Development of Assimilative Capacity and Carrying Capacity Models for Water Bodies utilized for Marine Bivalve and Caged Fish Farming

SARF012a

A REPORT COMMISSIONED BY SARF AND PREPARED BY

DR PAUL TETT
Abstract

This report describes the second phase of work to develop modelling tools for the estimation of capacity to assimilate waste from farmed fish and shellfish, and to supply food for shellfish, on CSTT’s zone ‘B’ (water body) scale in Scottish lochs and voes. It provides a guide to the ACExR-LESV model system, and examples of its use to estimate exchange rates, nutrient loading and mussel growth in lochs Creran, Fyne, Spelve and Torridon, and Sandsound Voe. Appendices give further details of equations and arguments, and guidance in using the software (in version ACEXR-LESV_eco3_AUG_2011).
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<td>definition or explanation</td>
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<tr>
<td>ACExR</td>
<td>Assimilative Capacity Exchange Rate (model)</td>
<td></td>
</tr>
<tr>
<td>ASSG</td>
<td>Association of Scottish Shellfish Growers</td>
<td></td>
</tr>
<tr>
<td>CSTT</td>
<td>(UK) Comprehensive Studies Task Team (and model)</td>
<td></td>
</tr>
<tr>
<td>DAIN</td>
<td>Dissolved Available Inorganic Nitrogen, the sum of ammonium, nitrite and nitrate</td>
<td></td>
</tr>
<tr>
<td>dCSTT</td>
<td>dynamic CSTT model (and mode of LESV)</td>
<td></td>
</tr>
<tr>
<td>dll</td>
<td>(Microsoft Windows) dynamic link library</td>
<td></td>
</tr>
<tr>
<td>ECE</td>
<td>Equilibrium Concentration Enhancement</td>
<td></td>
</tr>
<tr>
<td>GB98</td>
<td>A simple mussel model, taken from Grant &amp; Bacher (1998)</td>
<td></td>
</tr>
<tr>
<td>LESV</td>
<td>Loch Ecosystem State Vector (model and mode)</td>
<td></td>
</tr>
<tr>
<td>LESVSF</td>
<td>mode of LESV with shellfish</td>
<td></td>
</tr>
<tr>
<td>FRS</td>
<td>Fisheries Research Services</td>
<td></td>
</tr>
<tr>
<td>MATLAB</td>
<td>Matrix Laboratory software; a registered trademark of The MathWorks, Inc.</td>
<td></td>
</tr>
<tr>
<td>MLA</td>
<td>Marine Laboratory Aberdeen, previously part of FRS, now part of MSS</td>
<td></td>
</tr>
<tr>
<td>MSS</td>
<td>Marine Scotland - Science</td>
<td></td>
</tr>
<tr>
<td>NUE</td>
<td>Napier University, Edinburgh (now Edinburgh Napier University), a partner in phase 1</td>
<td></td>
</tr>
<tr>
<td>OAERRE</td>
<td>Oceanographic Applications to Eutrophication in Regions of Restricted Exchange, an EC Framework V research project</td>
<td></td>
</tr>
<tr>
<td>PML</td>
<td>Plymouth Marine Laboratory</td>
<td></td>
</tr>
<tr>
<td>POM</td>
<td>Particulate Organic Matter</td>
<td></td>
</tr>
<tr>
<td>SAMS</td>
<td>Scottish Association for Marine Science</td>
<td></td>
</tr>
<tr>
<td>SARF</td>
<td>Scottish Aquacultural Research Forum</td>
<td></td>
</tr>
<tr>
<td>sECE</td>
<td>seasonal ECE model (and mode of LESV)</td>
<td></td>
</tr>
<tr>
<td>SERAD</td>
<td>Scottish Executive Rural Affairs Department (as was; some of its functions now fall to MSS)</td>
<td></td>
</tr>
<tr>
<td>ShellSIM</td>
<td>Shellfish biology Simulation model</td>
<td></td>
</tr>
<tr>
<td>SPM</td>
<td>Suspended Particulate Matter</td>
<td></td>
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Table 2: **Main symbols used in this report.** SV = model state variable; p = model parameter; fv = model forcing variable; r = rate or other dynamic intermediate variable; oi = indicator value calculated from output.

<table>
<thead>
<tr>
<th>symbol</th>
<th>ACExR</th>
<th>LESV</th>
<th>explanation and typical units</th>
</tr>
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<tr>
<td>a</td>
<td>r</td>
<td></td>
<td>(optical model) PAR absorption coefficient, m$^{-1}$</td>
</tr>
<tr>
<td>b</td>
<td>r</td>
<td></td>
<td>(optical model) PAR scattering coefficient, m$^{-1}$</td>
</tr>
<tr>
<td>b</td>
<td>p</td>
<td></td>
<td>(shellfish model) allometric factor (dimensionless)</td>
</tr>
<tr>
<td>B</td>
<td>SV</td>
<td></td>
<td>biomass of a single mussel, mg organic C</td>
</tr>
<tr>
<td>C</td>
<td>SV</td>
<td>fv</td>
<td>salinity, psu ($\approx$ salt concentration)</td>
</tr>
<tr>
<td>$\frac{d}{dt}$</td>
<td></td>
<td></td>
<td>rate of change operator</td>
</tr>
<tr>
<td>e</td>
<td>p</td>
<td></td>
<td>excreted fraction of grazed (microplankton) nutrient (dimensionless)</td>
</tr>
<tr>
<td>E</td>
<td>oi</td>
<td></td>
<td>exchange rate: proportion of loch-box water exchanged with sea during 24 hours, d$^{-1}$</td>
</tr>
<tr>
<td>g</td>
<td>r</td>
<td></td>
<td>microplankton specific loss rate due to grazing/filter feeding by plankton and benthos, d$^{-1}$</td>
</tr>
<tr>
<td>h</td>
<td>SV</td>
<td>fv</td>
<td>layer thickness, m</td>
</tr>
<tr>
<td>$K_d$</td>
<td>r</td>
<td></td>
<td>diffuse attenuation coefficient for PAR, m$^{-1}$</td>
</tr>
<tr>
<td>$K_z$</td>
<td>r</td>
<td></td>
<td>eddy diffusivity, m$^2$ s$^{-1}$ or d$^{-1}$</td>
</tr>
<tr>
<td>N</td>
<td>fv</td>
<td></td>
<td>numbers of mussels (per 1 m segment)</td>
</tr>
<tr>
<td>q</td>
<td>p</td>
<td></td>
<td>yield, e.g. mg chl from mMol nutrient</td>
</tr>
<tr>
<td>Q</td>
<td>SV</td>
<td>fv</td>
<td>water fluxes, m$^{-3}$ s$^{-1}$ or m$^{-3}$ d$^{-1}$</td>
</tr>
<tr>
<td>r</td>
<td></td>
<td></td>
<td>generalized rate</td>
</tr>
<tr>
<td>S</td>
<td>SV</td>
<td></td>
<td>nutrient concentration, $\mu$M</td>
</tr>
<tr>
<td>V</td>
<td>SV</td>
<td>fv</td>
<td>layer volume, m$^3$</td>
</tr>
<tr>
<td>X</td>
<td>SV</td>
<td></td>
<td>chlorophyll concentration, mg m$^{-3}$</td>
</tr>
<tr>
<td>Y</td>
<td></td>
<td></td>
<td>generic state variable</td>
</tr>
<tr>
<td>$\beta$</td>
<td>r</td>
<td></td>
<td>biological flux, amount of SV m$^{-3}$ d$^{-1}$</td>
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<tr>
<td>$\Delta t$</td>
<td></td>
<td></td>
<td>time-step, s or d</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>r</td>
<td></td>
<td>aquacultural input or withdrawal, amount loch$^{-1}$ d$^{-1}$</td>
</tr>
<tr>
<td>$\eta$</td>
<td>p</td>
<td></td>
<td>heterotroph fraction of microplankton biomass</td>
</tr>
<tr>
<td>$\mu$</td>
<td>r</td>
<td></td>
<td>microplankton specific growth rate, d$^{-1}$</td>
</tr>
<tr>
<td>$\bar{\mu}$</td>
<td>p</td>
<td></td>
<td>mean cosine of downwelling PAR</td>
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<td>$\phi$</td>
<td>r</td>
<td></td>
<td>physical transport flux, amount m$^{-2}$ d$^{-1}$</td>
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<tr>
<td>$\psi$</td>
<td>p</td>
<td></td>
<td>diatom fraction of microplankton chlorophyll</td>
</tr>
<tr>
<td>$\theta$</td>
<td>SV</td>
<td>fv</td>
<td>water temperature, °C</td>
</tr>
<tr>
<td>$\zeta$</td>
<td></td>
<td>r</td>
<td>layer optical thickness</td>
</tr>
<tr>
<td>$\nabla$</td>
<td></td>
<td>r</td>
<td>divergence operator on physical flux vector</td>
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Part I
Report
1 Introduction & Rationale

Scottish sea-lochs and voes are used for the cultivation of fish (currently, mainly salmon) and shellfish (currently, mainly mussels), because they combine shelter with a good water circulation. The water removes waste and supplies oxygen and, in the case of filter-feeding shellfish, food. Nevertheless, each water body has a finite capacity for assimilating waste or supplying food and oxygen, and thus a finite capacity for carrying farmed fish or shellfish (Tett, 2008). The purpose of the work carried out under the SARF012 project, which started in July 2004, was to estimate the capacity of whole sea-lochs (the zone B scale of the Comprehensive Studies Task Team: CSTT, 1994) to assimilate fish-farm waste.

During the first phase of the project, the ACExR physical model, and the LESV microplankton biology model, were developed. The ACExR model estimated water exchanges between loch or voe and the sea, and between simulated layers in the loch (Gillibrand et al., ms). The LESV model included a component to simulate the input of plant nutrients, and the demand for oxygen, resulting from fin-fish farms (Portilla et al., 2009). Excess nutrients have the potential to stimulate phytoplankton growth, thus potentially leading to algal blooms and decreased water transparency: i.e., to eutrophication. The Scottish ‘Locational Guidelines’ on the environmental suitability of coastal areas for fish-farming currently use an ECE, or ‘Equilibrium Concentration Enhancement’ model (Gillibrand & Turrell, 1997; Gillibrand et al., 2002) to estimate eutrophication risk; the ACExR-LESV model was intended to increase the reliability with which this risk is estimated.

However, although the models had been developed and coded by the end of phase 1, in August 2007, there were known problems with the physical model’s ability to simulate all the lochs in the Scottish ‘Sea-loch Catalogue’ of Edwards & Sharples (1986), and the biological model had been tested only in Loch Creran. In addition, it seemed possible that co-cultivation of shellfish with fin-fish could result in nutrient removal by the shellfish (as a result of filtering phytoplankton that had absorbed nutrients) and so increase a loch’s capacity to deal with finfish farm waste. Thus the work was continued into a second phase (SARF 012A), starting in 2008.
2 Objectives & Partners

As proposed (in 2007) the research aimed to continue work done in the first phase of SARF 012. The ACExR and LESV models were to be improved and tested at additional sites. A sub-model for the growth of farmed bivalve molluscs was to be added to provide a tool for estimating bivalve carrying capacity on the water body scale and to investigate synergies between shellfish and fin-fish farming. In addition advice was to be provided to the shellfish and fin-fish farming communities on the use of these models and on the zone A or farm scale models evaluated during the ECASA project. The work was intended to relate to SARF’s aim of sustainable development of aquaculture, and the resulting models were intended to be useful to farmers as well as regulators. The partners in SAF012A were:

- Fisheries Research Service (FRS), now Marine Scotland:Science (MSS);
- Plymouth Marine Laboratory (PML);
- Scottish Association for Marine Science (SAMS; project leader);

The initial research objectives were:

1. Establish a data collection co-ordination group whose function would be to facilitate the process of acquiring the (Boundary Condition and in-loch) data required to validate these and similar models in future (SAMS, FRS);

2. Link an appropriate version of the PML ShellSIM model with the LESV model (SAMS, PML);

3. Assess constraints and advise on application of existing farm-scale and spatially-resolving shellfish models for farm scale (A) management (SAMS, PML);

4. Complete development of the improved bio-optical model in LESV, using samples and observations already made by FRS (SAMS, FRS);

5. Support use of ACExR and LESV models (SAMS);

6. Extend the physical boundary condition data base (FRS) and test the ACExR models at a wider range of sites (using the data already collected by FRS and new data) (SAMS);

7. Extend the chemical-biological BC data base (FRS) and test the LESV models at a wider range of sites (using the data already collected by FRS and new data) (SAMS);

8. Test the ShellSIM-LESV-ACExR combination against observations of mussel growth in at least one sea-loch (SAMS, PML).
3 Narrative Account of Work

Phase 2 (SARF012A) commenced in April 2008. Between the end of phase 1 in August 2007 and the start of phase 2, work funded from other sources was carried out by Napier University, Edinburgh (the leaders of the phase 1 project). This included finalizing the manuscript that was published as Portilla et al. (2009), and carrying out a study of the consequences of boundary condition uncertainty for estimates of assimilative capacity (see Tett et al., 2011).

The following summarizes what was done in relation to each of the SARF012A objectives from April 2008 through March 2011.

1. Establish a data collection co-ordination group. A meeting was held in Edinburgh in June 2008, with representatives from SARF and Scottish Government, to present the need for boundary condition data.

2. Link ShellSIM with LESV. Work included improvements (section 14) in the programming of ShellSIM (in the Microsoft, object-oriented, language C-sharp) before compiling into a dll, or dynamic-link library that includes executable code available for interfacing. MATLAB provides for such interfacing when run under Windows. Most MATLAB code will run under UNIX and MacOSX operating systems as well as Windows. The biological code was in development under MacOSX, and most of the development work on the link was done under this operating system. A number of visits were made to PML (in December 2008, June and November 2009) to discuss coupling, and gradually the scheme described in section 7 emerged. A simple mussel model (that of Grant & Bacher, 1998) was coded in MATLAB to provide a means of testing the coupling code and as a default when LESV could not be run under Windows. The link to ShellSIM is still to be made.

3. Advise on farm-scale models. The plan had been to hold a short workshop, early on in this phase of the project, where the ‘farm-scale’ models studied during the ECASA project, would be presented to the industry. It did not prove possible to arrange this during 2008, as originally intended; instead a presentation of ACExR-LESV was made to the ASSG annual meeting in November 2010, and was followed by small-group discussion with stakeholders.

4. Improve bio-optical model. The coding of the LESV function irradiance dealing with bio-optics was improved, and optical parameter values set to those estimated for UK seas by Devlin et al. (2009). Following a visit to MLA in September 2009, and the discovery that the MLA sub-marine irradiance sensor was of a design allowing direct estimation of absorption coefficient, it was decided to develop a 2-component irradi-
ance model and attempt to fit it to MLA data from loch Torridon. As described in section 12, some, albeit incomplete, progress was made.

5. Support use of ACExR and LESV. The main potential users of the model system have been, and are, MSS (who are partners in the project through MLA) and SEPA Modelling. A meeting involving SEPA, MLA and SAMS took place in Dingwall in January 2011 to consider what improvements were needed to the package to make it easier to use, and as a consequence a second rebuild of the code (section 13) was commenced. This allows multiple runs of the models, with recovery from error should this occur during any particular run.

6. Boundary conditions and testing of physical model. Improvements were made to the data-base of physical boundary conditions, and in data-base reading functions to deal better with absence of data, and ACExR was run successfully for 27 lochs and voes. As discussed in section 15, some run-time problems remain, and the model was not further tested against observations.

7. Boundary conditions and testing of biological model. The key achievement here was the setting up of a data-base to ensure that at least generic default boundary conditions were always available to the LESV model. The results of simulations are presented in sections 16 - 19, although further testing against observations was not achieved.

8. Test ACExR-LESV-ShellSIM against observations of mussel growth. At the time of writing, the coupling has not been completed. However, it was decided midway through the project that testing model growth predictions against observed mussel growth would not be an effective use of resources; instead a better test would be to compare predictions and observations of mussel harvest. This has been done only for one loch.

\[\text{1} \quad \text{Broom; Campbeltown; Carron; Claidh; Craignish; Creran; Duich; Etive; Ewe; Fyne, Gareloch; Gail; Greshornish; Inchard; Laxford; Leven; Long; Na Cille; Portree; Sandsound Voe; Shell; Snizort Bay; Spelve; Striven; Sunart; Tamanaray; Torridon.}
\[\text{2} \quad \text{This default boundary condition data had been prepared by EP in 2008, drawing on international data-bases. See: Portilla & Tett (2008). LESV-ACExR has been run for lochs Creran, Fyne, Spelve, Striven, Torridon, plus Sandsound Voe, under a variety of forcing conditions.}
\[\text{3} \quad \text{It had been proposed to analyse farmed mussels at regular intervals, whilst taking water samples near the farm for chlorophyll and POM. However, water samples would need to be very frequent to encompass natural variation; it was for a time envisaged that chlorophyll might be measured continuously using a SEPA recording fluorometer; but no suitable arrangements could be made with resources available. Meanwhile it became clear that ShellSIM’s algorithms for mussel (etc) growth had been extensively tested in laboratory studies, and that the priority should be to test the water-body-scale aspects of the ACExR-LESV-ShellSIM model - i.e. its predictions of mussel crop in a particular loch, given a certain seeding and harvesting schedule.} \]
As this summary makes clear, the actual work and its timing diverged from what had been intended. There were several reasons for this:

- as originally proposed, the available resources were spread rather thinly over the objectives;\(^4\)
- end-users’ developing requirements of the model system;
- staff changes.\(^5\)

It became apparent that the crucial task was to improve the coding of the model implementation in MATLAB, in order to: (i) allow interfacing with shellfish models; (ii) correct problems that were causing run failures in some lochs; (iii) load default boundary conditions when no others could be found; and (iv) to make the system more suitable for the needs of users. Most of the SAMS effort went to this task, and much of the remainder of this report describes that part of the work and its results.

