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Aquaculture

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<https://doi.org/10.1016/j.aquaculture.2023.739920>

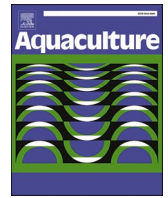
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From soil to sea: An ecological modelling framework for sustainable aquaculture

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ARTICLE INFO

Keywords:

Integrated modelling
Shellfish aquaculture
Catchment to coast
Land use
Short-term events
Carrying capacity
Eutrophication
Mussels
Oysters

ABSTRACT

An integrated framework is presented for carrying capacity assessment of aquaculture. The SUCCESS (System for Understanding Carrying Capacity, Ecological, and Social Sustainability) modelling framework uses a catchment to coast approach and is therefore able to partition organic and inorganic loading from disparate sources, resolve primary production, and simulate aquaculture carrying capacity.

An application of this framework to bivalve shellfish culture in Dundrum Bay, Northern Ireland, is used to illustrate: (i) how High-Impact-Short-Term (HIST) events such as pulse discharges from sewer systems can play an important role in changing environmental conditions in the receiving water; (ii) how changes in land-based loads can affect bay-scale nutrient enrichment and shellfish yields; and (iii) the role bivalves such as oysters and mussels can play in top-down control of eutrophication symptoms.

Our results show that in Dundrum Bay bottom-up control due to reduction of land-based loads can result in a 40% reduction in shellfish harvest, and that top-down control of phytoplankton and organic detritus by cultivated filter-feeders can reduce the percentile 90 of chlorophyll (i.e. the typical maximum) by over 20%. Both these results have important consequences for water quality and human use, and illustrate the complexity of integrated coastal management in multi-use systems.

The capacity of SUCCESS to analyse source apportionment from land, interactions at the open ocean interface, aquaculture production and environmental effects, and key biogeochemical processes at the bay scale, as a digital twin of the soil-to-sea continuum, makes it an important toolset for policy makers tasked with managing complex coastal systems.

1. Introduction

Over the last half century, aquaculture has undergone a number of paradigm shifts (see e.g. Ferreira et al., 2012a), which can be broadly grouped into four categories: (i) genetics and husbandry; (ii) structural technologies; (iii) social acceptance; and (iv) information technologies, including the Internet of Things (IOT).

A brief overview of these categories helps to place the present work in context. Given the diversity of aquaculture in terms of species, practices, and geographies, the rate of change in each category (i.e. the *shift*) is not uniform.

Progress in genetic selection varies widely across species, and the use of particular strains bred e.g. for disease resistance also differs markedly across nations. Hatchery-based stock, feed sourcing and control, biosecurity protocols, and pathogen containment also run the gamut from the most basic—often reactive—farming strategies in some parts of the world to sophisticated management for all these components in other areas (Gjedrem and Rye, 2016; Kelly and Renukdas, 2020).

Technology for cage structures, mooring systems, closed containment, and automated feeding has seen remarkable development over the last decades (Chu et al., 2020), but its application is extremely variable, from wooden cage grids in parts of Asia, South America, and Africa, in

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<https://doi.org/10.1016/j.aquaculture.2023.739920>

Received 12 May 2022; Received in revised form 23 June 2023; Accepted 23 July 2023

Available online 24 July 2023

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conditions where culture often exceeds ecological carrying capacity (e.g. Kluger and Filgueira, 2021; Liu and Su, 2015; Ross et al., 2013; see also Ferreira et al., 2012b for a general definition of carrying capacity), to sophisticated systems in Norway, Canada, and elsewhere, designed for offshore mariculture (Goseberg et al., 2017; Morro et al., 2021). A combination of costs, legislation and governance, and environmental awareness explains the worldwide variance in application of the cutting-edge cultivation systems that are presently available.

The social component is no less important for the industry as a whole: since 2013, farmed aquatic products have overtaken wild capture for human consumption (FAO, 2020; Lopes et al., 2017), so it is clear that social acceptance in the West, with respect to consumption, is in general well established and continues to increase—in the East this has never been in question. However, with respect to production, the situation is markedly different: the West imports the fish and exports the negative externalities and the jobs. The recognition in North America and Europe that there needs to be an increase in food security (NOAA, 2011a, 2011b; European Commission, 2018; European Commission, 2021) as the world population approaches ten billion has encouraged an expansion of production, but e.g. in China, greater environmental awareness has worked in the opposite direction, limiting the space available for aquaculture (Strand et al., 2021).

Finally, information technology has revolutionised aquaculture, in a similar way to how it has impacted terrestrial crops. Cybernetics optimises semi-automated offshore cage culture, food delivery (Føre et al., 2011) and net cleaning (Brijs et al., 2021; Føre et al., 2018), and recirculating aquaculture systems (RAS); Geographical Information Systems (GIS) are key to site selection (Aura et al., 2021; Ferreira et al., 2014; Falconer et al., 2017), and drones are regularly used for site selection and mooring analysis (Hamilton et al., 2020).

Mathematical models are applied to simulate transport of dissolved and particulate water properties (e.g. Peña et al., 2016), sediment interactions (Cromeey et al., 2002; Cubillo et al., 2016), growth (Brigolin et al., 2009; Cubillo et al., 2016; Ferreira et al., 2008; Filgueira et al., 2014; Santa Marta et al., 2020), environmental effects (Cubillo et al., 2018; Ferreira et al., 2012c; Ferreira et al., 2018), and pathogens (Taylor et al., 2011; Bidegain et al., 2017; Salama and Murray, 2011; Salama and Rabe, 2013). In the last decade, the Internet of Things (IOT) added sensor capability to this portfolio (Føre et al., 2016; O'Donncha and Grant, 2019), allowing the combination of real-time environmental data, organism response, and model application (Ferreira et al., 2021) to enable precision aquaculture. These models show great promise for bridging the present-day information divide, using web-enabled platforms, cloud processing, and distributed data to make complex tools available in under-resourced nations where much of the world aquaculture takes place.

An emerging area that has received less attention (but see Nobre et al., 2010 and Ferreira and Bricker, 2019) is the connection of catchment, estuary or bay, and adjacent ocean, through the application of end-to-end modelling tools to better understand the interactions of these complex systems and the consequences of e.g. changes in land use with respect to aquaculture performance. In particular, the explicit simulation of High-Impact-Short-Term (HIST) events such as pulse discharges of Combined Sewer Overflows (CSOs) or emptying of multiple shrimp ponds at the end of a culture cycle helps to understand water quality degradation through eutrophication spikes and effects on cultivated organisms such as growth spurts and accumulation of enteric bacteria in bivalves.

This is key to integrated catchment management and carrying capacity assessment in systems where finfish and/or shellfish cultivation exists or is planned. Fed aquaculture, whether land-based or in open water, is a net contributor of dissolved nutrients and particulate organics, and although bivalves are net sinks of carbon, nitrogen, and phosphorus, cultivation of mussels or oysters may result in a local increase of C, N, and P due to the release of fast-sinking faeces and pseudofaeces (Ferreira and Bricker, 2019). Taken as a whole, the

complexity of these systems and the need for policy-makers to deal with both source apportionment and internal biogeochemical processes were important considerations in the development of the present study.

The objectives of this work are to: (a) describe an integrated modelling framework that deals with the whole soil-to-sea continuum; (b) illustrate the application of this framework to an embayment where bivalve shellfish are commercially farmed; (c) analyse different loading and source apportionment scenarios and their consequences in terms of aquaculture production.

2. Methods

2.1. General modelling framework

The general framework developed for this work is shown in Fig. 1, together with examples of the models and other components it integrates. The SUCCESS (System for Understanding Carrying Capacity, Ecological, and Social Sustainability) modelling framework includes:

1. A hydrological model that addresses catchment loading of water, nutrients, and organic matter, from both rural and urban sources, including CSOs. In SUCCESS, the Soil and Water Assessment Tool (SWAT; Nunes et al., 2017) was applied, including a drainage area model (DAM) to deal with discharge of both sewage and stormwater from urban areas (Northern Ireland Water, pers. com.). SWAT is normally run with a daily timestep; for this work, the model was modified to use an hourly timestep (Boithias et al., 2017) in order to simulate HIST events for nutrient and bacterial loading;
2. A fine grid, high resolution, three-dimensional circulation model (Delft3D-Flow, e.g. Lesser et al., 2004) to capture the detailed hydrodynamics of bays or estuarine systems. A coarser grid 3D model was used to provide the boundary conditions at the ocean end-member;
3. A physiologically-based individual net energy balance (NEB) model (AquaShell) simulating growth and environmental effects of cultivated bivalve shellfish (Saurel et al., 2014; Cubillo et al., 2021);
4. The well-tested EcoWin.NET ecosystem model (Ferreira, 1995; Nobre et al., 2010; Bricker et al., 2018), which integrates all the components above and is able to simulate multiple aquaculture cycles at the decadal scale.

A number of these framework components have been previously described in the literature (Nobre et al., 2010; Nunes et al., 2011; Bricker et al., 2018); further details are provided below as necessary, together with calibration and validation outputs for the study area.

2.2. Study area

2.2.1. General features

Dundrum Bay (Fig. 2) is located in County Down, Northern Ireland, United Kingdom. The system consists of two interconnected bays: Inner Dundrum Bay (IDB) is predominantly intertidal, 6 km long and 1.4 km at its widest point, and is used for bivalve cultivation; IDB is connected to the more exposed south-facing Outer Dundrum Bay (ODB) by an inlet channel. Dundrum Bay (both Inner and Outer) is designated as a Special Area of Conservation (SAC) known as Murlough SAC and a small part is a nature reserve, attributable to the presence of dune systems, sandbanks, mud and sand flats, and saltmarshes, and due to the presence of the common seal (*Phoca vitulina*) as well as many species of waders, ducks, and geese (Clements and Service, 2015; DAERA, 2019).

