A dynamic CSTT model for the effects of added nutrients in Loch Creran, a shallow fjord

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Abstract

Despite a tendency for the complexity of physical–biological models to increase, simple coupled models remain useful for some applications and can provide insights into crucial links between physical and biological processes. This argument is illustrated with an account of a simple 3-box model intended to help assess the capacity of fjords to assimilate nutrients from fish farms. The model, a dynamic version of the UK “Comprehensive Studies Task Team” (CSTT) steady-state model for eutrophication, was applied to Loch Creran (Scottish Western Highlands) and was implemented using Stella 8 and tested using historical data from 1975 (before the installation of a salmon farm) and field data collected in 2003, during the period of operation of the farm. The model’s biological state variables are chlorophyll, dissolved inorganic nitrogen (DIN) and dissolved inorganic phosphorus (DIP), and it includes a simple run-off model to convert rainfall into river discharge. The physical processes involved in exchange between the loch and the adjacent waters of the Firth of Lorne were parameterised as a constant daily exchange rate.

Between 1975 and 2003, local inputs of nutrient increased but, despite this, there was little apparent increase in nutrient concentrations in the loch, and observed chlorophyll concentrations decreased substantially. Model simulations of chlorophyll and DIN agreed well with observations in 1975, as did DIN simulations in 2003. However, simulated chlorophyll was overestimated in 2003.

Some of the agreement between observations and simulations come from the use of observed boundary conditions to force the model. However, even when boundary conditions are subtracted from simulations and observations, the simulations in most cases retain a significant correlation with observations, demonstrating that the model’s ‘interior’ processes do add to its ability to replicate conditions in the loch.

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1. Introduction

This paper has two aims. The first relates to the protection of ecosystem quality in coastal Regions of Restricted Exchange (RREs) and, in particular, in those used as sites for finfish mariculture. Simple Equilibrium Concentration Enhancement (ECE) box-models have been used (Gillibrand and Turrell, 1997) to identify Scottish RREs at greatest risk from added nutrients. The OAERRE project (Tett et al., 2003) showed how developments of such models could be used to diagnose or predict eutrophication in European RREs. The
present paper describes a dynamic version of one of the OAERRE simple models and a preliminary test of this model in a shallow Scottish fjord, Loch Creran, as part of studies intended to develop tools for the assessment of the assimilative capacity of such RREs. Building these tools requires an understanding of ecosystem processes in RREs, and it is apparent that many of these processes are physically driven. Thus, models that couple physics and biology are required, even if both sets of processes and their coupling are described simply.

The second aim is more general and relates to the purpose of the Workshop on Future Directions in Physical–Biological Modelling. One theme in the development of such models has been a growth in complexity in both their physics and their biology, as well as in the number of links between the two. However, there is also a case for simplicity, especially if this is based in robustly parameterised descriptions of the key ecosystem interactions. Simple models sometimes work surprisingly well, and one reason for this is that, in many cases, model predictions are more strongly influenced by the boundary conditions of the modelled domain than by the details of representation of the interior processes. Thus, in addition to reporting the work in Loch Creran, general aspects of simplicity in models are also examined and, in particular, the importance of boundary conditions for model domains with little “interior” is shown (see Section 4 for further details).

2. Assimilative capacity

The capacity of a water body to sustain a stock of farmed fish without environmental damage depends, in part, on its ability to assimilate the by-products and waste products of fish farming. The by-products include chemicals and medicines used to treat fish diseases or prevent fouling of enclosing nets and are not further considered here. Waste products include uneaten fish food, faeces and mineralized nitrogen and phosphorus. The particulate wastes accumulate under fish cages in low energy environments or are transported by currents to settle elsewhere; in either case their decay consumes oxygen and releases mineral nutrients. It is the effects of these mineral nutrients, which are augmented by ammonium and phosphate excreted by the fish, that are the main concern of the model described in this paper. The reason for this concern is that these nutrients add to nitrate and phosphate from natural and other anthropogenic sources to bring about a risk of eutrophication, defined (C.E.C., 1991) as the “enrichment of water by nutrients especially compounds of nitrogen and phosphorus, causing an accelerated growth of algae and higher forms of plant life to produce an undesirable disturbance to the balance of organisms and the quality of the water concerned”.

Estimating an assimilative capacity for a water body thus requires a definition of what would constitute an undesirable disturbance in relation to nutrient enrichment. Current practice is to use Ecological Quality Objectives (EcoQOs) to define what is desirable. An assimilative capacity model can be seen as a tool capable of making reliable simulations of relevant conditions in a water body and thus, which can be used to explore loading scenarios to find those which do not result in a breach of the relevant EcoQOs. In the case of the Scottish fjords that are much used for salmonid farming, regulation, in relation to nutrient impact, presently derives largely from the requirements of OSPAR’s Comprehensive Procedure (part of its Strategy Against Eutrophication) and the EU Water Framework Directive (WFD) as implemented in the Water Environment and Water Services (Scotland) Act of 2003. Although there are some differences between the approaches of OSPAR and the WFD, both lead to objectives that require values of quality variables to be little disturbed from those of appropriate reference conditions. What constitutes more than a slight disturbance has yet to be defined in the context of the WFD. OSPAR considers that an increase in winter nutrient concentrations, either in maximum or average chlorophyll concentration of more than 50% over reference conditions, indicates a problem. The approach in the present paper has been to use a particular fjord as its own control, testing the model by comparing its predictions with conditions before and after the introduction of a salmon farm.

