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Hydro-epidemiological modelling of bacterial transport and decay in nearshore coastal waters

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Abstract

In recent years, society has become more aware and concerned with the environmental and human health impacts of population growth and urbanisation. In response, a number of legislative measures have been introduced within Europe (and globally), which have sparked much cross-disciplinary research aimed at predicting and quantifying these impacts, and suggesting mitigation measures.

In response to such measures this paper is focused on improving current understanding of, and simulating water quality, in the form of bacterial transport and decay, in the aquatic environment and particularly in macro-tidal environments. A number of 2D and 3D hydro-epidemiological models were developed using the TELEMAC suite to predict faecal bacterial levels for a data rich pilot site, namely Swansea Bay, located in the south west of the UK, where more than 7,000 FIO samples were taken and analysed over a two year period.

A comparison of 2D and 3D modelling approaches highlights the importance of accurately representing source momentum terms in hydro-epidemiological models. Improvements in 2D model bacterial concentration predictions were achieved by the application of a novel method for

24 representing beach sources within the nearshore zone of a macro-tidal environment. In addition,
25 the use of a depth-varying decay rate was found to enhance the prediction of Faecal Indicator
26 Organism concentrations in 3D models. Recommendations are made for the use of these novel
27 approaches in future modelling studies.

28

29 Keywords: Faecal Indicator Organisms (FIOs), bathing water quality, T90, decay rate, revised EU
30 Bathing Water Directive

31

32 **1 Introduction**

33 The health of nearshore coastal waters is a topic of great concern globally. As a result of population
34 growth and industrialisation, the number of polluted discharges into water bodies has increased
35 during the 20th and 21st centuries, with much detriment to the aquatic environment. Such
36 contamination has far reaching consequences, which include: human health impacts through
37 recreational activity (Weiskerger and Phanikumar, 2020) and the consumption of polluted food in
38 the form of shellfish, reduced tourism, and economic losses (DeFlorio-Barker et al. 2018; Bussi et
39 al. 2017; Given et al. 2006).

40

41 For example, domestic and international visitors to the coast contributed \$6 billion to the UK
42 economy in 2017 (BBC, 2017; Visit Britain, 2017). In a recent study, the Scottish Government
43 (2018) predicted a loss of \$3 million per year should bathing water quality not be maintained at
44 an acceptable level at popular beaches. Another financial incentive is the healthcare savings
45 associated with reduced exposure of beach goers to contaminated water (Given et al., 2006). For
46 example, DeFlorio-Barker et al. (2018) estimated that recreational waterborne illnesses cost the
47 US economy \$2.2 to \$3.7 billion every year. It is therefore important to address these issues by
48 determining the primary sources of pollution at any one location, developing an understanding of
49 the mechanisms which lead to adverse water quality, beach closure, and implementing mitigation
50 strategies.

51 To ensure protecting human health as highlighted above, legislative measures have been
52 introduced with regard to bathing water quality. The existing legislation applicable in the EU is the
53 revised Bathing Waters Directive (rBWD) (European Parliament, 2006) which ensures the
54 monitoring of water quality and defines acceptable standards, based on human health risk and
55 following guidelines released by the World Health Organisation on safe standards for recreational
56 waters (World Health Organization, 2003). The revised Bathing Waters Directive was introduced
57 by the European Parliament in 2007 requiring Member States to ensure all bathing waters were
58 of 'sufficient' quality by the close of the 2015 bathing season (European Parliament, 2006).
59 Compliance criteria are based on the monitored concentration of two Faecal Indicator Organisms
60 (FIOs); *Intestinal enterococci* and *Escherichia coli* (*E. coli*) in colony forming units per 100ml
61 (cfu/100ml). The directive requires the concentration of these organisms to be monitored over
62 consecutive bathing seasons (May to September), in accordance with a sampling calendar. Based
63 on the Directive 2006/7/EC of the European Parliament, samples showing abnormally elevated
64 concentrations, caused as a result of short-term pollution incidents, or contamination attributable
65 to a cause, expected to last less than 72 hours, such as high level of pollution following a heavy
66 rainfall may be disregarded and retaken (European Environment Agency, 2005). Efforts must also
67 be made to reduce the risk of bather exposure to contaminants in addition to providing regular
68 information on bathing water quality. Therefore, the directive requires the public to be made
69 aware of short-term pollution incidences in advance, in order for these events to be disregarded,
70 thereby making public health a key driver for prediction.

71

72 Due to the time lag between the collection and assessment of individual samples, monitoring in
73 this manner is not a practical way of providing rapid public feedback to prevent exposure (Feng
74 et al., 2015). To enable accurate and fast dissemination of information it is therefore in the interest
75 of the governing authority to develop predictive tools to provide water quality forecasts and
76 warning systems (Bedri et al., 2014, 2016; Chen and Liu, 2017; DHI, 2017a, b; Weiskerger and
77 Phanikumar, 2020). Not only would this comply with the rBWD but it could enable the

78 identification, reduction and removal of major pollution sources, increasing the likelihood of a
79 bathing water being assigned Blue Flag status (Bedri et al., 2015; Lea, 1996).

80 There are two main approaches to the development of predictive tools to provide water quality
81 forecasts and warning systems: data driven modelling based on extensive field measurements,
82 and process-based hydro-epidemiological models. Herein the latter approach is used, with the aim
83 being to improve our understanding of fundamental processes affecting the fate and transport of
84 bacterial pollution, in order to enhance the management of bacterial sources, development of
85 predictive tools, and assessing beach monitoring and management practices.

86

87 This study examines and investigates the use of two novel techniques, as well as the methods
88 which have been used to date for the prediction of bacterial decay in 2D and 3D model frameworks,
89 using a data rich macro-tidal bay as a study site.

90

91 **2 Methodology**

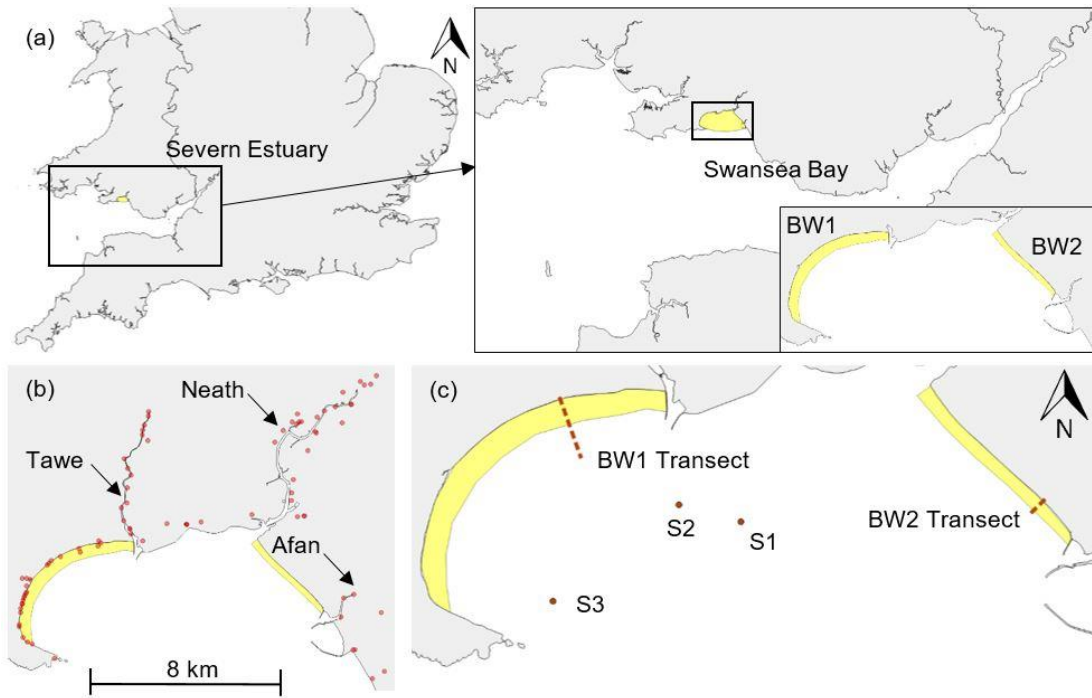
92 **2.1 Study Site**

93 Swansea Bay is situated on the north shoreline of the Bristol Channel, located in the south west of
94 the UK, and is a popular location among tourists and the local community (see Figure 1). The Bay
95 contains two bathing water sites: Swansea Bay and Aberafan, both of which received a 'good'
96 rating in the most recent bathing water assessment period. Swansea Bay was chosen for this study
97 due to the tidal nature of the Bay, the number of FIO point sources and, more importantly, a large
98 quantity of measured FIO data, where more than 7,000 FIO samples were taken and analysed over
99 a two-year period.

100

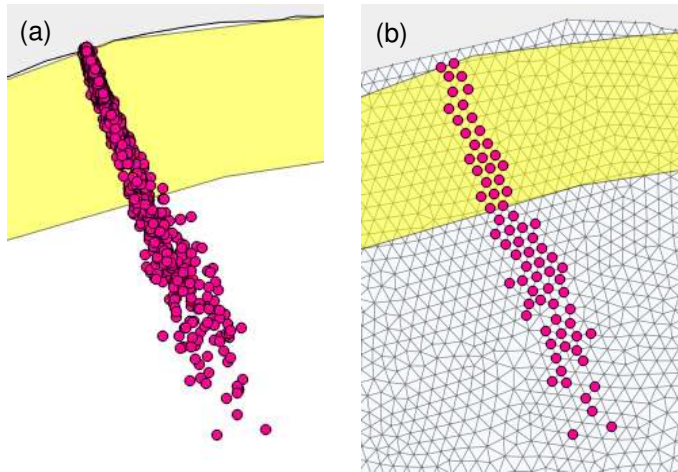
101 The Bay is subject to 85 different inputs (see Figure 1b) including three main rivers discharging
102 into the Bay: The River Tawe, River Neath and River Afan. There is a semi submerged barrage
103 located on the River Tawe, which only overtops at tides over 3.05 m above Ordinance Datum.
104 However, the River Neath and River Afan are tidal up to about 10 km and 1 km upstream from

105 the coast, respectively. Primary surface water and sewage discharges were recorded at 15-
106 minute intervals over the 2011 bathing season (May - September) and October - November 2012
107 for the Smart Coasts project (Aberystwyth University and University College Dublin, 2018) as
108 shown in Figure 1c, although data were unavailable for Combined Sewer Overflow (CSO) spills.
109 The rBWD requires samples to be taken at a minimum depth of 0.5 m (Bedri et al., 2016;
110 Bomminayuni, 2015) at the Designated Sampling Point (DSP) for each bathing water site.
111 However, the tidal range in the Bay exceeds 10 m and the tidal flats are exposed up to a distance
112 of 1500 m from shore during high spring tides. This prevents readings being taken at each
113 bathing water site at only one location for the rBWD. Therefore, the water quality at Swansea
114 Bay and Aberafan were monitored along BW1 and BW2 transects respectively as shown in
115 Figure 1c. Figure 1c also depicts the locations of offshore sampling points used for model
116 validation and calibration. The variability in the sampling location is shown in Figure 2 which
117 presents the sampling points along BW1, recorded throughout the 2011 bathing season at 30-
118 minute intervals from 07:00 to 16:00.



