

Modelling the Assimilative Capacity of Sea-Lochs (Final Report on SARF 012) *

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1 Introduction & Rationale

Commercial production of farmed finfish, primarily Atlantic Salmon, is an important industry for Scotland. It takes place mainly in sea-lochs, voes and coastal waters on the west coast of mainland Scotland, and around the the Western and Northern Isles.

Conventional cage fish farming practice does not involve the treatment of farm wastes before their discharge to the sea and therefore relies on natural dilution and degradation of these by-products. The capacity of the environment to assimilate waste is limited by the hydrodynamic and biological characteristics of the recipient water bodies. In order to minimise the risk from pollution and to maintain water and ecological quality, Scottish regulatory agencies - especially SEPA - have recognised a need for better predictive tools to match development more precisely to the assimilative capacity of the environment, taking into account inputs of potential pollutants arising from multiple sources within a management area (ACWG, 2004). The assimilative capacity models described in this report are intended to provide some of these tools.

Fish farms produce several sorts of wastes (Huntington et al., 2006). Fish faeces and uneaten food deposit on the seabed in waters of low dispersion. The decay of this organic waste consumes oxygen and can degrade chemical and biological conditions beneath a cage farm, and the deposition and impact can be simulated by models such as DEPOMOD (Cromey et al., 2002). This decay, and the metabolism of fish, also releases nutrients into the water column, with a consequential risk of *eutrophication*. This is defined in the Urban Waste Water Treatment Directive as:

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 present in the water and to the quality of the water concerned.

Although the algae thus stimulated can include the green and brown seaweeds that foul cages, the main problems associated with eutrophication are those due to the excessive growth of planktonic micro-algae. Such problems typically occur on the scale of water bodies - such as the basins of sea-lochs and voes, in the present case - in contrast to the obvious benthic impact of organic waste, which tends to be site specific (CSTT, 1994, 1997). This project has been concerned with CSTT's 'zone B', water-body, scale. Table 1 lists prior work relevant to

*Includes minor corrections to report of 9 October 2007.

modelling these ecosystem properties in *Regions of Restricted Exchange*, or **RREs** – a term that includes fjords, sea-lochs and voes.

Table 1: Studies relevant to the assimilative capacity of sea-lochs & voes

Studies of fish-farm impact, the potential yield of chlorophyll from nutrient, and water exchange	(Gowen, 1994; Gowen & Bradbury, 1987; Gowen & Ezzi, 1992; Gowen et al., 1992; Tett, 1986)
‘Strategic Simulation Model’ of a fjord ecosystem and the impact of nutrient enrichment	(Ross et al., 1993a; Ross et al., 1994; Ross et al., 1993b)
‘Equilibrium Concentration Enhancement’ and physical exchange modelling	(Gillibrand, 2001; Gillibrand & Turrell, 1997)
‘FjordEnv’ model for physical exchange and effects of fish-farming on transparency and oxygen in (Scandinavian) fjords	(Aure & Stigebrandt, 1990; Stigebrandt, 2001)
The ‘worst case’ and dynamic CSTT models applied to Regions of Restricted Exchange (RREs)	(Laurent et al., 2006; Tett et al., 2003)

2 Objectives

The objectives and achievements of the project are summarized in Table 2.

Table 2: Objectives and achievements of SARF012

Objective	Achievement
1. Improve the parameterization of water exchange and internal mixing in ECE models for application to inshore sites in sea-lochs and voes (i.e. in RREs) by incorporating mixing efficiency factors.	The ACExR model.
2. Establish a zone B scale ECE model, with appropriate exchange and mixing parameterizations, for new applications to offshore sites in more open waters.	The OWExR model.
3. Develop a time-varying ECE model which allows coupling to seasonally changing nutrient and organic inputs to zone B scale water bodies from rivers, fish-farms, and the sea.	The sECE model.
4. Combine the inshore and offshore ECE modelling approaches with that of a dynamic version of the CSTT model and develop this into an ESV model by addition of additional water and ecological quality variables which relate to appropriate EcoQOs.	The dCSTT and L-ESV models (RREs only).
5. Test the improved parameterizations and newly developed models against new and existing data sets from sites representing a range of ecohydrodynamic conditions appropriate for fish-farming.	RRE models tested for loch Creran; ACExR tested for loch Etive.

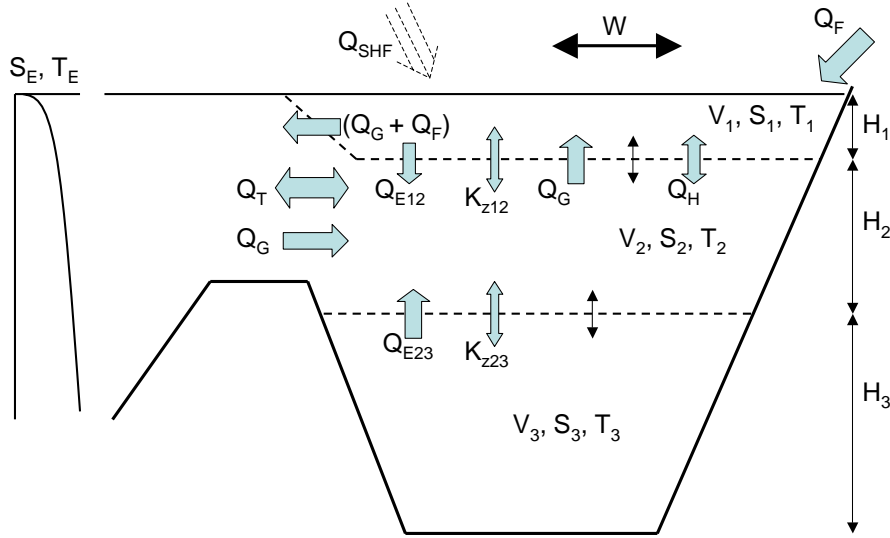


Figure 1: The three-layer conceptual model. Layer variables: thickness, H_i ; volume, V_i ; temperature, T_i ; salinity, S_i ; volume fluxes, $Q_T, Q_G, Q_H, Q_{E,ij}$; vertical turbulent diffusivity, $K_{z,ij}$. Forcing: river discharge, Q_F ; wind speed, W ; heat flux, Q_{SHF} ; external temperature & salinity profiles, T_E, S_E .

This final report deals with objectives 1 and 3 to 5. It gives an overview of the ACEXR physical, and sECE-dCSTT-LESV chemical-biological, assimilative capacity models developed for RREs (i.e., sea-lochs & voes) and examples of their testing and use to estimate assimilative capacity. A complete account of the work carried out in developing and testing models is given in the project's 5 milestone reports. Report 5 updates earlier reports 1, 3 and 4, and includes instructions for using the Matlab script packages to run simulations with the models. A complete account of the offshore OWExR model is available in the project's milestone 2 report.

3 Models

3.1 Introduction

The development of an applied model passes through 3 phases: conceptual, mathematical, and numerical, modelling.

The *conceptual model* of ACEXR divides a loch into three stacked layers, as shown in Figure 1. The thickness (and therefore the volume) of each layer can change. The conceptual model for L-ESV has a fish waste submodel, shown in Figure 2 connected to a CSTT chlorophyll model, and a pelagic ecosystem submodel shown in Figure 3 including its bio-optical component.

The *mathematical model* is summarized by the following equation in which V is the volume of a layer in the conceptual model, and Y is a generalized water quality variable – examples include salinity, nutrient and chlorophyll concentration – also called a *tracer*.

$$\frac{dY}{dt} = \frac{1}{V} \cdot \sum_k \Phi_{k,Y} + \beta_Y + \frac{1}{V} \cdot \Gamma_Y \quad (1)$$

On the right hand side:

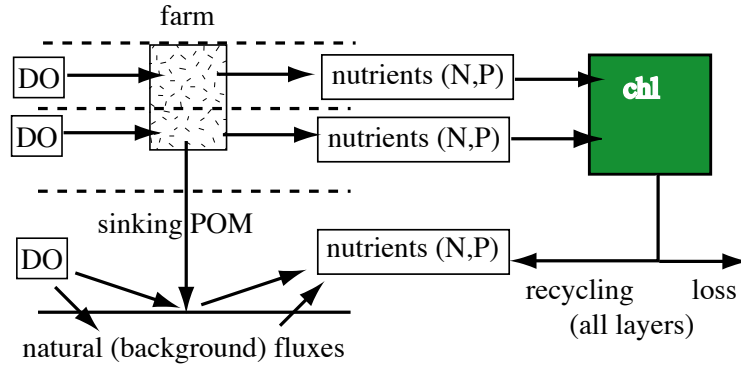


Figure 2: The farm-waste and dCSTT conceptual model. DO: dissolved oxygen; POM: particulate organic matter. Nutrients: fish excrete mainly ammonia and phosphate; seabed mineralization also releases nitrate.

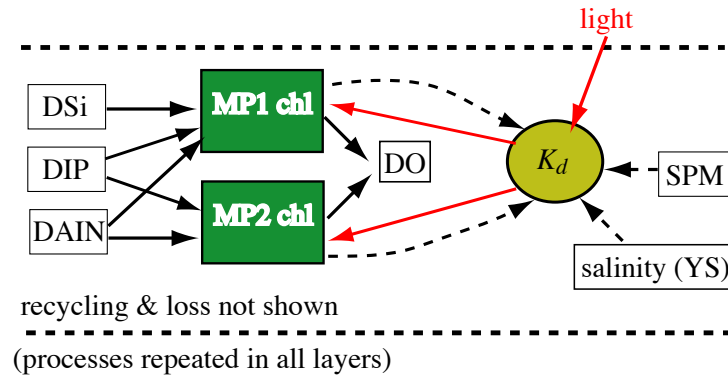


Figure 3: The LESV and bio-optical conceptual models.

- the first term gives the rate of change in the value of the variable as a result of a set of water exchanges, process k resulting in a flux $\Phi_{k,Y}$ into or out of the layer; the calculation of these processes is the function of the ACExR model;
- the second term (β_Y) is the sum of the **biological and chemical** rates of consumption and production of the variable in each cubic metre of the layer; the calculation of these fluxes is the subject of the L-ESV model or its dCSTT or sECE simplifications;
- in the third term (Γ_Y) gives the input of the variable by the **farm**, or its loss to the farm, totalled over the layer; it is also used for some other exchanges, such as benthic nutrient fluxes and surface heat flux, which take place into a layer from above or below.

