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A MODEL FOR OPTIMIZATION OF THE PRODUCTIVITY AND BIOREMEDIATION EFFICIENCY OF MARINE INTEGRATED MULTITROPHIC AQUACULTURE

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Abstract

Integrated multitrophic aquaculture (IMTA) has been proposed as a solution to nutrient enrichment generated by intensive fish mariculture. In order to evaluate the potential of IMTA as a nutrient bioremediation method it is essential to know the ratio of fed to extractive organisms required for the removal of a given proportion of the waste nutrients. This ratio depends on the species that compose the IMTA system, on the environmental conditions and on production practices at a target site. Due to the complexity of IMTA the development of a model is essential for designing efficient IMTA systems. In this study, a generic nutrient flux model for IMTA was developed and used to assess the potential of IMTA as a method for nutrient bioremediation. A baseline simulation consisting of three growth models for Atlantic salmon *Salmo salar*, the sea urchin *Paracentrotus lividus* and for the macroalgae *Ulva* sp. is described. The three growth models interact with each other and with their surrounding environment and they are all linked via processes that affect the release and assimilation of particulate organic nitrogen (PON) and dissolved inorganic nitrogen (DIN). The model's forcing functions are environmental parameters with temporal variations, which enables investigation of the understanding of interactions among IMTA components and of the effect of environmental parameters. The baseline simulation has been developed for marine species in a virtually closed system in which hydrodynamic influences on the system are not considered. The model can be used as a predictive tool for comparing the nitrogen bioremediation efficiency of IMTA systems under different environmental conditions (temperature, irradiance and ambient nutrient concentration) and production practices, for example seaweed harvesting frequency, seaweed culture depth, nitrogen content of feed and others, or of IMTA systems with varying combinations of cultured species (salmon, seaweed, sea urchins) and can be extended to open water IMTA once coupled with waste distribution models.

1. Introduction

The constantly increasing demand for seafood, during a period of overexploitation of the fisheries sector can only be met by sustainable growth of aquaculture. This growth is limited by the environmental impacts and economic requirements of intensive monoculture of fed species. Moreover, rapid and uncontrolled expansion of the aquaculture sector challenges the realization of an Ecosystem Approach to Aquaculture (Soto, 2008). If industry expansion is not regulated and developed appropriately, it has the potential to cause further damage to the environment. It has been proposed that expansion of marine aquaculture in parallel with environmental protection can be achieved using Integrated Multi-Trophic Aquaculture systems (IMTA) (Chopin et al. 2001; Neori et al. 2004). IMTA has the potential to be an economically viable solution to the problems of dissolved and particulate nutrient enrichment, since the waste from fed species aquaculture is exploited as a food source by extractive organisms of lower trophic levels giving added value to the investment in feed by producing a low input protein source as well as increasing the farm income. For example, in order to promote more resilient growth of the aquaculture industry in Scotland, a draft Seaweed Policy Statement that examines the cultivation of seaweed in general, and as part of IMTA systems was introduced in 2013 (Marine Scotland, 2013). Large-scale seaweed cultivation has been suggested as a means to mitigate the nutrient enrichment environmental impact of marine fish farms (Abreu et al. 2009; Fei et al. 1998; Wang et al. 2013). As a very large area is required for the cultivation of sufficient seaweed biomass for complete nutrient bioremediation, doubt remains as to whether complete bioremediation by seaweed cultivation is practically feasible (Broch and Slagstad, 2012). However, there is a general agreement that cultivation of seaweed as part of an IMTA is a promising way for partial removal of dissolved fish farm effluent (Broch et al. 2013; Jiang et al. 2010; Reid 2013; Wang et al. 2013). The amount of excess nutrients released from sea cages depends on the fish species and on farm practises. In salmon monoculture, approximately 62% of the nitrogen (N) and 70% of the phosphorus (P) input from feed is lost to the environment as feed wastage (non-consumed food) and fish excretory waste products (Wang et al. 2012). Particulate waste derived from intensive fed aquaculture is deposited in the proximity of sea cages and can lead to changes in sediment chemistry, oxygen availability and in the number and diversity of benthic species (Corner et al. 2006).

From a biological point of view, the choice of extractive species in an IMTA system is crucial because their physiology and their ecological attributes determine the rate of particle or nutrient consumption and assimilation, their growth rate and in capabilities in terms of biofiltration. Species are chosen based on specific culture performance traits, for which

quantitative information needs to be available, with respect to nutrient uptake efficiency and secondary considerations (e.g. yield and protein content). The marketability of the extractive species is largely dependent on the location, with the Western world showing less demand for food species that are low in the trophic chain. Nevertheless, dried seaweed products can always be exported and seaweeds can be processed to produce cosmetics, fertilizers, animal feed, biogas and others.

The environmental benefits, matter and energy flux within an IMTA farm as well as between the environment and the IMTA system, need to be qualified and quantified prior to the establishment of a marine IMTA system. The aim of this study was to provide a tool for designing IMTA farms at any site by creating a modelling tool that can be used to fine-tune IMTA designs for maximising yields and nutrient removal.

Without a thorough understanding of the system's dynamic, the environmental and economical benefits of IMTA cannot be achieved. However, field measurements of nutrient and Particulate Organic Matter (POM) concentrations in open-water systems are challenging due to the highly diluting, dynamic nature of open-water systems, presenting high spatial and temporal variation both diurnally and seasonally. The model described in this study determines the temporal availability of nutrients and POM released by the different IMTA components and thus the amount available for uptake by different groups of extractive organisms. Because of the site specificity of waste distribution, this model focuses on simulation of a virtually closed system, within which the nitrogen is homogenously distributed. The species used in this study are Atlantic salmon (*Salmon salar*), a sea urchin (*Paracentrotus lividus*) and the sea lettuce (*Ulva lactuca*), though it will be possible to re-parameterise for a range of different species.

2. Model development

The model was implemented using the visual simulation package Powersim™ Constructor Studio 8 (Powersim Software AS, Bergen), which supports structural construction, equation deduction and computer implementation of a conceptual model. The time horizon used was an 18-month period, to simulate the at-sea phase of salmon production cycle, which can last between 14 and 24 months (Marine Harvest, 2012). The model is typically operated with a one day time step and the model's differential equations were solved using a third order Runge-Kutta integration method. The selected time-step can reflect accurately all the

important time dependent environmental changes (accurate integration) with low computing effort.

An extensive literature review was carried out for model parameterization for *Ulva* (see Table 1) and for *Paracentrotus lividus* (Add_my_pet, 2014), while the model for *Salmo salar* was parameterized using data acquired from commercial Scottish salmon farms. For some parameters, a range of values was available in the literature in which case the most representative value was used. It is evident that the inclusion of many proxy variables from the literature propagates uncertainties through the model, which affects the overall model accuracy. Since the model presented in this study is deterministic, its output is entirely determined by the input parameters and structure of the model. Due to the high structural complexity of the model and high degree of uncertainty in estimating the values of many input parameters, a detailed sensitivity analysis was performed by varying each input parameter by ± 10% and quantifying the effect on eight output variables (Tables 3-6). The selected output variables reflect the objectives of the research with respect to nitrogen bioremediation and yield productivity. Within the sensitivity analysis all model parameters and initial values of state variables (50 input variables) were varied in order to determine the response of the following eight effect variables: harvested biomass of seaweed, salmon and sea urchin, nitrogen accumulated by the seaweed, salmon and sea urchin, DIN and PON available at the IMTA site at the end of the simulation. The sensitivity analysis results are presented as a normalized sensitivity coefficient (NS) (Fasham et al. 1990):

$$NS = \frac{DV/V_b}{DP/P_b} \quad (1)$$

where, DV = (V_b– V) is the change of a response variable, V_b is the value of a response variable for the base run, V is the value of a response variable for the sensitivity analysis run, DP = (P_b– P) is the change in a model parameter, P_b is the baseline value of a model parameter and P is the value of a model parameter for the sensitivity analysis run.

When the value of NS for a parameter +10% is negative then there is a negative correlation between parameter and effect. When it is negative for a parameter -10% then there is a positive correlation between parameter and effect.

2.1 Model outline

143 The model determines the nutrient recovery efficiency and biomass production of IMTA
144 systems based on a baseline simulation so that components of the model can be altered or
145 removed for the simulation of particular scenarios. Following re-parameterization, the model
146 can simulate IMTA systems consisting of different finfish, sea urchin (or other grazing
147 invertebrate) or seaweed combinations of species. The present model is for an IMTA system
148 comprising of Atlantic salmon (*Salmo salar*), seaweed (*Ulva* sp.) and sea urchins
149 (*Paracentrotus lividus*). It incorporates an ecosystem model consisting of three submodels
150 that interact with each other and with their surrounding environment via nutrient cycling (Fig.
151 1). The submodels consist of growth models for salmon, seaweed and sea urchin that include
152 nitrogen uptake and release via feed intake and excretion, and interact with each other through
153 modelled nitrogen release and subsequent assimilation (Fig. 1).
154
155 Insert fig. 1 here
156
157 Salmon growth was modelled using the Thermal-unit Growth Coefficient (TGC) (Iwama and
158 Tautz, 1981), the seaweed growth model is based on Droop's model for nutrient-limited algal
159 growth (Droop, 1968) and sea urchin growth was modeled using the Dynamic Energy Budget
160 (DEB) theory (Kooijman 1986). In principle, all three models are DEB models because the
161 TGC is a special case of the Von Bertalanffy equation (Dumas et al. 2010) which, along with
162 Droop's model for nutrient-limited algal growth (Kooijman, 2008), is a special case of the
163 DEB approach.
164
165 The TGC is a simple model widely used in aquaculture, based on three basic assumptions,
166 which may be violated under certain conditions (Jobling, 2003). Firstly, growth rate increases
167 linearly with temperature, secondly the length (L) and weight (W) relationship is $W \alpha L^3$, and
168 thirdly the growth in length for any given temperature is constant over time (Jobling, 2003).
169 The TGC can present errors when the temperature deviates far from the optimum for growth
170 (Jobling 2003), but this is not a setback given the temperature range used in the present
171 simulations. For the organic extractive organisms a bioenergetic model was used in order to
172 link the environmental variables, mainly food availability and temperature, with feed intake,
173 growth, excretion and faeces production. For the simulation of salmon growth and nutrient
174 uptake and release, the TGC was preferred to a bioenergetic model because under intensive
175 aquaculture conditions feed is not limiting growth. Furthermore, salmon is well studied and
176 daily time series data for the TGC and food conversion ratio (FCR) as well as sources of data
177 for excretions and faeces production were available in the literature. Finally, as salmon are