Because IDB has a small storage volume, mixing and advection processes in ODB and the adjacent shelf determine the fraction of Inner Bay water which gets re-incorporated in the next flood tide. In addition to the tide, wind, and coastal processes, IDB is influenced by the Ardilea, Blackstaff, Carrigs and Moneycarragh rivers, which contribute to the modulation of salinity and to the residual flow across the inlet.

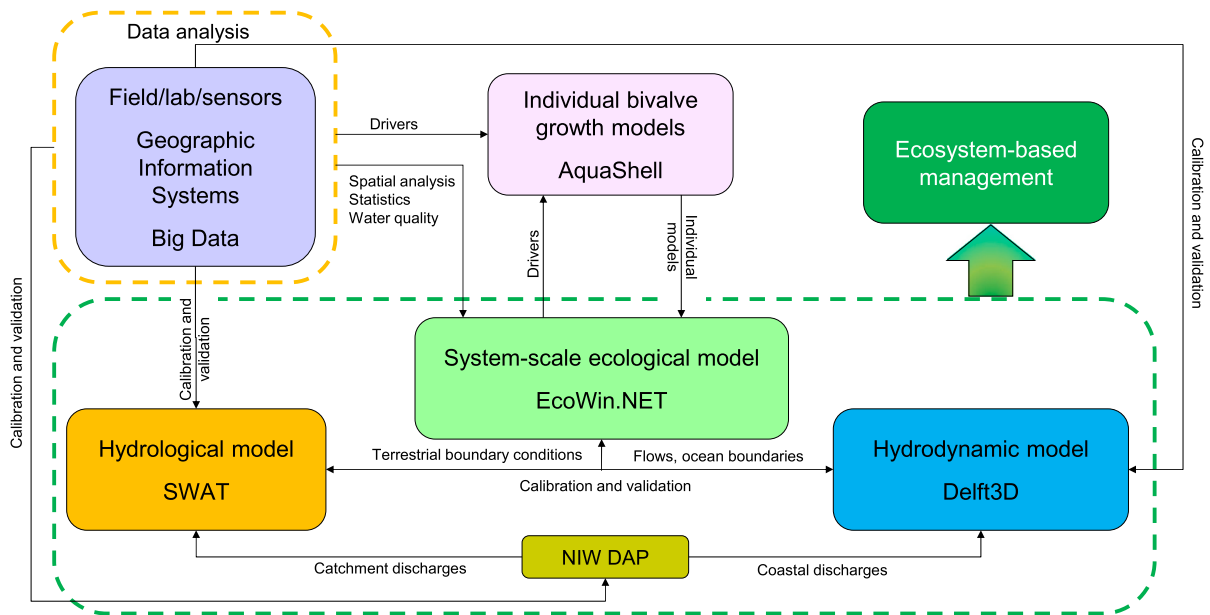


Fig. 1. Conceptual diagram of the SUCCESS (System for Understanding Carrying Capacity, Ecological, and Social Sustainability) modelling framework (NIW DAP: Northern Ireland Water Drainage Area Models).

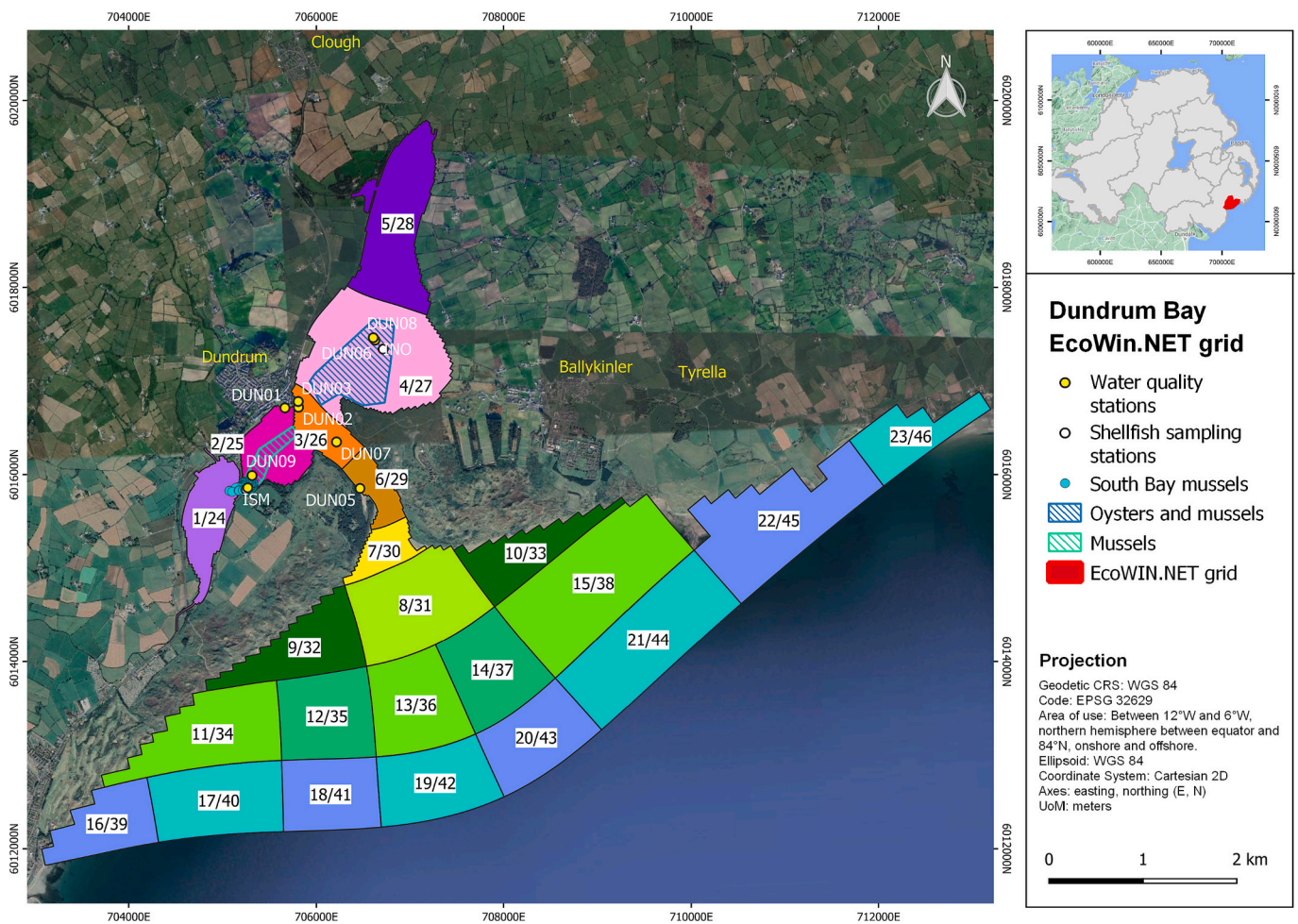


Fig. 2. Dundrum Bay, showing sampling stations, shellfish growing areas, and EcoWin.NET boxes (labelled 1–23 for Upper boxes and 24–46 for lower model boxes). Inner Dundrum Bay (IDB, upper part of the bay) is separated from Outer Dundrum Bay (ODB) by an inlet channel (boxes 6/26, 7/27, 8/28).

2.2.2. Shellfish cultivation

Designated shellfish waters in IDB cover an area of 2.12 km². Since 1980, bivalve aquaculture occurs in two licensed areas, covering 51.6 ha in the north and 11.8 ha in the south (Fig. 2). The north is licensed for Pacific oyster (*Magallana gigas*, currently 6 ha on trestles) and blue mussel (*Mytilus edulis*) and the south is licensed only for blue mussels (currently 12 ha bottom culture). An overview of the husbandry practice is given in Table 1.

2.2.3. Catchment and loading

Dundrum Bay has a catchment area of about 150 km². Land use is dominated by pastures, followed by natural grassland, moors and heathland, and mixed cultivation patterns. Along the coastal zone, land use consists of pastures, discontinuous urban fabric, agricultural activities, and recreational areas such as sport and leisure facilities and beaches.

Land use is 80% agricultural: predominantly sheep farming, followed by cattle, pigs, and poultry. Daily *E. coli* loadings per individual per day vary among species (Jones and Hobbs, 1996): sheep rank first (18.1 × 10⁹), followed by pigs (8.9 × 10⁹), cattle (5.4 × 10⁹), gulls (2 × 10⁹), humans (1.9 × 10⁹) and poultry (0.24 × 10⁹). There are 7 urban wastewater networks in the catchment: up to 65% of the major freshwater sources potentially affect the Inner South area and 35% the Inner North. The Dundrum wastewater treatment plant (WWTP) discharges directly into the Inner South Bay, within 70 m of the mussel aquaculture area, which is also affected by WWTP discharges into the Carrigs River (Annsborough and Leitrim). The Moneycarragh River also affects the Inner South area. The Inner North is affected by two small WWTP, Clough and Loughinisland, discharging to the Ardilea and Blackstaff Rivers respectively. There are a number of possible direct sources of untreated sewage into IDB from spills to the rivers, spills from the WWTP, and CSOs. Runoff from agricultural land also enters the bay directly or through the rivers.