The description is intended both to present the significant achievements of the project and to provide an introductory guide to users of the ACExR-LESV model system. Further details are included in the Appendices. By way of introducing this guide, we start in section 4 with a discussion of model reliability.\(^6\)

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\(^4\) Person-days available were: SAMS: 94; PML: 60; FRS: 28. It had been hoped that other sources of funding would augment this, as had been the case in phase 1 (ECASA); this did not prove the case in phase 2, although EP contributed to the work reported here on the basis of a Napier consultancy following the conclusion of his post-doc, and PG continued to work on the ACExR model after leaving SAMS.

\(^5\) During phase 1, most of the work on the physical model had been carried out by PG, who moved to NIWA (New Zealand) at the start of 2008 and subsequently to CSIRO in Tasmania. Most of the work on the biological model had been carried out by EP, who moved to ULPGC during phase 1, and was unavailable after the end of 2008. Given the 3-way split of funding, it was infeasible to appoint a new post-doc in phase 2. It was expected that PT, who had led phase 1 from NUE, would take over both the leadership of phase 2 from MI, and the detailed work on the model code, when - as was expected when the proposal was written - he moved part-time from NUE to SAMS in September 2008. In fact this move was delayed until May 2009, and substantial effort became possible only after February 2010 (when his work at NUE concluded). CC left SAMS to run his own consultancy in 2008, although remained available for public engagement work.

\(^6\) Some more history is relevant here. In August 2010 project officer MJ asked for an account of factors relating to uncertainty in model predictions to be included in the report. EP, who had trained as a bio-statistician, had already done some work on estimating the effect of boundary condition uncertainty on predictive reliability. And as a result of participation in the SPICOSA project (2007-2011), PT grew more aware that there were several technical steps to ensuring model reliability, and in addition that it might also be necessary to take account of social considerations bearing on model legitimacy.
4 Steps in building a reliable model

In order to evaluate the potential reliability of the ACExR-LESV model as a tool to help the optimum use of the natural resources in Scottish coastal waters, it is useful to explore the relationship between real systems and the models that attempt to describe and simulate them. Model-building involves several steps:

1. **Understanding the real system.** The starting point is the real sea-loch ecosystem; or, to be more precise, our presently imperfect understanding of the complex natural processes involved in the functioning of these systems.

2. **Making a conceptual model.** Conceptual models of these processes need to be both general (to apply to all lochs and voes) and simplified (to omit what is not relevant to aquaculture-environment interactions). The key decisions at this stage are the choice of model state variables (e.g. layer volume, chlorophyll concentration), main processes (e.g. water exchange, nutrient cycling), and the extent and grain of the model (where to place the external boundaries and internal partitions). With the exception of the shellfish-related components (Figs. 4, 5), these decisions were made in SARF012 phase 1 (Figs. 2 and 3).

3. **Mathematical modelling.** ACExR and LESV are formulated as differential equations in the state variables. These equations follow logically from decisions made at the conceptual modelling stage about which variables and processes to include. Secondary decisions concern how to calculate values for individual rate terms in these main equations, and in most cases required a choice to be made amongst several possible parameterization of the key processes. Again, most of these decisions were made in phase 1, and the equations are described and discussed in Gillibrand et al. (ms) and Portilla et al. (2009). Only a few examples (e.g. eqn. 1) are given in this report.

4. **Coding the numerical model.** The differential equations of ACExR and LESV must be solved to show how the values of the state variables (and associated rates) change with time. In general, this cannot be done analytically (i.e. by mathematical manipulation on paper) and instead requires numerical integration: repeated solution of the equations for small time-steps, each step building on values resulting from a previous step. In phase 1, sets of routines to do this for ACExR and LESV were written in the Matlab programming language. Much work in phase 2 has gone into improving this code, and adding routines for shellfish.
5. **Adjusting parameters and testing against observations.** Typical process equations - or parameterizations - include local constants as well as variables. The former are adjustable between computer runs and are referred to as *parameters*. Their values can be taken beforehand from the scientific literature, or adjusted over a series of simulations to give better agreement between observations and model results. Of course, data that are used for parameter adjustment cannot subsequently be used for assessing model reliability. ACExR and LESV contain few arbitrary parameters needing local adjustment, and hence comparisons of model results with relevant observations provide good tests of the models. Such tests were carried out in phase 1 for ACExR against observations in lochs Etive and Creran, and for LESV against observations in Loch Creran.

Using the model involves some further steps:

6. **Getting loch and boundary data.** Needed are data for the hypsometry and aquacultural loading of the loch that is to be simulated, and for the physical and chemical-biological boundary and forcing conditions for the loch and the year of the simulation. Much of the work in phase 2 has concerned assembling such data for LESV.

7. **Running a simulation.** A *simulation* is defined as a numerical integration of the (ACExR-LESV) model equations for a defined set of parameter values and of initial and boundary conditions. The result (also referred to as a simulation) is a set of time-series of values of the state variables. However, the numerical integration may fail, perhaps because it encounters an unexpected condition or a mathematical error such as attempting to divide a quantity by zero. Some of the work with the model code during phase 2 has concerned identifying the sources of these errors. In general, ‘bugs’ were fixed if they resulted from errors in coding algorithms, but not where faults were suspected in scientific understanding or process parameterization, or thought to result from an unrealistic jump in boundary conditions where the fundamental equations and model coding were correct. In these cases, the most recent version of the program traps and report an error, and then moves on to the next simulation.

8. **Interpreting the results.** At the least, interpretation requires plotting state variable time-series. In some cases the simulation results are further processed, perhaps by extraction of statistics (such as maxima and minima), indicator values (such as winter maximum nutrient concentration), or merging of data from several layers (for example to present values over a fixed depth range). In principle, it is up to the user to process simulation results as they wish. The ACExR-LESV
Errors or uncertainties can get into the results of the model in various ways. Incomplete knowledge of the real ecosystem processes, and imperfect simplification, can lead to an incorrect conceptual model. Since this is a matter of expert judgement or opinion, it is not easily tested by peer-review, although other experts’ opinions can be helpful. In the case of ACExR-LESV, we claim reliability on the basis of collective expertise in the fields of modelling physical systems, ecological systems, and shellfish. Correct formulation of state variable and process equations, and testing of model results against observations, are, typically, examined in the peer-review process, such as that applied to the manuscript of Portilla et al. (2009) before its publication. Coding the numerical model is, however, typically not checked during peer-review (Alexandrov et al., 2011) and thus, in most cases, including ours, relies on careful inspection and re-inspection of the code, checking of intermediate and final results in a variety of cases, and running test-cases where possible.

An important check carried out in phase 2 involved a comparison of simulations by two different codings of the physical transport equations. In the case of ACExR, the transport rate-of-change equations are set out in the function $\text{TracerSI}$ and integrated in the function $\text{CalcE}$ by a forward-Euler scheme with $\Delta t = 0.01$ day. In the case of LESV, they are set out in $\text{ScalarPhysics3}$ and integrated by the Matlab $\text{ode23}$ function using a Runge-Kutta scheme with adaptive time-step. Figure 1 shows good agreement between the results of the two schemes.

The approximations involved in preparing data sets for boundary conditions can also effect the results of numerical integration. Studies were carried out to discover how uncertainties in boundary condition data propagate through into simulations and indicators derived from them (see Tett et al., 2011). Finally, two sorts of tests were performed on the simulations of the model. As exemplified in Figure 1, one involves comparison between simulations, forced as far as possible by boundary conditions observed in a particular year, with observations made in the loch or voe in the same year. Such comparisons with physical data from lochs Creran and Etive, and biological data from loch Creran, were reported at the end of phase 1, and by Gillibrand et al. (ms) and Portilla et al. (2009). Currently, work is in hand (Gillibrand, CSIRO) to study the sensitivity of Creran and Etive simulations to varying some of the parameters of the ACExR model.\footnote{The parameters are those for wind entrainment, the estuarine circulation as a function of density difference between the loch and outside, and several coefficients in the algorithms for calculating vertical mixing. Initial results suggest that a higher value of the wind entrainment parameter, and a lower value of the estuarine circulation parameter, improves agreement between predicted and observed temperatures and salinities for Creran in 1978 and Etive in 2000.}
Figure 1: **Comparison of salinities** as calculated for the upper 2 layers of Loch Creran, 1978, by ACExR and LESV. ACExR computes salinities because they are state variables in the physical model. LESV re-computes salinities as a check that its `ScalarPhysics3` function (used to transport all biological state variables) achieves the same results as `TracerSI` in ACExR. The diagram also shows the salinity boundary conditions, which the layer 2 simulation tracks closely, and observations in Creran in 1978. Salinities observed at 4 m depth show good correspondence with those simulated for layer 1, median thickness 7 m. Those observed at 10 m were generally lower than those simulated for layer 2, which typically extended from 7 to 16 m.
5 Physical model science

Many of the inlets on the western and northern coasts of Scotland and its islands are fjords, river valleys deepened by glaciers and subsequently flooded by the sea, with a shallower sill region at the mouth. The ACExR model (Gillibrand et al., ms) treats such water bodies as containing three horizontally-uniform layers (Figure 2):

1. a superficial layer of lower density, with thickness determined in part by the balance between wind stirring and inputs of heat or freshwater buoyancy;
2. an intermediate layer, exchanging tidally with the sea;
3. basin deep water, isolated from the coastal sea by the entrance sill.

Figure 2: **ACExR physical model** conceptual diagram. Variables \( h, V, C, \theta \) give the thickness, volume, salinity and temperature of layer \( l = 1, 2, 3 \). \( C_E \) and \( \theta_E \) are profiles of salinity and temperature at the sea-boundary. \( W \) is the speed of the wind, which stirs layer 1. \( Q_{SHF} \) is heat flux; all other terms in \( Q \) are (water) volume fluxes: \( Q_E \) and \( Q_H \), entrainments from one layer to another; \( Q_K \) mixing due to eddy turbulence; \( Q_F \), freshwater input; \( Q_G \), the gravitational estuarine circulation with intermediate layer inflow and superficial layer outflow; \( Q_T \), tidal mixing.

Water exchanges amongst these layers, and with the sea, as a result of several processes. The following are simulated by ACExR, which solves equations for the water fluxes \( Q \) dynamically, based on calculated layer properties at each time-step and daily mean values of boundary and forcing conditions. The latter include river discharge \( Q_F \), wind speed, surface heat flux, and properties at the sea-boundary.
Gravitationally-driven estuarine circulation: river discharge into a fjord, at the head and along the sides, is mixed down by wind stirring and dilutes seawater, creating a brackish surface layer. The river water also raises sea level, forcing the surface layer to flow outwards. Seawater is entrained into the outflowing layer from below, leading to an inflow to the intermediate layer with volume flux $Q_G$.

Tidal mixing: on each rising tide, coastal seawater floods into the loch or voe. Because the external water is typically denser than the internal surface layer, it sinks beneath it into the intermediate layer. Only a part of this coastal water leaves on the ebb tide, the ebb volume also including water in the superficial layer as well older water in the intermediate layer. In ACExR, tidal mixing is modelled as an exchange of properties between the intermediate layer and the external coastal ocean, averaged over the cycle of flood and ebb to the flux $Q_T$.

Vertical entrainment: by an upper (more energetic) layer from a lower (less energetic) layer. The tide flooding into the intermediate layer entrains water from the layers above and below (the $Q_E$ terms in the model). During the ebbing tide, stratification increases and is assumed to inhibit entrainment. In opposition to tidal entrainment, simulated wind stirring at the surface drives entrainment $Q_H$ of water from the intermediate layer into the surface layer, leading to increased thickness and density of the surface layer. In this version of the model, basin deep water is renewed by entrainment from layer 2 into layer 3, which occurs when the density of the water inflowing to layer 2 exceeds that of the basin deep water.

Vertical turbulent mixing: Whereas entrainment is a one-way movement of water (and properties), mixing is a two way exchange of properties without changing layer volumes. Vertical turbulent mixing (simulated by the terms in $Q_K$) is generated by shear in horizontal currents and by internal waves.

Model equations are given by Gillibrand et al (ms) and are based on studies in Scandinavian fjords by Stigebrandt and co-workers (e.g. Stigebrandt 1980, 1981, 1985, 1999), culminating in the development of the FjordEnv model (Stigebrandt, 2001). ACExR builds on FjordEnv by incorporating time evolution of state variables rather than estimating an average steady state. It also includes refinements and additional exchange processes based on recent research in Scottish fjords (e.g. Inall and Rippeth, 2002; Cottier et al. 2004; Inall et al. 2005). Transport equations are given in Appendix A. In the case of a water body lacking an entrance sill (as is typical of Shetland voes), layer 3 processes are omitted from simulations.
6 Biological model science

The LESV biological model (Portilla et al., 2009) is summarized by Figure 3 and the rate-of-change equation for the generic state variable $Y$:

$$\frac{dY}{dt} = -\nabla \phi_Y + \beta_Y + \frac{\Delta \Gamma_Y}{V}$$ (1)

The actual state variables, implemented in all model layers, are three kinds of dissolved nutrient, two kinds of microplankton, several optical active constituents, and a simple tracer. The term $\beta_Y$ deals with the transformations of these variables. The term $\nabla \phi_Y$ gives their transports between layers of the physical model; it is calculated using the $Q$ terms from ACExR (see eqn. 9 in App. A). The term $\Gamma_Y$ is the total input to the water body of a

![Diagram of LESV biological model](image)

Figure 3: LESV biological model conceptual diagram. Part (a) illustrates the $\beta_Y$ terms and the optical submodel. It shows nutrient, oxygen, microplankton, and optical, variables in one layer of the model; chlorophyll can also be lost to grazing, which recycles some nutrients. The flagellates etc in MP2 do not use silica. Part (b) illustrates the set of $\Gamma_Y$ terms, showing the interactions between a fish-farm and each layer of the model.
substance (or its removal), broken down into fractions $\Delta \Gamma Y$ into each model layer, volume $V$.

LESV includes within it two earlier and simpler models for eutrophication: an equilibrium nutrient enrichment model (Gillibrand & Turrell, 1997) that has been used to rank Scottish lochs in terms of potential impact from farms; and a dynamic version (Laurent et al. 2006) of the UK ‘Comprehensive Studies Task Team’ eutrophication model (CSTT 1994; 1997; Tett et al. 2003a). A key feature of the CSTT model is its use of a chlorophyll yield parameter $q$ (Gowen et al. 1992; Edwards et al. 2003) for estimating the phytoplankton biomass that could grow from a given nutrient enrichment. The additional state variables in LESV result from the need to simulate some of the elements specified in Annex V of the Water Framework Directive for phytoplankton biological quality and general physico-chemical quality.

LESV is a microplankton rather than a phytoplankton model. ‘Microplankton’ refers to all pelagic micro-organisms capable of asexual reproduction by cellular fission. The community includes phytoplankton (pelagic micro-algae and cyanobacteria), some of which are now known to be myxotrophs, and pelagic microheterotrophs: bacteria, and ‘protozoa’ including ciliates, heterotrophic dinoflagellates, zooflagellates and mycoflagellates. The contents of a microplankton ‘box’ in the model may be thought of as a soup of chloroplasts (phytoplankters only) and mitochondria (all microplankton), and the parameterization takes account of the additional respiration of the microheterotrophs and the recycling of nutrients in the ‘microbial loop’ (Tett, 1987; Tett & Wilson, 2000; Tett et al. 2002; Lee et al. 2003).

LESV contains two microplankton boxes to simulate the seasonal succession of phytoplankton and associated microheterotrophs. ‘Microplankton 1’ has properties associated with Spring Bloom diatoms, including a requirement for silica, and a low content of micro-heterotrophs; ‘microplankton 2’ has properties associated with the recycling, microbial-loop dominated, plankton of Summer. The growth of each microplankton is modelled as the minimum of either linear dependence on illumination (Tett, 1990) or Monod-type dependence on seawater nutrient concentration, with nutrient removal coupled to growth by the inverse yield $q^{-1}$. Illumination in each layer is calculated by an optical submodel involving a diffuse attenuation coefficient calculated from simulated concentrations of ‘optically active constituents’ (including chlorophyll) by equations derived from Kirk (1984) by way of Bowers et al. (2000) and Devlin et al. (2009).

LESV avoids the need for state variables for mesozooplankton or benthos by parameterizing feeding losses to these as a single ‘grazing pressure’ parameter, which is multiplied by a function of water temperature to simulate seasonal changes both in activity and stock.

As in the case of ACExR, all LESV processes are parameterized in terms of 24-hour mean rates. Thus, microplankton growth rates are calculated by
LESV from average illumination without the need to resolve changing light during day and its absence during night.

On the water body ('zone B') scale simulated by ACExR-LESV, the environmental effects of aquaculture include:

1. input of nutrients (compounds of nitrogen and phosphorus, especially ammonium and phosphate) to, and removal of oxygen from, the water column as a result of the metabolism of cultivated animals;

2. input of nutrients, and consumption of oxygen, as the result of the mineralization at the seabed of organic waste from farms;

3. removal of microplankters and other particulate matter from the water column by filter-feeding shellfish, which use the organic particulates as food;

4. inputs to the water column of chemotherapeutants as a result of external treatments (mainly of farmed fish) and of antifouling compounds leached from farm gear;

5. release by the seabed of substances derived from food additives (including copper and internal chemotherapeutants) (mainly of farmed fish).