178 grown at sea for only for a part of their production, data are not required for the full life cycle,
179 which is the strength of the DEB approach.
180
181 The model includes daily time steps for better understanding of the process affecting the
182 IMTA productivity and nutrient removal efficiency. Due to the dynamic design of the model
183 the bioremediation potential of different production scenarios can be estimated by altering
184 various production parameters of the baseline simulation. These include site-specific
185 environmental conditions (temperature, irradiance and ambient nutrient concentration) and
186 production practices (seaweed harvesting frequency, seaweed culture depth, nitrogen content
187 of feed, initial stocking biomass of extractive organisms etc.). The maximum seaweed and sea
188 urchin biomass that can be sustained at any given time can also be estimated based on the
189 daily amount of nitrogen within the IMTA system that is available for uptake.
190
191 The complete model is used to determine the overall ability of the IMTA system to reduce the
192 nutrient and POM waste of fed-species monoculture taking into account the quantity of
193 nutrients and POM that are released and the quantity that could be potentially
194 absorbed/consumed by the extractive organisms if all the waste remained within the virtually
195 closed system. The only nitrogenous input to the seaweed and sea urchin submodels is the
196 daily waste released to the sea from the salmon submodel. This is used to calculate the
197 amount of particulate (suspended) and dissolved nitrogen released from the salmon farm for a
198 given fish production over 18 months, as well as the potential for decreasing the nutrient
199 released by converting salmon monocultures into IMTA systems. The model takes into
200 account fish growth and consequent feed input and waste release, and the uptake and release
201 of DIN and PON by the different IMTA components. The growth models are combined with
202 nutrient transfer/cycling and this way the virtually closed system bioremediation efficiency is
203 estimated (Fig. 1).
204
205 2.2 Salmon growth submodel
206 The growth rate of fish fluctuates throughout an individual's life cycle and is mainly
207 influenced by feed availability, temperature and photoperiod (Austreng et al. 1987; Brett,
208 1979). Salmon growth was simulated using a thermal growth coefficient:
209
210 $$TGC = 1000\ \frac{\sqrt[3]{W_t} - \sqrt[3]{W_0}}{T * t} \quad (2)$$
211
212 where, TGC is the thermal growth coefficient, W_0 is the initial wet weight of the smolt, W_t is
213 the wet weight of the fish at time t, T is the temperature and t is time in degree-days.

Solving for W_t we obtain:

$$W_t = \left[\sqrt[3]{W_0} + \frac{TGC*T*t}{1000}\right]^3 \quad (3)$$

The total salmon biomass was calculated as individual weight multiplied by the number of individuals. The model also accounted for natural mortality, modeled as a time series variable since mortality decreases with fish size, using empirical data from Scottish salmon farms.

The amount of waste released from the salmon farm in the form of excretion, faeces production and feed loss was assumed to be as calculated by Wang et al (2012) for Norwegian salmon farms. In detail, we assume that every day of the simulation 2% of the feed nitrogen is released in the environment in the form of feed loss, 45% in the form of dissolved excretions and 15% in the form of faeces, while the remaining 38% is assimilated into the salmon biomass and removed from the ecosystem when the fish are harvested. The nitrogen content of the feed was set to be 7.2% of the feed weight (Gillibrand et al. 2002).

2.3 Seaweed growth and nitrogen uptake

Seaweed biomass *(B)* increases with a varying growth rate and decreases due to both natural causes and periodic harvesting. The basic processes affecting seaweed biomass form the differential equation 4:

$$\frac{dB}{dt} = (\mu - \Omega) * B - (D + H) * B \quad (4)$$

where, μ is the specific growth rate, Ω the specific decomposition rate, D the loss rate due to environmental disturbance and H the harvesting rate. Biomass is calculated as wet biomass, for the conversion of seaweed wet to dry weight an 8.43 to 1 ratio was used (Angell et al. 2012; Neori et al. 1991). At the baseline simulation due to lack of data in the literature for the specific decomposition rate and the loss due to environmental disturbance for *Ulva* sp. the term mortality (M) is used, where M = Ω + D and Ω = D (Table 1).

The gross growth rate was defined as a function of water temperature, availability of Photosynthetic Active Radiation (PAR) and nutrient concentration in the water column and in the plant tissues. The joint dependence of growth on environmental variables is defined by separate growth limiting factors, which can range between 0 and 1. A value of 1 means the factor does not inhibit growth (i.e. light is at optimum intensity, temperature is optimum and

nutrients are available in excess). The limiting factors are then combined with the maximum gross growth rate at a reference temperature as in equation 5 (Solidoro et al. 1997):

$$\mu = \mu_{max(T_{ref})} * f(T) * f(I) * min(f(N), f(P)) \quad (5)$$

where, $\mu_{max(Tref)}$ is the maximum growth rate at a particular reference temperature (T_{ref}) under conditions of saturated light intensity and excess nutrients, $f(T), f(I), f(N, P)$ are the growth limiting functions for temperature, light and nutrients (nitrogen and phosphorus).

The major nutrients required for growth are nitrogen and phosphorus, while carbon is often available in excess and micronutrients such as iron and manganese are only limiting in oligotrophic environments. Typically, in marine ecosystems, nitrogen is the element limiting algal growth (Lobban and Harrison, 1994). Thus in the baseline simulation it is assumed that phosphorus is not limiting, so Eq. 5 becomes:

$$\mu = \mu_{max(T_{ref})} * f(T) * f(I) * f(N) \quad (6)$$

The Photosynthetic response to light is based on Steele's photoinhibition law (Steele, 1962):

$$\frac{P}{P_{max}} = \frac{I}{I_{opt}} exp\ \frac{1-I}{I_{opt}} \quad (7)$$

where, P is the photosynthetic response at a given light intensity I (W m^{-2}) for an organism that has a maximum photosynthetic rate P_{max} at the optimal (saturating) light intensity I_{opt} and I is the light intensity at a given depth (z). Light intensity at a given depth is an exponential function of depth, seaweed and phytoplankton standing biomass and is given by:

$$I(z) = I_0\, e^{-kz} \quad (8)$$

After mathematical integration of the light limitation factor Eq. 8 we obtain:

$$F(I) = \int_0^z \frac{P}{P_{max}} dz = \int_0^z \frac{I(x)}{I_{opt}} exp\ \frac{1-I(x)}{I_{opt}} dx = \int_0^z \frac{I_0 e^{-kx}}{I_{opt}} \exp \frac{1-I_0\, e^{-kx}}{I_{opt}}\ dx = \frac{1}{k} * \exp\left(\frac{1}{I_{opt}}\right) *$$

$$\left[\exp\left(-\frac{I_0}{I_{opt}} * \exp(-z * k)\right) - \exp\left(-\frac{I_0}{I_{opt}}\right)\right] \quad (9)$$

where, k is the light extinction coefficient (m^{-1}), z is the culture depth (m), I_{opt} is the optimal light intensity and P is the photosynthetic rate at a given light intensity I (W m^{-2}).

The temperature, like the light, limitation factor follows an inhibition law.

$$F(T) = q_{10}^{0.1(T-T_{ref})} \quad (10)$$

where, q_{10} is a temperature coefficient, T is the water temperature and T_{ref} is the reference temperature at which the seaweed growth rate was measured. The q_{10} temperature coefficient is a measure of the rate of change of a biological or chemical system as a consequence of increasing the temperature by 10°C (Raven and Geider, 1988).

The nitrogen limitation factor Eq. 11 is given by the range of internal nitrogen concentration, with a feedback effect on the uptake function (Aveytua-Alcázar et al. 2008; Coffaro and Sfriso, 1997; Solidoro et al. 1997; Trancoso et al. 2005; Zaldívar et al. 2009). It can range between 1, when $N = N_{max}$ and uptake is saturated and 0 when $N = N_{min}$ and maximum uptake rate is possible, all measured in mg N per g dry seaweed. Internal nitrogen quota/concentration *(N)* refers to the concentrations in the algal cells as opposed to external concentrations that refers to the concentration amount in the water column.

$$F(N) = 1 - \frac{N_{\max} - N}{N_{max} - N_{min}} \quad (11)$$

where, N_{max} is the maximum internal quota of nitrogen and N_{min} the minimum.

For calculation of the nitrogen quota *(N)*, a quota-based model was used developed from Droop's original formula (Droop, 1968):

$$\frac{dN}{dt} = V * F(N) - \mu * N \quad (12)$$

where, V is the nitrogen uptake rate (mg g^{-1}dw h^{-1}) and μ is the specific growth rate.

