

Report on dynamic CSTT (dCSTT) model for SARF012

Milestone 4:

Enrique Portilla*

Paul Tett†

School of Life Sciences, Napier University, 10 Colinton Road,
Edinburgh EH10 5DT, Scotland

November 30, 2006

*e.portilla@napier.ac.uk

†p.tett@napier.ac.uk

Abstract

This report describes the combined, dynamic, ECE-CSTT model and auxiliary models and their implementation as a Matlab script for the SARF012 project, ‘The development of modelling techniques to improve predictions of assimilative capacity of water bodies utilised for marine caged fish farming’. In this milestone report a biological term has been added to the nutrient terms in the sECE framework, together with some improvements of the physics of the ACEX model. An application of the dCSTT model, using phytoplankton chlorophyll, Dissolved Available Inorganic Nitrogen (DAIN) and Dissolved Inorganic Phosphorus (DIP), is shown for Loch Creran. Observations in 1975, before the introduction of a salmonid farm, are well simulated, but there are difficulties in accurately simulating observations from 2003, when a salmon farm was in place. These difficulties are discussed, and consideration is given to further model development and the use of the ACEX-sECE-dCSTT-IESV model series to establish assimilative capacity.

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1 Introduction

The report on the 3rd milestone for the SARF012 AC project introduced the idea of a sequence of models that were to be seen as solutions of the following generalized equation for the rate of change of a water quality state variable in the presence of fishfarming,

$$(1) \quad \frac{\partial Y}{\partial t} = -\nabla\varphi_Y + \beta_Y + \Gamma_Y \quad (\text{typical units: amount m}^{-3} \text{ d}^{-1})$$

where, on the right hand side:

- the first term deals with physical transports, being the divergence of the flux vector (φ_y), in which are included advective and diffusive terms in one or more spatial dimensions; the values of the fluxes at the boundary of the modelled domain must be specified;
- the second term (β_Y) is the sum of the biological and chemical sources and sinks for the variable;
- the third term (Γ_Y) gives the input of the variable by the farm, or its loss to the farm.

The third milestone report dealt with salinity and nutrients as state variables, and showed the importance of boundary conditions in controlling nutrient levels in the absence of biological and chemical sources and sinks. It gave accounts of the coupling into a seasonal ECE model of the 3-layer physical model of Figure 1 and milestone 1 report (Gillibrand and Inall, 2006), and of auxiliary models for catchment runoff and fish-farm nutrient input.

The present report, for the 4th SARF012 milestone, introduces the **dynamic CSTT model**. The model is thus called because it is a time-varying solution of equation (1) that draws on the main ideas of the eutrophication model proposed by the UK's Comprehensive Studies Task Team (CSTT, 1994, 1997; Tett, 2000; Tett et al., 2006). The dynamic CSTT (**dCSTT**) model adds one more state variable, phytoplankton chlorophyll, to the set of salinity and nutrient tracers in the seasonal ECE model. This requires a new equation of chlorophyll and a modification to the existing nutrient equations to deal with the removal of nutrient by phytoplankton.

This report describes the additional equations and their implementation as a Matlab script. As in the case of the milestone 3 script, the new script includes the ability to draw on data

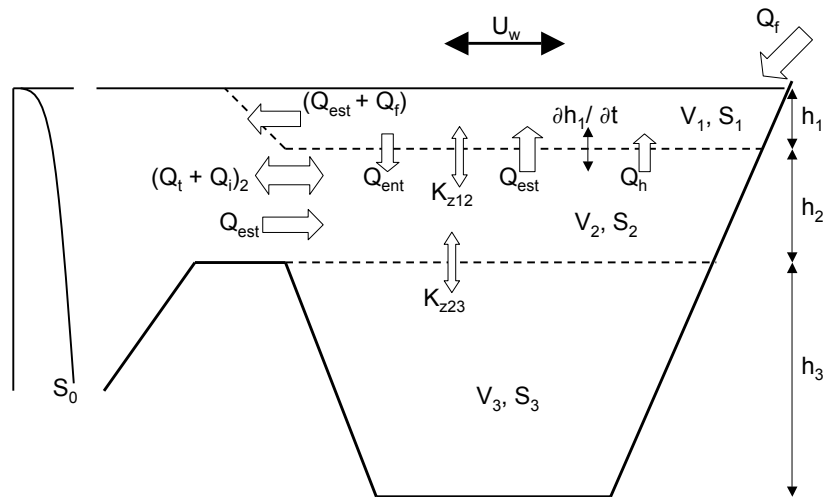


Figure 1: Schematic diagram of the three layer physical model. Volumes, fluxes and layer parameters are also represented. Extracted and upgraded from Gillibrand and Inall (2006)

bases of regional climatologies for boundary nutrient and chlorophyll concentrations and river nutrient concentrations and to run a simple catchment runoff-model driven by rainfall, in order to provide time-varying river flows. At present, the databases are populated only for Lorn (and the central Firth of Lorn) in Argyll, and the new simulations are tested against observations in loch Creran in Argyll. There are good sets of historic and recent data for loch Creran, and it provides a good site for testing models of the impact of mariculture.

In this report we deal at greater length than in the milestone 3 report with statistical issues involved in assessing the reliability of simulations of chlorophyll concentration. In addition, chlorophyll concentration is here considered the first of the *impact indicators* needed to assess the assimilative capacity of a water body, and the theory of such assessment is introduced here in terms of **pressure-impact** diagrams and exemplified for chlorophyll in loch Creran. The report commences with an introduction to two key ideas that form the basis of the theory of the CSTT model: the idea of the **yield** of chlorophyll from assimilated nutrient, and the idea of the **microplankton**, containing both phytoplankton and small pelagic consumers, as the main biological unit.

2 Exchange, Yield and Microplankton

The original CSTT model (CSTT, 1994) used several concepts to simplify the model equations. These concepts were : **exchange** between a mixed box and the sea; the use of **microplankton** rather than phytoplankton parameters; and the **yield** of chlorophyll from nutrient.

2.1 Exchange

The first idea, that of **mixed box exchange**, simplifies the description of the movement of tracers into or out of a simulated water body. The original CSTT model described a single box exchanging with the sea; the box was to be seen as being filled with many small packets of water, each containing phytoplankton and nutrient and having a daily probability p_i of being displaced from the box and replaced by a similar packet of seawater. The exchange rate was the bulk average of the individual probabilities,

$$(2) \quad E = \frac{1}{n} \sum_{i=1}^n p_i$$

The bulk tracer concentration was

$$(3) \quad Y = \frac{1}{n} \sum_{i=1}^n y_i$$

where a packet's content of a tracer was y_i . The effect of exchange on the tracer concentration was calculated from $-E \cdot (Y - Y_0)$, where Y_0 was the bulk concentration in the sea. This calculation requires

$$(4) \quad -E \cdot (Y - Y_0) = \frac{1}{n} \left(\sum_{j=1}^n (p_j \cdot y_{0,j}) - \sum_{i=1}^n (p_i \cdot y_i) \right)$$

to be true, which is only the case for a well mixed body of water receiving no other significant inputs of water. In reality the exchange probability is likely to vary depending on the position of a packet within the water body, and some sea-lochs receive a substantial river discharge.

The original CSTT model parameterized all the physical transport processes as a single exchange rate, and ignored displacement of water as a result of freshwater input. The

ACExR, sECE and dCSTT models resolve this exchange into a number of physical processes (Gillibrand and Inall, 2006) that can transport water, nutrients and phytoplankton and which do take account of the volume of freshwater discharged by rivers. Furthermore, they resolve the single CSTT box into a 3-layer structure. This increased physical resolution takes some account of the vertical inhomogeneities that are typical of sea-lochs, as well as the different transport processes operating on different layers. However, it neglects still neglects horizontal variability, and this neglect may need to be taken into account when comparing observed and simulated values of Y .

2.2 Microplankton

The second idea, that of the microplankton, concerns the biological particles that populate each layer in the model. Phytoplankton is the collective name for a community of phytoplankters, which are microscopic algae and photosynthetic bacteria able to assimilate nutrients from the water, absorb sunlight using chlorophyll, and consequently increase in numbers. Each phytoplankter is simple, consisting of either a single cell or a short chain of nearly identical cells. In a typical one litre water sample from a sea-loch, there are hundreds to millions of such cells. Feeding on the phytoplankters, or on organic matter leaked from them, are almost equally numerous pelagic bacteria and protozoans. Taken together, these bacteria, protozoa and phytoplankters make up the **microplankton**. In order to parameterize light-controlled growth, we can view the microplankton as a box to which photosynthesis (by the phytoplankters) provides an input of organic carbon and respiration (by everything) removes a fraction of that carbon. This leads to the following simple equation for the light-driven growth rate of the microplankton:

$$(5) \quad \mu(I) = \alpha \cdot (I - I_c)$$

In this equation, growth rate μ is the relative rate of increase of microplankton biomass. Biomass is quantified in the model as chlorophyll concentration, X , and hence

$$(6) \quad \mu(I) = (dX/dt) \cdot (1/X)$$

in the absence of other gains and losses of chlorophyll. The parenthetical term in $\mu(I)$ indicates that this equation calculates growth rate only in relation to the supply of light; it takes no account of other potential limiting factors. The gross efficiency of conversion of light into growth substance is given by α , photosynthetic efficiency. The final term

I_c is called the compensation illumination: it is the amount of light at which respiratory consumption of photosynthesate (by the entire microplankton) exactly balances the the gross production of this photosynthesate (by the phytoplankton), when both are totalled over 24 hours.

In all versions of the CSTT model, the photosynthetic efficiency and the compensation illumination are microplankton parameters, which can be calculated (Lee et al., 2003) from information about the relative amounts of phytoplankton (or **autotrophs**) and protozoa plus bacteria (**heterotrophs**) in the microplankton. The key parameter is the **heterotroph fraction** η , the ratio of heterotroph biomass to total microplankton biomass. Numerous other autotroph-specific or heterotroph-specific parameters are involved in the calculation, but for present purposes they can be treated as constants that are available from the literature. Values are presented later.

2.3 Yield

The third key idea is that of the yield, q , of chlorophyll from assimilated nutrient. Using S to refer to nutrient concentration, yield is defined as

$$(7) \quad q = -dX/dS$$

in the absence of any other processes changing nutrient concentration. As it is used in the CSTT model, q is a microplankton parameter: some of the nutrient taken up by phytoplankton is converted to protozoan or bacterial biomass, and hence the microplankton yield is less than the yield of chlorophyll from nutrient when only phytoplankters are present.

Following observations in sea-lochs (Gowen et al., 1992) and experiments in microcosms (Edwards et al., 2005, 2003), the value of the yield of chlorophyll from assimilated compounds of nitrogen (DAIN, 'dissolved available inorganic nitrogen') is quite well known. However, the yield from assimilated compounds of phosphorus is known well only for freshwater phytoplankton, and an attempt is made to estimate it, for marine coastal phytoplankton, in this report .

2.4 The steady state CSTT models

The original CSTT model predicted the maximum concentration of chlorophyll that could occur if all available nutrient were assimilated by microplankton. It is a steady state model, calculating equilibrium (enhanced) nutrient concentration S_{eq} from seawater concentration and local enrichment. Then,

$$(8) \quad X_{max} = X_0 + q \cdot S_{eq} \text{ but only if } \mu(I) > L + E$$

where L is local microplankton loss rate, due to, for example, filter feeding by the benthos. The nutrient equation is:

$$(9) \quad S_{eq} = S_0 + \frac{s_i}{E \cdot V}$$

where s_i is the local input of nutrient (from a river, fish farm or waste water discharge) and V is the volume of the simulated box.

This serves to introduce the dynamic CSTT model. As a development of the original, steady state CSTT model, it is described by two equations:

$$(10) \quad \frac{dS}{dt} = -\frac{\mu \cdot X}{q} + \frac{e \cdot L \cdot X}{q} + \frac{s_i}{E \cdot V} - E \cdot (S - S_0)$$

$$(11) \quad \frac{dX}{dt} = \mu \times X - L \cdot X - E \cdot (X - X_0)$$

The extra terms is e , the fraction of grazed nutrient that is recycled. This model was used by Tett et al. (2006) to derive the steady state equations and by Laurent et al. (2006). to simulate a sea-loch as a one-and-a-half box system. Details of the dCSTT version developed for the SARF012 project are given in the next section, writing the defining equations in a way that makes a formal difference between physical transport, biological, and anthropogenic processes.

3 The dynamic CSTT model

The general expression for any state variable introduced in equation (1) can be rewritten for phytoplankton chlorophyll (X) as follows:

$$(12) \quad \frac{\partial X_i}{\partial t} = -\nabla \varphi_{X_i} + \beta_{X_i} + \Gamma_{X_i} \quad (\text{typical units: mg chl m}^{-3} \text{ d}^{-1})$$

where i (1, 2 or 3) refers to physical layers (Gillibrand and Inall, 2006) (figure 1, from (Gillibrand and Inall, 2006)). The inclusion of phytoplankton chlorophyll in the modeling protocol implies that the Γ_X term is zero in the CSTT model, as fin-fish farms do not produce chlorophyll directly. Nevertheless, this term would be negative for a model dealing with phytoplankton-feeding shellfish.

In this introduction of the dCSTT model, we bring the phytoplankton chlorophyll as a state variable into use compared with the seasonal Equilibrium Concentration Enhancement (sECE) model. Seasonal Chlorophyll variation will be described by means of terms present in equation (12). Equally, limiting nutrients are also considered as state variables in our modelling approach interacting. The temporal variation and interaction between state variables will be described accordantly.

3.1 Biology in the dCSTT model

The main new term to consider in the dCSTT model in opposition to the sECE is β_{X_i} , describing the sum of the biological and chemical changes on a state variable. On phytoplankton chlorophyll this term can be described as follows:

$$(13) \quad \beta_{X_i} = \mu(S^N, S^P, I) X - L \cdot X$$

Where, L represents the Loss rate of phytoplankton to planktonic or benthic grathing. L is assumed to be temperature dependent and can be considered as a constant value or mimicked by a sinusoidal curve. The loss rate will be expanded in section (7). The $\mu(S^N, S^P, I)$ corresponds to the phytoplankton growth rate (see Tett and Wilson (2000) and later work with Forth estuary model). The final value is governed by the minimum

growth that phytoplankton experiment under limiting conditions:

$$(14) \quad \mu(S^N, S^P, I) = \min\{\mu(S^N), \mu(S^P), \mu(I)\}$$

where the three limiting factors considered here are dissolved nutrients (we use S to define generally the limitant nutrient in opposition to X for Chlorophyll) and solar radiation (denoted by I). For each of them the specific phytoplankton growth for each limiting factor can be expressed as:

$$(15) \quad \mu(S^N) = \mu_{max} \frac{S^N}{K_{SN} + S^N} \quad \text{For Dissolved Nitrogen}$$

$$(16) \quad \mu(S^P) = \mu_{max} \frac{S^P}{K_{SP} + S^P} \quad \text{For Dissolved Phosphorous}$$

$$(17) \quad \mu(I) = \alpha_{max}(I - I_c) \quad \text{For Light irradiance}$$

where μ_{max} is the maximum algal growth rate; K_{SN} and K_{SP} are concentrations of limiting nutrient (DAIN and DIP respectively) at which growth rate is half maximum and S^P and S^N are nutrient concentration (DAIN and DIP respectively). α_{max} is the effective photosynthetic efficiency. Further explanation on those terms will be made in section 5.

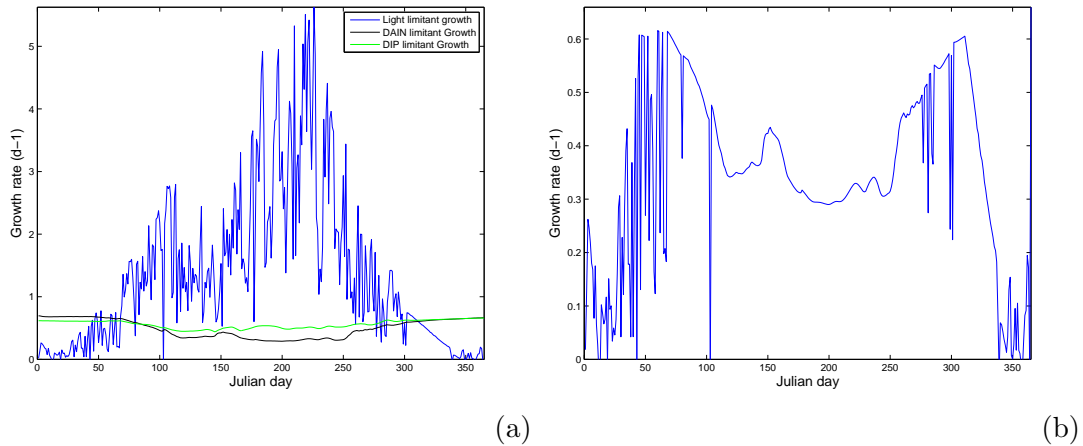


Figure 2: a) Microplankton growth as a function of three different limitant factors: Light, DAIN and DIP considered in the dCSTT model. b) Resultant Microplankton growth, which is the minimum growth from each limiting factor

Similarly, changes in nutrients due to biological and chemical mechanisms will be now expressed in the source-sink terms β_{Sj} (where j refers to each of the three potentially limiting nutrient elements, nitrogen, phosphorus or silicon). This term will update the idea of the seasonal equilibrium concentration enhancement (sECE) model of the 3rd SARF012 AC milestone report.