The models developed during this project are *dynamic*: each contains a set of state variables, exemplified by Y , and each state variable equation allows the calculation of the rate of change of that variable. The *numerical model* in the ACExR-LESV system is a set of programs (or ‘scripts’) written in the Matlab language to simulate annual time-series of the state variables, and at the core of these scripts are routine for ‘numerical integration’ of the rate-of-change equations. Use of a monospaced font, exemplified by ACExR or LESV, indicates reference to the numerical model, and, in some cases, particular Matlab scripts.

3.2 Physical model: ACEXR

The ACEXR model was based on research into exchange and mixing processes in Scandinavian fjords (Stigebrandt, 1980, 1981, 1985, 1999) which culminated in the development of the FjordEnv model (Stigebrandt, 2001). The physical dynamics of Scandinavian fjords are not dissimilar to Scottish sea lochs, and the mathematical framework of the FjordEnv model provided a proven basis on which to develop the Scottish sea loch exchange model. The present model incorporates refinements and additional exchange processes based on scientific literature and research conducted at SAMS (Cottier et al., 2004; Inall & Rippeth, 2002; Inall et al., 2005) and on descriptions of estuarine box models developed by other researchers (Babson et al., 2006; Li et al., 1999).

Because the model allows layer thicknesses and volumes to vary dynamically, the expansion of the physical exchange term in equation 3 requires two sets of equations. Both equations are written here in a manner that emphasizes conservation of properties. The first equation deals with layer volume V :

$$\begin{aligned} \frac{\partial V_1}{\partial t} - Q_H - Q_{E12} &= 0 \\ \frac{\partial V_2}{\partial t} - Q_H + Q_{E12} - Q_{E23} &= 0 \\ \frac{\partial V_3}{\partial t} + Q_{E23} &= 0 \end{aligned} \quad (2)$$

The second equation deals with the total amount VY of a tracer or scalar property in a layer:

$$\begin{aligned} \frac{\partial(V_1 Y_1)}{\partial t} - Q_G(Y_2 - Y_1) - Q_H Y_2 - Q_F(Y_F - Y_1) - Q_{E12} Y_1 \\ - Q_{K12}(Y_2 - Y_1) + \Gamma_Y &= 0 \\ \frac{\partial(V_2 Y_2)}{\partial t} - Q_G(Y_E - Y_2) + Q_H Y_2 - Q_T(Y_E - Y_2) - Q_{E12} Y_1 \\ - \delta Q_{E23} Y_2 - (1 - \delta) Q_{E23} Y_3 \\ + Q_{K12}(Y_2 - Y_1) - Q_{K23}(Y_3 - Y_2) &= 0 \\ \frac{\partial(V_3 Y_3)}{\partial t} + \delta Q_{E23} Y_2 + (1 - \delta) Q_{E23} Y_3 + Q_{K23}(Y_3 - Y_2) &= 0 \end{aligned} \quad (3)$$

The symbol Y gives the amount per cubic metre of the generalized tracer, scalar property, or model state variable, used in equation 1. In ACEXR the tracers are heat (or temperature) and salt, which interact dynamically within the model by means of their influence on water density. The biological models add additional state variables, which interact dynamically with each other and submarine light, but not with the physical model state variables. In all cases, division, at any particular time, of layer total VY by layer volume V gives a value of Y . Layer numbers are given by subscripts 1, 2 and 3; subscript F refers to the freshwater value and E to the external value, outside the entrance to the fjordic basin.

When Y refers to temperature, the term Γ_Y is the effect of net heat flux from sun and air, Q_{SHF} , into the surface layer. The other Q terms, listed in Table 3, are the rates ($\text{m}^3 \text{d}^{-1}$) at which water is exchanged between each layer and between the sea loch basin and adjacent coastal ocean, as a result of the main physical processes.

Values of these flows are calculated by ACEXR from data for tidal ranges, wind stress, density gradients and river discharge. Vertical mixing of scalar properties between layers is based on the theory of Lozovatsky et al. (2006). Vertical entrainment occurs when a layer increases in thickness by incorporating water from an adjacent layer. Its effect on the movement of mass

Table 3: Volume exchanges in ACExR

$Q_{E,ij}$	tidal & density driven entrainment between layers i & j
Q_F	freshwater discharged into the loch
Q_G	gravitational estuarine circulation
Q_H	wind-driven vertical entrainment
$Q_{K,ij}$	vertical mixing (eddy diffusion) between layers i & j
Q_T	tidal exchange

and scalar properties between layers is based on Turner (1986). Deep water mixing due to internal tide activity is included (Stigebrandt & Aure, 1989), and deep water overturn events are simulated by intensified vertical mixing. When the intermediate layer density, ρ_2 , becomes greater than the bottom density, ρ_3 , the switch δ in 3 is set to unity and the entrainment flux, Q_{E23} is made negative, resulting in a flux of water and associated properties from layer 2 into layer 3. The magnitude of the flux is set by the magnitude of the vertical mixing during the overturning event, i.e. $Q_{E23} = -Q_{K23}$. This flux continues until either $\rho_2 < \rho_3$ or the depth of the interface between layers 2 and 3 reaches sill depth, when δ is reset to zero.

3.3 Biological models: sECE, dCSTT, L-ESV

A sequence of ‘biological’ models were used to evaluate the β_Y term, and to include the fishfarming term Γ_Y , in eqn. 1. All used the output from ACExR to provide the physical transports, and hence they are applicable only to regions of restricted exchange such as lochs or voes. Coupling of the ‘biological’ models to the open water OWExR model has not been done.

The ‘biological’ models are best understood by looking at Table 4, which lists the chemical, biological and related state variables that substitute for the generic Y in eqn 1 and that are transported by the physical model as the tracers or scalar properties of equation 3. During model development, new variables were progressively added to the *seasonal Equilibrium Concentration Enhancement* model **sECE**, giving first the *dynamical Comprehensive Studies Task Team* model **dCSTT** (Laurent et al., 2006; Tett et al., 2003) and then the *Loch – Ecosystem State Vector* model **LESV**. In practice, the Matlab package **LESV** is a single suite of calculation routines for the full model, with switches that can be changed to simplify the variable set to those in **dCSTT** or **sECE**.

The **sECE**, or ‘seasonal ECE’ model has as its state variables only nutrients, and the ‘biological term’ β_Y is set to zero. This model thus allows simulation of seasonal variation in nutrient concentrations, in the absence of phytoplankton, as a result of the interaction between: physical exchange with sea-boundary conditions; river inputs; and fish farm inputs. Although unrealistic as a simulation of conditions in a water body, the results of the sECE model provide a means to quantify the input of fish farm nutrient in relation to other sources of nutrients. The steady-state solution is an ECE, or *Equilibrium Concentration Enhancement* model.

The **dCSTT**, or ‘dynamic CSTT’ model adds a rate-of-change equation for phytoplankton chlorophyll to the nutrient equations of the sECE model, and thus allows realistic simulation of seasonal changes in the total amount of phytoplankton in each layer. The steady-state solution is the *CSTT* model for the worst-case effects of nutrient enrichment.

The main new term added to the sECE model by the dCSTT model is β_{X_i} , describing the sum of the biological changes affecting phytoplankton/microplankton chlorophyll in each layer ($i = 1, 2, 3$). These changes are growth, driven by photosynthesis and nutrient assimilation, and

Table 4: State variables in the biological models

Variable	Symbol	Units	Models
<i>nutrients</i>			
DAIN dissolved available inorganic nitrogen	N	mmol N m ⁻³	sECE dCSTT L-ESV
DIP dissolved inorganic phosphorus	P	mmol P m ⁻³	sECE dCSTT L-ESV
DSi dissolved silica	Si	mmol Si m ⁻³	L-ESV
<i>microplankton chlorophyll</i>			
MP or MP1 total or diatoms	X or X_1	mg Chl m ⁻³	dCSTT L-ESV
MP2 flagellates	X_2	mg Chla m ⁻³	L-ESV
<i>other variables</i>			
DO dissolved oxygen	O	mmol O m ⁻³	L-ESV
SPM suspended particulate matter	A	g m ⁻³	L-ESV
Tracer non-interactive tracer with decay	(Y)	amount m ⁻³	L-ESV

loss to planktonic or benthic grazers. They are given by:

$$\beta_{X_i} = \mu(S_i^N, S_i^P, I_i) \cdot X_i - L \cdot X_i \quad (4)$$

where L represents the grazing loss rate and $\mu(S^N, S^P, I)$ gives the ‘specific growth rate’ of the microplankton as a function of nutrient concentration (DAIN, S^N , or DIP, S^P), and 24-hour layer-mean illumination I in layer i . In the original CSTT model, L was a constant. In the dCSTT model it is treated as an imposed variable dependent on temperature. Grazing recycles a fraction e of microplankton N or P. The equation for a generic nutrient (either DAIN or DIP) is:

$$\beta_{S_i} = -\mu(S_i^N, S_i^P, I_i) \cdot X_i \cdot \frac{1}{q} + e \cdot L \cdot X_i \cdot \frac{1}{q} \quad (5)$$

where the *yield* q specifies the ratio of chlorophyll synthesized to N or P removed from seawater (Edwards et al., 2005; Edwards et al., 2003; Gowen et al., 1992).

The **LESV**, or ‘Loch-Ecosystem State Vector’ model divides the chlorophyll variable of the dCSTT model into two and so allows simulation of seasonal changes in the ‘balance of organisms’. It adds dissolve silica as a nutrient state variable, to allow changes in N:Si or P:Si ratio to shift this balance. It adds dissolved oxygen as a state variable, and Suspended Particulate Organic Matter, and provides the basis for a better simulation of underwater light. The latter is needed for more reliable prediction of phytoplankton growth, and also because water transparency is a good indicator of water quality in relation to eutrophication. In addition we have added a simple tracer variable, which can decay, but which does not interact with any of the biological variables. It can be used in model tests, to represent dye added in mixing studies, or the zone B concentrations resulting from the use of treatment chemicals at a farm.

The dCSTT and LESV models both make use of the concept of *microplankton* (Lee et al., 2003; Tett, 1987; Tett & Wilson, 2000) to parameterize the ‘microbial loop’ (Williams, 1981). Each microplankton compartment in the models contains pelagic bacteria and protozoa

as well as phytoplankton; the effect is to increase respiration relative to photosynthesis and to decrease the yield of chlorophyll from nutrient, because the bacteria and protozoa take some of the nutrient uptaken by the phytoplankters, and respire organic matter gotten from them by grazing (protozoa) or uptake of dissolved organic matter (bacteria). In the case of the 2 microplanktons of LESV, we have used a simplified version of equations in the PROWQM model (Lee et al., 2002; Tett & Lee, 2005).