LESV averages these inputs (or withdrawals) over the whole loch, whilst dividing them between the layers of the simulation. Items (1) and (2) are implemented by a submodel based on Black (2001), in which monthly supplies of feed declared by salmonid farmers are converted into daily additions of nitrogen and phosphorus compounds to each of the dynamically changing layers of LESV. Oxygen is removed at the same time. Item (3) is dealt with in the next section. Items (4) and (5) are implemented by a generic tracer variable, with first-order decay, and there is provision for discrete or continuous addition of this variable to particular layers or to simulated freshwater inputs. The exact impact of the farm depends on its siting in the loch; LESV allows the vertical extent of the cage, and the depth of the seabed at the farm, to be entered as parameters in a model run.
7 Coupling shellfish models

Filter-feeding shellfish such as mussels take micro-organisms and other small particles from the water, and consume oxygen. As a by-product of metabolism they excrete nutrients, and they produce solid waste in the form of faeces (undigested material) and pseudofaeces (material rejected before ingestion). In principle, therefore, their activities can be represented by $\Gamma$ terms such as those in the Blackfish submodel for finfish. In practice, two sets of issues caused problems in linking shellfish models to LESV. They were to do with geometry and with numerical integration.

**Geometric issues** had been encountered in calculating how to assign the nutrient inputs and oxygen demands of salmon cages into particular layers of the ACExR-LESV model. They were encountered again in relation to filter feeding shellfish, which might be grown on the sea-bed, on posts or tables fixed to the sea-bed, or on ropes or bags dangling from buoys floating at the sea-surface. Whereas fish can swim, and were assumed to be equally spread throughout the cage depth, shellfish are attached. It was thus thought desirable to resolve their depth distribution into 1 metre bands, which could be mapped to the dynamic layers of the model, as shown in Figure 4. It

![Diagram of shellfish state variable vectors](image)

**Figure 4: The shellfish state variable vectors.** Each vector contains values for 1 m depth segments; $N$ is the total number of cultivated shellfish in the water body in each depth segment. The average size of a mussel in each segment is given by TFW (total fresh - or ‘wet’ - weight) and DTW (dry tissue weight).

was decided to implement shellfish models initially only for suspended-rope culture, which is the main practice in Scotland.
Numerical integration issues did not arise in the case of finfish farming. The input to the Blackfish model was the mass of feed supplied to farmed fish in each month, and the model calculated the daily rate at which this mass was converted to excreted nutrient etc. There was no need to simulate the fish themselves. In the case of shellfish, taking food from the water and growing as a result, it seemed necessary to have state variables for (i) number of shellfish in each depth segment and (ii) the average mass of a bivalve in each segment, with the former changing due to seeding, mortality and harvest, and the latter increasing as a result of feeding and decreasing as a result of metabolism.

For any state variable $Y$, the instantaneous relative rate of change is $r = \frac{dY}{dt} \cdot \frac{1}{Y}$. Implementation of a model aims to integrate this equation in order to calculate the time series $Y = f(r, t)$, given an initial value of $Y$ at $t = 0$. Because $r$ itself typically changes with time, in response to changing forcing conditions and other state variables, analytical integration is not possible. Instead, we rely on numerical integration, in which in which state variables are repeated recalculated as time is advanced in small steps $\Delta t$. The simplest method is the ‘forward-Euler’ scheme:

$$Y_{[t+\Delta t]} \approx Y_{[t]} \cdot (1 + r \cdot \Delta t)$$

The approximation becomes better as $r \cdot \Delta t$ is made smaller (and as $\Delta t$ approaches the infinitely small $dt$ of the differential equation).

There are more sophisticated numerical approximations that provide more accurate and stable solutions of the dynamical equations than ‘forward-Euler’ scheme, and these are often to be preferred. They include ‘Runge-Kutta’ schemes, and the ability to change the value of $\Delta t$ dynamically to deal with faster rates of change. Using such methods seemed vital for a model intended to estimate carrying capacity. Such a model must simulate accurately a system in which shellfish daily water clearance can be a substantial fraction of the volume of the water body. However, such schemes can encounter difficulties when dealing with discrete events, such shellfish seeding and harvesting, with large changes in $N$ occurring in a single day.

It was therefore decided to make:

- $N$ a forcing variable, requiring time-series of shellfish (in each depth segment) to be calculated in advance from information about seeding, natural mortality, and harvesting;

- individual shellfish biomass, one or more (dynamic) state variable(s) in each depth segment, with rate of change described by a ‘dynamic energy budget’ or DEB equation.

The next sections deal with such DEB models for individual shellfish.
8 Simple shellfish model science

In a DEB model, growth is the result of the balance between food acquisition and the use of food energy in metabolism. If food energy is assimilated at a faster rate than it is lost to respiration, organic material is available for growth. Many of the relevant processes depend on animal size, according to a general \textit{allometric law}, where the rate $r$ at given biomass $B$ is calculated from a reference rate as follows:

$$ r_B = r_{ref} \cdot \left( \frac{B}{B_{ref}} \right)^b \quad \text{factor } b < 1 $$

\begin{equation}
(2)
\end{equation}

Figure 5: \textbf{Simple Mussel Model} implemented by the function \texttt{GB98} and based on Grant & Bacher (1998).

The LESVSF code is intended to offer a choice of two shellfish models. ShellSIM is described in the next section. A simpler option is based on the ‘mechanistic’ mussel model of Grant & Bacher (1998). It is illustrated in Figure 5 and implemented in the vector function \texttt{GB98}, which operates simultaneously on all depth segments containing mussels. For each segment the function calculates a daily biomass increment for a typical mussel, measured as the organic carbon in mussel flesh. Conversion between carbon, DTW and TFW (including water and shell) can be made using constant factors. The total mussel biomass in each depth segment at a particular time is the product of the typical mussel biomass and the number of mussels in that segment.
Mussels get food by filtering water-born particles, which include phytoplankton or microplankton (preferred when available) and other suspended organic particles. Suspended inorganic particles are also collected by filtration, but rejected as pseudofaeces. Filtration rates decrease as the concentrations of these components increases. In addition to providing food for the mussels, such filtration also leaves the water more transparent, another benefit of mussel farming in relatively eutrophic waters. Some ingested organic matter is not assimilated but exported as faeces. Nutrient elements (N and P) contained in the organic particles are returned to the water as a by-product of respiration.

All these processes are simulated by GB98, which is called by the coupling function ShellFish that deals with mapping between ACExR-LESV layers and the depth segments used for shellfish variables. However, the current version of ShellFish does not do anything with the faeces and pseudofaeces, nor with Si in ingested diatoms. The Redfield stochiometry used for N and P excretion by GB98 takes no account of differences between C:N:P ratios in mussels, microplankton and POM. Finally, filtration and metabolic rates are not affected in GB98 by the physical environmental variables temperature and salinity. The more complex and better validated code of ShellSIM, the model described in the next section, improves over GB98 in a number of ways.
9 ShellSIM science

Simulation of the growth of suspension-feeding bivalve shellfish (including mussels, oysters, cockles, clams, scallops) is complicated by observations that filter-feeding and metabolism in shellfish are highly responsive to fluctuations in temperature, salinity, food availability and food composition, as frequently occur in near shore environments where most aquaculture takes place. These physiological adjustments affect growth of the individual. By influencing the relative biogeochemical fluxes of different particles and nutrients, they also affect ecosystem processes.

ShellSIM simulates functional interrelations between suspension-feeding bivalve shellfish and the environment, with outputs that quantify consequences for shellfish growth, water quality and ecological status. It is a dynamic model, and for individual growth it is based upon the common principles of energy balance illustrated in Figure 6, using differential equations that define physiological responses to environmental change. Time-varying rates of feeding and metabolism are simulated as component processes in the prediction of individual growth, reproduction and condition, the individual being treated as an input-output system with size and energy content as state variables.

Population dynamics are simulated using a standard conservation equation to calculate transitions between weight classes, accounting for seeding, settlement, harvesting and/or mortality as defined by the User.

Options have been integrated within a single tool to analyse consequences of culture practice; with ability for the User to define spatial distribution, environmental conditions and the relative composition of up to 14 commonly cultured shellfish species, whether located on the bottom, rope, pole or trestle.

Notably, whereas past models have been calibrated and optimized per species per site, ShellSIM is the first common model structure to simulate effectively upon calibration in separate species, and which can then be applied using the same calibration for each species reared in contrasting environments, thereby saving significant time and resources. ShellSIM accounts for differences that include body form and function, responses to food availability and composition, responses to temperature, salinity and other environmental variables, reproductive behaviour and metabolic conversion efficiencies, such that no two species will grow at the same rates under similar conditions, as is illustrated for different sympatric mussel species in Figure * below.

Figure 6: ShellSIM model principles: the physiological components of net energy balance.

Population dynamics are simulated using a standard conservation equation.

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8 ShellSIM is a mathematical shellfish model developed by Dr. A. J. S. (Tony) Hawkins of Plymouth Marine Laboratory, as a cost-effective tool for use by aquaculture growers, water-body managers and regulators. See: http://www.shellsim.com.
to calculate transitions between weight classes, accounting for seeding, settlement, harvesting and/or mortality as defined by the User.\footnote{This part is handled by the \texttt{ShellFish} function in LESV} The ShellSIM user can set options to define spatial distribution, environmental conditions and the relative composition of up to 14 commonly-cultured shellfish species, whether located on the bottom, rope, pole or trestle.

ShellSIM uses a common set of equations to simulate a number of species. It allows for differences in body form and function, responses to food availability and composition, responses to temperature, salinity and other environmental variables, reproductive behaviour and metabolic conversion efficiencies, such that no two species will grow at the same rates under similar conditions. The full list of environmental drivers that may be used by ShellSIM are summarized together with simulated responses in table 3.

### Table 3: ShellSim environmental drivers and responses

The variables in the first column collectively determine the variables in the second column.

<table>
<thead>
<tr>
<th>forcing variable</th>
<th>simulated response</th>
</tr>
</thead>
<tbody>
<tr>
<td>temperature</td>
<td>particle clearance</td>
</tr>
<tr>
<td>salinity</td>
<td>ammonia excretion</td>
</tr>
<tr>
<td>current speed</td>
<td>oxygen uptake</td>
</tr>
<tr>
<td>aerial exposure</td>
<td>faecal losses</td>
</tr>
<tr>
<td>dissolved oxygen</td>
<td>reproduction</td>
</tr>
<tr>
<td>food availability</td>
<td>growth</td>
</tr>
<tr>
<td>and composition*</td>
<td>condition</td>
</tr>
</tbody>
</table>

* chlorophyll, POM and inorganic SPM

Shellfish may selectively ingest and/or digest different particle types, whilst effecting compensatory adjustments that may help to maximize the utilization of particles rich in chlorophyll (Hawkins et al., 1999, 2001; Pascoe et al., 2009). ShellSIM distinguishes the processing of organic matter within three types of food: living phytoplankton (quantified by chlorophyll), other particulate organic matter (POM, bacteria, protozoans, colloids and detritus), and inorganic Suspended Particule Matter (SPM). For each of these dietary components, a separate functional relation simulates filtration, pre-ingestive rejection and ingestion within ShellSIM, affording prediction of absorption on the basis of the resulting organic content of ingested matter. ShellSIM takes into account allometric and ageing effects to simulate growth and its component physiological processes through full ranges of temporal and spatial variability in environments that extend from open water to turbid estuaries. An example simulation is shown in Figure 7.

The model can simulate individual growth to within 25% error even when applying a single standard set of species-specific parameter values across con-
Similarly, trans-site analysis of all measured and predicted data, using a single standard set of ShellSIM parameters, for a standard time stepsize (DT) is the interval of time between calculations by ShellSIM. ShellDIM affords the User choice of DTs that include 0.25, 0.5 and 1.0. Whilst Plymouth Marine Laboratory advises use of a single standard set of parameters to predict growth across a broad range of culture environments and practices. The robustness of ShellSIM’s mathematical and algorithmic structure is confirmed by successful calibration and validation in 14 species to date, exemplified in Figure 8 for the Pacific oyster.

Figure 7: ShellSIM simulation of the growth of cultivated oysters Crassostrea gigas in loch Creran. Oysters for analysis were supplied by the farmer at regular intervals, and food concentrations and other conditions were measured monthly from a research vessel during the KEYZONES project.

**Crassostrea gigas**

Figure 8: Validation of ShellSIM simulation. A single set of parameters was used to predict total fresh weight (TFW, g) at stages between 8 and 24 months during the normal culture of Crassostrea gigas in Sanggou Bay (China), Oosterscheldt (Netherlands), Strangford Lough (Northern Ireland), Carlingford Lough (Northern Ireland), Clew Bay (Republic of Ireland) and Loch Creran (Scotland). The predictions were compared with observations using the regression method given by Portilla & Tett, 2007: the fit is ‘excellent’ because the intercept does not differ significantly from 0, nor the slope from 1.

Trans-site analysis for M. edulis during normal culture at a variety of
sites in N-W Europe, shows fair agreement between observations and predictions (Figure 9).

Figure 9: Validation of ShellSIM simulation. A single set of parameters was used to predict shell length (mm) at various stages during the normal culture of *Mytilus edulis* in the Pertuis Breton (France), Oosterscheldt (Netherlands), Strangford Lough (Northern Ireland), Carlingford Lough (Northern Ireland), Lough Foyle (Northern Ireland), Belfast Lough (Northern Ireland) and Clew Bay (Republic of Ireland). The predictions were compared with observations using the regression method given by Portilla & Tett, 2007. $r^2 = 0.76; a = 6.6 \pm 2.3 (p = 0.006); b = 0.81 \pm 0.05 (p < 0.001)$.

In the terminology of Oreskes et al. (1994) the fit is ‘fair’ because although the model explains more than three-quarters of the variance in the observations, the intercept is significantly different from 0 and the slope significantly different from 1.
10 Initial and Boundary Conditions: in principle

Because models such as ACExR-LESV are discretizations of partial differential equations in which the independent variables are time and space, solutions typically depend on values at temporal origins and spatial boundaries. As explored in Appendix B, simulations are typically less sensitive to values chosen for initial conditions than to time-series of spatial boundary conditions. Thus, the computer model uses the initial boundary values as default start-up values for model state variables. This section considers the importance of spatial boundary conditions in general and through an example; the next section reports on work done to set up a data-base of default boundary conditions.

Boundary conditions are external conditions that can influence the state of a system. Systems can be closed (completely self-contained) or open to these external influences. Open boundary conditions are of two types. In the first type, quantities flow across the boundary, causing either a gain or a loss. In the second type, conditions at the boundary influence rates within the modelled system without transfer of substance. Because state variables obey conservation laws, it might be thought that fluxes should result in changes at the boundary. In reality, they must; but for modelling purposes it is assumed that beyond the boundaries lie infinite sources or sinks, so that withdrawals or additions have no effect. This assumption allows boundary data to be prepared independently of simulations.

Figure 10: Loch Creran Section constructed from CTD observations on 25 March 2009. The colours show water density.

Figure 10 shows an observed distribution of water density along a longitudinal section of loch Creran, and an interpretation in terms of water circulation. Superficial water from the Firth of Lorn enters Creran and, being denser than the upper water of the loch, sinks below it: entering layer 2 of the model in Fig. 2. It is the conditions in the Firth adjacent to Creran that provide the sea-boundary conditions for the loch.
There are also landward and other boundary conditions to take into account. Consider a physical state variable: salinity. This influences water density, and it is differences between loch and sea-boundary densities that drive the gravitational circulation. This circulation brings salt into the loch, as does tidal mixing (Figure 2). The landwards boundary condition is a flux of absence of salt, the freshwater discharge. There is a similar flux into the top of the box, due to rain. Finally, the bottom boundary of the loch is closed to salinity: neither salt nor freshwater enter or leave the sediments. Because the model simulates no internal processes removing salt, the average salinity of the loch is determined only by the boundary fluxes (although the salt content of each layers is influenced by other physical processes).

Chlorophyll concentration is an example of a biological state variable. The 5th row in Figure 11 shows the time-series at the sea-boundary and the resulting simulation of chlorophyll. The model simulates growth of microplankton in water that enters the loch and is entrained into the surface layer, giving rise to higher concentrations there. The growth uses nutrient, and so DAIN concentrations in layer 1 are typically less than those at the sea-boundary, as shown in row 6. Thus, both chlorophyll and nutrients exhibit linked dynamical behaviour within the simulated system, as implied by the $\beta$ term in eqn. 1. Nevertheless, much seasonal variation in these variables is prescribed by the seasonal cycle at the sea-boundary.

We assume that no freshwater microplankters survive exposure to seawater and hence that no chlorophyll is contributed by river discharge. This is however a source of nutrient. Nutrient also enters at the sea-bed as a result of mineralization. Finally, an important boundary influence is that of surface irradiance, which, after attenuation by its passage through the model layers, controls photosynthesis and hence microplankton growth rate.

The two columns in Figure 11 compare two sorts of forcing. The left column shows the results of forcing with boundary condition etc data for 1978, insofar as it is available. The right column shows the results of forcing with climatological data, which is most simply explained as the result of fitting smooth curves through one or more years of time-series of observations of the variable. The curves display seasonal trends without the day-to-day variability that characterizes the weather.

Figure 11: **Effect of boundary conditions on Creran simulations** with ACExR and LESV (but no aquaculture). Left column - 1978; right column - climatology. Total solar irradiance measured at Dunstaffnage; just under half is photosynthetically effective. 1978 water discharge from flow guaging of River Creran; ‘climat’ data estimated from rainfall on catchment. Sea-boundary nutrients and chlorophyll were climatological, even for the 1978 simulation.
med \( h_1 = 7.3 \) m
med \( h_{12} = 16 \) m
med \( V_1 = 88 \) M.m\(^3\)
med \( V_{12} = 157 \) M.m\(^3\)

depth, m

Sea−boundary sal & layer interfaces

med \( E_T = 0.324 \) d\(^{-1}\)
med \( E_G = 0.148 \) d\(^{-1}\)
med \( E_K = 0.222 \) d\(^{-1}\)

exchange rates for \( L_1 + L_2 \)

tidal \( E_T \)
estuar \( E_G \)
mixing \( E_K \)

Creran 70s envelope

nit BC
nit L1
nit river

total chlorophyll

corr. 70s envelope

Creran 78 observations

Corr. 78s replicate

corr. 78s replicate

total chlorophyll

nitrate

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11 Building a Boundary Condition data base

Simulation of conditions in a given loch or voe requires information about the shape and depth the water body and its connection with the sea. ACExR takes this from a digitized version of the Sea-lochs Catalogue of Edwards & Sharples (1986), included in the data base that accompanies the computer code, and read by the ACExR function ReadCatalogue. Table 4 lists the information on boundary and forcing conditions (excluding aquacultural inputs) that is, also, required for a simulation.