2.3. Data collection and model setup

2.3.1. Water quality and shellfish growth data

Bi-monthly surface and bottom samples were collected in Dundrum

Table 1

Culture practice data for blue mussel and Pacific oyster farming sites in Inner Dundrum Bay. These data were used to run the EcoWin model with environmental drivers from 2018.

	Inner Bay (South)		Inner Bay (North)	
	Blue mussel		Pacific oyster	Blue mussel
<i>Areas and layout</i>				
Total leased area (ha)	11.8		51.6	51.6
Farmed area (ha)	11.8		6.0	0.8
Culture structures	Bottom culture, 50% intertidal		Intertidal trestles	Intertidal trestles
<i>Economics and finance</i>				
Seed cost (£ kg ⁻¹)	–		5–10	–
First-sale price (£ kg ⁻¹)	–		11–15	–
<i>Culture practice</i>				
Stocking density (ind. m ⁻²)	1539		70	127
Seeding effort (ton ha ⁻¹ y ⁻¹)	0.6		21	0.83
Mortality (% cycle ⁻¹)	50		7	50
Seed weight (g live weight)	0.65		30	0.65
First seeding day	150 to 240		150 to 300	150 to 240
Culture period (days)	1095		550–730	1095
Harvest weight (g live weight)	–		>70	>10–12
Declared harvest (tons y ⁻¹)	–		173.1	2.77

Bay and Dundrum watershed between April 2018 and March 2019 for water temperature, salinity, total particulate matter, particulate organic matter, chlorophyll, dissolved nutrients, and bacteria. High intensity rainfall (HIR) events were monitored using automatic water samplers installed in the river network to help calibrate the SWAT model. A Sontek River Surveyor M9 (SONTEK San Diego, Ca.) was deployed to map the riverbed profile, water column velocity profiles, and measure current velocities to obtain discharge values for the four main rivers.

Hourly profiling of conductivity, temperature and depth was carried out using a SBE 19plus V2 SeaCAT (SEABIRD Scientific, Seattle, WA) at three additional stations over a full tidal cycle (Fig. 2): Dun07 in the inlet channel, Dun08 (Inner North Bay), and Dun09 (Inner South bay), to provide validation data for the Delft3D model.

Shellfish growth trials were performed in 2018 on blue mussels grown in both North and South bays. These growth trials provided partial growth curves, covering a size range of 38–57 mm. Growth data were also obtained for juvenile and half-grown Pacific oysters in Inner Dundrum North Bay, ranging from 40 to 100 mm shell length and 6.5 to 90 g live weight.

Laboratory experiments (see e.g. Ferreira et al., 2008) and data collected over the last four years in various Northern Irish loughs, including Belfast Lough, Lough Foyle, Carlingford Lough, and Dundrum Bay, were used to calibrate the individual bivalve models; measured growth data were used to validate the individual growth model for mussels and oysters, driven by synoptically collected water quality data from 2018 and 2019. The models aimed for generality in application to shellfish growing areas in Northern Ireland. The locations of the shellfish growth monitoring stations in IDB are shown in Fig. 2.

2.3.2. SWAT model

The SWAT model sub-basin definition was designed to match the EU Water Framework Directive (WFD, 2000/60/EC) freshwater basins (FB) delineation, with each FB represented by at least one sub-basin. The catchment delineation resulted in the creation of 11 sub-basins with an average area of 12.9 km² (Fig. 3). There are four main outlets, corresponding to the four main rivers discharging into the bay, that are inputs to the hydrodynamic and coastal models.

Hydrological Response Units (HRU) are a unique combination of land use, soil, and slope classes, and correspond to a subdivision of a sub-basin for which field scale processes can be simulated (e.g. water balance, nutrient cycling, plant growth) before being aggregated at the sub-basin level where they will be routed through the river network. HRUs are not spatialized units but represent a percentage of a sub-basin area with homogeneous properties. To calculate HRU statistics, SWAT requires information on land use, soil type, and slope (Fig. 3); Land use was provided by Corine Landcover 2012 (CLC, 2012), soil type by the European soil database (ESDB) and slope was calculated from the digital elevation model (DEM) used for sub-basin creation (EU-DEM, 25 m). In total, 66 HRUs were defined for the 11 sub-basins. Cattle density in pasture was defined based on the Northern Ireland Agricultural Census from the Department of Agriculture, Environment and Rural Affairs (DAERA, 2018) aggregated at the Dundrum watershed level. The annual quantity of agricultural slurry/manure (N and P) applied in pasture corresponds to the quantity of manure produced by livestock when housed and the annual quantity of chemical fertiliser applied was estimated using the fertiliser application statistics produced by DAERA for Northern Ireland.

In order to run SWAT at an hourly time step, hourly rainfall data are needed. Rainfall radar data were used to provide a good representation of the spatial-temporal variability of precipitation over the simulated area. Twenty-two rainfall time series were extracted from the Met Office radar data grid (Met Office, 2003) and hourly rainfall values were then combined into one representative rainfall time-series for each sub-basin using a spatially weighted average.

The hydrological component of the SWAT model was assessed using Nash-Sutcliffe efficiency criteria (NS), percent bias (PBIAS), and the

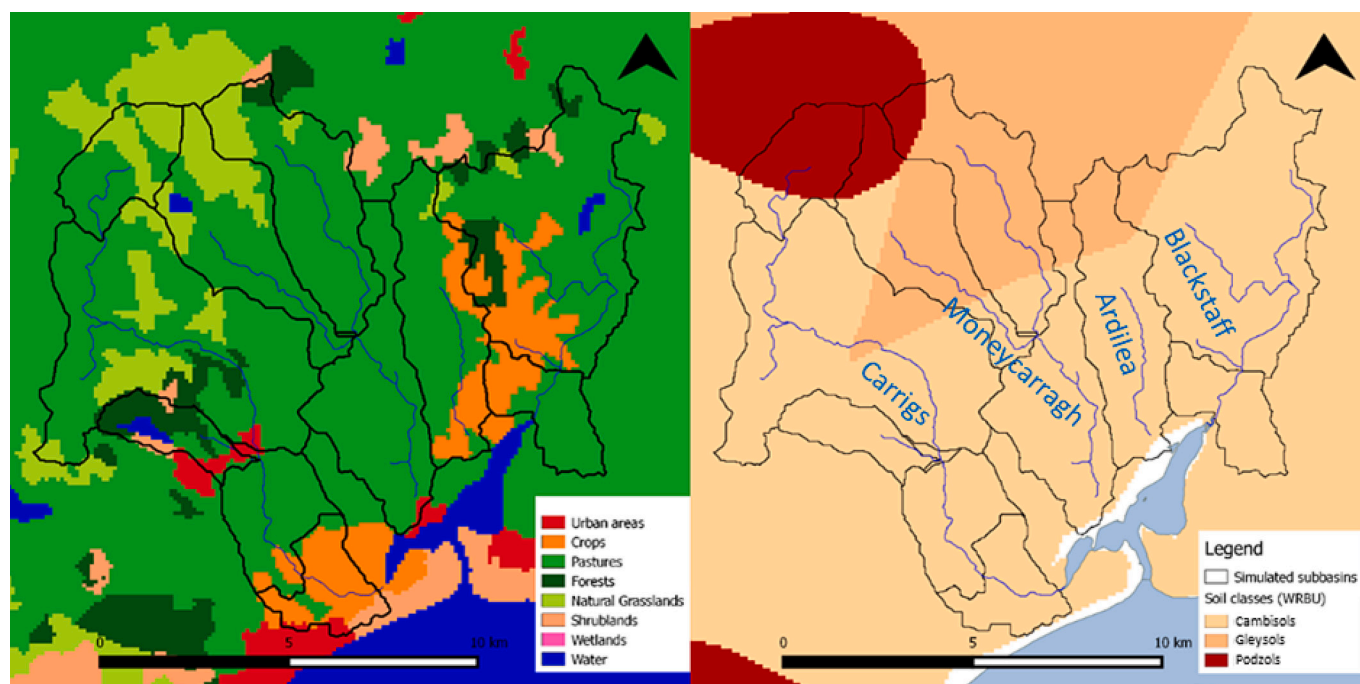


Fig. 3. Land-use (left) and soil (right) maps used to create the SWAT model hydrologic response units.

coefficient of determination (r^2), shown in Table 2. According to Moriasi et al. (2015), the model performance can be rated *Good* to *Very Good*. The water quality component of the model was assessed by a visual comparison between the simulated results and bi-weekly and HIR water quality data, including nutrient and bacterial concentrations.

2.3.3. Hydrodynamic model

Inner Dundrum Bay exchanges most of its volume every tidal cycle with the neighbouring shelf. Due to the small storage capacity of the IDB, most of the mixing and dispersion of water from the Inner Bay takes place in the outer area of Dundrum Bay. Hence, the water properties of IDB depend strongly on the flood tide water. A review of the currents in Inner and Outer Dundrum Bay showed that in Outer Dundrum Bay the tide is responsible for a maximum of 50% of the velocity's variance. Whilst the tide dominates transport in IDB, away from the influence of the tidal inlet, wind and stratification will be the main conditions determining the type of circulation: either barotropic and in the general direction of the wind or baroclinic when the wind action and heating allow stratification to develop. The oscillation between these two modes is important for dispersion of land-based discharges, such as enteric bacteria and nutrients that have a decay time greater than one tidal cycle. The existence or absence of an inner shelf condition (Lentz, 1995) or frontal systems can determine the residence time of flushed inner-bay water within the reach of the inlet's tidal excursion and thus affect the amount of IDB water re-incorporated in the next flood tide.