In each of the models, a submodel based on Black (2001) converts feed supplied to fish into releases of DAIN, DIP and oxygen demand into each layer of the model, as shown in Figure 2.

Finally, calculation of mean illumination in each layer uses simplifications discussed elsewhere (Tett, 1990; Tett & Walne, 1995). A linear relationship is assumed between growth rate and layer 24-hour mean photosynthetically effective irradiance, I_i (in $\mu\text{Einstein m}^{-2} \text{s}^{-1}$):

$$\mu(I) = \alpha \cdot (I_i - I_c) \quad (6)$$

where α is an appropriate *photosynthetic efficiency* and I_c is the *compensation irradiance* at which photosynthesis and respiration are equal when summed over 24 hours. The mean irradiance in layer 1 is calculated from

$$I_1 = m_1 \cdot I_0 \cdot \frac{1 - e^{-k_{D,1}H_1}}{k_{D,1}H_1} \quad (7)$$

This equation includes a parameter m_1 that corrects for non-linearities in the surface layer; modifications are used for deeper layers. The equations require a value of the *diffuse attenuation coefficient*, $K_{D,i}$ for photosynthetically active light in each layer. These are calculated, for each day, from

$$K_d = m_0^{-1} \cdot \sqrt{a^2 + k_m \cdot a \cdot b} \quad (8)$$

where m_0 is the mean cosine of underwater light in the absence of light-absorbing components, and a is, the beam absorption of light due to chlorophyll, suspended particulate matter (SPM) and dissolved ‘yellow substance’. The latter is estimated from salinity. The term b is the beam scatterance of light due to SPM. The equation is taken from submarine optical theory (Bowers et al., 2000; Kirk, 1994) with values for the parameters and the effects of unit amounts of chlorophyll, SPM and salinity taken from recent CEFAS/EA/AFBI/SEPA observations by M.Devlin and colleagues.

4 Methods

As already mentioned, the numerical models were implemented using Matlab, which allows programs (‘scripts’) to be exchanged between Windows, MacOS and Unix platforms. ACExR used a forward-euler integration method with a time-step of 0.01 day; LESV models used the Matlab `ode23` integration function. Running a simulation required:

- data with which to initialize the models
- boundary condition data

and evaluating the results of a simulation required

- observations with which to compare the simulation
- statistical methods for making the comparison

Obtaining adequate data, and putting it into the correct form, to provide good boundary conditions for the models, proved to be laborious and difficult, and some of these difficulties will be shown below. Because the numerical models are designed to calculate a year’s worth (365 daily values) of each state variable in each layer, the ideal boundary condition data set included 365 values of each state variable outside the basin and in the river, plus 365 values of meteorological variables, for the year to be simulated. The task was a little simplified because some variables (e.g. chlorophyll) had values of zero in rivers. Where sparser data were available for a particular year, we used various methods to interpolate to daily values. When flow gauge data were not available, river flows were calculated from precipitation data. When adequate data were not available for a site and specific year, we sought to make a *climatology* from data for several or many years. Detailed accounts of this work are given in milestone reports 3 – 5.

Simulations were run, and model tests were made, mainly for loch Creran, in which relevant observations were first made during the 1970s (Tett & Wallis, 1978) and again in the 2000s (Laurent et al., 2006) while a 1500 tonne farm was in place. Scottish Sea Farms provided feed data for this unit. ACExR was also used to simulate conditions in the inner basin of adjacent loch Etive, using data from SAMS studies in 1999-2001. Both these lochs lie on the west coast of Scotland, a little north of Oban, and exchange with the Firth of Lorne.

Initial conditions for the models were taken from typical values of the state variables in January. Loch hypsometry was taken from a digitized version of the ‘Sea lochs catalogue’ (Edwards & Sharples, 1986), which was read by the ACExR script.

Statistical assessment involved comparison of observations and simulations. Pairs of values of observed values of state variables, and the values simulated for the same day, were extracted. Linear regression was used to calculate the proportion, r^2 of (squared) observed variation that was explained by the model.

In the case of ACExR, the *root mean square error* between model and data, was then calculated. It is given by

$$E_{RMS} = \left[\frac{1}{N} \sum_{j=1}^N (p_j - o_j)^2 \right]^{\frac{1}{2}} \quad (9)$$

where p_j and o_j are predicted and observed values respectively and N is the number of data points in the calculation. Model skill was estimated from

$$d^2 = 1 - \frac{\sum_{j=1}^N (p_j - o_j)^2}{\sum_{j=1}^N (|p_j - \bar{o}| + |o_j - \bar{o}|)^2} \quad (10)$$

where \bar{o} is the arithmetic mean of the observed data. A perfect agreement between model and data would give $d_2 = 1$, with decreasing values indicating declining performance.

In the case of the LESV models, a *Major Axis Regression* (MAR) was fitted to the plots of observations against simulations, and the confidence intervals of the slope and intercept of this regression compared with the expectation of slope = 1 and intercept = 0 (Mesple et al., 1996; Portilla & Tett, 2007). A model is judged *excellent* if the slope of the MAR regression is not significantly different from 1 and the intercept is not significantly different from zero. *Good* refers to cases where either the intercept or the slope (but not both) differs significantly from the expectation. In the case of a *fair* model, both differ significantly from expectation, but a significant part of the variance is explained. A *bad* model is incapable of explaining any significant part of the variance.

5 Results

5.1 Overview

Table 5 summarizes years, lochs and models that have been tested. Full details are given in milestone report 5. Here we have space to show only the best case for ACExR and an ‘excellent’ and a problematic case for LESV.

Table 5: Tests of models. BC refers to (atmospheric, marine, and riverine) boundary conditions; RMS is the root mean square error; r^2 gives the proportion of observed variance that is explained by the model.

model	loch	year	results
ACExR	Creran main basin	1975	temperature RMS = 0.5°C , $r^2 = 0.97$, salinity RMS = 2.4, $r^2 = 0.15$; poor salinity fit due to poorly-known BCs: river flow from rainfall, sea-boundary climatology;
		1978	temperature RMS = 0.7°C , $r^2 = 0.95$, salinity RMS = 1.0, $r^2 = 0.67$; better salinity fit because better-known BCs: gauged river flow, observations in Firth of Lorne;
		2003	temperature RMS = 0.7°C , $r^2 = 0.96$, salinity RMS = 1.1, $r^2 = 0.06$; poor salinity fit due to poorly-known BCs, as in 1975
	Etive in- ner basin	2000	temperature RMS = 0.8°C , $r^2 = 0.89$, salinity RMS = 1.8, $r^2 = 0.85$; well-known BCs: see text
LESV	Creran main basin	1975	chlorophyll $r^2 = 0.68$, DAIN $r^2 = 0.88$, DIP $r^2 = 0.75$, MAR fit ‘excellent’ for all; some good BCs: see text
		2003	chlorophyll $r^2 = 0.48$, DAIN $r^2 = 0.97$, DIP $r^2 = 0.86$, MAR fit ‘excellent’ for nutrients; some good BCs: see text

5.2 ACExR, Loch Etive, 2000

The Restricted Exchange Environments (REES) experiment took place during 1999 to 2001. From July 1999 March 2001, SAMS undertook regular (approximately monthly) sampling trips in Loch Etive. During each trip, profiles of conductivity-temperature-depth (CTD) were made and water samples collected at 8 fixed station locations in both basins of the loch. This database was used to initialise and test the model performance.

For this simulation, river flows came from a gauge on the River Awe and was corrected to account for the whole Etive catchment. Wind speed data came from the Tiree meteorological station, and heat flux data were from Dunstaffnage, and the coastal temperature and salinity profiles came from a REES CTD station outside the entrance to Etive. However, attempts to simulate the whole of Loch Etive were not successful: the model failed to reproduce the mixing that occurs over the entrance sill at the Falls of Lora. Instead, the model was run for the upper basin of Loch Etive, upstream of the sill at Bonawe, with boundary data taken from a station in the deepest part of the lower basin. The forcing data are shown in Figure 4.

The simulation for 2000 is shown in Figure 5. The time series for each layer were compared with temperature, salinity and density data taken from fixed depths of 3 m, 15 m and 110 m and averaged over 5 stations, except for the bottom layer (115 m) which used data from the deepest station only. The model captured the observed seasonal cycle of temperature and salinity.

It simulated more high-frequency variability in both parameters, particularly for the surface layer, than is apparent from the monthly observations. It is also notable that the simulation reproduced the observed deep water renewal event that occurred in April-May 2000, which led to an initial decrease in temperature and increase in salinity of the bottom water followed by a gradual increase in temperature. The model also captured the effect of the seasonal heating cycle on the temperature of the surface layer.

The errors on the temperature, salinity and density predictions are presented in Table 6. The model captured over 80% of the variance in the observed signals and had an average skill level of over 0.9. The RMS error for temperature was less than 1°C, about 10% of the temperature range. Similarly, the RMS errors for salinity and density were less than 2, which is less than 10% of the observed range of values.

The simulations showed that the most important exchange flows were those due to tidal exchange (Q_T), the estuarine circulation (Q_G), and wind-stirred entrainment (Q_H). During the deep water overturning event of April-June 2000, and intermittently in the following period, the vertical mixing flux (Q_{K23}) dominated the flux of water properties. The entrainment flux due to wind stirring was much stronger in Loch Etive than in Loch Creran. Exchange rates for the surface layer were much stronger in Loch Etive than in Loch Creran, a result of the stronger freshwater flows, estuarine circulation and tidal entrainment (Q_{E12}) due to the stronger flows over the entrance sill. Conversely, the exchange rates in the intermediate layer were weaker than in Loch Creran. The range of exchange rates correspond to a range of flushing times from 0.4 days at the surface to 115 days in deep water.