119

120 *Figure 1: (a) Location of bathing waters within Swansea Bay, Severn Estuary, UK: BW1 - Swansea*
 121 *Bay, BW2 - Aberafan (b) Location of FIO inputs (c) Location of transects (dashed lines) and*
 122 *offshore monitoring points (dots)*



123

124 *Figure 2: FIO sampling locations throughout the 2011 bathing season (a) [Aberystwyth University*
 125 *and University College Dublin, 2018], and the respective 2D mesh nodes (b)*

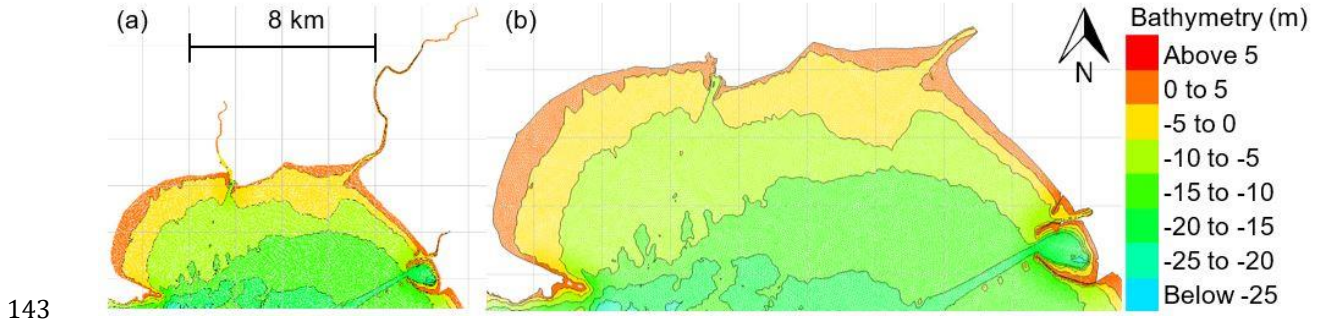
126 2.2 Hydrodynamic models

127 The open-source models TELEMAC-2D and TELEMAC-3D (Galland et al., 1991) were chosen for
 128 this study to compliment previous research applications in the field of hydro-epidemiological

129 engineering (Abu Bakar et al., 2017a, Bedri et al., 2013; Kopmann and Markofsky, 2000).
130 Developed by Electricité de France, the models solve the Navier-Stokes Equations over an
131 unstructured finite element grid (Hervouet, 2007). Further details are provided in the next
132 section.

133

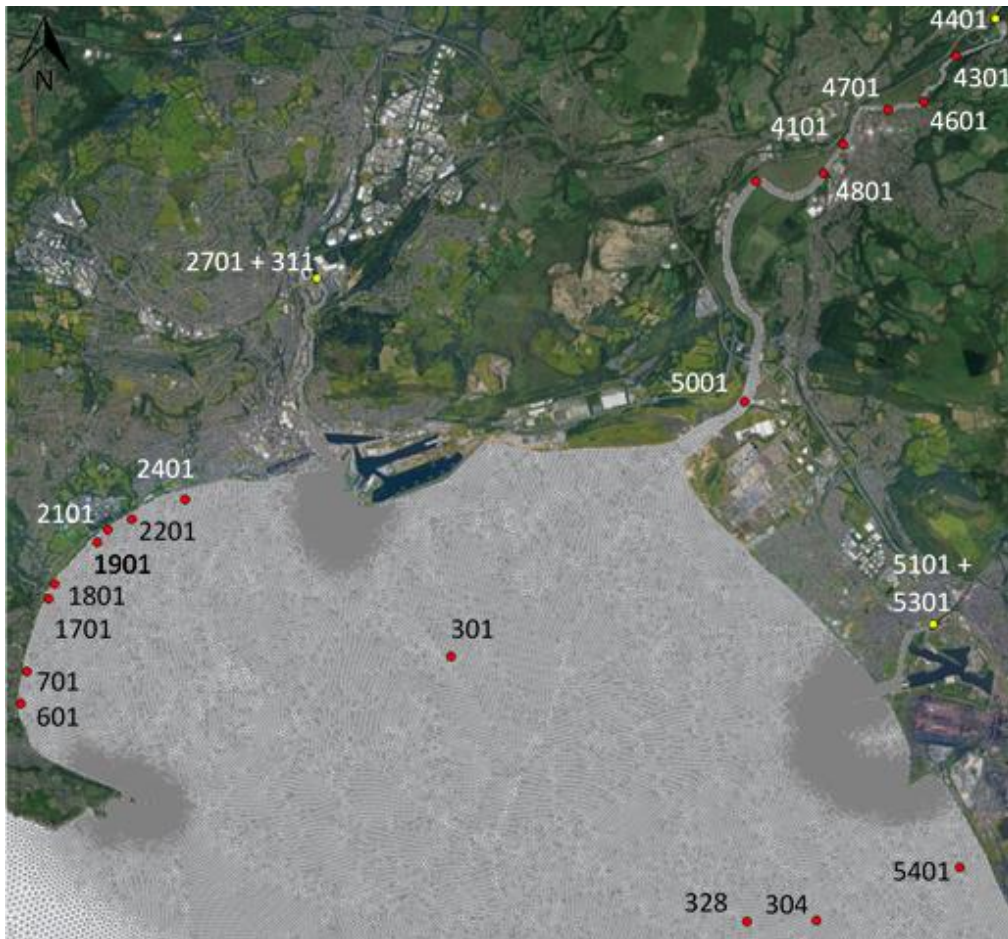
134 Two computational meshes of the Bristol Channel and Swansea Bay were created, one each for the
135 2D and 3D models. The 3D domain comprised a 2D mesh repeated over 5 uniformly distributed
136 sigma layers and extends over the same area apart from the rivers in Swansea Bay, as shown in
137 Figure 3. To remove the need for coupling with a 1D model, the 2D model was extended up the
138 River Tawe and to the tidal limits of the rivers Afan and Neath. However, these reaches were
139 excluded from the 3D model to reduce the computational time and unnecessary vertical
140 refinement in regions where 3D effects were of limited concern. Note that at the time of writing,
141 coupling between the latest release of TELEMAC-3D (v7p3r2), and the 1D river model TELEMAC-
142 MASCARET, was not possible.



144 *Figure 3: Extent of 2D (a) and 3D (b) unstructured computational meshes of Swansea Bay.*

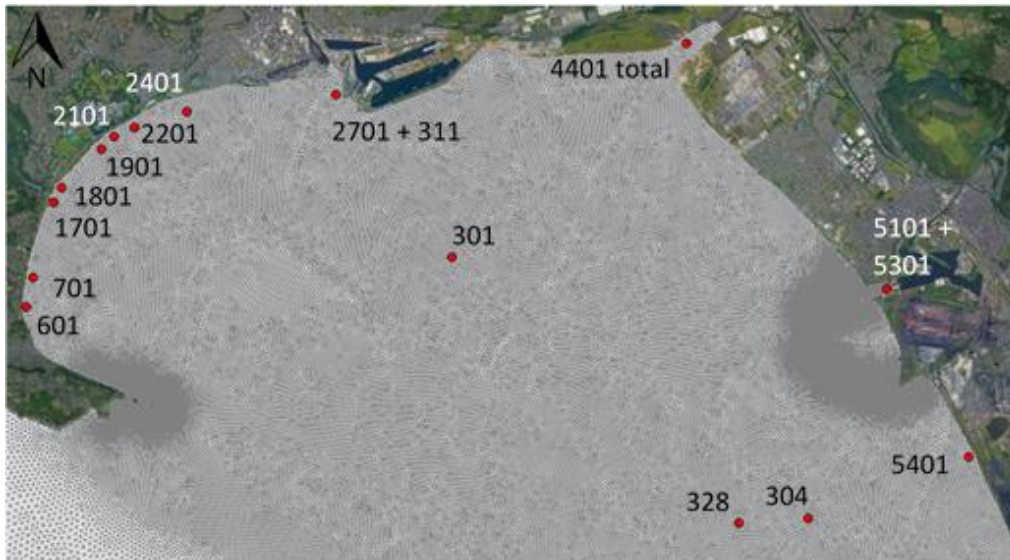
145 *Bathymetry relative to mean sea level (MSL)*

146 Bacterial sources were included as a concentration (cfu/100 ml) time series. Source locations
147 within each domain are shown in Figures 4 and 5, respectively. In the 3D model, the bacterial
148 source inputs distributed within each reach were combined into a single source point, whereas
149 those in the 2D model retained their true position.



150

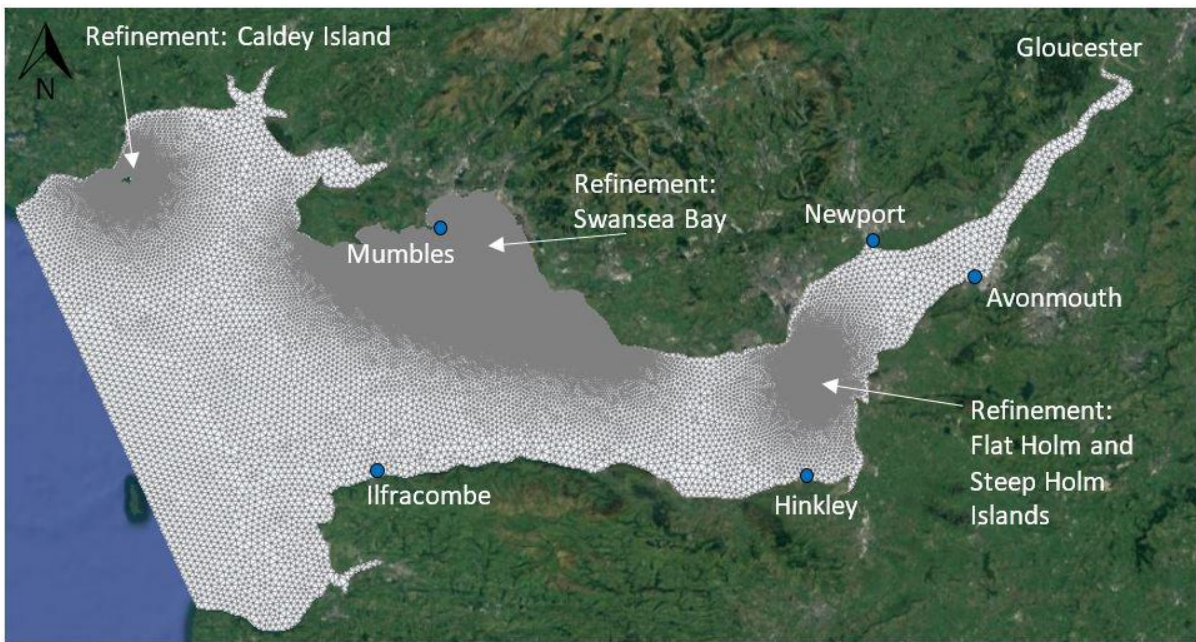
151 *Figure 4: Primary input locations of bacterial sources within the 2D model domain of Swansea Bay*
 152 *– year 2012; point sources (red dots) and boundary conditions (yellow dots) with the relative ID*
 153 *No.*



154

155 *Figure 5: Primary input locations of bacterial sources within the 3D domain – year 2012; point*
 156 *sources (red dots) with the relative ID No.*

157 Both meshes extend from the River Severn tidal limit close to Gloucester to the outer Bristol
 158 Channel close to Lundy Island, as shown in Figure 6, in order to capture the hydrodynamics of the
 159 Severn Estuary and Bristol Channel as has been widely used in previous studies (Ahmadian et al,
 160 2014, Coz et al., 2019 and Guo et al., 2020). Bathymetry data was obtained from EDINA Digimap,
 161 relative to chart datum (CD), at a 30 m grid resolution (The University of Edinburgh, 2016a, b). An
 162 open boundary with a tidal water level series is imposed along the westward edge of the domain
 163 where the Bristol Channel meets the Celtic Sea.



