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1 **Modelling the transport and decay processes of microbial tracers in a**  
2 **macro-tidal estuary**

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13  
14 **Abstract:** The Loughor Estuary is a macro-tidal coastal basin, located along the Bristol  
15 Channel, in the South West of the U.K. The maximum spring tidal range in the estuary is up to  
16 7.5 m, near Burry Port Harbour. This estuarine region can experience severe coastal flooding  
17 during high spring tides, including extreme flooding of the intertidal saltmarshes at  
18 Llanrhidian, as well as the lower industrial and residential areas at Llanelli and Gowerton. The  
19 water quality of this estuarine basin needs to comply with the designated standards for safe  
20 recreational bathing and shellfish harvesting industries. The waterbody, however, potentially  
21 receives overloading of bacterial inputs that enter the estuarine system from both point and  
22 diffuse sources. Therefore, a microbial tracer study was carried out to get a better understanding  
23 of the faecal bacteria sources and to enable a hydro-environmental model to be refined and  
24 calibrated for both advection and dispersion transport. A two-dimensional hydro-  
25 environmental model has been refined and extended to predict the highest water level covering

26 the inter-tidal floodplains of the Loughor Estuary. The validated hydrodynamic model for both  
27 water levels and currents, was included with the injected mass of microbial tracer, i.e. MS2  
28 coliphage from upstream of the estuary, and modelled as a non-conservative mass over several  
29 tidal cycles through the system. The calibration and validation of the transport and decay of  
30 microbial tracer was undertaken, by comparing the model results and the measured data at two  
31 different sampling locations. The refined model, developed as a part of this study, was used to  
32 acquire a better understanding of the water quality processes and the potential sources of  
33 bacterial pollution in the estuary.

34 **Keywords:** hydrodynamic modelling, mass transport, tracer studies, estuaries

35

## 36 **1. Introduction**

37 Water quality at recreational bathing and shellfish harvesting sites in coastal and estuarine  
38 waters are important to comply with the designated standards following the EU Directives  
39 (CEU, 2000). The failure to comply with these directives could cause pathogenic infections, as  
40 humans come into contact with polluted water or consume shellfish harvested in polluted water.  
41 In the 19<sup>th</sup> century, more than a quarter of infected diseases were due to consumption of mussel  
42 bio-accumulated pathogens (Kay *et al.*, 2008).

43 Pathogens enter coastal waters either through treated or untreated outfalls, or rivers as  
44 point sources, or from tidally inundated land as diffuse sources, such as grazing saltmarshes.  
45 Pathogens then go through complex estuarine processes, including particulate interactions with  
46 sediments, transport by the hydrodynamic processes, and through bio-chemical processes, such  
47 as decay. These processes and interactions make predicting the concentration and establishing  
48 the main sources of pathogens a complex challenge. Such predictions are more difficult in the  
49 Loughor Estuary due to the complex hydrodynamics in the region and the wide range of faecal  
50 bacteria sources, including primarily: Wastewater Treatment Works (WwTWs), Combined

51 Sewer Overflows (CSOs), and animal grazing and shellfish processing plant outfalls. This  
52 complexity is highlighted by differences in shellfish bed classifications as a result of faecal  
53 coliform and *E. coli* concentrations respectively, at the lower reaches of catchments and in  
54 shellfish flesh observed by the Environment Agency and Natural Resources Wales (Youell et  
55 al., 2013a; Youell et al., 2013b).

56 The research reported herein is focused on modelling microbial tracer transport and decay  
57 processes in the complex estuarine environment. Due to the distinct characteristics of the  
58 tracers used in these studies, modelling microbial tracers could be used for calibration and  
59 validation of the hydrodynamic and transport processes in hydro-environmental models, as  
60 well as for acquiring a better understanding of the links between sources and receptors of faecal  
61 indicator organisms (FIOs).

62

## 63 **2. Materials and methods**

### 64 ***2.1 Study area***

65 The Loughor is a macro-tidal estuary that flows into the Bristol Channel, with a maximum  
66 spring tidal range of up to 7.5 m near Burry Port (see Figure 1). The area is well-known for  
67 shellfish harvesting, with related processing industries being located in the vicinity of bathing  
68 water sites. Llanrhidian saltmarshes, located on the South bank of the estuary, are subjected to  
69 a number of designations (i.e. protection of natural ecosystems) which include a Site of Special  
70 Scientific Interest (SSI), Special Area of Conservation (SAC), Special Protection Area (SPA),  
71 a Ramsar Site (following an intergovernmental Ramsar treaty for the protection of wetlands)  
72 (TRCS), and a National Nature Reserve (NNR) (Youell et al., 2013a; Youell et al., 2013b).  
73 However, the saltmarshes are legally used for sheep grazing activities during low tides. The  
74 animal faeces left on the saltmarshes are suspected to be one of the main sources of pathogen  
75 inputs to the estuarine receiving waters after the saltmarsh floods on the rising tide. The other

76 main source of pathogen input to the estuary are the Llanelli and Gowerton WWTWs, as well  
77 as a few shellfish processing plants. An overview of the key sites in the Loughor Estuary,  
78 including the siting of these potential sources of faecal indicator organisms (FIOs) into the  
79 estuary is shown in Figure 1.