Although the bio-chemical term for limiting nutrients (β_{Sj} and that for phytoplankton chlorophyll (β_X) possesses identical processes (see $\mu(S^N, S^P, I)$ in equations 13 and 15), they include specific coefficients for each limitant nutrient for different ecosystems. They are the yield of chlorophyll from nutrients (q^j) and *in situ* nutrient recycling (e^j). In both cases the j subscript refers to the three potentially limiting nutrient. They will be treated with more detail in the following sections.

Therefore, when Nitrogen (N) is considered, the biological chemical process can be stated as follows:

$$(18) \quad \beta_{SN} = -\frac{\mu(S^N, S^P, I) X}{q^N} + \frac{e^N LX}{q^N}$$

Equally for phosphorous (N) :

$$(19) \quad \beta_{SP} = -\frac{\mu(S^N, S^P, I) X}{q^P} + \frac{e^P LX}{q^P}$$

We will omit Silicate for now when describing the dCSTT model. However its use will be suggested in the example case of Loch Creran.

3.2 physics in the dCSTT model

From equation (1), we identify the term which describes the physics in the dCSTT framework ($-\nabla\varphi_Y$). The physical term is estimated using the ACEX_R physical model developed for milestone 1 (Gillibrand and Inall, 2006). We have already apply the time-varying exchange with the adjacent sea water in the contest of the 3rd milestone report (Portilla and Tett, 2006).

The physical term, ($-\nabla\varphi_Y$), is given in full once for each of the three layer system simu-

lating horizontal and vertical exchange, as shown in figure 1, for a generalized variable Y (which is replaced by X , S_N or S_P). It considers 9 components of exchange, 6 of which act on the surface layer.

An important process that takes place in fjords water dynamic is the renewal of water from lower layers. Although, they are easy to implement within the framework of the physical model developed by Gillibrand and Inall (2006), the previous version of the ACExR model did not take account of such a processes. Nevertheless, the current version of the ACExR physical model used to couple the dCSTT model, contains an small script to take account of renewal events (`renewal.m`). They are easily trackable because there is an increase in salinity in layer 3.

Basically, the renewal event is simulated as a net import of external water, not an overturning event mixing only internal water (Gillibrand *pers. com.*). Therefore, values in the intermediate and deep layers take on external values, rather than being conserved. This suppose a problem with the adaptive numerical integration method used in the dCSTT modelling (`ode23`). Also the minimum value of the coefficient of vertical turbulent diffusion (denoted by K_z) is changed from the original in order to increase the exchange in the bottom layer. We treated these problems within section (8)

It should be noted that overturning occurs in the Clyde due to surface cooling. Although It might not be a widespread phenomena in other sea lochs, the analysis of physical profiles for different sea lochs within the context of this project might clarify this issue. Anyhow, since temperature is not at present a state variable in the model, overturning is not a possibility (since evaporation is unlikely to lead to density inversions). In further implementations, the inclusion of temperature as a state variable might increase the precision in the recreation of renewal events.

3.3 One equation to describe everything

The equation system will be therefore described by a set of equations contains temporal variation for the state variables considered in the dCSTT model, i.e. phytoplankton chlorophyl, and limiting nutrients. Here we only considered 2 limiting nutrients, but it can be extended by adding Silicate, for instance. The temporal variation of the state variables will be composed by the terms introduced previously, which are the physical term $-\nabla\varphi_{X_i}$, the Biology β_{X_i} and $\beta_{S_{j_i}}$ and the mariculture effect Γ_{X_i} and $\Gamma_{S_{j_i}}$

$$(20) \quad \begin{cases} \frac{\partial X_i}{\partial t} = -\nabla\varphi_{X_i} + \beta_{X_i} + \Gamma_{X_i} & (\text{typical units: mg chl m}^{-3} \text{ d}^{-1}) \\ \frac{\partial S_{N_i}}{\partial t} = -\nabla\varphi_{S_{N_i}} + \beta_{S_{N_i}} + \Gamma_{S_{N_i}} & (\text{typical units: mg DAIN m}^{-3} \text{ d}^{-1}) \\ \frac{\partial S_{P_i}}{\partial t} = -\nabla\varphi_{S_{P_i}} + \beta_{S_{P_i}} + \Gamma_{S_{P_i}} & (\text{typical units: mg DIP m}^{-3} \text{ d}^{-1}) \end{cases}$$

Therefore, as stated in the introduction our modeling approach can be resumed by the following formula:

$$(21) \quad \frac{\partial Y_{ki}}{\partial t} = -\nabla\varphi_{Y_{ki}} + \beta_{Y_{ki}} + \Gamma_{Y_{ki}}$$

where Y_{ki} subscript k corresponds to the state variable to considered (chlorophyll, DAIN or DIP) and i to the 3 different physical layers that we defined in a sea loch.

4 The simple optical model

4.1 Introduction

The equation for light-limited microplankton growth, given in previous sections, requires a value for I_i , the 24-hour mean PAR in the layer concerned. **PAR** stands for ‘Photosynthetically Active Radiation’, the part of solar radiation that has wavelengths between 400 and 750 nm and can be captured by chlorophyll (and other pigments) to drive photosynthesis. The calculation of each layer’s I is carried out in the procedure `SubmarineOptics.m`, which is largely based on Tett 1990.¹

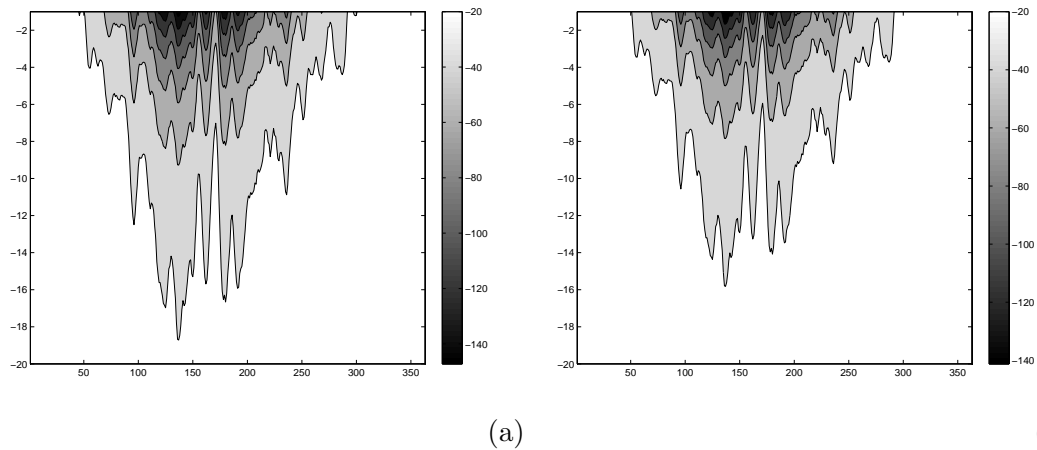


Figure 3: Seasonal change of PAR (x-axis) as a function of water depth (y-axis) under two different chlorophyll conditions (a) **No Chlorophyll** throughout the year (b) a constant value of chlorophyll equivalent to the **peak** observed in Loch Creran in 1975 (6.1 units??). The bar at the right of each figure represent the color scale of the Irradiance values in (units??)

What we are trying to highlight in the figure (3) is the effect of seasonal variation of PAR in the water column under different concentrations of chlorophyll. As it can be seen in the figure (3) , the radiation that can be observed at different depths along the year is function principally of the arriving solar radiation. Although a minor role, the chlorophyll concentration is also important in the Photosynthetically Active Radiation.

¹The use of the symbol I for irradiance (the flux of power or photons onto unit area) is out-dated, and modern works prefer the symbol E . However, we have appropriated E for water exchange, and so retain the older I

4.2 Calculation procedure

There are several steps in the calculation scheme:

1. Obtain a value for 24-hour mean total solar irradiance on a given day, either from meteorological data (as presently implemented) or from an astronomical model (not yet implemented here); the value should be given in units of Watts m^{-2} ; ‘total solar irradiance’ includes all the solar radiation that penetrates the Earth’s atmosphere to arrive at the surface of the sea;
2. Convert total irradiance (in W m^{-2}) to PAR (in $\text{microEinstein m}^{-2} \text{ s}^{-1}$) that penetrates the sea-surface; a microEinstein is a flux of photons whereas a Watt is a measure of power or heating ability ($1 \text{ W} = 1 \text{ J s}^{-1}$);
3. Calculate the mean PAR over layer 1 and the mean PAR at the base of layer 1, taking account of the **diffuse downwelling PAR attenuation coefficient** K_d in the layer; the coefficient is influenced by the amount of chlorophyll present (but not, in this version, by other light-absorbers);
4. Use the mean PAR at the base of layer 1 to calculate the mean PAR over layer 2 and at the base of layer 2;
5. Use the mean PAR at the base of layer 2 to calculate the mean PAR over layer 3

These are the equations:

$$(22) \quad K_{d,i} = K_{d,w} + m_3 \cdot (a_{PH}^* \cdot X_i) \text{ (attenuation in layer } i)$$

$$(23) \quad I_1 = I_0 \cdot (1 - m_0) \cdot m_1 \cdot m_2 \cdot \frac{1 - e^{-K_{d,1} \cdot h_1}}{K_{d,1} \cdot h_1} \text{ (layer 1 mean PAR)}$$

$$(24) \quad I_{1/2} = I_0 \cdot (1 - m_0) \cdot m_1 \cdot m_2 \cdot e^{-K_{d,1} \cdot h_1} \text{ (PAR at base of layer 1)}$$

$$(25) \quad I_2 = I_{1/2} \cdot \frac{1 - e^{-K_{d,2} \cdot h_2}}{K_{d,2} \cdot h_2} \text{ (layer 2 mean PAR)}$$

$$(26) \quad I_{2/3} = I_{1/2} \cdot e^{-K_{d,2} \cdot h_2} \text{ (PAR at base of layer 2)}$$

$$(27) \quad I_3 = I_{2/3} \cdot \frac{1 - e^{-K_{d,3} \cdot h_3}}{K_{d,3} \cdot h_3} \text{ (layer 3 mean PAR)}$$

The variables used in the irradiance estimations, with their longer names in the procedure `SubmarineOptics.m`, are:

- h_i : thickness of layer i , in metres

- I_0 (**Ibarbar0**) : sea surface 24-hr mean total solar radiation, all wavelengths, in W m^{-2}
- X_i : chlorophyll concentration in layer i , mg m^{-3}

The parameters and their values are:

- m_0 (**m0** = 0.06) : the albedo of the sea - the proportion of solar irradiance that is reflected, averaged over 24 hours;
- m_1 (**m1** = 0.46*4.15): the conversion from total solar energy to PAR photons; 0.46 is the PAR fraction of total solar radiation, and 4.15 is the mean microEinsteins/Joule of submarine PAR
- m_2 (**m2** = 0.37): the fraction of surface PAR that is penetrating light, explained and estimated by Tett (1990);
- $K_{d,w}$ (**Kdw**=0.215) the background diffuse PAR attenuation for loch Creran, in m^{-1} ; this is the attenuation in the absence of chlorophyll, but including ‘yellow substance’ and suspended inorganic matter, as estimated by Tyler (1984) by regression of K_d on X ; this is given as a parameter rather than a site-specific variable because in a future version of the optical model (which will make K_d depend on suspended particles and ‘yellow-substance’ as well as chlorophyll) it will be truly constant;
- m_3 (**m3**=1.25) : the reciprocal of the ‘mean cosine’ of underwater PAR, used in two ways - to convert a beam absorption value such as $a_{PH}^* \cdot X$ into a contribution to diffuse attenuation, and (in the biological code) to take account of the up-scattered light that can contribute to photosynthesis;
- a_{PH}^* (**astarPH** = 0.012) : the absorption cross-section of phytoplankton chlorophyll in loch Creran, with units $\text{m}^2/\text{mg chl}$; its value is further discussed below.

ere is the main part of the procedure **SubmarineOpticsF.m**. The procedure is called with daily values of the inputs. Note the preliminary calculation of optical thickness terms,

$$\zeta_i = K_{d,i} \cdot h_i$$

to speed the main calculations.

```
% -----
function [Ibarbar]=SubmarineOpticsF(Ibarbar0,h, X);
```

```

% -----
% inputs:
% Ibarbar0 = 24 hr mean solar radiation at the sea surface, W m-2
% h = vector of 3 layer thicknesses, m
% X = vector of chlorophyll concentrations in each layer
% output:
% Ibarbar = vector of mean irradiance in each layer, muE m-2 s-1
%
% calculate vector of diffuse attenuation coefficients, m-1
Kd=Kdw+m3.*(astarPH.*X);
% calculate vector of layer optical thicknesses
zeta=Kd.*h;
% calculate mean PAR, muE m-2 s-1, using scalar operations only
Isubsurface =(1-m0)*m1*m2*Ibarbar0;
Ibarbar(1)=Isubsurface*(1-exp(-zeta(1)))/zeta(1);
Ibottom(1)=Isubsurface*exp(-zeta(1));
Ibarbar(2)=Ibottom(1)*(1-exp(-zeta(2)))/zeta(2);
Ibottom(2)=Ibottom(1)*exp(-zeta(2));
Ibarbar(3)=Ibottom(2)*(1-exp(-zeta(3)))/(zeta(3));
% -----

```

4.3 Discussion

Some of the optical parameters (m_3 and a_{PH}^*) are used also in the procedure `microgrowthI.m` to calculate photosynthetic efficiency, and thus the simulated seasonal cycles of chlorophyll are sensitive to change in these parameters. Whereas the value of m_3 has been treated as fixed (and indeed would only have larger value for waters with a large load of light-scattering suspended particles, the value of a_{PH}^* depends on both the spectral distribution of light and the contribution of photosynthetic accessory pigments to light absorption. The greatest realistic value of a_{PH}^* is $0.04 \text{ m}^2 (\text{mg chl})^{-1}$, but using this resulted in excessive chlorophyll in Winter.

5 Microplankton growth parameters

5.1 Introduction

As described in an earlier section, the growth rate of microplankton is the minimum of growth rates calculated from light (PAR), nitrogen (DAIN) and phosphorus (DIP):

$$(28) \quad \mu^{mp}(S^N) = \mu_{max}^{mp} \cdot \frac{S^N}{k_S^N + S^N} \quad (\text{for DAIN})$$

$$(29) \quad \mu^{mp}(S^P) = \mu_{max}^{mp} \cdot \frac{S^P}{k_S^P + S^P} \quad (\text{for DIP})$$

$$(30) \quad \mu^{mp}(I) = \alpha_{max}^{mp} \cdot (I - I_c^{mp}) \quad (\text{for PAR})$$

These repeat earlier equations, except that some of the terms have been superscripted ^{mp} to emphasize that they are microplankton parameters or rates. In these equations:

μ_{max}^{mp} is the maximum microplankton growth rate;

k_S^N and k_S^P are concentrations of limiting nutrient (DAIN and DIP respectively) at which growth rate is half maximum;

α_{max}^{mp} is the microplankton photosynthetic efficiency and I_c^{mp} is the photosynthetic compensation illumination for the microplankton.

In the Matlab script, these equations are dealt with by the following functions:

`microgrowthN.m` for DAIN-limited growth

`microgrowthP.m` for DIP-limited growth

`microgrowthI.m` for PAR-limited growth

and these functions are explained, and parameter values given, in this section.

The dCSTT model equations for microplankton growth are derived from more primitive equations for the growth of phytoplanktonic micro-algae ('autotrophs') and pelagic protozoa and bacteria ('heterotrophs'), and the micro-algal equations are themselves simplified from a more complex theory for the growth of micro-algae under laboratory conditions. This section also sets out some of this underlying theory and derives some of the microplankton parameter values from it. Because of these multiple layers of theory, some of the samples used in this section are open to several interpretations, and annotations are used where it is necessary to specify the interpretation. These annotations include ^{mp} for microplankton parameters, and subscripts _a and _h specifying, respectively, autotroph and

heterotroph parameters. They are not applied where the context makes the interpretation clear and they are rarely used elsewhere in this report, where it may be assumed that parameters almost always refer to microplankton.

5.2 Simplifying algal growth theory

The dCSTT model is in part simplified from the **Cell-Quota** model for micro-algal growth. Droop (1968) introduced the model with a description of the relationship between the growth rate of a cultivated micro-alga and the algal cell content of a limiting nutrient, vitamin B₁₂. The model has since been shown to apply to a number of nutrients, including N, P and Si, as reviewed by Droop (1983), Tett and Droop (1988) and Tett et al. (2003). The algal cell quota Q is best defined as the ratio of cell nutrient content to cell biomass, although its estimates are usually based on bulk measurements of populations of algal cells. For example, Q^N is the atomic ratio of algal cell nitrogen to algal cell (organic) carbon, with values ranging from 0.04 to 0.25 atom N:atom C.