Table 6: Fit statistics for ACEXR simulations of loch Etive, 2000.

error	variable	layer 1	layer 2	layer 3	mean	
r^2	Temperature	0.97	0.83	0.88	0.89	explained
	Salinity	0.94	0.76	0.83	0.85	part of
	Density	0.93	0.75	0.80	0.82	variance
RMS	Temperature	0.85	1.24	0.42	0.84	°C
	Salinity	2.53	2.49	0.47	1.83	(psu)
	Density	2.03	1.85	0.24	1.38	kg m ⁻³
skill	Temperature	0.98	0.93	0.94	0.95	out
	Salinity	0.97	0.93	0.80	0.90	of
	Density	0.96	0.92	0.82	0.90	one

5.3 LESV, Creran, 1975 and 2003

Simulations with LESV were made for 1975 and 2003, using standard parameters and, for 2003, feed data provided by Scottish Sea Farms Ltd. Standard parameters include grazing loss rates of 0.1 d⁻¹ for both microplanktons. For boundary/forcing conditions, UKMO (via BADC) solar radiation and precipitation data recorded at Dunstaffnage during 1975 or 2003, were used, with precipitation corrected for higher values in the mountains around loch Creran (Tyler, 1984). A river flow model (see milestone report 3), calibrated against SEPA flow gauge data for 1978 in the river Creran, gave total freshwater discharges; they were multiplied by constant riverine nutrient concentrations, of 0.03 μM DIP, 10 μM DAIN and 6 μM DSi, to give nutrient discharges. Sea-boundary data for nutrients (DAIN, DIP and DSi) and chlorophyll in 1975 were based on Creran deep-water samples (Jones, 1979); for 2003 the data were taken from

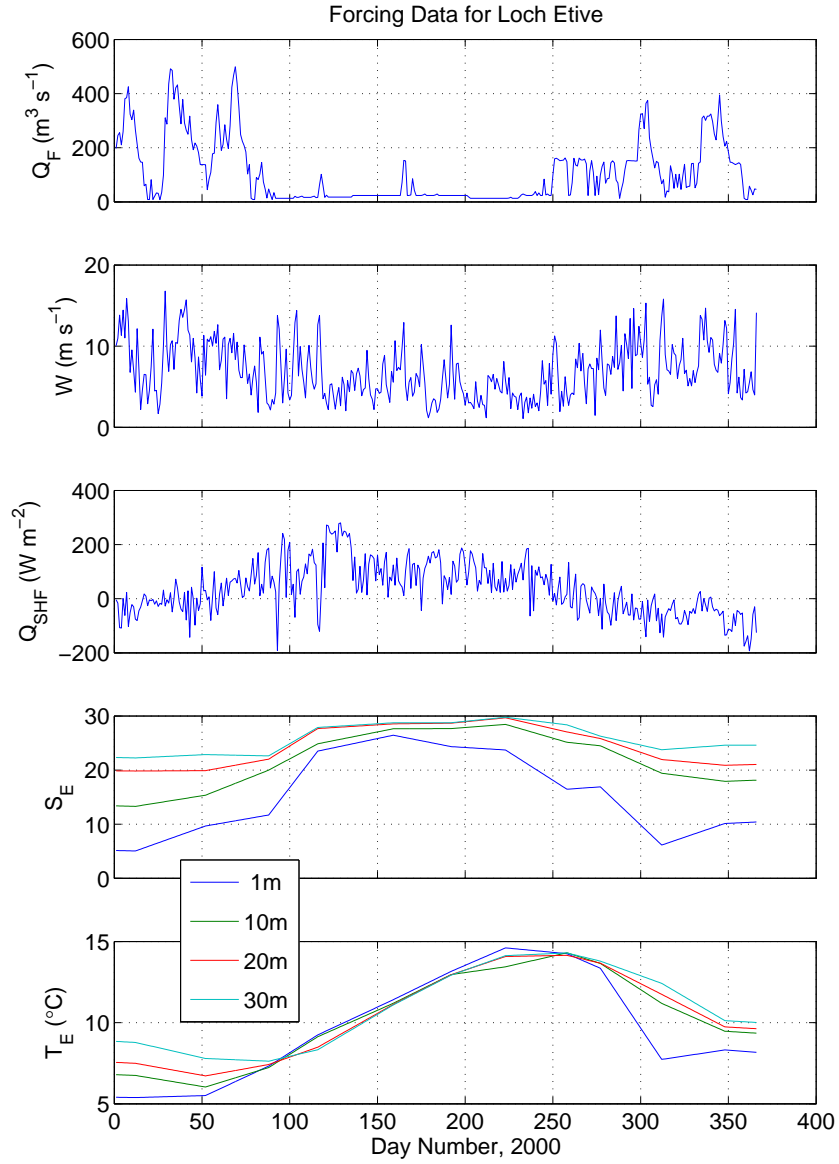


Figure 4: Daily boundary data for 2000 used to force the ACExR simulation of the upper basin of Loch Etive: riverine freshwater discharge (Q_F , $\text{m}^3 \text{s}^{-1}$), wind speed (W , m s^{-1}), net surface heat flux (Q_{SHF} , W m^{-2}), coastal salinity (S_E) and temperature (T_E , $^{\circ}\text{C}$) at 4 depths (1, 10, 20, 30 m).

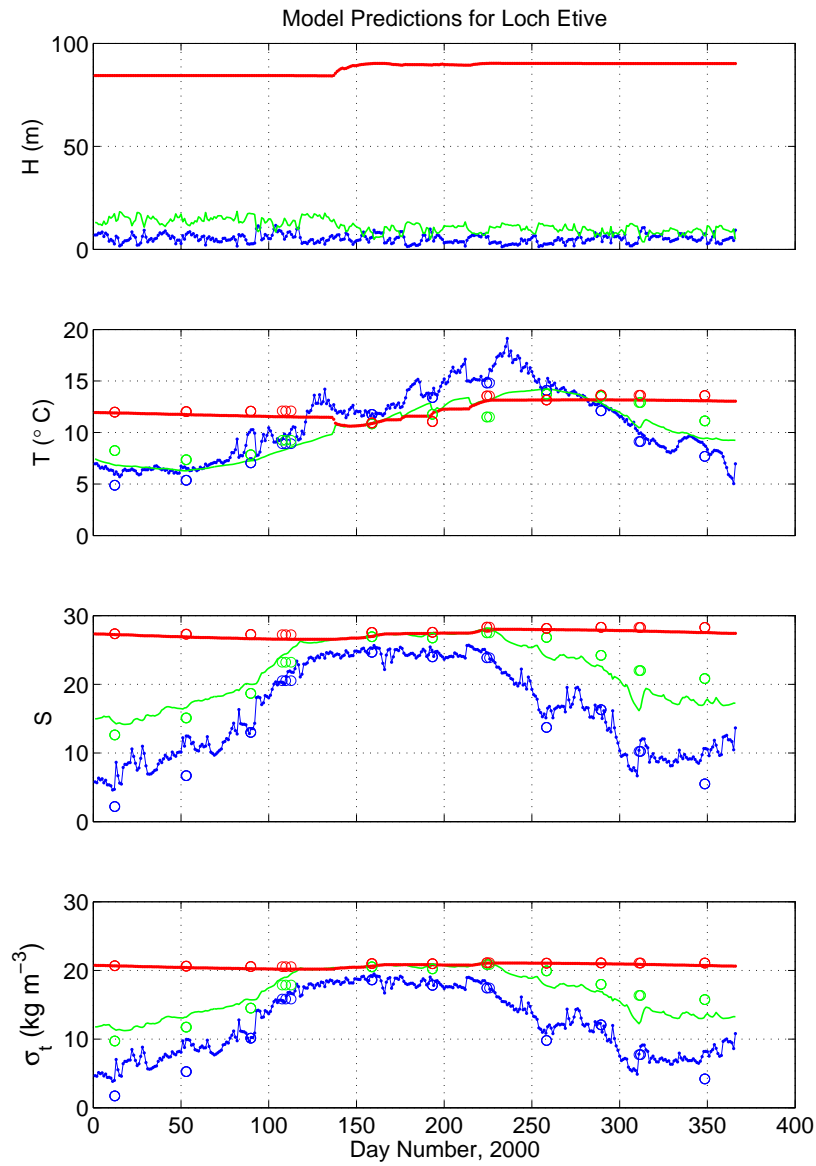


Figure 5: Daily layer parameters predicted by the physical exchange model from the simulation of Loch Etive for 2000: layer thickness (H , m), temperature (T , $^{\circ}\text{C}$), salinity (S) and density anomaly (σ_T , kg m^{-3}). Results for layers 1 (surface), 2 (intermediate) and 3 (deep) are coloured blue, green and red respectively. Model results (solid lines) and data from the SAMS REES experiment (open circles) are shown.

observations (Fehling et al., 2006; Laurent, et al., 2006) in the Firth of Lorne until day 150 and thereafter from climatology. Boundary ratios of microplankton 1 to microplankton 2 chlorophyll were taken from microplankton climatology based on observations in 1970-71 (Tett, 1973).

Observations of total chlorophyll and two dissolved limiting nutrients (DAIN and DIP) were those measured in samples collected from the upper layer of the main basin of Loch Creran in 1975 (Jones, 1979) and 2003 (Laurent et al., 2006). The chlorophyll data were log-transformed to correct for heterogeneity of variance (Tett & Wallis, 1978).

Results for 1975 are shown in Figure 6 and results for 2003 are shown in Figure 7. Statistics of fit were given in Table ???. The fit was ‘excellent’ for 1975, confirming the visual impression in Figure 6 of good agreement between the simulated and observed seasonal cycles. The results for 2003 are more problematic. The fit statistics were as good for DAIN and DIP in 2003 as in 1975, but the fit for chlorophyll was worse; the simulations substantially over-estimate the chlorophyll.

During the 1970s, loch Creran phytoplankton was dominated by diatoms (i.e. by MP1) (Tett et al., 1981, 1985)). Microscopic analysis of water samples taken between 2003 and 2007 suggests that there has been a major change. The important diatom, *Skeletonema costatum*, which formerly made up more than 90% of the spring phytoplankton bloom in the loch, has become several orders of magnitude less abundant, with the result that the season of phytoplankton dominance is now shorter. Although dinoflagellates and photosynthetic flagellates have increased to some extent, they have by no means compensated for the loss of diatoms. The simulations do not reproduce this change in the MP1:MP2 ratio, and it is presently unclear what has caused it.

6 Estimation of assimilative capacity

The models described in this report were developed to estimate the *assimilative capacity* of a sea-loch or voe. This capacity is defined, here, as the maximum rate at which a water body can receive a waste material without breaching one or more *Ecological Quality Objectives* (ECoQOs).

These Objectives are best understood in relation to the *DPSIR* system for relating human activities to impacts on ecosystems and the response made by society. As a result of a *Driver*, such as the development of fish-farming, an increase in a *Pressure*, such as nutrient loading, may change the *State* of an ecosystem, resulting in a *Impact* such as eutrophication that is deemed to be ecologically, socially or economically undesirable. Models can capture some of the changes in Pressure and State, and interpret the latter as Impacts. Table 7 lists some of the pressures and the state changes that can be investigated using the **L-ESV** model.

In addition, the **sECE** and **dCSTT** models, and the **tracer** mode, available within the LESV package, add other tools, as summarized in Table 8

The Ecological Quality Objectives in table 7 are merely indicative of possible values, and are stated to make our subsequent demonstrations more concrete. They are not meant to be recommended values - that is a different issue, which has been addressed by the SARF011 project (Crane et al., 2006). We have taken standards from the report of this project, adding some restrictions given in table 7.