80

## 81 **2.2 Modelling system**

82 The Telemac Modelling System (TMS) was used for the development of a hydro-  
83 environmental model in this study. The modelling system solves the two-dimensional (2D)  
84 Shallow Water Equations (SWEs) that are averaged from the Navier-Stokes Equations (NSEs),  
85 using the finite element method for iterations on an unstructured triangular mesh. The  
86 modelling system is designed to study the environmental processes in free surface waters for  
87 coastal and seas, estuarine and river water bodies, with the main applications regard to their  
88 modules-based being for hydrodynamic by Telemac-2D and -3D, water quality by Delwaq,  
89 sedimentology by Sisyphe, and water wave studies by Tomawac (Lang, 2010). The TMS,  
90 originally developed at the Research and Development department of Electricité de France  
91 (EDF), supports with the most available pre- and post-processing tools, i.e. BlueKenue,  
92 Tecplot, and Matlab.

93 The TMS solutions for the depth-averaged SWEs that derived from the NSEs require  
94 approximations for the simplification. The fluid is assumed to be Newtonian, incompressible  
95 and homogenous in the vertical plane, and the long wave approximation is adopted, i.e. the  
96 pressure remains hydrostatic in the vertical direction. The NSEs are averaged over the depth  
97 and Reynolds decomposition and stochastic averaging are applied for modelling the turbulence  
98 processes. Bottom friction is modelled by using non-linear laws for velocity, such as the Chezy,  
99 Strickler or Nikuradse friction laws. The SWEs implemented in the TMS use the non-divergent

100 form of the momentum equation, which are derived by substituting the continuity equation into  
 101 the two momentum equations in the x- and y-directions (Lang 2010).

102 Four equations are solved simultaneously within the TMS by considering the Telemac-  
 103 2D module, which are summarised below. Equation (1) is the continuity equation, Equations  
 104 (2) and (3) are the momentum equations in the x and y directions, respectively, and Equation  
 105 (4) is the transport equation, which is also used to model a tracer (Lang, 2010):

$$106 \quad \frac{\partial h}{\partial t} + \vec{u} \cdot \overrightarrow{grad}(h) + h \operatorname{div}(\vec{u}) = S_h \quad (1)$$

$$107 \quad \frac{\partial u}{\partial t} + \vec{u} \cdot \overrightarrow{grad}(u) = -g \frac{\partial Z_s}{\partial x} + F_x + \frac{1}{h} \operatorname{div}(h v_t \cdot \overrightarrow{grad}(u)) \quad (2)$$

$$108 \quad \frac{\partial v}{\partial t} + \vec{u} \cdot \overrightarrow{grad}(v) = -g \frac{\partial Z_s}{\partial y} + F_y + \frac{1}{h} \operatorname{div}(h v_t \cdot \overrightarrow{grad}(v)) \quad (3)$$

$$109 \quad \frac{\partial T}{\partial t} + \vec{u} \cdot \overrightarrow{grad}(T) = \frac{1}{h} \operatorname{div}(h v_T \cdot \overrightarrow{grad}(T)) + S_T \quad (4)$$

110 For the above equations:  $h$  is the depth of water,  $u$  and  $v$  are the horizontal velocity  
 111 components, in the x- and y-directions, respectively,  $T$  is the non-buoyant tracer or temperature,  
 112  $g$  is gravitational acceleration,  $v_t$  and  $v_T$  are the momentum and transport diffusion  
 113 coefficients, respectively,  $Z_s$  is the elevation of the free surface,  $t$  is time,  $x$  and  $y$  are the  
 114 horizontal coordinates,  $S_h$  is the source or sink term of fluid mass,  $F_x$  and  $F_y$  are the source or  
 115 sink terms of fluid momentum within the domain in the x- and y-directions, respectively, (with  
 116 the momentum source or sink terms including: the Coriolis force, bottom friction, and the wind  
 117 shear stress), and  $S_T$  is the source or sink of tracer or heat. The sink of tracer is used to represent  
 118 the microbial decay process which later is written  $k_b T$ , where  $k_b$  is the decay rate.