A set of three equations defines the original Cell-Quota model:

$$\begin{aligned} \frac{dQ}{dt} &= u - \mu \cdot Q && \text{(change in the cell quota)} \\ u &= u_{max} \cdot \frac{S}{k'_S + S} && \text{(nutrient uptake rate)} \\ \mu &= \mu'_{max} \cdot \left(1 - \frac{k_Q}{Q}\right) && \text{(nutrient-controlled growth rate)} \end{aligned}$$

where:

all the terms refer to micro-algae (only);

the units of uptake, u , are atoms of the nutrient assimilated per atom of (algal) carbon biomass per day;

u_{max} is maximum uptake rate, at nutrient (at C)⁻¹ d⁻¹;

k'_S is the concentration of ambient nutrient at which uptake rate is half of the maximum, using the same units as ambient nutrient concentration S ;

μ'_{max} is maximum (algal) growth rate, d⁻¹;

k_Q is the 'subsistence quota', the minimum (algal) cell nutrient content, at nutrient (at C)⁻¹;

The value of the subsistence quota is set, in the case of nitrogen as an example, by the

5.2 Simplifying algal growth theory5 MICROPLANKTON GROWTH PARAMETERS

minimum cellular content of protein and nucleic acids at which a cell is viable. Note the dashes on μ'_{max} and k'_S , which distinguish the values of these parameters in the cell-quota model from those in alternative algal nutrient-growth models.

The dCSTT simplification of the Cell-Quota model is based on the assumption of a steady state in which $\frac{dQ}{dt} \rightarrow 0$. Consequentially,

$$\begin{aligned}\mu &= \frac{u}{Q} \\ \text{and thus, } Q - k_Q &= \frac{u_{max}}{\mu'_{max}} \cdot \frac{S}{k_S + S} \\ \text{or, } \mu &= \frac{u_{max}}{Q} \cdot \frac{S}{k_S + S}\end{aligned}$$

The last formulation is that of the **Monod** growth equation, in which the reciprocal of Q is called the ‘yield’ (of biomass from nutrient) and is assumed to be constant, allowing $\frac{u_{max}}{Q}$ to be rewritten as the constant parameter μ_{max} (note lack of dash):

$$(31) \quad \mu = \mu_{max} \cdot \frac{S}{k_S + S}$$

A later addition to the Cell-Quota model was the idea of ‘threshold limitation’, so that for PAR and nutrients (nitrogen, phosphorus, etc):

$$\mu = \min\left\{f(I), f\left(\frac{Q^N}{k_Q^N}\right), f\left(\frac{Q^P}{k_Q^P}\right), \dots\right\}$$

which tells that the limiting nutrient is the one for which the ratio of cell quota to subsistence quota is lowest, unless growth rate predicted from PAR, $f(I)$, is even lower. The Cell-quota model also contains the idea of ‘yield limitation’, in which the biomass reached when an initial stock, S_0 , of ambient nutrient is exhausted, can be estimated from the minimum of S_0/k_Q evaluated over all potentially limiting nutrients. That is,

$$B_{a,max} = \frac{B_0 \cdot Q_0 + S_0}{k_Q}$$

repeated for each nutrient, the actual maximum carbon biomass $B_{a,max}$ being the least of those predicted.

From the Cell-Quota model, the dCSTT model takes the idea of threshold limitation. Its key simplification is to assume a constant yield of phytoplankton chlorophyll from nutrient,

so the analogous equation is

$$X_{max} = X_0 + q^{mp} \cdot S_0$$

5.3 Limiting nutrients

Microplankton growth as a function of limiting nutrients is estimated with the functions `microgrowthN.m` (for DAIN) and `microgrowthP.m` (for DIP). The main equations are:

$$(32) \quad \mu^{mp}(S^N) = \mu_{max}^{mp} \cdot \frac{S^N}{k_S^N + S^N} \quad (\text{for DAIN})$$

$$(33) \quad \mu^{mp}(S^P) = \mu_{max}^{mp} \cdot \frac{S^P}{k_S^P + S^P} \quad (\text{for DIP})$$

$$(34) \quad \mu_{max}^{mp} = \mu_{max,a} \cdot \frac{e^{k_\Theta \cdot (\Theta - 20)}}{1} (1 - \eta)(1.2 - \eta)$$

The first two of these equations are microplankton versions of the Monod equation that was derived in the preceding subsection. The relationship between μ_{max}^{mp} and $\mu_{max,a}$ was derived by Tett (1998) and Lee et al. (2003). The parameters, and their names and values in the functions, are :

- η (`eta = 0.4`); the heterotroph fraction;
- k_S^N (`kS = 2.0` in `microgrowthN`); concentration of DAIN (when limiting) at which growth rate is half the maximum; μM or mmol m^{-3} ;
- k_S^P (`kS = 0.2` in `microgrowthP`); concentration of DAIN (when limiting) at which growth rate is half the maximum; μM or mmol m^{-3} ;
- k_Θ (`ktheta = 0.069`); temperature coefficient, $(^\circ\text{C})^{-1}$; $e^{10 \cdot k_\Theta}$ is the biological temperature coefficient known as the Q_{10} ;
- $\mu_{max,a}$ (`mumaxa = 2.0`); maximum algal growth rate at 20°C ;
- Θ (`theta = 12.0`); water temperature, $^\circ\text{C}$; currently a constant, but will be made a variable in later versions of the model;

Here are the main parts of the code in `microgrowthN.m`. The first part provides a default temperature if the function is called without one.

```
% -----
function [muN]=microgrowthN(varargin)
```

```

% -----
% Variable input
% S: DAIN concentration
% theta: (optional) Water temperature
S = varargin{1};
if (length(varargin) == 2), theta=varargin{2};
else theta=12.0; end;
% calculation of maximum growth rate parameter
mumax=mumaxa*exp(ktheta*(theta-20))*(1-eta)/(1.2-eta);
% output: N-limited growth rate, d-1
muN=mumax.*(S./(kS+S));
% -----

```

The function `microgrowthP.m` is the same, but calls on the appropriate value of `kS`.

5.4 Light limited growth theory

The function of PAR in the Cell Quota model makes growth rate depend on gross, algal-biomass related photosynthetic rate, p_a^B less algal respiration rate, r_a :

$$\mu_a(I) = f(I) = p_a^B - r_a$$

Most theory for light-limited growth makes the $p^B(I)$ curvilinear, as exemplified by the Smith-Talling equation Tett et al. (2003):

$$p_a^B = p_{max,a}^B \cdot \left(\frac{I^2}{k_I^2 + I^2} \right)^{0.5}$$

where k_I is a parameter controlling the curvature of the approach to the ‘saturated’ maximum photosynthetic rate, p_{max}^B . The Cell-Quota model, however, adopted a linear relationship for $f(I)$:

$$\mu_a(I) = \alpha_{max,a}^B - r_a$$

The linear coefficient is that here called **photosynthetic efficiency** and is formally defined as:

$$\alpha_{max,a}^B = \left. \frac{dp_a^B}{dI} \right|_{I \rightarrow 0}$$

It can be related to the curvilinear equation parameters - for example, in the case of the Smith-Talling equation,

$$\alpha_{max,a}^B = \frac{p_{max,a}^B}{k_I}$$

or the equation can be rewritten:

$$p_a^B = \alpha_a^B \cdot I$$

where $\alpha_a^B = \alpha_{max,a}^B \cdot \left(1 - \frac{I^2}{k_I^2 + I^2}\right)^{0.5}$

The value of the algal photosynthetic efficiency depends on two fundamental bio-physical processes: the capture of photons by chlorophyll (and other photosynthetic pigments) and the conversion of photon energy into the chemical energy stored in organic matter. It is the second process that becomes less efficient at higher illuminations.

The photon capture process is quantified by the parameter a_{PH}^* , called the ‘absorption cross-section’ of chlorophyll because its typical units are $\text{m}^2 (\text{mg chl})^{-1}$. It is in principle estimated by the rate of light absorption (m^{-1}) divided by chlorophyll concentration (mg m^{-3}). Alternatively, consider a metre cube of seawater containing 1 mg of chlorophyll (in phytoplankton). Light falls on the upper surface of this cube. A typical value of a_{PH}^* of $0.02 \text{ m}^2 (\text{mg chl})^{-1}$ implies that 0.02 of this light is captured by the chlorophyll. Increasing the amount of photosynthetic accessory pigments (which also capture photons) in relation to the amount of chlorophyll, increases the value of a_{PH}^* .

The conversion process is quantified by the parameter Φ , called the ‘photosynthetic quantum yield’ because it specifies the number of atoms of carbon ‘fixed’ into organic matter for each PAR photon absorbed. Such ‘fixation’ follows the use of photon energy to split water molecules, releasing oxygen and making available hydrogen to reduce CO_2 to organic carbon ($(\text{CH}_2\text{O})_n$). In the best laboratory conditions a minimum of 8 photons is required to release one molecule of oxygen and fix one atom of carbon. In nature, some of the hydrogen is diverted to other purposes, and there are other inefficiencies, even under low-light conditions. Thus a realistic value for the maximum quantum yield, Φ_{max} is 0.04 atoms C fixed per absorbed photon. A gram-atom of carbon contains the same (Avogadro’s) number of atoms as an Einstein of PAR contains photons, and a mole of carbon dioxide also contains this number of atoms of carbon and molecules of the compound, and it is thus possible, and convenient, to express this efficiency as (in this example) 40 nmol C: μE PAR.

Combining the coefficients for the two processes,

$$\alpha_{max}^X = k \cdot \Phi_{max} \cdot (m_3 \cdot a_{PH}^*)$$

gives photosynthetic efficiency in relation to chlorophyll: $\text{mmol C (mg chl)}^{-1} \text{ d}^{-1} (\mu\text{E m}^{-2} \text{ s}^{-1})^{-1}$. The symbol k converts units, from nmol C to mmol C , and from seconds to days. For purposes of the dCSTT model however, the efficiency needs to be converted to units of $\text{d}^{-1} (\mu\text{E m}^{-2} \text{ s}^{-1})^{-1}$, and this requires division by a carbon:chlorophyll ratio, given the symbol χ . Thus,

$$(35) \quad \alpha_{max}^B = k \cdot \Phi \cdot (m_3 \cdot a_{PH}^*) \cdot \chi^{-1}$$

Using χ_a in this equation gives a value for $\alpha_{max,a}^B$, whereas using χ^{mp} results in a value for $\alpha_{max}^{B,mp}$, as further considered in the next section.

5.5 Light-limited growth

As previously described, the microplankton is composed of autotrophs and heterotrophs, with the variable η (the Greek letter ‘eta’) quantifying the ratio of heterotroph carbon biomass to total microplankton biomass. $\eta = 0$ would refer to phytoplankton in the absence of bacteria and protozoa; $\eta = 1.0$ would refer to a microplankton without any photosynthetic organisms. The first is unlikely, in the sea; the second is impossible, unless there is an external supply of organic matter to feed the bacteria and protozoa. A realistic range of values of η is from 0.1 to 0.8. The actual value can be estimated either from microscopic analysis of water samples or by finding the best fit of simulations with different values of η . The value changes during the year (e.g. Tett & Wilson, 2000), but in the dCSTT model we treat it as a constant, with a typical value obtained from observations in sea-lochs.

The equation for light-limited growth of microplankton is:

$$\mu^{mp}(I) = \alpha_{max}^{B,mp} \cdot I - r^{mp}$$

where r is the respiration rate of the microplankton, relative to their biomass In the microplankton model (Tett and Wilson, 2000; Lederman and Tett, 1981; Lee et al., 2003)res-

piration is composed of a basal and a growth rate-related component:

$$r^{mp} = r_0^{mp} + b^{mp} \cdot \mu^{mp}$$

which leads to: $\mu^{mp}(I) = \alpha_{max}^{B,mp} \cdot I - (r_0^{mp} + b^{mp} \cdot \mu^{mp}(I))$

and thus: $\mu^{mp}(I) = \frac{\alpha_{max}^{B,mp}}{1 + b^{mp}} \cdot I - \frac{r_0}{1 + b^{mp}}$

This gives the following, from which the ^{mp} superscripts have been omitted:

$$\text{giving: } \mu(I) = \alpha_{max} \cdot (I - I_c)$$

$$\text{where } \alpha_{max} = \frac{\alpha_{max}^B}{1 + b}$$

$$\text{and } I_c = \frac{r_0}{\alpha_{max}^B}$$

Given η , and taking account of the biophysics of photosynthesis as discussed in the preceding subsection, the three microplankton light-growth parameters can be calculated from:

$$(36) \quad \alpha_{max}^B = k \cdot \Phi_{max} \cdot (m_3 \cdot a_{PH}^*) \cdot q_a^N \cdot Q_{max,a} \cdot (1 - \eta)$$

$$(37) \quad r_0 = r_{o,a} \cdot (1 - \eta) + r_{o,h} \cdot \eta \cdot (1 + b_a)$$

$$(38) \quad b = b_a \cdot (1 + b_h \cdot \eta) + b_h \cdot \eta$$

The first of these equations is the result of combining:

$$\chi^{mp} = q_a^N \cdot Q_{max,a} \cdot (1 - \eta)$$

with eqn(??) above. This derivation of ths empirical relationship is explained by Lee et al. (2003)

A list follows for the parameters mentioned in these equations. The names are the forms used within the procedure `microgrowthI.m`. The list is divided into two parts:

... the first, for parameter values that were changed for some simulations, with their default values:

- η (`eta` = 0.4); the heterotroph fraction (biomass of protozoa and bacteria divided by total microplankton), which can vary between 0.0 - when the microplankton is solely phytoplankton - and about 0.8 - when it is mainly microheterotrophs;

- a_{PH}^* (astarPH = 0.012); absorption cross section for photosynthetic pigments, $\text{m}^2 (\text{mg chl})^{-1}$; the value can vary between 0.012 and 0.040, and is also used in `SubmarineOptics.m`

... the second for parameter values that were treated as always constant:

- k (k = 8.64E-02); units conversion: $\text{s d}^{-1} \text{mmol nmol}^{-1}$;
- Φ_{max} (phi = 40.0); photosynthetic quantum yield, $\text{nmol C } \mu\text{E}^{-1}$;
- m_3 (m3 = 1.3); reciprocal of mean cosine of angle of downwards photons in sea - also used in `SubmarineOptics.m`;
- Xq_a^N (XqNa = 2.2); algal chlorophyll:nitrogen ratio, $\text{mg chl (mmol N)}^{-1}$;
- Q_{max} (Qmaxa = 0.2); maximum algal nitrogen content, at N: at C;
- $r_{0,a}$ (r0a = 0.05); algal basal respiration rate, d^{-1} ;
- $r_{0,h}$ (r0h = 0.03); heterotroph basal respiration rate, d^{-1} ;
- b_a (ba = 0.5); slope of graph of algal respiration on growth rate, a ratio;
- b_h (bh = 1.5); slope of graph of heterotroph respiration on growth rate, a ratio;

Most of the values are taken from Lee et al. (2003), with that for Xq_a^N based on more recent, unpublished, work.

Finally, here are the main parts of the code of the function `microgrowthI.m`

```
function [muI]=microgrowthI(Ibarbar)
% inputs: Ibarbar: is solar radiation(PAR)
% outputs: muI: Light limited growth in d-1
% calculations of microplankton parameters
r0=r0a*(1-eta) + r0h*eta*(1+ba); % microplankton basal respiration, d-1
b=ba*(1+bh*eta)+ bh*eta; % microplankton respiration slope, ratio
alpha=k*phi*(m3*astarPH)*XqNa*Qmaxa*(1-eta);
% microplankton photosynthetic efficiency, d-1 (muE m2 s-1)-1
alphaB=alpha/(1+b);
% effective photosynthetic efficiency, d-1 (muE m-2 s-1)-1
Ic=r0/alphaB; % compensation irradiance, muE m-2 s-1
%
muI=alphaB.*(Ibarbar-Ic);%light limited growth
```

The name `alpha` corresponds to the symbol $\alpha_{max}^{B,mp}$ and the name `alphaB` to the symbol

variously written as α_{max} and α_{max}^{mp} . This is a little confusing, and we aim to make a clearer terminology for the final milestone report.

6 Yield of phytoplankton from nutrients

An important parameter to consider in both the CSTT model and subsequently, the dCSTT model is the yield of phytoplankton from Nutrients. This term is designed by q^j , being j the limitant nutrient to consider. This term was introduced explicitly in equations (18) and (19) and is calculated following the cell quote theory largely studied and tested (Droop, 1983).

