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

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Abstract: The Loughor Estuary is a macro-tidal coastal basin, located along the Bristol Channel, in the South West of the U.K. The maximum spring tidal range in the estuary is up to 7.5 m, near Burry Port Harbour. This estuarine region can experience severe coastal flooding during high spring tides, including extreme flooding of the intertidal saltmarshes at Llanrhidian, as well as the lower industrial and residential areas at Llanelli and Gowerton. The water quality of this estuarine basin needs to comply with the designated standards for safe recreational bathing and shellfish harvesting industries. The waterbody, however, potentially receives overloading of bacterial inputs that enter the estuarine system from both point and diffuse sources. Therefore, a microbial tracer study was carried out to get a better understanding of the faecal bacteria sources and to enable a hydro-environmental model to be refined and calibrated for both advection and dispersion transport. A two-dimensional hydro-environmental model has been refined and extended to predict the highest water level covering the inter-tidal floodplains of the Loughor Estuary. The validated hydrodynamic model for both water levels and currents, was included with the injected mass of microbial tracer, i.e. MS2 coliphage from upstream of the estuary, and modelled as a non-conservative mass over several tidal cycles through the system. The calibration and validation of the transport and decay of microbial tracer was undertaken, by comparing the model results and the measured data at two different sampling locations. The refined model, developed as a part of this study, was used to acquire a better understanding of the water quality processes and the potential sources of bacterial pollution in the estuary.

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

1. Introduction

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

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

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

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

2. Materials and methods

2.1 Study area

The Loughor is a macro-tidal estuary that flows into the Bristol Channel, with a maximum spring tidal range of up to 7.5 m near Burry Port (see Figure 1). The area is well-known for shellfish harvesting, with related processing industries being located in the vicinity of bathing water sites. Llanrhidian saltmarshes, located on the South bank of the estuary, are subjected to a number of designations (i.e. protection of natural ecosystems) which include a Site of Special Scientific Interest (SSI), Special Area of Conservation (SAC), Special Protection Area (SPA), a Ramsar Site (following an intergovernmental Ramsar treaty for the protection of wetlands) (TRCS), and a National Nature Reserve (NNR) (Youell et al., 2013a; Youell et al., 2013b). However, the saltmarshes are legally used for sheep grazing activities during low tides. The animal faeces left on the saltmarshes are suspected to be one of the main sources of pathogen inputs to the estuarine receiving waters after the saltmarsh floods on the rising tide. The other main source of pathogen input to the estuary are the Llanelli and Gowerton WWTWs, as well as a few shellfish processing plants. An overview of the key sites in the Loughor Estuary, including the siting of these potential sources of faecal indicator organisms (FIOs) into the estuary is shown in Figure 1.

2.2 Modelling system

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

The TMS solutions for the depth-averaged SWEs that derived from the NSEs require approximations for the simplification. The fluid is assumed to be Newtonian, incompressible and homogenous in the vertical plane, and the long wave approximation is adopted, i.e. the pressure remains hydrostatic in the vertical direction. The NSEs are averaged over the depth and Reynolds decomposition and stochastic averaging are applied for modelling the turbulence processes. Bottom friction is modelled by using non-linear laws for velocity, such as the Chezy, Strickler or Nikuradse friction laws. The SWEs implemented in the TMS use the non-divergent form of the momentum equation, which are derived by substituting the continuity equation into the two momentum equations in the x- and y-directions (Lang 2010).

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

$$\frac{\partial h}{\partial t} + \vec{u}.\overrightarrow{grad}(h) + h\,div(\vec{u}) = S_h \tag{1}$$

$$\frac{\partial u}{\partial t} + \vec{u}.\overrightarrow{grad}(u) = -g\frac{\partial Z_s}{\partial x} + F_x + \frac{1}{h}\,div\left(h\nu_t.\overrightarrow{grad}(u)\right) \tag{2}$$

$$\frac{\partial v}{\partial t} + \vec{u}.\overrightarrow{grad}(v) = -g\frac{\partial Z_s}{\partial y} + F_y + \frac{1}{h}\,div\left(h\nu_t.\overrightarrow{grad}(v)\right) \tag{3}$$

$$\frac{\partial T}{\partial t} + \vec{u}.\overrightarrow{grad}(T) = \frac{1}{h}\,div\left(h\nu_T.\overrightarrow{grad}(T)\right) + S_T \tag{4}$$

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

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

$$\frac{\partial k}{\partial t} + \vec{u}.\overrightarrow{grad}(k) = \frac{1}{h}\ div\left(h\frac{\nu_t}{\sigma_k}\overrightarrow{grad}(k)\right) + P - \varepsilon + P_{kv} \tag{5}$$

