Scenarios of intermittent *E. coli* contamination from sewer overflows to shellfish growing waters: the Dart Estuary case study

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Abstract

Sewage overflows (SOs) and Combined Sewer Overflows (CSOs) significantly contribute to the bacterial contamination of coastal waters, which is of especial concern for aquaculture, a growing industry worldwide. Hydrodynamic and water quality models were used to investigate impacts of CSO discharge frequency and duration, river discharge and tides on *Escherichia coli* levels at shellfish farming sites in the Dart Estuary (UK), being the employed methodology generally applicable. High *E. coli* contamination occurred during neap tides and high river discharges due to higher retention and lower bacterial decay. Synchronicity of CSO spills affected the duration of the pollution episodes rather than peak concentrations, more influenced by discharges of the neighbouring CSOs. During peak discharges, *E. coli* concentrations could be 10 times higher than during average flows. CSO spills were more frequent when rainfall was >20 mm. Model outputs combined with rainfall forecasts can indicate microbiological contamination risk in the aquaculture sites.

Highlights:

- A 3D-hydrodynamic and *E. coli* dispersal model was developed for the Dart Estuary.
- *E. coli* inputs from sewer overflows peak during neap tides and high river discharge.
- *E. coli* concentration is highly dependent on the decay model.
- Sewer overflow spills in the Dart are frequent when rainfall exceeds 20 mm.
- Model can be used to predict *E. coli* contamination at shellfish farming sites.

Keywords
Sewage contamination, Dart Estuary (UK), impact assessment, TELEMAC, faecal indicator organisms, shellfish health.

1. Introduction

Sewage contamination is one of the most important issues affecting coastal water quality and sewer overflows (SOs), i.e. overflows from combined (foul and surface water) sewers and from storm water holding tanks at sewage treatment works, feature as the second most important source affecting the quality of surface waters in Europe (European Environment Agency, 2018). To provide clarity, in this study we will use the term Combined Sewer Overflows (CSO), although both types exist. In the UK, a substantial proportion of serious pollution incidents to water are caused by CSOs (Environment Agency, 2016) and future improvements to these discharges are considered key to meet microbiological standards set out by water quality legislation (Defra, 2012). To achieve this, water quality managers require tools to characterise discharge frequency and volumes from CSOs, and the fate and transport of contaminants in receiving waters (Environment Agency, 2018). Modelling has been an integral part of many coastal pollution reduction programmes for characterisation of both quantitative and qualitative aspects of CSO discharge effects. Models used for these purposes usually comprise a hydrodynamic component to represent the advection and dispersion of the discharges and a water quality component to represent the quality of the discharge and subsequent contaminant fate (National Research Council, 2009). In general, the former is easier to calibrate and verify than the latter because contaminant fate and transport are more complex to simulate (National Research Council, 2009) and data are not readily available. This is particularly the case of contaminants such as *E. coli,* which are highly episodic and can vary by several orders of magnitude in very short time and space increments.

In this paper we focus on the Dart Estuary, located on the south west coast of England. Commercial use of the estuary includes shipping, marine services, fisheries and tourism, the latter being mostly water based (e.g. boating, fishing, canoeing). The cultivation of Pacific oysters (Crasostrea gigas) in the Dart Estuary dates to the 1960s and there are several sites currently used for this purpose at Waddeton and Long Wood (Cefas, 2011). UK water and sewerage companies have made substantial investments to improve the performance of wastewater treatment and reduce the number of water pollution incidents in shellfish water protected areas (SWPAs) (Environment Agency, 2018; Environment Agency & Natural England, 2017). In the Dart catchment, the largest sewage treatment works (STW), Totnes STW and Dartmouth STW, have been upgraded to include full treatment and ultraviolet (UV) disinfection or membrane bioreactors. However, despite these improvements, the SWPA in the upper Dart Estuary at Waddeton has not complied with the Guideline (G) microbiological standard of the Shellfish Water Protected Areas Directions (SWPAD) 2016 (formerly prescribed by the Shellfish Waters Directive) since its designation in 1999 (Environment Agency, 2015). Furthermore, there have been periodic downgrades in the microbiological classification of shellfish farming sites (Cefas, 2010), indicating that the shellfish have been frequently exposed to microbiological pollution in this part of the estuary. Currently, the SWPA is affected by CSO discharges to the estuary, particularly during prolonged rainfall events (Environment Agency, 2015). Shellfish in the Dart rapidly accumulate peak levels of *E. coli* and maintain these for several days after the rainfall events (Campos et al., 2011). This contamination pattern has been observed in other catchments in England where CSOs contribute a substantial proportion of microbiological contamination to coastal waters during high-flow events (Crowther et al., 2011). Policies introduced to mitigate the effect of CSO discharges include the permit system for shellfish waters, operated by the Environment Agency.

To reduce the number of CSO spills to an average of 10 spills/annum and help achieve the microbiological objective for the Dart SWPA by 2027, the Environment Agency (EA) recommended further work to reduce diffuse pollution from agricultural land and resolution of operational issues at STWs to reduce the frequency and duration of CSO spills (Environment Agency, 2015).

In this paper, we report results of a three-dimensional (3D) hydrodynamic and water quality model for the Dart Estuary to investigate the impacts of CSOs on the microbiological quality of the SWPA at Waddeton. The focus of this modelling study is *E. coli,* which is the bacterial indicator used to classify the extent of microbiological (faecal) contamination in shellfish harvesting areas (European Parliament and Council of the European Union, 2019) and verify compliance with the SWPA Directions G standard (Defra and Natural Resources Wales, 2016).

Hydrodynamic models in both 2D and 3D form have been used to simulate estuarine hydrodynamics in many countries for many years. The TELEMAC system in particular, is well suited to this type of study as its unstructured grid and finite element structure allows the best combination of high resolution and computational efficiency. By adopting a baroclinic, 3D version, we aimed to recreate processes of temperature and salinity development and the saltwater stratification and incursion during tidal cycle. These are important features to incorporate salinity and temperature into the computation of *E. coli* concentration in the flow. This is, to our knowledge, the first modelling study of this kind carried out in the Dart Estuary.

The model presented here was forced with averaged and peak CSO overflows from 28 discharge points to help us better understand the response of *E. coli* concentrations to variable water flows in the estuary (as determined by river discharges and tides). A preliminary study on the rainfall conditions that induced the CSO spills was also carried out, which constitutes a first step towards a forecasting system of *E. coli* pollution in the Dart Estuary. The model can be used as a tool to provide water resource managers with information to support pollution reduction measures and improve compliance of the shellfish water with microbiological standards and, consequently, to achieve better and more consistent microbiological quality of harvested shellfish.

2. Material and methods

2.1 Study site

The Dart Estuary and its catchment are located in Devon, on the south west coast of England (Fig. 1). Its catchment is an area of 470 km^{2,} with moorland drained by steep wooded valleys in the upper catchment and relatively low-lying undulating agricultural land in the lower reaches. The catchment is rural, relatively sparsely populated, with populated centres, Totnes at the head of the estuary, and Dartmouth at its mouth. The estuary is sheltered, branched with small tributaries, and narrows significantly towards its upper reaches. It has a macrotidal regime (5.2 m on spring tides; 1.8 m on neap tides) and is an ebb-dominant, type 3 ria (ABPmer and HR Wallingford, 2007). The upper tidal limit of the estuary is at Totnes, approximately 17 km upstream of Dartmouth. Sandflats, mudflats and a few areas of saltmarsh make up most of the intertidal area. In the lower reaches of the estuary, facilities such as slipways, marinas, moorings and boatyards are common.

The main freshwater input to the estuary is the Dart (mean flow=11.4 m^3/s measured at Austins Bridge), at the head of the estuary at Totnes (NERC, 2018). Rivers Hems and Harbourne contribute smaller volumes of freshwater. Discharge rates from all these rivers increase rapidly during rainfall, due to low absorption of the hard geology and steep topography of the upper catchment.

South West Water (SWW) operates sewerage networks serving five water company STWs within 10 km of the tidal limit. The largest discharge volumes are from Totnes STW [(dry weather flow (DWF)=3,967 m^3/day, number 8 in Fig. 1) and Dartmouth STW (DWF=4,644 m^3/day, number 26 in Fig. 1] (both receive UV disinfection) and from two small STWs (Harbertonford STW, DWF=242 m^3/day; Ashprington STW, DWF=98 m^3/day) (both receive secondary treatment) (Fig. 1). The network is also served by more than 20 CSOs, half of which discharge near Totnes at the head of the estuary and the other half discharge to rivers or directly to the estuary tidal waters, between Dittisham and Stoke Gabriel.

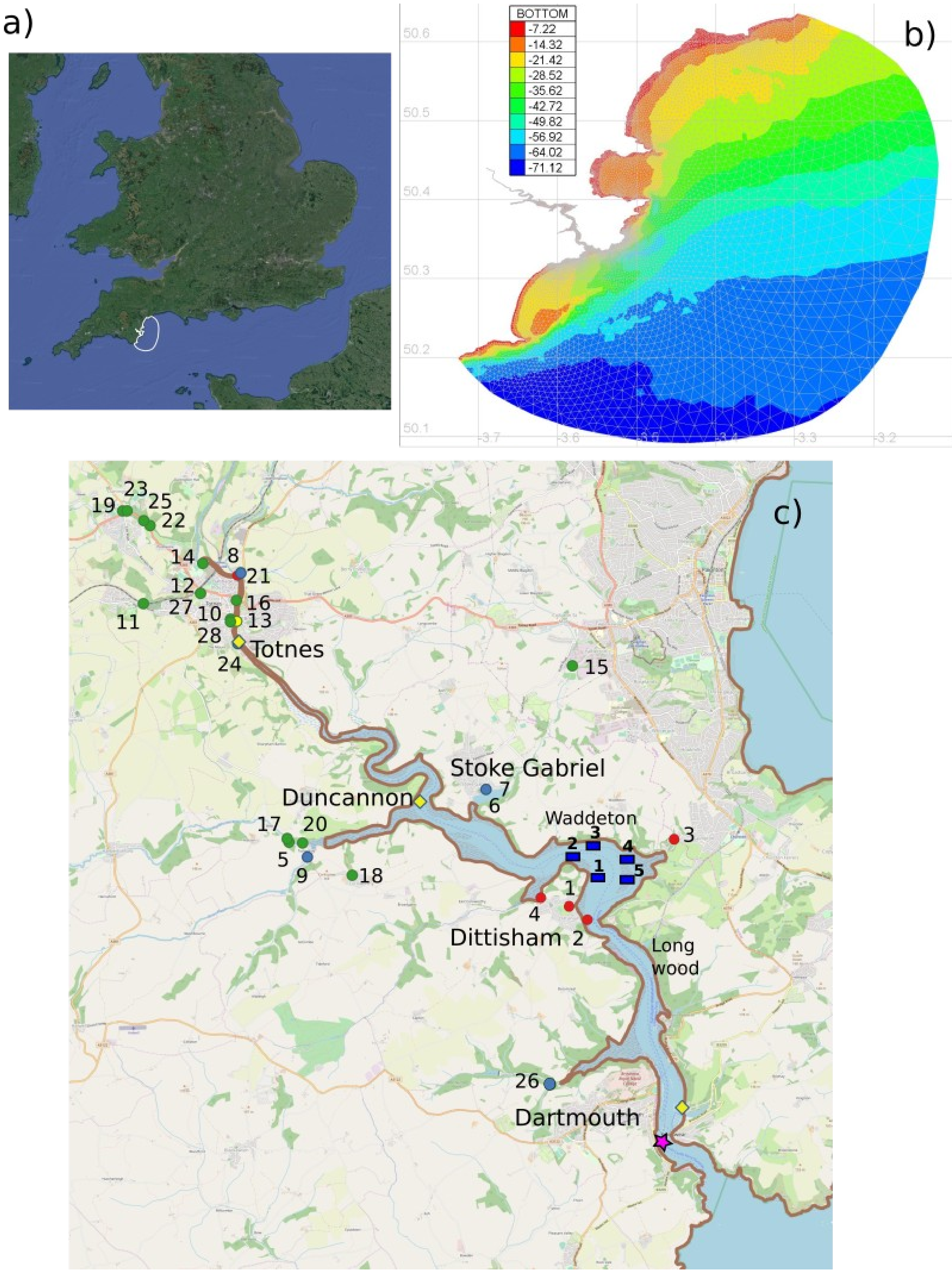

Fig. 1. Location of the study area (outlined in white) on the south west coast of England (a), model bathymetry and mesh (b), and Dart Estuary showing the location of the sewer overflows (CSOs) and shellfish farming sites considered in the study (c). The red circles indicate the CSOs for which spill frequency and duration data are available. The blue circles indicate the CSOs that were not considered in this study. The green circles indicate the remaining CSOs. The blue squares indicate shellfish

farming areas within the Waddeton shellfish water. The yellow diamonds are the locations of the tidal gauges for which water level data are available and the pink star is a location used to validate the model tidal currents.