3. Complexity and simplicity in physical–biological models of aquatic ecosystems

A generalised physical–biological model is described by the following set of equations for one or more state variables \( Y \):

\[
\begin{align*}
\frac{\partial Y}{\partial t} &= -\nabla \cdot \phi_Y + \beta_Y \\
\end{align*}
\]

where: \( \nabla \cdot \phi_Y \) is the divergence of physical transport (conservative) fluxes at a given point, and \( \beta_Y \) is the sum of non-conservative (chemical and biological) transformations at that point. \( Y \) might refer to a concentration of dissolved nutrient or phytoplankton chlorophyll, or the population abundance of a particular category such as
diatoms; in any case, to a bulk (or statistical) property rather than to a particular entity such as an organism itself. Although this equation cannot, therefore, be applied to models that simulate the properties and trajectories of individual particles, including plankters (e.g. Woods and Barkmann, 1993), there are many instances of models of bulk properties to which the generalised equation does apply. Applications of such models to the North Sea have been reviewed by Fransz et al. (1991) and Moll and Radach (2003). The links between physical processes and biology are implicit in both the transport term and the non-conservative term. As exemplified in the 1-D PROWQM model described by Lee et al. (2002), the transport term takes account of the turbulent mixing of nutrients and the turbulent mixing, sinking and resuspension of microplankton and other light-absorbing particulates. The \( \beta_Y \) term includes light-driven photosynthesis, temperature-regulated metabolism of all classes of plankters and the turbulence driven conversion of some classes of organisms into other, more-rapidly sinking, classes. These drivers of the biological processes may be taken from observations or from a parallel set of equations, a physical model, embodying physical state variables for velocity, momentum, kinetic energy and irradiance.

It is widely acknowledged that more work is needed on detailed aspects of some of these interactions, particle aggregation and disaggregation being a noted example (e.g. Jago et al., 2002). It is also argued that the main biological components of ecosystems should be represented in detail and that transport processes should be simulated by advanced models for flow and turbulence (exemplified in the case of the PROWQM model by Luyten et al., 2002). Such arguments for detailed representation of ecosystem physical and ecological complexity suggest that an assimilative capacity model may be made by combining a detailed fjord 2-D physical transport model such as that of Gillibrand (2001) with an ecosystem model such as ERSEM II (Baretta-Bekker and Baretta, 1997) for example.

However, models with many state variables and adjustable parameters, solved by numerical integration at many grid points, are laborious to implement for new locations and their necessary complexity renders their workings opaque except to experts and of little use to managers. A simpler approach was adopted by Ross et al. (1993a,b, 1994) in their ‘strategic simulation model of a fjord ecosystem’. This has several thick water column layers and represents concentrations of dissolved inorganic nitrogen, dissolved organic nitrogen, phytoplankton, zooplankton and detritus. Even simpler is the *equilibrium concentration enhancement* method, applied to estimate nutrient loadings of Scottish fjords by Gillibrand and Turrell (1997), which is a steady state, single-box model. The UK Comprehensive Studies Task Team used a similar, steady state, single-box approach to diagnose or predict eutrophication in transitional and coastal waters (CSTT, 1994; Tett, 2000). The CSTT model was further developed and applied to a range of RREs throughout Europe, between Spitzbergen and the Algarve in the OAERRE project (Tett et al., 2003). This project also used more complex physical–biological models but provided several arguments for the use of simple models. These arguments included transparency and relative ease of application to screen conditions at new sites—both important for management purposes. The simplicity, however, need not be primitive but can be secondary, based on bulk parameterisations derived from more elaborate models or empirically analysed data sets.

One of the simplest solutions for Eq. (1) is for a single asymmetrical grid-point or homogenous box representing an RRE, exchanging with the sea on one side only. The flux divergence term is:

\[
-\nabla \varphi_y = -E \cdot (Y - Y_0) + \frac{F}{V} (Y_F - Y)
\]

(units : amount m\(^{-3}\) day\(^{-1}\))

(2)

\( F \) is the discharge of river water into the RRE. \( V \) is the volume of the box. Two physical processes are parameterised here. The first process is relatively simple and is total land-derived freshwater inflow. The second involves exchange between the box and the adjacent sea (or adjacent boundary conditions) and is more complex because many physical processes may drive this exchange. They are parameterised here as the exchange rate \( E \), which is, loosely, the proportion of box volume replaced each day by water whose properties (and in particular the concentration \( Y_0 \)) are those of the adjacent boundary. Thus, a total amount of substance \( E \cdot V \cdot Y \) leaves the water body each day to be replaced by \( \left( E - \frac{F}{V} \right) \cdot V \cdot Y_0 \) from the sea and \( F \cdot Y_F \) from the river. (In fact, these statements are exactly true only of instantaneous rates.)

There is a well-known steady state equation to solve this for the case of a conservative substance, such as salt, whose box-averaged concentration is written here as \( C \):

\[
E = \frac{F}{V} \cdot \frac{C}{C_0 - C}
\]

(3)

Thus, the exchange rate parameter \( E \) can be obtained empirically from observations of salinity and river discharge, as reported by Tett (1986) for several Scottish
fjords. At the next level of complexity, $E$ can be estimated from empirically parameterised, theoretically based, equations for specific physical exchange processes. Finally, exchange can be calculated from detailed numerical simulations in 2-D or 3-D. Tett et al. (2003) discuss these options.

In the case of the biological model, there is wide acceptance that the nutrient-controlled growth of homogenous populations of planktonic algae is describable by a cell-quota model (Droop, 1983), which links the process of nutrient uptake from seawater and nutrient controlled growth through the cell quota or content of the limiting nutrient. Some, indeed, argue for more complex models (Flynn, 2001). Cell-quota models have been used increasingly in complex models (Tett, 1987; Tett and Droop, 1988; Baretta-Bekker and Baretta, 1997; Lee et al., 2002). Nevertheless, the phytoplankton–nutrient link can be alternatively and simply parameterised as a ratio of chlorophyll formed to nutrient assimilated, as proposed by Gowen et al. (1992), who gave this ratio the symbol $q$. Gowen et al. estimated the value of $q$ empirically from observations in Scottish fjords and coastal waters. Mesocosm experiments by Edwards (2001) and Edwards et al. (2003, 2005) have largely confirmed for Scottish waters the original, steady state, value suggested by Gowen et al.; and the CSTT model employs it to predict the worse case chlorophyll concentration that might result from a given nutrient loading.