164

165

166 *Figure 6: Extent of the unstructured computational mesh within the Bristol Channel and Severn*
 167 *Estuary, showing the water level monitoring locations (blue dots)*

168 Stapleton et al. (2007a) found that a coarse grid (600 m by 600 m), was incapable of capturing
 169 localised features, such as pollutant plume shapes. The minimum grid size in the bay was limited
 170 to 30 m to capture bathymetric features as closely as possible. Therefore, the mesh size in Swansea
 171 Bay was determined based on sensitivity analysis of the different meshes. Two computational
 172 meshes were developed; using a 25 m and 50 m mesh in Swansea Bay, and increasing at a uniform
 173 rate of 1.2 to 1,000 m in the outer Bristol Channel and the Severn Estuary. From the grid
 174 dependence model tests the model results were found to be insensitive to the mesh size for the
 175 grid resolutions studies and a 50 m grid size was therefore used within Swansea Bay to increase
 176 computational efficiency. Further refinements of the grid size to 10m were used at various
 177 locations within the Bay to capture shoreline complexities. The 2D mesh contained 142,533 nodes
 178 and 281,440 elements, the 3D mesh contained 133,341 nodes and 264,237 elements, repeated
 179 over 5 sigma layers giving 666,705 nodes and 1,059,648 elements in total. As for similar studies
 180 the Smagorinski turbulence closure model was used in the horizontal (Bedri et al., 2015, 2013,
 181 Abu Bakar et al., 2017b, Guo et al., 2020) and vertical directions.

182

183 **2.3 Fate and transport of bacteria: governing equations**

184 Bacteria was simulated in TELEMAC as a non-conservative passive numerical tracer, represented
185 by the advection-diffusion equation. Herein this is referred to as the tracer equation, written in 3D
186 as shown in Equation 1 (Hervouet, 2007):

187

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} + W \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left(\nu_T \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(\nu_T \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(\nu_T \frac{\partial C}{\partial z} \right) + S_C \quad 1$$

188

189 where C is the tracer concentration (units depend on the tracer but for bacteria it is cfu/100ml), t
190 is time (s), h is the water depth (m), U , V and W are layer averaged velocities (m/s) in the x , y and
191 z directions respectively, ν_T is the diffusion coefficient (m²/s). S_C is the source or sink term,
192 including both explicit and implicit terms. Bacterial decay is governed by the first order decay
193 rate k which is commonly written as shown in Equation 2 (Chapra, 1997; Thomann and Mueller,
194 1987).

195

$$\frac{\partial C}{\partial t} = -kC \quad 2$$

196

197 The decay rate k (1/d) is transposed into a T_{90} value, i.e. the time required for the concentration
198 to reduce by 90% (Guillaud et al., 1997), as shown in Equation 3. This is traditionally required as
199 a user input value in TELEMAC and many other models.

200

$$T_{90} = \frac{2.303}{k} \quad 3$$

201

202 Multiple methods exist to determine the T_{90} value, and which have been applied in a number of
 203 studies (Chapra, 1997; Droste, 1997; Mancini, 1978; Stapleton et al., 2007a; Ahmadian et al., 2010;
 204 de Brauwere et al., 2011; Bedri et al., 2013; Boye et al., 2015; Huang et al., 2015; Abu Bakar et al.,
 205 2017b). Two methods have been implemented in this paper: a pre-defined constant decay rate,
 206 and that proposed by Stapleton et al (2007a). The widely used approach proposed by Mancini
 207 (1978) was also used within the study but is not described herein due to its exclusion of sediment
 208 effects and the inclusion of non-site-specific data. For further information, see King (2019).

209

210 Stapleton et al. (2007a) carried out a study on water samples taken from the Bristol Channel and
 211 Severn Estuary to determine the impact of light intensity and turbidity on bacterial decay. As a
 212 result of laboratory experiments, the T_{90} decay rate for Enterococci was found to follow Equations
 213 4 to 8:

214

$$T_{90} = T_{90_2} + (T_{90_1} - T_{90_{*1}}) \quad 4$$

215

$$T_{90_1} = \frac{\ln 10}{K_B * 60 * I} \quad 5$$

216

$$T_{90_{*1}} = \frac{\ln 10}{K_B * 60 * I^{exp}} \quad 6$$

217

$$\text{Log}T_{90_2} = (0.0047 * \text{Turbidity}) + 0.677 \quad 7$$

218

$$\text{Turbidity} = 139.479 * \text{Log}(SS) - 244.736 \pm 32.678 \quad 8$$

219

220

221 where I is the sunlight intensity (W/m^2), I^{exp} is the fixed irradiance for the experiments (26,014
222 W/m^2), T_{90*1} is the sunlight dependent *Enterococci* mortality rate, T_{901} is the *Enterococci* mortality
223 rate obtained from laboratory experiments, T_{902} is the turbidity related *Enterococci* mortality rate
224 and $K_B = 1.1 \times 10^{-5}$ and SS is the suspended sediment concentration (mg/l). While Stapleton et al.
225 (2007a) only investigated the decay of *Enterococci*, the value for *E. coli* can be calculated using an
226 appropriate magnitude of K_B ($K_B = 1.3 \times 10^{-5}$) (Alkan et al. 1995).

227

228 **2.4 Model refinements**

229 **2.4.1 Depth-varying decay rate**

230 Bedri et al. (2013) published the first attempt at including a spatially and temporally variant decay
231 rate within TELEMAC-3D, using the decay formula proposed by Mancini (1978), but neglected the
232 ability of a 3D model to incorporate light attenuation throughout the water column. The decay rate
233 was calculated using Equations 9 and 10 (Bedri et al., 2013):

234

$$k_i = \alpha \bar{I} \quad 9$$

235

$$\bar{I} = \frac{I_a}{k_e H} (1 - e^{-k_e H}) \quad 10$$

236

237

238 where H is the water depth (m), I_a is the average daily light intensity (langleys/h), \bar{I} is the depth
239 averaged light intensity, α as a proportionality constant and k_e is the light attenuation coefficient
240 ($1/m$). Equation 10 is an integration of the Beer-Lambert law which, over the fully mixed water
241 depth (Xu et al., 2002; Chapra, 1997), can be expressed as:

242

$$I(z) = I_0 e^{-k_e H} \quad 11$$

243

244 where I_0 is the surface light intensity. The light attenuation coefficient k_e (1/m) may be calculated
 245 using (Chapra, 1997):

246

$$k_e = 0.55 SS \quad 12$$

247

248 where SS is the suspended solids concentration (mg/l). For a finite element model, such as
 249 TELEMAC, the governing equations are solved at each node and Equation 11 can be used without
 250 integration, such that the irradiance induced decay rate at depth is given by Equation 13 (Chapra,
 251 1997):

252

$$k_i(z) = \alpha I(z) \quad 13$$

253

254 where the light penetration at depth is given as a function of z , i.e. $I(z)$, and where this function is
 255 calculated using the Beer-Lambert law (see Equation 11). Experimental studies have confirmed
 256 this reduction in the decay rate at increasing depths below the water surface (Mattioli et al., 2017).

257 For completeness and to assist future studies a comparison is made with the application of
 258 Equation 11 in a finite volume model: the average light penetrating over each layer would be used.

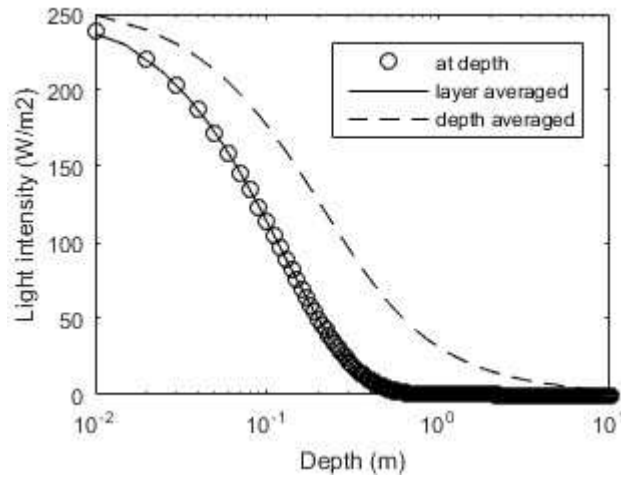
259 This can be calculated using the layer averaged Beer-Lambert law and using the mean value
 260 theorem for integrals:

261

$$\bar{I}_{layer} = \frac{\alpha I_0}{k_e (z_{bottom} - z_{top})} (e^{-k_e z_{top}} - e^{-k_e z_{bottom}}) \quad 14$$

262

263 where z_{bottom} and z_{top} , are the elevations at the bottom and top of the horizontal layer respectively.
264 Figure 7 presents depth-irradiance curves calculated using Equations 10, 11 and 14. Equations 11
265 and 14 exhibit a comparable reduction in light intensity with depth, whereas the rate of reduction
266 is less when using Equation 10 (i.e. a depth averaged representation). Since TELEMAC is a finite
267 element model, Equation 11 was used in this study.



268

269 *Figure 7: Comparison between irradiance at depth, calculated using: Equations 10 (depth*
270 *averaged), 11 (at depth), 14 (layer averaged) and k_e calculated using Equation 12 where $SS =$*
271 *84.82 mg/l*

272 2.4.2 Representation of beach sources

273 In modelling studies to date, bacterial sources such as CSOs and outfalls have been represented at
274 a single point source within numerical models. However, when the grid size is too coarse, a source
275 is distributed over a disproportionately large area and the local bathymetric features, such as that
276 shown in Figure 8, are not captured accurately.

277 Furthermore, in models such as TELEMAC, where the minimum permissible water depth is 0 m,
278 when these sources are released within shallow gradient regions the contaminated water spreads
279 over a large area in a thin film, as shown in Figure 9 (i.e. of depth less than 1 cm, up to 1×10^{-5} m).
280 For further details see King (2019).