2.2 Characterisation of storm overflows in the study site

In England, the EA applies a set of standards to the determination of permit (consent) applications for discharges that impact on shellfish waters. For shellfish waters impacted by multiple CSOs, the EA recommends aggregating spills by frequency and volume so that the combined impact of the aggregated spills does not exceed 10-spills per annum or 3% of the time on average (Environment Agency, 2003). However, spills do occur beyond those permitted by the regulations.

Twenty-eight CSOs were identified in the Dart catchment (Fig. 1 and Table 2) for this modelling study. Data on the frequency and duration of sewage spills from these overflows were available from SWW annual spill monitoring reports to the EA (relative to eight CSOs over the period 1 April 2006–31 March 2016, Fig. 2) and sewer network modelling reports (Frischmann, 2001; Hyder, 2012). Time series analysis of data taken from the EA annual reports shows that six CSOs (Totnes STW SO, Stoke Gabriel SPS, Higher Dittisham SPS, Galmpton PS, Ferry Boat Inn PS and Dittisham STW SO) have spilled over longer time periods and/or more frequently than the remaining ones (Fig. 2), with some overlapping among them. For the remaining CSOs, information on the number and duration of spills was obtained from modelling results. In particular, information for the Dartmouth STW was obtained from the Frischmann (2001) report, which briefly describes a model implemented for this CSO applying data for 2001. For the remaining CSOs, Hyder (2012) specifies that the catchment modelling software Infoworks was used to simulate the possible spills into the Dart Estuary from the different catchment areas for summer 2011 (since data were available for model validation in this period) and included a prediction for 2036. The data used to implement these models were: resident population connected to the sewerage catchment, rainfall records in the period 2008–2011 provided by the EA, SWW data obtained through the Supervisory Control and Data Acquisition (SCADA) and the EA Monitoring Certificate Scheme (MCERTS) systems, SWW spill monitoring reports, SWW record drawings and operations information, SWW 2008–2009 STW DWF Base Flow Study, EA defined agglomerations and South Hams District Council Local Plan Review (1995–2011).

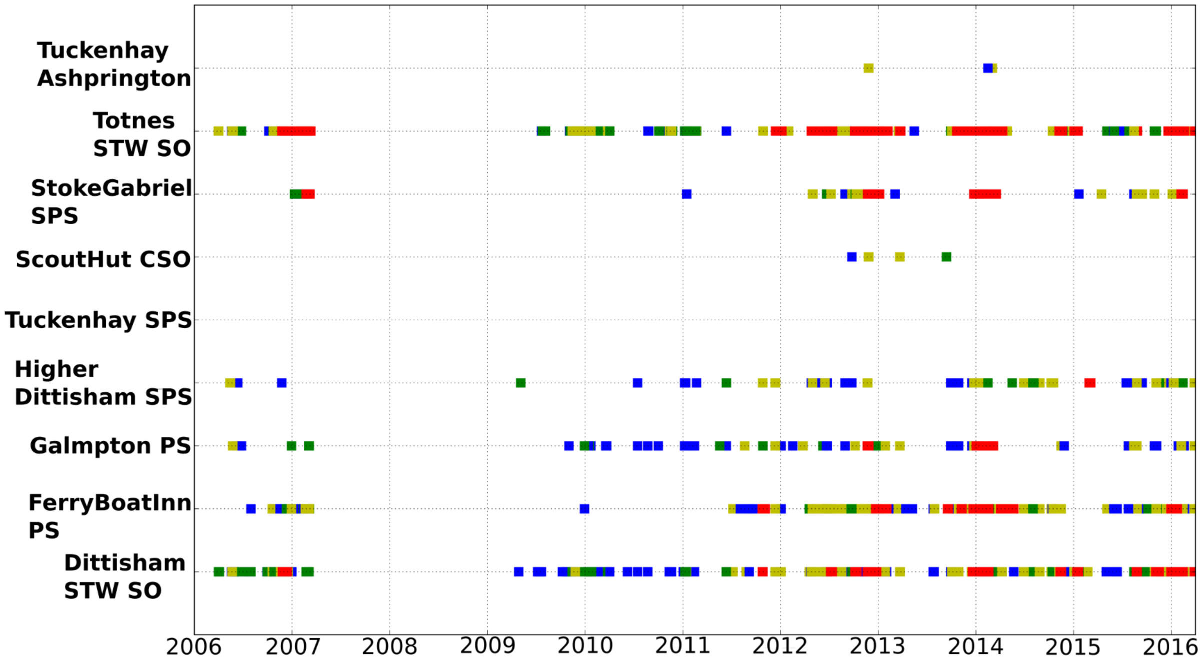

Fig. 2. Sewage spills from eight storm overflows in the Dart Estuary. In blue, spills < 12 h; in green, spills lasting 12–24 h; in yellow, those lasting 24–72 h and in red spills > 72 h.

2.3 Shellfish water regulations and improvements to storm overflows

The UK Government has identified water quality objectives and relevant statutory obligations that water and sewerage companies must observe to meet the requirements of the Water Framework Directive. For SWPAs, the objective is to endeavour to observe a microbiological standard of 300 *E. coli*/100 ml in shellfish flesh for 75% samples in a 12-month period (Defra and Natural Resources Wales, 2016), as determined by the SWPAD. In addition to this standard, the Food Hygiene Regulations (primarily Regulation (EC) No 627/2019) prescribe the harvesting area classification categories for products intended for human consumption. Under these regulations, the class A standard is 230 *E. coli*/100 g in 80% of samples with an upper limit of 700 in the remaining 20% of samples. Shellfish from production sites with *E. coli* concentrations ≤ 4,600/100 g (in 90% of samples, with no sample exceeding 46,000 *E. coli*/200 g) are class B.

For the purposes of water company investment planning for 2020–2025, the EA's design standard for intermittent discharges is ≤ 10 significant spills/year as 10-year average. For this, the significant spill volume for the asset or an agglomeration of assets (that impact collectively) needs to be determined, based on a shellfish water receiving water geometric mean of 5 *E. coli* cfu/100 ml. The affordability of improvements will be subject to cost/benefit criteria and ministerial approval. Where the scheme is not cost-beneficial, a possible future target for CSOs for use in planning investment in 2020–2030 is the 10 significant spills criterion against a geometric mean of 110 *E. coli* cfu/100 ml in the SWPA. This equates to meeting the class B standard of Regulation (EC) No 627/2019 in shellfish flesh.

In the environmental investment programme proposed by SWW for the period 2020–2025, several CSOs are identified for improvement in relation to the Dart SWPA (see Table 1).

Table1. CSOs identified for improvements by SWW in relation to the Dart SWPA in the period 2020-2025

STW/CSO Infrastructure	Figure 1 Reference
Ashprington STW SSO	5
Cornworthy STW SO	18
Fore Street CSO	10
Lower Collapark CSO	27
Northern Villages PS CSO	21
Quarry Close CSO	11
Scout Hut CSO	6
St Johns Terrace CSO	12
St Katherine's Way CSO	28
St Peter's Quay PS CSO	24
Steamer Quay CSO	13
Stoke Gabriel PSCSO/EO	7
Swallowfields Kevics CSO	14
Tor Park Road PS CSO/EO	15
Totnes STW CSO	8
Totnes Town PS CSO/EO.	16

2.4 Hydrodynamic model setup

A three-dimensional hydrodynamic model of the Dart Estuary was built using TELEMAC 3D (v7p2r2; EDF, 2017). The model domain comprises the estuary and the adjacent coastal and offshore waters to allow for a better propagation of the boundary conditions and to investigate the variability of the river plume (Fig. 1b). The domain was discretized by means of an unstructured grid with 12,054 nodes and 22,429 elements in the horizontal and 10 equally spaced layers in the vertical. The refinement in the grid varied spatially, with higher resolution inshore and coarser offshore (resolution range=13-3,843 m). The model bathymetry was mostly obtained from UKSeaMap (2010) with some modifications in the upper estuary to properly reproduce tidal propagation. The boundary conditions for the velocities and surface elevations on the offshore open boundary were obtained from the OSU TPXO European Shelf 1/30º regional model (11 tidal constituents: M2, S2, N2, K2, K1, O1, P1, Q1, M4, MS4 and MN4, see http://volkov.oce.orst.edu/tides/ES.html).

Temperature and salinity were kept constant in space and time along the boundary (12.2 ºC and 35.1, respectively). Freshwater inputs from the River Dart were accounted for in the model by imposing a time series of river runoff as measured at Austin's Bridge. Water temperature and salinity were set at a constant value of 12.2 ºC and 1.0, respectively. It must be noted that, since temperature was defined as a "constant" and no atmospheric forcing was considered in model simulations, water temperature remains constant over time. This approximation is believed not to affect the modelled water circulation in the estuary because the density structure of the water column is mainly driven by salinity variations, being the contribution of temperature negligible (see Priestley, 1998).

In this study, we considered the non-hydrostatic version of the Navier-Stokes equations. The κ-ε turbulence model was selected for the horizontal and vertical dimensions. Wetting and drying were included in the calculations due to the presence of tidal flats. Advection schemes that ensure conservative and monotonic behaviour were selected for tracers (scheme 14 in EDF, 2017). The model was run for a two-month period, starting on 1 December 2015, to capture periods of high and low river discharge and different tidal phases (Fig. 8). The initial seven days of model simulations were considered the spin-up period and hence were not used in the analysis.

2.5 Modelling E. coli transport and decay

The equation used to model the transport and decay of *E. coli* can be expressed as:

$$\frac{\partial EC}{\partial t}+\vec{u}.\vec{\nabla}(EC)=\left(\vec{K}.\vec{\nabla}(EC)\right)-k_d EC, \qquad (1)$$

where EC is the concentration of *E. coli* measured in cfu/100 ml, $\vec{u}$ is the flow velocity, $\vec{K}$ is the diffusion coefficient and k_d is the decay rate for *E. coli*. The left-hand side of Equation (1) represents bacterial advection, the first term on the right-hand side shows the diffusion and the last term accounts for the exponential decay of *E. coli*.

The die-off of faecal bacteria is often represented by a T_{90} parameter, which is defined as the time for bacterial concentration to reduce by 90%. T_{90} is related to the decay rate k_d by the following equation:

$$k_d=\frac{2.3}{T_{90}}. \qquad (2)$$

The decay rate of *E. coli* is a function of several environmental parameters such as temperature, salinity, solar irradiation or degree of sewage mixing (see, for intance Campos et al., 2013; Carneiro et al., 2018 or Alkan et al., 1995). Several models have been proposed to quantify either k_d or T_{90} as a function of some of these variables (see [Chan et al., 2015; Mancini, 1978] or the compilation of different models made by Feitosa et al., 2013), all of them adapted to the local conditions by means of certain parameters. An example of the application of this kind of model in UK waters is found in Gao et al. (2015). A simpler approach in which different constant decay rates for day and night have been considered is published in Abu-Bakar et al. (2017) and Huang et al. (2017).