The dynamic CSTT model described here has only three state variables (described in Table 1): the concentrations of phytoplankton chlorophyll and dissolved inorganic nitrogen (DIN) and phosphorus (DIP); and, in addition to the optical-photosynthetic model described below, only two crucial parameters: the site-specific exchange rate $E$ and the (almost-universal) chlorophyll yield $q$. However, such description is seriously incomplete without specification of boundary conditions (denoted by $Y_0$ above).

### 4. Boundary conditions and interiority

Eq. (1) cannot be solved analytically, except in very simple cases (such as that of Eq. (3)), and so its use commonly requires numerical integration. Such numerical solutions render explicit the need for initial and boundary conditions: the values of the state variables at time zero ($t=0$) and at the edges of the domain of simulation. In the present case, these edge-values must include time-series of concentrations in the adjacent sea and in the river, river discharges, and Photosynthetically Active Radiation (PAR) at the sea-surface.

In general, the exact or numerical solutions of differential equations have a dependency on the initial and boundary conditions that vary with ‘distance’ from these conditions, so it can be said that a solution has an ‘interior’ in which values of state variables depend more on the intrinsic parameters of the equation than on the boundary conditions. More specifically, Huthnance (1995) points out that wide continental shelves have ‘interiors’ in which their local dynamics are somewhat independent of shelf-ocean exchange. Of course, this omits the ubiquitous effect of changes in solar radiation (and other local meteorological variables) that control water column stratification as well as biological production. However, a well-stratified water column has considerable inertia (its upper layers have sufficient buoyancy to resist wind-stirring, for example) and so biological conditions can follow an intrinsically determined seasonal cycle that has been initiated by the vernal onset of stratification. Nevertheless, even in a large region like the North Sea, most ecosystem conditions are re-set or re-entrained once a year by lateral and superficial boundary conditions.

In the present case, we deal with fjordic water bodies in which the upper waters have residence times ranging from a few days to a few weeks (Tett, 1986) and hence we should expect the boundary conditions to have a substantial impact on numerical simulations. They are

### Table 1

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Definition</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorophyll concentration</td>
<td>$X$</td>
<td>Chlorophyll concentration inside the box considered, initialised with the typical winter value of 0.4</td>
<td>mg m$^{-3}$</td>
</tr>
<tr>
<td>DIN concentration</td>
<td>$NO_5$</td>
<td>Seawater DIN concentration, initialised with the typical winter value of 5.7</td>
<td>mmol m$^{-3}$</td>
</tr>
<tr>
<td>DIP concentration</td>
<td>$PO_4$</td>
<td>Seawater DIP concentration, initialised with the typical winter value of 0.7</td>
<td>mmol m$^{-3}$</td>
</tr>
<tr>
<td>Mean solar irradiance</td>
<td>$I$</td>
<td>Average solar irradiance in the RRE</td>
<td>$\mu$Einstein m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>Freshwater flow</td>
<td>$F$</td>
<td>Discharge of river water into the RRE</td>
<td>m$^3$ s$^{-1}$</td>
</tr>
<tr>
<td>Growth rate</td>
<td>$\mu$</td>
<td>Nutrient-controlled growth rate for phytoplankton</td>
<td>day$^{-1}$</td>
</tr>
</tbody>
</table>

See also Table 6 for a list of the variables used for the description of the boundary conditions.

* Initial values obtained from Jones (1979).
sometimes referred to as “lochs”, the Scottish word for a long thin body of water, typically either a glacially deepened lake or a salt-water fjord receiving freshwater inflow.

5. Study site and practical methods

The observation and modelling study was carried out on a shallow fjord: Loch Creran (Fig. 1). This site was chosen for three main reasons. Firstly, according to Landless and Edwards (1976), Loch Creran is close to the unrealised typical Scottish sea loch in dimensions and general hydrography; secondly, because it now contains a salmon farm of a size that is substantial in relation to its volume and thirdly, because there is a good body of historic data describing the hydrography and biology of the loch during the 1970s, before the installation of the fish farm. The loch also contains, nowadays, two large mussel farms. Prior to about 1990, it also received the waste from a seaweed processing plant.

Loch Creran is a small sea-loch situated on the north–west coast of Scotland (56°31.41 N, 5°21.12 W), approximately 15 km north of the town of Oban, Argyll. The loch connects to the larger fjord Loch Linnhe and eventually to the water of the NE Atlantic Ocean across the wide Scottish continental shelf. The loch is of a fjordic type, partially separated from the open sea by a sill and can be divided in two basins. The small (upper) basin is 3 km long by 0.8 km wide, with a maximum depth of 40 m, and the main (lower) basin is 11 km long by 1.5 km wide with a maximum depth of 53 m (Milne, 1972). These two basins are partially separated by a 3-m-deep sill. The main sill at the mouth of the loch is approximately 8 m deep. For modelling purposes, the loch and its approaches were divided into three boxes, as noted in Table 2 and shown in Fig. 2. The small basin of the loch was neglected; it was assumed that all rivers discharged directly into the surface layer of the main basin.