281

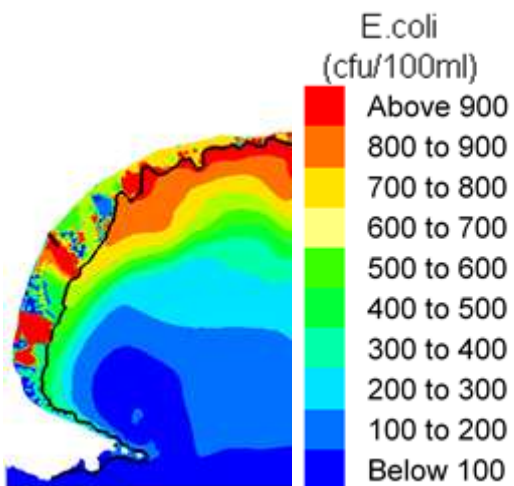
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283



284

285 *Figure 8: Stream track of beach source, South Wales, UK*

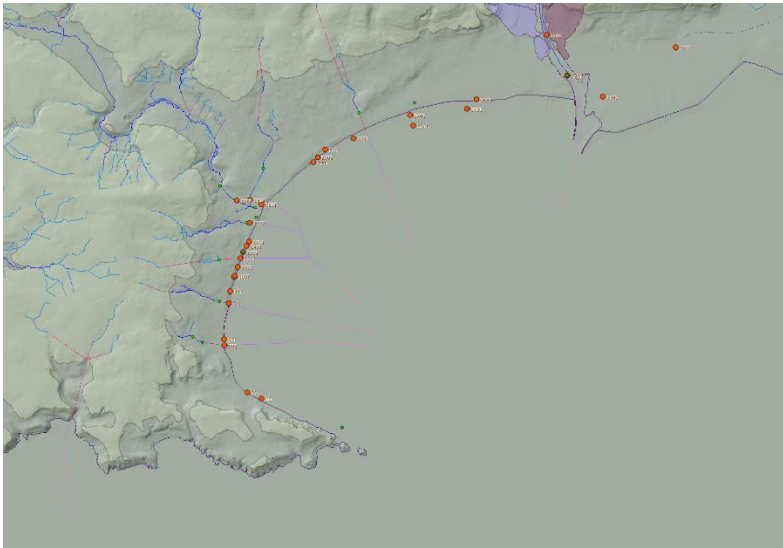


286

287 *Figure 9: Depth averaged E.coli concentration in Swansea Bay at mid-tide; black line indicates a*
288 *depth of 0.05m (i.e. the waterline)*

289 While inaccurate, this is necessary to ensure mass conservation. In reality, these inputs form small
290 streams in the beach sand (as illustrated in Figure 8), which run from the source point to the tide
291 line. These streams can run for up to a kilometre, from the sea defence wall to the tide line, at low
292 spring tide for this case study site. The major streams at Swansea Bay were tracked by staff at
293 Natural Resources Wales and Swansea City Council for this research study and as a part of Smart

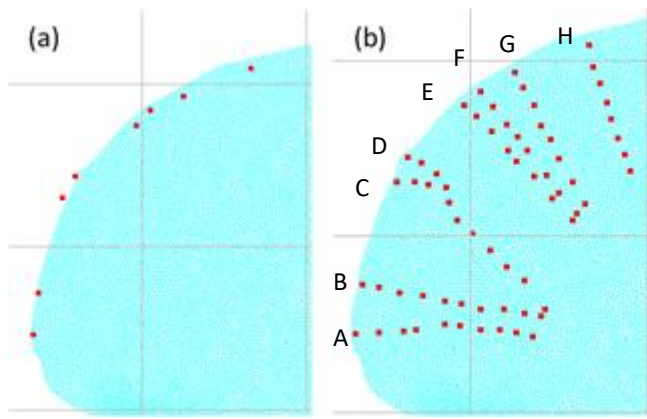
294 Coast project (Aberystwyth University and University College Dublin, 2018). The path of these
295 streams can be seen in Figure 10.



296

297 *Figure 10: Stream tracks of beach sources along Swansea Bay; purple lines and red dots respectively*
298 *(Aberystwyth University and University College Dublin, 2018)*

299 From Figure 10 it is clear that including sources at high water will not represent what happens in
300 the field and will cause inaccuracy in the predictions. The method proposed herein implements a
301 mobile source point which tracks the waterfront along the stream path and activates releases
302 based on the depth field. To achieve this, each source point is treated as a transect running from
303 the sea wall to the low water line based on the field tracking of that stream. Each transect is
304 represented by multiple source points, which discharge the same volume of water and
305 concentration of bacteria. The source release location is changeable to ensure release is always at
306 a point below the water line, mimicking transport within a stream. To ensure mass conservation,
307 modifications to the TELEMAC source code only permit one point to discharge per time step, i.e.
308 that which is closest to, and below, the waterline. Figure 11 shows the multiple source points
309 which were used along the transects for Swansea Bay. Up to 10 source points were selected on
310 each transect in this study as can be seen in the figure. However, more source points can be
311 considered if the path of the streams are more complicated.

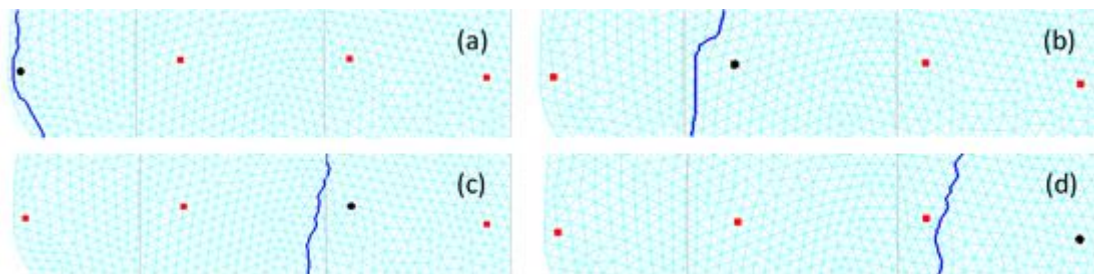


312

313 *Figure 11: Static source points at the outlet location and respective source transects along Swansea*
 314 *Bay beach; (a) and (b) respectively*

315 An illustration of this source representation for release at four different tidal phases is shown in
 316 Figure 12a to d. It can be seen as the tide recedes the 0.05 m depth threshold is activated at
 317 different source points along the transect (black dot). The source points along each transect were
 318 processed by multiple CPUs in parallel and the code was modified to implement this. Further
 319 information on the implementation of this method when using parallel computing methods can be
 320 found in King (2019). A similar approach was used by Feng et al. (2015), who developed a
 321 microbial transport model accounting for loading from beach sand and storm water run-off at a
 322 beach in Florida, U.S. However, the model was reduced to a 1D case for a single lumped source,
 323 and solved using the finite difference method. The grid followed a transect perpendicular to the
 324 straight uniform shoreline, which was assumed to be representative of the beach.

325



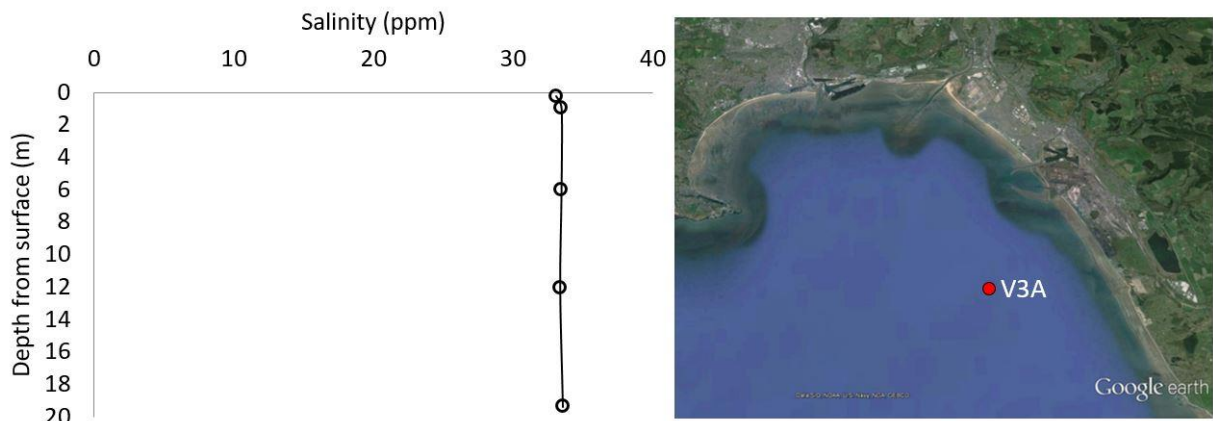
326

327 *Figure 12: Illustration of improved source representation at four different tidal phases for transect*
 328 *A in Figure 11; blue line = threshold depth (0.05 m) which retreats seaward (right) from figure a*
 329 *to d, red squares = transect points, black circle*

330

331 2.4.3 Parameter selection

332 Swansea Bay is well mixed (Ahmadian et al., 2013) with variations in temperature and salinity
333 being shown in Figure 13. As variations through the water column are negligible they were not
334 considered herein. Typically, in such environments a 2D modelling approach would be adopted,
335 thus making it an ideal environment to study the difference between using depth-averaged and
336 depth-varying approaches to calculate bacterial decay due to light intensity. Water temperature
337 and salinity were set at 15°C and 32 ppt respectively to match values used in previous studies
338 (Aberystwyth University and University College Dublin, 2018; White et al., 2014).

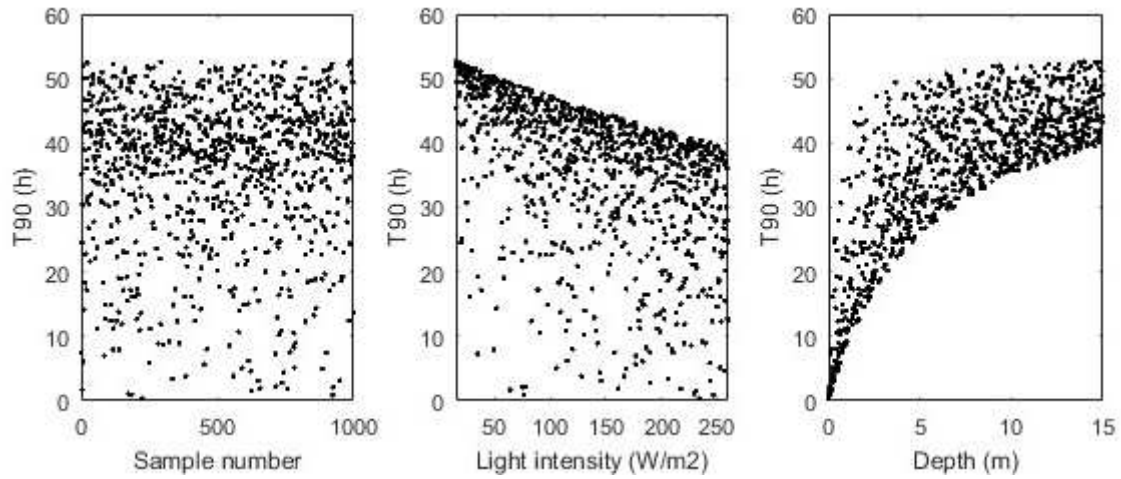


339

340 *Figure 13: Typical vertical salinity profile in Swansea Bay (location V3A; Ahmadian et al., 2013)*

341 The interaction between suspended sediment levels and FIOs has been studied previously and its
342 importance highlighted (Haung et al., 2015 and 2018, Ahmadian et al., 2010, Yang et al., 2008).
343 Since this study was mainly focused on implementation of the decay rate in the absence of
344 sediment data, sediment modelling was not considered as a part of this study. While surveys have
345 shown variations in suspended sediment concentrations throughout the water column, data are
346 sparse and a constant value of 84.82mg/l was assumed, based on measurements taken nearby at
347 Langland Bay and Porthcawl (Stapleton et al., 2007b). Based on this assumption Equations 4 to 8
348 are considered a function of light intensity and water depth. The relationship between the T_{90}
349 value and these variables is shown in Figure 14, using Latin hypercube sensitivity analysis (Iman,
350 2008; Stein, 1987). The water depth, which varied up to the maximum natural (i.e. not dredged)

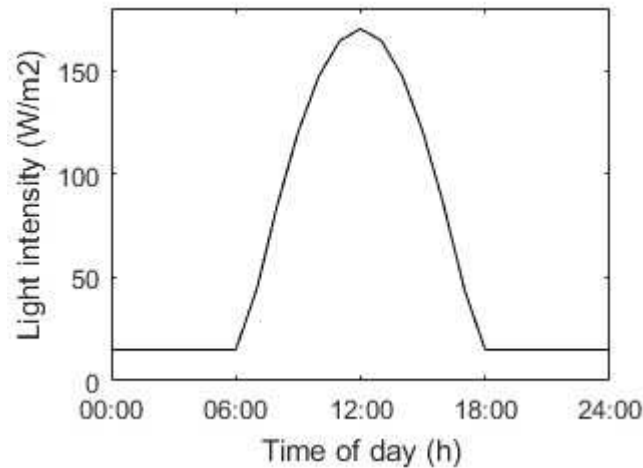
351 water depth in Swansea Bay and irradiance varied over the feasible parameter range from the
352 reviewed literature (Stapleton et al., 2007a) and site measurements (Aberystwyth University and
353 University College Dublin, 2018).