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

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

2.3 Model setup

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

The unstructured triangular mesh was generated to set up to cover the model domain, by using the BlueKenue mesh generator. The generated mesh also included the solid boundaries of Caldey Island at the outer Bristol Channel, and Flat Holm and Steep Holm Islands at the end of the Severn Estuary. To achieve high grids resolution within the Loughor Estuary, while maintaining the model efficiency, the edge length of the grids was set to vary from 1000 m close to the seaward open boundary and decreased down to 20 m in the Loughor Estuary, producing 711,106 unstructured triangular cells and 358,266 nodes. The bathymetric data in the horizontal plane were specified relative to Ordnance Datum Newlyn (ODN) and Universal Transverse Mercator (UTM) projection of Zone 30N respectively, with interpolation being used to provide data at the mesh nodes, using the inverse distance interpolation method. The generated mesh with the bathymetry interpolation of the model domain is shown as in Figure 2, with the deepest bottom elevation of approximately 65 m being shown near the model seaward open boundary and decreasing towards the eastern boundary in the River Severn.

2.4 Hydrodynamic calibration

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

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

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

2.5 Domain extension over intertidal marshlands

It was understood that the flooding processes over the intertidal floodplains, including marshlands, dunes and diffuse source pollutant inputs, at high tide could potentially have a significant impact on the water quality processes within estuaries (Grant *et al.* 2001; Weiskel *et al.* 1996; Evanson and Ambrose 2006; Sanders *et al.* 2005), including the Loughor Estuary. However, the entire intertidal floodplains, marshlands and dunes, which were flooded at high water, did not have bathymetric data. Therefore, it was decided to extend the existing model to include the marshlands and dunes using a high-resolution grid. Since the bathymetric data did not cover these areas with sufficient high quality, the extension had to be carried out by merging LiDAR (Light Detection And Ranging) and interpolation of bathymetric data. The LiDAR data for the topography covering the areas of Carmarthen Bay, the Loughor Estuary, and Swansea Bay, at the north-western side of the model domain, were provided by Environment Agency Geomatics (Natural Resources Wales, 2015). The topographic data were provided as the 'bare earth' Digital Terrain Models (DTM), with a resolution of 2 m in 1 km x 1 km tile sizes. The multiple data tiles were embedded into a tile size of 10 km x 10 km to ease the data processing. The data initially provided were referred spatially to the British National Grid coordinate system, which was re-projected onto the WGS 1984 UTM Zone 30N coordinate system, using the geographic transformation for petroleum to match the other parts of the domain. The data were referenced vertically, as for the bathymetric data relative to Ordnance Datum (OD) at Newlyn. The resolution of the projected data tiles was reduced to 8 m, to reduce the mapping time while maintaining a high resolution.

The projected data tiles were used to generate a new boundary line for extensions of the model domain in the regions of Carmarthen Bay, the Loughor Estuary, and Swansea Bay. Contour lines at 10 m level were generated from each data tile, with the shape file format provided being converted into a DXF file format. The merging work for a new shoreline of the domain extensions was carried out using the AutoCAD program. The original boundary lines at the areas for extension were extended to the new generated 10 m contour lines. The extended model covering the floodplains in Carmarthen Bay, the Loughor Estuary, and Swansea Bay is shown in Figure 3. The red dashed line in Figure 3 depicts the model boundary before refinement. The mesh generator of Blue Kenue software (Canadian Hydraulics Centre, 2011) was used to refine the grid in order to extend the domain. The new generated shoreline was used for the closed boundary, covering the areas of the domain extension. The grid size in the original model of 1000 m resolution was reduced to 200 m resolution for the offshore region surrounding Carmarthen Bay and Swansea Bay. The grid size in the Loughor Estuary was further refined from 200 m resolution to a minimum of 10 m, as shown in Figure 3. The grid size was set to be a linear function of the bottom elevation in the range between -5 and 5 m over the intertidal floodplains. The refinements obtained from the linear function, applied to the bottom elevation, were for accurately capturing the bathymetry-topography data to nodes of the mesh and representing complex geometries over the intertidal floodplains, especially with the finer grid resolution closer to the waterfront, where the wetting-and-drying processes occurred. The grid refinement across the intertidal floodplains, together with the natural and manmade features of the Loughor Estuary, are shown in Figure 4.

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

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

2.6 Tracer transport and decay modelling

The microbial tracer study was conducted for the Smart Coasts Sustainable Communities project within the Loughor Estuary, to examine connections between pathogen sources and impacts at locations of interest in the estuary and nearby bathing water designated sites (Wyer *et al.,* 2014). The microbial tracers were released simultaneously at four different locations, approximately one hour after high spring tides. The released sites were at Great Pill (site 101) – a tidal channel draining via Llanrhidian Marsh, the Morlais River (site 201) – a tidal channel at Crofty draining via Salthouse Pill, Loughor Bridge (site 501) – a bridge crossing the Afon Llwcher tidal channel, near the discharge from Gowerton sewage treatment works, and the Afon Lliedi (site 601) - a tidal channel draining via Llanelli into the estuary. These sites are shown in Figure 6 using purple triangles. Each microbial tracer was measured at 5 sampling sites, including Rhossili DSP (site 408), Broughton a potential designation site (site 409), the Loughor Boat Club at the upstream end of the estuary (site 410), Burry Port harbour, which is close to the shellfish beds (site 411), and Pembrey DSP (site 412), with these field monitoring sites being shown in Figure 6 with green circles.