A number of studies have been made on Loch Creran, including nutrient concentrations and phytoplankton growth (Jones, 1979), ecology of phytoplankton (Jones et al., 1978; Tett and Grantham, 1980; Lewis et al., 1985a,b; Tett et al., 1985; Tett, 1987), pigments (Tett and Wallis, 1978; Gowen, 1981; Gowen et al., 1983), carbon and nutrient budgets (Tyler, 1983, Tett et al., 1975), physical exchanges and dynamic of phytoplankton (Tett, 1986), hydrology and benthic community structure (Burrows et al., 2003; Nickell et al., 2003), ecotoxicology (Widdows et al., 2003) and mollusc ecology (Todd et al., 1998). Theses by Tyler (1983) and

Fig. 1. Map of Loch Creran showing the stations sampled in 1975 and 2003 (adapted from Jones, 1979).
Chlorophyll concentration was analysed by a method as close as possible to that used in the 1970s and described in detail by Tett (1987). A measured volume of seawater (about half a litre) was passed through a GF/F 47 mm filter. The filter was then folded and stored at −18 °C in a plastic centrifuge tube. Up to 6 months later, 90% acetone was added to the frozen samples and they were extracted overnight before measurement of their fluorescence before and after acidification, in a Turner fluorometer TD 700. The day-to-day calibration of this instrument was checked with a TD red solid standard (P/N: 7000-994) and, at intervals, a primary calibration was made with a solution of pure chlorophyll a (Sigma chemical co. ref. C5753)—the concentration of which had been determined in a spectrophotometer using a coefficient of 87.67 L g⁻¹ cm⁻¹ (Jeffrey and Humphrey, 1975).

For nutrients, 100 ml of seawater was filtered through a GF/F 47 mm filter in an all-glass filtration unit. The filtrate was bottled in acid-washed plastic containers and stored at −18 °C until analysis, using a Lachat Instruments QuickChem 8000 flow injector autoanalyser, for concentrations of nitrate and nitrite (measured together and referred to as DIN) and phosphate. The methods follow QuickChem (2001a,b). Random samples were run in triplicate in order to assess the variability of the instrument.

For modelling purposes, values obtained from all samples taken on 1 or 2 days within a given box (Table 2) were averaged. Where these data are used for comparison with simulations, the means are shown as points with bars giving ±1 S.E. of the mean. When used for boundary conditions, continuous time-series were generated by linear interpolation between nutrient means or logarithmic interpolation between chlorophyll means. A similar strategy was adopted with 1975 data.

Jones (1979) provide much information on the hydrography, nutrients and phytoplankton of the loch during the 1970s and the chlorophyll and nutrient data for 1975 used in the present paper are taken from Jones (1979).

During 2003, Loch Creran was sampled on a number of occasions (Table 3) using a small research vessel to work a longitudinal transect. In addition, a small boat was used to take samples close to the fish farm. An internally recording, portable SeaBird 19plus CTD was used to profile temperature and salinity at each station and NIO-pattern water bottles were used to take water samples at several depths for chlorophyll and nutrients (and other constituents not reported here). Near-surface samples were also taken from Barcaldine Pier and from the River Creran near Taraphocain.

### Table 2
**Details of Creran, including volumes, stations and thicknesses included in each box**

<table>
<thead>
<tr>
<th>Model</th>
<th>Geographical coordinates</th>
<th>Boundary box</th>
<th>Upper box</th>
<th>Lower box</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume (10⁶ m³)</td>
<td></td>
<td>980</td>
<td>98</td>
<td>98</td>
</tr>
<tr>
<td>Thickness (m)</td>
<td></td>
<td>12</td>
<td>7</td>
<td>7</td>
</tr>
</tbody>
</table>

### Stations and depths (m) for observations in 2003

| Greag Isles                  | 56°28.894N/5°30.084W     | 2, 5, 10     |
| Deepest                      | 56°31.001N/5°22.400W     | 2, 5, 10, 20, 30, 40 |
| Fish farm                    | 56°31.472N/5°20.972W     | 2, 5, 10, 20, 30 |
| Barcaldine                   | 56°32.027N/5°19.354W     | 2, 5, 10, 20  |
| Pier                         | 56°31.720N/5°19.050W     | 2            |

**Fig. 2. Graphical representation of the three-box model.**
Data from the station here called ‘Barcaldine’ for that year were taken from Jones (1979), who used the label ‘C5’. Sampling in 1975 was weekly during the Spring Bloom period, and monthly during the remainder of the year. Samples from 0 to 7 m depth provided the observations with which to compare the simulations in the ‘upper’ box of the model, while deeper samples characterized the ‘lower box’ and were used to provide the boundary conditions for this year.

6. Physical model

Loch Creran is a shallow fjord and contains no ‘basin deep water’ which is typically outside the normal circulation of water through the loch. In the implementation of the model reported here, the small basin was neglected. Much of the main basin of the loch shows characteristic salinity layering and, on the basis of this, its volume was divided into an ‘upper’ and a ‘lower’ layer, as shown in Fig. 2. Although the dynamics of water circulation through the main basin have not been analysed in detail, there is little evidence of the freshwater driven estuarine circulation that is apparent in the neighbouring Loch Etive (Wood et al., 1973). Instead, it is likely that the main driver of circulation in Loch Creran is the tidal regime, converted into a vertical circulation as a result of the density layering. Water entering the loch on the flood tide is normally saltier, and hence denser, than water already in the loch and so the inflow is deemed to enter the ‘lower’ box of the model. On the ebb tide, it is the less dense water in the upper layer than flows out over the shallow entrance sill (depth 8 m) of Loch Creran. However, the flushing time of Loch Creran, deduced from salinity budgets (Landless and Edwards, 1976; Tett, 1986) is about twice as long as implied by the tidal pumping model and it is thus likely that outflowing and inflowing water are mixed together in the loch’s entrance channel and adjacent waters, resulting in a tidal exchange efficiency of only about one half.