119 For modelling turbulence, the turbulent viscosity may be assigned by users as a constant  
 120 or using the Elder equation. The turbulent eddy viscosity can also be calculated spatially and  
 121 temporally using transport models for the turbulent kinetic energy and energy dissipation (i.e.  
 122 the  $k$ - $\varepsilon$  model) or the Smagorinski representation. The  $k$ - $\varepsilon$  transport model uses Equations (5)  
 123 and (6), respectively (Lang, 2010):

$$124 \quad \frac{\partial k}{\partial t} + \vec{u} \cdot \overrightarrow{grad}(k) = \frac{1}{h} \operatorname{div} \left( h \frac{v_t}{\sigma_k} \overrightarrow{grad}(k) \right) + P - \varepsilon + P_{kv} \quad (5)$$

$$125 \quad \frac{\partial \varepsilon}{\partial t} + \vec{u} \cdot \overrightarrow{grad}(\varepsilon) = \frac{1}{h} \operatorname{div} \left( h \frac{v_t}{\sigma_\varepsilon} \overrightarrow{grad}(\varepsilon) \right) + \frac{\varepsilon}{k} [C_{1\varepsilon}P - C_{2\varepsilon}\varepsilon] + P_{\varepsilon v} \quad (6)$$

126        The solute transport equation of the system satisfactorily conserves the transported mass  
 127 of a solute with the corresponding conservative transport schemes. The model can be used for  
 128 both conservative and non-conservative tracers, using a first-order kinetic decay rate for a non-  
 129 conservative tracer (such as FIOs).

130

### 131 **2.3 Model setup**

132        A two-dimensional hydrodynamic model has been set up for the area of the Severn  
 133 Estuary and Bristol Channel which covers an approximate area of 5,793 km<sup>2</sup>, as shown in  
 134 Figure 2. The seaward open boundary at the western side was located at the outer extremity of  
 135 the Bristol Channel, and extended to the eastern side of the River Severn, up to the tidal limit,  
 136 near Gloucester. The location of the seaward open boundary was specified along an imaginary  
 137 line from Stackpole Head to Hartland Point with the available tidal time series boundary  
 138 condition being located far away from the area of interest (i.e. the calibration and validation  
 139 sites) for minimizing any errors that might originate from the specified open boundary. This  
 140 large model domain was chosen to enable investigations to be undertaken of the potential links  
 141 between the water quality status within the Loughor Estuary and other key water bodies close  
 142 to this estuary, i.e. the bathing water sites along the Carmarthen Bay and Gower beaches.

143        The unstructured triangular mesh was generated to set up to cover the model domain, by  
 144 using the BlueKenue mesh generator. The generated mesh also included the solid boundaries  
 145 of Caldey Island at the outer Bristol Channel, and Flat Holm and Steep Holm Islands at the end  
 146 of the Severn Estuary. To achieve high grids resolution within the Loughor Estuary, while  
 147 maintaining the model efficiency, the edge length of the grids was set to vary from 1000 m

148 close to the seaward open boundary and decreased down to 20 m in the Loughor Estuary,  
149 producing 711,106 unstructured triangular cells and 358,266 nodes. The bathymetric data in  
150 the horizontal plane were specified relative to Ordnance Datum Newlyn (ODN) and Universal  
151 Transverse Mercator (UTM) projection of Zone 30N respectively, with interpolation being  
152 used to provide data at the mesh nodes, using the inverse distance interpolation method. The  
153 generated mesh with the bathymetry interpolation of the model domain is shown as in Figure  
154 2, with the deepest bottom elevation of approximately 65 m being shown near the model  
155 seaward open boundary and decreasing towards the eastern boundary in the River Severn.

156

#### 157 ***2.4 Hydrodynamic calibration***

158 The developed model was driven using a tidal time series, specified along the seaward  
159 open boundary, which drives the tidal circulation processes within the modelling domain, and  
160 using data obtained from the Proudman Oceanographic Laboratory (POL) (Heaps and Jones,  
161 1981). A typical mean value of the river discharges was specified across each river boundary  
162 for the main rivers based on data given by Stapleton et al. (2007) and Ahmadian et al. (2010).  
163 Due to the sensitivity of the transport processes to river discharges in the areas of interest, time  
164 series flows for the rivers and streams discharging into the Loughor Estuary were derived based  
165 on historical data (NRFA) and implemented in the model.

166 The initial condition for the water surface was set at a constant elevation across the  
167 domain, as governed by the level at the boundary at the starting time. The tidal currents were  
168 set to zero across the domain at the start of the simulation. The model was run for a cold start,  
169 with a tidal cycle from the boundary condition forcing the hydrodynamic processes within the  
170 model domain. The hydrodynamic model was run with a time step of 10 seconds, which  
171 resulted in a maximum Courant number of about 0.8.



172 For the first step, the large-scale model covering the entire domain was calibrated. The  
173 calibration of the hydrodynamic model was carried out by comparing predicted and measured  
174 water levels and tidal currents and using a constant bottom roughness coefficient across the  
175 domain. Manning's n was typically cited within the range of 0.01 to 0.1 in the literature (Ji,  
176 2008) and these values were used for calibration. The best fit of modelled results of water levels  
177 and tidal currents was found when the bottom roughness Manning coefficient was set to 0.025.  
178 Typical comparison between model predictions and observed data for water levels and currents  
179 within Swansea Bay is shown in Figures 11 and 12, respectively.