354

355 *Figure 14: Latin hypercube sensitivity analysis of decay rate based on depth and irradiance*
356 *variations with suspended solid concentrations, salinity and temperature being considered*
357 *constant*

358 Data recorded over the 2012 simulation period shows an average daily maximum of 170 W/m².
359 This fits within the 0 to 260 W/m² range of light intensity reported by Stapleton et al. (2007a). A
360 sine function, covering the range 0 to pi, was used to represent the variation in light intensity over
361 daylight hours (06:00 to 18:00), as proposed by Boye et al. (2015) and as shown in Figure 15.
362 Night-time values were recorded at 0.15 W/m². However, a lower limit of 15 W/m² was placed on
363 this value to prevent the T₉₀ value tending towards infinity as depth and solar intensity
364 approached zero.



365

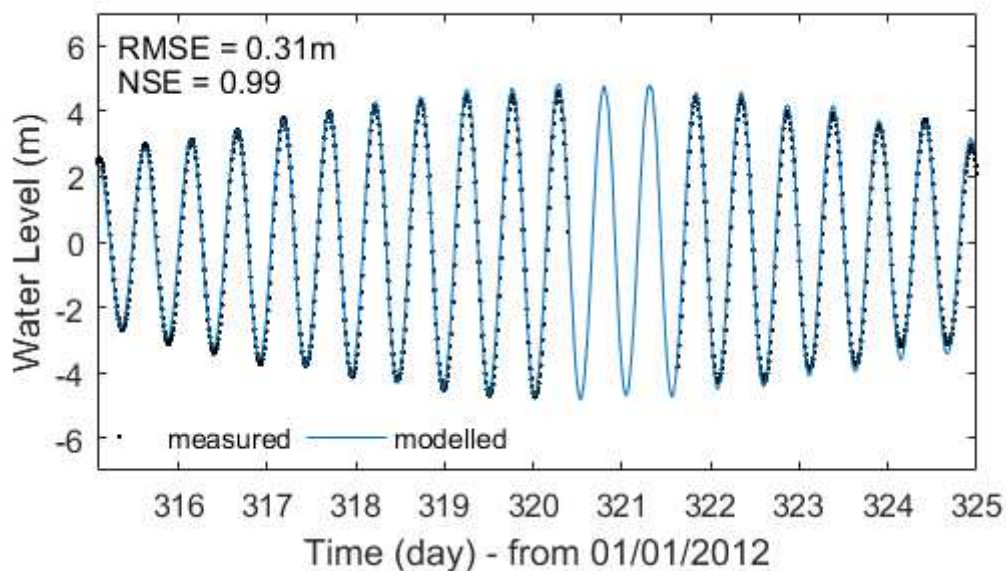
366 *Figure 15: Assumed light intensity function over a typical day*

367 **3 Hydrodynamic model validation**

368 A constant Manning's coefficient was used throughout the model domain. Based on the range of
 369 suggested roughness values presented in Chow (1959), water levels were calibrated by testing
 370 values of 0.02, 0.025 and 0.03 respectively, which were deemed suitable for excavated or dredged
 371 channels, and clean, straight main channels. The model was found to have low sensitivity to the
 372 bed roughness and a value of 0.025 was selected as that producing the best fit. Calibration and
 373 validation of water levels were initially carried out against tide gauge records provided by the
 374 British Oceanographic Data Centre (BODC) (<https://www.bodc.ac.uk/>), at four sites throughout the
 375 domain, as shown in Figure 6, over a spring-neap tidal cycle. Two sites, namely Illfracombe and
 376 Avonmouth, were used for model calibration and the sites at Mumbles and Hinkley Point were
 377 used for model validation. A plot comparing measured and predicted water levels at the Mumbles
 378 site, which is located at the Western edge of Swansea Bay, is shown in Figure 16. The Root Mean
 379 Square Error (RMSE) and Nash Sutcliffe Efficiency (NSE) (Nash and Sutcliffe, 1970; Coz et al.,
 380 2019) values were used to assess the correlation of the predicted and measured data. The RMSE
 381 and NSE values for the Mumbles site were 0.31 and 0.99, respectively, which showed good
 382 correlation between the measured and predicted data. There is a gap in the BODC data record for
 383 this site, which can be seen in Figure 16.

384

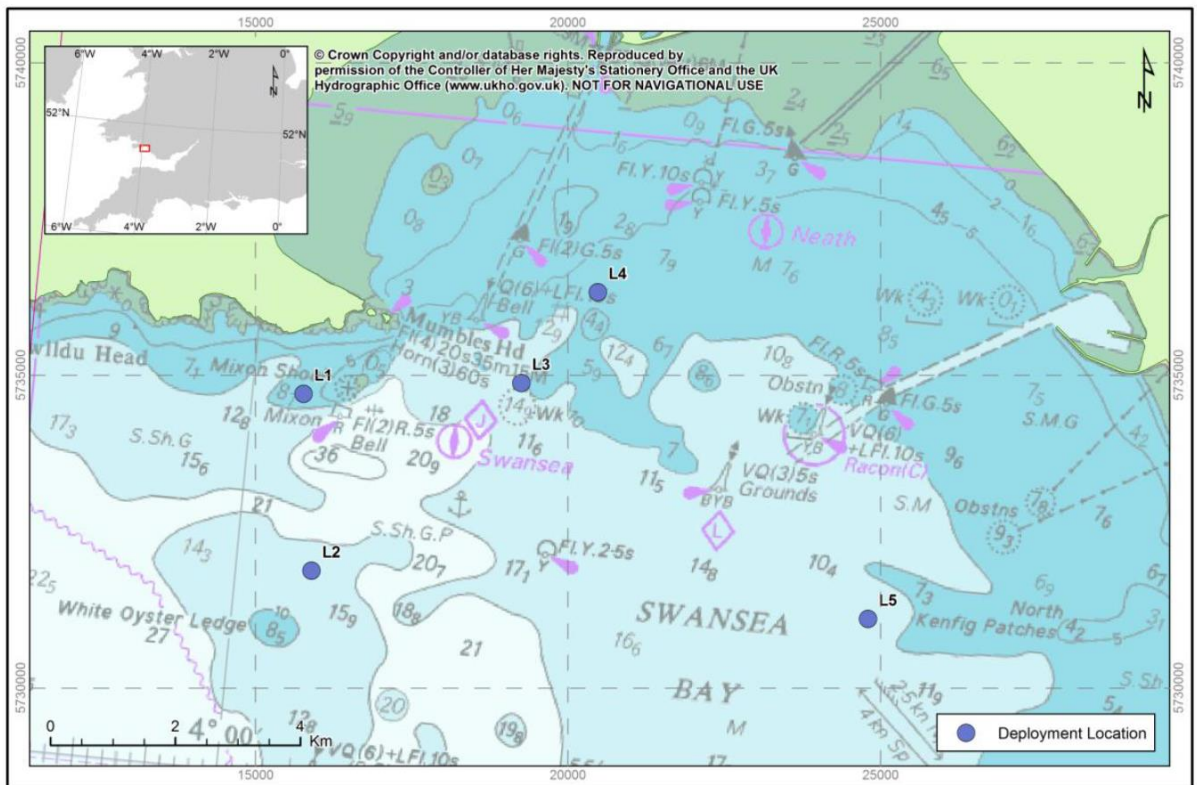
385 Further validation of water level predictions was carried out using Acoustic Doppler Current
386 Profilers (ADCP), deployed at 5 sites within Swansea Bay (as shown in Figure 17), from
387 21/07/2012 to 28/08/2012 (Aberystwyth University and University College Dublin, 2018; EMU
388 Limited, 2012) . The survey was carried out using a bed mounted Nortek Aquapro (EMU Limited,
389 2012). This further validation also confirmed good correlation between the measured and
390 predicted water levels. The velocity magnitudes and directions predicted by the model were
391 validated against the ADCP measurements, which were averaged over depth. The comparisons of
392 the measured and predicted velocity magnitudes and directions showed that model predictions
393 matched the measured data and that the model predictions were reliable. Typical comparisons of
394 measured and predicted velocity magnitudes and directions are shown in Figures 15 and 16.
395 Current direction are presented with respect to due north.



396

397 *Figure 16: Plot of calibrated water levels measured at Mumbles, adjusted relative to MSL, $n = 0.025$*

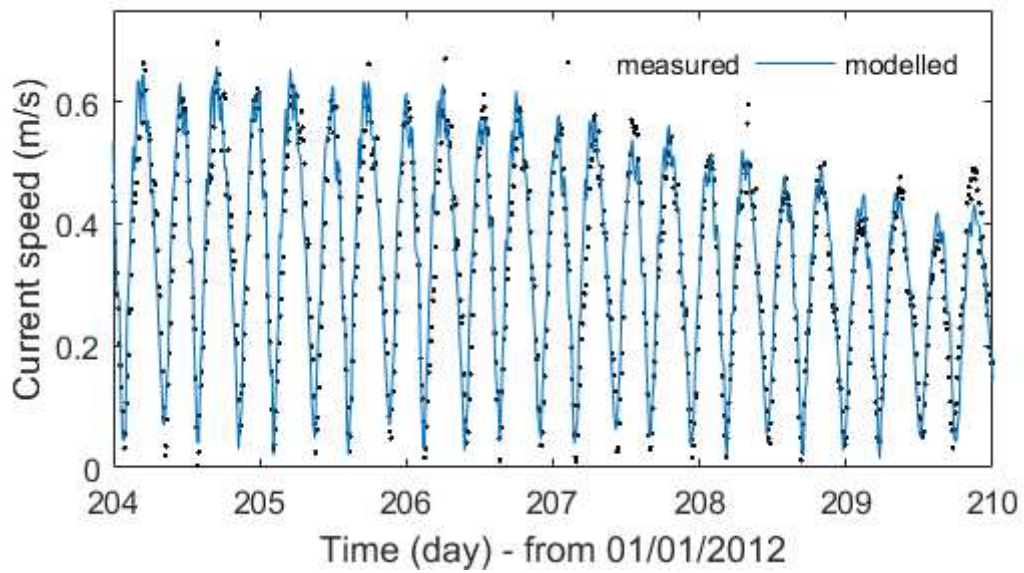
398



Map Document: (V:\J1012014_Swansea_Bay_Current_Monitoring\3_Plots\1_SurveyArray\Q2014_Deployment_Locations_RJM_20121024.mxd)
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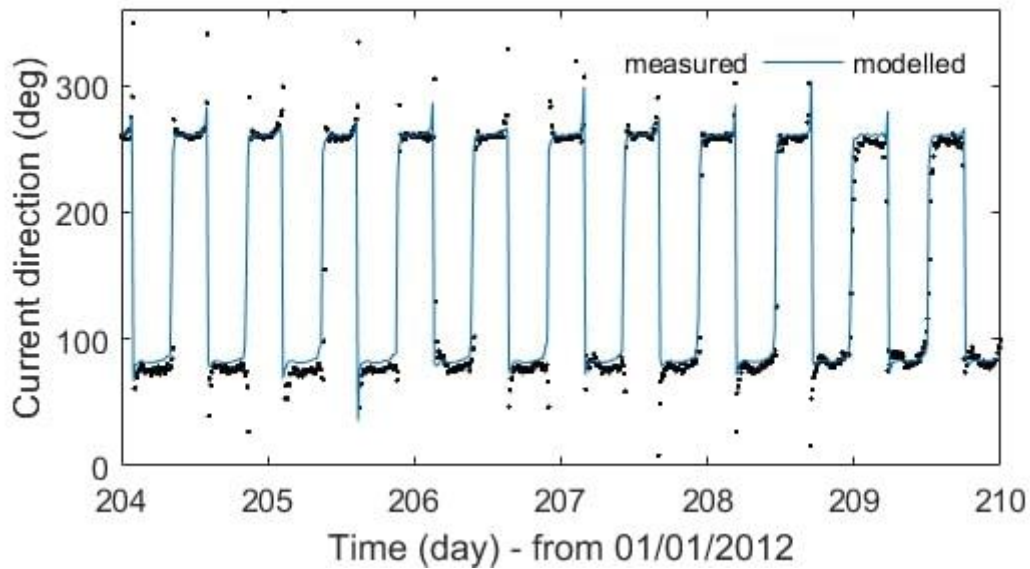
399