Although the model set-up shown in Fig. 2 allows tidal pumping and estuarine circulation processes to be simulated, the physics of the present version of the model are driven very simply by a single value (0.16 day$^{-1}$) of the exchange rate $E$, taken from Tett (1986). Thus, a daily volume $EV$ is assumed to flow out of the ‘upper’ box and to mix with water in the ‘boundary’ box, thus removing $EY$ of the state variables. At the same time, the ‘upper’ box receives a daily freshwater discharge of $F$ and hence inputs $FY_F$. A volume of $EV - F$ flows from the ‘boundary’ box by way of the ‘bottom’ box into the upper box, initially bringing $(EV - F)Y_B$ from the ‘boundary’ box, although subject to modification in the ‘bottom’ box. Finally, conditions in the ‘boundary’ box are relaxed towards the appropriate boundary conditions at a rate of 0.1 day$^{-1}$. The remaining part of the physical model deals with layer mean irradiance:

$$\bar{I} = m I_0 \left(1 - e^{-kd_h}\right)/(kd_h) \ \mu\text{Einstein m}^{-2} \text{s}^{-1} \quad (4)$$

where $I_0$ is 24-h averaged PAR at the sea-surface and $m$ corrects for surface reflection and hyperexponential decay (Tett, 1990). Layer thicknesses $h$ are given in Table 2. The diffuse attenuation coefficient $kd$ was computed from a constant background of 0.20 m$^{-1}$ and a chlorophyll-related component, using an attenuation cross-section of 0.029 m$^2$ (mg chl)$^{-1}$. The latter parameter is based on a reanalysis of measurements of diffuse attenuation and chlorophyll concentration reported by Tyler (1983), and corresponds to the absorption cross-section of 0.025 m$^2$ (mg chl)$^{-1}$ used in the biological model, given a

---

**Table 3**

Sampling dates and sites visited in 2003

<table>
<thead>
<tr>
<th>Date</th>
<th>Greag Isles</th>
<th>Entrance</th>
<th>Deepest</th>
<th>Fish farm</th>
<th>Barcaldine</th>
<th>Pier</th>
</tr>
</thead>
<tbody>
<tr>
<td>04/02/2003</td>
<td>v v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
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<td>v v v v</td>
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<tr>
<td>18/02/2003</td>
<td>v v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v</td>
</tr>
<tr>
<td>05/03/2003</td>
<td>v v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v</td>
</tr>
<tr>
<td>18/03/2003</td>
<td>v v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
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<td>v v v v v</td>
<td>v</td>
</tr>
<tr>
<td>01/04/2003</td>
<td>v v v v v v</td>
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<tr>
<td>08/04/2003</td>
<td>v v v v v v</td>
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<td>v</td>
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<tr>
<td>23/04/2003</td>
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<tr>
<td>13/05/2003</td>
<td>v v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
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<tr>
<td>03/06/2003</td>
<td>v v v v v v</td>
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</tr>
<tr>
<td>07/08/2003</td>
<td>v v v v v v</td>
<td>v v v v v</td>
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<td>v v v v v</td>
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</tr>
<tr>
<td>16/10/2003</td>
<td>v v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v v v v v</td>
<td>v</td>
</tr>
</tbody>
</table>
mean cosine for underwater light of 0.85. The parameters used in the physical model are defined, and their values given, in Table 4.

### 7. Biological model

The state variables of the biological model are: chlorophyll concentration \(X\) (mg m\(^{-3}\)), dissolved inorganic nitrogen (DIN) concentration \(\text{NO}_S\) (\(\mu\text{M}\)) and dissolved inorganic phosphorus (DIP) concentration \(\text{PO}_S\) (\(\mu\text{M}\)). (The naming convention follows Tett and Droop, 1988.)

In the case of chlorophyll concentration \(X\), the non-conservative term is:

\[
\beta_X = \mu(T, S) \cdot X - L \cdot X \quad \text{mg chl m}^{-3} \text{ day}^{-1}
\]

where \(\mu(I, S)\) is the intrinsic growth rate (day\(^{-1}\)), a function of compartment mean irradiance \(I\) and nutrient concentration (either DIN or DIP, see below) and \(L\) is the rate of loss to grazing by zooplankton and benthos. A constant value was assumed for each model box (Table 5).

Growth rate is a threshold function of PAR and the two dissolved nutrients:

\[
\mu(T, S) = \min \left\{ \alpha \cdot (I - I_c), \mu_m \cdot \left( \frac{\text{NO}_S}{\text{NO}_S + \text{PO}_S} \right) \right\}
\]

where the parameters are defined, and their values given, in Table 5. Although the equation can be applied equally to phytoplankton and to microplankton, the values used were those for microplankton, the mixture

### Table 4

Physical parameters definitions and values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Definition</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exchange rate</td>
<td>(E)</td>
<td>Tidal water renewal rate in Loch Creran</td>
<td>0.16</td>
<td>day(^{-1})</td>
</tr>
<tr>
<td>Volume of the box</td>
<td>(V)</td>
<td>Volume of the box considered</td>
<td>980 \cdot 10^6</td>
<td>m(^3)</td>
</tr>
<tr>
<td>Layer thickness</td>
<td>(h)</td>
<td>Thickness of the layer of water considered in each box</td>
<td>7</td>
<td>m</td>
</tr>
<tr>
<td>Diffuse attenuation coefficient</td>
<td>(k_D)</td>
<td>Diffuse attenuation of light in mixed layer</td>
<td>0.1</td>
<td>m(^{-1})</td>
</tr>
</tbody>
</table>

