Improving Assimilative Capacity Modelling for Scottish Coastal Waters: I. A Model of Physical Exchange in Scottish Sea Lochs

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Introduction

This report describes progress towards achieving the first milestone of the project entitled "The development of modelling techniques to improve predictions of assimilative capacity of water bodies utilised for marine caged fish farming" which was funded by the Scottish Aquaculture Research Forum (Project code SARF012). The first milestone is to consider, and develop a model of, physical exchange in Regions of Restricted Exchange (RRE). In Scotland, sea lochs and voes are the RRE where marine fish farming is primarily located, and the model described in this report has been designed with the sea loch environment, both with and without internal sills, in mind.

In this report, we describe the conceptual framework for the model, describe the equations that govern the exchange, in both diagnostic and prognostic forms, and explain the implementation of the model and how it can be coupled to ecological models to predict the evolution of biological state variables over an annual cycle. For ease of reading, the technical aspects of the report, e.g. the governing equations and descriptions of each module in the code, have been placed in Appendices.

Description of the Model

Conceptual Framework

We assume, as the basis for sea loch exchange, a three-layer system (Figure 1). This classical approach encapsulates the fundamental processes of horizontal and vertical exchange in these fjordic systems (e.g. Edwards and Edelsten, 1976; Stigebrandt, 2001). Freshwater water discharge from rivers into the fjord is mixed into the underlying saline water to form a brackish surface layer, of varying depth, which is assumed to flow persistently seawards (averaged over time scales of several tidal cycles). The depth of this surface layer is controlled by the quantity of freshwater discharge (Q_f) and the strength of wind mixing. In the model, changes in the depth of the surface layer are implemented by means of a vertical flux of water, denoted Q_h.

As it flows seaward, the surface layer entrains water from the intermediate layer below. In the intermediate layer, therefore, there is a compensating landward flow (again, averaged over several tidal cycles) that replaces the water lost to the surface layer. This net circulation is commonly known as the estuarine circulation: landward flow in the intermediate layer, entrainment into the surface layer, and seaward flow in the surface layer. It therefore creates persistent, unidirectional flow in both layers and is represented in model by the symbol Q_{est}.

Superimposed on the estuarine circulation is the exchange due to tides. In Scotland, tides in the coastal regions are dominated by the semi-diurnal constituents and particularly by the M_2 and S_2 tides. The combination of these two constituents produces a strong spring-neap cycle, during which the tidal range can vary by a factor of more than 2. Tidal exchange affects both the surface and intermediate layers. We have used the tidal prism method to calculate the volume of water involved in the exchange process, as has been used in previous ECE (Equilibrium Concentration Enhancement) models (e.g. Gillibrand and Turrell, 1997). However, we have improved this tidal exchange model by implementing the method described in Wells and van Zeijst (2003). They have developed the jet-sink model of estuarine exchange, first proposed by Stommel and Farmer (1952), to give an estimate of the efficiency of tidal exchange. The details of the method are given later in this report. Tidal exchange in the model is denoted by Q_t.

We have included in the model the option of simulating the "intermediary circulation" and the exchange that results. The intermediary circulation derives from oscillations of the pycnocline in the coastal waters adjacent to the fjord entrance. Such oscillations drive baroclinic currents into and out of the surface and intermediate layers of the fjord. This exchange process is thought to be particularly important in Scandianavian fjords (Stigebrandt, 2001), which often have deeper sills and weaker tidal currents than Scottish fjords. It may be that barotropic exchange in Scottish fjords dominates this baroclinic effect; however, we have incorporated the intermediary exchange in the model which will allow the relative magnitude of the terms to be assessed. The intermediary circulation is denoted by Q_i.

The circulation field created by the estuarine and tidal circulations will generate a velocity shear between the surface and intermediate layers. The intermediate layer will have stronger landward flows, and the surface layer stronger seaward flows. We propose that during the flood tide, as surface waters of coastal origin enter the intermediate layer (enhancing the estuarine circulation induced flow in that layer), water will be entrained from the surface layer into the intermediate layer. This will induce a flux of mass and any associated scalar properties into the intermediate layer water. This flux is denoted by Q_{ent}.