In this modelling study, we used two approaches to calculate *E. coli* decay rates:

1. An "explicitly variable" decay rate (EVDR) dependent on temperature (T, in degrees Celsius), salinity (S) and solar irradiation (I, in Watts/m2), based on Mancini, (1978). Namely,

$$k_d(T,S,I,z)=[0.8+0.017S]\times 1.07^{(T-20)}+0.086\times I\times e^{-k_z z}, \qquad (3)$$

where z is the water depth and k_z is the light extinction coefficient, which in TELEMAC 3D is calculated as $1.7/z_{SD}$, with z_{SD} the Secchi disk depth, fixed at a value of 0.9 m for this study. Note that Mancini's equation is based on data from New York estuary data. Although Gao et al. (2015) equation is based on UK estuaries, we did not consider it in this paper because not all the values of the equation coefficients were included in the paper.

2. An "implicitly variable" decay rate (IVDR) considering the values for estuarine waters of Huang et al. (2017): one constant value of T_{90}=8.6 h for day time and another one of 30.64 h for night time. These values are within those reported by Abu-Bakar et al. (2017) in a different UK estuary (T_{90} ranged between 2.5 and 20 h for day time and between 30 and 60 h for night time).

Both approaches were implemented in the TELEMAC subroutine SOURCE_TRAC. In the first case (EVDR), the waqtel process 5 (atmosphere-water exchange) was activated, and the solar irradiation (I) in Equation (3) was calculated by means of the TELEMAC subroutine SOLRAD. The inputs provided to SOLRAD were the latitude, longitude and cloud coverage (obtained from ECMWF ERA-interim - www.ecmwf.int/en/research/climate-reanalysis/era-interim - in the geographical centre of the computational domain). The date and time of the day is automatically read during the model calculations.

2.6 Data and assumptions on sewer overflows considered in the model

Overflow discharge volumes and average spill duration for each CSO were used as input into the model by combining the information in Section 2.2 (Table 2). The annual average discharge volumes (m^3/day) were calculated using data reported by Frischmann (2001) (for Dartmouth STW) and Hyder (2012) (the remaining CSOs, based on the 2011 modelling results). The peak discharges (m^3/day) were provided by SWW. The average spill duration was extracted from the SWW annual reports, when available (CSOs number 1-9 in Table 2) and from the Frischmann (2001) (for Dartmouth STW) and Hyder (2012) reports for the rest of the CSOs.

Information on average spill duration and/or average flow was not available for six CSOs (identified with an asterisk in Table 1). Of these, Stoke Gabriel SPS, St. Peter's Quay, Ashprington Nº1 and Northern Villages were removed from the simulations; the first three because they do not spill during annual events and the last one for being an emergency overflow, meaning that it should only operate during pump or rising main failure. For Tuckenhay and Ashprington SPS Nº2 and Malsters SPS, missing information was assigned the median of the data for the remaining CSOs used in the model simulations (indicated with two asterisks in Table 2).

Monitoring of *E. coli* in effluents from CSOs is not required under the EA discharge consenting policy (Environment Agency, 2003). Therefore, we used as input concentrations into the model the reference *E. coli* concentrations for different treatment levels and individual types of sewage-related effluents under different flow conditions reported by Kay et al. (2008), which are the result of a study undertaken across the UK in 15 study areas over an 11 year period (1995-2005) at 205 river/stream monitoring points. Totnes STW-SO and Dittisham STW-SO (stored settled sewage) were assigned a *E. coli* concentration of 8 x 10^5 cfu/100 ml, while the remaining CSOs were assigned a concentration of 2.5 x 10^6 cfu/100 ml (storm sewage overflows). Effluent from Dartmouth STW is UV disinfected and has a reported mean *E. coli* concentration of 95 cfu/100 ml, which is several orders of magnitude lower than those in CSO discharges. For this reason, this discharge was excluded from the modelling.

Table2. Summary of discharge information for twenty-eight sewer overflows considered in the modelling study.

Name of storm overflow	Figure 1 reference number	Average spill duration (hours)/number of spills	Average discharge volume (m^3/day)	Peak discharge (m^3/day)	*Assigned E. coli* concentration (cfu/100 ml)
Dittisham STW SO	1	21.3 / 326	568	4,838.4	8 x 10^5
Ferry Boat Inn PS SPS	2	23.8 / 258	77.7	4,147.2	2.5 x 10^6
Galmpton PS SPS	3	14.7 / 179	785.9	5,529.6	2.5 x 10^6
Higher Dittisham SPP	4	7.8/ 190	87	2,505.6	2.5 x 10^6
Tuckenhay and Ashprington SPS No2*	5	0.2 / 4	301.6**		2.5 x 10^6
Scout Hut CSO	6	7.5 / 12	858	18,144	2.5 x 10^6
Stoke Gabriel SPS*	7	47/ 69			2.5 x 10^6
Totnes STW SO	8	48.8 / 271	201	8,812.8	8 x 10^5
Tuckenhay and Ashprington SPS No 1*	9	4.5 / 16			2.5 x 10^6
Fore Street CSO	10	7.1	217	26,265.6	2.5 x 10^6
Quarry close CSO	11	2.4	226	11,923.2	2.5 x 10^6
St. Johns Terrace CSO	12	0.5	358	5,270.4	2.5 x 10^6
Steamer Quay CSO	13	3	1,344.9	41,904	2.5 x 10^6
Swallowfields Kevics CSO	14	5.3	253.3	12,873.6	2.5 x 10^6
Tor Park Road PS/CSO/EO	15	1	640	1,209.6	2.5 x 10^6

Totnes Town PS/CSO/EO	16	10	1,581.9		2.5×10^6
Ashprington STW SSO	17	17	34	2,160	2.5×10^6
Cornworthy STW SO	18	5.2	22.4	1,900.8	2.5×10^6
Dartington School 2 CSO	19	4.8	301.6	18,230.4	2.5×10^6
Malsters SPS*	20	5.3**	301.6**		2.5×10^6
Northern Villages PS/EO*	21				2.5×10^6
Queens Arms CSO	22	6.8	107	604.8	2.5×10^6
Shinner's Bridge SCO	23	5.1	97	1,296	2.5×10^6
St. Peter's Quay PS/CSO*	24				2.5×10^6
Textile Mill CSO	25	9	303	5,011.2	2.5×10^6
Dartmouth STW	26	1.1	540,072		9.5×10^1
Lower Collar Park	27	4	428.5	26,784	2.5×10^6
St. Katherine's Way	28	2.8	641.7	41,212.8	2.5×10^6

* Some data were not available for the CSO.

** Value assumed to be equal to the median of all other CSOs.

NB. Sewer overflows with missing data on average spill durations and/or average discharge volumes were not considered in the model simulations.

2.7 Model scenarios

To investigate the impact of CSO discharges on the Dart Estuary, we considered the seven scenarios listed in Table 3. The specific aims of these scenarios were to study:

- The effects of river discharge and tidal phase on the fate and transport of *E. coli* (Scenarios 1–4).
- The effect of CSO spills from all discharges occurring simultaneously (worst-case) (Scenario 2 versus Scenario 5).
- The difference between average and peak discharge conditions (Scenario 2 versus Scenario 6).
- The effect of *E. coli* decay rate on modelling results (Scenario 2 versus Scenario 7).

Table 3. Details of the modelling scenarios considered in the study.

Scenario Number	River discharge	Tidal phase	Sewer overflows considered	*E. coli* decay rate	Simulation start date and time	Simulation length (days)
1	High	Neap	Five quasi-simultaneous spills in Fig. 2 (Totnes_STW_SO, Stoke Gabriel SPS, Higher Dittisham SPS, Galmpton PS, Ferry Boat Inn PS and Dittisham STW SO. Notice that Stoke Gabriel SPS has been removed as explained in Section 2.6) spilling at average flow rates	EVDR	04/01/2016 (13:00)	5
2	Low (Fig. 8(a)–(b))	Neap	Five quasi-simultaneous spills in Fig. 2 spilling at average flow rates	EVDR	19/01/2016 (13:00)	5
3	Low	Spring	Five quasi-simultaneous spills in Fig. 2 spilling at average flow rates	EVDR	13/01/2016 (09:00)	5
4	High (Fig. 8(a)–(c))	Spring	Five quasi-simultaneous spills in Fig. 2 spilling at average flow rates	EVDR	26/01/2016 (07:00)	5
5	Low	Neap	All the CSOs in Table 1 for which data are available, except Dartmouth STW spilling at average flow rates	EVDR	19/01/2016 (13:00)	5
6	Low	Neap	Five quasi-simultaneous spills in Fig. 2 spilling at peak flow rates	EVDR	19/01/2016 (13:00)	5
7	Low	Neap	Five quasi-simultaneous spills in Fig. 2 spilling at average flow rates	IVDR	19/01/2016 (13:00)	5

2.8 Data for model validation

As a general comment, the data available for model validation were scarce in time and space, except for the water levels. Some of the data presented in this section were not directly used for the model validation but are included to illustrate the range of values that are expected for different variables in the Dart Estuary.

2.8.1 Water levels

Water levels (m) at Totnes (tidal limit), Duncannon (mid-estuary) and Dartmouth (estuary mouth) were obtained from DartNet (https://www.valeport.co.uk/InsideValeport/DartNetTides, see Fig. 1(c) for their location) (Valeport, 2018). Tidal prediction data provided by the UK Hydrographic Office (UKHO) were also obtained from the website. Generic current velocity data published in the peer reviewed literature (Thain et al. 2004) were used for model validation because detailed data were not available (see Section 3.1.2).

2.8.2 Salinity

Salinity data available for eight cross-river transects in the upper estuary for five days (20–25 March 2003) during a period of low river discharge (<10 m^3/s) were used for model validation. Each transect consisted of several stations (the number depending on the transect width) where salinity was measured using hand-held CTD profilers from a small boat. Each station was sampled at different stages of the tidal cycle at a frequency of 1 s for approximately 3 minutes. Fig. 3 shows salinity results along transect 7 (greater freshwater influence) and 0 (greater marine influence). Salinities were lower and less variable at station 7 than at station 0 indicating the penetration of seawater on the flood and influence of freshwater discharges on the ebb. CTD casts taken at a number of sites in the upper part of the estuary on 19 March 2003 indicate a degree of stratification. It should be reminded that the available salinity data are representative of periods of low river discharge and therefore do not reflect the full range of salinity variation expected in the estuary.

Few data exist to describe the variability of water column stratification in the Dart Estuary. The existing data are mostly representative of the estuary mouth. For instance, Priestley (1998) analysed the stratification using data from a telemetered monitoring buoy deployed at approximately 2 km upriver from the estuary mouth over three weeks in March–April 1998 to study water column stratification during a spring tide-neap tide-spring tide cycle. Thain et al. (2004) took CTD casts to measure the water column stratification during spring tide on 13 March 2002 and neap tide on 22 March 2002. Both studies have shown that the Dart is a partially mixed estuary with a complete stratification/destratification cycle during the spring/neap tide transition.