180

### 181 ***2.5 Domain extension over intertidal marshlands***

182 It was understood that the flooding processes over the intertidal floodplains, including  
183 marshlands, dunes and diffuse source pollutant inputs, at high tide could potentially have a  
184 significant impact on the water quality processes within estuaries (Grant *et al.* 2001; Weiskel  
185 *et al.* 1996; Evanson and Ambrose 2006; Sanders *et al.* 2005), including the Loughor Estuary.  
186 However, the entire intertidal floodplains, marshlands and dunes, which were flooded at high  
187 water, did not have bathymetric data. Therefore, it was decided to extend the existing model to  
188 include the marshlands and dunes using a high-resolution grid. Since the bathymetric data did  
189 not cover these areas with sufficient high quality, the extension had to be carried out by merging  
190 LiDAR (Light Detection And Ranging) and interpolation of bathymetric data. The LiDAR data  
191 for the topography covering the areas of Carmarthen Bay, the Loughor Estuary, and Swansea  
192 Bay, at the north-western side of the model domain, were provided by Environment Agency  
193 Geomatics (Natural Resources Wales, 2015). The topographic data were provided as the 'bare  
194 earth' Digital Terrain Models (DTM), with a resolution of 2 m in 1 km x 1 km tile sizes. The  
195 multiple data tiles were embedded into a tile size of 10 km x 10 km to ease the data processing.  
196 The data initially provided were referred spatially to the British National Grid coordinate

197 system, which was re-projected onto the WGS 1984 UTM Zone 30N coordinate system, using  
198 the geographic transformation for petroleum to match the other parts of the domain. The data  
199 were referenced vertically, as for the bathymetric data relative to Ordnance Datum (OD) at  
200 Newlyn. The resolution of the projected data tiles was reduced to 8 m, to reduce the mapping  
201 time while maintaining a high resolution.

202 The projected data tiles were used to generate a new boundary line for extensions of the  
203 model domain in the regions of Carmarthen Bay, the Loughor Estuary, and Swansea Bay.  
204 Contour lines at 10 m level were generated from each data tile, with the shape file format  
205 provided being converted into a DXF file format. The merging work for a new shoreline of the  
206 domain extensions was carried out using the AutoCAD program. The original boundary lines  
207 at the areas for extension were extended to the new generated 10 m contour lines. The extended  
208 model covering the floodplains in Carmarthen Bay, the Loughor Estuary, and Swansea Bay is  
209 shown in Figure 3. The red dashed line in Figure 3 depicts the model boundary before  
210 refinement. The mesh generator of Blue Kenue software (Canadian Hydraulics Centre, 2011)  
211 was used to refine the grid in order to extend the domain. The new generated shoreline was  
212 used for the closed boundary, covering the areas of the domain extension. The grid size in the  
213 original model of 1000 m resolution was reduced to 200 m resolution for the offshore region  
214 surrounding Carmarthen Bay and Swansea Bay. The grid size in the Loughor Estuary was  
215 further refined from 200 m resolution to a minimum of 10 m, as shown in Figure 3. The grid  
216 size was set to be a linear function of the bottom elevation in the range between -5 and 5 m  
217 over the intertidal floodplains. The refinements obtained from the linear function, applied to  
218 the bottom elevation, were for accurately capturing the bathymetry-topography data to nodes  
219 of the mesh and representing complex geometries over the intertidal floodplains, especially  
220 with the finer grid resolution closer to the waterfront, where the wetting-and-drying processes

221 occurred. The grid refinement across the intertidal floodplains, together with the natural and  
222 manmade features of the Loughor Estuary, are shown in Figure 4.

223 The LiDAR data acquired from the Environment Agency Geomatics (Natural Resources  
224 Wales, 2015) are shown in Figure 5. As can be seen there are flat areas close to some convex  
225 points, which do not seem to be accurate. These inaccuracies were confirmed through site  
226 observation and discussion with the Smart Coast and NRW colleagues, who have a good  
227 working knowledge of the site. These errors are mainly thought to be caused by carrying out  
228 LiDAR surveys not at low water at these sites, but when water had flooded the flood plains.  
229 The errors associated with the processed topographic data were eliminated before the  
230 topography data were merged with the bathymetric data. The polygon with the best merging  
231 outline between the different datasets was used to extract the processed data. The multiple  
232 datasets were allowed to merge at overlapping edges of 50 m or more, to preserve continuity  
233 of the bottom elevation between the different data sources. The datasets were then mapped onto  
234 the new mesh and were used as the geometry for the improved simulations.

235 The model was then run using the refined extended bathymetry with a smaller time step  
236 of 1 sec to maintain a maximum Courant number of about 0.8. The simulation time of the  
237 refined 2D model was over 125 hours on a single core, or about 2 hours on 64 cores using  
238 Cardiff University's High Performance Computing facilities, i.e. Raven (ARCCA), for 456 hr  
239 of simulation time. A constant bottom Manning roughness coefficient of 0.025 was used across  
240 the domain, based on the previous hydrodynamic calibration.