All the volume fluxes described above act on the surface and intermediate layers. In a silled fjord, the deep basin landward of the sill is filled with water that is isolated from the tidal and estuarine circulation (Figure 1). This water is exchanged only though vertical turbulent diffusion, which gradually exchanges scalar properties of the bottom water with those in the intermediate layer. In this model, we assume that there is no net exchange of mass, so the volume of the bottom water remains constant. The coefficient of vertical turbulent diffusion is denoted by K_z.

The conceptual framework of this model is illustrated in Figure 1, where each of the terms discussed above is shown. Next we discuss the equations that govern the exchange of each layer and its inherent scalar properties.

Governing Equations

The equations used in this model come from a variety of sources. The fundamental mathematical framework is derived from the FjordEnv model, developed for Scandinavian fjords by Stigebrandt (2001). However, we have utilised other theories and analytical solutions where appropriate to develop a package that is more appropriate for the mesotidal environments of Scottish fjords. The equations are presented in Appendix A. Here we describe how the equations fit into the conceptual framework given above.

The FjordEnv model of Stigebrandt (2001) developed an analytical solution for the exchange of the brackish surface layer of a fjord. The solution is stationary for fixed values of river flow and wind speed. In the present model, we have developed a time-dependent model that can simulate the exchange over an annual cycle (i.e. January – December). In addition, we have extended the model to predict the exchange of the intermediate layer and included interactions between the three layers. Thus the model we have developed here can be used to describe the layer-dependent temporal evolution of any scalar property over an annual cycle. In terms of salinity, the model can be used in either a diagnostic mode, where the FjordEnv equations (Appendix 1, Eqn 2) are used to determine the surface layer salinity, or in fully prognostic mode, where the salinity is treated as a scalar property and calculated by Eqns 4 and 5.

Solution Sequence

The model solution proceeds as follows:

1. Physical data for the system e.g. topography, tidal range etc, is extracted from the sea loch database, which is based on the catalogue of Edwards and Sharples (1986). [Module ReadCatalogue.m].

2. A hypsographic function is derived for the loch. At present, this function assumes that the loch has the shape of an inverted pyramid, with a volume, surface area and mean depth that match those of the real system. Values of horizontal planar area, vertical cross-sectional area, and volume are calculated as functions of depth. [Module Hypsography.m]

3. Boundary data are acquired. At present, we do not have available a database of river discharge, wind forcing and ocean salinity profile for regions around the Scottish coast. For the present model, we have created smoothly-varying (sinusoidal curves) time series of river flow and wind speed for an annual cycle (Figure 2). Both river flow and wind speed are at a maximum at the start and end of the year and at a minimum at the end of June. For the salinity profile, we have assumed a linearly varying depth profile, with typical values for Scottish coastal waters (i.e. surface salinity = 34). [Module ReadForcing.m].

4. The model is initialised. Surface layer values are set to zero i.e. the surface layer does not exist in the initial state. Intermediate layer values are controlled by the depth of the sill nearest to the entrance to the fjord i.e. the intermediate layer thickness is set to the sill depth, the volume is set accordingly based on the hypsographic function, and the salinity is set to the external salinity at sill depth. The bottom layer is defined by the mean depth of the fjord and the remaining volume. Salinity is set by the external salinity at the mean fjord depth. In the absence of a sill, the initial state is that of no surface layer, with the initial values of the intermediate layer determined by the hypsography and the external forcing at the mean depth of the fjord. A number of constants and parameters from the FjordEnv model are calculated (e.g. M and N) and the datum of some of the variables from the sea loch database is set to Mean Sea Level (MSL) rather than the Low Water mark. [Module Initialise.m].