Nutrient uptake rates *(V)* are proportional to nutrient concentration in the water column according to Michaelis–Menten kinetics:

$$V = \frac{V_{max}S}{K_N + S} \quad (13)$$

where, V_{max} is the maximum nitrogen uptake rate under the prevailing conditions at the site (mg g^{-1}dw h^{-1}), S is the total DIN concentration in the seawater (mg l^{-1}) and K_N is the half-saturation coefficient for the uptake of nitrogen (mg l^{-1}).

By combining Eqs. 11, 12 and 13 we obtain:

$$\frac{dN}{dt} = \frac{V_{max}\, S}{K_N + S} \frac{N_{\max} - N}{N_{max} - N_{min}} - (\mu * N) \quad (14)$$

The bioremediation effect of IMTA is closely dependent on the biomass of extractive organisms harvested. However, the maximum biomass is restricted by culture practicalities such as the potential alteration of water currents and by the availability of nutrients. The maximum biomass is site and species dependent, and for the baseline simulation presented in this study the maximum seaweed biomass permitted to be on site at any given time was set at 35 tonnes wet weight. The area required for the culture of 35 t of *Ulva*, with stocking density of 1.6 kg/m^2 and two layers of seaweed one at the sea surface and one 3 m deep would be 10,937 m^2. This stocking density was selected because the maximum density permitted to guarantee the greatest uptake of nutrients in *U. lactuca* is 1.9 kg m^{-2} (Neori et al. 1991). The area required for the seaweed culture is used for the estimation of the virtually closed IMTA site's water volume, which is estimated using the following formula:

'IMTA site volume' = 'Average depth' * 'Number of salmon cages' * 'Sea cage area' + 'raft area' * 'number of rafts' * 'Average depth'.

Seaweed is lost due to mortality, harvesting and natural biomass loss (seedling mortality, grazing, epiphytism, sediment abrasion and smothering and removal by wave action). Managing the harvesting rate is of paramount importance for achieving high productivity rates. For optimal results, in the present model, when the seaweed biomass reaches a predefined level (35 t in the baseline simulation) the seaweed is harvested at regular time intervals. The biomass harvested depends on the forecasted growth and natural mortality rate of the forthcoming days. A discrete flow in the model controls the loss of seaweed biomass due to harvesting; the rate of the flow (harvest rate) is regulated by the following instruction:

*IF (start harvesting = 0, 0 ton, IF (current time step * timestep = stoptime - starttime, seaweed biomass, IF (accrued part of 10 days = 1, seaweed biomass – maximum seaweed biomass, IF (accrued part of 10 days = 0, seaweed biomass – maximum seaweed biomass, 0 ton))))*

where, '*start harvesting*' is a level that allows harvesting to start only when the seaweed biomass has surpassed the value of a constant that defined as maximum biomass that can be on site (maximum seaweed biomass). The level 'start harvesting' changes from 0 to 1 when the level '*seaweed biomass*' is equal to or larger than the constant '*maximum seaweed biomass*'. '*Current time step*' is a level that counts the time steps, starting from zero. *Timestep* is a Powersim built-in function that returns the time step of the simulation, *starttime* and *stoptime* are Powersim built-in functions that return the start-time and stop-time of the simulation, respectively. In the final time step all the seaweed in the level *'seaweed biomass'* is transferred to the level *'harvested seaweed'*. '*Seaweed biomass*' is a level that shows the seaweed biomass. *'Accrued part of 10 days'* is a level used for the calculation of 10-day periods. When the value of this level is one, all the seaweed is harvested apart from *'maximum seaweed biomass'*.

The model is effective for perennial seaweed species. However, as the gametophyte stage of *Ulva*, lasts only for a few months, frequent reseeding will be necessary at time intervals dependent on the environmental conditions, epiphytic growth or disease. The numerical parameters used in the seaweed model are summarized in Table 1.

Insert Table 1 here

2.4 Sea urchin growth and nitrogen uptake and release

The sea urchin growth submodel is based on the Dynamic Energy Budget (DEB) theory (Kooijman, 1986). A DEB model describes and interconnects the physiological processes that occur within an individual as a function of the state of the individual and the environment (Kooijman, 2001). DEB theory is based on two state variables: structural volume (V) and energy reserves (E) and on two forcing variables: temperature (T) and food density (X). The basic concept of the theory is that from the food ingested a certain amount is released as faeces and the rest is assimilated. All the assimilated food enters a reserve compartment. From there a fixed fraction will be spent on maintenance and the rest will spend on maturity or reproduction (Kooijman, 1986). A detailed description of the DEB can be found at Kooijman (2008). Most of the species-specific parameters used for this DEB model were obtained from (Kooijmann, 2014).

The initial structural length/diameter of the sea urchin juveniles was set to 10 mm, because at this size hatchery reared sea urchins can be transferred to sea successfully (Kelly et al. 1998). At this length *P. lividus* individuals are characterized as sub adults (Grosjean et al. 1998), so in the baseline simulation the DEB model simulates the growth from late juveniles to mature adults. The physical length (L_w) was converted to volumetric length (L):

$$L_w = L/\delta_M \tag{15}$$

where, δ_M is the shape coefficient.

For this simulation the notation from Kooijman (2000) was used. All rate variables are dotted above, all variables that are expressed per unit volume and per unit surface area are given between square brackets and braces, respectively. Additionally, the expression (x)+ is defined as: [x]+ = x for x > 0, [x]+ = 0.

Most of the processes described by the DEB model are influenced by the effect of temperature on the metabolic rate *(K(T))* according to Eq. 16:

$$K(T) = K_o\, e^{\left(\frac{T_A}{T_o} - \frac{T_A}{T}\right)} * \left[1 + e^{\left(\frac{T_{AL}}{T} - \frac{T_{AL}}{T_L}\right)} + e^{\left(\frac{T_{AH}}{T_H} - \frac{T_{AH}}{T}\right)}\right]^{-1} \tag{16}$$

where, K_o is the reference reaction rate at 288 K, T_A is the Arhenius temperature, T_o is the Reference temperature, T_{AL} and T_{AH} are the Arrhenius temperature at lower and upper boundary, respectively, T_L and T_H are the lower and upper boundary tolerance, respectively and T is the water temperature (simulated as a time series variable).

The DEB model starts with the ingestion of PON ($mgN\ d^{-1}$) by the sea urchins. This is based on ingestion rate ($\dot{J}_x$) ($mgC\ d^{-1}$) divided by the C/N ratio of the aquaculture waste (Eq. 17). Ingestion rate is proportional to the surface area of the structural volume and follows type-II function response depending on the density of PON.

$$\dot{J}_x = K(T) * f * \{\dot{J}_x\} * V^{2/3} \tag{17}$$

where, $K(T)$ is a temperature dependent rate, $\{\dot{J}_x\}$ is the maximum surface area-specific ingestion, V is the structural volume and f is the functional response that can range between 0 and 1 and is given by:

$$f = \frac{X}{X+X_K} \quad (18)$$

The saturation coefficient *(X_K)*, is analogous to a Michaelis-Menten constant, in this case being the food density at which the ingestion rate is half the maximum. For the calculation of the food density in the environment *(X)*, the concentration of PON is converted to organic carbon concentration.

DEB models assume that the assimilation rate, ($\dot{P}_A$), is independent of the ingestion rate:

$$\dot{P}_A = K(T) * f * \{\dot{P}_{Am}\} * V^{2/3} \quad (19)$$

where, $K(T)$ is a temperature dependent rate, f is the functional response, $\{\dot{P}_{Am}\}$ is the maximum surface area specific assimilation and V is the structural volume.

The food that is ingested but not assimilated as biomass will be released to the environment as faeces or as excretion by diffusion. The DEB model enables estimation of the potential amounts of faeces released by the sea urchins by estimating the hourly production of faeces released into the surroundings using Eq. 20 for the faeces production in ($mgC\ d^{-1}$) and Eq. 21 for the excretion rate in ($mgN\ d^{-1}$). Eq. 20 is then divided by the C/N ratio in order to calculate the amount of PON that is in the sea urchin faeces, which is assumed to be immediately added to the PON and DIN pools and is thus available for consumption by the sea urchins and seaweed, respectively.

$$\dot{F} = \dot{J}_x - \dot{P}_A/\mu_{cj} \quad (20)$$

where, $\dot{J}_x$ is the consumption rate, $\dot{P}_A$ is the assimilation rate and μ_{cj} is the ratio of carbon to energy content.

$$\dot{D}_{excr} = \left\{\left[\dot{P}_c - (1-k_R) * \frac{dE_R}{dt} - \mu_V * \rho * \frac{dV}{dt}\right] * Q + \dot{P}_A * (Qs - Q)_+\right\}/\mu_{cj} \quad (21)$$

where, $\dot{P}_c$ is the catabolic rate, k_R are the reproductive reserves fixed in the eggs, E_R are the reproductive reserves, μ_V is the structural energy quota, ρ is the biovolume density, V is the structural volume, Q is the sea urchin N quota, $\dot{P}_A$ is the assimilation rate, μ_{cj} is the ratio of carbon to energy content and Qs is the sediment N quota (calculated as the ratio of organic nitrogen to organic carbon in the sediment). The *P. lividus* N quota (*Q)* was set to

127 $mgN\ mgC^{-1}$ (Tomas et al. 2005) and sediment N quota (*Qs)* is site specific it was set to 7, which is a representative value for an average Scottish salmon farm site.