For demonstration purposes we have started from the 2003 standard run of LESV for loch Creran. However, because this simulation over-estimated chlorophyll, as reported above, and because we have some reservations about some of the parameter values used in this run, we refer to the simulated water body as *loch Erewhon*. For demonstration purposes it has been given a higher turbidity, and a lower deep-water mixing rate, than is likely to be the case for water bodies of the size and depth of loch Creran.

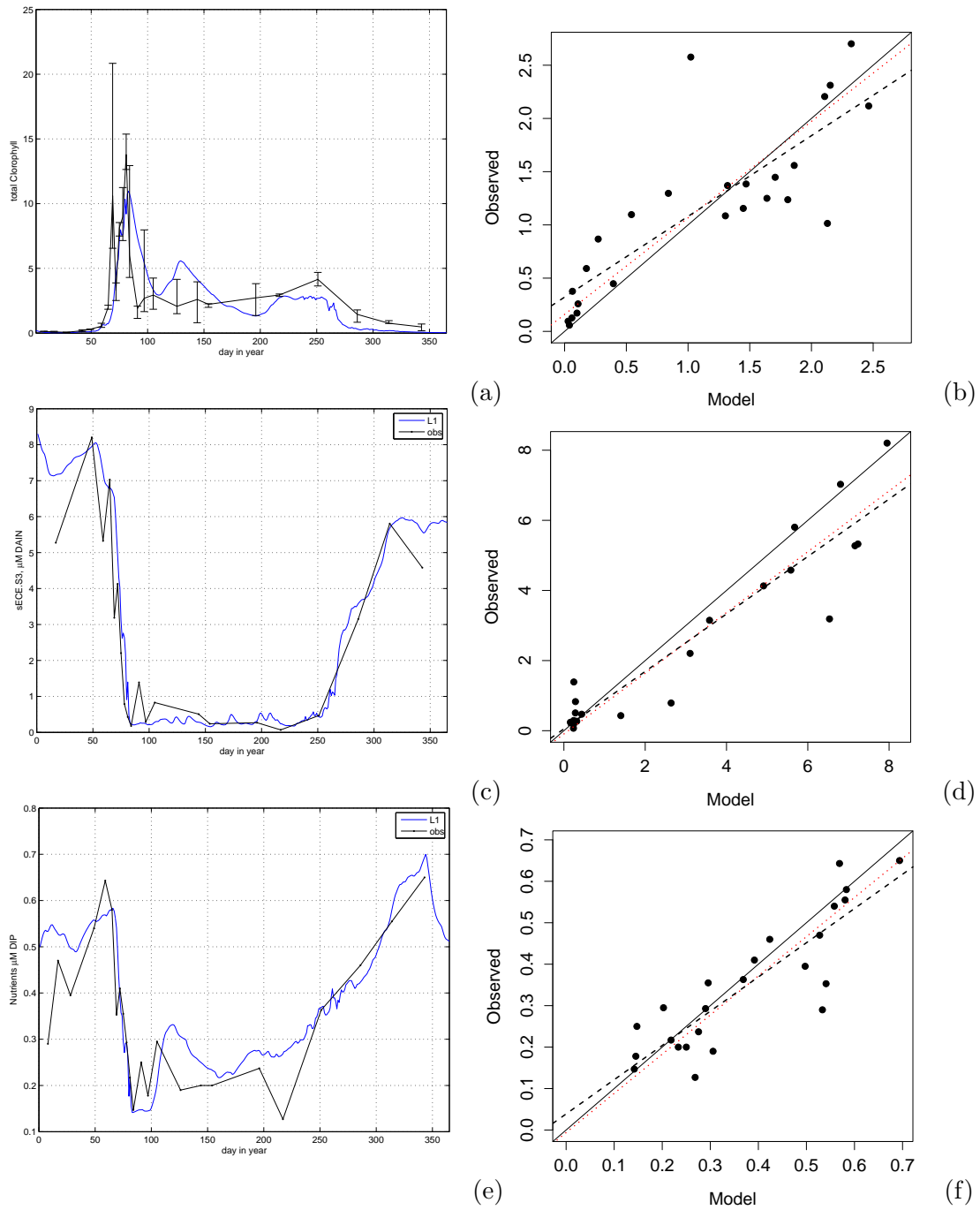


Figure 6: Test of the LESV model for 1975. The left column contains the time series of observed values (black) and simulated values (blue) for total chlorophyll (a) DAIN (c) and DIP (e). The error bars in (a) span quantiles 5 to 95, so they contain 90% of the data. The right column contains plots of simulated values on the x-axis versus observed median values on the y-axis for $\ln(\text{mg chl m}^{-3} + 1)$ (b) $\mu\text{M DAIN}$ (d) and $\mu\text{M DIP}$ (f). The continuous line is the 1:1 relationship expected in the case of a perfect fit. The broken black line is the relationship found by least squares regression and the dotted red line is the relationship found by MAR regression.

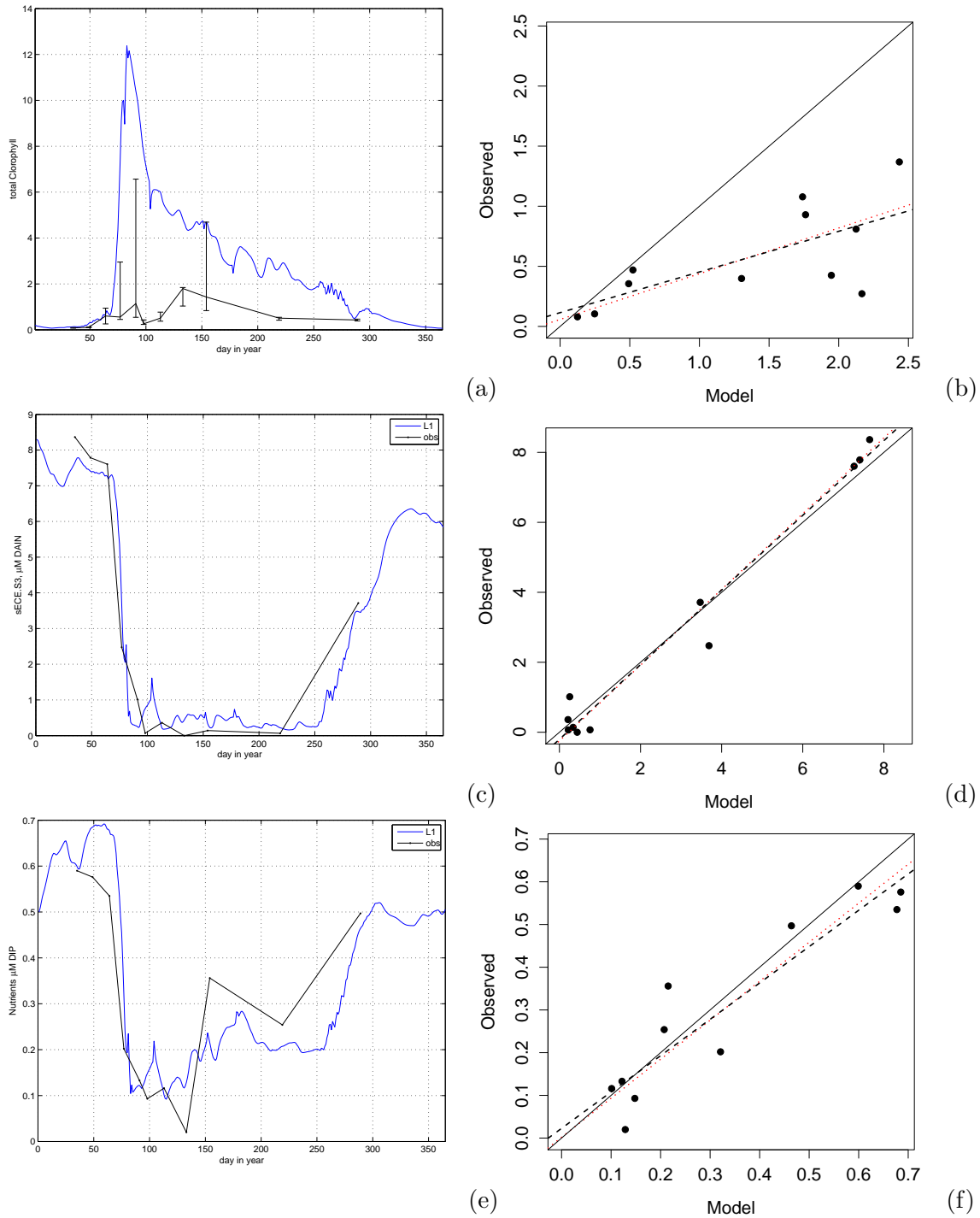


Figure 7: Test of the LESV model for 2003. The left column contains the time series of observed values (black) and simulated values (blue) for total chlorophyll (a) DAIN (c) and DIP (e). The error bars in (a) span quantiles 5 to 95, so they contain 90% of the data. The right column contains plots of simulated values on the x-axis versus observed median values on the y-axis for $\ln(\text{mg chl m}^{-3} + 1)$ (b) $\mu\text{M DAIN}$ (d) and $\mu\text{M DIP}$ (f). The continuous line is the 1:1 relationship expected in the case of a perfect fit. The broken black line is the relationship found by least squares regression and the dotted red line is the relationship found by MAR regression.

Table 7: Pressures and State changes that can be studied with L-ESV

Loading	Pressure	L-ESV state variable that might change	Indicative EcoQO(s)
Fish respiration and organic waste input	consumption of oxygen	dissolved oxygen	dissolved oxygen shall not fall below 5.7 mg L^{-1} (Crane)
pelagic N and P excretion by fish and benthic input from mineralized organic waste	increase in DAIN and DIP	increase in phytoplankton biomass as chlorophyll	DAIN shall not exceed $10 \mu\text{M}$ (Crane); maximum (summer) chlorophyll shall not exceed 10 mg m^{-3} (Crane + restriction to summer)
	change in elemental ratios, especially N:Si	'balance of organisms' in MP1 and MP2	(winter) N:Si ratio shall not exceed 2:1 (Crane + restriction to winter); ratio of MP1 chl to MP2 chl shall not change by more than 50% from a reference condition
decay of extra primary production	consumption of oxygen	dissolved oxygen	dissolved oxygen shall not fall below 5.7 mg L^{-1} (Crane)

Table 8: Use of LESV options in relation to Assimilative Capacity

Model or mode	Use
sECE	to compare lochs in terms of nutrient enrichment in the absence of phytoplankton use, and to estimate AC relative to a nutrient EcoQO
dCSTT	to compare lochs in terms of maximum chlorophyll and to estimate AC relative to a chlorophyll EcoQO
L-ESV	to estimate AC against a number of EcoQOs, as described in Table 7
tracer	to estimate the AC for a decaying tracer against a zone B EQS for that tracer

A series of simulations of Erewhon were made, in which the feed input for a farm of 1500 tonnes annual production was multiplied by 0, 1, 2, 4, 6, 8 and 10. Example results for x1 and x10 are shown in figures 8 and 9. Most of the sub-plots include a threshold derived from an EcoQO in table 7.