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

Four types of microbial tracers were released at each of these locations to represent the microbial source tracking from different pollutant sources (Wyer *et al.,* 2014). *Serratia marcescens* phage was released at site 101 over 14 minutes, with a total dose of 2.75E+16 pfu. *Enterobacter cloacae* phage was released at site 201 over 7 minutes, with a total dose of 4.50E+16 pfu. MS2 coliphage was released at site 501 over 11 minutes to produce a total dose of 4.00E+17 pfu. The ϕX174 phage was released at site 601 over 3 minutes, with a total dose of 2.00E+15 pfu. Table 1 summarises details of the released microbial tracers into the Loughor Estuary. The application of bacteriophage as a source for tracking and similar work have been conducted elsewhere, such as Simpson *et al.,* (2002); Shen *et al.,* (2008).

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

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

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

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

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

$$k_b = -\frac{\ln 10}{T_{90}} \tag{8}$$

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

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

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

$$C_t = C_0 \exp^{-kt} + C_0{'} \exp^{-k't} \tag{9}$$

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

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

3. Results and discussion

3.1 Hydrodynamic modelling process

Figure 9 illustrates a typical comparison between model predictions and measured field data, for water levels at Ilfracombe, Mumbles, Hinkley Point and Newport, with the locations being shown in Figure 2. The data for validation of the water levels was acquired from the National Oceanography Centre, with the Bristol Channel Admiralty Chart 1179 being used for validation of the tidal currents and a typical comparison of the predicted and measured tidal current speeds and directions being shown in Figure 10. The results of the hydrodynamic validation during spring tides are shown in Figures 9 and 10 for water level and tidal currents, respectively. The modelled water levels and tidal currents agree well with the measured and referred data, for both spring and neap tides. The validated hydrodynamic model gave confidence in proceeding to the next modelling stage, both spatially and temporally.

3.1.1 Hydrodynamic process at intertidal marshland

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

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

3.1.2 Hydrodynamic process at release and sampling locations

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

3.2 Tracer transport and decay modelling processes

3.2.1 Transport calibrations

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

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

The zones with higher bottom roughness locally decreased the advective transport of the tracer mass when compared to the base value. However, limited currents data in the main channels and the marshlands were available to accurately validate the roughness values for the various zones. This is due to the tidal range and limitations of the main channel and the nature of the marshlands. Since there only one source of tracer existed in the estuary (Wyer *et al.*, 2014), microbial tracer could be used to validate the model hydrodynamics and the roughness values used for the various zones. This was based on the view that accurate tracer predictions required accurate hydrodynamic model predictions. The tracer concentration results at the estuarine transport scale using different roughness scenarios are illustrated in Figure 22. This Figure shows a significant reduction in the lateral transport rates with increased bottom roughness values from the middle of estuarine channels to the marshlands, but slightly increased transport rates longitudinally, with decreased bottom roughness values from the upstream channel to the estuarine downstream region. The reduction in the tracer concentration at Loughor Boat Club was deemed to be more significant, in comparison with the concentration at Burry Port Harbour with the increased bottom roughness values, as illustrated in Figure 23. However, these changes in the roughness reduced the tracer concentration at significant amounts for the zones of sand dunes and marshlands at the Southern region of the estuary. Calibration of the hydrodynamics based on tracer transport required tracer monitoring at various points in each zone. Due to the lack of this type of tracer concentration observations, tracer concentrations could not be used in selecting an accurate value for each roughness zone in this study. Therefore, variable bed roughness values could not accurately be justified and subsequently were not utilised in this study.

3.2.2 Decay calibrations

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

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

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

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

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

Figure 26 illustrates the transport results of the modelled microbial tracer after considering the two-stage decay processes at Loughor Boat Club and Burry Port Harbour. From the results of the two-stage decay, the first peak of concentration of the tracer at Burry Port Harbour was overestimated when compared with the measured data, but the subsequent peaks in concentration closely matched the measured data. This is because the first peak results from the first stage mass of the 3 hours T_{90} value. The T_{90} value of less than 3 hours for the first stage decay could be used for modelling correctly the process at Burry Port Harbour.

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

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

4. Conclusion

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

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

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

A mass balance analysis of the model was then undertaken for the tracer to ensure that the tracer was conserved within the model. It was thought that removal of tracer from the system due to mortality or, interaction with the sediments, vegetation or some other water quality constituent could affect the tracer transport processes and the corresponding predicted concentrations (Malham *et al.*, 2014). This removal process was modelled using a first-order decay rate, followed by different day and night time decay rates, and a two-stage decay process. Finally, model predictions indicated that the tracer did not flush out of the estuary immediately, with this result having important implications in terms of faecal bacteria residence times within the estuary. However, this needs to be studied further by implementing a well calibrated model.

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