### Table 5

Biological model parameter definitions and values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Definition</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absorption cross-section</td>
<td>(a^*)</td>
<td>Relative absorption of light beam by photosynthetic pigment</td>
<td>0.025</td>
<td>(\text{m}^2\ \text{mg Chl}^{-1})</td>
</tr>
<tr>
<td>Slope term</td>
<td>(b)</td>
<td>In microplankton model (Tett et al., 2002, 2003). Value for (\eta=0.125)</td>
<td>0.781</td>
<td>N/A</td>
</tr>
<tr>
<td>Photosynthetic quantum yield</td>
<td>(\Phi)</td>
<td>Conversion of photons into fixed carbon</td>
<td>40</td>
<td>(\text{nmol C \mu E}^{-1})</td>
</tr>
<tr>
<td>Chlorophyll to carbon ratio</td>
<td>(\chi)</td>
<td>Chlorophyll to carbon ratio, value of 0.525 calculated from microplankton model with (\eta) of 0.125, and assuming maximum cell nutrient content</td>
<td>0.525</td>
<td>mg Chl mmol C(^{-1})</td>
</tr>
<tr>
<td>Microplankton basal respiration rate</td>
<td>(r_0)</td>
<td>0.057 for (\eta) of 0.125 and standard microplankton parameters</td>
<td>0.057</td>
<td>day(^{-1})</td>
</tr>
<tr>
<td>Loss rate</td>
<td>(L)</td>
<td>Rate of loss to grazing by zooplankton and benthos</td>
<td>0.2</td>
<td>0.1 day(^{-1})</td>
</tr>
<tr>
<td>Photosynthetic efficiency</td>
<td>(\alpha)</td>
<td>((\alpha_m-m) \cdot \Phi \cdot \chi \cdot (86,400/1,000,000) \cdot (1+b)^{-1}) where (m=0.85) is mean cosine of submarine irradiance</td>
<td>0.03</td>
<td>day ((\mu \text{E m}^{-1} \text{s}^{-1}))</td>
</tr>
<tr>
<td>Compensation illumination</td>
<td>(I_c)</td>
<td>(R_0/(\alpha \cdot (1+b)))</td>
<td>1.1</td>
<td>N/A</td>
</tr>
<tr>
<td>Maximum nutrient-controlled growth rate</td>
<td>(\mu_m)</td>
<td>(1)</td>
<td>1</td>
<td>(\mu \text{E m}^{-1} \text{s}^{-1})</td>
</tr>
<tr>
<td>Half saturation concentration for growth</td>
<td>(k_S)</td>
<td>For nitrate</td>
<td>2</td>
<td>mmol m(^{-3})</td>
</tr>
<tr>
<td></td>
<td></td>
<td>For phosphate</td>
<td>0.2</td>
<td>N/A</td>
</tr>
</tbody>
</table>
of phytoplankters and pelagic protozoa and bacteria (Tett and Wilson, 2000; Lee et al., 2002). The main difference is the compensation irradiance $I_c$ for microplankton is greater than that for phytoplankton (Tett et al., 2002). The microplankton parameterisation takes account of losses of primary production to pelagic microheterotrophs, thus avoiding the need for a separate protozoan compartment in the model.

The values of photosynthetic efficiency $\alpha$ and compensation irradiance $I_c$ were calculated using standard parameters of the microplankton model of Tett et al. (2002, 2003) and a value of the heterotroph fraction of 0.125, which was that chosen for a diatom-dominated microplankton in the PROWQM model of Lee et al. (2002). The value of photosynthetic efficiency derives from an assumed photosynthetic quantum yield of 40 nmol C mmol$^{-1}$, and the absorption cross-section was 0.025 m$^2$ (mg chl)$^{-1}$, as mentioned in relation to the physical model. Further details are given in Table 5.

The non-conservative term for DIN concentration is:

$$\beta_{\text{NOS}} = \frac{-\mu_{(T,S)} X}{N q} + \frac{N e \cdot L \cdot X}{N q} \text{ mmol m}^{-3} \text{ day}^{-1}$$

where $N e$ is the proportion of grazed nitrogen that is locally recycled and $N q$ is the yield of chlorophyll from nitrogen, taken as 2.5 mg chl (mmol N)$^{-1}$ on the basis of the results of microcosm experiments with Loch Creran water reported by Gowan et al. (1992). This value corresponds more closely to the peak yields of 1.8–3.0 mg Chl/mmol N obtained by Edwards (2001) and Edwards et al. (2003, 2005) than to the steady state yield of 1.1 mg chl (mmol N)$^{-1}$ used in the equilibrium CSTT solution of these dynamic equations. The peak value was thought to be more appropriate in a dynamic model, and it corresponds more closely to that deduced using the microplankton model standard parameters for a diatom-dominated microplankton. The CSTT steady state solution was devised for summer conditions in which the heterotrophs of the microplankton took a greater share of available nitrogen.

The DIP term is similar:

$$\beta_{\text{POS}} = \frac{-\mu_{(T,S)} X}{P q} + \frac{P e \cdot L \cdot X}{P q} \text{ mmol m}^{-3} \text{ day}^{-1}$$

where the yield $P q$ is set at 30 mg chl (mmol P)$^{-1}$ on the basis of modelling by Tett (1998) of microcosm experiments by Jones et al. (1978) and re-analysis of Loch Creran 1973 chlorophyll and particulate data given by Tett et al. (1975).

8. Model implementation

The model was implemented using High Performance System’s Stella 8 software. The equations of the model were integrated using Euler’s method. Although less precise than the Runge–Kutta integration, this method is advised when using switches in the model (as in the case of Eq. (6)). The integration time-step was 0.125 day, and the reliability of the numerical solutions checked against known test cases and by testing the conservation of simulated DIN. In the case of DIN for example, the numerical error term was less than 0.4% of the annual budget and is too small to show in Fig. 7.

Data were output from the simulations at 1-day intervals, the displayed data being the final values obtained each day. Time-series of boundary condition data (irradiance and freshwater inputs as well as the boundary concentrations) were supplied in the form of Stella ‘graph’ variables—actually as tables of values with intervals of 1 to 3 days; Stella interpolated linearly between these values.

The program was run to simulate the seasonal cycle in 2 years: 1975 and 2003—the differences between the years being set by the boundary conditions, as considered below.

9. Boundary conditions

Boundary conditions are summarized in Table 6 and some are illustrated in Fig. 3.

Daily values of total solar irradiance were taken from a solarimeter on the roof of the Dunstaffnage Marine Laboratory (DML), about 15 km from the Barcaldine site in Loch Creran. Values for 1975 were tabulated by Tyler (1983); values for 2003 were obtained from the UK Meteorological office by way of the British Atmospheric Data Centre (BADC). It was assumed that PAR made up 46% of total radiation and this part of solar energy was converted to photons at 4.15 $\mu$Einstein J$^{-1}$ (Tett, 1990).