400 *Figure 17: ADCP survey locations in Swansea Bay*



401

402 *Figure 18: Plot of validated current speed in Swansea Bay at location L2*



403

404 *Figure 19: Plot of validated current direction in Swansea Bay at location L2*

405 **4 Results**

406 The model performance was next assessed using the *E. coli* records taken on 15th November 2012
 407 (Aberystwyth University and University College Dublin, 2018). Monitoring at the Swansea Bay and
 408 Aberafan DSPs was done along the transects shown in Figure 1. The measured and predicted
 409 values were compared using the new developments discussed in 2.4.1 and 2.4.2, to assess the
 410 performance of each method. For supplementary data omitted from this paper for brevity, see
 411 King (2019).

412

413 Figure 20 presents a comparison between the 2D and 3D modelled *E. coli* concentration
 414 predictions at the Swansea Bay DSP, using stationary point sources and a depth-averaged decay
 415 function. To mirror the sampling strategy used in the field the predictions shown are taken at the
 416 shallowest transect point greater than or equal to the sampling depth (0.5 m, see Section 2.1 and
 417 Figure 2b). Thus, the line plots shown correspond to multiple locations. Note that all 3D results
 418 presented herein have been averaged over the vertical layers to provide an indication of the
 419 concentration throughout the water column, rather than within a single layer. It can be seen in
 420 Figure 20 that the 2D model predicts higher concentrations than the 3D model.

421

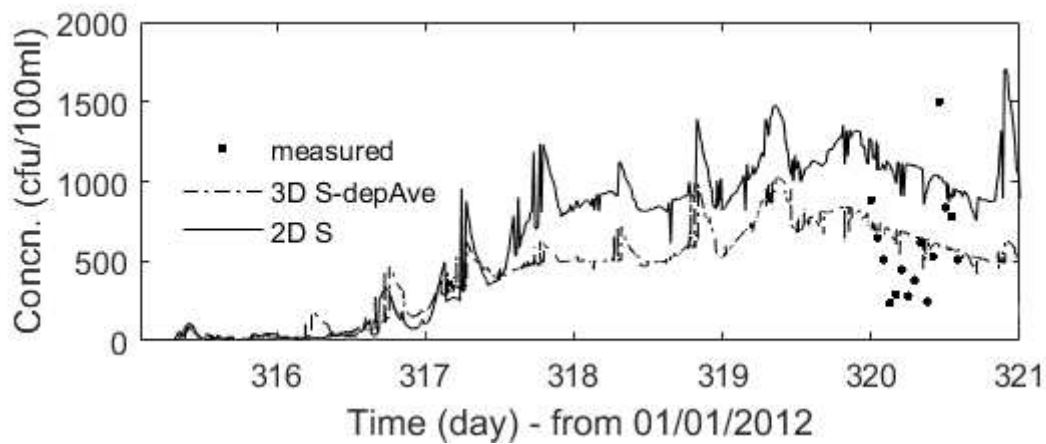
422 The predicted concentrations using the depth averaged decay function at all points along the DSP
423 transect within the 2D model are plotted in Figure 21, while the concentration plots around the
424 DSP and the monitoring points along the DSP transect are shown in Figure 22. It can be seen in
425 Figure 21 that at any point in time, there are significant spatial differences in the predicted *E. coli*
426 concentrations at each transect point, with a range of up to half the magnitude of the highest
427 predicted concentrations. The point which is considered a best fit to the measured data has been
428 highlighted.

429

430 Figure 23 presents a comparison between the measured and predicted *E.coli* concentrations at the
431 Swansea Bay DSP using depth-averaged and varying decay rates. It can be seen that lower
432 concentrations were predicted when using the depth-varying decay function.

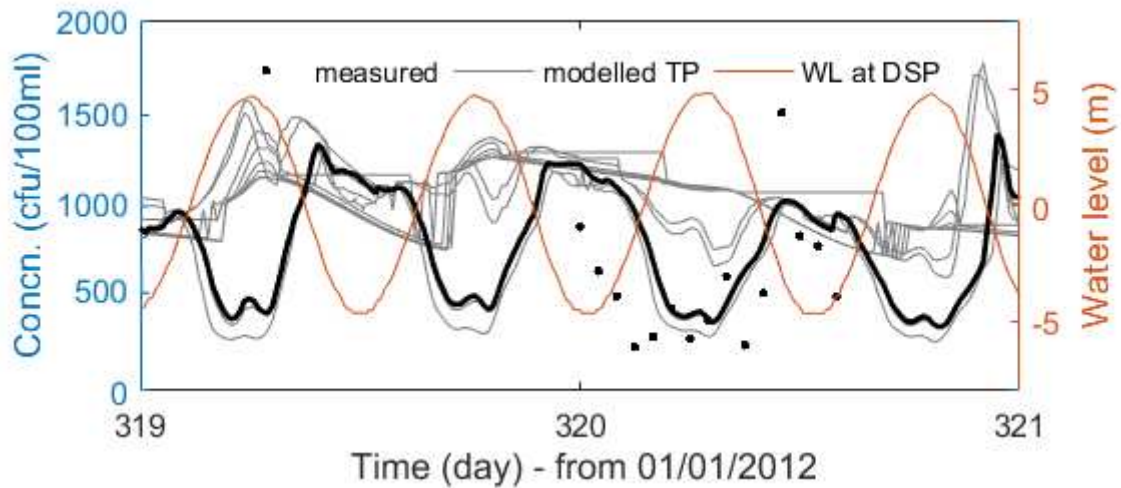
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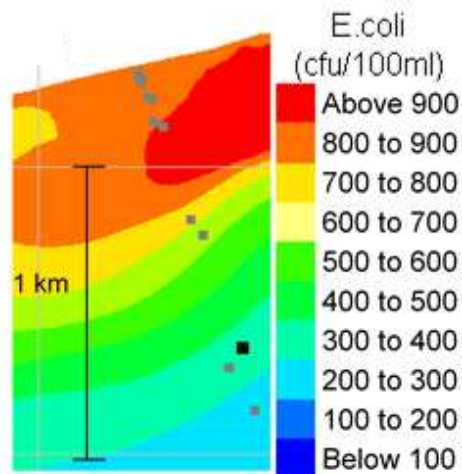
435

436 *Figure 20: Comparison between the measured and predicted E.coli concentrations at the Swansea*
437 *Bay DSP, using the Stapleton et al. (2007a) (S) decay function in the 2D and 3D models*



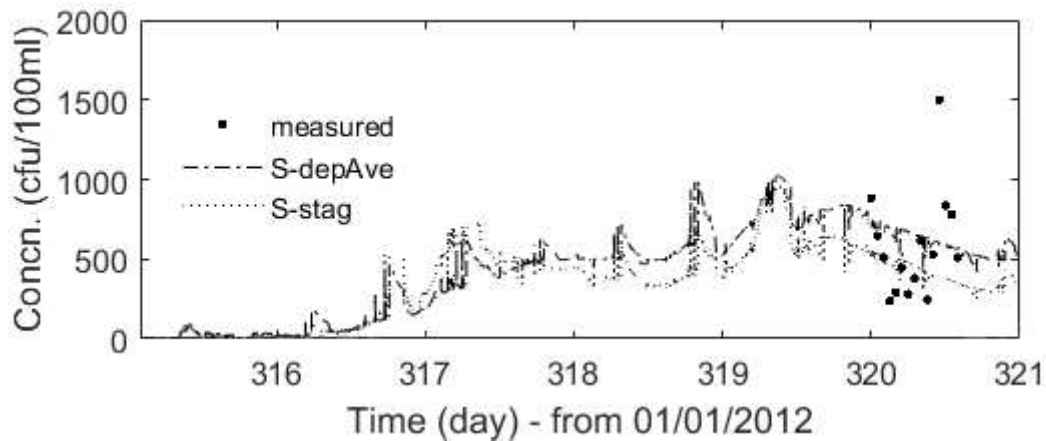
438

439 *Figure 21: Comparison between the measured and predicted E. coli concentrations at each*
 440 *monitoring location along the Swansea Bay DSP transect (TP), using the Stapleton et al. (2007a)*
 441 *decay function in the 2D model. Plotted alongside the predicted water level at the most offshore*
 442 *monitoring location*



443

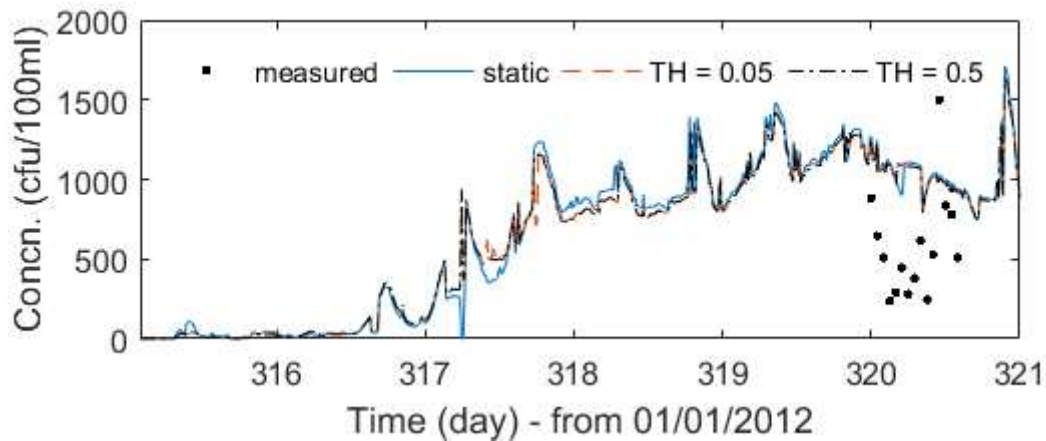
444 *Figure 22: Surface plot of the predicted E. coli concentrations along the Swansea Bay DSP transects,*
 445 *using the Stapleton et al. (2007a) decay function in the 2D model at 19:11:57 on 15/11/12 (high*
 446 *tide)*