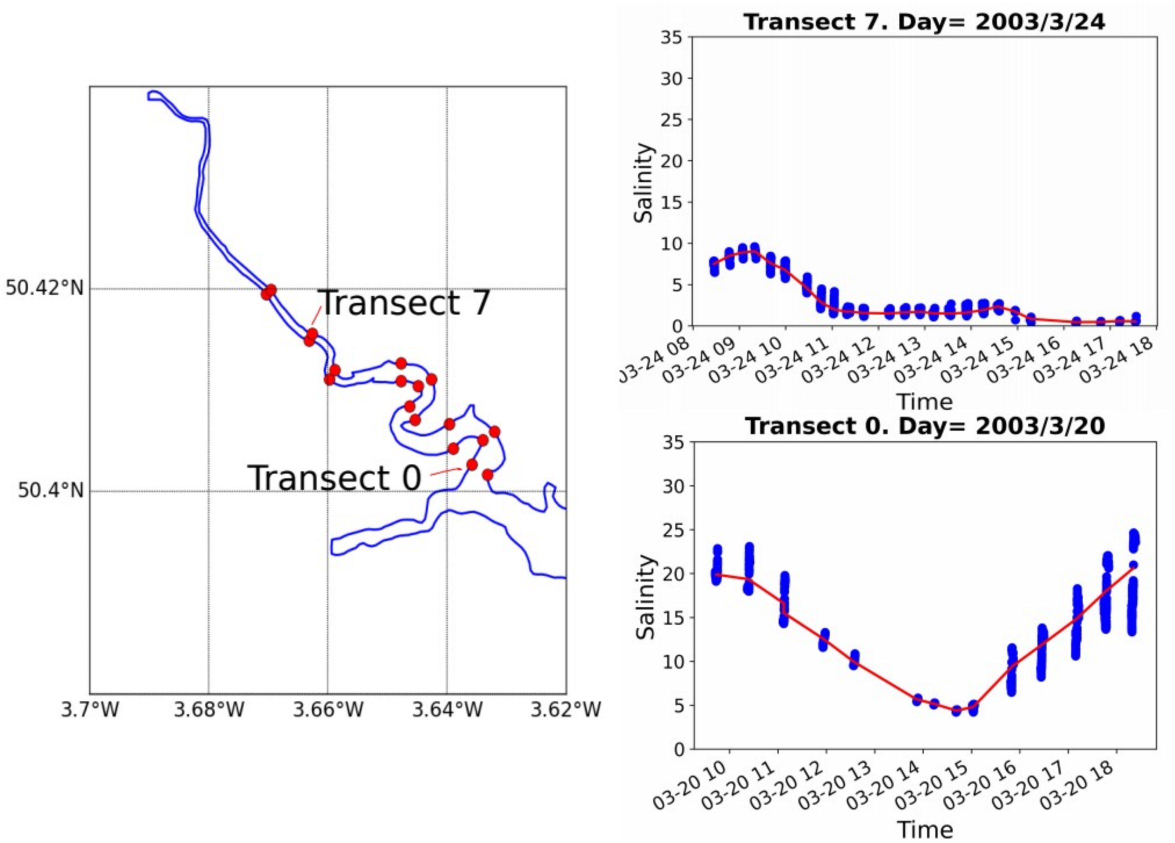

Fig. 3. Measured salinity at sites along transects 0 and 7 on 20 and 24 March 2003. At each site (corresponding to each time cluster) the high resolution raw data (one observation every second for approximately three minutes) measured in the first 40cm of the water column are depicted in order to show the range of variability. The red line shows the average of each time cluster. The Time format in the x axis is mm-dd hh.

2.8.3 E. coli *concentrations*

E. coli concentrations quantified in surface water samples taken weekly at nine sites along the estuary during six months (June–December 2000) were used in this study. Fig. 4 shows that the measured *E. coli* concentration at Waddeton, which is close to the shellfish farming areas (Fig. 1(c)) exceeded 2,000 cfu/100 ml in August, November and December, and 7,000 cfu/100 ml in December. However, since the time when these samples were taken, the sewerage infrastructure has been upgraded and tertiary treatment installed at Totnes STW and Dartmouth STW. Hence, these values may not be fully representative of the current levels of contamination in the estuary, even in the event of spills and changes in degree of diffuse input of *E. coli* from farming sources.

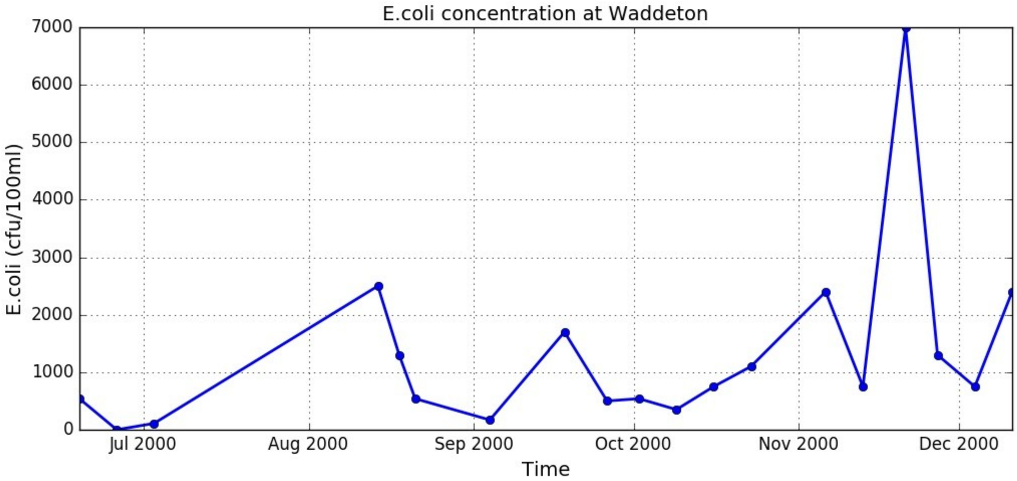

Fig. 4. *E. coli* concentrations in surface water samples taken at a site in the Waddeton shellfish water. Data from Allen (2001).

2.8.4 Rainfall

In order to do a preliminary assessment of the correlation between rainfall and CSO spills, daily cumulative rainfall data were obtained from ECMWF ERA-Interim (www.ecmwf.int/en/research/climate-reanalysis/era-interim) at the geographical centre of the computational domain and are displayed in Fig. 5 together with the sewage spills from Higher Dittisham and Dittisham STW SO during the period 2013–2015. In most of the cases, the sewage spills occurred during rainfall events. Higher volume spills generally coincided with periods of high rainfall.

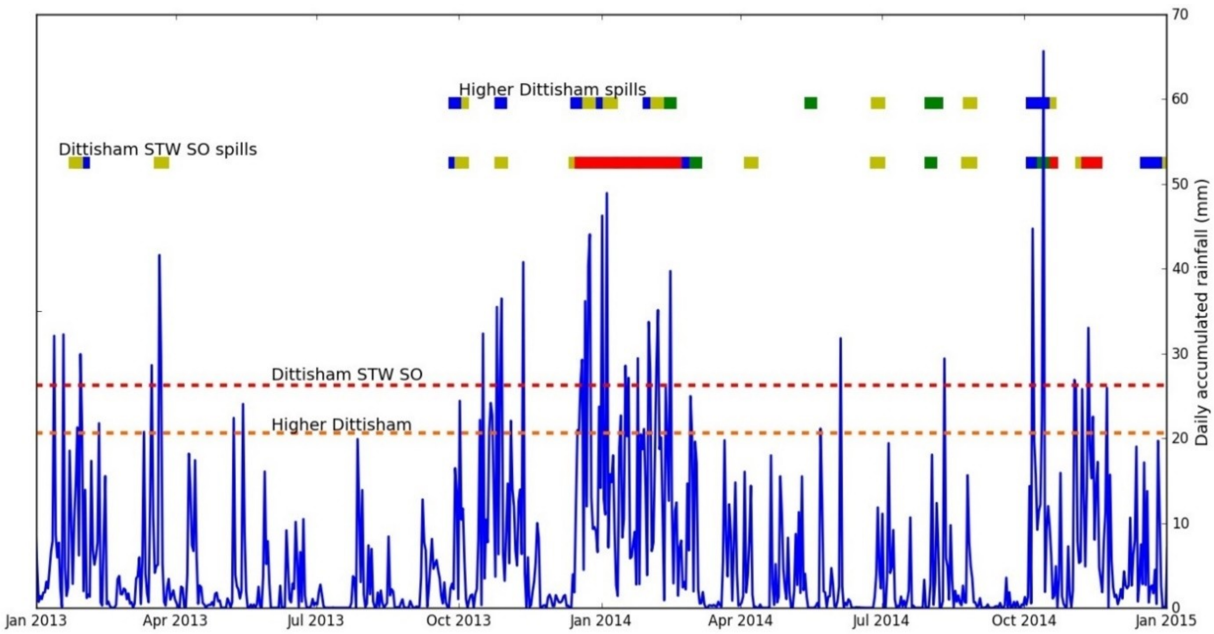

Fig. 5. Daily cumulative rainfall in the Dart Estuary catchment (mm) and sewage spills from Higher Dittisham CSO and Dittisham STW SO, January 2013–December 2014. The dashed lines represent the averaged cumulative rainfall over spill duration. Rainfall data from ECMWF ERA-Interim.

3. Results

3.1 Validation of the hydrodynamic model

3.1.1 Water levels and current velocities

Figs 6(a), 6(c) and 6(e) compare model results with observed data on water levels at the three tidal gauges described in Section 2.8.1 (see Fig. 1 for their locations). The predictions from the UKHO area are also included for reference. Figs 6(b), 6(d) and 6(f) show the relationships between modelled and predicted observations. Model skill was quantified by means of bias, Root Mean Square Error (RMSE) and correlation (Table 4). The results show that the model reasonably reproduced the tidal cycle at all validation sites, although with certain anomalies (i.e. 11 cm mean underestimation at Dartmouth, 11 cm mean underestimation at Duncannon and 1.8 cm mean underestimation at Totnes). Some events such as the high water levels registered simultaneously around the 8th of January 2016 at all tidal gauges were not captured by the model. Some events such as the high water levels registered simultaneously around the 8th of January 2016 at all tidal gauges were not captured by the model. The differences between our model and the observations were very similar to those obtained by the UKHO prediction (Table 4), but variable depending on the location. In both cases (our model and the UKHO prediction), the differences can be attributed to the fact that the observations contain the effect of variable meteorological conditions (i.e. changes in pressure or wind) that affect the water levels, which are not included in the UKHO predictions nor in our model. Differences can also be attributed to reduced propagation of the tidal signal over the extremely variable bathymetry of the Dart Estuary.
Although no direct observations of current velocities were available to validate our model, data from the literature indicate that, in the estuary mouth, characteristic velocities on the flood phase of spring and neap tides are ≈0.6 m/s and ≈0.3 m/s, respectively (Thain et al., 2004). Figs 7(c), and 7(d) show modelled current velocities at a site in the estuary mouth (marked with a star in Fig. 1(c)), which are in close agreement with these values.

Table 4. Statistics of modelled and observed results for three tidal gauges considered in the study.

	Totnes		Duncannon		Dartmouth	
	Model	UKHO	Model	UKHO	Model	UKHO
Bias (cm)	-1.8	0.13	-10.31	-22.38	-11.17	-11.04
RMSE (cm)	30	41.84	32.28	30.24	56.27	26.52
Pearson Correlation	0.95	0.91	0.97	0.99	0.91	0.98

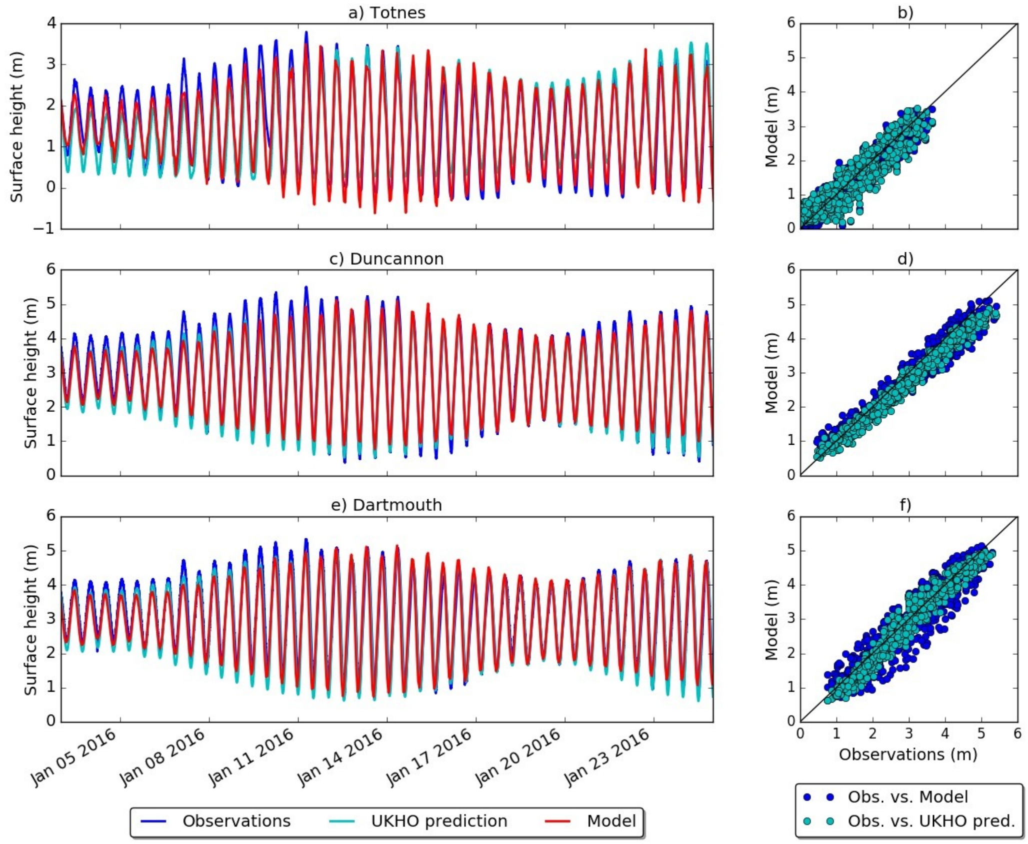

Fig. 6. Time series of modelled and observed water levels at three tidal gauges in the Dart Estuary.