In the present implementation, information on freshwater runoff was needed only to provide an estimate of land-derived nutrients. Runoff was calculated from rainfall using a simplified version of the hydrological component of the CHUM model (Tipping, 1996). In this version, the catchment was divided into two boxes, each containing a reservoir of a certain size. Outflow from the reservoir to the next box, or into the ‘upper’ box of the Loch Creran model, was governed by Darcy’s Law. In addition, surface runoff occurred when the soil reservoirs were full and evapotranspiration was assumed to be driven by absorbed solar radiation. The
run-off model was tested against daily flows measured in the River Creran during 1977 and 1978 and tabulated by Tyler (1983). The rainfall data used to drive the model was taken (by way of the British Atmospheric Data Centre, BADC) from Meteorological Office records for DML, corrected for increased rainfall in the hills forming the loch’s catchment, according to factors tabulated by Tyler (1983). River nutrient concentrations for 1975 were taken from Jones (1979). Concentrations in 2003 were obtained from samples taken in the River Creran.

Fish farm nutrient input in 2003 was calculated from monthly values of food supplied to the fish which totalled 2147 tons during the year. The budgetary model of Black (2001) was used to convert this to daily rates of ammonium and phosphate added to the water column (and input to the ‘upper’ box of the model) and to rates of ammonium, nitrate and phosphate mineralised by the sediment (and input to the ‘lower’ box of the model). Even if only oxidised nitrogen was measured in Loch Creran in 2003, it has been shown by Edwards (2001) that in spring, the yield of chlorophyll from ammonium was similar to the yield of chlorophyll from nitrate and that, in summer and autumn, the yield values showed only little variations. The state variable used in the dynamic CSTT model is DIN. Although only nitrate and nitrite were measured, it is rather unlikely that much nitrogen was missed by omitting ammonium measurements.

The remaining boundary conditions are those supplied as time-series of chlorophyll and nutrient concentrations to which the ‘boundary’ box relaxes in the model. No data for conditions outside the loch were available in 1975 and so observed concentrations in the deep water of Loch Creran were used to provide the relaxation time-series. This was also done in 2003 (run A), but some data were also available for the Greag Isles station (see Fig. 1 for position) and, in run B, these data were used for the relaxation boundary conditions. In the case of chlorophyll concentrations, daily values were obtained by logarithmic interpolation while linear interpolation was used for the nutrient data.

10. Results

Fig. 4 shows the results of a comparison between the chlorophyll and nutrient concentrations simulated by the model and those observed in the loch. The comparison presented here is for the upper layer of the main basin of Loch Creran.

The 1975 simulation (Fig. 4a) shows good agreement between simulated and observed values of all three variables in winter and spring, with the amplitude of the peaks or falls, as well as their phase, matching the observed data. Agreement is also good in summer and autumn for the description of the nutrient concentrations, with only slight discrepancies towards the end of the year. For the chlorophyll however, the simulated concentrations in summer and autumn are slightly different from the corresponding observed data. The simulations are too low in summer (1 to 2 mg m$^{-3}$ as opposed to the 2 to 3 mg m$^{-3}$ observed) and, in autumn, a simulated chlorophyll peak appears at around day 300, which was not observed in the loch.

The 2003A and 2003B simulations (Fig. 4, parts b and c), derived with different data for boundary conditions, present similar patterns and will be described together.

In both cases, simulated chlorophyll concentrations match the observations well only in winter. The timing
of the simulated spring bloom agrees with the observed bloom, but the simulated amplitude is four times higher. In summer, the simulated concentrations remain high (2.5 to 6 mg m\(^{-3}\)) whereas the observations showed concentrations of only 0.3 to 2 mg m\(^{-3}\). In autumn, both simulations include a second chlorophyll peak of high amplitude (up to 8 mg m\(^{-3}\)) and long time span (up to 100 days). These peaks were not observed in the field.

The simulated nutrient concentrations are in better agreement with the observations. Simulations slightly exceed observations in late winter and during part of the summer, then lag the observed increase in the autumn.

Figs. 5 and 6 exemplify for 1975 the method used to assess agreement between observations and simulations. The top row of Fig. 5 includes the boundary conditions used to force the simulation. In the lower row of graphs are plotted the values minus the simultaneous boundary value; this difference is, in the case of the simulations, what the model ‘interior’ adds or subtracts to chlorophyll or nitrate concentration in the water arriving from the sea. Fig. 6 presents scatter plots of observed values against values simulated for the same day. A good fit would be indicated by points plotting close to a line of unit slope. A weaker criterion of agreement is given by the correlation coefficient, which shows whether the simulated and observed
values co-vary rather than whether they agree numerically.

Table 7 summarizes the agreement statistics for all years. Simulations agree with observations for all variables, except chlorophyll in 2003. The agreement between simulations and observations corrected for boundary conditions (BCs) is always significant for DIN but only significant for DIP in one case out of 3. In the case of chlorophyll, the correlation is significant when Creran deep water values are used for boundary conditions, even in the case of the 2003 data. Finally, there are a few cases in which the slope of the plot of observed on simulated variables is significantly less than one. This is most marked for BC-corrected chlorophyll in 2003, but is true of chlorophyll and BC-corrected DIN in 1975.

Fig. 7 compares simulated budgets for dissolved inorganic nitrogen in 1975 and 2003. The ‘source’ terms are those of: DIN input from the sea (the ‘boundary’ box of the model) to the bottom water of Creran (the model’s ‘lower’ box); DIN in river discharge; DIN from the fish farm, both direct input to the ‘upper’ box and input of mineralized particles to the ‘lower’ box; and recycling of nitrogen in phytoplankton (or microplankton) lost to grazers. The latter is low because the loss rate in the ‘upper’ box was deemed to be small. The ‘sink’ terms are those of: DIN loss from the loch’s surface layer to the sea,
and uptake of DIN in the ‘upper’ box as the result of light-driven growth. In both years, the exchange with the sea dominates the simulated budget during autumn and winter, and provides the main source of nitrogen during the spring and summer in 1975. During spring and summer 2003, however, the farm input of nitrogen is important, balanced by a greater phytoplankton nutrient uptake (see Table 8).