241

## 242 ***2.6 Tracer transport and decay modelling***

243 The microbial tracer study was conducted for the Smart Coasts Sustainable Communities  
244 project within the Loughor Estuary, to examine connections between pathogen sources and  
245 impacts at locations of interest in the estuary and nearby bathing water designated sites (Wyer

246 *et al.*, 2014). The microbial tracers were released simultaneously at four different locations,  
247 approximately one hour after high spring tides. The released sites were at Great Pill (site 101)  
248 – a tidal channel draining via Llanrhidian Marsh, the Morlais River (site 201) – a tidal channel  
249 at Crofty draining via Salthouse Pill, Loughor Bridge (site 501) – a bridge crossing the Afon  
250 Llwyher tidal channel, near the discharge from Gowerton sewage treatment works, and the  
251 Afon Lliedi (site 601) - a tidal channel draining via Llanelli into the estuary. These sites are  
252 shown in Figure 6 using purple triangles. Each microbial tracer was measured at 5 sampling  
253 sites, including Rhossili DSP (site 408), Broughton a potential designation site (site 409), the  
254 Loughor Boat Club at the upstream end of the estuary (site 410), Burry Port harbour, which is  
255 close to the shellfish beds (site 411), and Pembrey DSP (site 412), with these field monitoring  
256 sites being shown in Figure 6 with green circles.

257 Each of the release sites represent major bacterial inputs to the estuary, while each of the  
258 sampling sites are major receiving sites and were selected because of the interest in these sites.  
259 Each of these sites represents a different characteristic from the hydrodynamic perspective and  
260 which impacts on the transport of the microbial tracer.

261 Four types of microbial tracers were released at each of these locations to represent the  
262 microbial source tracking from different pollutant sources (Wyer *et al.*, 2014). *Serratia*  
263 *marcescens* phage was released at site 101 over 14 minutes, with a total dose of 2.75E+16 pfu.  
264 *Enterobacter cloacae* phage was released at site 201 over 7 minutes, with a total dose of  
265 4.50E+16 pfu. MS2 coliphage was released at site 501 over 11 minutes to produce a total dose  
266 of 4.00E+17 pfu. The  $\phi$ X174 phage was released at site 601 over 3 minutes, with a total dose  
267 of 2.00E+15 pfu. Table 1 summarises details of the released microbial tracers into the Loughor  
268 Estuary. The application of bacteriophage as a source for tracking and similar work have been  
269 conducted elsewhere, such as Simpson *et al.*, (2002); Shen *et al.*, (2008).

270 To establish the baseline concentrations in the field, the microbial tracers were sampled  
271 prior to being released at all five monitoring locations, over 120 hours and at hourly intervals.  
272 The released tracers were used as input sources in the modelling of mass transport in the  
273 Loughor Estuary and surrounding waters. The MS2 coliphage, which was released from the  
274 Loughor Bridge, was used for calibration of the mass transport, as its location was at the most  
275 upstream point of the estuary and best represented the transport processes within the estuary.  
276 Initially, the tracers were considered to be conservative and the model was setup and run for  
277 the transport processes of advection and dispersion. The evaluation on grid sizes has been  
278 conducted for the mass dispersion sensitivity for a molecular diffusivity of  $10^{-10}$  m<sup>2</sup>/s (Chapra,  
279 2008), with refinements in the Loughor using resolutions of 100 m and 20 m respectively, for  
280 the coarse and fine grids. The evaluation has been further conducted for estimating the  
281 longitudinal dispersion of  $10^1 - 10^3$  m<sup>2</sup>/s eddy diffusivity (Chapra, 2008).

282 The transport sensitivity of MS2 coliphage mass by the advection process has been  
283 evaluated by assigning multi friction zones over the floodplains, particularly where the natural  
284 features vary significantly. The inter-tidal areas have been divided into four zones with  
285 different natural bed features, and the estimation on Manning's n values across the floodplains  
286 have been calculated using the following equation (George and Schneider, 1989):

$$287 \quad n = (n_1 + n_2 + n_3) \quad (7)$$

288 where  $n_1$  is the base value referring to the natural bare soil across the floodplains, which is  
289 assumed to be in the range of 0.025 – 0.032 for firm soil;  $n_2$  is the value of the degree of  
290 irregularity, i.e. the rises and dips across floodplains, which is in the range of 0.030 – 0.045;  
291 and  $n_3$  is the vegetation value which accounts for growth density and average flow depth, in  
292 the range of 0.010 – 0.050 (Hall and Freeman 1994). The zones have been characterized as the  
293 estuarine downstream, tidal channel, sand dunes, and marshland areas, and are illustrated in  
294 Figure 7.