447

448 *Figure 23: Comparison between the measured and predicted E.coli concentrations at the Swansea*
 449 *Bay DSP using depth-averaged and varying Stapleton et al. (2007a) (S) decay functions in the 3D*
 450 *model*

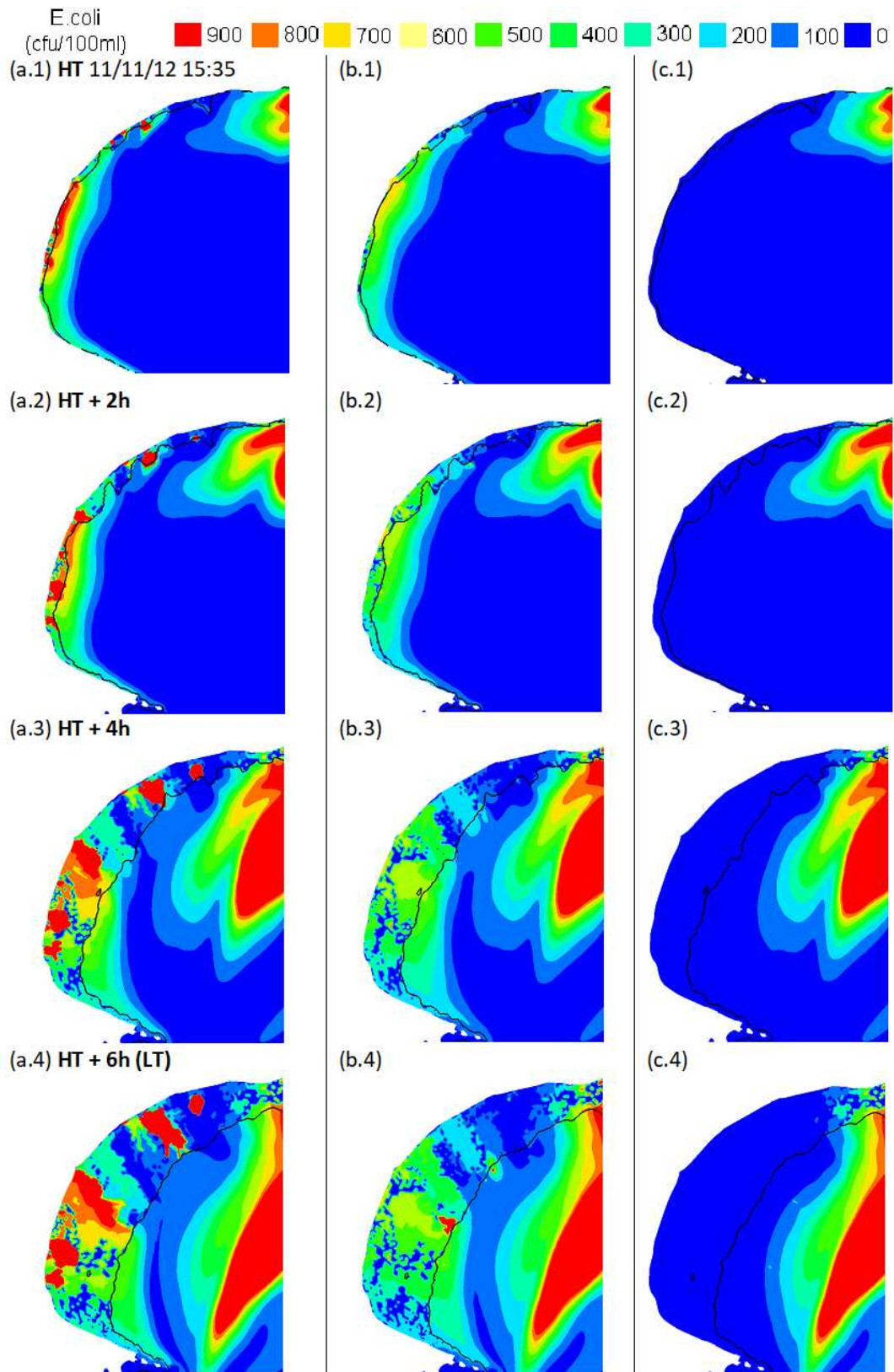
451 Plots comparing the measured and predicted *E.coli* concentrations at the Swansea Bay DSP using
 452 the static and improved source release models are shown in Figures 24 and 25. Figure 24 presents
 453 this comparison at the Swansea Bay DSP whereas Figure 25 includes the wider Bay area and
 454 highlights the spatial variability in concentration predictions between the methods.



455

456 *Figure 24: Comparison between the predicted E. coli concentrations at the Swansea Bay DSP, using*
 457 *static sources, and improved source representation with two threshold depths (TH)*

458



459

460 *Figure 25: Comparison of the predicted E. coli concentration distributions in Swansea Bay, using the*
 461 *2D model with static sources, improved source representation (TH = 0.05), and deep water sources;*
 462 *(a), (b) and (c), respectively*

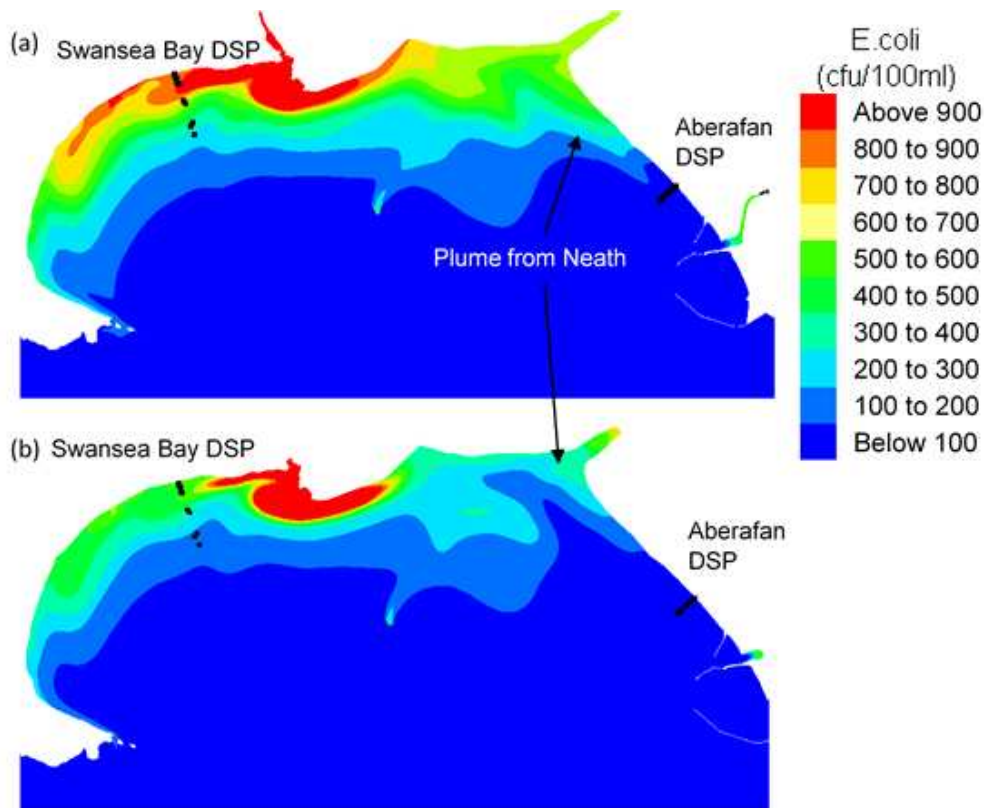
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464

465 5 Discussion

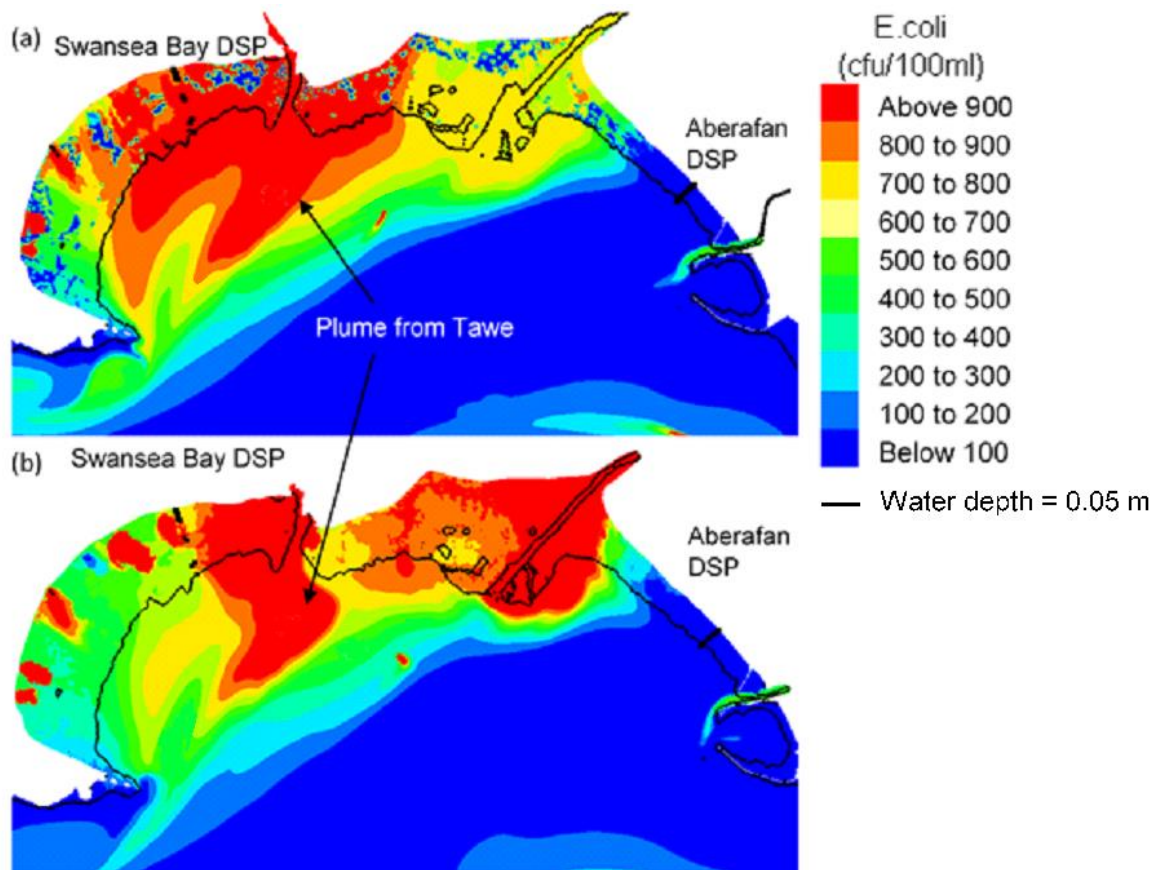
466 5.1 Comparison of 2D and 3D decay model setup

467 It can be seen in Figure 20 that the 2D model predicts higher bacterial concentrations than the 3D
468 model. This can be partly attributed to the method used in inclusion of the rivers Tawe and Neath
469 in the 2D model, which were included in the 3D model by accumulating the flow and bacterial input
470 at a single point due to computational time issues, and can be explained by looking at Figures 26
471 and 27.



