAPE (Fig. 4a) and the relative percentage error (Fig. 4b) something similar to what  
 254 happens with absolute error occurs. As the number of variables and the complexity of the model  
 255 increases, errors decrease, reaching the values indicated in the 12 variables model and the  
 256 complexity 90 of  $27.1 \pm 4.1\%$  and  $0.370 \pm 0.055$  for MAPE and relative percentage error, respectively.  
 257 However, when the number of variables increases to 13 variables, the mean error is very similar to

258 the 11 variables model but the standard deviation increases. For example, for complexity 90, the  
 259 MAPE of 13 variables model is  $38.3 \pm 5.7\%$  and the relative percentage error is  $0.372 \pm 0.056$ .

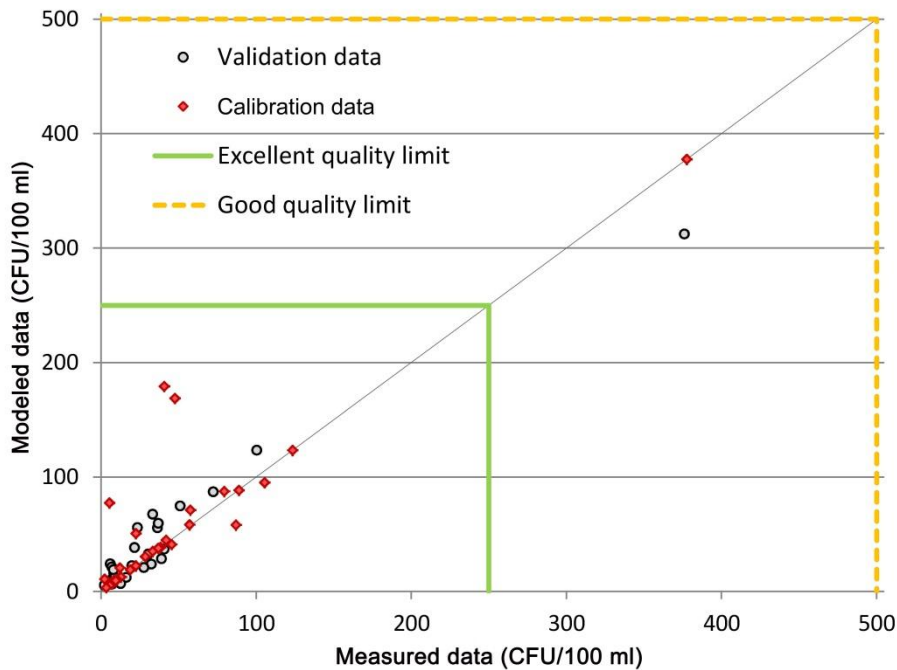


260  
 261 **Fig. 4. a) MAPE and b) relative percentage error, for each of the studied models.**

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



270  
 271 **Fig. 5. a) Absolute error and b) MAPE, for validation data.**



272  
273 Fig. 6. Measured and modeled data during the model (12 variables and complexity 70) calibration and  
274 validation, for the 30 beaches used for validation.

275 **5. Discussion**

276 Several studies have shown that there is a relationship between gastrointestinal symptoms and the  
277 quality of recreational waters, which is determined by measuring the number of bacteria (Prüss,  
278 1998). Therefore, given the popularity of the use of coastal waters for recreational purposes, quality  
279 minimums must be met (Sardá and Fluvía, 1999). In order to avoid endangering the health of users,  
280 regulators set limits on the maximum concentrations of faecal bacteria in the water. In Europe these  
281 values are described in Directive 2006/7/EC. To know the concentration of faecal bacteria during the  
282 bathing season, regulators carry out costly microbiological analyses once every 2 weeks. In this  
283 study, a model was generated to obtain the concentration of *E. coli* in coastal bathing waters, in  
284 order to reduce the number of microbiological analyses.

285 First, the bivariate correlations between the analysed variables and the concentration of *E. coli* were  
286 studied (Table 2). The variables with the highest direct correlation are: sun hours (-0.349),  
287 precipitation (0.335) and goat cattle (0.308), so these variables are in all models. To these three  
288 variables were added other variables following the criterion described in section 3.2. Thus, the first  
289 model that presented significant results was the 6 variables model (sun hours, rainfall, goat cattle,  
290 presence of *Posidonia oceanica*, population density and UV), with values of  $R^2$  between 0.396-0.504  
291 (Fig. 2), and average absolute error of 25.9 CFU/100 ml. From the PCA, is extracted that there are no  
292 strong relationships between the explanatory variables that have been used later to generate the  
293 models. It is observed that there are no correlation between variables that a priori can be thought  
294 that are possibly correlated to each other, as can be the temperature, the hours of sun and the  
295 ultraviolet radiation. Although, it is true that there is a certain relationship between ultraviolet  
296 radiation and temperature, neither of the two variables has been used together in the generated  
297 models.