To simulate this, a model is required: (i) with a full 3-dimensional

Table 2
Model performance criteria for the hydrological component of the SWAT model.

Stations	Performance criteria	Value
Moneycarragh	NS	0.72
	PBIAS	-7.7%
	r^2	0.75
Feedwell (Carrigs)	NS	0.78
	PBIAS	-2.6%
	r^2	0.81
Sissy's Point (Carrigs)	NS	0.81
	PBIAS	6.34%
	r^2	0.82

domain to give a good description of the vertical structure; (ii) forced by space-varying atmospheric momentum to account for direct wind forcing and wind curl, key to establish mixing and stratification conditions; (iii) incorporating heat exchange with the atmosphere to allow a good description of the stratification cycle; and (iv) forced at the boundary by a mesoscale model to allow for mesoscale thermohaline structures to propagate inside the domain and to provide a more stable and predictable simulation of the seasonal stratification.

The Delft3D-Flow model (Lesser et al., 2004; Deltares, 2010) was used to build the hydrodynamic and transport models for Dundrum Bay. The model uses curvilinear grids appropriate for domain decomposition, allowing two or more models to be set up and executed simultaneously, each providing boundary information to the other. In order to describe processes both at the Irish Sea mesoscale and at the Inner Dundrum small scale we developed two subdomains: the Western Irish Sea and Dundrum domains.

The Western Irish Sea domain has a horizontal grid of 146×112 cells, with resolution that varies from 500 m along sections of the coast to 3000 m at the adjacent shelf (Fig. 4), and with 8 vertical, terrain-following, sigma layers. To the north the grid extends approximately 25 km north of Larne Lough and south of Carlingford Lough, and 40 km offshore. The bathymetry adjacent to Carlingford Lough and Dundrum Bay was obtained from the UK Hydrographic Office (UKHO). Further north, General Bathymetric Chart of the Oceans (GEBCO) data were used. The model is forced at its lateral boundary by the Marine Institute Northeast-Atlantic ROMS (NEA_ROMS; Nagy et al., 2020) model for subtidal water level, full velocity spectrum, salinity, and temperature. The NEA_ROMS model has 1.1 km horizontal resolution and 40 vertical sigma levels with the highest concentration of levels at the surface and the bottom. The tidal water levels were obtained by synthesis of the FES2014b tidal constituent atlas (Carrere et al., 2016; Lyard et al., 2021) and incorporated with the NEA_ROMS subtidal water levels and velocity in the form of Riemann invariants at a 6-min time step. Atmospheric forcing in the form of momentum input from the wind, atmospheric pressure and heat-exchange parameters were provided by the European Centre for Medium Range Weather Forecasts (ECMWF) with a 3-hourly time step, at a 0.125° horizontal grid, the same solution used by the NEA_ROMS.

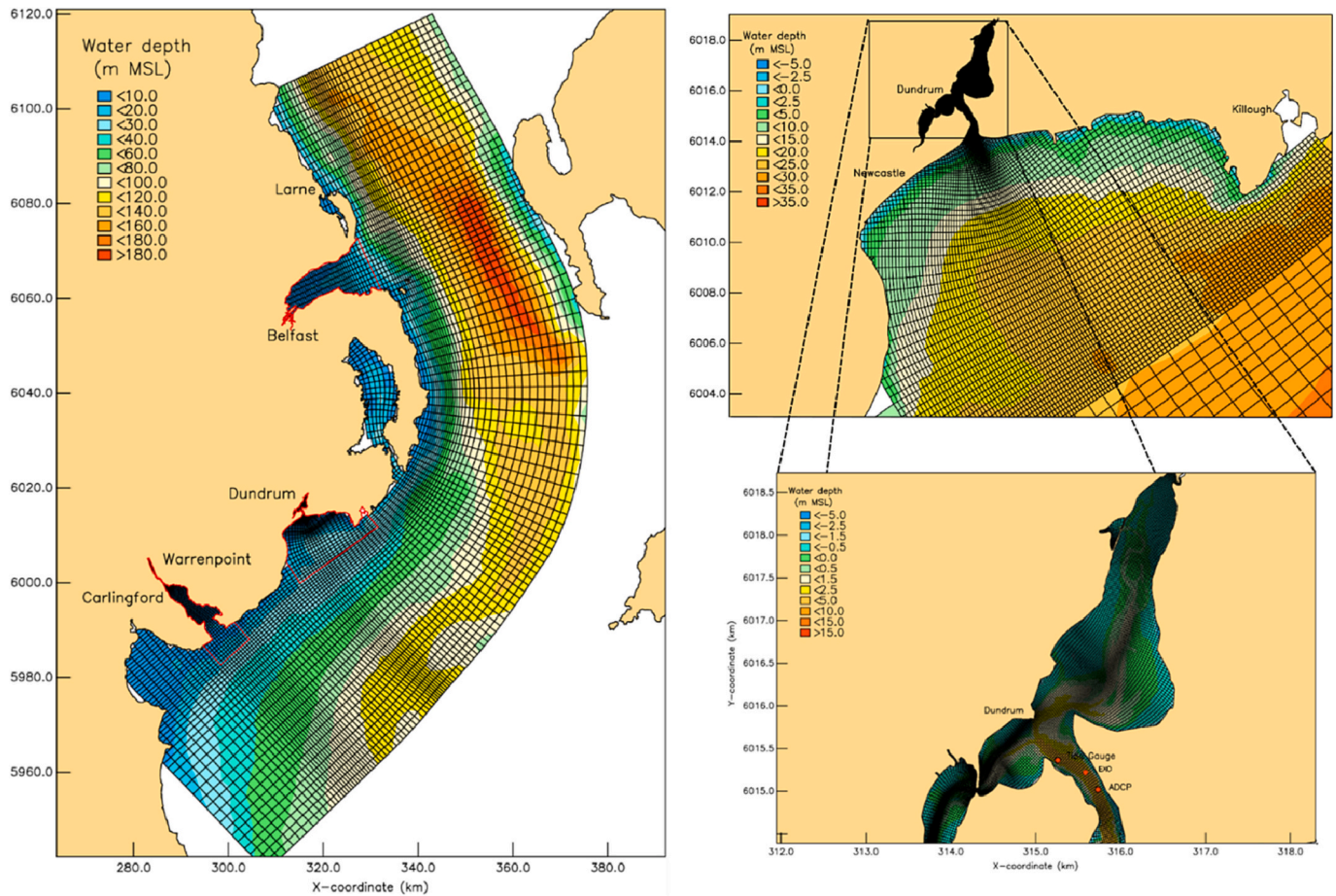


Fig. 4. Delft 3-D computational grid for Dundrum Bay and the Irish Sea model grid (UTM coordinates for display purposes). The grid in the inner bay appears black due to the high number of grid cells.

The Dundrum Bay domain has 350×167 cells in the horizontal, 8 vertical sigma layers, and is designed so that the grid sizes are refined to a size of ~ 13 m along sections of the main channels in the bay, ~ 20 m along the inlet channel and ~ 250 m at the adjacent shelf where it connects to the Western Irish Sea domain. The bathymetry was constructed from (i) photogrammetry drone survey (inner bay); (ii) boat surveys (inlet channel) and; (iii) the UKHO base (Outer bay and adjacent shelf).

Circulation and transport were validated by comparing salinity and temperature at a stage when the model outputs are independent from the initial condition after a 6-month spin-up (Table 3 and Fig. 5) In the Western Irish Sea domain, water levels were validated at the mouth of Belfast Lough, Dundrum Bay, and Carlingford Lough, while salinity and temperature were cross-validated with the NEA_ROMS model for the full domain (validation of NEA_ROMS model reported in Nagy et al., 2020).

Fig. 5 e) and f) show that the Western Irish Sea model adequately represents the salinity and temperature profiles at the mouth of Belfast Lough, Dundrum Bay, and Carlingford Lough, lends confidence with respect to the good depiction of the mesoscale dynamics (yearly RMSE $< 1^\circ\text{C}$ and < 0.2 PSU for temperature and salinity respectively).

The hydrodynamic response of the Dundrum Bay subdomain was calibrated against water level and velocity measurements at the inlet by adjusting the bottom roughness in the Inner Bay and making small changes in local bathymetry where there was uncertainty about the actual depth at the time of the calibration data was collected.

Water levels, temperature, and salinity in Dundrum Bay were validated at the inlet channel. Fig. 5 (a to d) shows the good fit of the depth-averaged velocity at inlet channel during a complete fortnightly cycle (RMSE $< 5\%$ of the range and skill > 0.99). The model also presents a

Table 3

Hydrodynamic and transport performance indicators for the Western Irish Sea and Dundrum domains.