295 Although the released microbial tracers were isolated from the seawater and sewage, the  
296 literature suggested that they were undergoing decay processes in space and time due to the  
297 dynamic estuarine environment (Kay *et al.*, 2005). In this modelling work, the decay process  
298 of the tracers is presented as a simple first order degradation, with the decay rate being  
299 represented by  $T_{90}$  values (Schnauder *et al.*, 2007) as in the following equation:

$$300 \quad k_b = -\frac{\ln 10}{T_{90}} \quad (8)$$

301 Initially, the decay process of the microbial tracers was modelled at the constant rates of  
302 spatial and temporal resolution, with the  $T_{90}$  values tested in the range of 2.5 – 20 hours. The  
303 constant decay rate reduced the total mass of the released microbial tracers exponentially with  
304 time, with the effects of the estuarine environmental dynamics being excluded to gain an  
305 understanding of the impact of the decay process.

306 In considering the effects of the estuarine environmental dynamics, especially the  
307 inactivation of microbial tracers with sunlight, the decay process was modelled using different  
308 rates during day and night times. The  $T_{90}$  value was set as a spatial constant in the range of 2.5  
309 – 20 hours during day time, and increasing in the range of 30 – 60 hours during night time. The  
310 process was modelled from 6 am to 6 pm using the day time decay, then followed by the night  
311 time decay for the next 12 hours etc.

312 The simple first order degradation is an approach used to represent the survival of the  
313 microbial tracers in natural waterbodies but, in reality, the process is non-linear as microbial  
314 inactivation interacts with the dynamic environment. Several studies of the bacterial survival  
315 in a natural waterbody have suggested that bacteria undergo a two-stage degradation as they  
316 are exposed (Bowie *et al.*, 1985; Crane and Moore, 1986). The model equation used for this  
317 modelling work can be written as:

$$318 \quad C_t = C_0 \exp^{-kt} + C_0' \exp^{-k't} \quad (9)$$

319 where  $C_t$  is the bacteria concentration at time  $t$ ,  $C_0$  and  $C_0'$  are the initial microbial  
320 concentrations for two hypothetical stages, and  $k$  and  $k'$  are the constant decay rates for two  
321 hypothetical microbial stages. The decay rates can also be represented by the  $T_{90}$  values, as  
322 given in Equation 8. Figure 8 illustrates the total mass balance for the typical bacteria after  
323 undergoing the two-stage decay process.

324 The two-stage microbial decay is a process of combining the two first-order kinetic decay  
325 processes that occur simultaneously, with the two hypothetical microbial groups that decay at  
326 different rates. The first stage decay process takes place with the microbial group with higher  
327 initial counts and with a higher decay rate. This decay process, which occurs over a short  
328 period, also considers the environmental shock effect to the bacteria as they are introduced to  
329 the natural waterbody for the first time. The second stage decay results in the remaining bacteria  
330 being of a lower initial count, with the lower rate. The rates for both the first and second stage  
331 decay rates are functions of salinity, temperature, and solar radiation and turbidity. Table 2  
332 illustrates the specific values of parameters used for the two-stage microbial decay model of  
333 this work.

334

### 335 **3. Results and discussion**

#### 336 ***3.1 Hydrodynamic modelling process***

337 Figure 9 illustrates a typical comparison between model predictions and measured field  
338 data, for water levels at Ilfracombe, Mumbles, Hinkley Point and Newport, with the locations  
339 being shown in Figure 2. The data for validation of the water levels was acquired from the  
340 National Oceanography Centre, with the Bristol Channel Admiralty Chart 1179 being used for  
341 validation of the tidal currents and a typical comparison of the predicted and measured tidal  
342 current speeds and directions being shown in Figure 10. The results of the hydrodynamic  
343 validation during spring tides are shown in Figures 9 and 10 for water level and tidal currents,

344 respectively. The modelled water levels and tidal currents agree well with the measured and  
345 referred data, for both spring and neap tides. The validated hydrodynamic model gave  
346 confidence in proceeding to the next modelling stage, both spatially and temporally.

### 347 *3.1.1 Hydrodynamic process at intertidal marshland*

348 The hydrodynamic model predictions were validated using measured data. Model  
349 predictions were validated within the main domain, which showed similar comparisons to those  
350 shown in Figures 9 and 10. There were very limited data available to perform a comprehensive  
351 model calibration and validation study in the main area of interest, i.e. the Loughor Estuary.  
352 This was expected to impact on the quality of the calibration and validation of the model and  
353 therefore the model predictions, particularly in such a complex part of the model domain. The  
354 model water level and tidal current predictions at Burry Port, Llanelli, and Lliw were compared  
355 to the measured data as shown in Figure 13. It was observed that the predicted tidal currents at  
356 Burry Port were improved by implementing the refined and improved bathymetry and  
357 topography across the Loughor Estuary, although the predicted water levels did not  
358 significantly change between the unrefined and refined modelling domains, as shown in  
359 Figures 14 and 15. However, more current data are required for a comprehensive calibration  
360 and validation of the model, with the bottom roughness representation in this area being  
361 particularly significant since the bathymetry has been refined, particularly across the  
362 marshlands and dunes.