The assimilated energy from the food enters the reserve pool. The energy density *[E]* in an organism may vary between 0 and the maximum energy density $[E_m]$ depending on the food density in the environment.

$$\frac{d[E]}{dt} = \dot{P}_A - \dot{P}_c \quad (22)$$

where, $\dot{P}_A$ is the assimilation and $\dot{P}_c$ the catabolic rate.

The sea urchin catabolic rate) ($\dot{P}_c$) denotes the energy utilised by the structural body and is given by:

$$\dot{P}_c = K(T) * \left[\frac{[E]}{[E_G]+K*[E]}\right] * \left(\frac{[E_G]*\{\dot{P}_{Am}\}*V^{2/3}}{[E_M]} + \left[\dot{P}_M\right] * V\right) \quad (23)$$

where, $K(T)$ is a temperature dependent rate, $[E]$ is the reserves, $[E_G]$ the volume specific cost of growth, K the catabolic flux to growth and maintenance, $\{\dot{P}_{Am}\}$ the maximum surface area specific assimilation, V the structural volume, $[E_M]$ the maximum reserve density and $\left[\dot{P}_M\right]$ the volume specific maintenance rate.

The rate of maintenance cost of the animals ($\dot{P}_M$) is proportional to the body volume and calculated with Eq. 24. Since the sea urchins will be mature the maturity maintenance *Pj* is also used Eq. 25:

$$\dot{P}_M = K(T) * \left[\dot{P}_M\right] * V \quad (24)$$

$$\dot{P}_j = \min\left(V, V_p\right) * \left[\dot{P}_M\right] * \frac{1-k}{k} \quad (25)$$

where, $K(T)$ is a temperature dependent rate, $\left[\dot{P}_M\right]$ is the volume specific maintenance rate, V is the structural volume, V_p is the structural volume at puberty and K is the catabolic flux to growth and maintenance.

The sea urchin structural volume growth (V) is given by:

$$\frac{dV}{dt} = \frac{(k*\dot{P}_c - \dot{P}_M)_+}{[E_G]} \quad (26)$$

where, K is the catabolic flux to growth and maintenance, $\dot{P}_c$ is catabolic rate, $\dot{P}_M$ is the maintenance rate and $[E_G]$ is the volume specific cost of growth.

In this model we are also interested in the body mass (W) of the sea urchins, in order to calculate the total biomass of the stock. To convert volume to dry weight Eq. 27 is used:

$$W = \mathrm{V} * \rho + \frac{(E + E_R * k_R)}{\mu_E} \quad (27)$$

where, V is the structural volume, ρ is the biovolume density, E and E_R are reserves and reproductive reserves, respectively, k_R are the reproductive reserves fixed in the eggs and μ_E is the reserve energy content.

The total biomass was calculated as individual weight multiplied by the number of individuals. Once an individual has reached the volume *(V_p)* at sexual maturity, a portion of the total energy reserve is stored in the sea urchin reproductive reserves *(E_R):*

$$\frac{dE_R}{dt} = (1 - k) * \dot{P}_c - \dot{P}_j \quad (28)$$

where, K is the catabolic flux to growth and maintenance, $\dot{P}_c$ is the catabolic rate and $\dot{P}_j$ is the maturity maintenance

The DEB model simulates the process within individuals. However for this model it is necessary to know how a non-reproducing stock *(N)* will decrease in size with time, due to mortality. The decrease of the sea urchin stock size is calculated in Eq. 29 where due to the planktonic nature of sea urchin larvae, it is assumed they will be dispersed from the IMTA site and thus reproduction will represent a net energy loss and restocking of the sea urchins will be necessary. However, the release of the larvae will contribute to restocking the native sea urchin population.

$$\frac{dN}{dt} = -\delta_r * N - \delta_h * N \quad (29)$$

where, δ_r and δ_h are the natural and harvest mortality of sea urchins, respectively. The harvest mortality (δ_H) was zero and at the last time step of the simulation all sea urchins were harvested, same as in the salmon and seaweed submodels. The natural mortality (δ_r) was set to 0.00102 individuals d^{-1} for sea urchins with test diameter smaller than 2 cm and 0.00056 individuals d^{-1} for sea urchins with test diameter larger than 2 cm (Turon et al. 1995).

During the grow-out stage of *P. lividus* juveniles, the stocking density is approximately 400 individuals m^{-2} (Carboni, 2013). Space is not an issue for the organic extractive component of the IMTA, since for the production of 560,525 individuals only 1,401 m^2 would be required and this area would be directly underneath the fish cages and the seaweed rafts.

2.5 Assumptions and simplifications

The overall model's key assumption is that all nitrogen released by the various IMTA components is dispersed homogenously within a quantified water volume defined as the IMTA site water volume (see section 2.3). It is also assumed that all the nitrogen available in the IMTA site volume is in a form suitable for uptake; thus the model does not distinguish between nitrate and ammonium. Correspondingly, the model does not take into account the interactions between nitrate and ammonium within the environment and organisms, such as the role of sediment and water in the nutrient dynamics or denitrification. The increase of light limitation due to increased self-shading as the seaweed grows was not considered, neither was the shading caused by phytoplankton. Data from Broch and Slagstad (2012) could be used to derive a seaweed self -shading formula from which an add-on model could be used to simulate the changes in k. In this study the light extinction coefficient (k) was a constant (k=1). In the seaweed growth submodel the small biomass loss due to mechanical damage caused by harvesting was not included. It is also assumed that nitrogen is the only nutrient limiting seaweed growth. Additionally, the seaweed biomass used as initial biomass is assumed to have an average $\left({}^{(N_{min} + N_{max})}/_{2}\right)$ N quota (this can be regulated by using nitrogen deprived seedlings). When seaweed is harvested it is assumed that the N quota of the harvested seaweed is equal to the maximum N quota due to the high availability of DIN in the virtually closed system. The assumption that the seaweed harvested has this high nitrogen quota might lead to overestimation of the bioremediation efficiency and the effect of lower N quota at harvest was examined in the sensitivity analysis (Tables 5 and 10). From a farm practice perspective it is assumed, that the relative position of the extractive organisms in relation to the fish cages is such that it ensures high O_2 availability for the fish. For the

559 salmon growth model, excretion, faeces production and feed loss were assumed to be steady
560 during the 18 month production period while in reality they change as the fish grow.
561
562 2.6 Production specifications of the baseline simulation
563 The results presented are from the IMTA baseline simulation, which was parameterized using
564 data acquired from the literature and from commercial salmon farm sites. The environmental
565 data such as monthly variations in seawater temperature and irradiance were acquired from
566 empirical databases for the West coast of Scotland and the production-specific input data
567 from Scottish commercial salmon farm sites (Figs. 2 and 3). Typically, S1 smolts are
568 transferred to sea in spring (April-May), so April is set as simulation time 0 and the model
569 then runs for 18 months. The test scenario farm consists of nine 90 m circular salmon cages
570 with the extractive organisms placed in immediate proximity to those cages. The model
571 simulates a farm that produces 1,000 t of Atlantic salmon in 18 months on-growing, a farm
572 size representative of the Scottish industry (FAO, Scottish Fish Farm Production Survey
573 2011).

574
575 Insert Fig 2 and Fig 3
576
577 3 Results
578 3.1 Growth performance of IMTA components at the baseline simulation
579 The baseline simulation run estimated that the mean individual fish biomass after 540 days
580 (18 months) was 3.78 kg (Fig. 4a) and the salmon stock decreased by 16,525 individuals
581 from 280,883 to 264,358 individuals (Fig. 4b).
582
583 Insert fig. 4 here

584
585 During the 18-month production period, 348 t of seaweed and 50 t of sea urchins were
586 produced and harvested as well as the targeted 1000t of salmon (Table 2). The seaweed
587 achieved high growth rates, especially during the summer months (Fig. 5). The effect of the
588 growth limitation factors on the seaweed growth rate is presented in Fig. 6. The lower
589 seaweed growth rate during the first 300 days (10 months) of the simulation (Fig. 5) can be
590 mainly attributed to low levels of nitrogen available for uptake (Figs. 6 and 10). It is clear that
591 in the hypothetical baseline model scenario, during the first 300 days of the simulation
592 seaweed growth is mainly limited by the availability of nitrogen. Temperature limits growth
593 more during the colder months (October – April) while, the effect of light intensity is rather

stable throughout the year (Fig. 6). It should be emphasized here that site specific shading caused by phytoplankton or seaweed self shading does not contribute to light limitation in the baseline simulation (see section 2.5 for more details).

Insert Fig. 5 and fig. 6 here

The aim of the IMTA model developed was to achieve high bioremediation efficiency. Sustaining the seaweed biomass at a high density at all times, using the harvesting instruction (described at section 2.3), played an important role in achieving this (Fig. 7). The first seaweed harvesting occurred 330 days after the simulation start, following which there was enough nitrogen available due to the large size of the fish and the environmental conditions were also favorable for the remaining seven months of the simulation (April – October) (Figs. 3 and 6) thus ensuring constant high growth rate and harvesting at 10-day intervals (Fig. 7).

Insert Fig.7 here

At the beginning of the IMTA simulation the site was stocked with 827,900 sea urchins. During the 18-month production period 50 t (wet weight) of sea urchins of the species *P. lividus* were produced with average test diameter 4.47 cm (Table 2, Fig. 8). As a result 1.01 t of nitrogen were assimilated in the sea urchin biomass and removed from the ecosystem via the process of harvesting.