The yield of phytoplankton from inorganic Nitrogen (q^N) for Scottish waters was firstly given from field work by Gowen et al. (1992). q^N was estimated regressing Dissolved Available Inorganic Nitrogen in spring for a bulk of Scottish Sea Lochs as a function of phytoplankton chlorophyll. In the laboratory the result were similar and tested in a laboratory experiment in Edwards et al. (2003). The value found in those studies was similar ($q^N=1.1$) and will be used here. On top of htis, we performed ourselves a similar study to that of Gowen et al. (1992) but also including other limiting nutrients that might contribute to the correct estimation of yield. For this porpoise we used field data recollected in the Graig island between 1970 to 1980 and between 2000 to 2003. The updated approach also provide estimate of yield of phytoplankton from phosphorous.

The yield of phytoplankton from inorganic phosphorous (q^P) is difficult to estimate. In previous studies q^P , has been taken from Fresh water studies. Therefore, a new value for this yield will be re-estimated in the context of this report. *Three* different approach will be taken in order to feed the dCSTT model with values of yield of phytoplankton from phosphorous.

Firstly, the yield of phytoplankton from inorganic phosphorous, will be recalculated using the methodology employed by Tett et al. (1975) ; secondly,the value of q^P estimated followed a similar approach of that of Gowen et al. (1992) but also including other limiting nutrients that might contribute to the correct estimation of yield. Finally by iteration too, but in this case we will not minimize the difference between observed and predicted values of the state variables, but the differential change of the state variable recorded in the field assuming that the only process that takes place is defined by equation (20) (in section (3.3)). In other words, what values of q^P will minimise the sum of square of errors of the quotient $\Delta Y/\Delta t$ (from direct observation) and the right hand side of equation (20) for DIP. This is a modification of what some people will call model tuning (Rykiel, 1996). All methods will be explained and illustrated with an example for Loch Creran below.

7 Loss Rate

In this section we extend the Loss rate term of phytoplankton. We aim to assume by this rate the loss due to benthos grazing or shell farm effects. As introduced before, the loss rate of phytoplankton is dependent on temperature, which in the current version of the dCSTT model was assumed as variable throughout the season (Figure 4), simulated by a sinusoidal curve. This assumption contrast with the previous uses of the dCSTT model (Laurent et al., 2006), where 10 °C was assumed the constant temperature value in loch Creran.

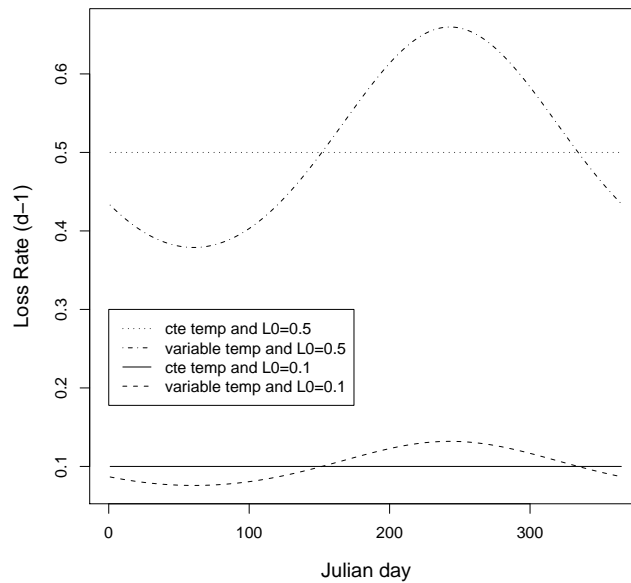


Figure 4: Loss rate of phytoplankton chlorophyll throughout the year. Different rates are displayed as a function of Temperature (constant or time varying temperature) and basal rate at temperature 10 °C.

The loss rate of phytoplankton due to planktonic or benthic grazing is expressed in units of d^{-1} . It is assumed that this value combine Loss rate of microzooplankton due to mesozooplankton and bentic grazing. The contribution in terms of grazing by farmed shellfish, is also included in the parameters. However, its contribution can be improved by using better physiological models for shellfish-famrs.

The paramters of the Loss rate module is highly dependent on the basal loss rate L_0 , or the Loss rate at the average temperature of 10 degrees. parameter was the only one included

in Laurent et al. (2006) in order to include grazing.

For the 1975 simulation, a value of L_0 equal to 0.1 was found optimal, and concordant with Laurent et al. (2006). Nevertheless, Several values were used in the 2003 simulation in order to decrease the overall predicted concentration of phytoplankton chlorophyll. It was assumed that an increase in the grazing pressure has been produced in the last years in Loch Creran (Ana Sequeira *pers. com.*). The instalation of a Shellfish farm in loch creran might be the responsible for such change.

The range of values used for L_0 were from 0.1 to 0.6. those found suitable varied from 0.2 to 0.5. However the one that was kept for the final realisation of the dCSTT model was $L_0 = 0.2$. The criteria used to employ such values was relatively fuzzy, and further study and improvement is required for the the optimal estimation of the Loss rate.

Other parameters used for the estimation of Loss rate, which we can assumed constant, where, a) the biological rate increase factor for a 10 degree C temperature increase, commonly taken as 2.0 (Q_{10} , and b) reference temperature (T_{ref}), in our case, 10 degrees Celsius.

The last parameters constitute a factor that should make the loss rate equal to L_0 at the reference temperature and double it in an increase of 10 degrees.

$$(39) \quad Factor = \exp \left(\log(Q_{10}) \cdot \frac{T - T_{ref}}{10.0} \right);$$

the final equation has this form:

$$(40) \quad L = L_0 \cdot Factor;$$

8 Renewal events in layer 3

In this section we will explain the strategy followed to simulate renewal events in layer 3 for the three state variables considered in the dCSTT model. As introduced earlier, renewal events in layer 3 are determined by salinity values becoming similar to that of layer 2 at a certain level. This equalisation of salinity produce the same process for the state variables, which will diminish the accumulation of nutrients in deep water by the fish farm.

We want highlight in this section the difference in the layer composition if the renewal events are taken into consideration within the physical model. Firstly we present the figures of the dCSTT model when the physics described in the sECE is used (Figure 5). Secondly, we employed the same parameters to run the dCSTT model but now, the upgraded version of the physical model with present a renewal event for deep water (Figure 6). This second attempt implies a modification on the code of the `dcstt.m` matlab script. It will be showed below.

Finally an increase in the mixing flux between layer 2 and 3 has been done my modifying accordantly the script `Kz23.m` (figure 7). This new version is located in the folder `SARFACv2/ACExRrenewal/`

Two issues are considered in the integration of the dCSTT model. Firstly, we need to track the daily salinity record so that exists an indication of a renewal event occurring (signalled by an increase in layer 3 salinity).

Secondly, and specific to the dCSTT model structure, we have to take account of the numerical integration of layer 2 and 3 in the moment of renewal. We need to considered that when an event occurs, the differential increase or decrease for an state variable Y in layer 3 at time t is that of layer 2 at the same time, i.e. $\partial Y_3/\partial t = \partial Y_2/\partial t$. Moreover, this differential change needs to be added to previous integrated value of layer 2 at time $t - 1$, i.e. $Y_3(t) = Y_3(t - 1) + \partial Y_2/\partial t$. To illustrate this we write explicitly part of the code used to simulate a renewal in layer 3.

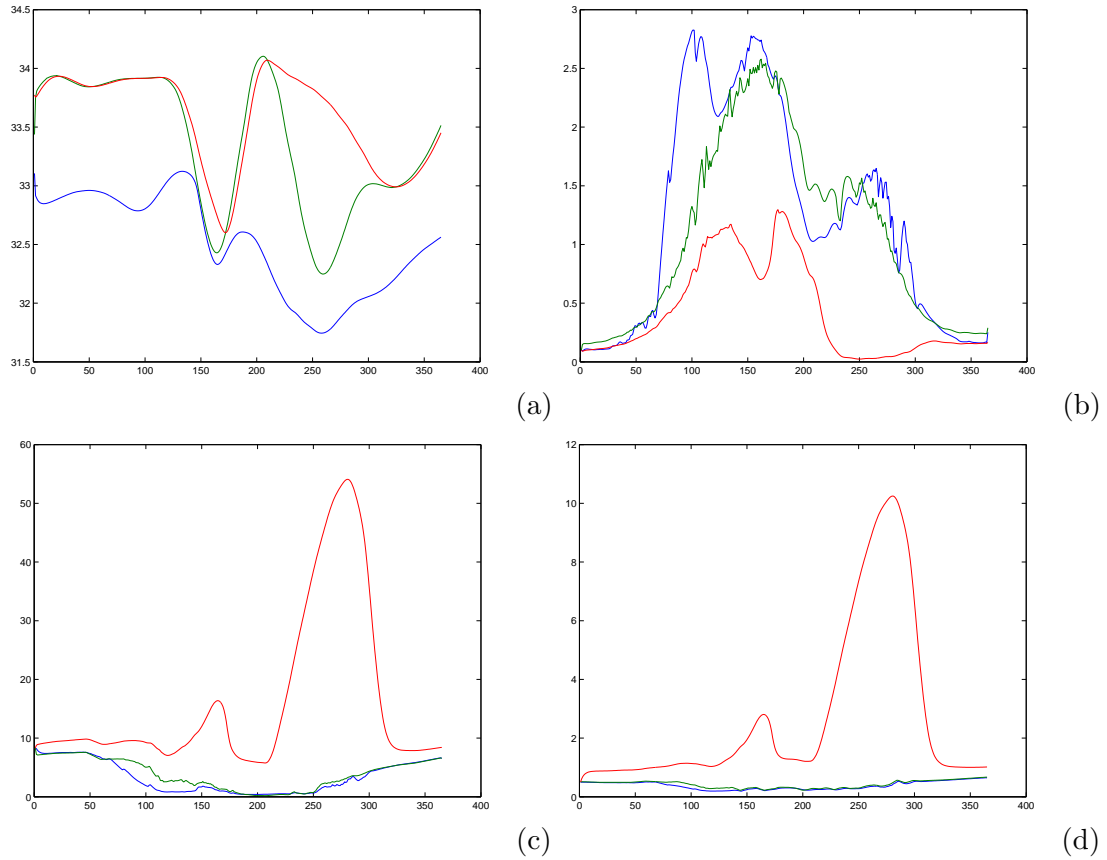


Figure 5: Predicted seasonal variation for salinity (a); phytoplankton chlorophyll (b), DAIN(b); and DIP (d) in 2003. The simulation was performed coupled with the physical model but without taking into account renewal events. The seasonal variability is represented for the three layers of water: layers one in blue, two in green and three in red

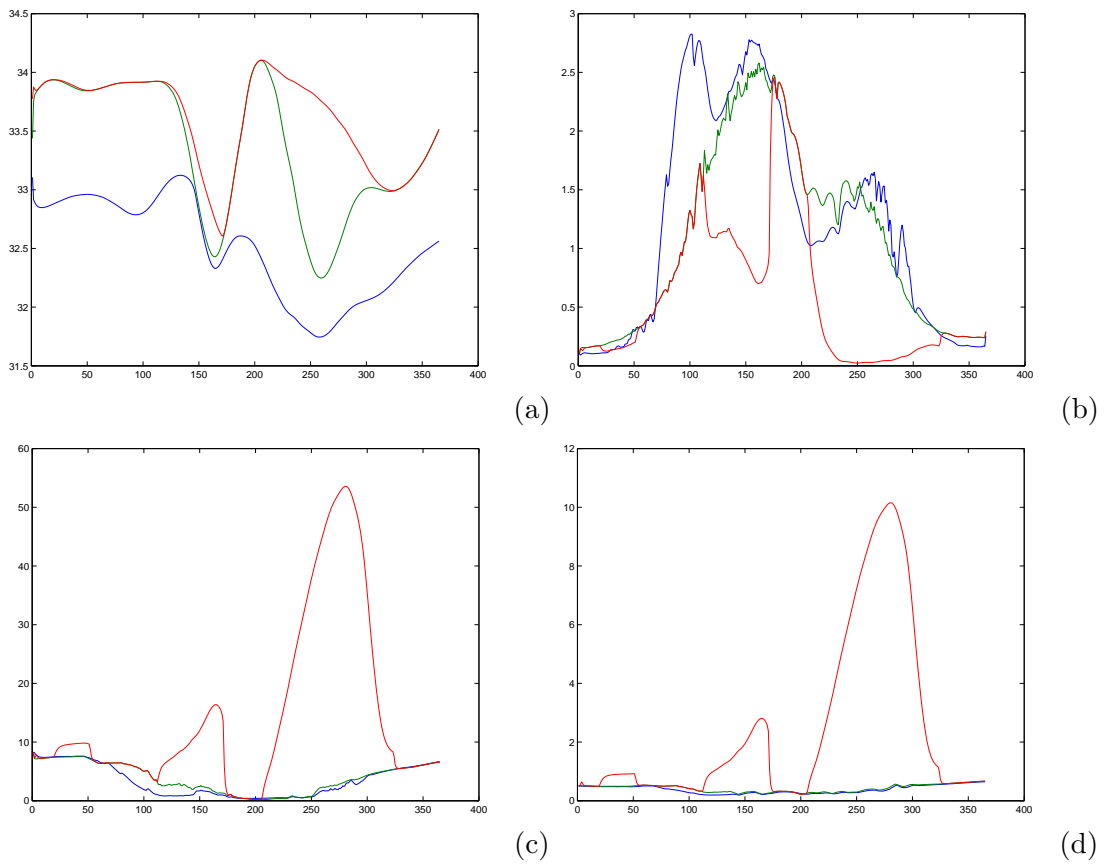


Figure 6: Same as figure (5), but in this case we coupled the biology with the physical model which makes allowances for renewal events

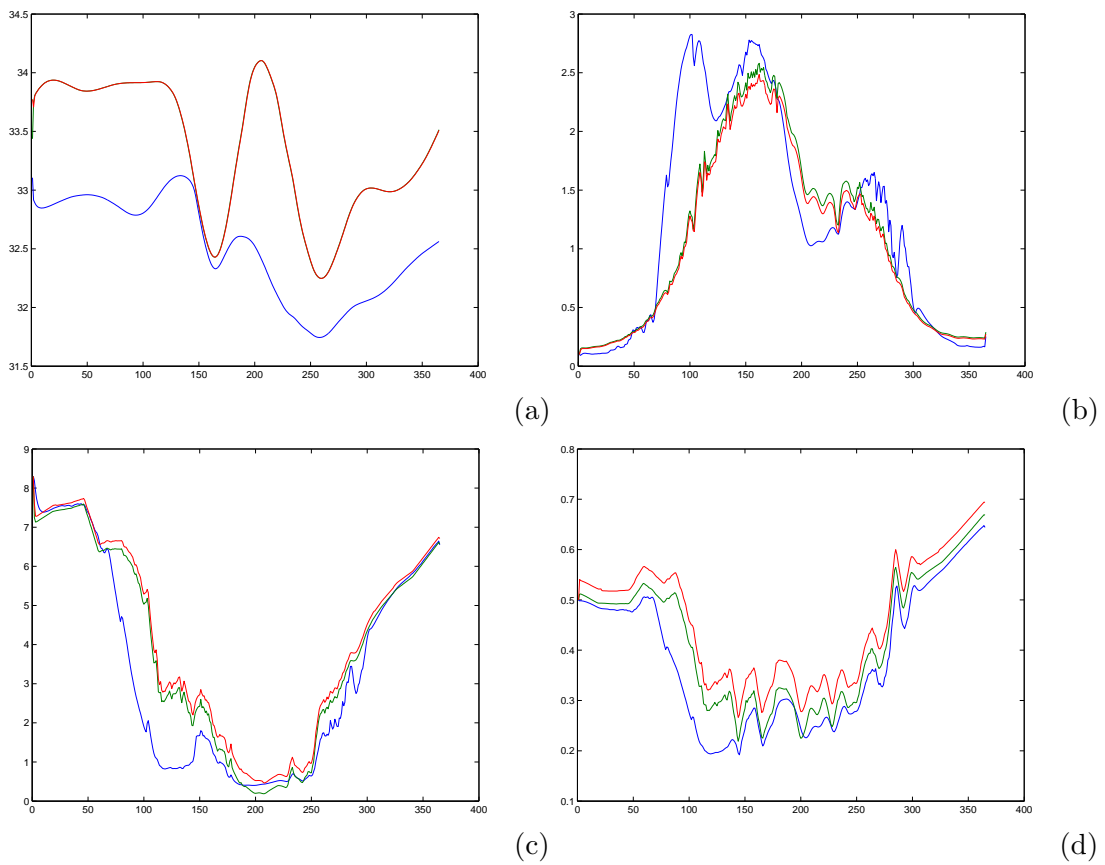


Figure 7: Same as figures (5) and (6), but now the renewal events are simulated by using a modified version of Kz23.m from Gillibrand and Inall (2006)

```

newsal=sall'+SAL;%integrated sal at time t
    %newS=X.S'+XX.S;
    %newP=X.P'+XX.P;
    % renewal events
    if(newsals(2)>newsals(3))
        %display a message
        %disp([num2str(newsals) 'at t = ' num2str(t)])

        %do something to make Y(3)=Y(2)
        %What i will be doing is subtracting the initial value
        %of the state variable for layer 3 (y03) and then I will
        %change it for the initial value of state var. in layer
        %2 (y02). to put the change, i add the diffierential
        %change on time of state variable in layer 2 (dy2/dt).
        XX.S(3)=(XX.S(2)+X.S(2))-( X.S(3));%DIN
        XX.P(3)=(XX.P(2)+X.P(2))-( X.P(3));%DIP
        XX.X(3)=(XX.X(2)+X.X(2))-( X.X(3));%chl
        SAL(3)=(SAL(2)+sall(2))-( sall(3));%salintiy
    end

```

As a main conclusion that we can extract, by comparing figures (5 and 6), is that several times of the year, there is a renewal effect in layer 3. In those moments, the layer become similar to layer 2. however, the pattern do not change greatly compared with the early solution, and there are times of the year, where the fish farm nutrient input in layer 3 become an important issue. Nevertheless, the accumulation of nutrients in layer 3 is diminished by using the upgraded version of the script Kw23.m (figure 6). This is the result of increasing the overturn rate in the diffusive term is the responsible for such change.