<table>
<thead>
<tr>
<th>boundary</th>
<th>ACExR</th>
<th>LESV</th>
</tr>
</thead>
<tbody>
<tr>
<td>seabed</td>
<td>none</td>
<td>fluxes of nutrients (into), and oxygen (from), each layer</td>
</tr>
<tr>
<td>land</td>
<td>freshwater discharge $Q_F$; salinity $C[F] = 0$; temperature $\theta[F] = \theta[1]$</td>
<td>freshwater nutrients ${S^m[F]}$; chlorophylls ${X^{mp}[F]} = 0$; SPM $M^{SPM}[F] = 0$; dissolved oxygen $O[F] = O[1]$</td>
</tr>
<tr>
<td>land</td>
<td>wind speed $W$; air-sea heat flux $Q_{SHF}$</td>
<td>surface PAR $I_0$; $O[A] = O_{sat}[1]^*$</td>
</tr>
<tr>
<td>sea</td>
<td>density $[E, 1, 2]$ calculated from profiles of: salinity $C[E, z]$ &amp; temperature $\theta[E, z]$</td>
<td>nutrients ${S^m[E, 2]}$; chlorophylls ${X^{mp}[E, 2]}$; SPM $M^{SPM}[E, 2]$; dissolved oxygen $O[E, 2] = O_{sat}[1]^*$</td>
</tr>
<tr>
<td>sea</td>
<td>* calculated from oxygen saturation at salinity $C[1]$ and temperature $\theta[1]$.</td>
<td></td>
</tr>
</tbody>
</table>

The most accurate simulation should result from using a set of intensive time-series of boundary conditions for the given loch in a particular year. Rarely, however, are full sets of intensively measured BCs available, and it often necessary to interpolate between sparse observations, to substitute data from other sites for the same year, or to use climatological data obtained by averaging available values over a number of years. Figure 11 compares the results for loch Creran simulation of using forcing from 1978 with those from using climatological forcing. In fact, even the 1978 forcing was incomplete: there were insufficient nutrient and chlorophyll data available from 1978 to allow an adequate boundary condition time-series to be
constructed for this year, and so the simulations used climatological series for these variables.

Part of the work in phase 2 of the project was to set up a **data-base for boundary and forcing conditions**, such that a simulation would never fail to run because of lack of these data. Systematic and step-wise searching methods were therefore programmed into the function `ReadDBForcing2` in ACExR, and the function and `LoadData2` in LESV.

In the case of ACExR, `ReadDBForcing2` expected data-file names to be supplied to `RunLESVBatch`. If a file was not found, its name was replaced by a climatological default. In most cases, `ReadDBForcing2` searched for the nearest station for which data were available for the specified year or climatology.

Where no *river-flow data* were available, freshwater discharge was computed as a fixed fraction of daily rainfall over the land catchment and loch surface. Areas were available from the Sea-lochs Catalogue, and the precipitation data-base was searched for the nearest site for which rainfall data were available. The graphs in the second row of Figure 11 show the differences in runoff obtained in these two ways. They result from several imprecisions in the method using rainfall: the use of a fixed fraction to convert precipitation into run-off does not allow for any retention in the catchment nor for seasonal variation in the amount of evapotranspiration; and there was no allowance for local variations in rainfall due to topography, such as explored by Tyler (1983) for the loch Creran catchment.

**Sea-boundary hydrography** was mostly supplied from a UK Hydrological Office climatological data base, which provides monthly values in 0.25° rectangles. Profiles of temperature and salinity were interpolated to give daily time series for each metre of the water column. The difference between such data, and that obtained by observation in a given year, can clearly be seen in row 3 of Figure 11. 10

**Wind speed** data were those reported at open sites, such as Tiree airport. The effective wind may be less, depending on wind direction and loch topography.

LESV needed a different approach. Whereas the UK Hydrological office data base covers the whole of Scotland, albeit at low resolution, and UKMO data (obtained by way of BODC) provides meteorological data at characteristic locations across the highlands and islands, there was (and still is) no simple analogue for chemical and biological data, although there is quite a lot of relevant data. LESV therefore employed a data-base struc-

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10 1978 observational data were interpolated to daily values from CTD profiles at station LY1 reported by Tyler (1983) at intervals of about 2 weeks.
ture involving directories for water-bodies (such as ‘Creran’), regions (such as ‘LORN’) and provinces (such as ‘ScotNW’): see Figure 12. The idea of dividing aquaculturally-relevant waters into two major areas came from a statistical analysis of spatial variability described by Portilla & Tett (2008). The regionalization of source waters was based on expert knowledge of the western coastal waters of Scotland and on the known or likely existence of sufficient data for making boundary conditions time-series.

For example, the region ‘LORN’ refers to the inner part of the Firth of Lorne which provides boundary conditions for lochs Creran, Etive, and Spelve, amongst others. A station near the southern end of Lismore has been sampled by SMBA/SAMS in many years starting in 1970, and conditions here have been taken as representative of boundary conditions throughout the region. In principle the search routines in LoadData2, tasked with finding boundary nutrient data for loch Creran and year 1978, would start in directory NCnut, subdirectory Creran and look for a file called BCnut1978. In default of this, the function would continue search within NCnut, looking first for LORN/BCnut1978, then for LORN/BCnutclimat, and finally for ScotNW/BCnutclimat. Currently the function decides the regional and provincial directories in which to search by checking a loch’s latitude and longitude against limits prescribed for each region and province: for example, default boundary condition data any loch or voe with an entrance east of 3°W would be sought in the ScotNE directory.

Figure 13 shows some of the results of a detailed statistical analysis of variation at the south Lismore (LY1, Greag Isles) station that had been made in phase 1 (Portilla & Tett, 2006a,b). All available data from the upper part (0-10 m) of the water column were used. A (Generalized, non-linear Additive Model, or GAM) was fitted with components for long-term trend, seasonal variation, and ‘noise’ or higher-frequency variation (Portilla et al., ms 2008). The chlorophyll data were log-transformed. The seasonal variation components - shown by the ‘seasonal cycle’ lines in the figure - were used for the ‘LORN’ regional climatology.

Some effort was put into getting data for the ‘NORTHMINCH’ region, regularly sampled near Loch Torridon by FRS/MSS, but analysis was incomplete at the time of writing this report. Boundary condition data for the ‘CLYDE’ region were obtained from the analysis (Slesser & Turrell, 2005) of Clyde Sea data for chlorophyll and nutrients in the FRS data-base.

11 To be precise, using some placeholder names and the Mac OSX and Unix separator /, the current search pattern for the nutrient example is: <Loch>/BCnut<year>; <Loch>/BCnutclimat; <REGION>/BCnut<year>; <REGION>/BCnutclimat; <Province>/BCnut<year>; <Province>/BCnutclimat; OTHER/BCnutclimat. In the case of loch Creran, the LORN conditions are the same as the Creran conditions, but this is not always so.

12 It is, however, planned to assign all lochs and voes in the Sea-Lochs Catalogue to a region and province using a look-up table containing expert opinion about source-water.
The main effort in phase 2 went to the ‘final default’ sea-boundary conditions, and involved a detailed analysis of information in the Hydchem data base of ICES. Two provinces were defined (Figure 12(b)). Many data were available for the period 1970 through 2003 (exemplified in Figure 12(c)). They were filtered to exclude samples taken at depths greater than 10 m and in water columns of greater than 100 m: i.e. to include near-surface samples from continental shelf waters. A GAM method was used, to identify long term trends and seasonal cycles in each province (Portilla & Tett, 2008), with corrections for aggregation of sampling in certain seasons and areas.

Boundary condition data for particulates other than chlorophyll are discussed in the next section. The remaining important sea-boundary condition was that which sets the ‘balance of organisms’ in the microplankton, i.e. the ratio ψ, defined as $X/(X^{mp1} + X^{mp2})$. Microscopic observations of phytoplankton from LY1 (Tett, 1973) and the FRS station offshore from Stonehaven (Bresnan et al., 2008) were used to compute time-series of this ratio, calculating chlorophyll from cell volumes and assumed values of the heterotroph fraction η for each microplankton. LY1 results were used for ‘LORN’ and ‘ScotNW’, and the Stonehaven results for ‘ScotNE’.

Figure 14 presents and compares some of these sea-boundary conditions.

Finally, there was a need for information about conditions at other boundaries, in particular on nutrients in freshwater and about the ‘background’ sea-bed fluxes. ‘Default’ data files were assembled for nutrients, using annual average concentrations of each nutrient as found in the river Creran. This could be improved using SEPA data, although only one catchment that is regularly sampled by the Harmonized Monitoring Scheme is typical of both highland drainage and the short rivers of the west coast and islands (Anderson et al., 2010).

The ‘background’ exchanges of nutrients and oxygen between the seabed and the water column are currently treated as a boundary condition, independent of conditions inside lochs, although they might be better modelled as a function of sedimenting organic material that mineralizes in the sea-bed. Based on work during the OAERRE and related projects, a constant value of each flux is assumed, independent of loch, water depth or time of year. The background fluxes are currently implemented within the LESV function Blackfish so that they can be combined with fluxes resulting from aquacultural waste.

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Figure 12: Regions and Provinces in the LESV data-base  (a) shows part of the west coast of Scotland and the coastal water regions used in the LESV data-base. (b) shows the two provinces: W - ScotNW and N = ScotNE. Circles show lochs and voes in the Sea-lochs Catalogue. (c) shows the positions of DIN samples (taken between 1970 and 2003) for which data were obtained from the ICES data-base and used to construct the default climatology for this variable.
Figure 13: Climatology for nitrate and chlorophyll in the Firth of Lorne Station: LY1, near the Greag isles towards the south-east of Lismore. Data from several sources: Paul Tett (SAMS) measured chlorophyll in 1970-71; Brian Grantham (SMBA) was responsible for nutrient and chlorophyll measurements in 1979-1983, Johanna Fehling (UHI/SAMS during PhD studies in 2000-2003, and Celine Laurent (Napier) during PhD studies in 2003-2005. The dashed lines include 95% of the observations.
Figure 14: Comparison of Boundary Conditions. The ‘CLYDE’ and ‘LORN’ regions are mapped in Figure 12(a), and the ‘ScotNW’ and ‘ScotNE’ provinces are mapped in part (b) of that figure. N:Si is the atomic (or molar) ratio of dissolved nitrate to dissolved silicate. The diatom proportion of microplankton chlorophyll is $X^{mp} / X$.
12 Optics and particulates

An marine optical sub-model is an important part of LESV because of the need to simulate light, or, more precisely, *photosynthetically active radiation* (PAR), in each layer. At the heart of this sub-model is $\zeta$, the ‘optical thickness’ of a model layer. It is calculated by multiplying layer thickness $h$ by the diffuse attenuation coefficient $K_d$. The attenuation coefficient is the proportion of PAR lost as it passes through 1 metre of water; it is inversely proportional to transparency and can itself be used as a water-quality indicator. The optical sub-model has two main components:

- algorithms (Kirk, 1994; Bowers et al. 2000) for calculating the value of $K_d$ from the coefficients $a$ (absorption) and $b$ (scattering):

  \[ K_d = \mu_0^{-1} \cdot \sqrt{a^2 + k \cdot a \cdot b} \]  

  (3)

  The values of $a$ and $b$ result from summing the products of the absorption, or scattering, cross-sections and the concentrations of the optically active constituents (OACs): seawater itself, dissolved ‘yellow-substance’, chlorophyll-containing phytoplankters, and other particles;

- algorithms for calculating 24-hr mean PAR $I_{[l]}$ averaged over each layer, given 24-hr mean PAR $I_{0-}$ just beneath the sea-surface:

  \[ I_{[l]} = I_{t+} \cdot \frac{1 - e^{-\zeta_{[l]}}}{\zeta_{[l]}} \]  

  where: \( \zeta_{[l]} = K_{d,[l]} \cdot h_{[l]} \)  

  (4)

  and $I_{t+}$, the effective PAR at the top of each layer, is:

  \[ I_{1+} = m \cdot I_{0-} \]  

  \[ I_{2+} = I_{1+} \cdot e^{-\zeta_{[1]}} \]  

  \[ I_{3+} = I_{2+} \cdot e^{-\zeta_{[2]}} \]  

  (5)

  Exponential (Beer-Lambert) decay of light with depth is assumed in layers 2 and 3. It is, however, typically observed that PAR decays faster than exponential near the sea-surface, and this effect is approximated by the factor $m$ (Tett, 1990).

  The near-surface hypergeometric decay results from the more rapid absorption of certain wavelengths of light as PAR penetrates the upper part of the sea (Kirk, 1983).  

  This analysis suggests that an improved model could use two PAR components:

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14 The Beer-Lambert law assumes monochromatic light of uniform angular distribution in a water column homogenous with respect to OACs. Kirk (1983) points out that, in the absence of scattering, $K_d = a/\cos \theta$, where $\theta$ is the zenith angle of the light beam in the water. In waters containing many light-scattering particles, $K_d$ for monochromatic light can increase with depth, compensating for hypergeometric decay.
The most penetrating light, which we’ll call \textbf{green}, although the actual colour depends on the optical type of the water. The parameter \( m \) in eqn. 5 is this component’s fraction, just below the sea-surface, of PAR.

The less-penetrating light, mostly absorbed near the sea-surface. We’ll call this \textbf{red}, although it will often include some blue light, and it also implicitly includes shallow-angle green photons.

Each component has its own rate of decay with depth, with \( K_{d,\text{red}} > K_{d,\text{green}} \) and \( K_{d,\text{green}} \) corresponding to \( K_d \) in the one-component model. A revised model will therefore need red and green values of the absorption and scattering cross-sections for each OAC.

When the single-component model was updated for phase 2 of the project, the values of the absorption and scattering cross-sections were taken from Devlin et al. (2009). They had been estimated by non-linear fit of a set of equations, including 3 above, to estimates of \( K_d \) obtained from regression of submarine PAR on depth, excluding depths at which less-penetrating light was important. The independent variables were salinity (a proxy for yellow-substance), chlorophyll, and total \textit{suspended particulate material} (SPM). The data were obtained in estuaries and coastal waters around the U.K.

The plan in phase 2 of SARF012 was to repeat Devlin’s study using data obtained by MLA (FRS, now MSS) in coastal waters and sea-lochs of N-W Scotland. This work has not been completed, but some progress was made using data from Loch Torridon. Although not appreciated at the time of the phase 2 proposal, the FRS light sensor (attached to a CTD) follows the design of Højerslev (1975) by having upper and lower hemispherical light collectors. According to Kirk (1983): adding the signals from the two collectors gives a response proportional to \textit{scalar irradiance}, \( E_0 \); subtracting the lower signal from the upper gives a response proportional to \textit{net downwards irradiance}, \( \vec{E} \). The attenuation coefficient \( K_E \) is obtained from the rate of change of \( \ln(\vec{E}) \) with depth, while the attenuation coefficient \( K_0 \) is estimated by \( \Delta \ln(E_0) / \Delta z \).\footnote{Scalar irradiance, \( E_0 \), is “the integral of the radiance distribution at a point over all directions from the point” (Kirk, 1983). Planar irradiance, \( E \), is the radiant flux per unit area of surface, and is measured with a flat plate collector of photons with a response proportional to the cosine of the angle (to a line at right-angles to the surface of the plate) at which the photons arrive. Such a flat plat detector, lying parallel to the sea-surface and pointing upwards, measures \textit{downward} irradiance, \( E_d \); if turned over, it measures \textit{upward} irradiance, \( E_u \); \textit{net downwards} irradiance \( \vec{E} = E_d - E_u \). \( K_d = \Delta \ln(E_d) / \Delta z \).

The benefit of being able to estimate these two forms of attenuation coefficient is that they, in turn, allow direct estimation of (beam) \textit{absorption coefficient}, \( a \), and \textit{mean cosine}, \( \bar{\mu} \):\footnote{Following convention, we use the symbol \( \mu \) for (microplankton) specific growth rate and \( \bar{\mu} \) for the mean cosine of the angle made by underwater photons to the vertical. The context (and the overbar) should make clear which meaning is intended.}

\[
a = K_E \cdot \frac{\vec{E}}{E_0} = K_E \cdot \bar{\mu} \tag{6}
\]
Figure 15 shows an example profile from Loch Torridon. The first panel presents the (calibrated) outputs from the two hemispherical light collectors. The second panel shows the analysis of these data to give values of $K_E$, $a$ and $\bar{\mu}$ from differences between outputs in successive 1-metre depth increments. The third panel shows water-column structure (as density), chlorophyll concentration estimated by fluorescence, and red beam attenuation measured by a transmissometer and proportional to total SPM.

Figure 15: **Optical measurements** and derived variables at station S1 in Loch Torridon on 4 September 2005. FRS data. $dPAR$, $uPAR$ and $sPAR$ refer to downwards, upwards and scalar PAR. $K_E$ is the attenuation coefficient for net downwards PAR, $\mu$ (strictly, $\bar{\mu}$) is the mean cosine of the angles made by downwards photons to the vertical, and $C$ is salinity relative to the minimum observed value. Beam attenuation $c_{red}$ was measured by a red beam transmissometer, and shows water turbidity increasing near the sea-bed. The horizontal line across all the panels shows the depth at which water was sampled, and the dashed horizontal line shows the depth of minimum estimated (PAR) absorption coefficient. Note that the values of $\bar{\mu}$ seem too high for a profile made at $\sim 57^\circ$N and 3 hours before local noon.