Insert fig. 8 and fig. 9 here

3.2 Test scenario bioremediation potential

For the production of 1,000 t of salmon with average feed conversion ratio (FCR) of 1.02 and feed nitrogen content 7.2%; the model shows that 80 t of nitrogen are introduced into the system over the 540 day simulated production period. From this 80 t, only 38% will be accumulated by the fish and incorporated into their biomass. The remaining 62%, which under the production scenario described above (production of 1000t of salmon) is 49.6 t, will be released into the environment as dissolved and particulate nitrogen. Under the environmental conditions and production method of the test scenario the total nitrogen released to the environment from the IMTA site would be 36% less (31.8 t instead of 49.6 t) than what would have been released from a salmon monocutlure farm of the same capacity. In detail, the amount of nitrogen released from salmon monoculture would be 62% of the exogenous nitrogen input but only 39% in the IMTA system since a large proportion of the

630 nitrogenous waste will be assimilated by the extractive organisms and removed from the
631 ecosystem via harvesting (Figs. 9 and 10). Fig. 10 shows the gradual increase in nitrogen
632 within the IMTA system over the simulated production period.
633
634 3.3 Sensitivity analysis

635 All biological, environmental and production parameters were analysed in terms of
636 uncertainty and their relative importance in the model. Due to the large number of input and
637 response variables used in the sensitivity analysis, the results for only those that were shown
638 to be the most sensitive parameters (absolute values) to operation of the model are
639 summarized in Tables 3 to 6. Those parameters were therefore classified as potential critical
640 assumptions and thus require accurate estimation and/or calibration.
641
642 In the salmon submodel, the growth and nutrient uptake is most sensitive to change in the
643 TGC and secondarily on variation in the FCR (Table 3).
644
645 Insert Table 3 here
646
647 In the seaweed submodel, all output variables were most sensitive to parameters affecting
648 growth and nutrient uptake either indirectly through nitrogen uptake and nitrogen content of
649 the seaweed tissues, wet/dry ratio and the culture depth or directly through maximum growth
650 rate, temperature and nitrogen input from salmon excretion. These results show the overall
651 importance of temperature and nitrogen uptake for seaweed growth (Table 4). All parameters,
652 apart from culture depth that was negatively correlated with seaweed biomass harvested, were
653 positively correlated with the output variables. Also, increasing parameter values mirrored the
654 effect on the model output of decreasing parameter values, which indicates that most
655 parameters affected growth linearly.
656
657 Insert Table 4 here
658
659 In the sea urchin submodel the output variables were most sensitive to parameters related to
660 temperature. Other sensitive parameters included the maximum surface-specific feeding rate
661 (Table 5), the volume specific cost of growth and the ratio of carbon to energy content. An
662 increase in the value of T_L had a strong negative effect on the output variable 'harvested sea
663 urchin biomass' (sensitivity -9.96), while a reduction caused a weak positive effect
664 (sensitivity 0.08). Overall, this analysis revealed that the DEB model was most sensitive to
665 increases in T_L. The model also showed a high sensitivity to increases or decreases in other

parameters (Table 5) while changes in the remaining DEB input variables had little effect on growth (sensitivity < 1).

Insert Table 5 here

Table 6 summarizes tables 3 to 5 in the context of the overall model. The most sensitive parameters within the salmon and seaweed sub-models are also the most sensitive to outcomes of the overall model. The most sensitive parameters of the DEB sub-model do not play such an important role within the overall model performance due to the sea urchin biomass being very small in comparison to that of salmon and seaweed (Table 6).

Insert Table 6 here

4. Discussion

The aim of this study was the development of a dynamic tool for relative comparison of different IMTA scenarios at a given production site, rather than the generation of absolute bioremediation and production estimates. The model results presented are derived from a baseline simulation, which can be re-parameterised to simulate different scenarios.

Results from IMTA studies similar to the one presented here, have shown bioremediation potential of a similar scale to the output generated by the present model. Broch and Slagstad (2012) estimated that 0.8 km^2 of *Saccharina latissima* biomass would be needed to sequester all the waste released from a salmon farm producing 1,000 tonnes a year and Abreu et al. (2009) estimated that a 1 km^2 *Gracilaria chilensis* farm would be needed to fully sequester the dissolved nutrients released from a salmon farm producing 1,000 tonnes a year. Sanderson et al. (2012) estimated that 0.01 km^2 of *S. latissima* could remove 5.3-10% of the dissolved nitrogen released from a salmon farm producing 500 t of salmon in two years. However, the results presented, as the results from any other IMTA model or trial, cannot be directly compared with output from similar studies due to the fact that the productivity of an IMTA farm depends on local environmental characteristics, the species combination used, the duration of the grow out seasons and other factors. Moreover, linear interpolation of results from studies with shorter durations can lead to misestimating results. Thus a large variance in production and bioremediation results is natural. The results of this study are in the same order of magnitude as the results acquired from the studies mentioned above; however they suggest higher bioremediation potential, possibly largely due to the harvesting method applied. Specifically, it was estimated that 35% of the total nitrogen released from a salmon

farm, with the specifications of the simulated scenario, will be accumulated by the 0.01 km^2 of *Ulva* sp suggesting a very high bioremediation efficiency. Aiming to achieve 100% bioremediation (i.e. no available nitrogen above the ambient concentration occurs at any given time), especially without the addition of external feed sources for the extractive organisms and while sustaining the quality of the extractive organisms, is unrealistic and might only be possible in a fully closed system such as a Recirculating Aquaculture System (RAS). Nonetheless, even at lower bioremediation efficiencies, the model already demonstrates the environmental benefits of IMTA.

The simulated growth for juvenile and adult sea urchins showed good correspondence with empirical data, although the reference temperature for which all the DEB constants were calculated was 20°C (Table 2) which is significantly higher than the average temperature (11° C) at the modelled IMTA site during the 18 month grow out period. The sea urchin growth model output is comparable to the results of Cook and Kelly (2007) who concluded that *P. lividus*, with an initial test diameter of 1 cm, deployed adjacent to fish cages need approximately 3 years to reach market size (> 5.5 cm test diameter). The sea urchins will be around 1 year old when they are deployed and 2.5 years old at the end of the grow out phase at which point their test diameter will be 4.47 cm. At the end of the 18-month grow-out phase of the salmon, the sea urchins will have reached the lower limit of their target market size. The growth rate achieved in this study was similar to that achieved directly adjacent to the sea cages (Cook and Kelly, 2007) and higher than that achieved by Fernandez and Clatagirone (1994) (1.41 mm per month) where the sea urchins were fed with artificial feed containing fish meal and fish oil at higher water temperature than this study (5-33°C). After the sea urchins have reached market size a two to three month period of market conditioning at controlled environment is required (Carboni, 2013; Grosjean et al. 1998).

In the first eight to ten months of the IMTA baseline scenario, seaweed and sea urchin growth is limited by nitrogen (Figs. 6 and 8b), since the fish are still small and thus require a relatively low feed input. From the eleventh month onwards mainly light and to a lower extend temperature are limiting the seaweed growth. From that point onwards the seaweed growth rate is high as can be seen in Fig. 5. For successful high bioremediation efficiency, at an IMTA farm seaweed growth should not be limited by light or temperature but only by nutrient availability. For this reason IMTA systems could be more efficient in sites further south than the one used for the baseline simulation. It can be seen clearly in Fig. 10 that there is a constant increase of the residual DIN and PON remaining at the IMTA site. This high waste output particularly during the last months of the salmon production is a challenge for

738 achieving very high bioremediation efficiency. The ratio of salmon to extractive organisms
739 (especially for sea urchins) used at the test scenario is very low (Table 2). From the
740 perspective of space requirement there is the potential for increase of the amount of sea
741 urchins produced, however the quantity of waste available for consumption by the sea urchins
742 decreases with distance from the sea cages and thus increasing the production would mean
743 that some sea urchins would be potentially too far from the food source. Furthermore, limited
744 market demand for marine invertebrates might also pose limitations.
745
746 The results of the sensitivity analysis indicate that the model is robust, since variation of key
747 model parameters by ±10% does not cause unexpected changes in the effect parameters. The
748 various model parameters have a different relative influence on the model's output, both in
749 terms of harvestable biomass and in terms of nitrogen bioremediation. Thus, depending on
750 users' specific study objectives, one should consider the precision with which certain
751 parameter values are determined, and whether further tuning is required. This model
752 sensitivity analysis is a useful means for assessing which are the key parameters that increase
753 model uncertainty. Those parameters with high sensitivity have a big impact on the output of
754 the model (e.g. thermal sensitivity parameters T_L in the sea urchin DEB submodel, T in all the
755 submodels and μ_{max} in the seaweed submodel), and therefore future efforts should focus on
756 methods for improving their estimation. In contrast, because parameters with low sensitivity
757 have little influence on the output of the model, their estimation could be simplified.
758 Consequently, despite the large variability observed in some of the parameters, their relative
759 importance may be minor if their sensitivity is low.
760
761 The model presented here is highly adaptable as all the submodels can function
762 independently. By altering model variables the submodels can simulate growth and nutrient
763 assimilation under different environmental conditions or for different species. Altering the
764 values of constants can also help assess their effect on the IMTA system and in some cases
765 these values can be optimised. For example, all the values related with production practices at
766 the IMTA site, such as seaweed harvesting frequency, maximum seaweed biomass allowed,
767 initial biomass of seaweed or sea urchins, seaweed culture depth and seaweed density, can be
768 optimised for the achievement of higher bioremediation efficiency and/or higher extractive
769 organism production.
770
771 Apart from achieving the major objectives described the model can be used for the
772 accomplishment of more general objectives such as: optimization of IMTA culture practices
773 (e.g. timing and sizes for seeding and harvesting, in terms of total production), assessment of