9 Boundary conditions

Boundary conditions belongs to one of the 3 different external types of data-sets necessary to run the dCSTT model. Those already introduced in the 3rd milestone report (Portilla and Tett, 2006) are the forcing variables and the initial conditions. The boundary conditions describe how the state variable are influenced from outside the model domain, in the case of the dCSTT model, the new state variable considered is the phytoplankton chlorophyll input from open ocean.

The dCSTT model simulates limiting nutrient and phytoplankton chlorophyll concentrations variation throughout the season. In this milestone, It has been implemented for Loch Creran because of the great quantity of data describing its hydrography and biogeochemistry. Loch Creran connects to the larger fjord Loch Linnhe, the Firth of Lorn, and eventually to the open sea. Most of the boundary conditions come from the station situated in the Greag Islands as a proxy of open ocean value for nutrients.

Following the same statistical analysis and methods described in third milestone report (Portilla and Tett, 2006), we were interested in seasonal and long term patterns for concentration of Dissolved Available Inorganic Nitrogen (DAIN), Dissolved inorganic Phosphorous (DIP) and Phytoplankton Chlorophyll (chl_a) at the Greag Islands sampling site. The available data for these variables derives from seasonal samples between 1979 and 1983 and more frequent samples from 2000 (Grantham, 1983a,b,c; Grantham et al., 1983; Fehling, 2004)² (figure 8).

Seasonal variation of nutrients was presented and studied in the previous milestone report. They will not be object of more analysis than the display of the raw values and the summarized seasonal pattern found by using harmonic regression (figure 8a)b)). However, phytoplankton chlorophyll was analysed in more detail in the context of this report. We display the seasonal pattern found for phytoplankton chlorophyll, together with the 95 % confidence interval. Because the nature of the variable, we were forced to transform phytoplankton chlorophyll in the log scale. Therefore, the envelope for the raw values (figure ??c) where asymmetrical compared to that of the transformed variable (figure ??d).

There was not found a long term trend in the concentration of chlorophyll in the boundary conditions. The figure (9) shows the predicted seasonal pattern for station LY1 in the Graig Islands for all the years of recorded samples. However, an interesting process seems to take

²Brian Grantham (SMA) was responsible for chemical measurements in 1979-1983, Johanna Fehling (UHI/SAMS during PhD studies in 2000-2003, and Celine Laurent (Napier) during PhD studies in 2003-2005

place between the early seventies compared to the recent years (2001 onwards).

Although a slightly statistically significant effect, a change in chlorophyll was observed other than a long term change. A model was fitted to the phytoplankton chlorophyll in order to account to changes in the seasonal pattern from year to year. The results showed that there is a change in the timing of the two seasonal peaks between 1970 to 2003 figure (10) . However, this change can be misleading, because there is no sufficient data in between those years to confirm the observed change.

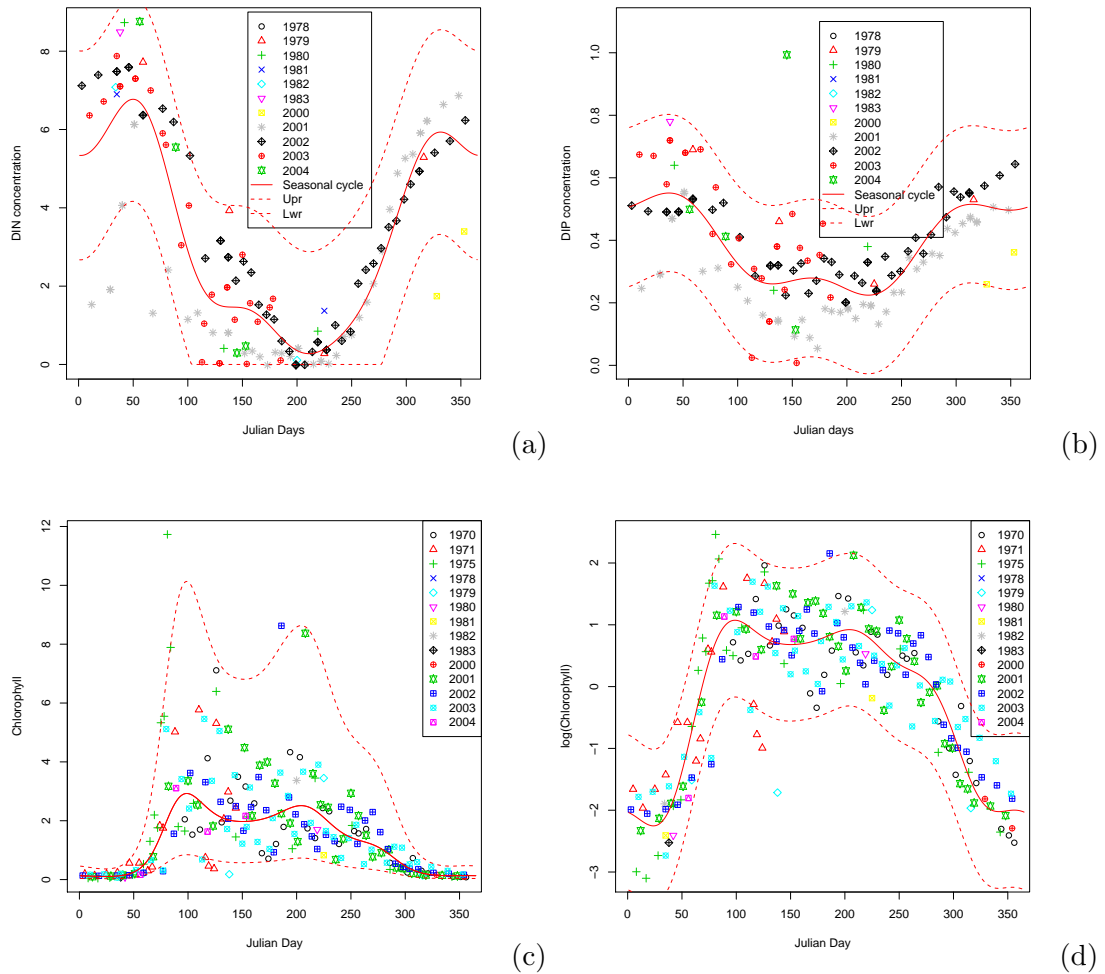


Figure 8: Boundary conditions for Loch Creran for the 3 state variables included in the dCSTT model (colored dots) and its modeled seasonal pattern (lines). a) DAIN, b) DIP, c) phytoplankton chlorophyll d) log of phytoplankton chlorophyll,

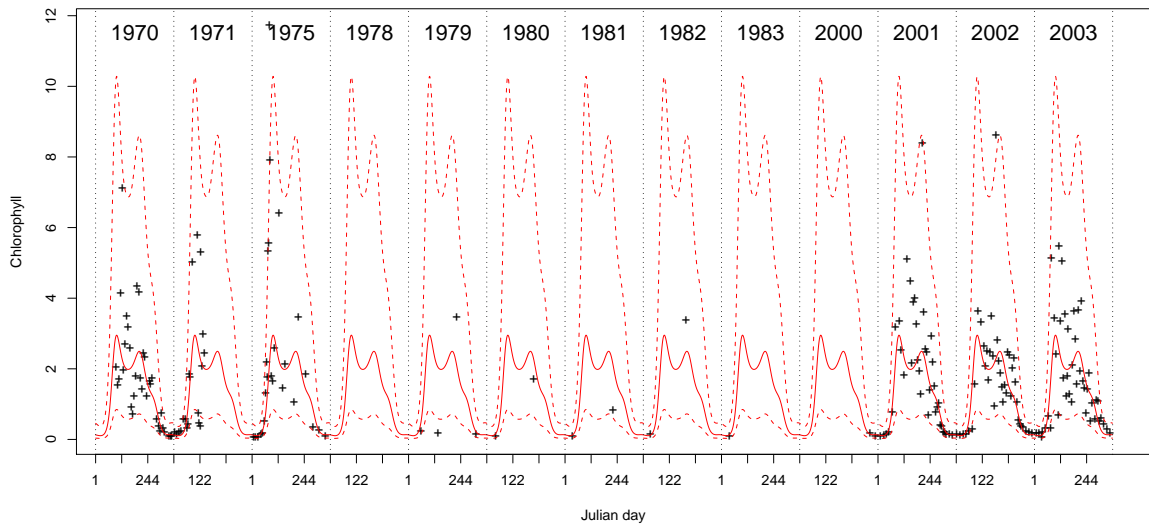


Figure 9: Time series of the concentration of phytoplankton chlorophyll between 1970 and 2001. The continuous line correspond to the fitted seasonal pattern and considering year as not having a long term trend. The dotted line correspond to the 95 % envelop of the data.

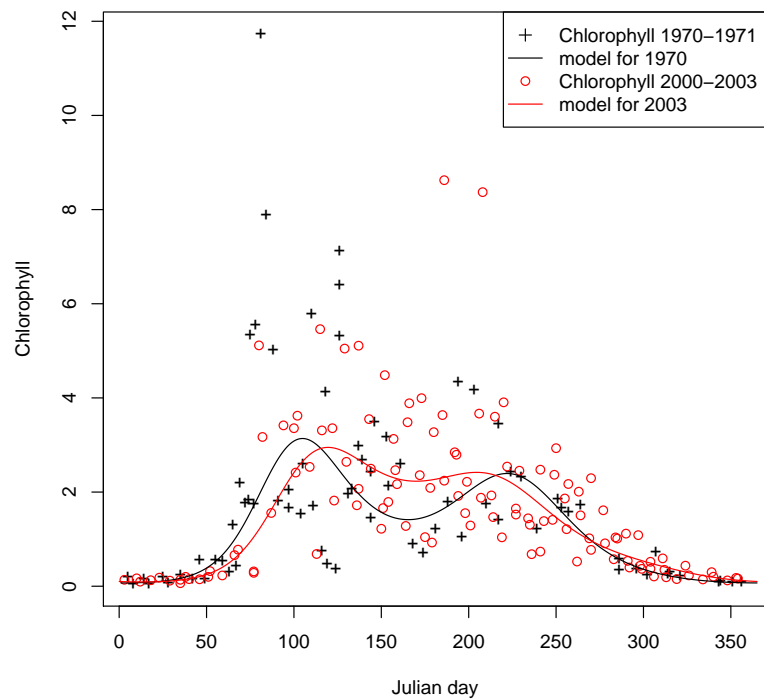


Figure 10: Concentration of phytoplankton chlorophyll in the Graig Islands for two sets of data: early seventies (black crosses) and early 2000 (red circles). Seasonal pattern in for 1970 (black line) and 2003 (Red line) is overimposed. The two continuous line correspond to the fitted seasonal pattern and considering year as interacting with the seasonal not only on the long term trend.

10 Statistical methods

In this section we describe some statistical tools used in the report. We will introduce the method employed for the assessment of model reliability, which involves regression between model and observed records. Similarly we used regression in order to evaluate the relationship between limiting nutrients and phytoplankton chlorophyll.

We also used harmonic regression for the description of seasonal patterns on boundary conditions, but its rationale was described in detail in Portilla and Tett (2006).

10.1 Model validation

Assessing the reliability of the model system described here is especially important because the system may be used to regulate fishfarming. Several statistical matters are involved:

- estimating values of model parameters from relationships between observed variables;
- testing whether a simulation is a good fit to some observations
- estimating the confidence limits of predictions made by the model system

The milestone 3 report (Portilla and Tett, 2006) described a method for testing goodness of fit that involved the regression of observed values of state variables upon values predicted by a model. This method also leads to estimates of the confidence limits of predictions. However, the use of standard linear regression requires a single, normal, distribution of errors about the Y-axis variable. Incorrect estimates of fit and confidence can result if this assumption is not satisfied. Similar difficulties also arise in the estimation of parameter values from relationships between observed values, and an example of such difficulties, and their resolution, is considered in the next subsection.

10.2 Weighted regression and estimation of weights

In this subsection we use the general form of the linear regression equation, $\hat{y}_i = a + b \cdot x_i$. Weighted regression differs from the traditional linear regression in allowing the residual errors, $\epsilon_i = \hat{y}_i - y_i$, to be heterogenous. If the variances of each y_i change at each x_i , then we can weight each observation by the reciprocal of an estimate of its variance (σ_i), as

follows:

$$(41) \quad w_i = \frac{1}{s_i^2}$$

where s_i is an estimate of σ_i and w_i is the weight introduced in the least square minimization, $\min(\sum_{i=1}^n w_i (y_i - \hat{y}_i)^2)$.

In order to weight the regression, different strategies can be chosen, which we will call methods one to four. **Firstly** we can weight the regression (figure 15) by using the absolute value of the residual from a prior model ($|\epsilon_i|$). An alternative is to group nearby observations, but the problem lies knowing how many observations to include in each group. We explored a modification of this last approach using a bootstrap (re-sampling) method on grouped samples to estimate s_i . We will call it method two. A comparison between the first approach and the last one is shown in figure (12a).

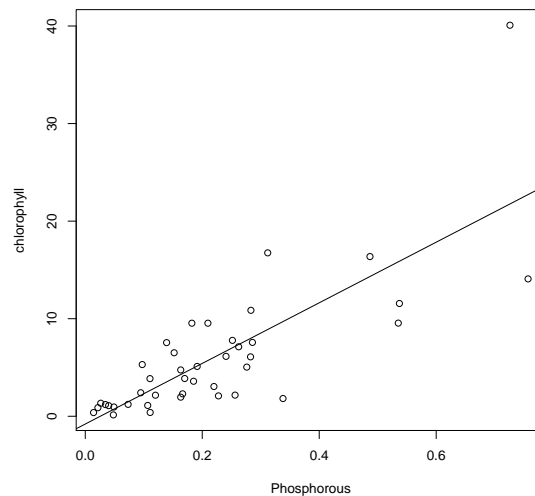


Figure 11: Chlorophyll as a function of phosphorous. The regression model represented by a continuous line is used in order to make the first estimation of the standard error of the response variable y (chlorophyll)

In **method two**, the data were grouped in bins progressively increasing numbers of samples. Within each bin, a resampling was carried out. When each resampling was complete, standard errors were estimated for each bin. To explain this in more detail, let's assume we are considering an observation in position y_2 . Firstly we chose the bin formed by the

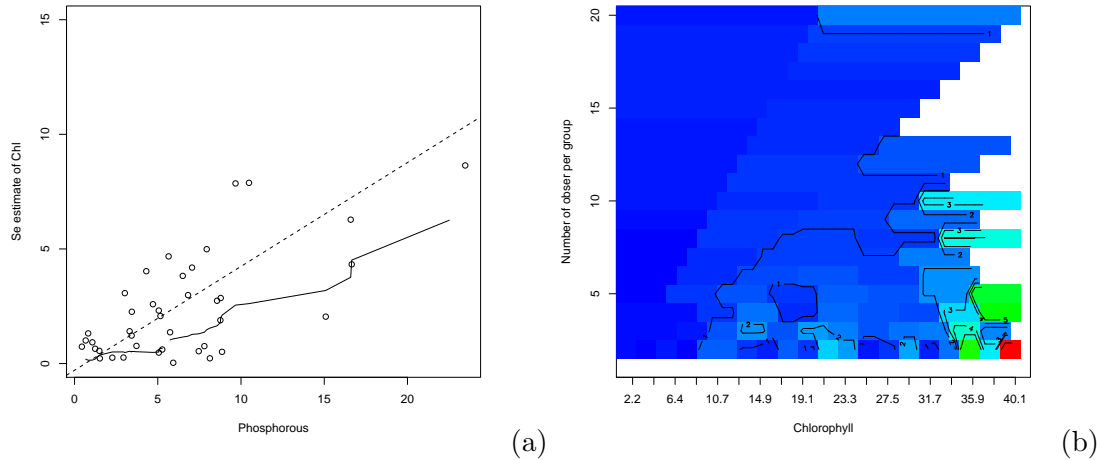


Figure 12: Standard error estimation for phosphorus using different methods. (a) methods 1 and 2: using absolute value of residuals (open circles) and grouped samples (line). A linear models is over-imposed (broken line) to relate relates absolute error ($|e_i|$) as a function of Phosphorous (Method three) (b) method 2a: using bins of progressively increasing number of samples, from 2 to 20 (y axis) for each value of Chlorophyll (x -axis)

grouped samples y_1, y_2 and y_3 . For the position y_3 , the group will be formed by samples y_1, y_2, y_3, y_4 and y_5 . Within each group the standard error, i.e. standard deviation normalised by the number of samples within group is estimated by bootstrapping. It should be noted that by using this technique the number of samples within group (inside the bins) increases until the samples $n/2$, where n is the number of observations of variable y . After this the number of samples decrease until the standard error of sample y_n is again 0.