Table 9: Indicators

Indicator	Layer	Derivation	during Days	standard
Maximum winter DAIN	1	Maximum (daily) value	1 - 90	10 μM
Maximum Summer chlorophyll	1	Maximum (daily) value	91 - 270	10 mg m^{-3}
Maximum diffuse attenuation	1	Maximum (daily) value	1 - 365	none
Minimum dissolved oxygen	3	Minimum (daily) value	1 - 365	5.7 mg L^{-1} , 170 μM

Some of the time-series in these Figures have been analysed for the extraction of values of statistics that may be used as the indicators of *pressure*, *state* or *impact* listed in Table 9. Values of these indicators have been plotted against feed multiplier in Figure 10. They suggest that it is the capacity of loch Erewhon’s deep water to assimilate oxygen-consuming wastes that is the most limiting to the size of a farm.

Loch Erewhon’s capacity to assimilate nutrients (or dilute them by exchange with sea-water) is relatively greater, and the use of a ‘Winter Nutrient’ EcoQO would allow a several-fold increase in the size of the existing farm. In this particular version of loch Creran, chlorophyll concentrations never breach a summer EcoQO, whatever the farm nutrient input, because microplankton growth is self-limiting. Under the turbid conditions that have been simulated for Erewhon, self-shading restricts submarine light and thus slows growth of the flagellate microplankton. Simulated silica limitation during summer restricted growth of diatom microplankton. Together, these limitations prevented summer chlorophyll from exceeding 7 mg m^{-3} .

Another approach to setting an assimilative capacity is to consider the extent to which the natural pattern of fluxes are disturbed by the emplacement of a fish-farm. The model allows the calculation of changes in each state variable due to known processes. Figures 11 and 12 show the contributions of physical, biological and farm processes to changes in DAIN and dissolved oxygen. Each flux has units of amount $\text{m}^{-3} \text{ d}^{-1}$, and includes the components shown in Table 10. Where the flux includes an exchange with the sea-bed, air or boundary, the quantitative effect depends on layer volume, which changes from day to day.

Table 10: Explanation of the fluxes

biological	the relevant β_Y term, including microplankton use or production, and pelagic recycling
farm	the relevant $\Gamma_Y \cdot V^{-1}$ term, including farm input to water column and via sediment, and background benthic fluxes
physical	the relevant physical transport flux divergence $V^{-1} \cdot \sum \Phi_Y$, including river inputs, exchange with sea-boundary conditions, and air exchange

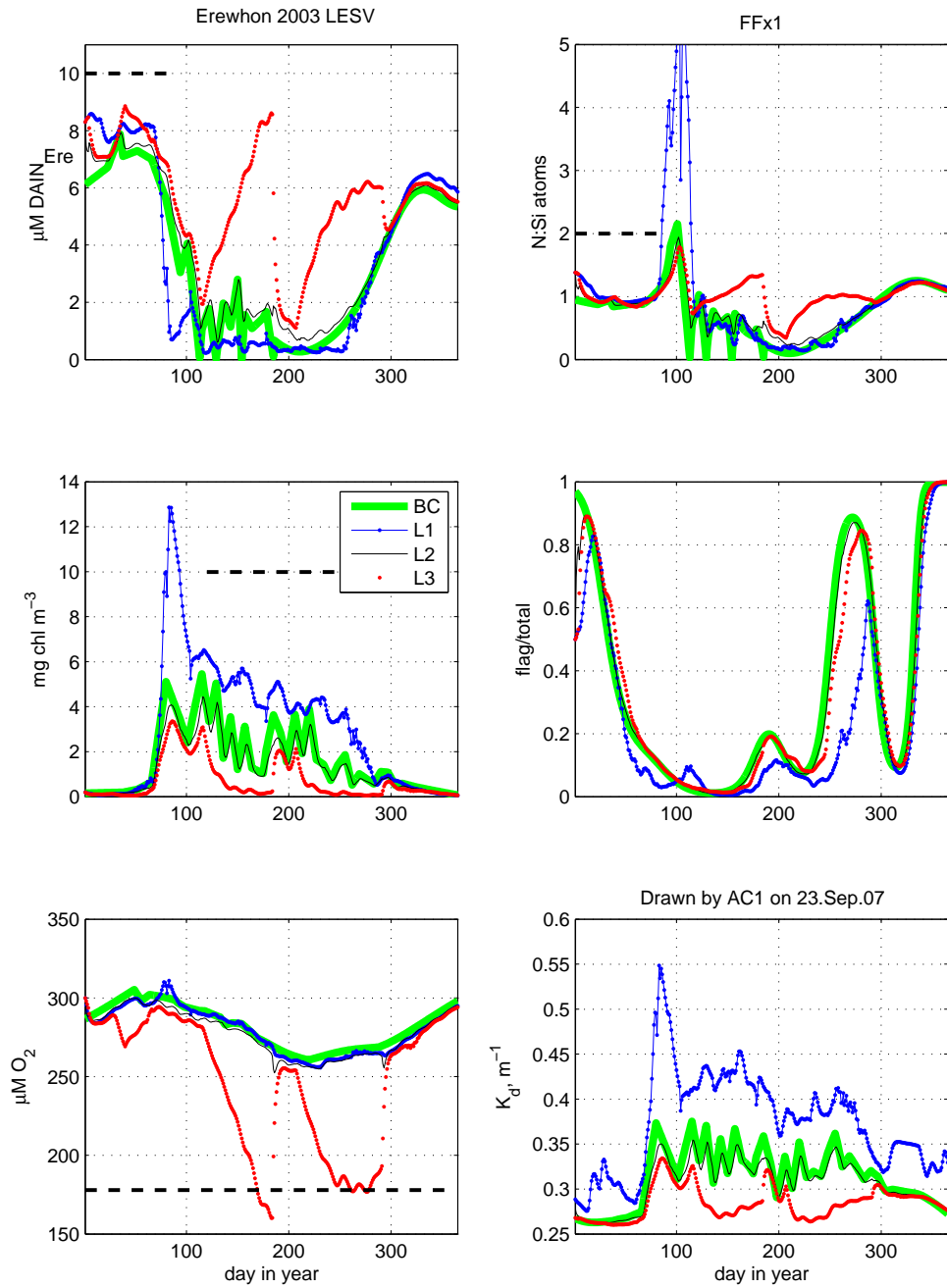


Figure 8: Loch Erewhon with 1,500 tonne farm. The dashed lines in some sub-diagrams show thresholds taken from Table 9). In each sub-diagram, simulated annual time-series are plotted for the sea-boundary conditions (BC in the legend); and for layers 1 to 3 (L1, L2, L3 in the legend).

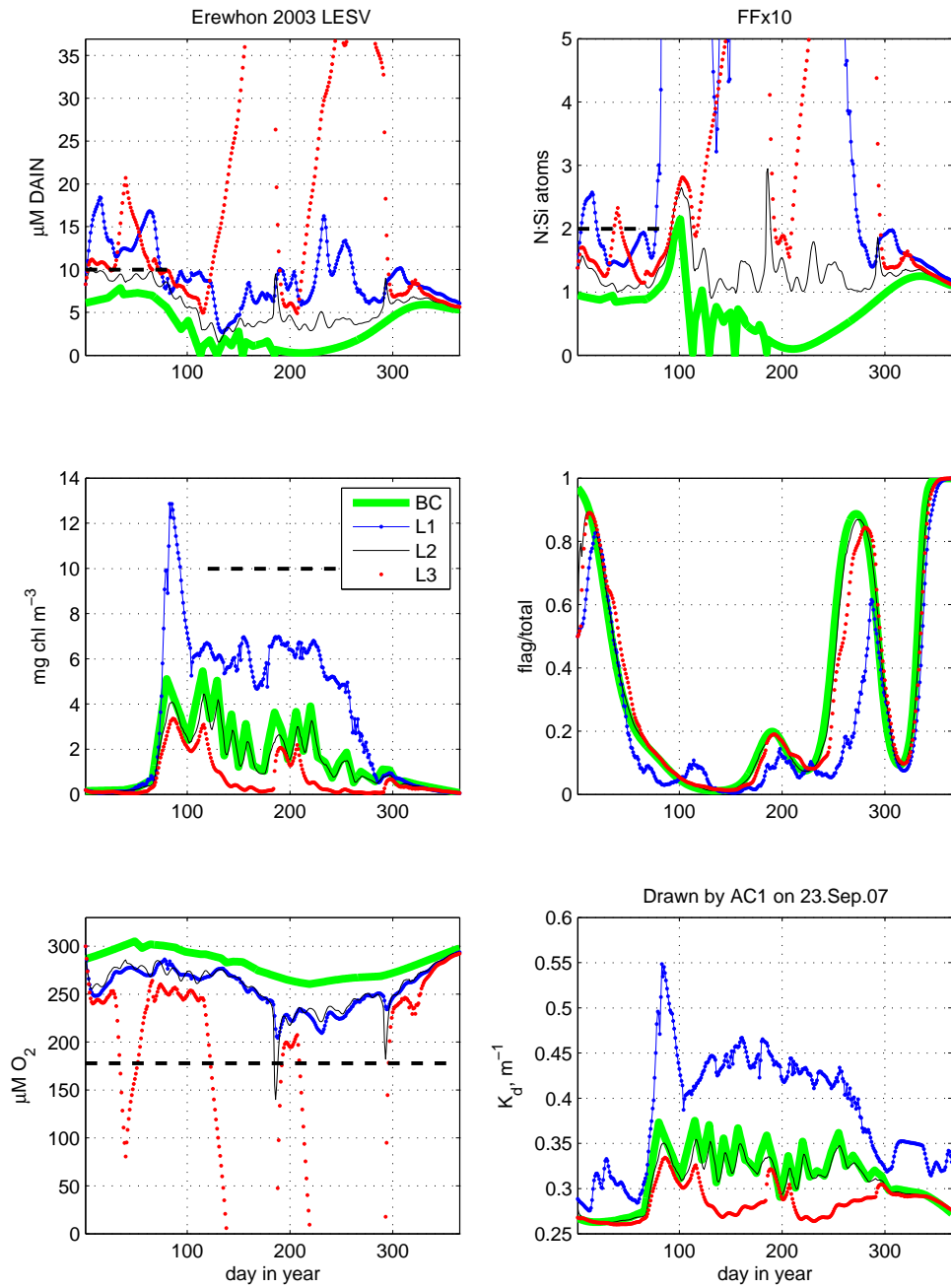


Figure 9: Loch Erewhon with 15,000 tonne farm. The dashed lines in some sub-diagrams show thresholds taken from Table 9). In each sub-diagram, simulated annual time-series are plotted for the sea-boundary conditions (BC in the legend); and for layers 1 to 3 (L1, L2, L3 in the legend).