In a homogenous water column, the minimum value of absorption ($a_{min}$) could be equated with $a_{green}$ and the difference $a_{PAR} - a_{min}$ could be taken as the red absorption. Then, given data from a number of profiles, each ab-
sorption coefficient could be related to concentrations of OACs by multiple regression, in order to estimate a pair of absorption cross-sections (red and green) for each OAC. Most observed water columns were however not homogeneous with respect to OACs, as figure 15 shows, and it will therefore be necessary, in addition, to calibrate measurements by CTD sensors against OAC contained in the water samples taken in the surface layer.

Concerning these OACs,

- **yellow-substance** (YS): its salinity proxy is dynamically simulated by ACExR, but the MLA data, which include direct measurements of YS absorption at a standard wavelength, will allow investigation of the salinity-YS relationship; in addition, calibration of salinity against YS will allow salinity profiles to be interpreted as YS profiles, as required for the overall analysis;

- **chlorophyll** is directly simulated by LESV, and calibration of the CTD-fluorometer allows fluorescence profiles to be interpreted as chlorophyll profiles, as shown in figure 15;

- **SPM** was included as a single variable in the original version of LESV, and is been kept as a single variable when LESV is run in dCSTT mode. There are no in-loch dynamics. When LESV is run in LESVSF mode it simulates two components that are subject to removal by filter-feeding shellfish: inorganic suspended particulate matter (iSPM) and organic suspended particulate material (more commonly called particulate organic matter: POM). The latter excludes anything (such as living micro-heterotrophs) that are correlated with chlorophyll. The two components can be estimated by combusting SPM samples: the organic part burns away and the remainder is iSPM, and a correction can be made to the POM for material related to measured chlorophyll. In addition, it should be possible to calibrate the signal of the CTD-transmissometer against sample (total) SPM, so as to obtain depth profiles of SPM.

As we’ll see, POM is of importance to mussel growth, and it will be desirable to improve its simulation in the LESV model (by adding $\beta$ terms) and to get better boundary condition data for it. Existing MLA data should give some additional information on seasonal cycles of POM and iSPM as well as allowing the better parameterization, envisaged here, of the optical sub-model.
13 Re-engineering ACExR-LESV

At the conclusion of phase 1, the ACExR-LESV system as published in the package LESV_1_3 (17 October 2007), had these two main components:

- a set of functions for running ACExR, called from ACExR and including an initial set of meteorological and hydrological data-bases to allow the physical model to be run for lochs Creran and Etive; the main function was CalcE that ran the time-step loop to simulate changes in layer properties and exchange rates during a year.

- a set of functions for running LESV, called from LESVsolver and including an initial set of boundary condition and farm-feed data to allow the biological model to be run for loch Creran; if ACExR had already been run, LESV loaded the physical model output, otherwise it called ACExR; the matlab function ode23 was used to provide numerical integration and called LESV which contained the top-level equations for the biological model.

During phase 2, the package structure went through two major rebuilds:

1. The first improved the boundary condition data available to LESV, built the interface function ShellFish to shellfish models, and improved the ability of ACExR to simulate a variety of water bodies, including sill-less fjords and voes. The result was published to Drop-Box as the package ACEXR-LESV_eco2_AUG_2010 on 17 August 2010.

2. The second resulted from a user meeting in Dingwall in January 2011, and aimed to allow multiple runs of ACExR-LESV within a single batch job, directed by a configuration file, and recovering from errors during particular runs. As shown in Figure 16, the new version uses the function LESVBatch. Results from each run are saved to a pair of mat-files (one for ACExR and one for LESV results) named by loch and simulation year, and these become available to user-written programs for data visualization and analysis. Although not all planned changes have been fully implemented, the reworked code will be published to Drop-Box on 5 August 2011 as the package ACEXR-LESV_eco3_AUG_2011. It contains a ‘read-me’ file giving minimum details for set-up and run, as paraphrased in Appendix I.

What remains to be done is:

- linking the pre-compiled ShellSIM.dll with the LESV interface function Shellfish;
- completing code for reading configuration and parameter XML files.
Figure 16: Flow diagram of the function LESVBatch, which can be used to make multiple runs of the ACExR and LESV models, by calling RunACExR (Fig. 24) and RunLESV (Fig. 25).

- Function LESVBatch
  - OutputDir (name), where
  - Parameters selected for screen or log-file output.
  - Function iterates through config_row() to config_row(config_row()) in iteration n.
  - Structure config is config_row(config_row()) in iteration n.
  - Fields in config_row include:
    - config_file (keyword),
    - SetF (set configuration file),
    - SetW (set working directory),
    - SetC (set configuration file),
    - SetL (set log file),
    - SetS (set script file).
14 Advances in programming ShellSIM

A key advance in the programming of ShellSIM, undertaken by Plymouth Marine Laboratory to help integration with ACExR-LESV and other models, has entailed developing the capability for a floating time-step.

Time-step ($\Delta t$) is the interval of time between calculations by ShellSIM, expressed in days. The ShellSIM package uses the Euler algorithm (see section 7). The revised version of ShellSIM, written in the C$^\#$ language and compiled using the Microsoft.NET framework to a dynamic linked library or dll, allows the user to set a variable timestep of between 1 and 0.01 day, subject to any changing requirements of linked software, such as ACExR-LESV.

Model results have been calibrated and validated for a standard time-step of 0.25 days, which had been found suitable for the processes involved in shellfish growth. Increasing $\Delta t$ from 0.25 to 1 results in cumulative overestimation in the lifetime prediction of growth of less than about 1.5%, compared with cumulative underestimation in the lifetime prediction of growth of less than about 0.5% when using shorter time-steps (down to 0.01).

It is necessary to distinguish the numerical integration time-step ($\Delta t$) from the ‘frequency window’ used to examine or analyse observations, including forcing data. Conditions at real shellfish farms change continuously, but most of this change occurs as a result of tidal processes and diel variation, and, on the longer term, from weather-related day-to-day variability, the spring-neap cycle, and the cycle of the seasons. ShellSIM can simulate physiological responses in shellfish over time intervals of 30 minutes, the minimum response time for which predictions have been calibrated. Thus it could be coupled with an ecosystem model that provides for changing tidal conditions, as well as temperature, during the course of a day. Although ACExR uses $\Delta t = 0.01$ day, and LESV employs a variable timestep that is typically a fraction of a day (see section 4), both these models deal in daily-averaged processes. Thus LESV will supply ShellSIM with values of environmental conditions that are averaged over tide and day.

Calculation of aerial exposure, although not an issue within the current application of LESV-ShellSIM to suspended-rope culture, illustrates subtle problems that might arise because of this coupling. Filtering ceases when shellfish are exposed to air (because they close their valves). A bivalve at mean tide level will spend half its time in air and half its time submerged. This does not mean that food acquisition is a half of what it would be if the animal was sited below low-water of spring tides. Although species differ, it is known that a mid-tide animal might compensate through faster feeding, and so acquire, say, two-thirds of what the permanently-submerged animal

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17 To be precise, the values supplied each time that the LESV function Shellfish issues a call to a shellfish model are the result of a smooth interpolation through daily-mean values: there is no abrupt change at midnight!
might get. Given the potential for physiological acclimation, a challenge in model-making is thus to *parameterize* over different time-scales.

All environmental variables needed by ShellSIM can be supplied as time-series of at least daily resolution. But in addition, when data are limiting, ShellSIM has been designed to accept single average values such as may be representative of seasons or sites. This is convenient, for example, because current speeds influence filtration rates, and ACExR is a water-body scale model, and so cannot predict flows that are local to a particular site. Instead, it is possible to input a single value to ShellSIM, perhaps based on a series of current-meter measurements at the site under typical conditions.
15 Simulating exchange in a variety of water-bodies

During phase 2, ACExR was successfully run for 26 water bodies, including a simulation of conditions in Loch Sunart during the last thousand years. The combination of ACExR and LESV has been successfully run for the diversity of water bodies listed in Table 5. The bugs detected and fixed during this work included those affecting the simulation of water bodies (most voes) that are without entrance sills and hence possess only two effective layers. There remain some water bodies and forcing conditions for which simulation fails, for example because of a divide-by-zero error generated when a layer ceases to exist (i.e. \( h \rightarrow 0 \)). We are beginning to understand what causes such events (Appendix E), but fixing them has not proven easy, and we have been reluctant to add error traps to the code (e.g. by ensuring a minimum layer thickness) that may implicitly break physical laws.

Table 5 summarises results from the physical model that are relevant to waste-assimilative and shellfish-carrying capacities. There is much variation between lochs and, as the Creran results show, inter-annually. Whereas the part of exchange due to tidal mixing (\( Q_T \)) remains much the same from year to year, the part due to fresh-water driven estuarine circulation (\( Q_G \)) was much less in the dry 1978 than in the more typical 1975.

Table 5: Median values of Exchange rates and related variables. \( E_1 V_{[1]} = Q_G + Q_H + Q_{K12} \). \( V = V_{[1+2+3]} \). See Appendix A for further details.

<table>
<thead>
<tr>
<th>water body</th>
<th>( h_{[1]} )</th>
<th>( E_1 V_{[1]} )</th>
<th>( E_1 )</th>
<th>( Q_F V_{[1]} )</th>
<th>( Q_G V_{[1+2]} )</th>
<th>( Q_T V_{[1+2]} )</th>
<th>( Q_{K23} V_{[3]} )</th>
<th>( V_{[3]} )</th>
<th>( V )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>m</td>
<td>Mm(^d)</td>
<td>d(^-1)</td>
<td>d(^-1)</td>
<td>d(^-1)</td>
<td>d(^-1)</td>
<td>d(^-1)</td>
<td>( V )</td>
<td></td>
</tr>
<tr>
<td>Creran 1975</td>
<td>6.5</td>
<td>20</td>
<td>0.280</td>
<td>0.011</td>
<td>0.115</td>
<td>0.289</td>
<td>0.862</td>
<td>0.266</td>
<td>214</td>
</tr>
<tr>
<td>Creran 1978</td>
<td>7.3</td>
<td>11</td>
<td>0.120</td>
<td>0.003</td>
<td>0.041</td>
<td>0.285</td>
<td>0.790</td>
<td>0.267</td>
<td>214</td>
</tr>
<tr>
<td>Creran clim</td>
<td>6.5</td>
<td>22</td>
<td>0.279</td>
<td>0.012</td>
<td>0.130</td>
<td>0.286</td>
<td>0.856</td>
<td>0.285</td>
<td>214</td>
</tr>
<tr>
<td>Fyne 2003</td>
<td>18</td>
<td>29</td>
<td>0.011</td>
<td>0.000</td>
<td>0.002</td>
<td>0.044</td>
<td>0.003</td>
<td>0.457</td>
<td>10246</td>
</tr>
<tr>
<td>Sandsound Voe 2003</td>
<td>14</td>
<td>7</td>
<td>0.107</td>
<td>0.002</td>
<td>0.072</td>
<td>0.103</td>
<td>-</td>
<td>0</td>
<td>86</td>
</tr>
<tr>
<td>Spelve 1981</td>
<td>4.6</td>
<td>13</td>
<td>0.344</td>
<td>0.004</td>
<td>0.092</td>
<td>0.359</td>
<td>0.158</td>
<td>0.493</td>
<td>177</td>
</tr>
<tr>
<td>Torridon 2003</td>
<td>12</td>
<td>33</td>
<td>0.041</td>
<td>0.001</td>
<td>0.006</td>
<td>0.119</td>
<td>0.011</td>
<td>0.239</td>
<td>4287</td>
</tr>
</tbody>
</table>

Typical mussel ropes extend to a depth of 10 metres, and thus in most cases lie within the model’s top layer. The flushing of this layer removes soluble wastes and supplies food from outside the loch or voe. This aspect of
carrying capacity increases with daily flux through the surface layer ($E_1 V_{[1]}$). Finfish farms impact on layer 2 as well as layer 1, and the table shows that tidal mixing is the largest single component of flushing when layers 1 and 2 are considered together. Finally, lochs in which ‘basin deep water’ exists are vulnerable to de-oxygenation here. This is influenced in ACExR-LESV by mixing between layers 2 and 3. Relative mixing rates are lowest in the deep lochs Fyne and Torridon, although the low exchange rates are offset by the large volumes of deep water. Also relevant is the alternation of periods of stagnation and renewal. The former are shown in the examples in Figure 17 by decreasing layer 3 volume, the latter by increasing volume. Also, as the Figure shows, the simulation of deep-water behaviour is dependent on the kind of sea-boundary data supplied, since simulated and real renewal events follow increases in density of external water at sill depth.

Figure 17: Changes in the relative volume of layer 3 in loch Creran in (a) 1978, with ACExR forced by gauged river flows and observed hydrographic conditions at the sea-boundary, and (b) forced by climatological runoff and sea-boundary conditions.
16 Simulating nutrient enhancement

Tett et al (2011) demonstrated how the ACExR-LESV model could be used to estimate a loch’s assimilative capacity for waste from fin-fish farming, by extracting indicator values (such as maximum summer chlorophyll concentration) from simulations at different farm loadings (Figure 18).

Figure 18: Estimation of Assimilative Capacity for waste from finfish farming in the imaginary Loch na Rerc. From Tett et al., 2011. Feed data from the second year of the productive cycle for a farm with a consented maximum biomass of 1500 tonnes were used. This loading was multiplied by values from 0 to 10 in different simulations, and indicator values extracted from simulations were plotted against the feed loading. Some parts of the diagram show indicative thresholds for quality standards: for example, summer chlorophyll not to exceed 10 mg m\(^{-3}\). Waste assimilative capacity is exceeded when the simulated indicator values cross these thresholds. In this hypothetical example, the chlorophyll threshold is not exceeded, and the assimilative capacity is set instead by the effect of the farm on deep-water oxygen.

This is an elaborate procedure, however, and for accuracy requires good boundary condition data. A simpler alternative is to use the Equilibrium Concentration Enhancement or hotspot approach of Gillibrand & Turrell.
LESV can be run in sECE mode, which does not calculate the $\beta$ terms in eqn. 1. The simulation still takes account of physical exchanges, of nutrient fluxes from the sea-bed and fish farm, and of nutrients at the sea-boundary and in freshwater. Switching off the $\beta$ terms thus enables the effect of a farm on nutrient concentrations to be examined in the absence of microplankton and without data for their boundary conditions.

Figure 19: **sECE simulation for loch Creran** in 1978. (a) shows concentrations of DAIN at the sea-boundary (BC) and in the upper 10 metres of the loch during run 1 (no fish-farms) and run 1 (1 standard farm, 1500 tonnes). (b) shows the DAIN enhancement by the farm, calculated as the difference between the run 2 and run 1 time-series. (c) shows the molar ratio of DAIN to DSi in the three conditions.

Figure 19 exemplifies results for DAIN in Loch Creran, showing the potential effects of the waste from a ‘standard farm’ of 1500 tonnes maximum consented biomass. Enrichment exceeded 1.2 $\mu$M on 10% of days, the highly enriched days occurring between May and August when nutrient-nitrogen is otherwise naturally scarce. Enrichment also perturbs the ratio of N:Si. Gen-
erally speaking, a molar ratio of 1:1 is considered optimal in that it should adequately support the growth of diatoms as well as other algae; higher ratios, especially those above 3 (Tett & Lee, 2005), can result in the ‘balance of organisms’ moving towards flagellate- or dinoflagellate-dominated systems, of concern because of the greater proportion of harmful species found in these groups. It is a striking feature of chemical conditions in the coastal waters of Argyll (at least) that nitrogen is comparatively scarce, and as the Figure illustrates, becomes depleted in Summer relative to silicon, which is supplied in freshwater discharge and by mineralization in the deep water of fjords (Grantham & Tett, 1993). So the addition of nitrogen by fish farms tends to move conditions closer to the optimal balance.

Use of the sECE mode enables lochs, such as those in Table 6 to be ranked in terms of the contribution of a ‘standard farm’ of 1500 tonnes to nutrient levels. The simulated farm impact is least in Torridon, the loch with the largest value of $E_1V_1$ (Table 5), and greatest in Sandsound Voe, which has the smallest value of $E_1V_1$. The Creran illustrate interannual variability as well as the consequences of using different sorts of boundary condition data.

Table 6: Enrichments resulting from the simulation by LESV in sECE mode of the addition of a standard salmon farm. $\Delta N$ and $\Delta P$ are the 90th percentile values of the excess of a simulation with 1 standard farm over a simulation with no farm. The figures in parenthesis are the average summer concentration of the nutrient at the sea-boundary, to allow the enrichment to be seen in context. The N:Si and N:P molar ratios are the summer means for run 2; the values in parenthesis are the equivalent means at the sea-boundary. ‘Summer’ was taken as June, July and August.

<table>
<thead>
<tr>
<th>loch</th>
<th>$\Delta N$ (BC)</th>
<th>$\Delta P$ (BC)</th>
<th>N:Si (BC)</th>
<th>N:P (BC)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\mu$M</td>
<td>$\mu$M</td>
<td>mol:mol</td>
<td>mol:mol</td>
</tr>
<tr>
<td>Creran 1975</td>
<td>0.73 (0.66)</td>
<td>0.06 (0.25)</td>
<td>0.54 (0.26)</td>
<td>5.1 (2.6)</td>
</tr>
<tr>
<td>Creran 1978</td>
<td>1.17 (0.66)</td>
<td>0.09 (0.25)</td>
<td>0.66 (0.26)</td>
<td>6.0 (2.6)</td>
</tr>
<tr>
<td>Creran 2003</td>
<td>0.73 (0.66)</td>
<td>0.06 (0.25)</td>
<td>0.53 (0.26)</td>
<td>5.0 (2.6)</td>
</tr>
<tr>
<td>Creran climate</td>
<td>0.67 (0.66)</td>
<td>0.06 (0.25)</td>
<td>0.55 (0.26)</td>
<td>5.3 (2.6)</td>
</tr>
<tr>
<td>Fyne 2003</td>
<td>0.49 (3.03)</td>
<td>0.03 (0.40)</td>
<td>1.36 (1.69)</td>
<td>11.4 (7.4)</td>
</tr>
<tr>
<td>Sandsound 2003</td>
<td>3.89 (1.36)</td>
<td>0.31 (0.27)</td>
<td>2.45 (1.03)</td>
<td>8.9 (4.9)</td>
</tr>
<tr>
<td>Spelve 2003</td>
<td>0.81 (0.66)</td>
<td>0.08 (0.25)</td>
<td>0.58 (0.26)</td>
<td>4.9 (2.6)</td>
</tr>
<tr>
<td>Torridon 2003</td>
<td>0.38 (2.57)</td>
<td>0.02 (0.33)</td>
<td>1.32 (1.31)</td>
<td>8.6 (7.8)</td>
</tr>
</tbody>
</table>

52
17 Simulating chlorophyll and microplankton

The simulations reported in the previous section do not predict observed nutrient concentrations in lochs: the purpose of the sECE mode is to calculate loadings rather than their consequences. In reality, much of the added nutrient will be used by phytoplankton and thus appear as chlorophyll rather than as extra DAIN or DIP. This effect is simulated in the LESV mode, which implements the biological model of section 6. Since results and tests of this model have been reported in detail for loch Creran in the phase 1 report and by Portilla et al. (2009), and since no further precise tests have been carried out using data from other lochs, this section is included mainly to complete the story.