5. Calculations of exchange then begin [Module CalcE]. Initially, calculations are performed for Day 1 of the annual cycle. Here, no previous parameter values are available (since there has been no previous time step), and the solution is based on the analytical solution of FjordEnv. Calculations are then made for the remaining days in the simulation. The solution sequence is as follows:

    a. Obtain a first estimate of h_1 from Eqn A1. Based on the estimated displacement of the interface from its previous location, a vertical flux of water, Q_h, is derived.
    b. Calculate the volume of the surface layer, V_1, based on the hypsography and h_1.
    c. Calculate S_1 using Eqn A2.
    d. Calculate Q_t, Q_{est}, Q_{ent} and Q_i for day 1.
    e. Calculate K_z for day 1.
    f. Repeat steps a-f for the remaining days of the simulation, except that:
        i. Salinity is calculated last, following the calculation of K_z
        ii. Following step d, h_1 and h_2 are calculated from Eqn A3.

    In step f, the calculations for Q_{est}, Q_{ent}, Q_h and K_z use parameter values (e.g. layer salinities) from the previous day. Thus the model steps forward iteratively with a time step of 1 day, solving for layer thickness (Eqn A3) and associated volume fluxes.

The sequence described above provides time series of layer depths, volumes and salinities, volume fluxes, and the vertical turbulent diffusion between the intermediate and bottom layers. The solution sequence is illustrated in Appendix D.

We have developed a model with two possible modes of operation, which we call diagnostic and prognostic. These determine how the salinities of each layer are calculated, which has implications for the calculation of volume fluxes. In the following sections, we describe these two modes of operation, and provide examples of output from the model, with Loch Creran having been chosen as the example location.

For the example case of Loch Creran, we used sinusoidally-varying time series of river flow, with values of 4.5–13.5 $m^3 s^{-1}$, and wind speed, with values of 5–10 $m s^{-1}$ (Figure 2). The external salinity increased linearly with depth from a value of 34 psu at the surface, to 34.75 psu at 150m depth. The intermediary circulation was not included in these simulations ($\Delta M = 0$).

Diagnostic Model

In the diagnostic version of the model, salinity in the surface layer, S_1, is calculated from the FjordEnv equation A2. Salinities in the intermediate and bottom layers, S_2 and S_3, are not modified but are set according to the external salinity profile as performed in the module Initialise.m; these values are therefore constant throughout the simulation.

The predicted layer depths, volumes and salinities are presented in Figure 3. The surface layer depth varies from approximately 5 m in winter to 2 m in summer, when wind stirring and freshwater input are lowest. The intermediate layer depth compensates for the change in layer 1 thickness; note that the total layer thickness $h_1 + h_2$ remains constant. The layer volumes are not calculated independently, but are merely derived from the hypsography based on layer thickness; the time series of volume therefore follows the corresponding layer thickness.

The salinity in the diagnostic case is constant in layers 2 and 3 (intermediate and bottom). In the surface layer, the salinity varies smoothly from just over 32 in winter to 31.5 in summer. Eqn A3 determines the surface layer salinity from the wind speed, river flow and intermediate layer salinity; the time series in Figure 3, therefore, varies smoothly like the time series of wind and runoff.

The volume fluxes predicted by the diagnostic model are dominated by the tidal exchange (Q_t, Figure 4). The estuarine circulation (Q_{est}) provides a significant contribution to the volume flux, but the remaining three components are all very small. The tidal exchange includes a calculated efficiency coefficient of 0.85, and also incorporates a spring-neap cycle, where the tidal range at neap tides is assumed to be 40% of that at spring tides.

The total volume flux, Q_j, affecting each layer, j, is shown in the middle panel of Figure 4. The fluxes shown here for layers 1 (surface) and 2 (intermediate) are the sum of the pertinent volume fluxes affecting that layer, as derived from Eqn A5. The fluxes vary over the annual cycle in response to the changing forcing from wind and river flow, and to the change in layer thickness and volume. The effect of the volume fluxs on the flushing times of each layer is shown in the bottom panel. Here we have calculated the flushing time of layer j, T_{Fj} according to:

$$T_{Fj} = V_j / Q_j \qquad (1)$$

and T_{Fj} is converted to days.