298 The results of this model (6 variables) confirm the relationship, established by other authors,  
299 between these six variables and the concentration of *E. coli*. For example, according to Abdelzaher *et al.*  
300 *al.* (2010); Whitman *et al.* (2004); Zagarese *et al.* (1998) the concentration of *E. coli* decreases with  
301 UV, and increases with the low temperatures which is directly related to the hours of sunlight  
302 (Bathingwatercommittee, 2009; Bogosian *et al.*, 1996; Brettar and Höfle, 1992; Sampson *et al.*, 2006;  
303 Smith *et al.*, 1994). Other authors, such as Rijal *et al.* (2009) indicate the importance of the volume  
304 of precipitation. Higher precipitation influences *E. coli* concentration in the following ways: i) allows  
305 an increase in bacteria dilution, which could reduce the concentrations (Cho *et al.*, 2010); ii) modifies  
306 salinity conditions of water; iii) runoff waters clean the land surface and drag the pathogens toward  
307 the coast, increasing the bacterial concentration in coastal waters; and iv) Increases the flows of  
308 rivers, ravines, rainwater, which flow out to sea with all kinds of contaminants, such as animal  
309 defecations (Gibbs, 2001). This last point, could explain the high correlation obtained between the  
310 goat cattle and the *E. coli*, since in the studied area, goats usually freely graze on pastures (Meseguer  
311 and Espín, 2001), while the other livestock (bovine, porcine, etc.) are characterized by intensive,  
312 farms, and their excreta accumulate in the barn and are used as manure in agriculture (Ferrer *et al.*,  
313 2000). Meanwhile, Hammami *et al.* (2013) and Luzi *et al.* (2016) observed that *Posidonia oceanica*  
314 has an antibacterial function against *E. coli* bacteria.

315 Moreover, population density during the bathing season has a significant influence on bacterial  
316 concentration, due to the drastic increase in the number of users (Ariza *et al.*, 2010). Also, urban  
317 development in the beach environment generally worsens the water quality of the beach. Ariza *et al.*  
318 (2008) observed that urban sandy beaches are the most affected by bacterial contamination since  
319 they are more accessible and accommodate more bathers. In addition, several recent studies  
320 indicate that bacterial indices may be associated with sewer leakage (generally ubiquitous in urban  
321 areas) due to aging infrastructure (Sercu *et al.*, 2009). The type of sediment also influences the  
322 concentration of bacteria, because *E. coli* is able to reproduce in the sand if the necessary conditions  
323 of nutrients, predators and environmental conditions occur (Alm *et al.*, 2006; Yamahara *et al.*, 2007),  
324 where it can persist for longer and then be transferred to the sea. In addition, the smaller the  
325 sediment size, the greater the number of particles that can be suspended when the waves break,  
326 making it difficult to purify water by UV (Abdelzaher *et al.*, 2010; Haugland *et al.*, 2005; Salcedo *et al.*  
327 *al.*, 2002). The degree of urbanization and the sediment type has a significant influence on bacterial  
328 concentration, as confirmed by the results of the 8 variables model, which decreases the absolute  
329 error by 30%, although it is higher than 16 CFU/100 ml (Fig. 3).

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

342 the trapping of fertilizers and contaminants of the irrigation waters, as well as to the lack of  
343 regulation and control in the discharge of these waters into the sea.

344 The incident wave ( $H_{s, 12}$ ) and its related period are intimately linked to the discharges and their  
345 distance to the beach, since currents may move the discharges onshore or offshore. It has also been  
346 observed that, generally, beaches whose coasts are parallel to the wave front have a higher  
347 concentration of bacteria (Palazón *et al.*, 2017), perhaps because of the turbidity that is generated  
348 when the wave breaks. This explains the improvement that occurs in the modelling by including the  
349 wave height as input variable. Although the absolute error is similar to that of the 11 variables model  
350 (11.4 vs. 12.8 CFU/100 ml, Fig. 3), the MAPE is much lower (29.3% vs. 43.8%, Fig. 4a). However,  
351 including the period in the models does not improve the results, they are even slightly worse (11.35  
352 vs. 13.09 CFU/100 ml, Fig. 3).

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

361 Finally, the analysis of the models shows that there are two types of variables: i) variables directly  
362 related to humans or their activity (population density, livestock, level of urbanization and  
363 purification ratio); and ii) variables related to the environment (rainfall, UV, sunshine hours,  
364 *Posidonia oceanica*, sediment and salinity). Therefore, we can affirm that except for important  
365 modifications in the analysed variables, the concentrations of *E. coli* will remain more or less stable.  
366 In that case, the model can replace microbiological analysis, which could be performed only once  
367 during each bathing season (rather than every two weeks) in order to corroborate the model results.  
368 This study also shows that in order to further improve the results of the models, the effect of  
369 currents, tides, or sediment transport should be included in future studies.

## 370 **6. Conclusion**

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

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

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