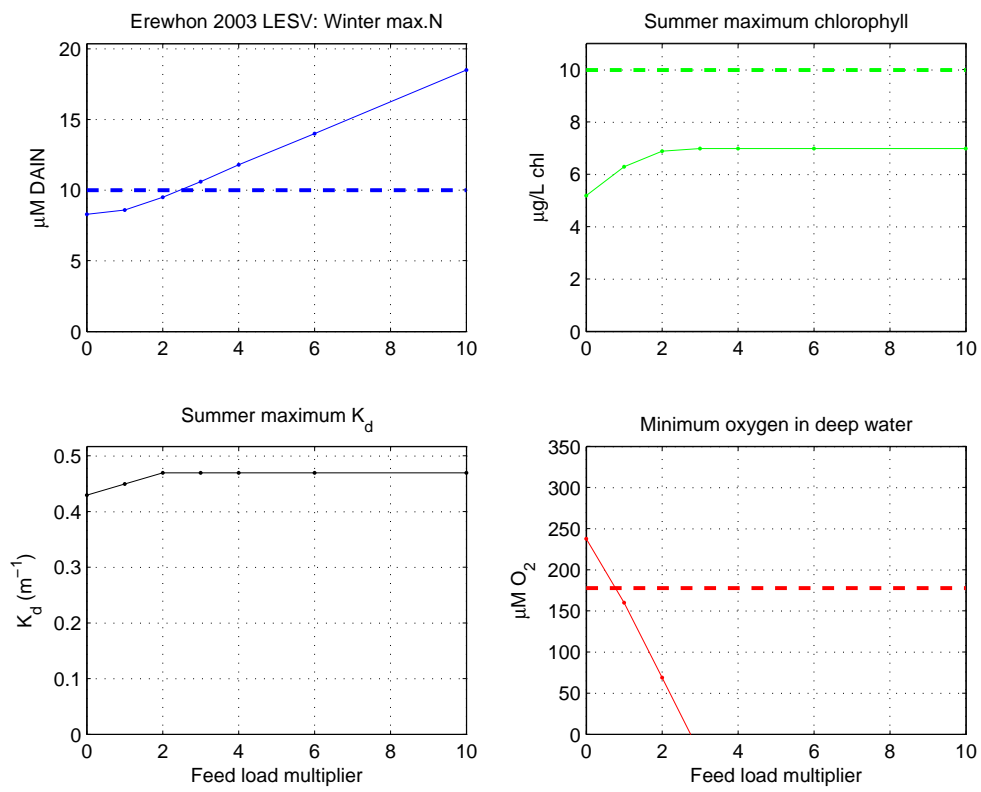


Figure 10: Estimation of assimilative capacity for Loch Erewhon. Thresholds (from Table 9) shown by dashed lines.

At a loading (x1) corresponding to a 1,500 tonne consented production (figure 11), the simulated farm has an effect on the fluxes in loch Erewhon, but the natural balance is preserved. This balance is that between physical transports and biological consumption or production. Under normal conditions, water movements, on average, bring nutrients into the loch, where they are removed by the biological processes in layer 1. Similarly, water transport of oxygen, and air-sea gas exchange, are balanced by oxygen produced by photosynthesis in layer 1 and consumed by decay in layer 2 and 3.

In contrast, at a loading of x10 (figure 12), the effect of the farm overwhelms the other fluxes – which is to say that the balance between removal and supply is now struck between, on the one hand, the effects of the farm, and on the other, the physical transports and biological processes. In this case, loch Erewhon becomes an exporter of nutrients, rather than an importer. This, and the changes in ecosystem function implied by the new balances of fluxes, labels the farm effect as undesirable, irrespective of specific EcoQOs or detailed assumptions used in the simulations..

7 Discussion

7.1 ACEXr and physical modelling

ACEXr parameterizes known physical processes in Scottish sea lochs to simulate annual cycles of temperature, salinity and exchange rates. Given the simple nature of the model (relative to, say, a three-dimensional hydrodynamic model), the model performs well in reproducing observed time series of temperature and salinity from two sea lochs, Creran and Etive, from a total of four years of observations. RMS errors for temperature and salinity were typically less than 1 ° C and of the order of 1 respectively. Net exchange in both systems tended to be a balance between tidal exchange, the estuarine circulation and vertical mixing. Other volume fluxes, due to entrainment and wind stirring, tended to be an order of magnitude less. The model has also demonstrated a capability to simulate the effects (though not the dynamics) of deep water overturn events, when the bottom water in a sea loch basin is flushed out and replaced by denser incoming coastal water.

Some discrepancies between model and data inevitably remain. The model failed to reproduce major freshening events during 1978 that lowered the intermediate and deep water salinities in Loch Creran. In the 1975 simulation, lowered salinities during the first 30 days of the year were not reproduced, and in 2003, the modelled salinities throughout the water column were too high. The model appears to under-predict the exchange between the surface layer and the underlying intermediate layer, and possibly to over-predict the exchange between the intermediate and deep layers. Entrainment is modelled according to the results of laboratory studies (Turner, 1986), but recent studies (Princevac et al., 2005) have suggested that these experiments underestimate the entrainment in natural flows because the laboratory flows have been conducted at much lower Reynolds Numbers ($Re < 10^3$) than occur in natural flows ($Re \sim 10^7$). A revision of the entrainment algorithm utilised in the ACEXr model may lead to enhanced exchange between surface and intermediate layers. This may also go some way to explaining why the model was unable to simulate the salinity transition across the Falls of Lora in Loch Etive, where the vertical exchange of water from surface to depth is very high.

The model results also indicate that, in order to hindcast observed time series, the choice and quality of boundary forcing data are very important. The simulation of Loch Creran in 2003 suggests that using rainfall data from a local observation station may severely underestimate the total river discharge into the loch. Rainfall can be highly spatially variable, and the resulting river flow data unrepresentative of actual flows. In addition, the use of a year-averaged factor

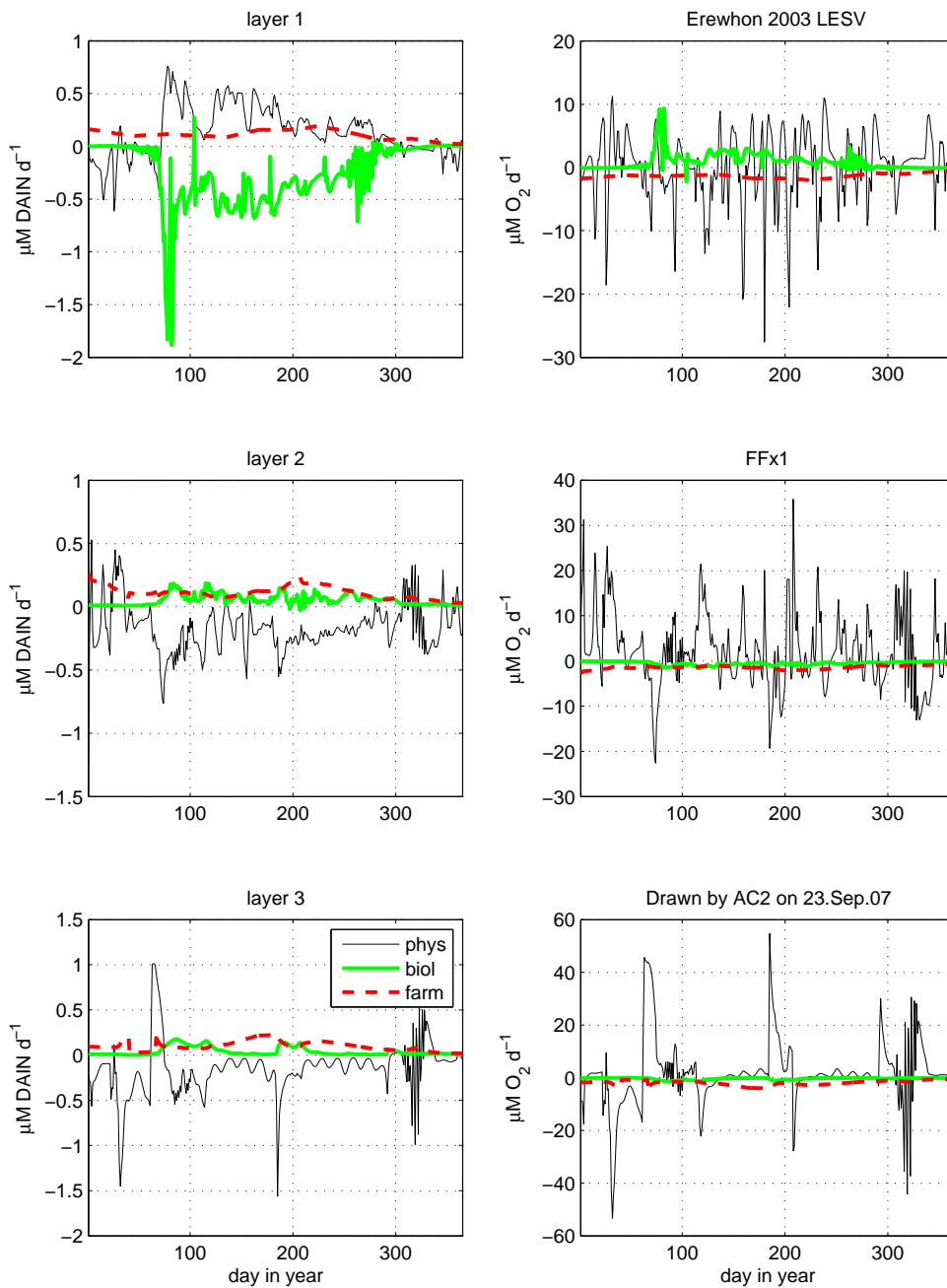


Figure 11: Fluxes: Loch Erewhon with 1,500 tonne farm. Rows show layers. Left hand column for DAIN flux, right hand column for fluxes in dissolved oxygen. See Table 10 for components of **physics**, **biology** and fish **farm** and benthic fluxes. A +ve flux is a gain to that layer. In the simulation without a fish-farm (not shown), the state of the loch resulted from a balance between physical transports of nutrients or oxygen (black lines), and the consumption or production of nutrients or oxygen by biological processes (green lines). This is still largely the case with a simulated 1,500 tonne farm, although the effects of the fish-farm (red dashed lines) disturb the balance somewhat in layers 2 and 3.