Exploring the relationship between standard error estimated from the first linear model ($|e_i|$), we can try to formulate an equation to estimate the standard error of the response variable (Chlorophyll) as a function of phosphorous. Consequently, we will try to find a function $\sigma_i \sim g(x_i, \theta)$, where θ is the unknown parameters that link the prediction variable x and the variance of the response variable y , i.e. $\hat{\sigma}_i$.

After computing the approach number two it is valid to think that a linear model over the residuals will be sufficient. Therefore, we can assume that the standard error of the response variable increase linearly with the x variable (**method three**).

We finally used an approach in order to support the idea variance increase by grouping the variable y_i . Bins of data composed of 2, or more was grouped until each bin has a total number of observation of $n/2$. The assessment of the variance by this method

(**Method four**) is described in figure (12b), but the method was de-estimated for the final estimation of variance and the porpoise we showed it here were only to compare with the other methods.

11 The estimation of yield

11.1 Introduction

Yield was defined in a previous section as:

$$(42) \quad q = -\frac{dX}{dS}$$

If the yield is constant, then a linear relationship between observed chlorophyll concentration, X , and observed nutrient concentration, S , is to be expected, and the slope of that relationship can be used to estimate a value of q , as was done by Gowen et al. (1992). That is,

$$(43) \quad X = c - q \cdot S$$

where c is a constant. However, a difficulty in making an unbiased estimate of q is that the response variable, chlorophyll, X , has a clearly skewed distribution, with the scatter of values increasing with the mean value. Another way to state this problem is that the predictive errors in X , given by:

$$(44) \quad \epsilon_i = \hat{X}_i - X_i$$

are not homogenous - that is, not drawn from a single normal distribution. Since the postulated linear relationship between X and S prohibits transformation of X , we instead used weighted regression to deal with this problem of heteroscedastacity.

11.2 Estimation from field data

We performed multiple regression of chlorophyll as a function of the 3 limiting nutrients in the Graig Island Station (LY1), in order to estimate yield of phytoplankton from nutrients. We followed a similar strategy to that of Gowen et al. (1992).

In Gowen et al. (1992), data of chlorophyll concentrations from Scottish sealochs were regressed successfully with nitrate with decreasing slope. The estimate absolute value of the significant estimated t slopes represented the yield (q) of chlorophyll from nitrogen assimilable by microalgae. The median value there estimated was 1.05, however, the range of observed slopes were from 0.25 to 4.4.

We now concentrated in a more restricted area (only the Firth of Lorn) with a much limited quantity of data. This might cause that the differences will only be caused by the inherent variability. Moreover, we divided up the data set into two groups as a function of year: 1) early data, which is the smallest data-set, composed by 8 samples taken between 1970 and 1980, 2) the recent data, composed by 73 samples taken between 2000 onwards. For the second data-set, only data between March and October were analysed since they suppose to contribute in phytoplankton growth under no light limitation.

The estimations of yield by multiple regression were optimised by using weighted regression (section 10.2). The weights used here are simply the absolute of the residuals from a previous fitted model. We could have used other type of approach in order to estimate the variance of the response variable, chlorophyll. Nevertheless because there are involved several covariates in the modelling procedure, we decided to use the simplest of all the methods proposed. Indeed, it is more difficult to estimate a function involving the 3 variables than one only composed by a single covariate.

The modelling framework postulated here included more limiting nutrients apart from DAIN. Any process that limits growth other than nitrate availability, result in diminution of yield. We tried to include other factors which contribute to that diminutions. Clearly the slope estimates changed by the inclusion of some of those factors.

We would like to believe that although the data analyzed here is smaller than that of Gowen et al. (1992), they predicted the specific contribution of each nutrient to the phytoplankton growth when information on covariates is included.

Yield of phytoplankton from nitrogen estimated to be equal to 0.85 ($se = 0.0963$) in the early dataset is equal to 0.51 ($se = 0.12$) for the late years. Although the estimated values were within the range of the study by Gowen et al. (1992), they are slightly lower. Besides, the estimation of yield from nitrogen in the recent data-set was the only to be statistically different from that of Gowen et al. (1992).

For phosphorous, the estimation of yield was 13.90 ($se = 0.62$). This estimate was only possible to compute from the data collected in the 70's and 80's. Yield of phytoplankton from phosphorous, was not possible to perform for the recent data. The value obtained was not statistically different from zero, so the number here presented lacks of any value.

Gowen et al. (1992) also found non significant slopes that related nitrogen and chlorophyll. This might be the case shown here, where the lack of significance is a legitimate outcome, only due to nature variability. However, the differences in the values of yield might be also

Table 1: Estimated yield of chlorophyll from 3 limiting nutrients in the Graig Islands between 1970 to 1980 and 2000 to 2000.

Nutrient	Estimate	Std. Error	t value	Pr(> t)
<i>Historic data: 1970-1980</i>				
(Intercept)	7.1705	0.2235	32.08	0.0001
DAIN	-0.8548	0.0963	-8.88	0.0030
DIP	-13.8994	0.6223	-22.34	0.0002
DAIN:DIP	1.6661	0.1402	11.89	0.0013
<i>Recent data: 2000-2003</i>				
(Intercept)	4.6135	0.1235	37.36	$p < 0.0001$
DAIN	-0.5104	0.1208	-4.22	0.0001
DIP	-1.4063	1.1045	-1.27	0.2074
Si	-0.6611	0.0937	-7.06	$p < 0.0001$
DAIN:DIP	0.9038	0.2807	3.22	0.0020
DAIN:Si	0.0048	0.0262	0.18	0.8559
DIP:Si	0.2979	0.3443	0.87	0.3900

caused by differences in the compositions of populations that grow in the Firth of Lorn. This change was also supported by the swift on bloom timing highlighted in section (9)

We do not have clear the contribution of the interaction terms in the yield estimation. factors associated to the interaction terms are always positive. Statistically, express the increase on the response variable (chlorophyll) when there is a simultaneous increase of both values involved in the interaction term. We might postulate, that this term is the responsible for the cell growth in in a small time scale. An increase on the concentration of the source nutrients, might cause the increase on the concentration of chlorophyll in a first step. Thereafter, the main process that will take place is the reduction of nutrients as a result of this growth of algae.

As a result of the figure here analysed, higher concentration of nutrients will not forcibly mean high concentration of chl_a but more complicated interaction. In figure (13) we display graphycally this interaction for the data collected between 2000 and 2003 in the Graig Islands.

It should be noted that the inclusion of silicate was not possible when estimated the yields for the early data (table 1). Although Silicate concentration was measured together with phosphorous and nitrate, the small amount of samples obliged us to restrict the number of cofactors to use in the model (low degrees of freedom available).

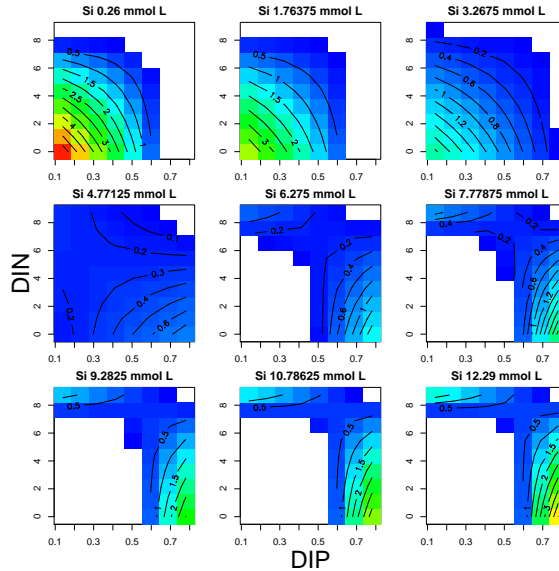


Figure 13: Predicted concentrations of chlorophyll at different levels of Nutrients (DAIN, DIP and Si), using a linear model allowing interaction of the 3 terms

11.3 Re-estimation of q^P from Tett et al. (1975)

By reanalyzing the field data published by Tett et al. (1975), we recompute several values of yield of chlorophyll from phytoplankton.

In those studies particulate phosphorous in the water column was estimated by a chemical method. Thereafter, It was estimated the part of this particulate phosphorous corresponding to detritus, i.e. non-living material. Consequently, the reminding particulate phosphorous measured in the samples was attributed to particulate phosphorous in the phytoplankton cells.

The estimation of chlorophyll yield is made by simply dividing the observed concentration of chlorophyll by the concentration of phosphorous in the cells. The rationale behind this operation follows the cell quote theory described by Droop (1983).

The histogram of the observed values of yield by computing the previous division is shown in figure (14). Two different values of yield can be extracted from this distribution: a) the mean value equivalent to 27.08 ($se=2.34$). b) the median value equivalent to 25.51(IQR=17.04, which is the difference between quartiles 0.25 and 0.75)

Alternatively to the measures of frequency of yield (figure 14), we can estimate this parame-

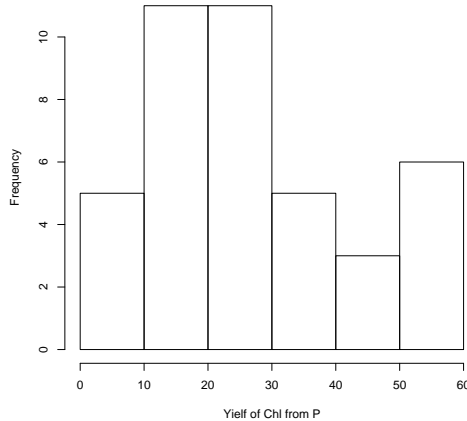
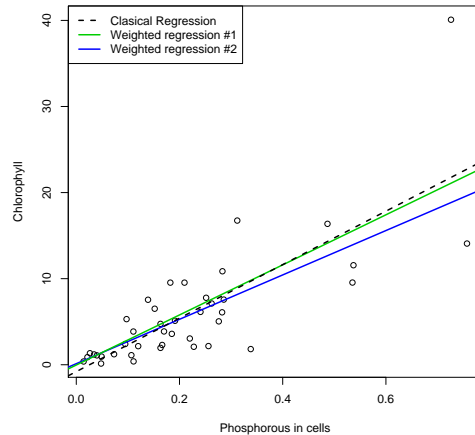


Figure 14: Histogram of estimated values of yield of chlorophyll from phosphorous from Droop (1983)

ter by regressing the concentration of chlorophyll in the water column and the concentration of phosphorous in the phytoplanktonic cells (figure 15). This can be done by assuming that there are concentration zero of chlorophyll in the water column when the concentration of phosphorous is zero in the cells (Do not allowing the linear model to use an intercept different from zero). Alternatively, we can make an allowance for the regression model to estimate an intercept different from zero.

When we do not make allowance for an intercept, the estimated slope of the model correspond to a value of yield equivalent to 28.8 ($se=2.47$). In opposition to that, when we make allowance for an intercept the estimated value was 31.07($se= 4.00$). Both estimates of yield are not statistically significant different amongst them, neither they are from the previous estimated values.

Likewise when using weighted regression (figure 15), the differences weren't specially big. The estimates of yield with weighted regression and approach 1 was 29.08 ($se=0.35$), whereas the estimated using approach 3 was 25.78 ($Se=2.99$). The standard error associate to the estimation indicates that the yield of Chlorophyll from phosphorous using Tett et al. (1975), can be taken between 25.78 and 31.07.



(a)

Figure 15: Regression to estimate yield of phytoplankton from phosphorous in phytoplankton cells by using linear regression (black broken line) and weighted regression (blue and green lines). The two examples of weighted regression correspond of methodologies 1 and 3 from section 10.2

11.4 Estimation by iteration

As introduced before, the estimation of the yield of chlorophyll from nitrogen was estimated by means of an iterative technique. The software R (R Development Core Team, 2005) was used to Determine the nonlinear least-squares estimates of the model parameter q^N .

Firstly, we performed a simulation for Loch Creran in 1975. The value of q^P was set initially to 30 and the fluxes involved in the dCSTT model were stored separately. Once we have all these information, Field data for 1975 was rearranged to display the daily change of Phosphorous in the upper layer. We set this as the response variable. The response variable will be composed by a combination of fluxes (equation 20) and a value of q^N such as minimise the least square estimate. This is done by iteration within the routine `nls` (R Development Core Team, 2005).

Then the new estimate of q^P will be set as the initial value for the yield in order to run the dCSTT. Once the fluxes are stored, the new estimation of q^P using `nls` is computed. This will be done until the value stays stable (figure 16).

The starting value of the simulation was 30. The following computed yield was estimated to be 44.93 ($se = 16.44$). The second try produced an estimate of yield equal to 48.79 ($se=16.44$). Finally the third estimate of yield was equal to 49.05 ($se = 16.41$).

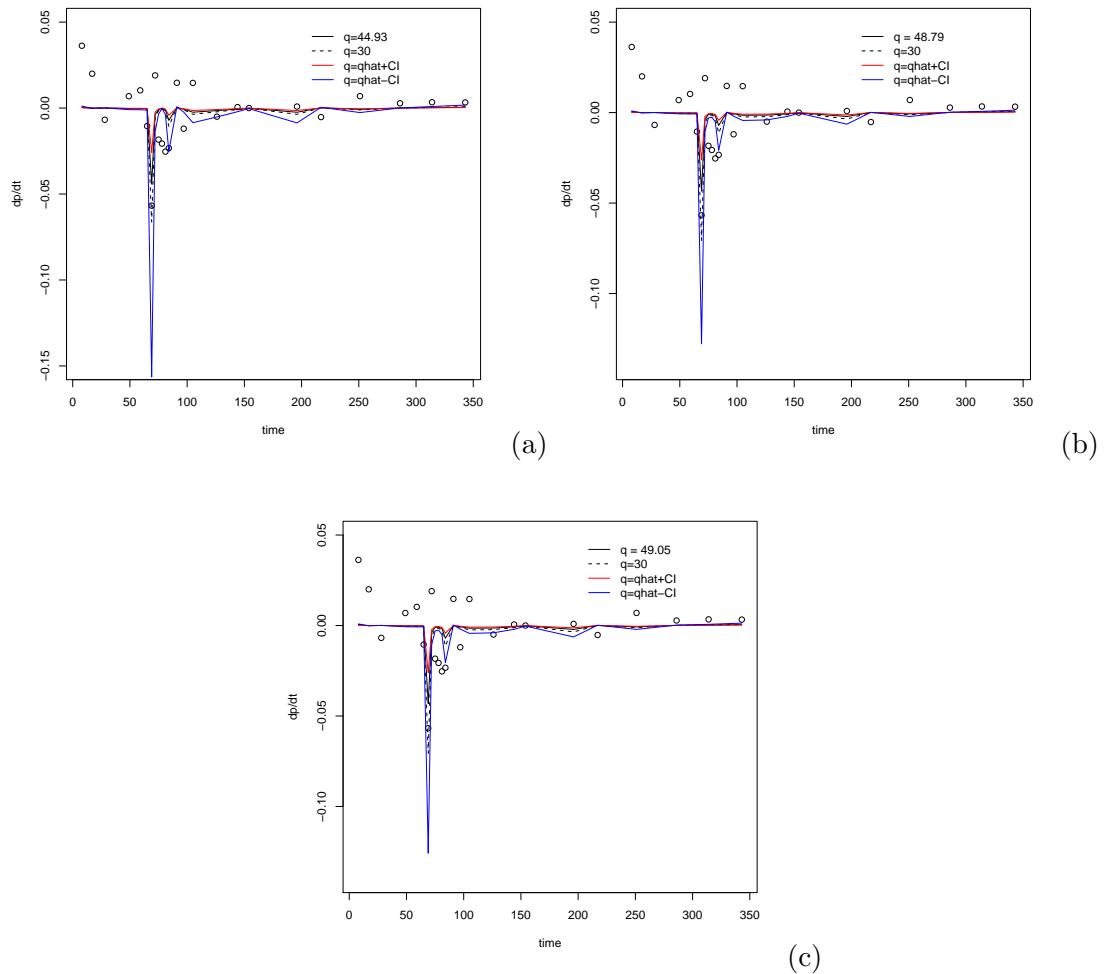


Figure 16: Estimation of q^N by iteration using non linear least squares. Open circles represent the observed daily variation of phosphorous in loch Creran in 1975. Several values were tried until the value seems to stays stable at the value of 50. In all the panels the predicted daily variation of phosphorous with the reference value of q^P equal to 30 (typical value for fresh water algae) is displayed (broken black line): a) predicted daily change with yield equal to 44.93, b) predicted daily change with yield equal to 48.79, c) predicted daily change with yield equal to 49.05.