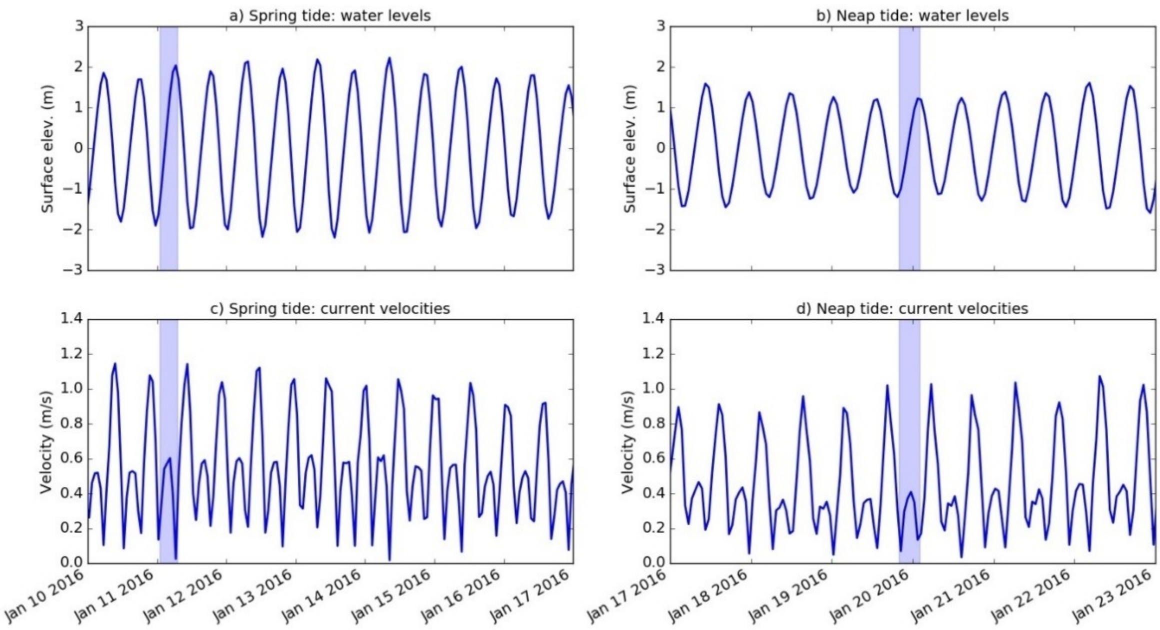

Fig. 7. Modelled current velocities on spring and neap tides in the Dart Estuary mouth, 10–17 January 2016.

3.1.2 Salinity and water column stratification

Fig. 8 shows the variations of water levels at Dartmouth, river discharge, surface salinity at a site in the middle of transects 0 and 7 (located in the upper estuary, Fig. 3), and the surface and bottom salinities at Dartmouth. The results show the effect of river discharges in modulating the amplitude of salinity levels during flood and ebb tides. Salinities in Fig. 3 reach higher values than those predicted by the model because the river discharge during the modelled period (minimum≈20 m^3/s, Fig. 8(b)) was much higher than that recorded during the period when the salinity data displayed in Fig. 3 were sampled (≈5 m^3/s).

Averaged daily salinities at surface and bottom of the water column are shown in Fig. 8(d). The results show that the tidal regime plays an important role in the stratification/destratification of the water column, as described by Thain et al. (2004) and that this is also determined by the river discharge. This effect is illustrated for three time periods: period (A), when freshwater discharges remain relatively constant and the stratification increases during neap tide; period (B), when high freshwater discharges coincide with neap tide and stratification strengthens to maximum levels; and period (C), when freshwater discharges coinciding with spring tides are sufficiently high to cause stratification of the water column.

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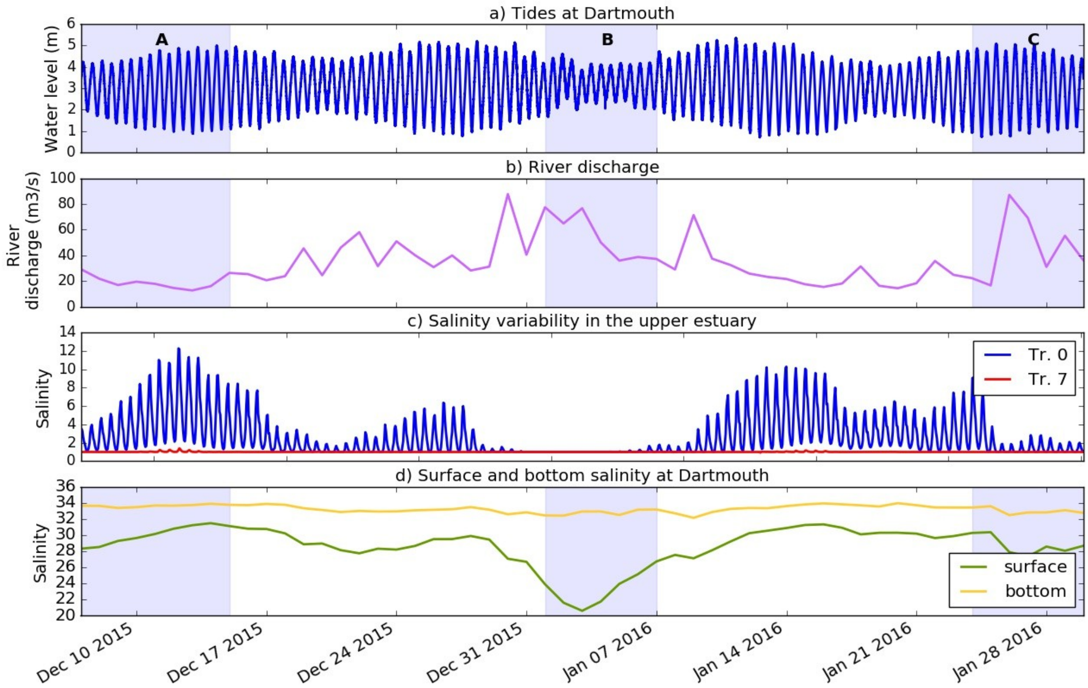

Fig. 8. Time series of water levels at Darmouth (a), river flows (b), salinity at transects 0 and 7 in the upper estuary (c) and salinity at two depths measured at the estuary mouth (d), 10 December 2015–28 January 2016.

3.2 Modelling scenarios

3.2.1 Effect of tides and river discharge on E. coli concentrations

This section reports results on the effect of hydrodynamic conditions (tidal phase and river discharges according to Scenarios 1–4 in Table 3) on the fate and transport of *E. coli* in the Waddeton SWPA following CSO spills. Time series of *E. coli* concentrations at the five shellfish farming sites (Fig. 1(c)) within the shellfish water following spills from five CSOs (red dots in Fig. 1(c)) are shown in Fig. 9 in log scale. Average bacterial concentrations at individual sites and the corresponding time of exposure at different concentrations are presented in Table 4. The *E. coli* maxima occurred within the first 24–36 h, which is the time when most discharges stopped spilling (Fig. 9(a)). Totnes STW SO continued to spill for a further 24 h, but this did not appear to affect bacterial levels in the shellfish water as much as the remaining four CSOs, which discharge near the shellfish farming sites. The highest *E. coli* concentrations were predicted at the farming sites 4 (1,600 cfu/100 ml) and 5 (2,500 cfu/100 ml) (Figs 9(e) and 9(f), respectively). These sites are the closest to Galmpton PS SPS CSO, which is a very significant source of contamination locally in terms of discharge volume (Table 2).

Scenario 1 represents the highest average and instantaneous *E. coli* concentrations at the shellfish farming sites (Fig. 9, Table 5) and corresponds to high river discharge volumes and neap tide. Under these conditions, the transport of *E. coli* to the upper reaches of the estuary on the flood tide is constrained by the outflowing river discharges, and thus bacterial contamination persists for some time in the shellfish water. During neap tides and high river discharges, salinity is at its lowest level (Table 5), which reduces the *E. coli* decay rate and this might contribute to maintain elevated *E. coli* concentrations in the water.

Scenario 2 shows higher peak and average concentrations than any other scenarios at all farming sites, except Scenario 1. This is because under this scenario *E. coli* retention in the estuary is high, although bacteria can still be transported further upstream along the estuary. In addition, the *E. coli* decay rates in Scenario 2 were faster than in Scenario 1 due to higher salinities (Table 5).

Scenarios 3 and 4 represent high influence of marine waters in the estuary on spring tides and variable river discharges. Scenario 3 represents lower river discharge and shows longer exposure time of *E. coli* contamination in the SWPA than Scenario 4. The *E. coli* decay rates are also higher in Scenario 3 due to higher salinities. However, the average *E. coli* concentrations in both scenarios are relatively similar (Table 5) with Scenario 3 showing slightly higher concentrations, probably due to longer exposure time of bacterial contamination.

Consideration of these results in relation to the SWPAD and Regulation (EC) 627/2019 shows that an *E. coli* concentration in the waters of 110 cfu/100 ml, which is equivalent to the Class B standard under the regulation, was exceeded for several hours at all the farming sites under Scenarios 1 and 2 (the maximum is 22h under Scenario 1 at farming site 5). Under Scenarios 3 and especially 4, the threshold is not achieved at some farming sites (Table 5). The *E. coli* threshold of 5 cfu/100 ml (equivalent to the Class A standard) was exceeded for several days (up to 4 days at site 2 under Scenario 1) under all scenarios at all the farming sites (Table 4).

The spatial distribution of *E. coli* concentrations in the estuary after 24 h (left column) and 48 h (right column) of CSO spill start time under Scenarios 1–4 are shown in Fig. 10. The estuarine areas affected by *E. coli* concentrations greater than 110 cfu/100 ml are enclosed by a white isoline in plots (a) and (c). After 24 h of the beginning of the spills, the Class B standard was only exceeded under Scenarios 1 and 2, especially at the shellfish farming areas (Figs. 10(a) and (10c)), with Scenario 2 showing a broader area of exceedance at this particular time. After 48 h of the beginning of the spills, bacterial concentrations decreased below this threshold across the SWPA under all scenarios..