Location	Skill	RMSE	Bias (%)
Water level calibration Dundrum inlet	0.996	0.14 m ($< 5\%$)	0.74
Velocity calibration Dundrum inlet	0.998	0.12 m/s ($< 5\%$)	0.01
Water level validation Dundrum inlet	0.996	0.16 m ($\sim 5\%$)	1.01
Water level validation Belfast (Bangor)	0.987	0.14 m ($< 5\%$)	-0.95
Water level validation Carlingford (Greenore)	0.991	0.16 m ($\sim 5\%$)	-0.07
Temperature validation Belfast offshore (yearly)	0.89–0.92	0.8–0.9 $^\circ\text{C}$	-3 to -6%
Temperature validation Dundrum offshore (yearly)	0.92–0.94	0.7–0.8 $^\circ\text{C}$	-3 to -6%
Temperature validation Carlingford offshore (yearly)	0.92–0.96	0.6–0.9 $^\circ\text{C}$	0 to -2%
Salinity validation Belfast offshore (yearly)	0.87	0.1–0.2 psu	-13%
Salinity validation Dundrum offshore (yearly)	0.83–0.86	0.1–0.2 psu	-2 to -5%
Salinity validation Carlingford offshore (yearly)	0.81	0.1–0.2 psu	-2 to -3%
Salinity validation Dundrum inlet	0.94	3.38 psu (12%)	-3%

good response to river flow input matching the response from the catchment, most felt at low water slack, and the changing of the ambient shelf water in Outer Dundrum bay during flood tide (Fig. 5 g and h). This indicates a good representation of the mixing and dispersion outside of the inlet, showing the reincorporation of Inner Dundrum Bay water and

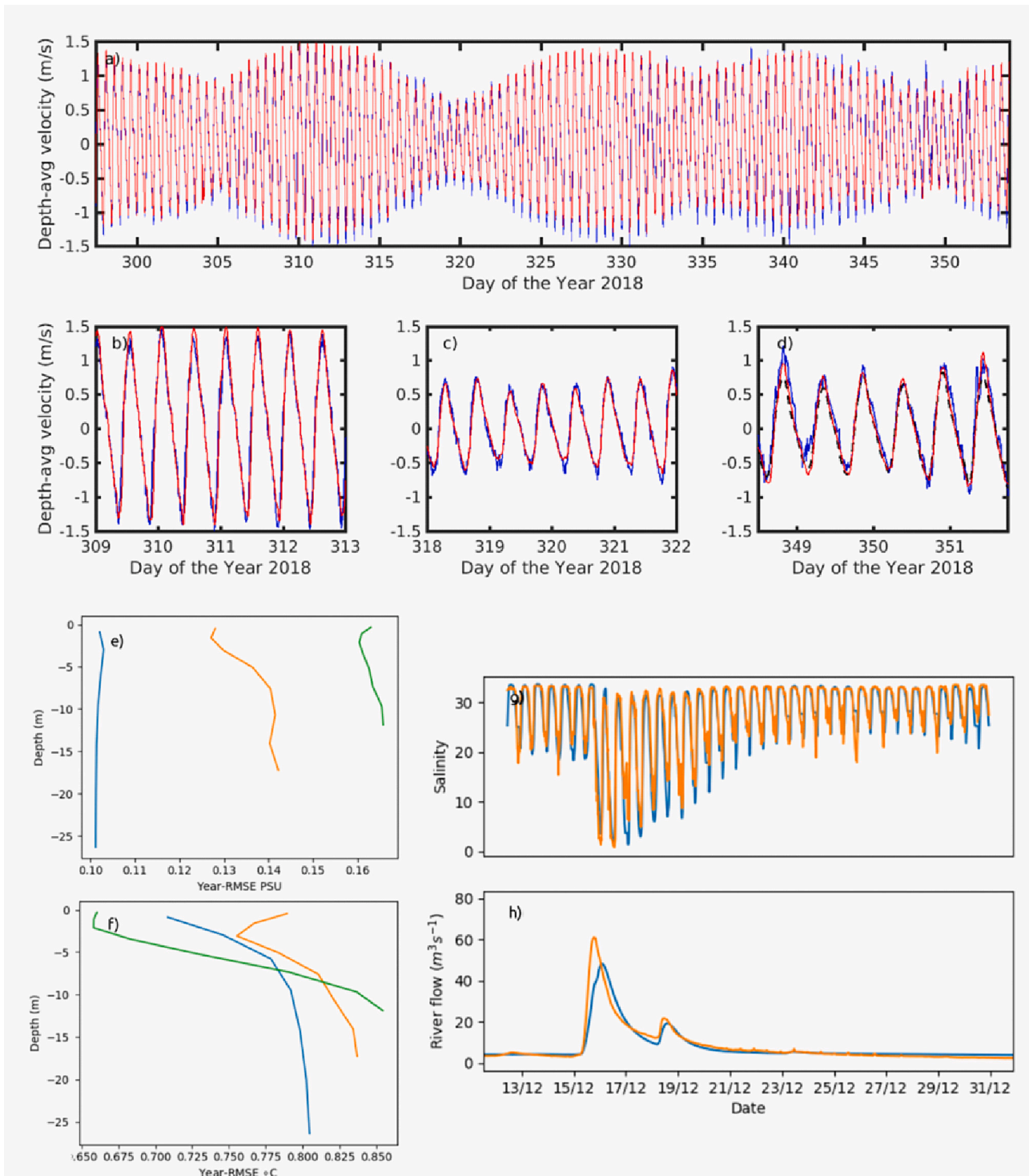


Fig. 5. Hydrodynamic model fitness: (a) to (d) comparison of measured and modelled velocity in the Inner Dundrum Bay inlet channel for: (a) the full validation period; (b) a spring tide; (c) a neap tide; and (d) mid-cycle. Velocity measurements are in blue (raw) and black (tidal velocity only), and model results are in red; (e) and (f): Western Irish Sea year-long vertical RMSE comparing the modelled salinity (e) and temperature (f) with the NEA_ROMS model at the mouth of Belfast Lough (orange), Dundrum Bay (Blue), and Carlingford Lough (green); (g) salinity validation for Dundrum bay: observed (orange) and modelled (blue) salinity; (h) observed (orange) and SWAT-modelled (blue) river flow. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

thus simulating the flushing of the bay proficiently (skill 0.94 and RMSE of 12% of the range for salinity).

2.3.4. Bivalve individual model

2.3.4.1. AquaShell model development. Filter-feeding bivalves have complex interactions with their environment. The impact of these interactions depends on a number of variables, including population

density, water quality, and food availability. To model the positive and negative interactions of bivalves with the ecosystem it is necessary to simulate physiological response and growth at the individual level.

The individual shellfish models used in SUCCESS are part of the generic AquaShell™ framework, which has been developed and parameterized for multiple shellfish species and validated for different locations across Northern Ireland (e.g. Ferreira et al., 2008; Ferreira et al., 2018), Ireland (e.g. Nunes et al., 2011; Sequeira et al., 2008), and elsewhere (e.g. Bricker et al., 2018; Cubillo et al., 2018, 2021; Nobre et al., 2010; Saurel et al., 2014).

These individual growth models use a net energy balance (NEB) approach and have been published elsewhere for the species farmed in Dundrum (see e.g. Cubillo et al., 2017 for blue mussels and Ferreira et al., 2012a, 2012b, 2012c for Pacific oyster).

Improvements to these individual shellfish growth models have led to greater accuracy in simulating both shellfish production and environmental effects. This improved approach for modelling blue mussels and Pacific oysters has been successfully tested in various European systems (Ferreira et al., 2021; Cubillo et al., 2021), and in other Northern Irish Loughs such as Belfast Lough, Carlingford Lough, and Lough Foyle.

The main disadvantage of previous individual modelling approaches is the lack of flexibility to deal with the wide range of food conditions encountered in nature, from oligotrophic to highly eutrophic waters.

The objective of the new AquaShell™ framework was to produce a more generic model, able to deal with the range of food conditions found across Northern Irish loughs. To achieve this, the feeding behaviour simulation of the individual model was modified as follows:

- Limitation of bivalve food intake by establishing a maximum ingestion rate based on the gut capacity/gut volume, related to animal size through an allometric relationship, and gut passage time, following Scholten and Smaal (1998, 1999).
- Limitation of ingestion rate by the pseudofaeces production rate, which is estimated in different ways as: (i) the difference between filtration rate and the maximum ingestion rate—when the maximum ingestion rate limits food intake; or (ii) a function of particulate organic matter (POM) and a half-saturation constant for rejection (K_c), through a Michaelis-Menten formulation.

The validation of AquaShell™ model outputs for different sampling stations and oyster sizes is shown in Fig. 6.

The improved parameterization of environmental effects of shellfish culture on the environment, in particular the net removal of phytoplankton and non-phytoplankton organics, and a more robust nutrient mass balance, provide added value by including regulatory ecosystem services of shellfish in the modelling framework. The individual shellfish models are then used at the ecosystem scale in EcoWin.NET to determine