12 Results for loch Creran

12.1 Model realizations

For years 1975 and 2003 we run the dCSTT model in order to compare predicted and observed chlorophyll, DAIN and DIP, with conclusions about model reliability and sources of error (figure 17). The list of parameters used for the two years is displayed in table (2).

Table 2: default

Parameter	matlab script	1975 Value	2003 Value
q^N , Yield of nitrogen	Biology.m	30	16.2
q^P , Yield of phosphorous	Biology.m	1.1	0.7
L_0 , Loss rate	LossRate.m	0.1	0.2
K_{wd} , background diffuse attenuation	SubmarineOpticsF.m	0.214	0.5

The main lecture we can extract from the simulations performed is that the dCSTT model performed a relatively good fit for year 1975 (figure 17a), when the fish-farm was not established. However, the simulation for the year 2003 (figure 17b), predicted an overall too high concentration of chlorophyll. There is also a peak on the concentration earlier in the season than that compared to field data. This caused a depletion of limiting nutrients more quickly than that observed in the field data.

Several coefficients were changed with table (2) a notable improve on the predictions when compared with the previous simulation for 2003 (figure 17c).

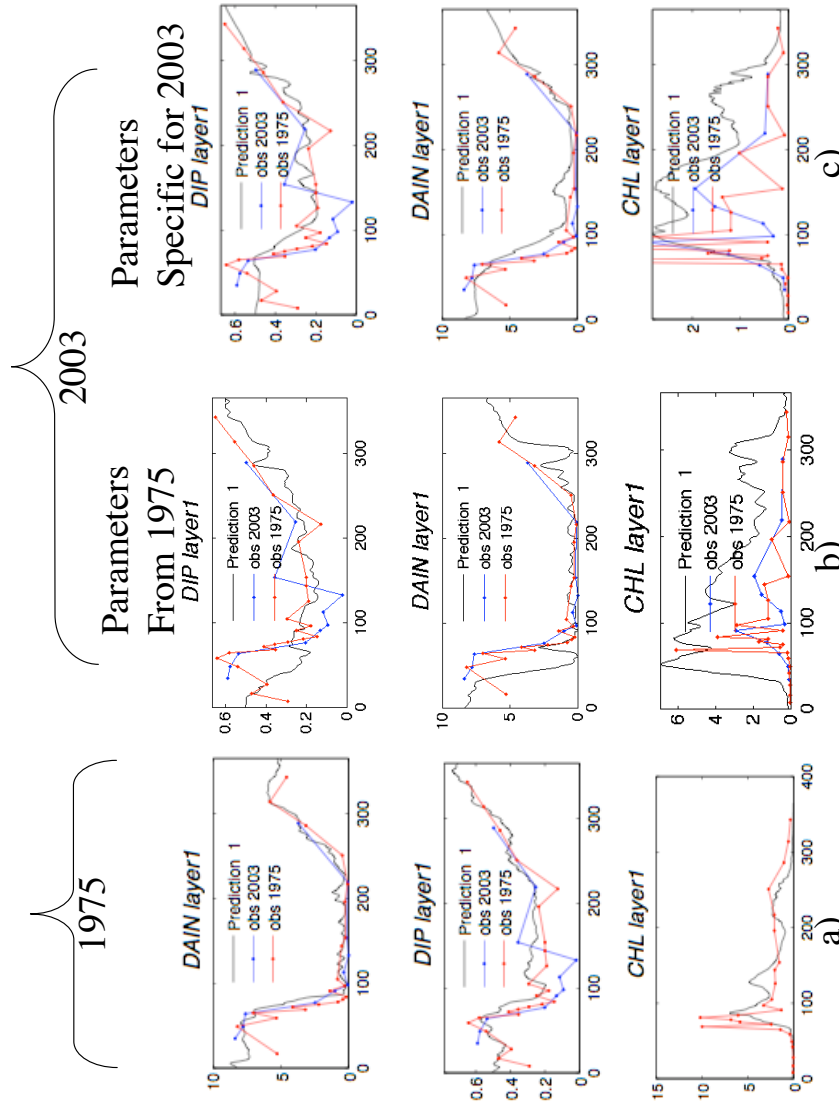


Figure 17: Realizations of the dCSTT model for DAIN, DIP and phytoplankton chlorophyll in years 1975 and 2003. Simulation for 2003 (b) was made firstly with the parameters used in 1975 (a) and a new set of parameters described in table (2) (c)

12.2 Comparison between model and data

The dynamic cstt model was run using forcing data from 1975 using a constant exchange rate. This result is similar to that of Laurent et al. (2006), because the new physical ACExR routine was not employed. Nevertheless the conclusion extracted from examining that realisation can be also applied to that of the dCSTT model coupled with the ACExR model. Here only the state variables Chlorophyll and DIP were compared against field data. In the following sections, we aim to assess whether or not there is a relationship between what was modelled for Chlorophyll and DIP in Loch Creran in 1975 and what was actually measured in that year.

We want to set the criteria to evaluate models in function of the scores on the different goodness of fit values for the linear regression. Models will be classified as Excellent, good, fair or poor, as a function of : (1) values of slope and intercept of the regression, (2) performance in Percentage of variance explained (r^2)

- 1 **Excellent:** When Slope and intercept are not significant different from one and zero respectively. the r^2 value should be is reasonable high
- 2 **Good:** When the slope or intercept are different from one or zero, but one at a time. The r^2 value is high but does not reach the levels of an Excellent model.
- 3 **Fair:** When neither the slope or the intercept are equal to one nor zero. however, The slope should be significant different from zero and the r^2 value is high but does not reach the levels of an Excellent model.
- 4 **Poor:** When slope is not significant different from 0 , or the variance explained (r^2) is lower than zero.

The dCSTT prediction for loch Creran in 1975 is shown in figure 18. Visually, we can argue a fair agreement between observed values and prediction in the time series. Trend was captured for both chlorophyll and DIP consistently with peaks in spring and autumn for chlorophyll and high concentrations during winter, and low during summer and spring for DIP .

Assessment with linear regression

Several models are fitted here (Table 3). Firstly, a fit of the row numbers was computed for Chlorophyll and DIP. Later a transformation in the log scale was performed for Chloro-

phyll.

For Chlorophyll, when compared with field data the first model summary indicates both coefficients estimates (β_0 and β_1) are different from 0 and the slope different to 1 (t -test $p < 0.001$).

For non transformed values of Chlorophyll, not only the model fails to provide prediction in low values, but also there is a difference in the output proportional to the actual measured value. The higher the model value estimated, the lower the real observation is. Nevertheless, a fair amount of variance is explained by the model and the slope is significant different from 0. Therefore we classify it as a **fair** model.

When the observation and model outputs are both log-transformed, the slope is significantly different from 0 (t -test $p < 0.001$, and the intercept (β_0) do not differ from 0. When removing the intercept, the new model possess parameter β_0 is different from both, 0 and 1 (t -test $p < 0.001$). Therefore, if data is log-transformed, we could classify the model for chlorophyll as a **good** model.

By log-transforming data analysed, model and observations agreement increases to provide consistent estimates. However, the fact that the slop is not equals to 1, indicates, that there is a proportion of the value which is missed consistently from the model. Also note that the fact that the model prediction and field data are transformed indicates a certain degree of failure from the model to predict Chlorophyll.

For DIP, the regression indicates a fair agreement between model output and field data (Table 3). The intercept of the regression indicates a value different from 0. The slope is different from both 0 and 1 ($p < 0.001$), and its value is even higher than that of non-transformed chlorophyll. Nevertheless the coefficient of determination r^2 is lower for DIP (0.291) than it is that of Chlorohyll (0.647). We therefore classify this model as **fair**.

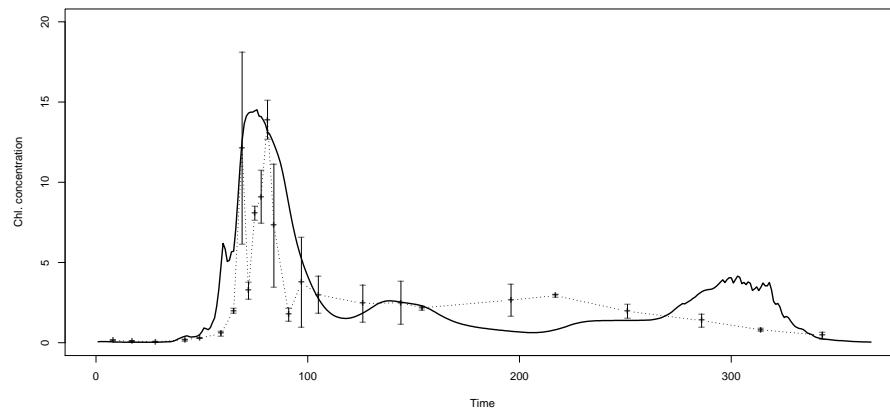
Envelope

Once the linear regression has been done, It can be possible to draw an envelop that contains a certain percentage of the sampled population. Figure 20, show the interval containing 95 % of the bulk of observations and CSTT model predictions. Note in this time all available field samples was used, instead of using standard errors (Figure 19 and 18).

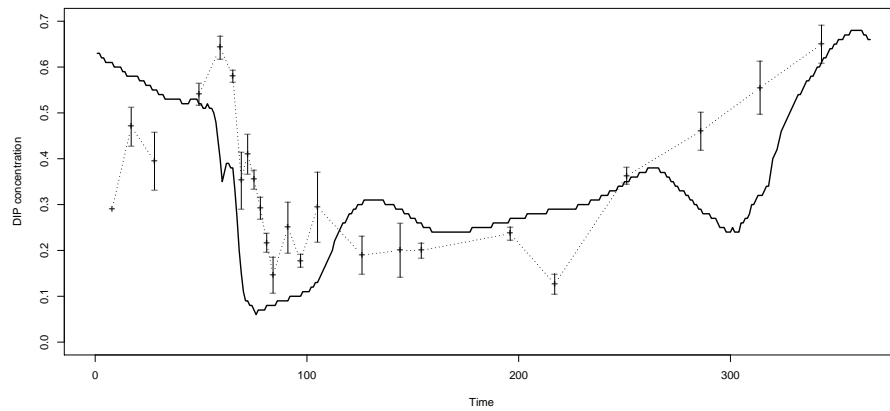
Note the differences in area estimated for both variables. Although the envelop drown for

chlorophyll seems to show a clear seasonal pattern, the wider envelop observed for DIP it can be a cause of concern.

To illustrate this problem we propose an example. Lets assume that we want to predict DIP value for Julian day 130 (Figure 20d). The model output predict a low value for DIP when compared with the seasonal cycle. Now it can occurs that we observe a value of DIP of 0.6, which is the second highest value. This observation will be included within the predicted bounds and will be taken as part of the inherent variability. Therefore any peak occuring at this time of the year and with this level, will be missed out by the model. This is a clear example where both, high variability and mismatch between predicted and observed values (i.e. circa julian day 300), decreases performance of a model.



(a)



(b)

Figure 18: Modelled vs Observed Chlorophyll concentrations a) and Dissolved inorganic phosphorous b) in Loch Creran expressed as a function of time

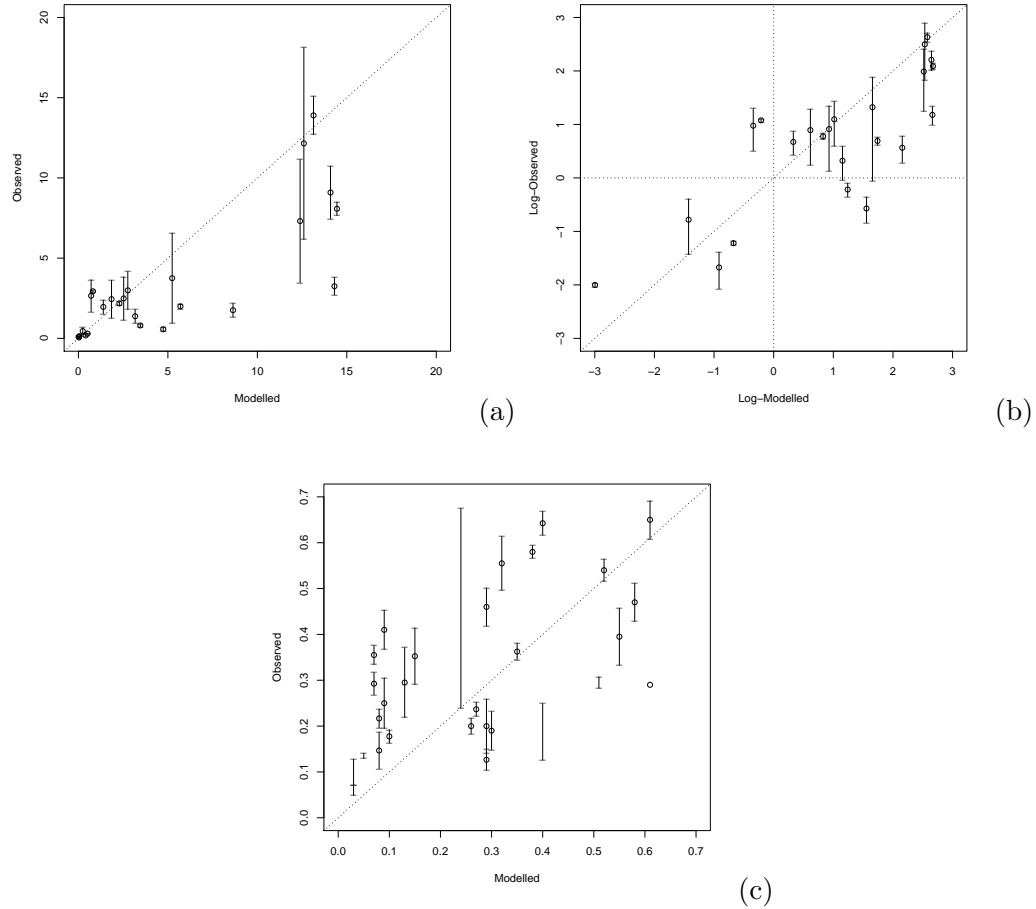


Figure 19: Modelled vs Observed Chlorophyll concentrations in Loch Creran expressed as 1:1 relationship of raw values (a) 1:1 relationship of log-transformed values (b) . Modelled vs Observed DIP concentrations (c)

Table 3: Assessment of cstt model outputs and observation by linear regression. A linear model is fitted investigating the 1to1 relationship. For the classification of model in classes, see Portilla and Tett (2006)

Model	Estimate		Standard error		Case
	β_0	β_1	β_0	β_1	
<i>Chlorophyll</i>					
$Y = \beta_0 + \beta_1 X$	0.110 **	0.373***	0.037	0.087	case 3
<i>Log Chlorophyll</i>					
$\log(Y) = \beta_0 + \beta_1 \log(X)$	0.341*	0.709***	0.160	0.093	case 2/3
<i>DIP</i>					
$Y = \beta_0 + \beta_1 X$	0.144 *	0.74***	0.055	0.186	case 3

Note: $p < 0.001$ ***, $0.001 < p \leq 0.01$ **, $0.01 < p \leq 0.05$ *, $0.05 < p \leq 0.1$ •

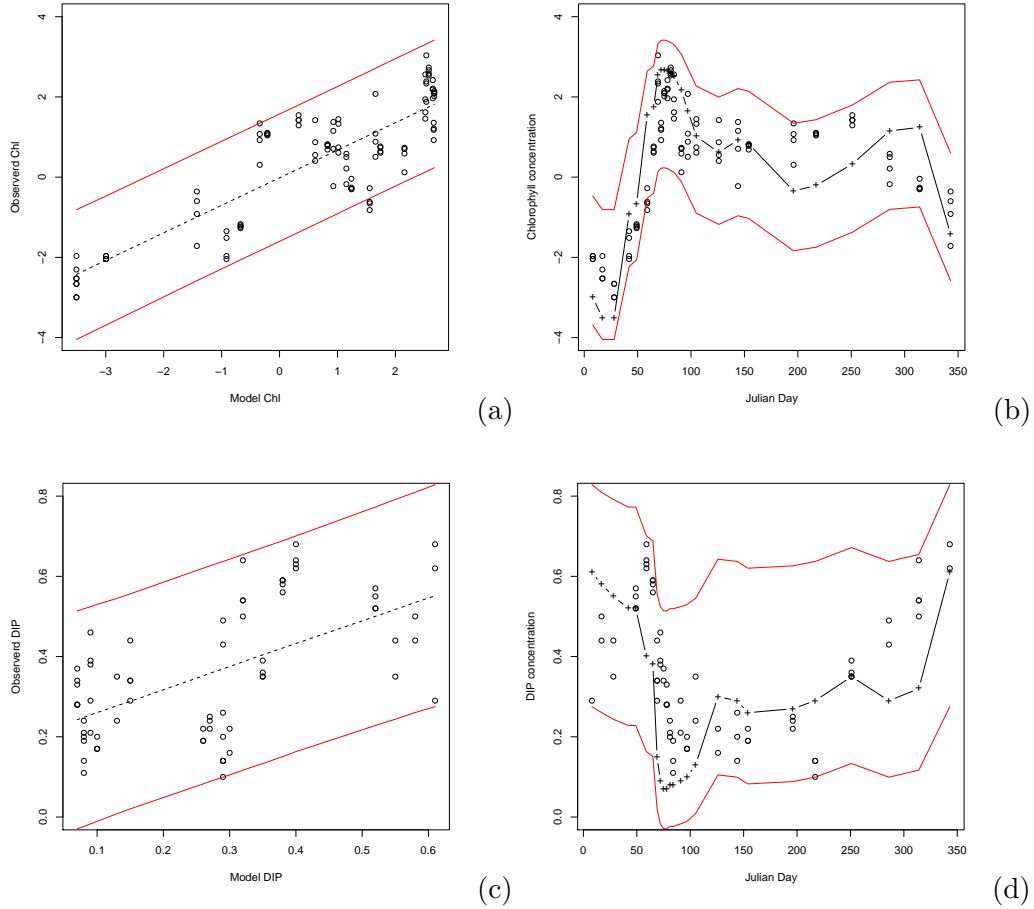


Figure 20: Prediction bounds containing 95% of the data made of bootstrapping all the data available (replicates) and fitting a linear model each time. a) Modelled Log-transformed Chlorophyll data as a function of observed data are represented by circles. Prediction interval (wider bound) and predicted line (discontinuous line) are also displayed b) For the time series of log-transformed Chlorophyll, once the bound (Red line) was computed for each modelled value, it is placed in time, and the interval is drawn. Time series of Model prediction (continuous thick line) and field data (circles) are also over imposed. c) Same as a but for Modelled data of DIP as a function of Observed values. d) same as b) but with time series of model predictions for DIP and field observations.