11. Discussion

Between 1975 and 2003, local inputs of nutrient from rivers and the fish farm increased (Fig. 3) but despite this there was little apparent increase in nutrient concentrations in the loch, and observed chlorophyll concentrations decreased substantially (Fig. 4). The results support the report of a decrease in observed chlorophyll in Creran because of the care taken to calibrate 2003 measurements so as to make them comparable to those in 1975, and also because those made in 2003 at the Greag Isles station outside the loch.
are similar to those made there in 1970–1971 by Tett (unpublished). The decrease in Loch Creran is contrary to expectations of a nutrient-stimulated increase in phytoplankton biomass, and the causes are currently being studied. The 2003 simulation (Fig. 4) displays the increase in chlorophyll expected to result from additional nutrient inputs, especially by the fish farm and thus highlights the low concentration of chlorophyll observed during the year. This low concentration contrasts with the expectation that adding nutrients to an aquatic ecosystem will typically result in increased amounts of phytoplankton and therefore an increase in water-column chlorophyll.

So far as the model is concerned, nitrate in both years, and chlorophyll in 1975, are well simulated (Table 7). Although some of these good agreements are the results of the importance of boundary conditions, removing them (Fig. 5) leads to correlations that remain significant for nitrate and chlorophyll in both years. This shows that the model’s representation of ‘interior’ processes does possess ‘skill’ in replicating conditions in the loch. However, there is also the matter of ‘hyperlinearity’, by which we mean the over-estimation of values in simulations compared with observations, shown by slopes of less than 1:1 when observations are plotted against simulations (Fig. 6 and Table 7). The model’s over-estimation of chlorophyll is most marked in 2003. The parameter values that gave good agreement for 1975 hindcast too much chlorophyll in 2003. Because observed and simulated DIN remain in good agreement in 2003, it can be concluded that phytoplankton growth and removal of DIN have been simulated correctly, but that either the yield of chlorophyll from nitrogen is lower, or the loss rate of phytoplankton is higher, in 2003 compared with 1975.

Whereas DIN is well simulated by the model, and the discrepancies in chlorophyll simulation in 2003 suggest interesting if as yet unknown changes in the loch’s pelagic ecosystem, DIP concentrations are less well hindcast. This may be because of difficulties in simulating concentrations of a non-limiting nutrient, or because of aspects of the estuarine biogeochemistry of phosphate (e.g. Zwolsman, 1994) that are not described in the model. In any case, the value of the chlorophyll yield from phosphorus (30 g Chl/mol P) needs more attention.

As the budgets in Fig. 7 show, boundary exchanges (and thus the sea-boundary conditions) are the most important contributors towards nitrogen dynamics during autumn and winter, while internal, biogeochemical processes of nutrient uptake becomes relatively more important during spring and summer. River inputs are relatively small, whereas the fish farm in loch Creran, which consumed 2147 tons of food during the year, made a significant contribution (shown in Table 8) to spring and summer nutrients. However, the rapid flushing of the loch prevents substantial increases in observed nutrient concentrations, which are not significantly greater in 2003 than in 1975.

In conclusion, this simple model shows promise of simulating conditions in a fjord sufficiently well to be

![Fig. 7. Budgets for daily gains and losses of dissolved inorganic nitrogen in 1975 and 2003 (A boundary condition). The budgets are summed over the ‘upper’ and ‘lower’ boxes of the model; inflow is that from the ‘boundary’ box to the ‘lower’ box; outflow is that from the ‘upper’ box to the ‘boundary’ box. Uptake occurs only in the ‘upper’ box, because it is assumed to be linked to light-driven growth. It was computed from $\mu_3 \cdot X_3 \cdot N_q^{-1} \cdot V_3$.](image)

Table 8

<table>
<thead>
<tr>
<th>Year</th>
<th>From sea</th>
<th>From river</th>
<th>From fish farm</th>
<th>Recycled</th>
<th>To sea</th>
<th>Uptake</th>
</tr>
</thead>
<tbody>
<tr>
<td>1975</td>
<td>33.4</td>
<td>1.2</td>
<td>0.0</td>
<td>0.7</td>
<td>31.6</td>
<td>3.8</td>
</tr>
<tr>
<td>2003</td>
<td>35.0</td>
<td>1.6</td>
<td>8.8</td>
<td>3.1</td>
<td>31.5</td>
<td>15.2</td>
</tr>
</tbody>
</table>
useful in estimating assimilative capacity. After further model development, it will be possible to explore scenarios for nutrient loading and to find conditions for which the loch’s nutrient and phytoplankton levels satisfy ecological quality objectives such as those of the CSTT and OSPAR, or those that are likely to emerge from WFD considerations.

The first step towards an assimilative capacity model will be to select suitable indicators for an accurate description of the environmental health of the system considered. When a wide range is available, only the ones most representative and easiest to test will be selected. Once few indicators have been chosen, the threshold for “undesirable disturbance” will have to be defined and quantified in order to set ecological quality objectives (EQOs) for the RRE considered. For example, in the case of Loch Creran, winter nutrient concentrations (DIN and DIP) could be considered as good indicators of environmental health. The Bergen Declaration (2002) states that “Winter DIN and/or DIP should remain below elevated levels, defined as concentration >50% above salinity related and/or region-specific natural background concentrations”. In the case of Loch Creran, these could be the concentrations measured in Loch Linne (represented by the “boundary” box of the dynamic CSTT model). In some cases, these could also be the concentrations measured at the same site but several years before, if enough historical data are available; this would be possible in the case of Loch Creran since this site has been widely studied throughout the 1970s and early 1980s. The assimilative capacity model could then be used to predict the conditions under which the system would go beyond the set EQOs. This last step will involve running the model under different scenarios and assessing the relative importance of all variables and parameters.

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