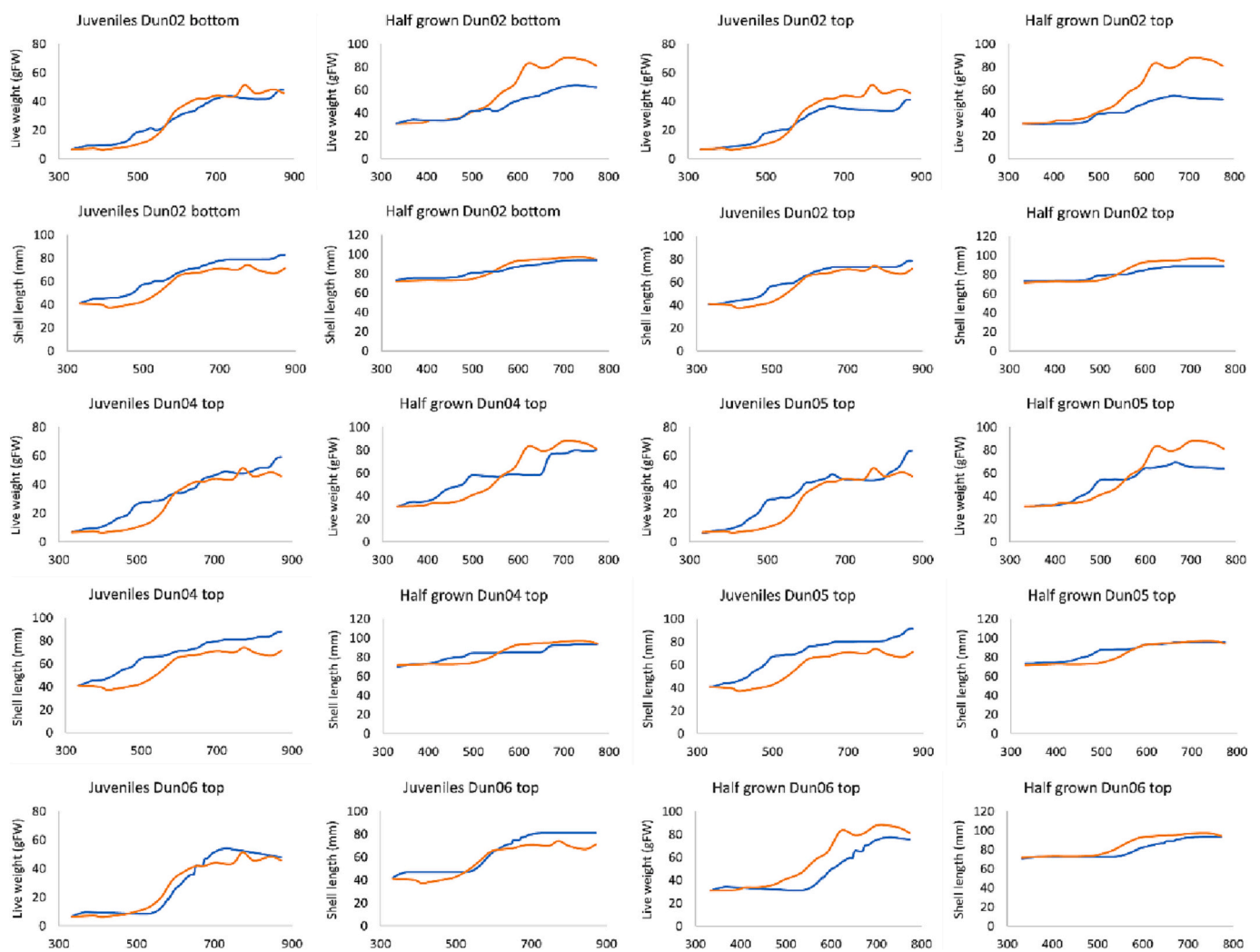


Fig. 6. Comparison of measured growth in juvenile and half-grown *Magallana gigas* cultivated on trestles in Inner Dundrum Bay North (orange lines) with predicted growth from AquaShell (blue lines) at sampling stations Dun 02, 04, 05, and 06. Upper (top) and lower (bottom). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

both shellfish production and environmental effects at the bay scale: removal of suspended particulate matter, particulate organic waste, excretion of dissolved nitrogen, and oxygen consumption.

2.3.5. Ecological model

The ecological model for Dundrum Bay was developed using the well-tested EcoWin.NET (EWN) application (see e.g. Nobre et al., 2010; Bricker et al., 2018).

The EWN model domain (Fig. 2) was divided into functionally uniform boxes according to a multi-criteria approach based on physics, water quality, WFD water bodies, and aquaculture leases, yielding areas that span 10–100's Delft3D-Flow calculation cells. The Delft3D-Flow subdomain was subset to the area of influence of the Inner Bay plume and then divided into 23 horizontal boxes. The 8 σ layers from Delft3D were aggregated into 2 vertical layers based on the ratio of stratification depth to water column depth at the mouth of Dundrum Bay, to give a total of 46 individual computation units.

The flow across the Delft3D-Flow cells at the boundary between EWN boxes was aggregated to provide water exchanges at the box boundaries with a 30 min timestep. A trend correction was applied to each yearly run to compensate for the residual flow, thus allowing the production of decadal runs by repeating a single year of circulation outputs.

The model developed for Dundrum runs for ten years, therefore dealing with multiple aquaculture cycles, and contains less complexity in the physics, partly because of the large number of processes and pelagic and benthic state variables simulated, when compared to Nutrient, Phytoplankton, Zooplankton and Detritus (NPZD) models such as ROMS or Delft-WAQ, which are fundamentally designed for the coastal ocean.

EWN was calibrated using four different approaches:

1. Calibration of external model components, and validation of these against measured data;

2. Calibration of internal model components based on measurements and/or declarative data;
3. Calibration of internal model parameters based on measurements and literature;
4. Development of bespoke objects that extend the EWN model library.

The external model components are part of the SUCCESS framework shown in Fig. 1, i.e. the SWAT, Delft3D-Flow, and AquaShell models, dealing with hydrology and nutrient loading, coastal circulation, and shellfish growth respectively.

EWN boundary conditions for nutrient concentrations and chlorophyll were taken from monthly sampling campaigns and Copernicus data. Some data on conservative variables such as salinity was taken from the broader scale NEA ROMS model described above. Parameters such as P_{max} , the maximum light-limited production rate, I_{opt} , the optimal light energy, and K_s , the half-saturation constant for nutrient uptake were calibrated based on typical values measured for Belfast, Strangford, and Carlingford Loughs (Ferreira et al., 2008; Capuzzo, 2011).

Bespoke model 'objects' (EWN is programmed using an object-oriented approach, or OOP; see Ferreira, 1995 for the original concept) were developed to reflect particular conditions in Dundrum Bay.

The model was validated for nutrients and chlorophyll based on measured data (Fig. 7 and Fig. 8).

The fortnightly or monthly data sets miss the effect of CSO discharges, seen as model spikes in the winter months; these correspond to HIST events rarely detected in regular sampling campaigns. Box 4 was usually sampled at low tide and samples reflect river properties, which accounts for the poor model fit to some of the data. On the other hand, a correlation analysis between observed and simulated chlorophyll for the warmer part of the year (days 100–300) for box 6 and box 29 shows r is equal to 0.75, with a probability of significance >99% ($P_{<0.01} = 0.623$).

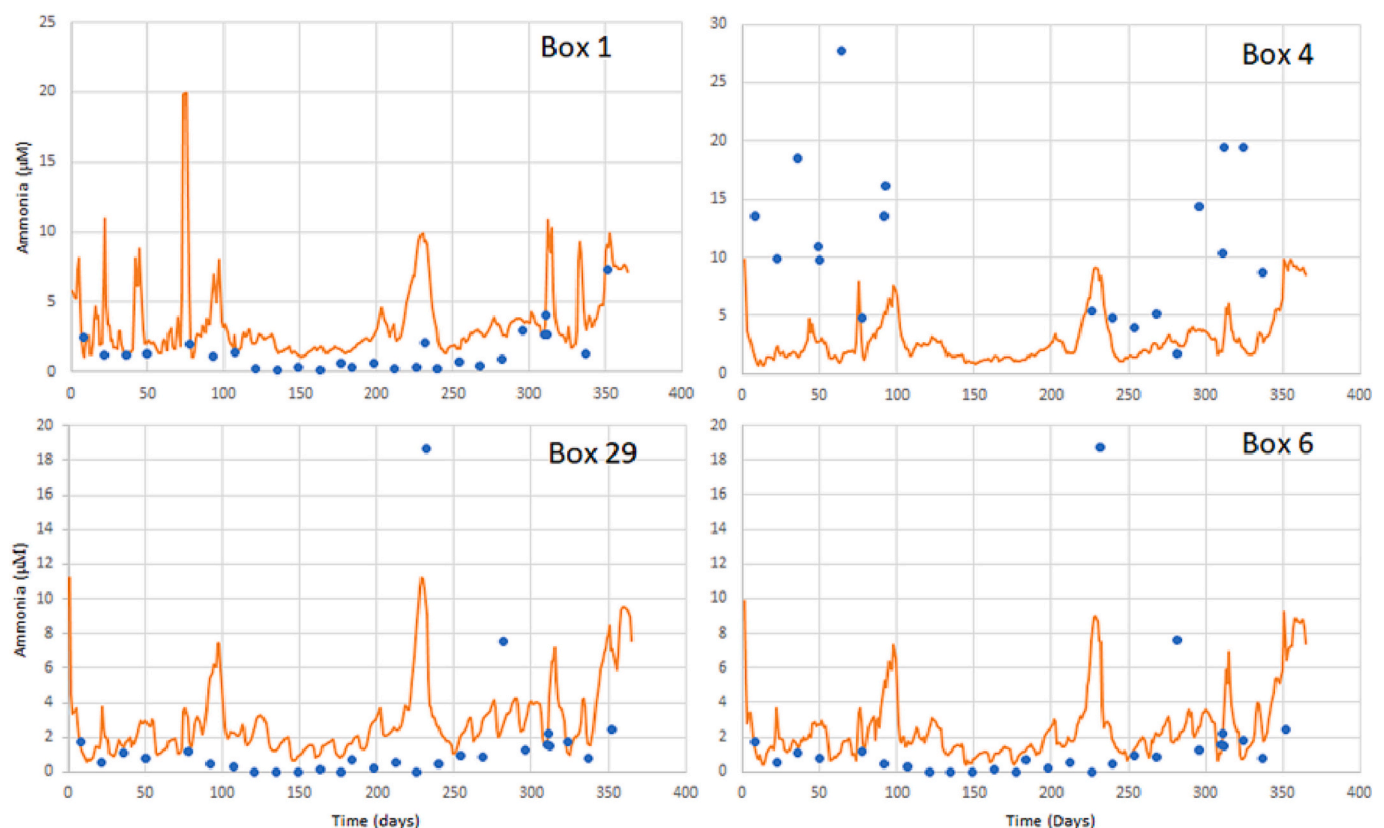


Fig. 7. Ammonia concentration in four model boxes (Inner Dundrum Bay and inlet channel).