363 The flooding process predictions over the intertidal floodplains of the Loughor Estuary,  
364 for high and low water, are shown in Figures 16 and 17, respectively. The figures show that  
365 Llanrhidian Marsh, located on the Southern bank of the estuary, was flooded to a level in excess  
366 of 10 cm depth during high water. This emphasises the importance of implementing the  
367 extended bathymetry for this study site.

### 368 *3.1.2 Hydrodynamic process at release and sampling locations*



369 Figures 18 and 19 illustrate the predicted water depths and/or water levels, and tidal  
370 current speeds and directions at the release and sampling locations, respectively. It is worth  
371 noting that the hydrodynamic processes at the release sites are dependent on the tidal process,  
372 together with the river discharges from upstream of the Loughor catchment.

373

### 374 **3.2 Tracer transport and decay modelling processes**

#### 375 *3.2.1 Transport calibrations*

376 The results, as illustrated in Figure 20, show the grid sizes were less sensitive with mass  
377 molecular diffusivity at areas of higher advective transport (sites 408 – 412), but there were  
378 significant effects at areas of lower advective transport (i.e. on the floodplains with dunes and  
379 marshlands). Calibration studies were further conducted to estimate the longitudinal dispersion  
380 values considered of  $10^1 - 10^3$  m<sup>2</sup>/s eddy diffusivity (Chapra, 2008), with results showing the  
381 grid sizes were much more sensitive, even at areas of higher advective transport (sites 408 –  
382 412). The sensitivity analysis reflected that by decreasing the grid size pollutant transport by  
383 dispersion varied more significantly than by advection, thereby highlighting the need to  
384 represent the contribution of the natural bed features as accurately as possible.

385 Figure 21 illustrates the calibration results of dispersion transport for a range of estuarine  
386 longitudinal dispersion coefficients and based on comparisons with the measured data. At  
387 Loughor Boat Club, the result shows the effect of residual turbulent dispersion on the transport  
388 of the pollutant in the upstream direction, while advection by the ebb current occurs for the  
389 ebbing flow.

390 The zones with higher bottom roughness locally decreased the advective transport of the  
391 tracer mass when compared to the base value. However, limited currents data in the main  
392 channels and the marshlands were available to accurately validate the roughness values for the  
393 various zones. This is due to the tidal range and limitations of the main channel and the nature

394 of the marshlands. Since there only one source of tracer existed in the estuary (Wyer *et al.*,  
395 2014), microbial tracer could be used to validate the model hydrodynamics and the roughness  
396 values used for the various zones. This was based on the view that accurate tracer predictions  
397 required accurate hydrodynamic model predictions. The tracer concentration results at the  
398 estuarine transport scale using different roughness scenarios are illustrated in Figure 22. This  
399 Figure shows a significant reduction in the lateral transport rates with increased bottom  
400 roughness values from the middle of estuarine channels to the marshlands, but slightly  
401 increased transport rates longitudinally, with decreased bottom roughness values from the  
402 upstream channel to the estuarine downstream region. The reduction in the tracer concentration  
403 at Loughor Boat Club was deemed to be more significant, in comparison with the concentration  
404 at Burry Port Harbour with the increased bottom roughness values, as illustrated in Figure 23.  
405 However, these changes in the roughness reduced the tracer concentration at significant  
406 amounts for the zones of sand dunes and marshlands at the Southern region of the estuary.  
407 Calibration of the hydrodynamics based on tracer transport required tracer monitoring at  
408 various points in each zone. Due to the lack of this type of tracer concentration observations,  
409 tracer concentrations could not be used in selecting an accurate value for each roughness zone  
410 in this study. Therefore, variable bed roughness values could not accurately be justified and  
411 subsequently were not utilised in this study.

### 412 3.2.2 Decay calibrations

413 By modelling the microbial tracer decay with constant rates in space and time, this basic  
414 decay process is incapable of simulating any interactions between the tracer decay and the  
415 dynamic estuarine environment. The  $T_{90}$  values tested were from 2.5 to 20 hours, as illustrated  
416 in Figure 24, however reducing the magnitude of the predicted tracer concentrations to the level  
417 of measured data, suggested the correct range of microbial decay rates for the estuarine  
418 environment.

419 The exponential mass reduction of the microbial tracer for constant rates continuously  
420 decreased the tracer concentration at the sampling locations, but these values were not suitable  
421 in comparison with the measured data for longer periods. The results also suggested that the  
422 decay rate of the microbial tracer was higher during the early release and reduced gradually  
423 with time as the mass was transported, in an analogous manner to the environmental shock  
424 process.

425 Following the decay modelling of the microbial tracer using different decay rates for day  
426 and night times, the approach showed an improvement to the modelled results, for the alternate  
427 lower and higher ranges of the  $T_{90}$  values during day and night times respectively. The  
428 improvement in the modelled results, however, only occurred for a duration period of less than  
429 12 hours.