472

473 *Figure 26: Comparison of the predicted E. coli concentration distribution in Swansea Bay, at 19:16*
474 *on 15/11/12 (HT), using the Stapleton et al. (2007a) decay function in the 2D (a) and 3D (b)*
475 *models. Depth-averaged decay function used in the 3D model*



476

477 *Figure 27: Comparison of the predicted E. coli concentration distribution in Swansea Bay, at 12:09*
 478 *on 15/11/12 (LT), using the Stapleton et al. (2007a) decay function in the 2D (a) and 3D (b)*
 479 *models. Depth-averaged decay function used in the 3D model. The black line represents a water*
 480 *depth of 0.05 m.*

481 Based on the location of the model *E. coli* inputs (see Figures 4 and 5), it can be reasoned that the
 482 plume from the River Tawe is responsible for the water quality at the Swansea Bay DSP. While this
 483 input is included accurately within the 2D model, it is represented as a point source at the river
 484 mouth in the 3D model, without an assigned velocity. In this case the flow speed is greatly reduced
 485 and the plume does not extend far enough into the Bay during the ebb tide. This highlights the
 486 importance of including source term momentum when representing bacterial inputs in 3D models.
 487 This may be either by assigning a velocity to point sources or linking 1D river models with the 3D
 488 coastal model, with momentum transfer across the linked boundaries.

489

490 **5.2 Spatial and temporal variability**

491 It is suggested that because of the spatial variance in bacterial concentrations shown in Figures 21
492 and 22, when modelling and sampling it may be prudent to predicted and record FIO levels at
493 multiple locations to ascertain the spatial distribution in bacterial concentration and adequately
494 determinate the risk to bathers. Not doing so may lead to under prediction of this risk and
495 erroneous calibration of the hydro-epidemiological models.

496 In addition, Figure 21 shows a diurnal pattern in the predicted *E. coli* concentrations at the
497 Swansea Bay DSP. On day 320 this is also seen in the measured data. This diurnal pattern is
498 expected to be due to the accumulative impact of decay during the day following an increase in the
499 solar radiation, as shown in Figure 15. However, other influential factors might be affecting the
500 diurnal pattern, such as a contribution from the sources, tidal dilution or interaction with
501 sediments, and which need to be considered in more detail.

502

503 High spatial, and potentially diurnal, variations are seen along all other transects too, thus
504 highlighting the variability of the concentration along a beach and at different times. Therefore,
505 although this highlights a potential limitation of the model to calculate processes which take place
506 at a high spatial resolution, it may also be prudent to consider different methods of classifying
507 bathing water sites based on a non-stationary DSP.

508

509 **5.3 Depth-varying decay**

510 It can be seen in Figure 23 that lower concentrations were predicted when using the depth-varying
511 decay function. To discuss the reason for this reduction in concentration and highlight the
512 applicability of the depth-averaged decay approach, a simplified vertical 1D case is considered.
513 Equation 15 represents a simplified form of Equation 1, reduced to 1D in the vertical and with zero
514 vertical velocity.

515

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z} \left(v_T \frac{\partial C}{\partial z} \right) - kC \quad 15$$

516

517 In this situation the problem is reduced to one controlled by turbulent and molecular diffusion
518 between the layers and decay. This can be further reduced to Equation 2 by setting the turbulent
519 diffusion term to zero. The analytical solution of Equation 15 is then given in Equation 16:

520

$$C(t) = C_0 e^{-kt} \quad 16$$

521

522 where $C(t)$ is the concentration at time t , C_0 is the concentration at time $t = 0$ and k is the decay
523 rate (1/d). For a simple 5-layer problem, with a node spacing of 1 m, we look at the decay of an
524 initial tracer (bacteria) concentration of 1,000 (dimensionless) over 2 days. The equation was
525 solved at a time step of 1 minute using the finite different method, with a first order forward
526 difference scheme in time and a second order central difference scheme in space. The boundary
527 value problem was solved at the surface and bed introducing phantom layers, with a value equal
528 to the adjacent real boundary. Thus, diffusion only acts within the domain. Values for suspended
529 sediment concentration, salinity and temperature were set as those used in the Swansea Bay
530 study, and with the light intensity fixed at 260 W/m².

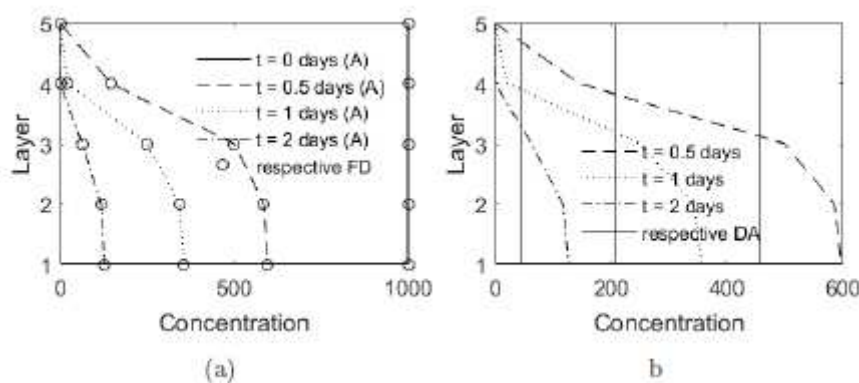
531

532 A comparison of the concentrations over depth predicted by the analytical solution and two
533 different decay approaches used in this study is illustrated in Figure 28. As can be seen there is
534 good agreement between the analytical solution and the finite difference solutions, using a depth-
535 varying decay, when the tracer diffusion term is set to zero. This result confirms the validity of this
536 method. For further information, see King (2019) wherein the data plotted in (a) is presented in
537 tabular form. Comparing the use of the depth-varying and depth-averaged decay functions, it can
538 be seen in (b) that the overall concentration in the water column is less when a depth-varying

539 approach was used. This is because the exponentially larger decay rate in the surface layers causes
540 a greater reduction in the concentration than that predicted at depth (see Figure 7).

541

542 Due to the increased transport of bacteria from regions of high concentration at depth to lower
543 concentrations at the surface, this results in higher concentrations in the surface layers, reduced
544 concentrations at depth and a reduction in total concentration in the water column. Bacteria in the
545 surface layers continues to decay at a faster rate, increasing the concentration gradient and hence
546 the movement of bacteria between layers.



547

548 *Figure 28: Solution of simplified 5 layer decay problem; (a) comparison between analytical and*
549 *finite difference (FD) solutions using a depth-varying decay rate, where $T = 0$; and (b)*
550 *comparison between FD solutions using depth-averaged (DA) and varying solutions*

551 This interchange between layers will be further increased by including the velocity term in
552 Equation 15, where there is an upward flow such as in Swansea Bay, and in the vicinity of long
553 sea outfall diffusers with a vertical orientation.

554 **5.4 Moving discharge**

555 The following section presents a comparison between the use of static and non-stationary
556 bacterial point inputs in the 2D model of Swansea Bay. In considering the predicted surface
557 concentration distributions (see Figure 25), there are clear differences observed when comparing
558 the two approaches over a tidal cycle. At high tide there are elevated concentrations in the static
559 discharge model and the *E. coli* plume extends a greater distance into the western region of

560 Swansea Bay. During the ebb tide the differences become more pronounced as the plume spreads
561 over a larger beach area above the water line. In comparison, the predicted concentrations in the
562 improved source model are greatly reduced and the plume below the water line is reduced in size.
563 There are also small regions with high *E. coli* concentrations immediately below the waterline, and
564 in the vicinity of the source points, which have more serious implications on the predicted risk to
565 bathers. Therefore, implementation of the mobile source point could significantly impact the
566 results and should be considered in future studies. With regard to the *E. coli* distribution above the
567 water line, this will have a greater implication if the beach sand is considered as a diffuse bacterial
568 source and sink, in a similar manner to how Abu Bakar et al. (2017b) modelled inter-tidal
569 marshland in the Loughor Estuary, UK. Furthermore, these regions may aid in providing more
570 accurate predictions of the location of 'safe' and 'no go zones', on the beach and in the water, which
571 is of utmost importance when disseminating bathing water information to beach goers, as advised
572 in the rBWD.

573 As shown in Figure 24, for the majority of the simulation period, use of the improved source model
574 results in lower concentrations. This is due to increased dilution as the tracer is released into
575 deeper water. While it is not possible to discern a difference between the two improved source
576 models using different threshold depths, it can be seen in Figure 25 that if all release locations are
577 moved to a point below the low tide line, *E. coli* concentrations in the nearshore region are under
578 predicted throughout the tidal cycle, due to increased dilution. This indicates that correctly
579 modelling the beach sources is important in order to predict accurately the dynamics governing
580 bacterial transport. It is therefore suggested that the apparent invariance between the static and
581 improved source release models seen in Figure 24 is due to the distance of the DSP from the
582 bacterial beach source locations (see Figure 1), as well as the influence of the River Tawe on the
583 DSP as previously explained.

584 It can be seen from these results that although using the new model results in minor
585 improvements in *E. coli* concentration predictions at the DSP and within Swansea Bay, the

586 differences between model predictions are not significant enough to warrant the choice of one
587 method over the other for this case study, or at this stage in model development.

588

589 **6 Conclusions**

590 Two computational models, one 2D and one 3D, were set up using the TELEMAC suite of models
591 to implement new enhancements in simulating the transport and decay of *E. coli* in a data rich case
592 study site. The models and the data were then compared for a range of different modelling
593 approaches. The case study site was Swansea Bay, located in South West of the UK, where over
594 7,000 samples were taken during 2011. The 3D model was found to under predict bacterial
595 concentrations due to the inclusion of the Rivers Neath and Tawe as point sources, and without
596 momentum conservation. The application of a 3D model in a well-mixed marine environment,
597 where a 2D depth averaged approach is usually adopted, highlights the impact of a vertically
598 variable decay through the water column. Application of this method is an important step in
599 improving the reliability of 3D deterministic epidemiological models, to ensure that decay
600 processes are represented realistically. Of the two methods used to calculate decay throughout the
601 water column in the 3D model, namely depth-varying and depth-averaged, the depth-varying
602 approach was found to predict lower bacterial concentrations due to the exponential decrease in
603 light intensity with depth and the associated effect on the decay rate. It is therefore suggested that
604 in 3D modelling studies a depth-varying decay model should be used as it provides a more
605 accurate representation of the vertical spatial variation in bacterial die-off rates. Using the 2D
606 model, an improved method of representing beach sources was developed to mimic the streams
607 discharging along the Swansea Bay beach. Rather than being considered stationary, the sources
608 were moved along a transect throughout the simulation period, to ensure they discharged just
609 below the waterline. This provided more accurate predictions of the spatial distribution of *E. coli*
610 within the domain, with the most significant effects noticed above and near the waterline, such as
611 zones of elevated bacterial concentration where the beach streams enter the water. In addition, it
612 highlights the limitations of using TELEMAC to model static beach sources on shallow gradient

613 beaches, subject to wetting and drying throughout the tidal cycle. Spatial and diurnal variations in
614 bacterial concentrations were seen along the Swansea Bay Designated Sampling Point transect,
615 highlighting the variability of water quality along the beach and at different times. Therefore, it is
616 suggested that bathing water monitoring based on a stationary Designated Sampling Point may
617 lead to incorrect classification of the bathing water quality and provide a false indication of the
618 risk of infection. In addition, it highlights a potential limitation of bacterial models to calculate
619 processes accurately, which take place at a high spatial resolution.

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629 coastline shapefile used to create Figure 1 was provided by the OpenStreetMap project
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