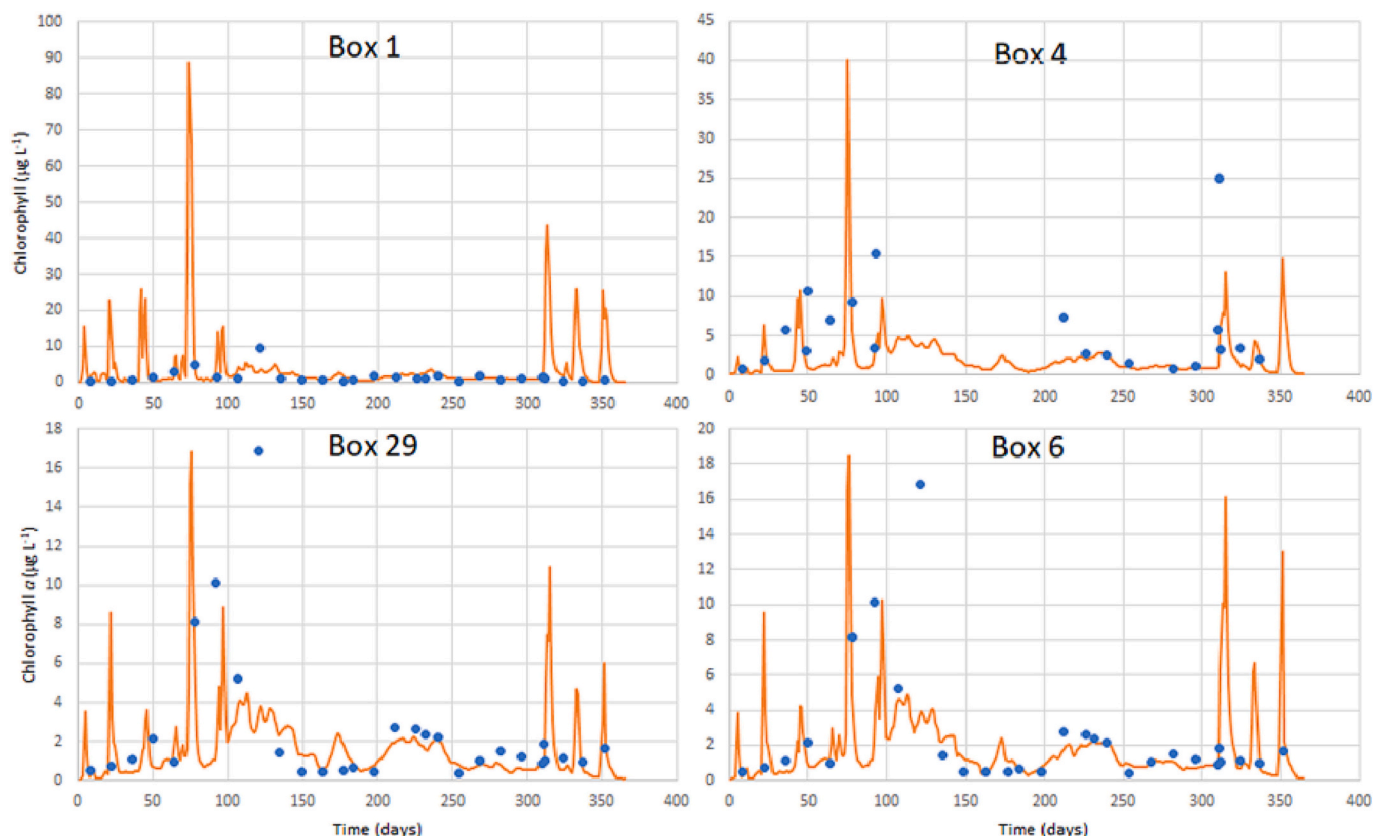


Fig. 8. Chlorophyll concentration in four model boxes (Inner Dundrum Bay and inlet channel).

In box 29, $r = 0.72$, allowing rejection of the null hypothesis with an equally high probability.

The key drivers for shellfish growth, i.e. phytoplankton chlorophyll and particulate organic matter, are considered to be simulated with sufficient quality to drive the shellfish growth models.

Harvestable biomass of shellfish is one of the key indicators that EcoWin provides to support management decisions. There are no intermediate data points that can be measured for this kind of output, so verification is based on the declared harvest. In Dundrum Bay, as in any other system where aquaculture takes place, there are interannual fluctuations in harvest. Data on shellfish landings were analysed for both species over a period of several years in order to arrive at the best estimate of mussel and oyster harvest.

Table 4 shows the validation outputs obtained for the standard model. Differences between declared and simulated harvest are minimal, and the model is considered as correctly reproducing the aquaculture activity in Inner Dundrum Bay.

On the basis of the overall validation of EWN, the standard model

Table 4
Validation of modelled shellfish production in Dundrum Bay.

	Box 25	Box 27	Box 27
	Blue mussel (<i>Mytilus edulis</i>)	Blue mussel (<i>Mytilus edulis</i>)	Pacific oyster (<i>Crassostrea gigas</i>)
Cultivation area (ha)	11.80	0.80	6.0
Cultivation period (days)	1095	1095	550
Seed weight (g live weight)	0.65	0.65	30
Declared harvest (t live weight)	–	2.77	173.08
EcoWin simulated harvest year 9 (t live weight)	–	2.91	169.93
Δ between declared and simulated harvest (%)	–	5.1	–1.8

was accepted as suitable for exploring the ecological behaviour of the bay, within the scope of the state variables EWN includes, and for analysing a range of management scenarios.

3. Results and discussion

The focus of this section is on the outcomes for shellfish aquaculture and water quality obtained through the application of the SUCCESS modelling framework and in particular EcoWin.NET. These include system behaviour analysed (i) from the results of the standard model; and from two different scenarios common in coastal ecosystems: (ii) land-based loading control; and (iii) changes to shellfish aquaculture.

In addition, some SWAT model outputs are shown, but detailed results and scenarios for the land-based modelling are given in Bernard-Jannin et al. (submitted).

3.1. Standard model

SWAT results indicate that the relative contributions of urban and diffuse sources are similar and represent 54% and 46% of the total *E. coli* exports, respectively. Two urban sources (Annsborough Park WWTP CSO and Clough CSOs) can be identified as major sources of bacteria as they account for 43% of the total *E. coli* exports. The other urban sources are less significant and 23 of the 28 urban sources contribute to <1% of the total bacteria exports.

Zones of influence for these sources of enteric microorganisms can be derived from such data, but the translation of bacterial loads into water column concentrations is challenging because a very fine-scale (grid cells of the order of 10×10 m) hydrodynamic model would be required to resolve the peak values. Water column concentrations depend not only on loading but on a combination of complex (see e.g. Tiwari et al., 2019) physical (e.g. ultraviolet radiation at the surface, sedimentation), chemical (e.g. survival in a dilute, nutrient-poor medium,

osmoregulatory issues), and biological (e.g. antibiosis by phytoplankton, competition with autochthonous bacteria), and although proxies such as the T_{90} coefficient (reduction of concentrations by an order of magnitude) are often used, there would be a wide variation in bacterial concentrations e.g. between low water and high water, and between spring and neap tides.

Furthermore, the translation of water column concentrations (the indicator used in the US) into shellfish gut concentrations (the indicator used e.g. in the WFD) is extremely complex (e.g. Dabrowski et al., 2014), and possibly more closely associated with feeding behaviour and its drivers than with the concentration in the receiving water. As a consequence, the microbial component is not taken further herein, since more research is required to ensure a modelling framework can make dependable forecasts for use by policy makers.

Fig. 9 shows the response of Box 1 in Inner Dundrum Bay to the HIST discharges from combined sewer overflows. Short-term peaks can be seen in nutrients and organic particulates—the latter are an energy source for bivalves. The water quality in the southern part of IDB is affected by CSO discharges from both north and south, but not much change (<5%) is observed to shellfish growth because sewer overflow is largely a winter phenomenon.

The CSO discharges and periodic deposition of agricultural slurry/manure will however have a detrimental effect on shellfish harvesting (e.g. EC /2073/2005) because of the resulting spike in enteric bacteria. Simulation of inter-valvar and tissue (gut) concentration of enteric bacteria in mussels and oysters presents significant challenges—it is likely that gut accumulation of these pathogens has a stronger dependency on feeding behaviour than on the concentration in the water.

3.2. Scenario analysis

The EWN model was used to test the response of key ecosystem indicators to two different scenarios: (i) bottom-up; and (ii) top-down control of primary production. These scenarios address the balance between source control, which acts to reduce eutrophication but reduces secondary production, and the role of bivalves in reducing or avoiding secondary symptoms of eutrophication (sensu Bricker et al., 2003) such as hypoxia. Fig. 10 shows the response of IDB (Box 4) to the removal of land-based sources of ammonia and chlorophyll. The warmer part of the year shows little change, but the reduction in phytoplankton concentration in the colder months (November–March) is striking.