774 the role of IMTA in nutrient waste control and used as input for the evaluation of economic
775 efficiency of various system designs. The present model can be used as a decision support
776 tool for open-water IMTA only after being coupled with waste distribution modelling and
777 environmental sampling for model parameterization. Future versions of the model can link the
778 virtually closed IMTA system to hydrodynamic models for spatial analysis of the waste
779 dispersion and nutrient dilution. Such a model could help develop a balance among the
780 components of the IMTA system and assist in developing an IMTA design for maximum
781 waste uptake in "open environment systems", as water exchange rate is the key factor
782 influencing the assimilative performance, thus enabling prediction of the effectiveness and
783 productivity of open water IMTA systems.
784
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786
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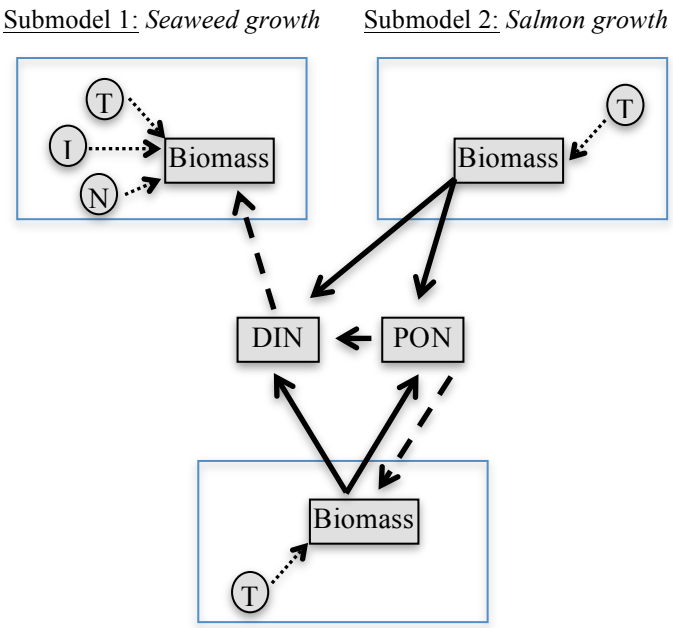

Fig. 1: Conceptual diagram of the model showing the major state variables (squares) and forcing functions (circles) of each submodel as well as the interactions among the submodels. The dashed lines represent nitrogen assimilation and the solid lines nitrogen release. *T, I* and *N* represent temperature, irradiance and nitrogen, respectively.

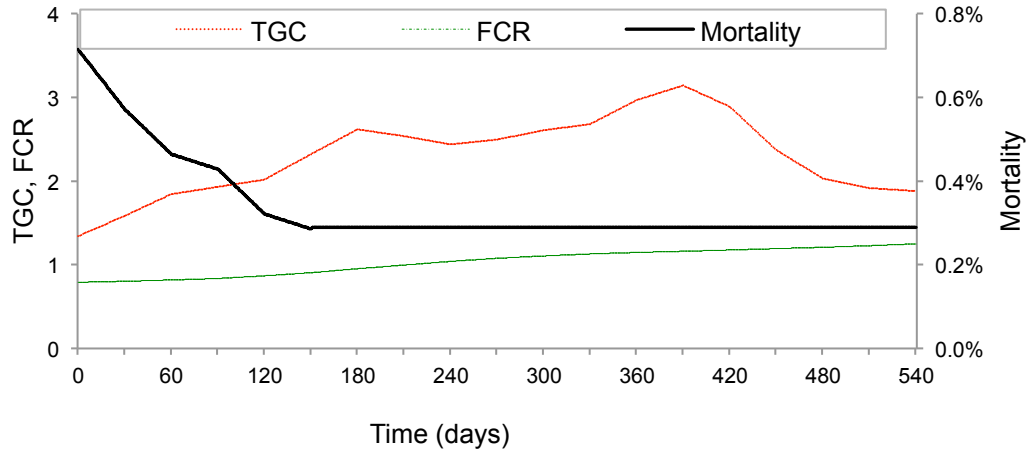

Fig. 2: Production scenario values of the time series variables, TGC, FCR and salmon mortality.

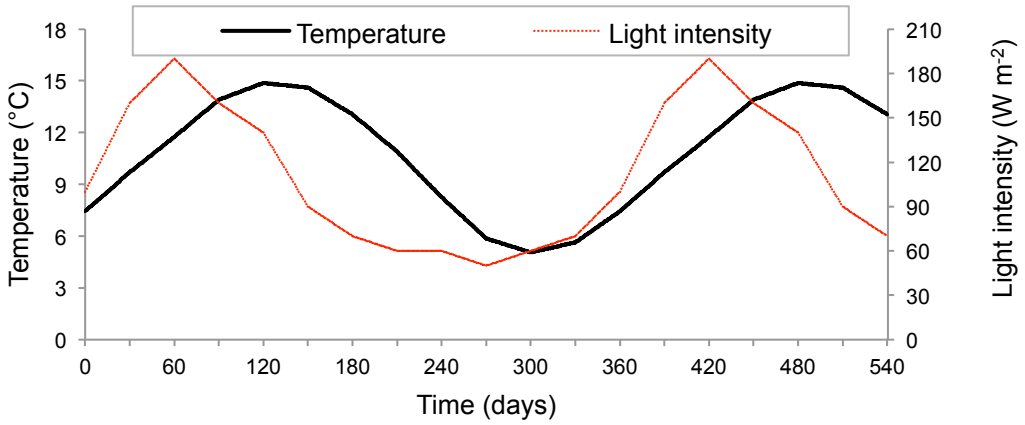

Fig. 3: Production scenario values of the time series variables, water temperature and light intensity.

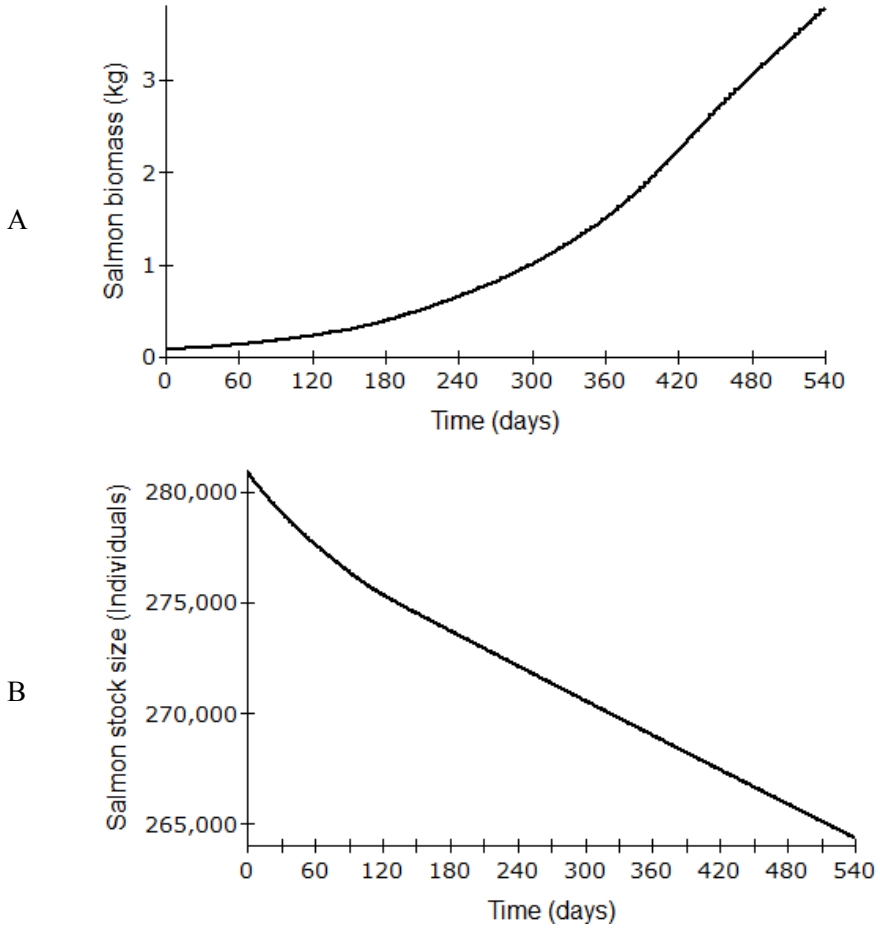

Fig. 4: Simulated output of the salmon: a) individual average biomass, b) stock size, during the 540 days of culture at sea.

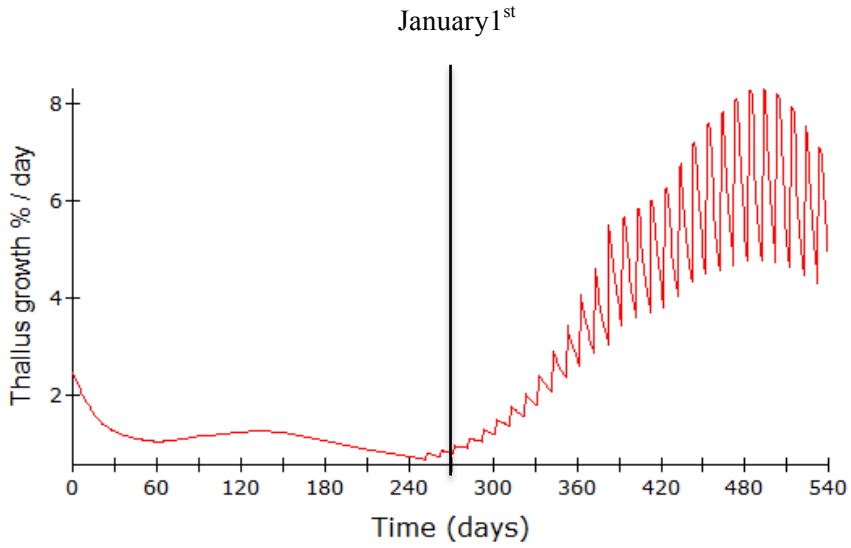

Fig. 5: Seaweed specific growth rate for *Ulva* sp. during the test scenario production conditions.