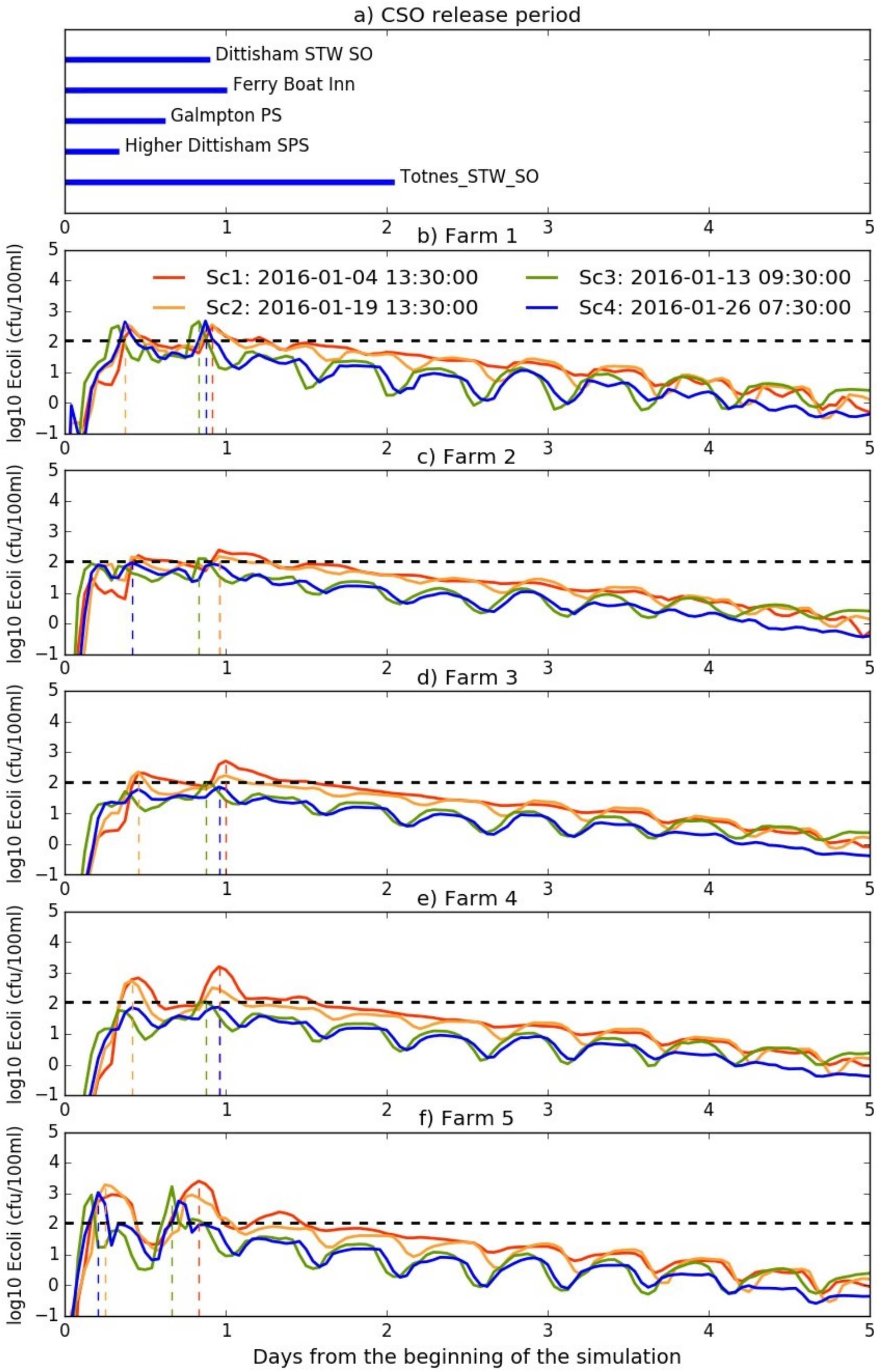

Fig. 9. Modelled *E. coli* concentrations at five shellfish farming sites (see Fig.1 (c)) for five days of model simulations under Scenarios 1–4. The dashed black line represents the threshold of 110 cfu/100 ml in the water equivalent to the Class B standard in shellfish flesh. The vertical dashed lines

represent the time when peak *E. coli* concentration is achieved. Notice that at the farming site 2, the peak concentration for Scenarios 1 and 2 is achieved at the same time.

Table 5. *Mean salinities, E. coli concentrations and times of expos*ure *to E. coli concentration greater than 110 cfu/100 ml and 5 cfu/100 ml at five shellfish farming sites* during *four contamination scenarios.E. coli in cfu/100 ml.*

	Scenario 1				Scenario 2				Scenario 3				Scenario 4			
	Mean sal	Mean *E. coli*	Time (h) *E. coli* > 110	Time (h) *E. coli* > 5	Mean sal	Mean *E. coli*	Time (h) *E. coli* > 110	Time (h) *E. coli* > 5	Mean sal	Mean *E. coli*	Time (h) *E. coli* > 110	Time (h) *E. coli* > 5	Mean sal	Mean *E. coli*	Time (h) *E. coli* > 110	Time (h) *E. coli* > 5
Farm 1	9.21	39.58	12	86	18.63	37.66	8	87	21.63	23.78	5	68	15.43	21.33	4	59
Farm 2	6.45	41.68	14	95	16.77	34.64	5	93	20.53	17.31	2	74	12.81	16.29	0	63
Farm 3	8.13	54.43	21	90	18.00	32.44	7	90	20.97	13.40	0	73	14.34	12.045	0	61
Farm 4	9.56	93.74	22	90	19.09	43.28	10	88	21.98	13.43	1	7	15.34	11.99	0	58
Farm 5	12.39	144.32	22	91	21.79	101.07	13	87	24.01	39.12	7	61	18.05	35.29	5	57

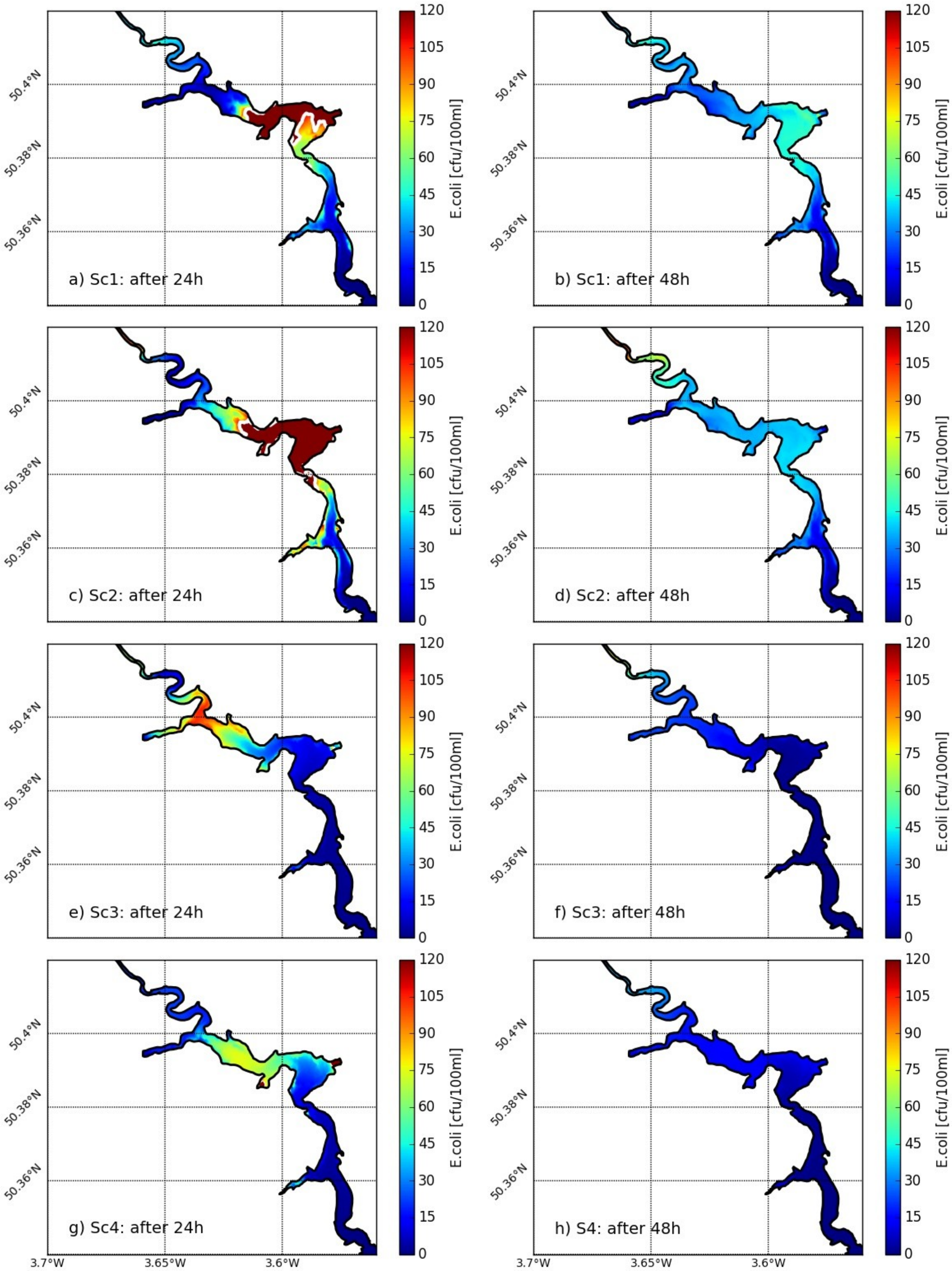

Fig. 10. Modelled concentrations of *E. coli* in the Dart Estuary. The left column shows bacterial concentrations at 24 h after the beginning of the CSO spills; the right column shows the same information at 48 h after the beginning of the spills. The white lines in plots (a) and (c) represent the 110 cfu/100 ml *E. coli* concentration isoline.

3.2.2 Effect of all storm overflows spilling concurrently (Scenario 5)

A modelled scenario with all CSOs spilling concurrently showed *E. coli* concentrations increasing to a peak level within approximately 24 h after spill start time and reducing thereafter under all scenarios at most farming sites (Fig. 11). However, the *E. coli* concentration response to the spills differed between sites. Farming sites 4 and 5 showed the highest *E. coli* concentrations. Under Scenario 5 at site 2, *E. coli* concentrations peaked at 48 h after spill start. During the first three days after the spills, *E. coli* concentrations exceeded for several hours a day the 110 cfu/100 ml threshold. Although most CSOs stopped spilling within 24 h (except Totnes STW SO), *E. coli* concentration remained above this limit for a few days at most farming sites.

3.2.3 Effect of five storm overflows spilling at peak volume (Scenario 6)

In this section, we analyse the modelling results of *E. coli* concentration in water at the five shellfish farming sites with five CSOs spilling simultaneously at peak flow rates. Although this is a possible scenario, it is likely that the duration of these peak events would be shorter than the one considered here. Under peak flow discharge conditions, the water quality concentration equivalent to class B standard (110 *E. coli*/100 ml) was frequently exceeded over four days after spills. *E. coli* concentrations of 16,000 cfu/100 ml were predicted for the shellfish farming site 5 (Fig. 12(e)). At the remaining four sites, the peak *E. coli* concentrations ranged from 200 cfu/100 ml to 4,500 cfu/100 ml. These are around 10 times higher than the concentrations obtained under average discharge conditions (low river discharge and neap tide, Scenario 2).