A synthesis of some key indicators of bottom-up control is provided in Table 5 for three different EWN boxes in the inner bay. An example of the change in chlorophyll percentile 90 is shown for boxes 4, 25, and

27—other boxes show a similar downward trend. In these three boxes, the reduction is over 30–40%.

An analysis of the consequences for shellfish weight and harvest is shown for boxes 25 and 27, where the cultivation takes place (although no harvest takes place in Box 25 at present). Mussels are more sensitive to the reduction in load, with decrease in growth of 10% in Box 25 and 6.9% in box 27, and an overall decrease in harvest of 41%. The difference is due to the much higher harvestable biomass in Box 25.

Oysters do not show a significant difference in the bottom-up control scenario tested. The overarching message appears to be that mussel production would be significantly affected by a drastic reduction in nutrient loading from land. For both species, the consequent reduction in bacterial load would have a major impact on shellfish quality with respect to microbiological contamination (see e.g. bacteriological quality standards subsumed into the EU WFD from the European shellfish waters directives).

Table 6 shows the effect of shellfish cultivation on the percentile 90 of chlorophyll in three EWN boxes: Box 25 and Box 27 are the boxes where shellfish are grown, and Box 6 is in the centre of the inlet channel.

The increase in the typical Chl maximum ranges from 5.8 to 21.6%. For the boxes where cultivation takes place, the southern part of the inner bay shows a much higher difference, but more interestingly, the inlet channel shows the second highest difference—these results suggest that the effect of top-down control occurs in a broader area of the bay, since the benthic filter-feeders are removing food from the water passing through the cultivation sites. Changes to cultivation practice will thus be reflected in a more general way on bay-scale eutrophication.

4. Conclusions

Open-water aquaculture, whether in marine, brackish, or freshwater environments, cannot be dissociated from other water uses, including land-based discharges. Legislative frameworks in many parts of the world (e.g. EU WFD and MSFD, US Clean Water Act, Canada Water Act, China Water Pollution Control Law) mandate environmental standards for receiving waters (as opposed to end-of-pipe thresholds) that must be met by water managers, and are the result of multiple human pressures, accompanied by internal processing within the ecosystem and exchange of dissolved and particulate materials at the sediment and open boundaries.

Policy decisions for systems subjected to multiple pressures are thus extremely complex, both because the relationship between pressure and state (Elliot et al., 2017; Elliot and O'Higgins, 2020) is usually non-linear and because source apportionment presents a major challenge. In

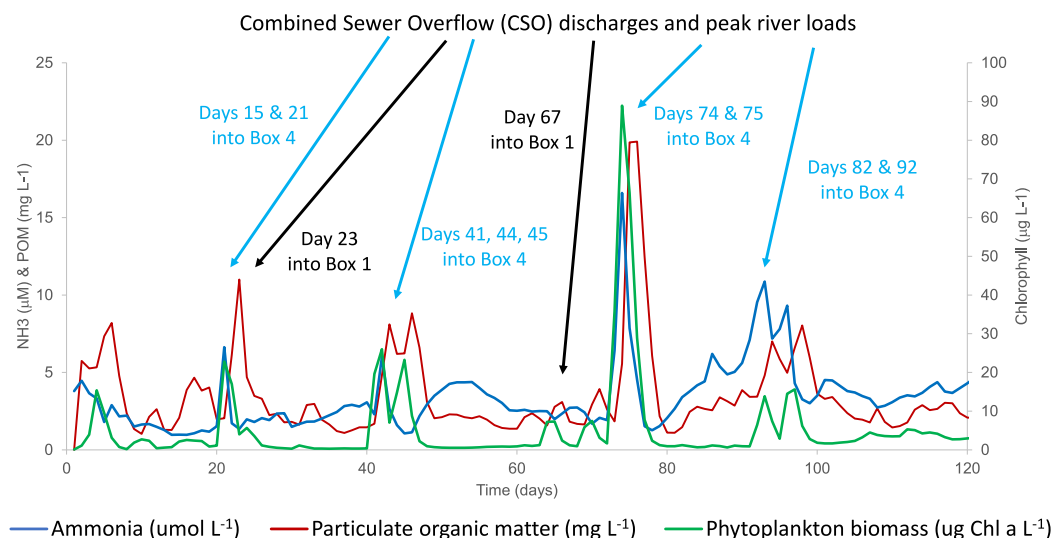


Fig. 9. Ecosystem response (EWN Box 1) to NH_3 loading from rivers and CSOs (Model Year 9).

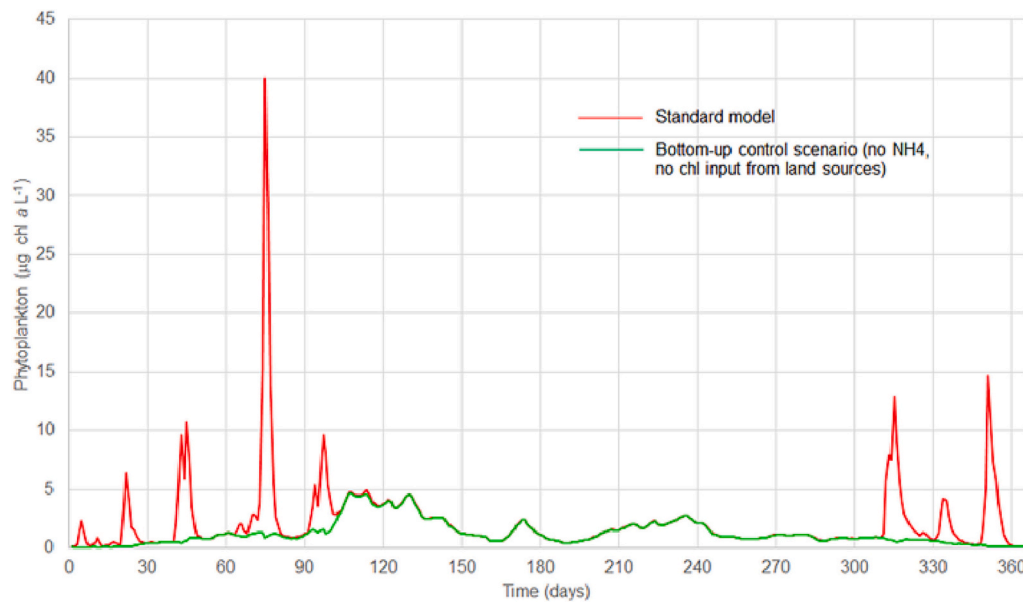


Fig. 10. Chlorophyll concentration in Box 4 (Year 9) for the standard model and for a scenario with no ammonia or chlorophyll loading from land.

Table 5
Comparison of key indicators for three different EWN boxes located in Inner Dundrum Bay.

Key indicators	Box 4	Box 25	Box 27	Total
Standard model chlorophyll P ₉₀ (µg chl L ⁻¹)	4.42	3.89	3.84	–
Bottom-up scenario chlorophyll P ₉₀ (µg chl L ⁻¹)	2.58	2.20	2.59	–
Difference (%)	–41.66	–43.43	–32.63	–
Standard model mussel live weight (g)	–	15.93	15.41	–
Bottom-up scenario mussel live weight (g)	–	14.32	14.34	–
Difference (%)	–	–10.09	–6.93	–
Standard model mussel harvest (t)	–	23.28	2.91	26.19
Bottom-up scenario mussel harvest (t)	–	13.04	2.33	15.37
Difference (%)	–	–43.99	–19.93	–41.31
Standard model oyster live weight (g)	–	–	89.69	–
Bottom-up scenario oyster live weight (g)	–	–	87.01	–
Difference (%)	–	–	–2.99	–
Standard model oyster harvest (t)	–	–	169.93	–
Bottom-up scenario oyster harvest (t)	–	–	169.07	–
Difference (%)	–	–	–0.51	–

Table 6
Top-down control of eutrophication in inner Dundrum Bay and the inlet channel.

	Box 25	Box 27	Box 6
Standard model with shellfish P ₉₀ (µg chl L ⁻¹)	3.9	3.8	3.9
No top-down control by shellfish P ₉₀ (µg chl L ⁻¹)	4.8	4.1	4.6
Difference (%)	21.6	5.8	16.8

parallel, aquaculture requires clean water, so the effect of the environment on aquaculture is an additional constraint—an excessive load of enteric microorganisms has important economic consequences for fish and shellfish farmers. In the latter case, this is a frequent source of conflict between industry and water authorities and increasingly the agricultural sector. The modelling approach described above is key to understanding source apportionment of these loads.

The SUCCESS modelling framework exemplifies how an appropriate combination of field data, process-oriented studies, and a range of complementary mathematical models can provide the basis for more

holistic decision-making. We have shown that simulation of High Impact Short Term events can explain water quality spikes that are not captured through conventional sampling—although this does not seem to have a significant effect on shellfish growth, it is likely to condition the microbiological quality of the harvested animals.

Perhaps the most important role of this kind of framework is to bring the ‘soil-to-sea’ paradigm closer to managers and contribute to the removal of siloes; in so doing, the relative importance of nutrient and organic sources can be better understood, and in the case of coastal waters or inland lakes used for farming, realistic progress towards the Ecosystem Approach to Aquaculture (sensu Soto et al., 2008) can be achieved.

Author statement

None.

Declaration of Competing Interest

None.

Data availability

The authors do not have permission to share data.

Acknowledgements

The authors acknowledge various sources of direct or indirect funding, including the EU Horizon 2020 GAIN (G.A. 773330) project, and the AFBI Dundrum Bay project. We are grateful to three reviewers for comments on an earlier draft.

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