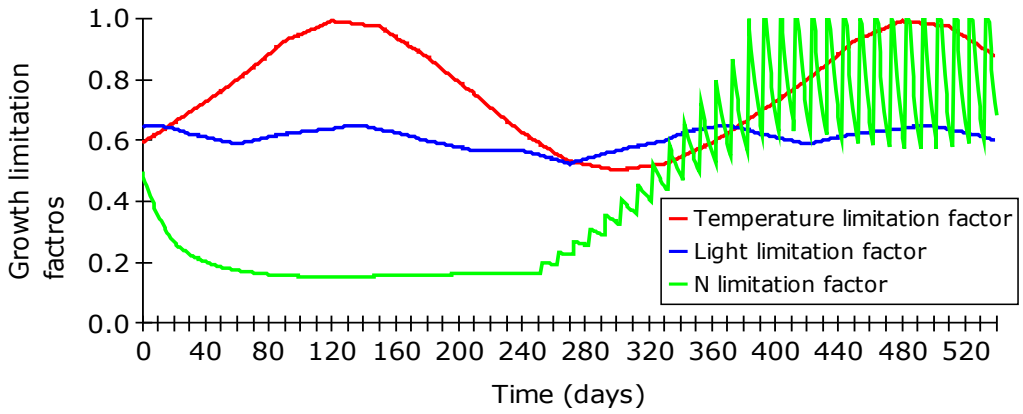

Fig. 6: Seaweed growth limitation factors, under the test scenario production conditions. The limitation factors can vary between 0 and 1; where a value of 1 means that the factor does not inhibit growth.

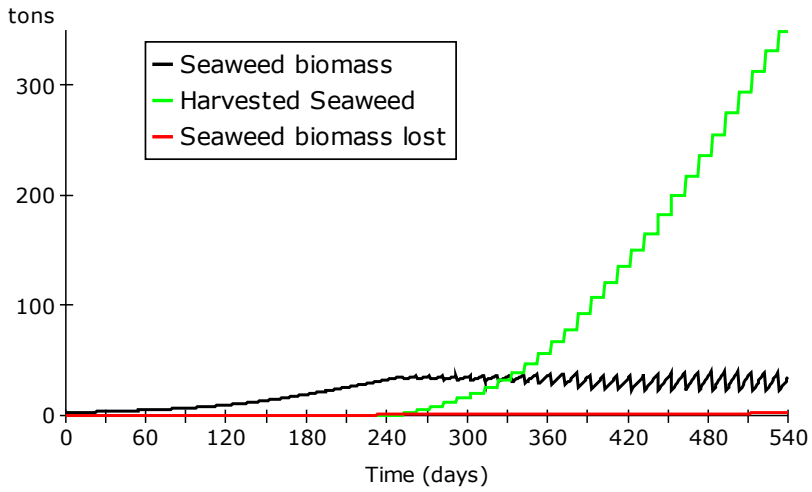

Fig. 7: Seaweed submodel simulation output for *Ulva* sp. produced under the test scenario conditions. It illustrates the biomass change over time, the cumulative amount of seaweed biomass lost due to natural causes and the cumulative amount of seaweed biomass harvested.

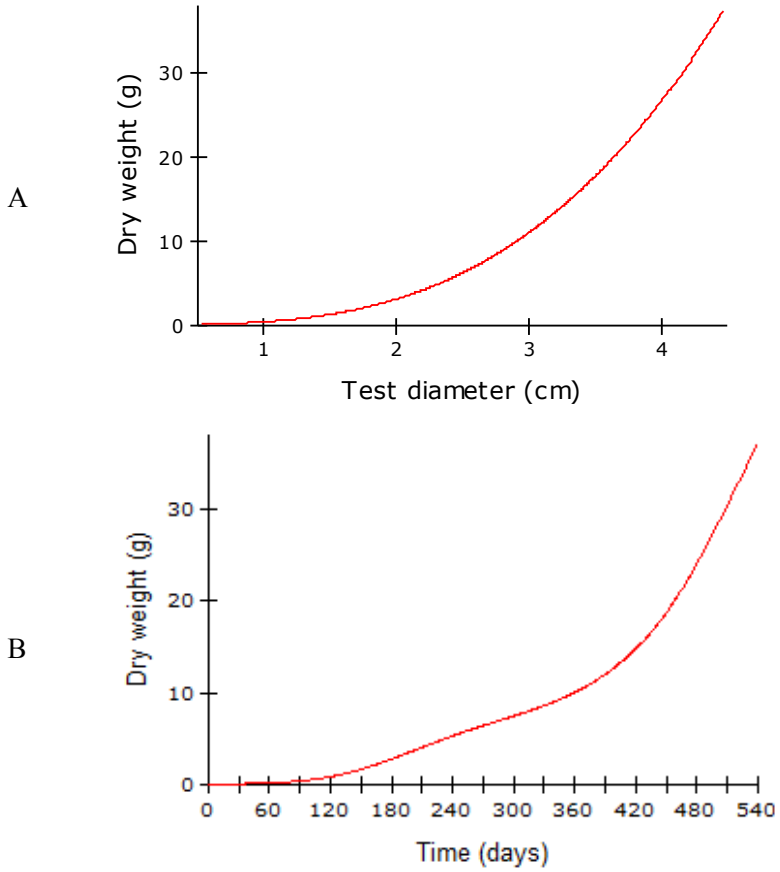

Fig. 8: Sea urchin submodel simulation output for: a) the length - dry weight relationship of *P. lividus* b) *P. lividus* dry weight

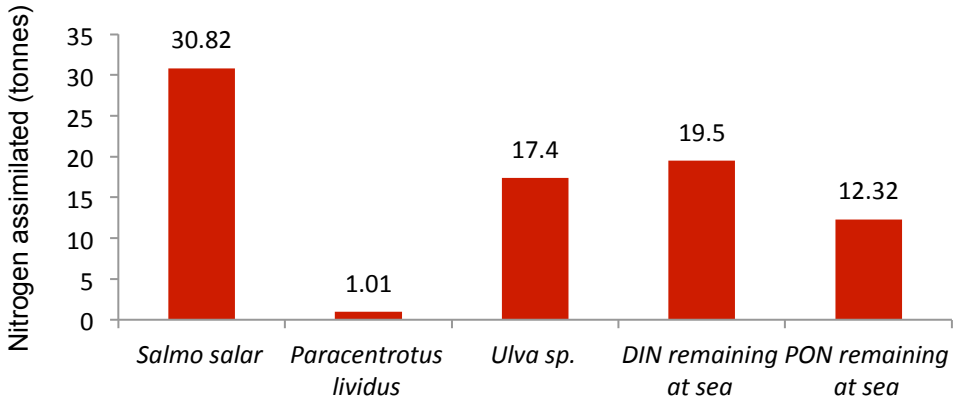

Fig. 9: Modelled output of nitrogen assimilated (in harvested biomass) in the different IMTA components and the amount of DIN or PON remaining at the virtually closed IMTA site area (above the ambient seawater nutrient concentration) over a 540 day simulated production period.

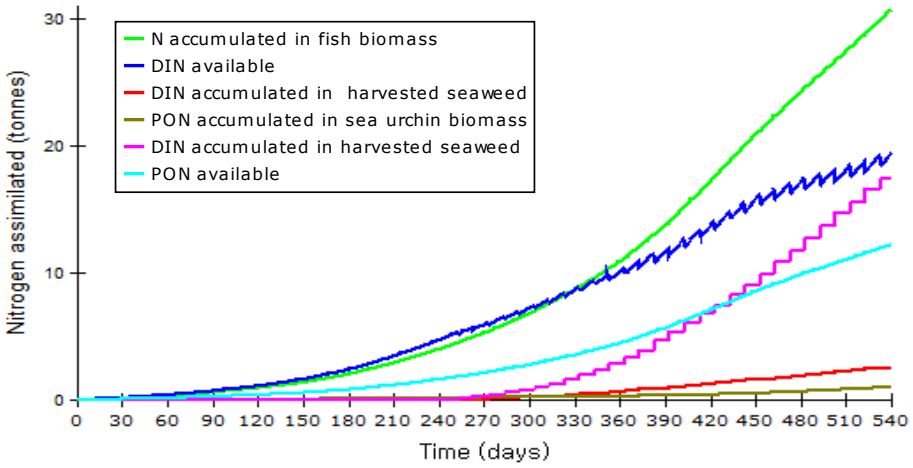

Fig. 10: Modelled output of cumulative amount of nitrogen assimilated by the different IMTA components and the amount of DIN or PON remaining at the IMTA site area at each time step.