Figure 20: LESV simulation for loch Creran in 1978 without aquaculture. Values for loch averaged over upper 10 m. In the two left-hand panels, simulations (chl loch, DAIN loch) are compared with envelopes containing 95% of values observed in the loch during the 1970s: (Tett & Wallis, 1978; Jones, 1979). The upper right-hand panel shows simulated chlorophyll associated with diatoms as a proportion of total chlorophyll, and the lower right-hand panel compares simulated nutrient (molar) ratios with Redfield ratio values.

Figure 20 reproduces part of the ‘standard results page’ (see Appendix J) from a simulation for loch Creran without aquaculture. Comparison of the simulated time-series for boundary conditions with those for the loch’s upper

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18 LESV can also be run in dCSTT mode, in which a single microplankton box depends on only N and P amongst nutrients. This corresponds to the dynamical CSTT model of Laurent et al. (2006) and Tett et al. (2003). The LESV mode adds silicon dynamics and splits the microplankton into ‘diatomy’ (silica-requiring) and ‘flagellatey’ (other) compartments.
layer, suggests that Creran is naturally a ‘source for plankton and a sink for nutrient’ - that is to say, it provides an environment that is better for phytoplankton growth than the sea outside, so that nutrients are converted into planktonic algae, despite losses of the latter to grazers. One concern about the use of sea-lochs for aquaculture is that they will flip, becoming sources for nutrients and sinks for phytoplankton. We examine this in section 19.

The diagram includes a weak test of the reliability of chlorophyll and DAIN simulations, showing that these fall within envelopes constructed from observations in the upper water of the loch during the 1970s. The argument for such a test, as contrasted with the direct comparisons of simulations and observations by Portilla et al. (2009) is that, even in the case of 1978, the year for which there are the best boundary condition data available for Creran, the biological model forcing had to be provided by climatological data. However, the comparison climatology was derived from all observations, whereas a stricter test would involve comparison with a climatological envelope of loch mean chlorophyll or nutrient. Such an envelope is harder to make, because it requires frequent systematic sampling at representative stations within the loch. Such sampling did take place in Creran during some years in the 1970s and again in the 2000s. MLA sampling in some of the lochs of the North-West Highlands during the 2000s should allow such envelopes to be calculated also for these sites.

The time-series of nutrient element ratios are here plotted inverted from their previous representation. This allows a watch to be kept for occasions when time-series of Si:N and P:N cause concern by falling significantly below the ‘Redfield’ values of 1:1 and 1:16. Such low values are not shown in these Creran simulations, and the relative abundance of Si and P relative to N explains the dominance throughout most of the simulation of diatomy microplankton. In Loch Fyne and the Firth of Clyde, flagellates and dinoflagellates are comparatively more abundant during Summer (Figure 21).

Figure 21: **LESV simulation for loch Fyne** in 2003 without aquaculture. Values for loch averaged over upper 10 m. See also legend to Fig. 20.
18 Simulating mussel farming

Use of a shellfish model embedded in an ecosystem model can help farmers understand and manage their farms in relation to the food available in the water. It can also help farmers collectively, and regulators, understand and quantify the limits on the amount of shellfish that could be produced in a given water body, and can be used to explore synergies between shellfish and finfish farms. The last point is dealt with in the next section. The results presented in this section provide some insights in mussel growth and maximum potential harvest. They were made using the less detailed GB98 model, so should not be treated as definitive until they have been redone with ShellSIM. And they are very dependent on the assumptions about seeding and harvesting practice that were used to set up a simulation, so we’ll start with those.

Most mussel cultivation in Scotland uses vertical ropes (‘dropers’) suspended beneath surface buoys. The ropes are exposed to mussel spat at a suitable site, and then incubated at the farm for several years. The model calculates a time-series of flesh weights (measured in mg C) for a typical mussel in each 1 metre section of a droper. Because the ACExR-LESV model system is set up for 1-year simulations, the outputs show mussels during the final year of cultivation, assuming that on 1 January (at the start of the simulation) all these typical mussels had a biomass of 80 mg C, corresponding to a wet weight (including shell) of 1.6 grams.

Figure 22: Simulation of mussel cultivation in Sandsound Voe in 2003 with 1 standard fish farm and 1 standard mussel farm. Horizontal axis gives days since 1 January.

The right-hand panel of Fig. 22 shows the changing biomass of typical mussels at selected depths in Sandsound Voe. The left hand panel shows a time series of mussel numbers under cultivation in the voe. Multiplying biomass by numbers harvested, and assuming 50% discards, allows calculation of the wet weight harvested each day.19

19 A ratio of 20 g wet weight to 1 g flesh C was assumed.
The time-series of numbers was set up in advance of the simulation. The harvest was assumed to take place uniformly between days 200 and 300 (late July until end of October). The aim was, allowing for 50% discards, to harvest 200 wet tonnes of mussels from this ‘standard farm’, which, at 100 mussels per wet kilogram, required an average final weight of 500 mg C per mussel. The mussels in Sandsound Voe didn’t achieve this required body mass and the harvest was only 87 tonnes. That wasn’t known when the forcing time-series was calculated, by extrapolating backwards from the supposed final weight and harvested numbers, and assuming a natural daily mortality of 1%, to obtain the required numbers at the start of the year: just over 46 million small mussels. This may be an oversimplified account of the reality of growing mussels, but it provides a time-series of mussel numbers for a ‘standard farm’, and thus gives a basis for comparing the ability of different lochs to produce mussels (Table 7).

Table 7: **Simulated mussel harvests** using LESV in **LESVSF** mode. A ‘standard shellfish farm’ (SF=1) sets out about 400 million mussels of 80 mg carbon biomass on January 1, as detailed in the text. The simulations are for 2003 and include 1 ‘standard finfish farm’ providing nutrient enrichment in the loch or voe. ‘Winter’ is Jan-Mar, ‘Spring’ is Apr-Jun. Means of chl and POM over upper 10 m.

<table>
<thead>
<tr>
<th>loch or voe</th>
<th>Creran</th>
<th>Fyne</th>
<th>Sandsound</th>
<th>Spelve</th>
<th>Torridon</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>SF = 0</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mussel harvest</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Winter chlorophyll</td>
<td>1.8</td>
<td>0.5</td>
<td>0.9</td>
<td>1.4</td>
<td>1.5</td>
</tr>
<tr>
<td>Spring chlorophyll</td>
<td>4.4</td>
<td>5.1</td>
<td>5.4</td>
<td>3.9</td>
<td>3.9</td>
</tr>
<tr>
<td>Winter POM</td>
<td>1.46</td>
<td>1.07</td>
<td>1.11</td>
<td>1.48</td>
<td>1.20</td>
</tr>
<tr>
<td>Spring POM</td>
<td>1.47</td>
<td>0.72</td>
<td>1.08</td>
<td>1.49</td>
<td>1.07</td>
</tr>
<tr>
<td><strong>SF = 1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mussel harvest</td>
<td>1039</td>
<td>90</td>
<td>87</td>
<td>827</td>
<td>424</td>
</tr>
<tr>
<td>Winter chlorophyll</td>
<td>1.4</td>
<td>0.6</td>
<td>0.8</td>
<td>1.1</td>
<td>1.5</td>
</tr>
<tr>
<td>Spring chlorophyll</td>
<td>3.6</td>
<td>5.0</td>
<td>5.0</td>
<td>3.3</td>
<td>3.7</td>
</tr>
<tr>
<td>Winter POM</td>
<td>1.13</td>
<td>0.97</td>
<td>0.72</td>
<td>1.15</td>
<td>1.05</td>
</tr>
<tr>
<td>Spring POM</td>
<td>1.10</td>
<td>0.60</td>
<td>0.74</td>
<td>1.13</td>
<td>0.89</td>
</tr>
<tr>
<td><strong>SF = 3</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mussel harvest</td>
<td>1194</td>
<td>81</td>
<td>56</td>
<td>900</td>
<td>484</td>
</tr>
<tr>
<td>Winter chlorophyll</td>
<td>1.3</td>
<td>0.7</td>
<td>0.7</td>
<td>1.0</td>
<td>1.5</td>
</tr>
<tr>
<td>Spring chlorophyll</td>
<td>3.5</td>
<td>4.9</td>
<td>5.0</td>
<td>3.1</td>
<td>3.6</td>
</tr>
<tr>
<td>Winter POM</td>
<td>0.89</td>
<td>0.83</td>
<td>0.54</td>
<td>0.92</td>
<td>0.89</td>
</tr>
<tr>
<td>Spring POM</td>
<td>0.98</td>
<td>0.48</td>
<td>0.70</td>
<td>1.01</td>
<td>0.79</td>
</tr>
</tbody>
</table>

--- SF = 0 ---

--- SF = 1 ---

--- SF = 3 ---

--- SF = 0 ---

A function `MakeSFN` was written to do this.
It is evident that from the table that the harvest differs between lochs and does not increase in proportion to mussels laid. Some of the differences may be artefactual, the result of the description of mussel growth in the GB98 model. As Figure 23 shows for loch Creran, the model predicts that in some cases mussels grow infeasibly large. There are biological constraints, not built in to the model, that will prevent this; in addition, it is likely that overlarge mussels will fall from the cultivation ropes.

Another cause of differences between lochs is the supply of food in Winter. At this time, phytoplankton abundance is low, and mussels survive by using POM. The limited data available to us, suggests that coastal waters and lochs differ in amounts of this substance. In addition, in the model, the only supply is from the sea outside the loch. In slow-flushing lochs, supply can be insufficient, with the consequence that, during Winter, mussels burn more stored food reserve than they acquire, and so decrease in size until the arrival of the Spring phytoplankton bloom. This is shown in Fig. 22 for mussels in Sandsound Voe.

Another control on mussel growth is provided by the balance between diatoms and other algae. LESV includes mussel preferences for the two kinds of phytoplankter, and in the simulations reported here, the preference for ‘flagellatey’ microplankton has been set to zero. The effects of this on a simulated mussel in Loch Fyne, where dinoflagellates are an important part of the phytoplankton in Summer, are shown in panel (b) of Fig. 23).

These results suggest that potential mussel harvest is likely to vary between lochs as a result of flushing, POM availability and phytoplankton composition. They argue the need for improvements both in the description of POM dynamics in the LESV model, and the information about POM in coastal seawater. Simulations could also be improved by using ShellSIM as an alternative to GB98, giving more realistic relationships between mussel growth and food, temperature, etc. Finally, there is a need to check both the simulated cultivation practices and the mussel harvest against reality in a number of lochs.
19 Synergies

Finfish excrete compounds of nitrogen and phosphorus into the water column, and faecal decay adds more by way of the seabed. These nutrients have the potential to stimulate phytoplankton growth and, in excess, to cause eutrophication, defined by the Urban Waste Water Treatment Directive as an ‘accelerated growth of algae and higher forms of plant life [that produces] an undesirable disturbance to the balance of organisms present in the water and to the quality of the water concerned’. Natural and cultivated filter feeders can remove some of this phytoplankton and the nutrient it contains. Thus there is a potentially positive synergy between shellfish and finfish farms, ameliorating a potential bad - too much phytoplankton - and turning it into a good - an enhanced supply of food for mussels. Table 8 contains estimates of nutrient removal as simulated by LESV. They are of course dependent on the growth model used and assumptions made about cultivation practice.

Table 8: Shellfish as nutrient-strippers in LESV simulations for 2003. See section 18 for details.

<table>
<thead>
<tr>
<th>1 standard fish farm (section 16) releases</th>
<th>tonnes N</th>
<th>tonnes P</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 standard mussel farm (section 18) harvests in:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Loch) Creran</td>
<td>104</td>
<td>25</td>
</tr>
<tr>
<td>(Loch) Fyne</td>
<td>18</td>
<td>2.5</td>
</tr>
<tr>
<td>Sandsound (Voe)</td>
<td>1.6</td>
<td>0.2</td>
</tr>
<tr>
<td>(Loch) Spelve</td>
<td>1.5</td>
<td>0.2</td>
</tr>
<tr>
<td>(Loch) Torridon</td>
<td>15</td>
<td>2.0</td>
</tr>
<tr>
<td>(Loch) Torridon</td>
<td>7.5</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Although some of the nutrient atoms removed in this way will have come from other sources, and shellfish themselves also excrete ammonium and phosphate, the harvesting of shellfish biomass can help to offset nutrient enrichment, as has been argued by Lindahl et al., 2005 and implemented by the Swedish town of Lysekil (Gren et al., 2009).

The LESV model can also be used to explore negative synergies, such as the possibility that finfish and shellfish farms will together increase N:Si ratios, and, by shellfishes’ differential filtration, stimulating flagellate blooms. This is currently being investigated as part of SARF053.

21 In the Creran simulation reported here, the nutrient-nitrogen taken up by phytoplankton, and not recycled by local zooplankton grazing, totalled 149 tonnes over a year. The sources of this DAIN included the sea, river discharge, benthic remineralization and recycling by cultivated shellfish themselves. The latter - the excretion of N that mussels got from phytoplankton - was 47 tonnes. 244 tonnes of DAIN-N entered the loch from the sea and 50 tonnes from river discharge. There was an outflow of 344 tonnes, and hence, in this simulation, the loch was a net exporter of DAIN-N.
20 Discussion and Conclusions

1. Re-engineering the ACExR-LESV code has resulted in a more robust program that is able to carry out multiple simulations of seasonal cycles in a variety of lochs and voes and to find at least default boundary conditions for all lochs and voes in the Sea-Lochs Catalogue (section 13). There remain some conditions that cause the physical model simulations to fail to complete, and there remains the need to complete the XML reading routines and the coupling of ShellSIM.

2. As discussed in section 4, building a reliable model, and showing that it is realistic, is a complex task. We have not, in this phase of the project, done much to compare simulations with observations. Given the scarcity of full sets of actual-year boundary condition data, the best way to test LESV might be to compare simulations with climatological envelopes of loch-averaged observations of the model state variables. In the case of shellfish modelling, there is a need for stakeholder engagement to allow comparison of simulated with actual cultivation practices and harvests.

3. The combination of the ACExR model and the LESV model in sECE mode should allow more precise estimation of the nutrient enhancement of lochs and voes by finfish farming (section 16). The LESV blackfish function may need updating in response to changes in feed composition and delivery practices.

4. Because phytoplankton growth is light-limited in some lochs, it will be important to complete the optical analysis of section 12.

5. Simulations suggest that the supply of POM for over-wintering shellfish is a key factor in setting carrying capacity (section 18). The supply depends both on flushing rates (which we think adequately estimated by ACExR), and the sea-boundary concentrations of POM (for which better data are needed). It also seems desirable to improve the simulation of POM dynamics within LESV.

6. Simulations also suggest that the harvesting of cultivated shellfish can remove a small but useful portion of finfish N and P (section 19).

7. Linking a shellfish model into LESV proved a difficult task, for several reasons (sections 3 and 7). Using the simple model GB98 proved useful both during the coupling work and in understanding the relationships between farming practice, shellfish growth, and the sea-loch ecosystem (section 18). Use of GB98 has also made clear why a more realistic shellfish model is needed, the better to predict growth, harvestable biomass and nutrient recover. ShellSIM, once linked to and tested in LESV, should provide this better model.
21 Potential for use and development

The variety of Scottish sea-lochs and voes is documented in the Sea-Lochs Catalogue of Edwards & Sharples (1986). The shape and size of each loch or voe interacts with weather, drainage basin characteristics, and zone C conditions to determine water layering and exchange, the sensitivity of the water body to fishfarm waste, and its ability to provide food for cultivated shellfish. The ACExR-LESV model system is: (i) a formal statement of present understanding of the relevant physical and biogeochemical processes in sea-lochs; (ii) a set of hypotheses about these processes for further scientific testing; and (iii) a tool for management and prediction of aquacultural effects and capacities. Thus it might be of interest to educators, research scientists, and aquaculturalists and their regulators.

ACExR and LESV parameterize processes that more detailed models simulate by solution of primitive equations, requiring specific adaption of 2D or 3-D grids to the detailed hypsography of each water-body. Because they draw on the digitized Sea-Lochs Catalogue, and have a data-base that is capable of providing at least default boundary conditions for all lochs in this catalogue, the ACExR-LESV model can be applied without the need for further data, although in most cases getting some local measurements will improve application precision. Thus ACExR-LESV package is simpler to use, and in suitable circumstances - for example as the engine of a game ‘to explore and manage your local loch’ - might be seen as a tool for community engagement in efficient use of natural resources, as well as software to help specialists in environmental management (Appendix L). Militating against this at present are the general obstacles arising from the need to run a computer program from a command-line interface, and the specific problems of using proprietary software and of intellectual property rights in the model, its components, and the data-base.