The flushing times of both layers vary from about 1 day in winter up to 2.5 days in summer. These values compare well with the flushing time of 3 days given by Edwards and Sharples, which probably applies to the water column above sill depth (i.e. the surface and intermediate layers combined). The spring-neap cycle clearly affects the flushing time of both layers, which can double during neap tides.

Prognostic Model

In the prognostic version of the model, salinity is treated as a conservative scalar property and the layer salinities are calculated using Eqns A4 and A5. Eqn A2 is not used at all in this version of the model. The calculated salinities S_1 and S_2 feed back into the calculations for Q_{est} and Q_h.

In terms of layer thicknesses and volumes, the prognostic model produces essentially identical results to the diagnostic model (Figure 5). However, the predicted salinities are noticeably different. Here, time series of salinity reflect the spring neap-tidal cycle. The surface layer salinity stays remarkably constant during the whole simulation, despite the decrease in river flow and wind stirring. The intermediate and bottom layer salinities become slightly fresher in summer, before increasing again to winter values. These results are somewhat unexpected, and need further analysis.

It is also worth noting the instability of the prognostic model during the first few days of the simulation. This is not abnormal for time-stepping models; if the prognostic model is adopted, it may be necessary to run the model for two years, taking the results from the second annual cycle as output. The fact that the model overcomes the stability indicates that it is intrinsically stable.

The exchange rates are of a similar magnitude to the diagnostic model results (Figure 6), but the estuarine circulation now also reflects the spring-neap cycle through its dependence on S_1 and S_2. The tidal and estuarine fluxes continue to dominate exchange in the surface and intermediate layers.

Flushing times again vary from 1 – 2.5 days for both layers, as was the case for the diagnostic simulation.

Exchange Efficiency

The efficiency of tidal exchange has long been a source of difficulty for box models of the type described here. The simplest version of the tidal prism exchange method, described by Dyer (1997), assumed that tidal exchange was 100% efficient, an assumption known to be improbable but one that was difficult to improve without resorting to unproven exchange coefficients. In this model we used the method of Wells and van Heijst (2003) to estimate the exchange efficiency; their method in turn was strongly based on the work of Stommel and Farmer (1952).

The method invokes a jet-sink style of estuarine exchange, whereby flood water is injected into the semi-enclosed basin through a narrow entrance at a relatively high velocity, forming a jet of length $L = UT/2$ in the basin. In contrast, during the ebb, the water drawn through the entrance is sourced from a semi-circle, centred on the entrance, with a radius r. The exchange is illustrated in Figure 7. The development of Wells and van Heijst concentrated on the formation of dipoles during the flood tide and the effect of the exchange of the estuary should the dipoles escape from the flood jet and not be drawn back into the ebbing tide. The effect of escaping dipoles was found to significantly increase the efficiency of tidal exchange, and was based on a relatively simple criteria, that

$$W/UT < 0.13 \tag{2}$$

where U is the tidal velocity of the jet, T is the tidal period and W is the width of the channel.

From Figure 7, the water entering the basin on the flood tide is described by LW. The water leaving the basin on the subsequent ebb tide is described by $\frac{1}{2}\pi r^2$. On each tidal cycle, therefore, a portion of the flooding water remains within the basin, given by roughly $(L-r)W$. This water constitutes the effective exchange volume.

By equating the flood tide and ebb tide volumes i.e.

$$\tfrac{1}{2}\pi r^2 = LW \tag{3}$$

we get

$$r = (2LW/\pi)^{1/2} \tag{4}$$

The efficiency of tidal exchange, ε, is given by

$$\varepsilon = (L-r) / L = 1 - r / L \tag{5}$$

and by inserting (4), we get

$$\varepsilon = 1 - (2W/\pi L)^{1/2} \tag{6}$$

or

$$\varepsilon = 1 - (4W/\pi UT)^{1/2} \tag{7}$$

We use Eqn 7, with an additional condition based on Eqn 2 that

$$\varepsilon = 1 \qquad \text{when } W/UT < 0.13 \tag{8}$$

Entrainment

In the conceptual model flooding tidal flow over the sill is pushed under the fresh surface layer, creating a zone of potentially high shear between layers 1 and 2, extending over some horizontal distance from the sill. If the shear is sufficiently high and stratification sufficiently weak, in other words if the bulk Richardson Number is sufficiently small, then entrainment from layer 1 into layer 2 will occur. The consequences of this entrainment will be to decrease h_1 and S_2, and increase h_2, which will in turn affect the estuarine circulation Q_{est}. In the model this entrainment flux is parameterised as an entrainment velocity, W_{12}, expressed as a function of the Richardson Number (Turner, 1986), viz:

$$W_{12}(x,t) = \begin{cases} \Delta U(x,t)\dfrac{a - bRi(x,t)}{1 + cRi(x,t)}, & Ri < 0.8 \\ 0, & Ri \geq 0.8 \end{cases} \tag{9}$$

where, a, b, and c are tunable parameters, set here to a=0.08, b=0.1, c=5, ΔU is the velocity difference between the layers, and Ri is the bulk Richardson Number. The shear (ΔU) is formed from the difference between the combined out-flowing estuarine and freshwater fluxes in the upper layer and the combined in-flowing estuarine and tidal flow in the lower layer. Tidal flow is clearly a function of time (over a tidal cycle) and space (decreasing with distance from the sill). Entrainment is calculated at 20 minute time intervals over the flood tide and 20 m space intervals from the sill to a distance equal to the tidal excursion. The resultant mean entrainment velocity, W, is then converted into an entrainment volume flux from layer 1 into layer 2, Q_{ent}.

Lower Layer Diffusion

Below sill depth the isolated deep layer is assumed to be subject to gradual diffusive mixing from above. Measured diffusivities are generally several orders of magnitude above the molecular value, and the presumption is that the diffusive flux is driven by shear instability across the base of layer 2. Favourable conditions for developing shear instability, and thus local turbulent mixing, occur when the Richardson Number falls below a critical value, Ri_{cr}. Traditionally such turbulence is parameterised in terms of an exchange coefficient known as the vertical eddy diffusivity, K_z. The coefficient is assumed to be: 1) constant (K_{z0}) for $Ri \ll Ri_{cr}$, 2) dependent on Ri for intermediate values of Ri, and 3) decrease to molecular values at $Ri \gg Ri_{cr}$. Many parameterisations of this nature have appeared in the literature; the parameterisation used here (Pacanowski and Philander, 1981) is typical of the many which have been published. For application to sea lochs a value of K_{z0}=0.0001 m^{2}s^{-1} is chosen (see, for example, (Inall and Rippeth, 2002). The shear across the interface between layer 2 and 3 is determined by combined in-flowing tidal and estuarine flows in the intermediate layer over a stagnant lower layer. Lower layer flow decreases to zero towards the head of the basin, and thus *Ri* varies along the axis of the basin. An analytic expression for the integral of $K_z(x)$ is evaluated at each time step to give a value for K_{z23}, which then allows the tracer conservation equations for layers 2 and 3 to be solved at each time step.

Application of the Model

The model has been developed in Matlab, and is supplied as a suite of functions. The root function is called ACExR.m and is called in the following way:

[E, Param] = ACExR(Lochname)

where Lochname is a string containing the name of a sea loch contained in the sea loch database e.g. Lochname = 'Creran'.

The model will return the variables E and Param, which contain all the layer parameters and exchange rates that are needed to determine the evolution of a state scalar variable within the chosen loch.

Each module can be called independently e.g. the boundary forcing data can be obtained by entering:

Bdata = ReadForcing(LochData)

Where LochData is an output from ReadCatalogue.m and Bdata contains the boundary forcing data (see Appendix C).

Further Work

Some further work is required before the model can be considered completed. However, the work required is not expected to fundamentally alter the outputs of the model as it currently stands. The model needs to be calibrated by, and tested against, observed data from a number of lochs, including real hypsographic data from a sub-selection of lochs. This part of the work will continue throughout the lifetime of the project, and will be reported under milestone 5.