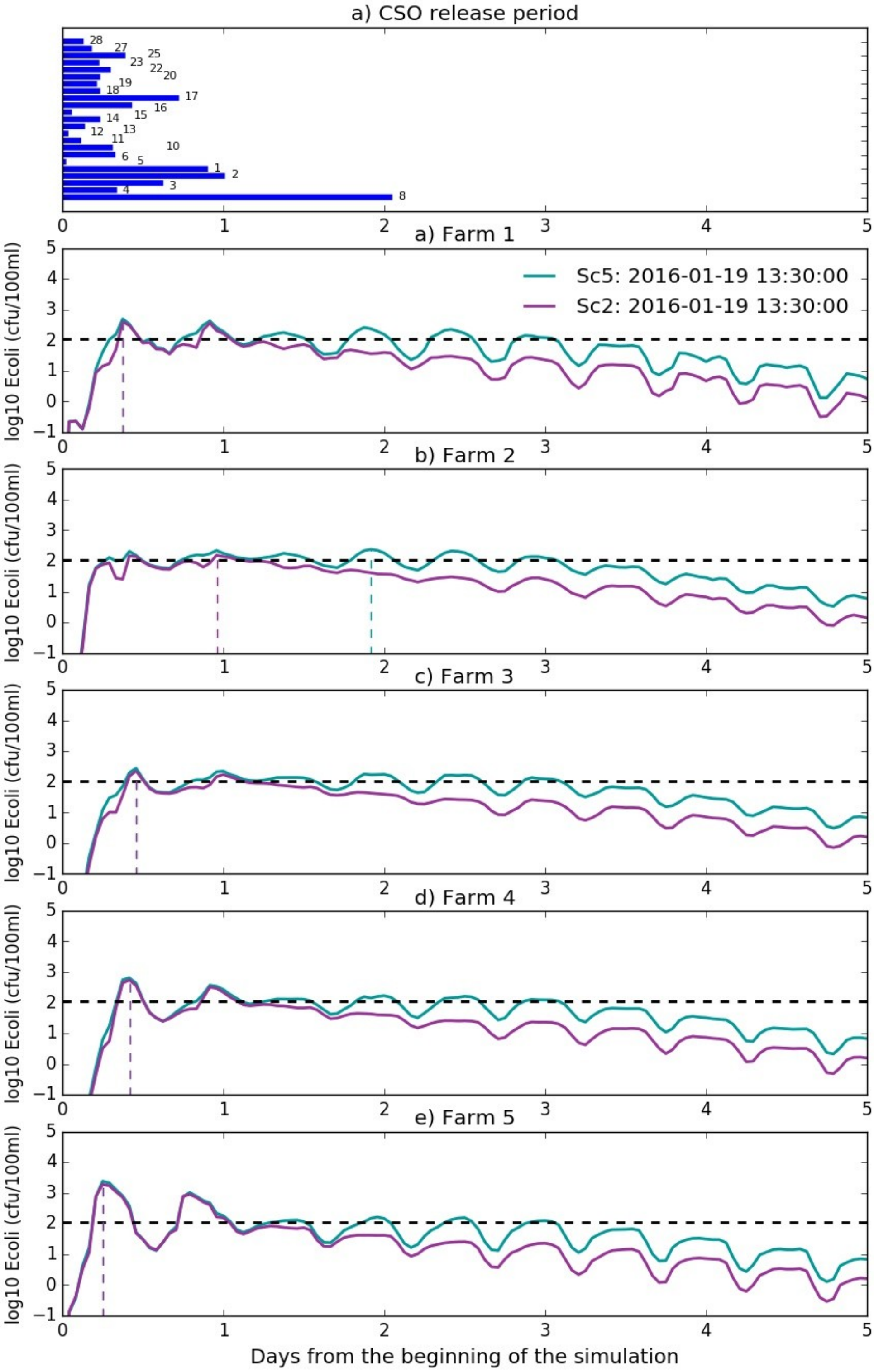

Fig. 11. Concentrations of *E. coli* at five shellfish farming sites considering all the CSOs spilling concurrently (Scenario 5) or only the five for which spill information is available (Scenario 2). Both scenarios are based on the same hydrodynamic conditions. The dashed black line represents the threshold of 110 cfu/100 ml in water (equivalent to the Class B standard in the shellfish). The vertical

dashed lines represent the time when peak *E. coli* concentration was achieved. Notice that the peak was achieved at the same time for both scenarios at all farming sites, except for Farm 2.

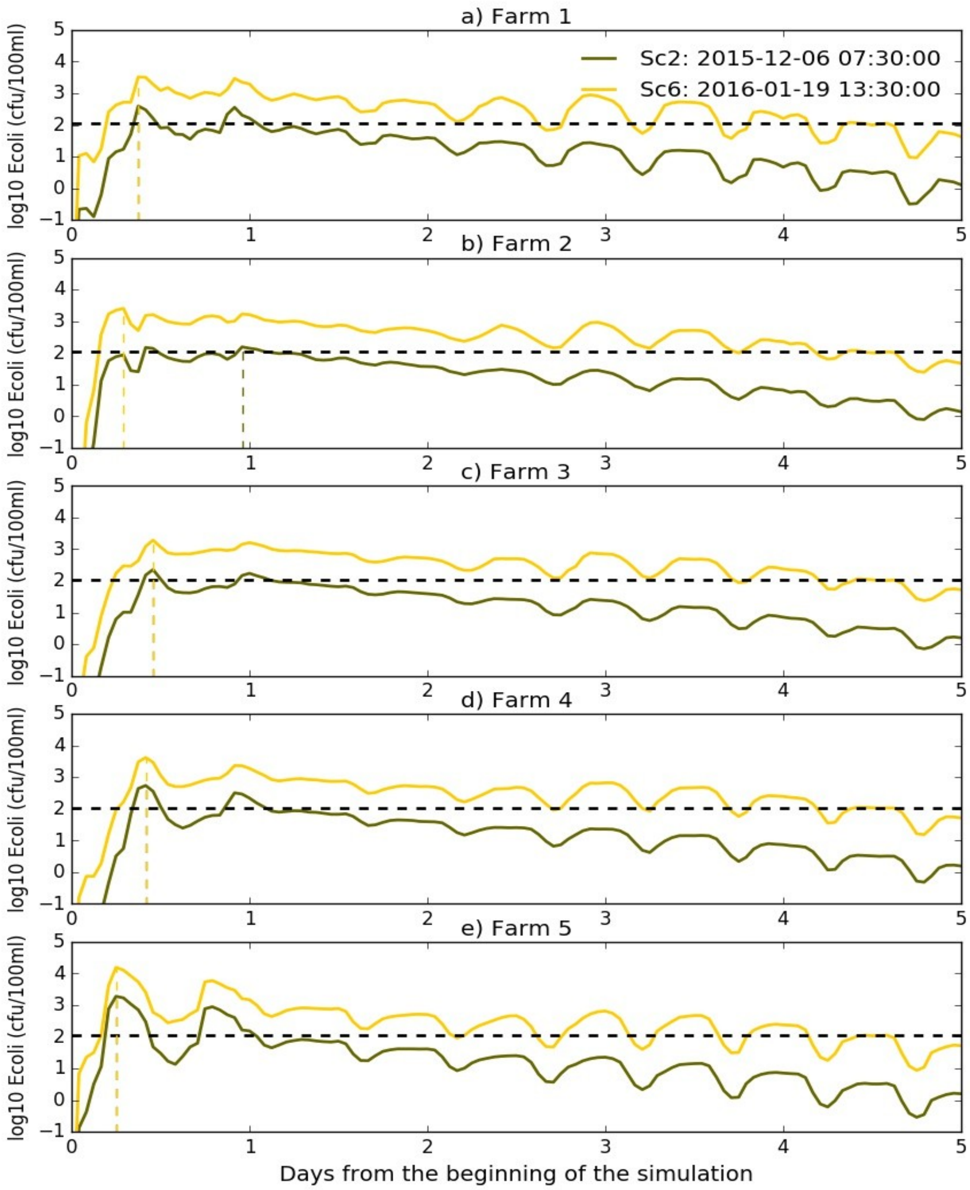

Fig. 12. Modelled concentrations of *E. coli* at five shellfish farming sites over five days following sewage spills under peak flow discharge (Scenario 6) and average discharge (Scenario 2) conditions. The same hydrodynamic conditions were considered in all model runs. The dashed black line represents the threshold of 110 cfu / 100 ml in water (equivalent to the Class B standard in the shellfish). The vertical dashed lines represent the time when peak *E. coli* concentration was achieved. Notice that the peak was achieved at the same time for both scenarios at all farming sites, except at Farm 2.

3.2.4 Effect of varying E. coli decay rates

This section reports on the effect of the two *E. coli* decay rates introduced in Section 2.5 on the model results. Fig. 13 shows *E. coli* concentrations at the five shellfish farming sites predicted by the model for the explicitly variable decay rate (EVDR; Scenario 2) and the implicitly variable decay rate (IVDR; Scenario 7). The results show that the IVDR leads to much higher decay rates and hence to lower concentrations of *E. coli* in water. At farming sites 2, 3 and 4, *E. coli* concentrations did not exceed the threshold of 110 cfu/100 ml when the IVDR was considered. Bacterial concentrations for IVDR were approximately four times lower than those for EVDR. At farming sites 1 and 5, the 110 cfu/100 ml threshold was exceeded when IVDR was used, but the *E. coli* concentrations were approximately half of those obtained with an EVDR.

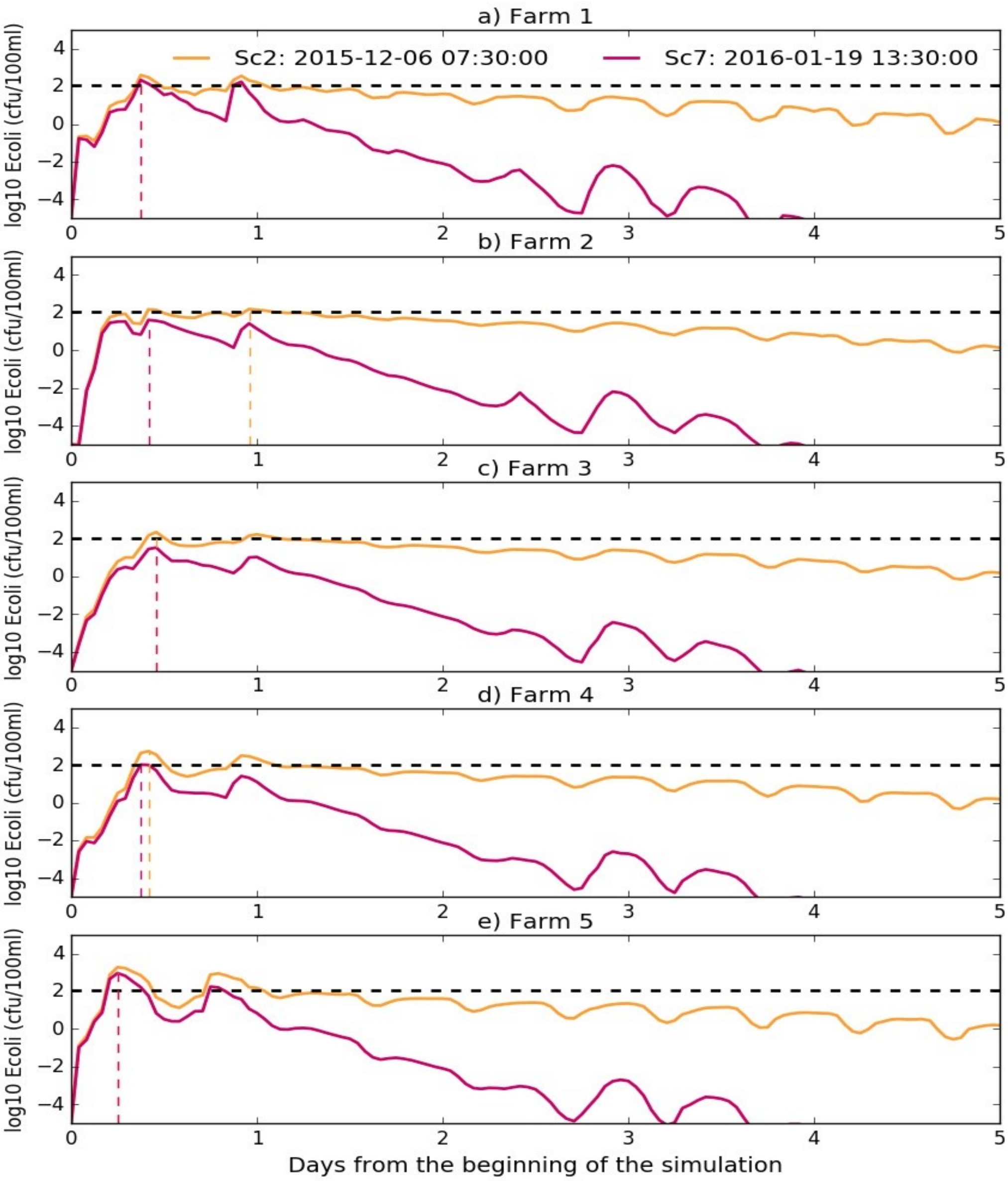

Fig. 13. Modelled concentrations of *E. coli* at five shellfish farming sites over five days of model

simulation under two bacterial decay rates. EVDR - explicitly variable decay rate (Scenario 2); IVDR - implicitly variable decay rate (Scenario 7). The same hydrodynamic conditions were considered in all model runs. The dashed black line represents the threshold of 110 cfu/100 ml in water (equivalent to the Class B standard in the shellfish). The vertical dashed lines represent the time when peak *E. coli* concentration was achieved. Notice that the peak was achieved at the same time for both scenarios at all farming sites, except for Farm 2. The y axis has been truncated at a concentration of 10^{-5} cfu /100 ml (-5 in the log scale).