It is proposed to place a current version of the ACExR-LESV source code, data-base, example outputs, and some documentation, on a public web-site, probably that of SAMS, for downloading and use ‘as is’ by any person or institution, private, commercial or public, who wish to examine and perhaps apply it, and who have access to Matlab™. Before doing this we need to formalize and agree the rights of the holders of intellectual property in the system. Meanwhile, the ACExR-LESV files (excluding ShellSIM, for which, see Appendix K) are available through the DropBox web-site to invitees, currently the project members (including MSS) plus SEPA modellers. It is likely that the model system will be used, during the next year, in sECE mode, to revise nutrient aspects of the ‘Locational Guidelines’.

\[\text{The IP in the model as developed in phase 1 was to be shared between SARF, FRS, NUE and SAMS; phase 2 brought in PML, which reserves rights in ShellSIM; and the data-base includes meteorological data obtained, by way of BADC, for research purposes.}\]
References


• Portilla, E. & Tett, P. (2008) Boundary conditions for Assimilative Capacity models of lochs and voes on the northern and western coasts of Scotland., Edinburgh: Napier University,


• Stigebrandt, A. (1981) A mechanism governing the estuarine circulation in deep, strongly stratified fjords, Estuarine Coastal and Shelf Science, 13, 197-211.


• Stigebrandt, A. (2001) FJORDENV - a water quality model for fjords and other inshore waters, Gteborg: Earth Sciences Centre, Gteborg University, pp. 41

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Part II
Appendices
A Transport equations and box models

This section presents the transport equations that are used by both ACExR (in the function TracerSI) and LESV (ScalarPhysics3) to move physical quantities (heat and salt) and biological quantities (microplankton, nutrients, oxygen, SMP) amongst layers or between them and the sea. These equations conserve volume (of water) and mass (of tracers).

Layer volumes (and hence layer thicknesses) change only as a result of entrainment, and always sum to a constant total, because the models average over tidal cycles.

\[
\begin{align*}
\frac{dV_1}{dt} &= +Q_H + Q_{E12} \\
\frac{dV_2}{dt} &= -Q_H - Q_{E12} + Q_{E23} \\
\frac{dV_3}{dt} &= -Q_{E23}
\end{align*}
\]

Transports result from the processes discussed in section 5 and are written in terms of rates of change of layer total quantities:

\[
\begin{align*}
\frac{d(V_1 Y_1)}{dt} &= +Q_G \cdot (Y_2 - Y_1) \quad \text{(gravitational circulation)} \\
&\quad +Q_F \cdot (Y_f - Y_1) \quad \text{(freshwater)} \\
&\quad +Q_H \cdot Y_2 + Q_{E12} \cdot Y_1 \quad \text{(entrainment)} \\
&\quad +Q_{K12} \cdot (Y_2 - Y_1) \quad \text{(mixing)} \\
\frac{d(V_2 Y_2)}{dt} &= +Q_G \cdot (Y_0 - Y_2) \quad \text{(gravitational circulation)} \\
&\quad +Q_T \cdot (Y_o - Y_2) \quad \text{(tidal mixing)} \\
&\quad -Q_H \cdot Y_2 - Q_{E12} \cdot Y_1 + Q_{E23} \cdot (\delta \cdot Y_2 - (1 - \delta) \cdot Y_3) \\
&\quad -Q_{K12} \cdot (Y_2 - Y_1) + Q_{K23} \cdot (Y_3 - Y_2) \quad \text{(mixing)} \\
\frac{d(V_3 Y_3)}{dt} &= -Q_{E23} \cdot (\delta \cdot Y_2 - (1 - \delta) \cdot Y_3) \quad \text{(entrainment)} \\
&\quad -Q_{K23} \cdot (Y_3 - Y_2) \quad \text{(mixing)}
\end{align*}
\]

The wind-driven entrainment \(Q_H\) is always either zero or positive in the model, and makes layer 1 deepen at the expense of layer 2. It is opposed by the tide-driven entrainment \(Q_{E12}\), which is either zero or negative, and takes water from layer 1 into layer 2. The indicator \(\delta\) is 1 when deep water renewal is occurring, otherwise it is zero.

In equation 1, the effects of transport are presented as a flux divergence term. This relates as follows to the terms in eqn. 8:

\[
-\nabla \phi_Y = \frac{d(VY)}{dt} \frac{1}{V} - \frac{dV}{dt} \frac{Y}{V} 
\]
In the case of an **ECE model**, the \( \beta \) term is omitted from eqn. 1, so that only physical transports and (finfish-)farm inputs are taken into account.

In the case of an **ECE box model**, the water body is assumed to be a single box of volume \( V \), exchanging with the sea at relative rate \( E \). Eqn. 1 becomes, for box nutrient concentration \( S \):

\[
\frac{dS}{dt} = E \cdot (S_o - S) + \frac{Q_F}{V} \cdot (S_f - S) + \frac{\Gamma S}{V} \tag{10}
\]

In the ECE model used by Gillibrand & Turrell (1997), freshwater nutrients were ignored and eqn 10 solved for the steady-state, giving the equilibrium enrichment:

\[
S_{ECE} = S_{eq} - S_o = \frac{\Gamma S}{E \cdot V} \tag{11}
\]

Gillibrand & Turrell estimated \( E \) from average tidal exchange, i.e. from (in our symbols) \( Q_T/V_{1+2+3} \), but calculating \( Q_T \) on the assumption that the inflow prism fully replaced loch water on each tide.

Building on eqn. 11 is the **static CSTT model** (Gowen et al., 1992; CSTT, 1994; Tett et al., 2003) for ‘worst-case’ chlorophyll:

\[
X_{max} = q \cdot S_{eq} + X_o \tag{12}
\]

In the case of the dynamical, or dCSTT, model of Laurent et al. (2006), the \( \beta \) terms of eqn. 1 are retained but are simple. The following pair of equations give rates of change for nutrient \( S \) and chlorophyll \( X \) in Laurent’s ‘upper’ box:

\[
\frac{dS[u]}{dt} = E_u \cdot (S[l] - S[u]) - \frac{(\mu - \epsilon \cdot g)}{q} \cdot X[u] + \frac{Q_F}{V[u+l]} \cdot (S[f] - S[u]) + \frac{\Gamma S}{V[u+l]} \tag{13}
\]

\[
\frac{dX[u]}{dt} = E_u \cdot (X[l] - X[u]) + (\mu - g) \cdot X[u] \quad \text{where:} \quad X_u = E \frac{V[u+l]}{V[u]} \]

Laurent’s boxes had fixed volumes, and a constant value of the ‘whole-loch’ exchange rate \( E \) was used, estimated from the loch’s observed salt content and freshwater flows (Tett, 1986).

Operated in **sECE** and **dCSTT modes**, the LESV model simplifies biological process to those shown in eqns. 10 and 13, but retains the complete set of ACExR transport equations and hence the dynamic three-layer description of loch state and water exchange. It should thus provide more reliable estimates of seasonally-changing nutrient and chlorophyll enhancement resulting from finfish farming. In this context, it is useful to re-arrange the physical transport equations further, the better to understand the relative
importance of the several exchange processes. The equations that follow were derived by substituting appropriate parts of eqns. 7 and 8 into eqn. 9.

Layer 1. In many cases, rope-grown mussels are exposed mainly to layer 1, and thus it will be useful to define an exchange rate $E_1$ for this layer.

\[
\frac{d\bar{Y}_{[1]}}{dt} = \frac{Q_G}{V_{[1]}} (Y_{[2]} - Y_{[1]}) + \frac{Q_H}{V_{[1]}} (Y_{[2]} - Y_{[1]}) + \frac{Q_{K12}}{V_{[1]}} (Y_{[2]} - Y_{[1]}) + \cdots \\
+ \frac{Q_F}{V_{[1]}} (Y_{[f]} - Y_{[1]})
\]

(14)

where: $E_1 = \frac{Q_G}{V_{[1]}} + \frac{Q_H}{V_{[1]}} + \frac{Q_{K12}}{V_{[1]}}$  

(15)

$E_1V_{[1]}$ thus specifies the daily amount of water circulating through layer 1. Carrying capacity should be, in part, proportional to this amount, since it brings phytoplankton and DOM from outside the loch.

Layers 1 and 2. The waste of salmon farms typically goes into both upper layers. There is no simple exchange term for the combination, but eqn. 16 shows the importance of estuarine circulation $Q_G$ and tidal mixing $Q_T$. The terms in square brackets are omitted for a 2-layer water body.

\[
\frac{d\bar{Y}_{[1,2]}}{dt} = \frac{Q_G}{V_{[1+2]}} (Y_{[o]} - Y_{[1]}) + \frac{Q_T}{V_{[1+2]}} (Y_{[o]} - Y_{[2]}) + \cdots \\
+ \frac{Q_F}{V_{[1+2]}} (Y_{[f]} - Y_{[1]}) + \frac{Q_{K23} + (1 - \delta)Q_{E23}}{V_{[1+2]}} (Y_{[3]} - Y_{[2]})
\]

(16)

Layer 3. The analogous equation (17) for this layer is simpler: properties change as result of mixing with layer 2 and, intermittently, as a result of deep water replacement (when $\delta = 1$).

\[
\frac{d\bar{Y}_{[3]}}{dt} = + \frac{Q_{K23} + \delta Q_{E23}}{V_{[3]}} (Y_{[2]} - Y_{[3]})
\]

(17)

Except during replacement, layer 3 is eroded by entrainment into layer 2, and in many cases a key physical phenomenon is the alternation of decreasing $V_{[3]}$ with comparatively rapid restoration from layer 2 (and the marine inflow to the loch). During the erosion period, waste products tend to increase, and oxygen to decrease, in the layer, because $Q_{K23}/V_{[3]}$ tends to be small, and the most critical indicator of condition is thus the time since the last replacement episode. This depends partly on the mixing term (which reduces the density difference between layers 2 and 3) but mainly on changes in density at the sea-boundary.
B Initial and Boundary Conditions examined

Considering Creran as a box, there are also landward boundary conditions - freshwater discharges - and conditions along the top and bottom boundaries to take into account. Let’s consider a physical state variable, *salinity*. This influences water density in the loch and at the sea-boundary, and it is differences between these densities that drive the gravitational circulation. This circulation brings salt into the loch, as does tidal mixing (Figure 2). The matching landwards boundary condition is in effect a flux of absence of salt, the freshwater discharge. There is a similar flux into the top of the box, due to rain. Finally, the bottom boundary of the loch is closed so far as salinity is concerned: neither salt nor freshwater enter or leave the sediments. Because the model contains no process removing salt or freshwater, the average salinity of the loch is determined only by the boundary fluxes (although the distribution of salt between layers is influenced by other physical processes). Indeed, the mean salinity $C_{eq}$ under steady state conditions is:

$$C_{eq} = C_{[o]} \left(1 + \frac{Q_F}{E \cdot V}\right)$$ (18)

where $E$ is the average rate at which loch water exchanges with the sea as a result of gravitational and tidal circulations (see Appendix A) and $C_{[o]}$ is the boundary salinity.

In the case of microplankton chlorophyll $X$ there can be chlorophyll fluxes across the sea-boundary and in the freshwater discharge. The former that provides the starting point of changes that occur within the loch as the sea-water mixes with loch-water and freshwater, as phytoplankton grow, increasing chlorophyll and removing nutrients. The analog of eqn. 18 is:

$$X_{eq} = \frac{X_{[o]} + \frac{Q_F \cdot X_{[f]}}{E \cdot V}}{1 + \frac{Q_F}{E \cdot V} + \frac{g - \mu}{E}} \approx \frac{X_{[o]} \frac{g - \mu}{E}}{1 + \frac{g - \mu}{E}}$$ (19)

The term $\frac{g - \mu}{E}$ might be said to represent the ‘interiority’ of the model: the processes that are determined by in-loch conditions and not by boundary fluxes. If the relative rate of grazing ($g$) on microplankton by mesozooplankton and benthos (including, in this simplified case, cultivated shellfish) exceeds the local relative rate ($\mu$) of microplankton growth, the loch will act as a sink for phytoplankton etc, displaying lower concentrations of chlorophyll than those in the sea. On the other hand, if $\mu > g$, the loch will contain more chlorophyll than the sea. 23

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23 As the equation is written, it is possible for $\frac{\mu - g}{E}$ to equal or exceed 1, resulting in a meaningless value of $X_{eq}$. But such a case could not occur, because other factors - for example, nutrient supply - would restrict the growth of microplankton.
One of the independent variables in the partial differential equations mentioned at the start of this section is, of course, time. Integration with respect to time requires a set of starting values of the state variables, i.e. a prescription of initial conditions. However, knowledge of these conditions proves to be less important than knowledge of boundary conditions, for most lochs and voes. Suppose (in an experiment with the model), a loch is initially filled with freshwater. Its salinity will evolve towards the steady state value of eqn. 18 at a rate that depends on $E^{-1}$. For the upper waters of most lochs and voes, $E$ is of order $10^{-1} \text{ d}^{-1}$, so that after a month the simulated salinity is within $e^{-3}$, or 0.05, of $C_{eq}$. In effect, if numerical simulation starts at 1 January, by 1 February the model has largely ‘forgotten’ its starting conditions and is dominated by the current boundary conditions. Because of this, the code for starting an ACExR-LESV simulation takes, as default, the initial values of state variables from the boundary values on day one.

C Methods used in analysing LORN boundary conditions

The principles and initial results of the analysis of boundary data sets were reported by Portilla & Tett (2006a) during phase 1 of SARF012. They involved estimation of the parameters of an empirical model composed by a long term trend, a seasonal term and some noise. Climatologies were taken from the seasonal components.

Meteorological data were taken from the British Atmospheric Data Centre (BADC), for Air temperature, Solar radiation and Rainfall as recorded at the Dunstaffnage meteorological station. With some corrections for the effects of mountains, these data can be treated as representative of the northern part of Argyll, including loch Creran. The analysis used around 30 years worth of such data, starting with 1970 or 1971 and ending with 1996 or 1999 (depending on the variable).

Air temperature and solar radiation showed relatively consistent seasonal patterns from year to year, although radiation showed much day-to-day variability, treated as ‘noise’. Rainfall patterns showed similar noise and also greater year-to-year variability, implying that a rainfall climatology is less reliable than those for the other two variables. There was a significant long-term trend in temperature, amounting to an increase of about 0.6°C between 1970 and 2000. There was also some evidence of a long-term increase (of about 5% over the 3 decades) in rainfall. These trends were ignored in making the climatologies, which were based solely on the seasonal component of

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24 Meteorological data are collected by the UK Meteorological Office, who make some of it available to BADC by arrangement with NERC, under a licence that restricts its use to research.
the data.

Data for the concentration of the **nutrients** DAIN and DIP were available from the Greag Islands (LY1) sampling site, from seasonal sampling between 1979 and 1983, more frequent sampling from 2000 to 2002, and intermittent samples in 2003 and 2004. DAIN values are shown in Fig. 13(a). Because of the changing frequency, it was not possible to estimate a long term trend with any reliability: however, there does not seem to have been any increase in concentrations. Fig. 13(a) displays both the seasonal component (the climatology) for the DAIN example, and also a seasonal envelope that takes account of ‘noise’ by including 95% of all values.

Data for the concentration of **chlorophyll** were also available from the Greag Islands, for most nutrient surveys and also for the years 1970-1971. The data, the seasonal pattern and the 95 % confidence interval are shown in figure 13(b). It was necessary to transform phytoplankton chlorophyll into a logarithmic scale before carrying out the analysis, and therefore the envelopes are asymmetrical.

There was no obvious long term trend in the concentration of chlorophyll in the boundary conditions. There was however some evidence of change in the timing of the two seasonal peaks between 1970-1 to 2000-2003 figure. In particular, the peak in 1971 was larger, and came earlier, than in 2000-2003. This could however have resulted from the dominant sampling depth (about 0.5 m) in 1970-71 and that (about 10 m) in 2000-2003.

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25 Brian Grantham (SMA) was responsible for chemical measurements in 1979-1983, Johanna Fehling (UHI/SAMS during PhD studies in 2000-2003, and Celine Laurent (Napier) during PhD studies in 2003-2005
D Structure of the ACExR Matlab code

As shown in Figure 16, the function RunACExR4 is called from LESVBatch for each waterbody and set of run parameters. After loading necessary data, RunACExR4 calls CalcE to perform the numerical integration (Figure 24).

None of the ACExR functions below RunACExR4 receives or returns explicit parameters; instead, these are passed in the global structures named below. RunACExR4 returns them explicitly to LESVBatch, where they are given different names.

Figure 24: Structure of ACExR model code. Function names are bold.

<table>
<thead>
<tr>
<th>RunACExR4</th>
<th>LESVBatch</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LochData</td>
<td>LD</td>
<td>Data loaded from Sea-lochs catalogue</td>
</tr>
<tr>
<td>Bdata</td>
<td>PF</td>
<td>Boundary and forcing data</td>
</tr>
<tr>
<td>E</td>
<td>Q</td>
<td>Water exchange flux time-series</td>
</tr>
<tr>
<td>Param</td>
<td>V</td>
<td>Layer property time-series</td>
</tr>
</tbody>
</table>
E  Divide by zero errors in ACExR

The problem of $h_{[1]}$ (layer 1 thickness) tending to zero and causing instability is difficult to eradicate without enforcing a minimum value of this thickness. The problem is caused by difficulties in describing two processes:

(i) **Tidal entrainment** ($Q_{E12}$) which transfers water from Layer 1 to Layer 2, without regard to the remaining volume of Layer 1. One way to solve this would be to weaken entrainment as Layer 1 becomes thin. We have tried supposing that the entrainment velocity is a function only of the velocity in Layer 2: i.e. by assuming that the seagoing flow in layer 1 is arrested by the incoming tide and is stationary - the shear therefore comes from the current speed in Layer 2. In that case, as more water is entrained into Layer 2, Layer 2 becomes thicker and the velocity (and therefore the entrainment) becomes weaker. However, it hasn’t yet proven possible to code this into a stable but robust process description.