Although we have incorporated a calculation for the efficiency of tidal exchange, the efficiencies produced by that calculation need to be assessed. To do that, in collaboration with partners at FRS Aberdeen, we plan to use a three-dimensional numerical model of an idealised sea loch to investigate the efficiency of exchange and to test the parameterisation and, if necessary, seek a new parameterisation. Similar work is being conducted presently by researchers investigating exchange in Hood Canal, a branch of Puget Sound (M. Kawase, pers. communication).

We will continue to test the prognostic version of the model described above. The model currently appears to be very sensitive to the mixing between the intermediate and bottom layers, and we need to investigate further to understand the cause of the sensitivity and, if necessary, to address it.

The description of Milestone 1 states that we will carry out an analysis of the lochs listed in the sea loch catalogue and group them into physio-topographic classes. We have not performed this analysis yet. The development of the conceptual framework for the model described in this report took longer than anticipated, since we had to considerably develop the model beyond the basis provided by the FjordEnv model. We are now satisfied that the conceptual framework and the model developed to date provide a significant improvement on the existing models of exchange in Scottish fjords, and we expect that additional work will merely be a case of fine-tuning the existing code.

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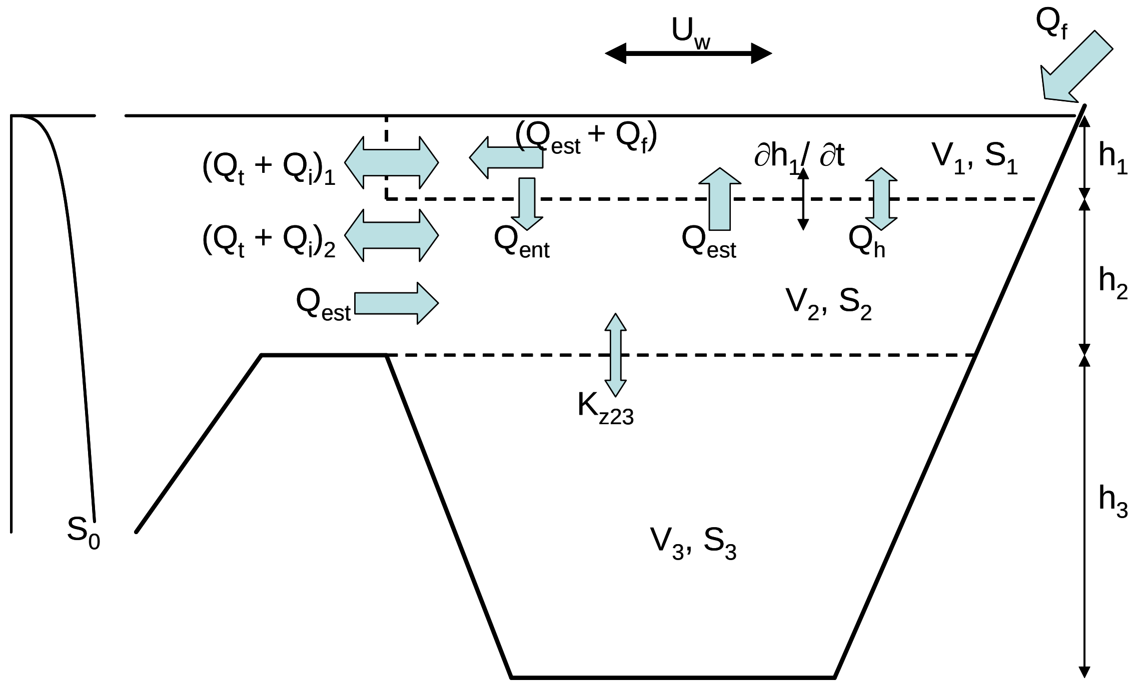

Figure 1. Schematic diagram of the three-layer conceptual model and the volume fluxes and layer parameters calculated. The layer parameters of thickness (h_j), volume (V_j) and salinity (S_j) are indicated, as are the fluxes Q_t, Q_{est}, Q_i, Q_h, Q_{ent} and the vertical turbulent diffusivity (K_{z23}). The symbols are explained in the text. Also shown are the forcing data of river discharge (Q_f), wind speed (U_w) and external salinity (S_0).