3.3. Comments on E. coli forecasting

Information on the association between rainfall and spill occurrence, frequency and duration can inform decisions on management of microbiological contamination risks in SWPAs/shellfish farming sites. In this study, we carried out an initial analysis of cumulative rainfall levels that may trigger spills from the five CSOs considered in the model simulations. This is, those for which spill frequency and duration data are available (Fig. 2). The rainfall data available for the period 2010–2016 described in Section 2.8.4 were used for this analysis. A summary of results is compiled in Table 6.

The results indicate that, in general, a 3-day rainfall accumulation of 20–25 mm is likely to trigger a spill. On the day the spill commences, an accumulation of between 12 and 20 mm is established and rainfall remains greater than 20 mm for the duration of the spill at each CSO. Galmpton and Higher Dittisham spill at higher cumulative rainfall (28.4mm and 26.2 mm, respectively), which may be related to the greater capacity of these CSOs to store sewage (74 m^3 and 20 m^3, respectively). In contrast, Dittisham and Ferry Boat Inn have lower storage capacity (7 m^3 and 4.4 m^3, respectively) and therefore are more likely to spill at lower rainfall. The position at Totnes is in strong contrast with the other four stations. Totnes serves an urban area with a population of ~8,000; the much higher consented storage capacity of 3,520 m^3 at Totnes STW reflects the much greater accumulations possible over paved areas of the town.

To assess factors that may help “predict” the occurrence of a spill, we calculated the number of days for which the accumulated rainfall was equal or exceeded the mean value during the spill (column 4 in Table 6) and the percentage of time (days) that coincided with the occurrence of a spill. This analysis shows that this was the case in more than 64% of cases, reaching 83% at Dittisham. The exception was Higher Dittisham, where a value of less than 50% was obtained, although discontinuities exist in the dataset of spill occurrence and duration in coincident periods where other CSOs register medium to long term duration spills, (i.e. winter 2003 see Fig. 2 and Fig. 5). Applying the same analysis to rainfall events > 50mm coincident with the occurrence of a spill results in a lowest value of more than 70% coincidence, and for some CSOs, 90% or even 100% coincidence (Dittisham).

The relationship between accumulated rainfall over the previous 3 days and the occurrence of a spill was not very strong (<37% coincidence), except for Totnes STW SO, where 57% coincidence between rainfall and spill occurrence was obtained. In summary, these results suggest that although the occurrence of a spill is affected by rainfall falling on previous days (which takes up capacity of the sewerage network to store sewage), the best indicator of spill occurrence seems to be rainfall of the day.

Table 6. Summary statistics of association between cumulative rainfall and sewer overflow spills.

Name of sewer overflow	Accumulated rainfall (3 days prior to spill)		Accumulated rainfall (beginning of spill)		Accumulated rainfall (spill duration/day)		Percentage of rainfall events ≥ Mean accumulated during spill	Percentage of rainfall events ≥ Mean (resulting in a spill on the same day or within 2 days)	Percentage of rainfall events ≥ 50 mm (resulting in a spill on the same day or within 2 days)
	Mean (mm)	95th Conf. level	Mean (mm)	95th Conf. level	Mean (mm)	95th Conf. level			
Dittisham STW SO	20	2.4	14.5	1.6	26.2	6.4	83	37	100
Ferryboat Inn PS	23	3.3	12.7	1.7	22.1	5.6	64	35	70
Galmpton PS	24	3.3	20.8	2.5	28.4	9.0	72	24	70
Higher Dittisham	26	3.9	18.4	2.4	20.6	2.7	48	17	70
Totness STW SO	22.5	2.9	15.9	2.1	21.5	16.4	81	57	90

4. Discussion

A three-dimensional hydrodynamic model (TELEMAC 3D) was developed and successfully applied to simulate the effect of the intermittent sewage discharges (CSOs) on the fate and transport of *E. coli* in the Dart Estuary. Our interest lies in these bacteria because their presence indicates potential human health risk from exposure to enteric pathogens via recreational contact with water and consumption of contaminated shellfish. The model combines all the components that drive the distribution of contamination and helps assess relative impact and associated health risk by simulating different modelling scenarios. The wide range of riverine fluxes, variation in temperature and salinities, and large tidal range in the estuary and the arrangements and operation of the CSOs themselves in the catchment made this a complex problem to analyse.

Results show that the hydrodynamic conditions were key for the retention of *E. coli* in the SWPA/farming sites, with neap tides and high river discharges leading to the highest *E. coli* concentrations. Also, the distance from the CSOs to the farming sites, the duration and intensity of the spills and whether the spills were concurrent were all shown to affect the resultant concentrations. *E. coli* experiences a decay through time due to increased mortality, and this depends on many factors (Campos et al. 2013). This non-conservative behaviour was implemented in the model through two methods, which resulted in very different *E. coli* concentrations at the farming sites: the more sophisticated EVDR method results in higher concentrations and relies on the application of a fully baroclinic 3D model to acquire the fully resolved temperatures, salinities and irradiation; and the less complex IVDR, that leads to lower concentrations, and parametrises decay rates based on varying the rate in periods of day and night, which may be suited to a simpler, 2D modelling approach. A model of this type was applied by Robins et al. (2019) on the river dominated part of the Dee Estuary (North Wales) to examine the transport of adenovirus through the river system. This research did not include ephemeral storm discharge from CSOs along the river but used sampling and stochastic methods to gauge the extent of dispersal which were highly dependent upon river and tidal conditions. Examples of scenario-based modelling approaches similar to ours involving CSOs in other rivers can be found in Even et al. (2007) and Björklund et al. (2018).

Unfortunately, a sustained dataset of *E. coli* concentrations in water does not exist for the Dart Estuary, which hindered the task of the model calibration and validation and constrained the operational use of the model. The only observational data available at Waddeton. were approximately measured between farming sites 3 and 4 in Figure 1 (c) and are not likely to reflect current conditions in terms of microbiological pollution in the estuary. Comparable concentrations to those detected in the waters were only obtained when the CSOs were spilling at peak flow conditions.

The model presented here focuses on scenarios designed based on available data and/or previous modelling results, and potentially constitutes a valuable tool for managers to understand the conditions under which water/shellfish standards may be exceeded and for how long those exceedances are likely to occur, as well as to plan actions to improve the water quality of the Dart Estuary. However, some improvements to make the model more realistic and adapted to the local conditions would be needed before the model scenario outputs presented here can be used with confidence by water resource managers in the Dart. Some of these are: a) including wind forcing, since it influences the hydrodynamic circulation; b) explicitly calculating the 3D temperatures (now considered constant in time and space), which would result in a better characterization of the water column structure and would allow to account for the variability in temperature in the *E. coli* decay rates and c) acquiring further monitoring data to validate the model, parametrise *E. coli* decay and characterise CSO discharge effects over time. Given all these uncertainties, the results shown here should be taken with caution, especially with regard to the exceedance of regulatory levels. Nevertheless, it seems that for average CSO spill frequency and duration, it is likely that the 110 cfu/100 ml concentration in water corresponding to the Class B standard of Regulation (EC) No 627/2019 will be exceeded for several hours in the Dart Estuary. This generally occurs within the first day after the beginning of the spill and especially at the shellfish farming sites closer to the CSOs (i.e. site 5) and under certain hydrodynamic conditions, even when faster decay rates are considered (IVDR). For the slower decay rates (EVDR) the period of exceedance would be longer. The *E. coli* concentration of 5 cfu/100 ml (equivalent to Class A standard of the regulation) is likely to be exceeded during the first day after CSO spill start times (when IVDR decay rates are considered), increasing up to 4 days (depending on the hydrodynamic conditions and location of farming sites in relation to the CSOs) when EVDR decay rates are considered. These results are consistent with the lag time of 3–4 days between the occurrence of rainfall and *E. coli* maxima detected at the shellfish farming sites in the Dart, as reported by Campos et al. (2011).

A preliminary study was also undertaken to characterize the rainfall conditions that would lead to the occurrence of CSO spills in the Dart Estuary. Model outputs demonstrated that spills generally occurred with average rainfall > 20 mm, that variability in response to rainfall event exists between individual CSOs, and that the response of these discharges to a rainfall event is faster during the first day of the event than when accumulated rainfall over previous days is considered. The absence of a time series of spill data did not allow for a full characterization of CSO spill variability in relation to the magnitude of rainfall. Moreover, the rainfall data were obtained from ECMWF ERA-Interim, which has a relatively coarse resolution of 0.75 degrees and therefore cannot provide summary statistics for specific parts of the catchment. Undoubtedly, rain gauge data in the vicinity of the CSOs would have provided a better characterization. In addition to the rainfall, other factors such as the catchment area, population connected to the network or storage capacity of each overflow influence spill frequency and magnitude. Therefore, an operational forecasting system for water quality in the Dart Estuary would ideally couple a Storm Water Management Model (SWMM) to represent the catchment and sewer system, with a hydrodynamic model such as the one reported here. Some examples of these coupled models can be found in the literature (De Marchis et al., 2013; Locatelli et al., 2019).

5. Conclusions

The three-dimensional hydrodynamic model of the Dart Estuary reported in this paper can reproduce water levels and current velocities, as well as periods of stratification and mixing generated by tides and varying river discharge in the estuary. The model was used to investigate the fate and transport of *E. coli* from CSOs. The model incorporates constant flow volumes and average spill duration to simulate a set of discharge scenarios according to varying hydrodynamics, spill frequency and duration and *E. coli* decay rates. From these modelling scenarios, it was concluded that:

- High volumes of river discharge at neap tides lead to larger areas of *E. coli* contamination impact in the SWPA and longer exposure of shellfish to peak *E. coli* concentrations due to a combination of high retention and, to a lesser extent, lower *E. coli* decay rates.
- In extreme rainfall events, if all CSOs spill at average flow volumes and are coincident in time, the peak *E. coli* concentrations in the water column do not increase significantly in magnitude when compared to a scenario of spills from a reduced number of CSOs, i.e. those located near the shellfish farming sites. However, elevated levels of *E. coli* in the water, exceeding the equivalent of class B standard in shellfish flesh, are likely to occur over longer periods of time at the farming sites.
- During peak spill volumes, *E. coli* concentrations in the SWPA can increase up to 10 times the concentration predicted under average flow conditions.
- Rainfall events greater than 20 mm are likely to trigger spills from CSOs which will affect microbiological contamination in the SWPA.
- Model outputs for time periods when tidal and river flow conditions dictate elevated *E. coli* concentrations combined with rainfall forecasts for the Dart catchment can provide a good indication of microbiological contamination risk in shellfish farming sites and recreational waters.

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Author contributions

L.G., C.C., S.K., A.Y. and J.B. designed the research and drafted the manuscript; L.G. and J.B. analysed the data and conducted the modelling studies.

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