430 As illustrated in Figure 25, at Loughor Boat Club, the modelled concentration converged  
431 to the measured data for the duration of 12 hours, beginning from 281 JD (Julian date) at 6 pm  
432 with day-night  $T_{90}$  values of 5-60 hours, followed for the next 12 hour duration with day-night  
433  $T_{90}$  values of 7.5-60 hours, and continuously in the same pattern. The predicted concentrations  
434 at Burry Port Harbour also improved in comparison with measured values when different day  
435 and night time decay rates were used.

436 The microbial tracer inactivation by sunlight is dynamic in time and space, which depends  
437 on the intensity of radiation due to both atmospheric conditions and light penetration through  
438 the water column. However, a simplification of this process is required to gain an  
439 understanding of the decay sensitivity due to the effects of sunlight.

440 Figure 26 illustrates the transport results of the modelled microbial tracer after  
441 considering the two-stage decay processes at Loughor Boat Club and Burry Port Harbour. From  
442 the results of the two-stage decay, the first peak of concentration of the tracer at Burry Port  
443 Harbour was overestimated when compared with the measured data, but the subsequent peaks

444 in concentration closely matched the measured data. This is because the first peak results from  
445 the first stage mass of the 3 hours  $T_{90}$  value. The  $T_{90}$  value of less than 3 hours for the first  
446 stage decay could be used for modelling correctly the process at Burry Port Harbour.

447 The modelled microbial tracer concentrations at Loughor Boat Club were estimated  
448 closely and within the range of measured data for all of the concentration peaks, which  
449 represented the correct initial tracer mass of 99% for the second stage decay within the  $T_{90}$   
450 value range of 50 to 125 hours. The significant decrease from the second to the third peak  
451 concentration at Loughor Boat Club is thought to be due to the effect of solar radiation and the  
452 dispersion process.

453 The results of the modelled microbial tracer during slack and low tides at Loughor Boat  
454 Club are estimated correctly compared to the measured data, which also represents a proper  
455 flushing effect from the upstream discharge of the river catchments, at  $5 \text{ m}^3/\text{s}$  that being  
456 included for this modelling work. Elliot *et al.* (2012) also estimated the average river discharges  
457 to be approximately  $5 \text{ m}^3/\text{s}$  from the upstream catchments.

458

#### 459 **4. Conclusion**

460 A hydro-environmental model of the Severn Estuary and Bristol Channel was set up to  
461 study microbial tracer transport processes within the basin and, in particular, the Loughor  
462 Estuary. Due to the complex nature of the bacterial sources in the estuary, such as diffuse  
463 sources from the marshlands, the model was extended to include the entire wetted area of the  
464 estuary by merging the bathymetry and LiDAR data over the floodplains etc. Due to  
465 inaccuracies in the available LiDAR data, associated with surveys undertaken during high  
466 water, various sources of data and interpolation were used. To model all of the complex  
467 features in the estuary accurately, the extended model was refined to a high resolution of about

468 10 m. This increased the computational cost significantly and required the use of the High  
469 Performance Computing (HPC) facilities at Cardiff University, namely Raven.

470 The refined model was calibrated against water levels and current data available for the  
471 Loughor Estuary. However, it was clear that the available data were limited and more water  
472 levels and current speeds and directions are required for any more comprehensive model  
473 calibration and validation study in the future. These sources were included in the model, and  
474 the concentration of tracers at each of the five different sampling locations, were predicted  
475 using the model. These predictions were compared with the measured data to calibrate and  
476 validate the model and improve on our understanding of the governing transport processes in  
477 the estuary. Initially the tracers were assumed to be conservative and the model was setup and  
478 calibrated for transport by the dispersion processes. The model was also setup using varying  
479 bottom friction zones to improve the on the representation of the hydrodynamic and tracer  
480 advection processes. It was noted that the tracer transport processes were influenced by  
481 including different bottom friction representations in the model, which highlighted the potential  
482 for implementing tracer studies for future validation studies of hydrodynamic simulations. In  
483 particular, implementing a varying bed roughness coefficient was shown to be more realistic  
484 in representing the changing bed roughness characteristics, known to occur across the estuary  
485 from visual inspection and historical observations. However, different roughness zones could  
486 not be validated due to a lack of available tracer observations at these zones. Changes in  
487 concentrations as a result of different zones were more significant over the dunes and  
488 marshlands, which highlights the future need for further data for improved model calibration  
489 and validation across these region.

490 A mass balance analysis of the model was then undertaken for the tracer to ensure that  
491 the tracer was conserved within the model. It was thought that removal of tracer from the  
492 system due to mortality or, interaction with the sediments, vegetation or some other water

493 quality constituent could affect the tracer transport processes and the corresponding predicted  
494 concentrations (Malham *et al.*, 2014). This removal process was modelled using a first-order  
495 decay rate, followed by different day and night time decay rates, and a two-stage decay process.  
496 Finally, model predictions indicated that the tracer did not flush out of the estuary immediately,  
497 with this result having important implications in terms of faecal bacteria residence times within  
498 the estuary. However, this needs to be studied further by implementing a well calibrated model.

499

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