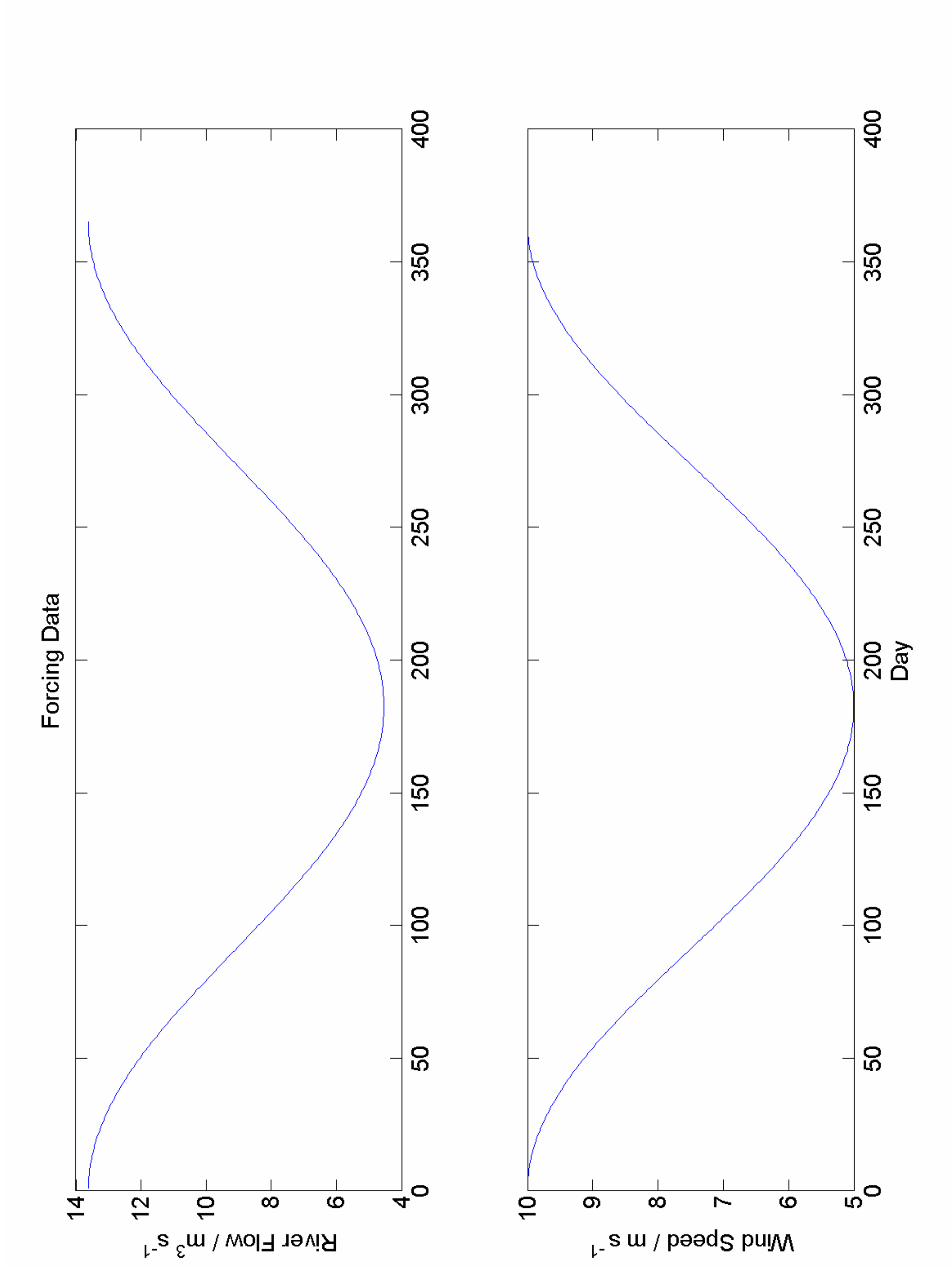

Figure 2. Time series of river flow and wind speed used to drive the exchange model.