13 Assimilative capacity

In this section we begin to consider how the models developed during this project may be used to estimate the capacity of sea-lochs and voes to assimilate the waste from fishfarming.

13.1 Introduction

The assimilative capacity of a sea-loch, voe or coastal water is its ability to absorb the waste products associated with mariculture without harming the local marine ecosystem or the farmed fish. It is undesirable to measure harm by allowing it to happen and observing it, because it may be difficult for the marine ecosystem to recover quickly from the damage. The mathematical models developed by this project are tools that allow potential harm to be predicted, and avoided. Such prediction can be made either as part of the processing of licensing a site, or as part of site management.

The models simulate changes induced in water quality variables by fish farm wastes. The final objective of this project is an **L-ESV** (Loch - Ecological State Vector) model, in which the variables are: the concentrations of dissolved plant nutrients (dissolved compounds of nitrogen, phosphorus and silicon) and dissolved oxygen; the transparency of seawater; the amounts of phytoplankton (measured as chlorophyll) and the balance between the two main types of phytoplanktonic micro-organisms. So far we have added dissolved nitrogen and phosphorus nutrients (in the sECE model) and phytoplankton chlorophyll (in the dCSTT model reported here) to the physical ACExR model.

A generalized strategy for model use is shown in the diagram.

This diagram is based on the DPSIR (Driver-Pressure-State-Impact-Response) concept of anthropogenic impact on ecosystem. The causative agent of ecosystem change is the ecological pressure, measured by an indicator that could be a measure of nutrient loading; the (undesirable) effect of this pressure appears as changes in an impact indicator, such as the amount or composition of phytoplankton. The modelling work is aimed to provide information about the pressure-impact relationship, shown by the thick dashed line, together with an estimate of uncertainty in this relationship.

In addition to the modelling results, it is necessary to have some externally-defined **Eco-QOs** (Ecological Quality Objectives), which can be translated into (impact) Ecological Quality Standard (**EQS**). One such standard is shown as a horizontal line that should not

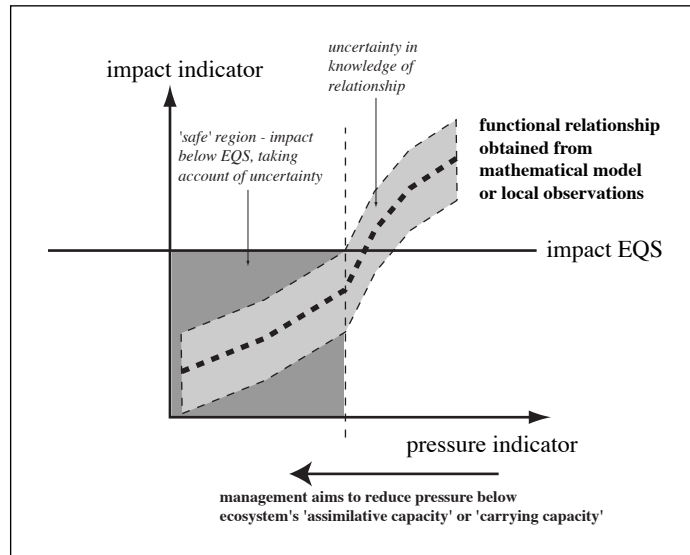


Figure 21: The relationship between ecological pressure and impact indicators can be quantified by models, which thus provide a tool for managing pressure in order to avoid breaching Ecological Quality Standards

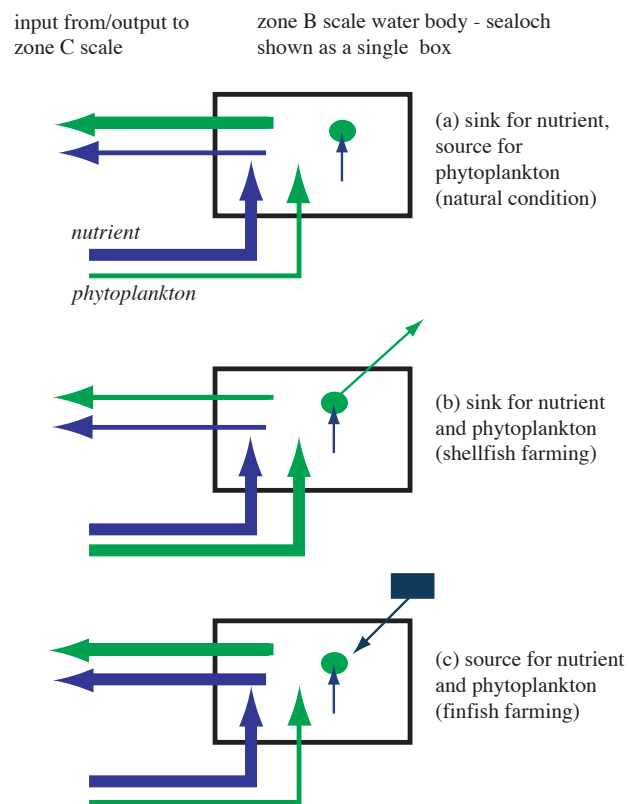
be transgressed - that is, the regulator who consents to a fish farm development, or the manager who runs the farm, should ensure that the impact EQS is not exceeded.

This raises the question of how the EcoQOs are to be defined. There are some existing standards (such as the CSTT's upper limit of 10 mg chl m^{-3} in summer) which are being altered and extended by work for the WFD and OSPAR. In addition, the modelling work itself may provide some insights into 'natural' rather than purely human-defined standards, by drawing on concepts of ecosystem health and disturbance as discussed by Tett et al. (2007).

The next subsection gives some examples of pressure-impact relationships, and the final subsection addresses the question of disturbance to ecosystem health. Both parts are work in progress, and the ideas will become better developed as the project moves towards completion.

13.2 Undesirable disturbance

How will we define the health of a system? One way to answer this question is to consider how the input and output of nutrients can change the system (figure 22).



Perturbations of RRE ecosystems by mariculture:

Impacts become undesirable when condition (a) is substantially changed to (b) or (c). (Combining (b) and (c) might restore (a)).

Figure 22: Sources and sinks and definition of undesirable disturbance

We can analyze the system seasonally, when most of the variation occurs. At this stage we might define what New production and old production is in terms of nutrients and phytoplankton. New and old production relates phytoplankton growth to two different sources of nutrients and times of the year. On the first hand, New production stands for the growth of phytoplankton in arrives in spring and it is based on the availability of nitrate external to the system. On the other hand the old production is based on ammonium remineralised from to in nitrate and nitrite, in the summer.

In open systems when there is not external input of nutrients and the growth of phytoplankton depends exclusively from the external input from the platform (mainly in spring) or the local remineralisation (mainly in summer), there are different moments and time scales where an equilibrium or steady state is achieved. We define equilibrium when the increment of a variable over a fraction of time is zero.

Steady state situations occurs over the time scale of one year, when uptake and removal of any state variables is balanced and reset to the original conditions (figure 23). Steady state also occurs during the summer when remineralisation is balanced out by the growth of phytoplankton and vice-versa. Any modification of both steady state situations can be defined as a undesirable disturbance.

An undesirable disturbance situation can be experienced when there is a local input of nutrient that become more important to what naturally observed (figure 24). For instance, during the summer when the external inputs of nutrients due to natural conditions is very low and its only source is local regeneration, any loading such as those of the fish farm can become an issue. Steady state is violated and there is an value of the ratio $\delta Y/\delta t$ higher than 0 for nutrients followed by the subsequent effect in phytoplankton.

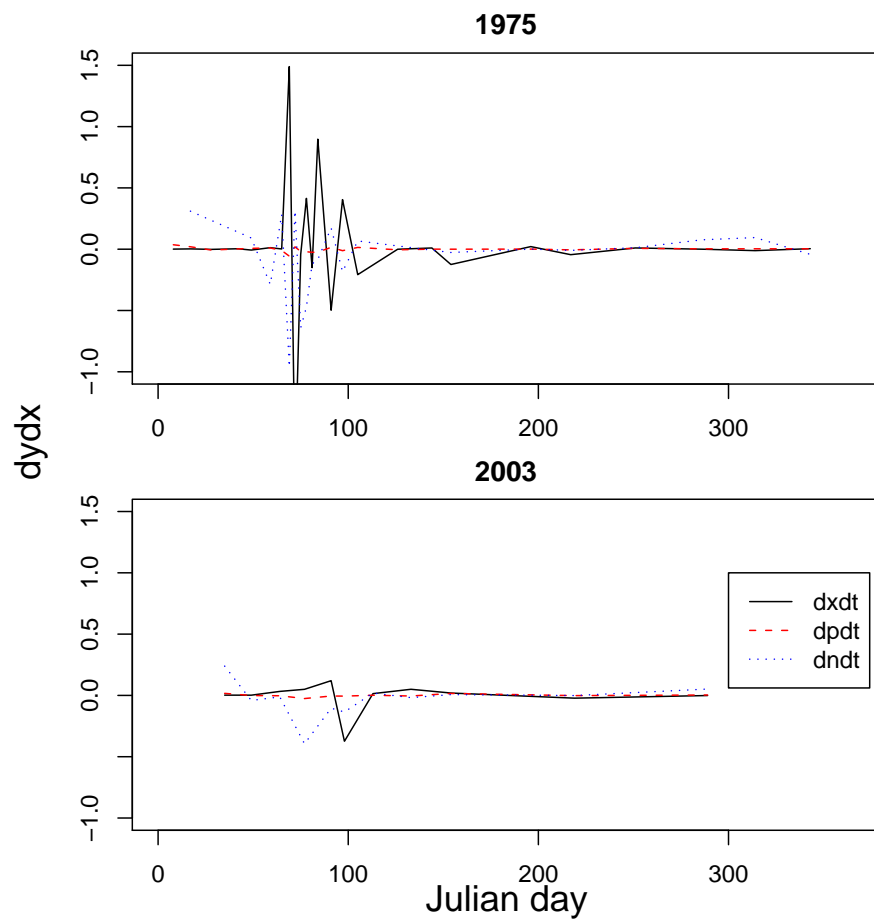


Figure 23: Seasonal variation of the balance equations for the three state variables studied in the context of the dCSTT model. The two panels represent field observation in 1975 and 2003 in the upper layer of Loch creran. The three state variables employed are: Chlorophyll (black line; $dxdt$), DIP (red broken line, $dpdt$), and DAIN(green pointed line, $dndt$).

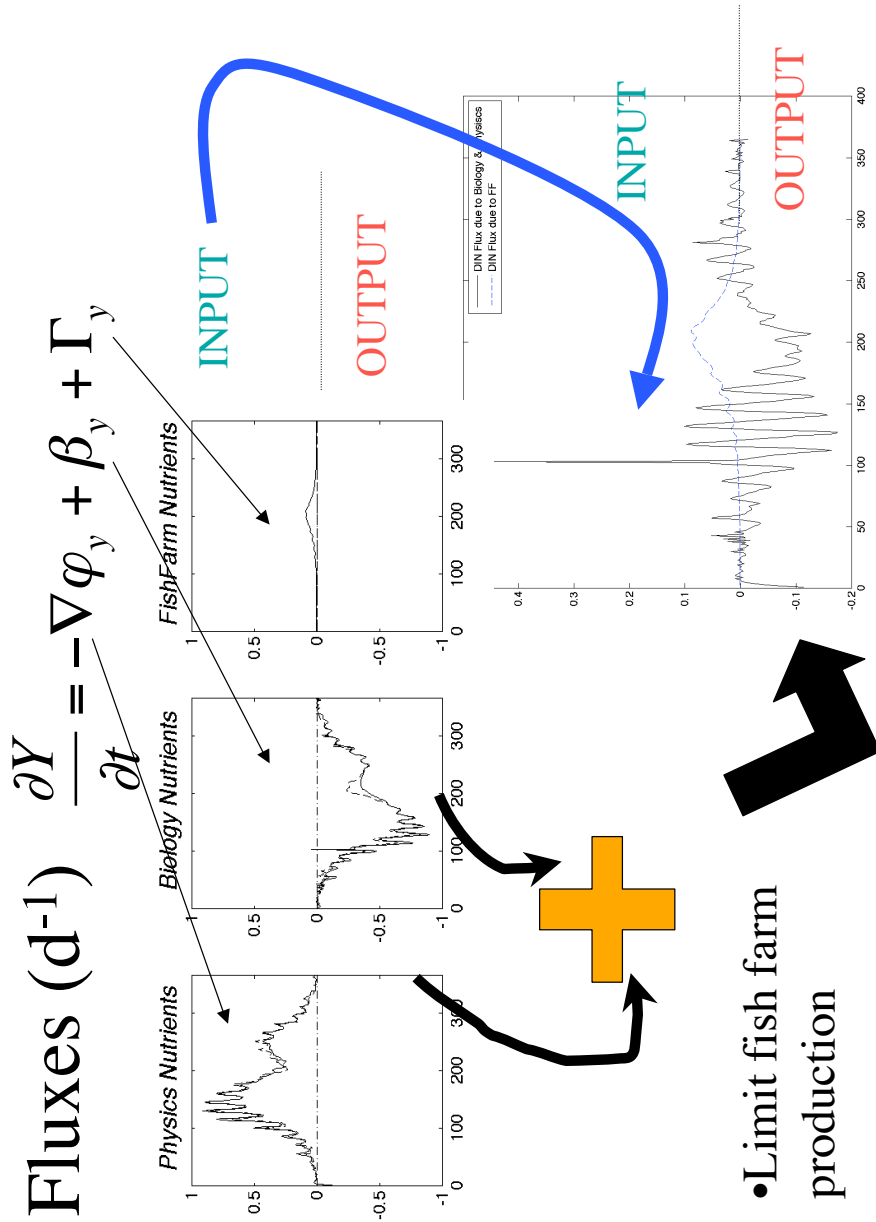


Figure 24: Display of different fluxes contributing to the Seasonal variation of the nutrients state variable. this figure tries to emphasize the relative contribution of each flux as stated in section (1) to the final value of nutrients and the effect than the fish farm has in summer.

14 Discussion

We think that something is happening between 1975 and 2003. To begin with, The model was not able to predict similar values for 2003 using the same parameters than in 1975. Secondly, although the model is able to fit seasonably well the data for 1975, it is unable to predict correct values for 2003. Finally, whatever the combination of parameters is, in order to make closer predictions, there is an overall overestimation of chlorophyll in Loch Creran.

Direct observations also confirm this issue. There is less chlorophyll in Loch Creran in 2003 than it was in the seventies.

We have started to identify where the difference might be between both years. Also we introduced different approaches in order to estimate parameters. However, they are not definitive and need the inclusion of other state variables such as Silicate and to differentiate the phytoplankton population.

We might want to identify different causes for this. It is unfeasible to differentiate clearly cause effect mechanisms. One is possible cause is the difference in the nutrient relative proportion between both years. This relationship has not been showed within the context of this milestone report. Nevertheless a clear change on pattern has been observed. This might be corroborated by the fact that timing on phytoplankton blooms has changed between the early seventies and the early 2000.

However, it is not clear if this change in proportion is caused by the change in the phytoplankton number/proportion/timing or vice-versa.

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