1000 Table 1: Parameterization of constants and time series variables used at the seaweed growth submodel.

Variable	Description	Value range in literature	Value used	Units	Reference
μ_{max}	Maximum growth rate	0.8-18	10	% Day^{-1}	Neori et al., 1991; Luo et al., 2012; Perrot et al., 2014
N_{max}	Maximum intracelular quota for N	36-54	50	mg^{-1}N g dw^{-1}	Fujita, 1985; Bjornsater and Wheeler, 1990; Cohen and Neori 1991; Perrot et al., 2014
N_{min}	Minimum intracelular quota for N	10 to 13	10	mg^{-1} N g dw^{-1}	Fujita, 1985; Bjornsater and Wheeler, 1990; Cohen and Neori 1991; Perrot et al., 2014
T	Water Temperature	Site specific	6.8-13.7*	°C	n/a
q_{10}	Seaweed temperature coefficient	2	2	n/a	Aveytua-Alcázara et al., 2008
I_0	Water surface light intensity	Site specific	50-190*	W m^{-2}	n/a
I_{opt}	Optimum light intensity for macroalagae	50	50	W m^{-2}	Perrot et al., 2014
k	Light extinction coefficient	Site specific	1	m^{-1}	n/a
z	Culture depth	Farm practice	2	m	n/a
V_{max}	Maximum N uptake rate	0.44-2.2	1.32	mgN g^{-1} dw h^{-1}	Lapointe and Tenore 1981; Perrot et al., 2014
K_N	N half saturation	0.06-0.55	0.31	mg L^{-1}	Perrot et al., 2014
Wet/Dry	Wet to dry weight ratio	6.7-10.15	8.43	n/a	Neori et al., 1991; Angell et al., 2012
M	Mortality	0.009-0.02	0.015	d^{-1}	Aveytua-Alcázara et al., 2008; Perrot et al., 2014
T_{ref}	Reference temperature for seaweed growth	n/a	15	°C	Neori et al., 1991; Luo et al., 2012; Perrot et al., 2014

Ω	Decomposition rate and natural biomass loss	n/a	M / 2	d^{-1}	n/a
D	Loss rate due to environmental disturbance	n/a	M / 2	d^{-1}	n/a
S	DIN concentration in sea water	Site specific	0.594	mg m^{-3}	n/a

* Time series variable

Table 2: Test scenario output illustrating the initial and final wet biomass of each IMTA component, as well as the salmon to extractive organism weight ratios required for achieving the bioremediation effect described above.

Biomass (wet)	Initial (tonnes)	Final (tonnes)
Ulva sp.	2	348
P. lividus	0.09	50
Salmo salar	22.47	1000
Ratio		
Salmo salar / *Ulva sp.*	11.24	2.87
Salmo salar / *P. lividus*	249.67	20

1010

1011 Table 3: Most sensitive parameters (with NS ≥ 1) for the effect variables *N accumulated in*
1012 *harvested salmon* and *Harvested salmon biomass*, by descending absolute normalized
1013 sensitivity coefficient (NS) for either + or – 10% of the effect parameter's value. The baseline
1014 values of the effect variables *N accumulated in harvested salmon* and *Harvested salmon*
1015 *biomass* were 30.82 and 1000 tonnes, respectively.

1016

Parameter symbol	Parameter name	Parameter baseline value	Effect for parameter + 10%	NS for parameter +10%	Effect for parameter -10%	NS for parameter -10%
N accumulated in harvested salmon: effect baseline value is 30.82 tonnes						
TGC	Thermal-unit growth coefficient*	2.33	38.24	2.41	24.42	2.08
FCR	Feed conversion ratio*	1.04	33.91	1	27.74	1
Harvested salmon biomass: effect baseline value is 1000 tonnes.						
TGC	Thermal-unit growth coefficient*	2.33	1233	2.33	798	2.02

1017

1018

1019 Table 4: Most sensitive parameters (with NS ≥ 1) for the effect variables *DIN accumulated in*
1020 *harvested seaweed* and *harvested seaweed biomass*, by descending absolute NS value for
1021 either + or – 10% of the effect parameter's value. The baseline values of the effect variables
1022 *DIN accumulated in harvested seaweed* and *Harvested seaweed biomass* were 17.55 and
1023 347.97 tonnes, respectively.

Parameter symbol	Parameter name	Parameter baseline value	Effect for parameter + 10%	NS for parameter +10%	Effect for parameter - 10%	NS for parameter -10%
DIN accumulated in harvested seaweed: effect baseline value is 17.55 tonnes						
N_{state}	Nutrient state of seaweed at harvest**	10	3.63	-7.93	10.59	3.97
μ_{max}	Max seaweed growth rate	0.13	21.38	2.18	13.96	2.05
T	Water Temperature*	10.89	21	1.97	14.83	1.55
V_{max}	Maximum N uptake rate	1.32	19.98	1.38	14.59	1.69
W/D	Wet / dry ratio	8.43	20	1.40	14.68	1.64
z	Culture depth	2	20	1.40	15.41	1.22
N_{excr}	Nitrogen lost via excretion	0.45	18.25	0.40	15.64	1.09
Harvested seaweed biomass: effect baseline value is 347.97 tonnes						
μ_{max}	Max seaweed growth rate	0.13	424.57	2.20	293.53	1.56
T	Water Temperature*	10.89	416.95	1.98	293.60	1.56
V_{max}	Maximum N uptake rate	1.32	396.47	1.39	288.71	1.70
W/D	Wet / dry ratio	8.43	397.21	1.42	290.29	1.66
z	Culture depth	2	296.91	-1.47	305.13	1.23
N_{min}	Min intracellular quota for N	10	320.95	-0.78	387.64	-1.14
N_{max}	Max intracellular quota for N	50	327.78	-0.58	387.43	-1.13

1024

Table 5: Most sensitive parameters (with NS ≥ 1) for the effect variables *Nitrogen accumulated in harvested sea urchin biomass* and *Harvested sea urchin biomass,* by descending absolute NS value for either + or – 10% of the effect parameter's value. The baseline values of the effect variables *Nitrogen accumulated in harvested sea urchin biomass* and *Harvested sea urchin biomass* were 1.01 and 20.86 tonnes, respectively.

Parameter symbol	Parameter name	Parameter baseline value	Effect for parameter +10%	NS for parameter +10%	Effect for parameter -10%	NS for parameter -10%
Nitrogen accumulated in harvested sea urchin biomass: effect baseline value is 1.01 tonnes						
T	Water Temperature*	10.89	11.98	3.46	9.8	2.58
$\{Px\}$	Maximum surface-specific feeding rate	578.55	1.21	2.9	0.71	2.44
K_o	Reference reaction rate at 288 K	1	1.19	2.72	0.72	2.33
T_A	*P. lividus* Arhenius temperature	8000	0.77	-1.74	1.14	-2.13
$[E_G]$	Volume specific cost of *P. lividus* growth	2748	0.82	-1.23	0.94	-0.01
μ_{cj}	Ratio of carbon to energy content	83.30	0.85	-0.91	1.04	-1.10
Harvested sea urchin biomass: effect baseline value is 20.86 tonnes						
T_L	*P. lividus* lower boundary tolerance	273	0.09	-9.96	21.02	-0.08
T	Water Temperature*	10.89	27.77	3.31	15.65	2.50
$\{Px\}$	Maximum surface-specific feeding rate	578.55	26.95	2.92	15.76	2.44
K_o	Reference reaction rate at 288 K	1	26.30	2.61	16.16	2.25
T_A	*P. lividus* Arhenius temperature	8000	17.36	-1.68	25.14	-2.05
$[E_G]$	Volume specific cost of *P. lividus* growth	2748	17.96	-1.39	21.48	-0.30

1033 Table 6: Most sensitive parameters (with NS ≥ 1) for the effect variables *DIN available at the*
1034 *IMTA site* and *PON available at the IMTA site*, by descending absolute NS value for either +
1035 or – 10% of the effect parameter's value. The baseline value of the effect variables *DIN*
1036 *available at the IMTA site* and *PON available at the IMTA site* were 19.50 and 12.32 tonnes,
1037 respectively.
1038

Parameter symbol	Parameter name	Parameter baseline value	effect for parameter + 10%	NS for parameter +10%	effect for parameter - 10%	NS for parameter -10%
DIN available at the IMTA site: effect baseline value is 19.50 tonnes.						
N_{state}	Nutrient state of seaweed at harvest**	10	33.41	7.13	26.45	-3.56
TGC	Thermal-unit growth coefficient*	2.33	27.72	4.22	12.34	3.67
FCR	Feed conversion ratio*	1.04	22.51	1.54	15.59	2.01
N_{excr}	Nitrogen lost via excretion	0.45	22.45	1.51	15.64	1.98
μ_{max}	Max seaweed growth rate	0.13	15.67	-1.96	23.08	-1.84
$N_{content}$	Nitrogen content in feed	0.07	22.41	1.49	15.68	1.96
T	Water Temperature*	10.89	16.04	-1.77	22.22	-1.39
V_{max}	Maximum N uptake rate	1.32	17.07	-1.25	22.46	-1.52
W/D	Wet / dry ratio	8.43	17.04	-1.26	22.36	-1.47
z	Culture depth	2	17.05	-1.26	21.64	-1.10
N_{min}	Minimum intracellular quota for N	10	20.85	0.69	17.51	1.02
PON available at the IMTA site: effect baseline value is 12.32 tonnes						
TGC	Thermal-unit growth coefficient*	2.33	15.49	2.57	9.59	2.22
FCR	Feed conversion	1.04	13.63	1.06	11.01	1.06

	ratio*					
$N_{content}$	Nitrogen content in feed	0.07	13.59	1.03	11.05	1.03

* Time series variable. The time series parameters where increased/decreased by 10% at each time step

** For the parameter "Nutrient state of seaweed at harvest" we used N_{min} instead of N_{max} at the column labelled as +10% and $(N_{min} + N_{max})/2$ at the column labelled as -10%