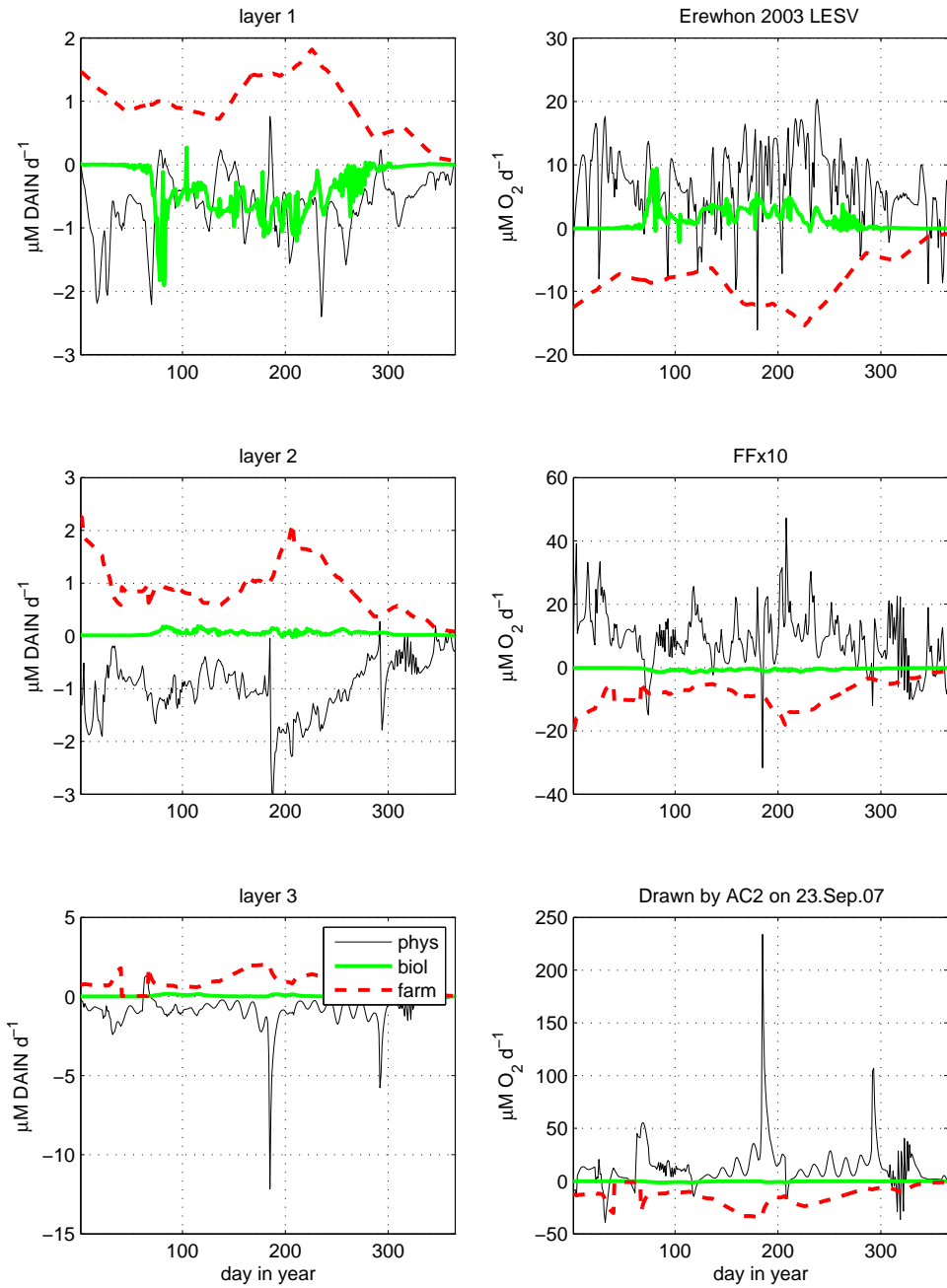


Figure 12: Fluxes: Loch Erewhon with 15,000 tonne farm. Rows show layers. Left hand column for DAIN flux, right hand column for fluxes in dissolved oxygen. See Table 10 for components of **physics**, **biology** and fish **farm** and benthic fluxes. A +ve flux is a gain to that layer. In the simulation without a fish-farm (not shown), the state of the loch resulted from a balance between physical transports of nutrients or oxygen (black lines), and the consumption or production of nutrients or oxygen by biological processes (green lines). The fluxes due to the fish-farm (red dashed lines) disturb this balance very substantially.

to account for evapotranspiration suppresses some seasonal variation in flow. The effect of boundary conditions, particularly the use of the climatologies, on predicted exchange rates need further investigation.

The comparison between modelled and observed temperature was generally better than that for salinity, largely due to the overriding effect of the seasonal heating cycle which dominates both the local surface heat flux and the coastal ocean temperature. Temperature is an important parameter for primary productivity in coastal waters and accurate simulation is essential for the ecological models.

Finally, the model results are critically dependent on the hypsography of sea lochs. Hypsographic data has been assembled for many sea lochs in the catalogue by Edwards and Sharples (1986). During the course of SARF012, we identified physical parameters that were not available from the catalogue. These were: the cross sectional area of the sill at mean tide, the wetted area of the seabed and the horizontal area of the loch at any given depth (to allow volume calculations of deep, middle and surface boxes in the model).

Although some digitised bathymetry was already available for Scottish sea lochs (e.g. digibath 250 data-set; SeaZone data-sets), some lochs have not been described in sufficient detail to allow these calculations to be performed. A preliminary assessment of the available data-sets has suggested that there were at least an additional 31 lochs supporting aquaculture that required digitisation.

FRS have re-analysed 104 sea lochs and voes by using a combination of existing digitised data (digibath 250 dataset from BGS) and manually digitising from raster Admiralty datasets within ArcMap. The digitised bathymetry was then rasterised and 3D spatial analyst software was used to calculate all the hypsographic parameters required. These data have been compiled into a database. Comparisons have been made with the data in the original sea loch catalogue and some differences observed. It is felt that the recent digitisation process has produced more accurate information on sea loch parameters that more closely matches the areas being used by e.g. Locational Guidelines.

7.2 LESV and assimilative capacity

Given adequate boundary condition data, the LESV model was well able to simulate seasonal cycles of nutrients and chlorophyll in Creran in the year 1975, which were typical of conditions in the 1970s. It simulated DAIN and DIP cycles equally well in 2003, but failed to hindcast total chlorophyll correctly, or the ratio of microplankton 1 to microplankton 2. As already mentioned, there has been evidence of a major shift in the ‘balance of organisms’ amongst Creran microplankton between the period 1970 - 1983 and from 2003 onwards. Although a small shift from diatoms towards flagellates is to be expected in cases of enrichment with dissolved N and P relative to dissolved silica, the most striking change is the loss of diatoms rather than the increase in flagellates. We are using the LESV mode to explore possible causes of the change, under the constraint that we should not markedly worsen the good fit to nutrient concentrations that we obtained using standard parameters. It is likely that more work needs to be done on the model’s equations and parameter values that determining the MP1:MP2 ratio. A detailed analysis of the model’s sensitivity to changes in parameter values, and interactions between parameters, has been set in hand with ECASA funding, and may shed light on this problem.

The loch Erewhon simulated in Figures 8 to 9 is only one of the possible lochs that resemble loch Creran. Loch Erewhon may be a water body that is more turbid than loch Creran, and in which deep water vertical mixing is weaker than in typical lochs of this depth and size. Furthermore, there is the matter of the over-estimation of chorophyll compared with

observations in loch Creran 2003. Nevertheless, we have shown the results in the Figures because they help us to make a number of points about Assimilative Capacity. The results should not, however, be taken as setting a capacity for the real loch Creran.

The mention of turbidity takes us to the need to calibrate, better, the optical model in LESV, just as the discussion of deep-water oxygen leads back to the need to consider, further, matters of mixing and overturn in bottom water in shallow lochs such as Creran. ACEXR was able to simulate, correctly, the replacement of loch Etive bottom water, so the problem for Creran may lie partly in the climatological boundary conditions that were used for temperature and salinity outside Creran and which, very likely, were insufficiently variable. So far as the optical model is concerned, measurements made in northern lochs by FRS during the SARF012 project, should allow the present UK-wide calibration to be made more relevant to use in lochs and voes.

7.3 Conclusions

The Matlab scripts that allow simulations with the combined model are available for distribution and provide a substantially improved tool for estimating the environmental impact of caged-fish-farming on the water-body scale. Wide and reliable application will need further development of the hypsographic data in the 'Sea-lochs' catalogue and in the provision of sea-boundary, river flow, and meteorological data to force the model. Some further development of the model is also desirable - especially in relation to deep-water exchange, calibration of the bio-optical sub-model, and the relative properties of the 'diatomey' and 'flagellatey' microplanktons. Finally, it might be feasible to add a sub-model for the growth of bivalve molluscs, thus allowing the estimation of lochs' carrying capacities for cultivated mussels and oysters and a study of synergies between finfish- and shellfish- farming.

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Milestone reports

1. Gillibrand, P.A. & Inall, M.E. (2006). Improving Assimilative Capacity Modelling for Scottish Coastal Waters: I. A Model of Physical Exchange in Scottish Sea Lochs. Marine Physics Report No. 167, March 2006. Scottish Association for Marine Science, Dunstaffnage Marine Laboratory, Oban.
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3. Portilla, E. & Tett, P. (2006a). Report on the Seasonal Equilibrium Concentration Enhancement (sECE) model, August 2006. School of Life Sciences, Napier University, Edinburgh.
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5. Portilla, E., Tett, P., Gillibrand, P., Inall, M., Gubbins, M. & Amundrod, T. (2007) Report on the Loch – Ecological State Vector (L-ESV) and component models for SARF012 milestone 5. December 2007. School of Life Sciences, Napier University, Edinburgh.

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