(ii) **Wind stirring during a retreating regime.** If the wind speed ($W$) drops to (or close to) zero, the entrainment velocity is negative and the surface layer thickness reduces to a thickness given by the Monin-Obukhov length scale. But this length scale is directly related to $W$, so if $W \to 0$, the length scale also tends to zero, and the surface layer will become vanishingly thin. This might be avoided by setting a minimum thickness for $h_{[1]}$, or by greatly increasing the time scale that the retreat occurs over (which is arbitrary anyway).
F  Structure of the LESV Matlab code

RunLESV4 is called from LESVBatch (Figure 16). It uses the MATLAB ode23 solver to numerically integrate the equations programmed into LESV4 and its child functions (Figure 25).

![Diagram](image)

**Figure 25: Structure of LESV model code.** Function names are bold.

RunLESV4 is called by the following line in LESVBatch:

```
[outB outB2 outFF outSF BF] = RunLESV4(loch, year, cs, Q, V, LD, PF);
```

where `cs` is a structure containing control variables, and `Q`, `V`, `LD`, `Bdata` are structures from RunACExR4. The RunLESV4 outputs are the structures:

<table>
<thead>
<tr>
<th>RunLESV4</th>
<th>LESVBatch</th>
<th>Description (time series of)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Out</td>
<td>OutB</td>
<td>state variables (x(t)) returned by solver</td>
</tr>
<tr>
<td>Out2</td>
<td>OutB2</td>
<td>biological rates (internally: (Brates))</td>
</tr>
<tr>
<td>OutFF</td>
<td>OutFF</td>
<td>fish-farm fluxes (internally: (FFfluxes))</td>
</tr>
<tr>
<td>OutSF</td>
<td>OutSF</td>
<td>shellfish numbers etc (internally: (SF))</td>
</tr>
<tr>
<td>BF</td>
<td>BF</td>
<td>biological forcing (internally: (Forcing))</td>
</tr>
</tbody>
</table>
Excepting the matrix of state variables $x(t)$, which are created by the running of ode23, the structures are passed to child functions mainly as globals. Filling of some values with data depends on LESV mode. The control structure includes a field `cs.mode`, which can take the following (string) values:

<table>
<thead>
<tr>
<th>mode</th>
<th>what it does</th>
<th>how it’s done (mostly in RunLESV4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>sECE</td>
<td>Biological ($\beta$) terms are effectively switched off whilst finfish $\Gamma$ is retained; SPM is total</td>
<td>IC for MP1 and MP2, and BC for MP1, MP1 and POM set to 0</td>
</tr>
<tr>
<td>dCSTT</td>
<td>Single MP box, constant $\eta$, SPM is total; otherwise as default</td>
<td>IC and BC for MP2, Si, and POM set to 0</td>
</tr>
<tr>
<td>LESV</td>
<td>Default state, as shown in Fig. 3 and eqn. 1</td>
<td>normal IC and BC loaded for nutrient, microplankton, DO and particulate state variables (distinguishing iSPM and POM)</td>
</tr>
<tr>
<td>LESVSF</td>
<td>Default plus shellfish $\Gamma$ terms</td>
<td>adds a vector of initial shellfish individual biomass to IC, and shellfish equations are active in in LESV4</td>
</tr>
<tr>
<td>Tracer</td>
<td>Biological state variables replaced by a tracer concentration variable with first order decay</td>
<td>IC and BC for all usual state variables set to zero, special BC files for tracer added</td>
</tr>
</tbody>
</table>

IC = initial conditions, BC = boundary conditions, MP = microplankton

The structure `Coef`, containing biological parameters, is passed to child functions as a global. It corresponds to the global `paramBio` passed from LESVBatch and in principle loaded from an XML file. Some aquacultural parameters, part of the control structure `cs`, are added to `Coef`. Some of the biological parameters must be supplied as a 3-dimensional matrix, as exemplified for the nutrient concentrations that half-saturate growth, held in `Coef.ks(l,nt,mp)`: $l$ refers to layer number (1 . . . 3, as set by ACExR), $nt$ to nutrients (1=N, 2=P, 3=Si) and $mp$ to microplankton (1=MP1, 2=MP2). The $ks$ values do not differ between layers, but do of course differ between nutrients and may differ between microplanktons.

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26 As in some other cases, the xml read code has not yet been implemented. Instead, LESVBatch loads the matfile `paramBio.mat` in which the parameter values have been saved from the structure (also called `Coef`) that was generated in the function LESVparlist2 contained in older packages.
G Physical Boundary Conditions

Function ReadDBForcing2 takes the following boundary condition data from the directory BCdataP.\(^{27}\)

- **River discharge** (in daily mean \(m^3\ s^{-1}\)) in file named by Bdata.Qf_file. Brate.QF_switch must be set to 1. If the file contains rainfall data (in mm \(d^{-1}\)), Brate.QF_switch must be set to 0, instructing the function to compute run-off from rainfall and loch catchment area. The latter is available in the Sea-lochs Catalogue.

- **Wind speed** (in daily mean \(m\ s^{-1}\)) in file named by Bdata.Wind_file.

- **Sea-boundary temperature and salinity** profiles in file named by Bdata.OB_file.

- **Daily mean meteorological data needed to calculate surface heat flux** in file named by Bdata.SHF_file. Only needed if Param.SHFlux == 1.

Example filenames are shown below. Each is a spreadsheet, saved in csv format. The arrangement of data in the files differs according to data type (consult ReadDBForcing2 for details). Some of the files contain data for multiple sites. In these cases, the function searches for the site closest to the latitude and longitude of the mouth of the loch or voe, as given in the Sea-lochs Catalogue.

The function checks for the existence of the named data files and the existence of data for a specified year. If the required data cannot be found, the function loads data from the default file.

<table>
<thead>
<tr>
<th>variable</th>
<th>example filename</th>
<th>default filename</th>
</tr>
</thead>
<tbody>
<tr>
<td>runoff</td>
<td>Creran_modelled_flow_1975</td>
<td>Climatology_rainfall_1970-2004</td>
</tr>
<tr>
<td>rainfall</td>
<td>ACmodel_rainfall_database</td>
<td>Climatology_rainfall_1970-2004</td>
</tr>
<tr>
<td>wind speed</td>
<td>ACmodel_windspeed_database_editted</td>
<td>Climatology_windspeed_1970-2004</td>
</tr>
<tr>
<td>sea-boundary</td>
<td>Etive_RE6_2000</td>
<td>ukhoclimateology (edit)</td>
</tr>
<tr>
<td>hydrography</td>
<td>ACmodel_heatflux_database_Dunstaffnage</td>
<td>Climatology_heatflux_Dunstaffnage_1970-2004</td>
</tr>
</tbody>
</table>

\(^{27}\)Details refer to function as at 7 April 2011.
H Biological Boundary Conditions

Function `LoadData2` takes boundary condition data mostly from subdirectories within the directory `data`. Each subdirectory contains a set of subdirectories named for regions or provinces. As explained in section 11, subdirectory search takes place based on the string in `LochData.Name` and the year (or the string `climat`) in the variable `year` explicitly passed to `LoadData2`. The search (performed by the function `fdf3`) seeks the most precise and relevant data-file available, defaulting stepwise to a generic climatology for that variable.

Files are in csv format, starting with comment rows (i.e. following ‘%’) giving header information. The first column of data is, unless otherwise stated, day number (1 = January 1). In the case of 2-column files, the second column gives the daily values of the variable. The variables are:

- **Solar radiation** (in daily mean W m$^{-2}$, including infrared and UV as well as visible), in a 2-column file within subdirectory `SolarRadiation`.

- **River nutrient concentrations** (in µM), in a 4-column file within subdirectory `RNut`. Columns 2-4 give, respectively, concentrations of DAIN, DIP and DSI. In all cases the values are, currently, generic for highland rivers and display no seasonal variation.

- **River particulates and salinities**, which are (currently) set to zero.

- **Sea-boundary conditions for nutrients** (in µM), in a 4-column file within subdirectory `BCNut`. Columns 2-4 give, respectively, concentrations of DAIN, DIP and DSI.

- **Sea-boundary conditions for particulates** (in mg m$^{-3}$), in a 4-column file with name commencing `BCpart` within subdirectory `BCPart`. Columns 2-4 give, respectively, concentrations of chlorophyll, iSPM and POM. The iSPM and POM data are in most cases generic estimates, and need improvement.

- **Sea-boundary conditions for ψ**, diatom chlorophyll as a proportion of total chlorophyll, in a file with name commencing `BCpsi` within subdirectory `BCPart`.

- **Finfish aquacultural data**: food supplied to salmon over a 2-year cycle, in a 4-column file within the subdirectory `Food`; the columns are month number, central day number, year, and amount (in tonnes per month), converted by `LoadData2` to kg d$^{-1}$;
- Shellfish aquacultural data, in files within shellfish: the file structure is complex, with the first column giving day number, the penultimate column the total number of mussels harvested that day, the final column the daily mortality rate, and all intermediate columns the numbers of mussels in 1 m thick depth cells; the first row of data are the initial biomasses (in mg flesh carbon) in each depth cell.\textsuperscript{29}

- Tracer forcing, which is, currently, set explicitly within LoadData2 as time-series of concentrations in the loch, river and sea; this allows simulation of the effects of spike additions of material.

The syntax for the function is:

\[
[DD] = \text{LoadData2} (\text{LochData}, \text{year}, \text{mode})
\]

where the output DD is a structure with fields as listed in the introductory comments in the function. Each field contains a vector of values of the forcing variables.

\textsuperscript{29} A function MakeSFN, in directory Auxiliary programs, can be used to generate this file.
I Using LESVBatch

These instructions apply to the current published version of the ACExR-LESV package, called ACExR-LESV_eco3_AUG_2011. This package is designed around the function LESVBatch, which can make multiple runs of the ACExR and LESV models under the control of a configuration file (see Fig. 16). However, as suitable XML files and reading routines were not completed when this package as made, the configuration information is contained in a script TestLESVBatch in the form of a structure that is written to a matfile and then read by LESVBatch when that starts. It is recommended that, for the time being, TestLESVBatch is edited according to the lochs and conditions for which the models are to be run. Note that LESVBatch detects existing model output for given lochs and conditions, and does not repeat runs. If you wish to repeat, remove output mat-files from the directory LESVBatchTest.

The following is a minimum set of instructions:

1. You need Matlab software; the package was prepared with Matlab 7.8 (2009) running under MacOSX and has been tested in Matlab 7.11 (2011) running under Windows 7. No special toolboxes were used.

2. Unzip the package ACExR-LESV_eco3_AUG_2011.zip and install it in an appropriate directory. Read ReadMeFirst.txt in directory documentation.

3. Open the function a_script_to_set_the_path and edit the line that names the directory in which the package has been placed. Now run this function and accept Matlab’s option to ‘change folder’. (This should be done at the start of each Matlab session with ACExR-LESV or after any crash in the program or accessory (interpretational) functions.)

4. Edit TestLESVBatch as desired, and then run this script. If you have selected whereOP = 1 in TestLESVBatch, output will be directed to the command window, so that you can track what is happening. Results are written to mat-files (one each for physics and biology) in the directory LESVBatchTest.

5. Use one of the provided functions in directory Output Processing to visualize and interpret the output from one run of ACExR-LESV, or write your own function. See appendix J.
J Output processing with ShowLESVresults2011

Analysis of results is in principle a user responsibility. However, the directory Output Processing contains some functions written for this purpose. As an example, the function ShowLESVresults2011 generates a ‘standard results page’ (a multipart diagram) saved as pdf, and some statistics and indicators printed to the Matlab Command Window. The syntax for the function call is:

\[
\text{ShowLESVresults2011(OutputDirName, Loch, Year, Row, h, pt)}
\]

and an example call (from the MATLAB Command Window) is:

\[
\]

where:

- **OutputDirName** names the directory containing the ACExR and LESV mat-files output from LESVBatch;
- **Loch** names the loch (or voe) for which results are to be analysed;
- **Year** gives either the year, as an integer, or the string ‘climat’, for which results are to be analysed;
- **Row** gives the integer row number in the structure `configg` (eventually, in the XML configuration file corresponding to the file `1_Config.mat`) corresponding to the simulation that has produced the results for analysis;
- **h** gives the thickness of the layer (starting at the sea-surface) over which results are to be averaged;
- **pt** specifies the form in which diagrams will be saved: options include ’pdf’, ’ps’, ’ai’.

Within the output directory, simulation filenames are `<Loch><Year><B or P>.mat`, where the ending B names LESV (biological) output and the ending P names ACExR (physical) output.
K Using ShellSIM with ACExR-LESV

It is only possible to run the MATLAB LESV-ShellSIM combination under Windows. In the absence of the ShellSIM dll, or if running under a Unix-type OS (including MacOSX), the shellfish model will default to GB98.

1. Obtain a copy of the ShellSIM dll\(^{30}\) and install WHERE?

2. Set the following values in the configuration file:
   ```
   configg.row(n).mode = 'LESVSF';
   configg.row(n).SFmodel = 'ShellSIM';
   n is the row number.
   ```

3. INSTRUCTIONS WILL BE COMPLETED IN A LATER VERSION OF THIS DOCUMENT

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\(^{30}\) See: www.shellsim.com. Availability of the dll is subject to Plymouth Marine Laboratory’s (PML) Licence Agreement for nominal fee of £50 within the context of collaborative work, and which fee is negotiable within commercial contexts, subject to any required training from PML. A Demonstration Version of ShellSIM with limited capability is available for no fee subject to User Registration alone, using the Software as a Service (SaaS) approach that enables the User to run ShellSIM remotely from anywhere with an internet connection, accessing ShellSIM behind a firewall on a server at the Plymouth Marine Laboratory.
A discussion of mechanisms for further use

The ACExR-LESV package is a loch management tool and a library of expertise and data. Its development so far (since the start of SARF012 in 2004) has taken about 7 scientist-years, excluding most work on ShellSIM. The package represents an intellectual capital acquired at an estimated ‘full economic cost’ of about 0.7 M£ for the time of the post-docs and senior scientists involved, funded by SARF012A, EC ECASA and the institutions (SAMS, NUE, FRS) that contributed staff time from general budgets.\(^{31}\)

The contribution that the model system can make to assessing assimilative and carrying capacities has been sketched in the body of this report. In principle, use of the model can lead to economic benefits through more efficient use of finite ecosystem services. To get some idea of what these benefits might be, we refer to a NERC study of the benefits of the DEPOMOD benthic impact model.\(^{32}\) The study pointed out that the output value of the aquaculture industry was 367 M£ ‘at the farm gate’ in 2008, and that the use of DEPOMOD allowed an increased salmon farm approval size equivalent to 521 tonnes per 101 regulated sites, or a marginal benefit to the industry of 78 M£ in additional annual output. Although the figures are spuriously precise, and might be better evaluated within a framework of contrasting scenarios which cost externalities as well as industry benefits, there would seem little doubt that the intellectual investment in DEPOMOD has been repaid many times over by benefit to industry and environment. A similar argument can be made for the ACExR-LESV system.

The options that have been considered, or can be envisaged, for continued use of ACExR-LESV, fall into two groups, which can be broadly categorized as ‘use by specialists’ and ‘use in the community’.

**Expert use.** It is the requirement for specialized equipment (such as the Matlab software) and knowledge, as well as motivation, that traditionally restricts use of mathematical models to specialists, sited within the scientific research, higher education and policy-advice communities. In terms of the sociology of institutions, these communities are part of, or linked to, societal governance, even in cases where their work is funded by market methods. Possibilities include

- use as a tool in other funded scientific research: it is likely that ACExR

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\(^{31}\) Also excludes the effort involved in getting the original data that has been mined for the data-bases, and prior work on the ideas used in the model. EP was the main post-doc, employed for 3.6 years by NUE; senior scientists included PG and MI (SAMS), PT (SAMS and NUE, about 1.5 years) and FRS staff. Costing assumes 50 K£/year average direct costs per scientist, with overheads (including travel and consumable) at 100%.

at least will continue to be used in SAMS studies of sea-lochs, with LESV helping in understanding the changes in the planktonic flora of loch Creran;

- continued (commissioned) research use, as a consequence of a successful knowledge exchange proposal to a national funder;

- take-over by professional end-users (who have Matlab etc) within SEPA or Scottish Government, who see uses in the regulation of salmonid aquaculture, or in the longer term, in moving towards multiple farming uses of sea-loch resources; it is certainly envisaged that ACExR-LESV will be used in the sECE mode to help improve the Locational Guidelines;

- use as a practical tool to allow HE students to explore interactions between sea-loch physics and biology, for example under scenarios of climate change.

Community use. By this is meant usages that are not centrally directed, but governed either by market mechanisms or the ‘big society’. DEPOMOD provides a good example of a model, originally developed within the scientific community for policy purposes, which has been made available to the fish-farming industry (and indeed anyone who wishes to run it), with SAMS requiring only registration but offering (along with others) training or advice in use. ‘Stakeholders’ (see Tett et al., 2011) are all those, in the industry or local communities with a legitimate ‘interest’ in aquaculture or its impacts. Many of these stakeholders have HE qualifications, and most are familiar with using complex software through windows or touch-screen interfaces. Thus it can be argued that models such as ACExR-LESV could be diffused into this community for use by concerned stakeholders, given appropriate vehicles. Possibilities include

- open-source availability (for users who have Matlab and appropriate experience) by placing a copy of the package on the web;

- the user-friendly, or game, interface approach - a user-friendly web-site, which in effect, takes orders to run ACExR-LESV on a separate hardware device;

- the approach of expert engagement with stakeholders in order to run (and sometimes to modify) the models to simulate issues of concern to them; this could be done either through a commercial (consultancy-type) model, or by ‘outreach’ from specialized institutions (for which there is currently no suitable funding model).

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