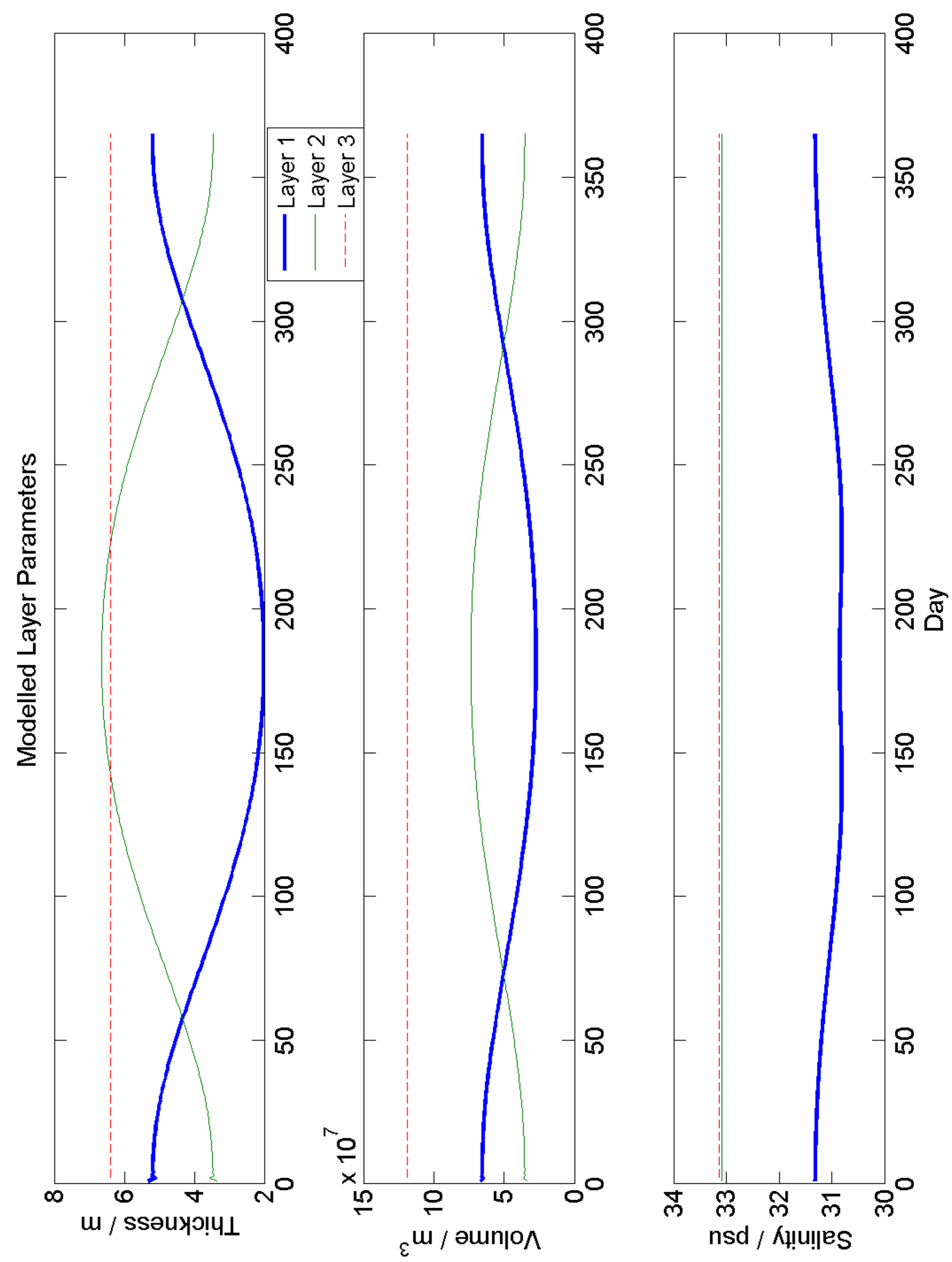

Figure 3. Example results of predicted layer parameter values from the diagnostic exchange model for Loch Creran over an annual cycle.

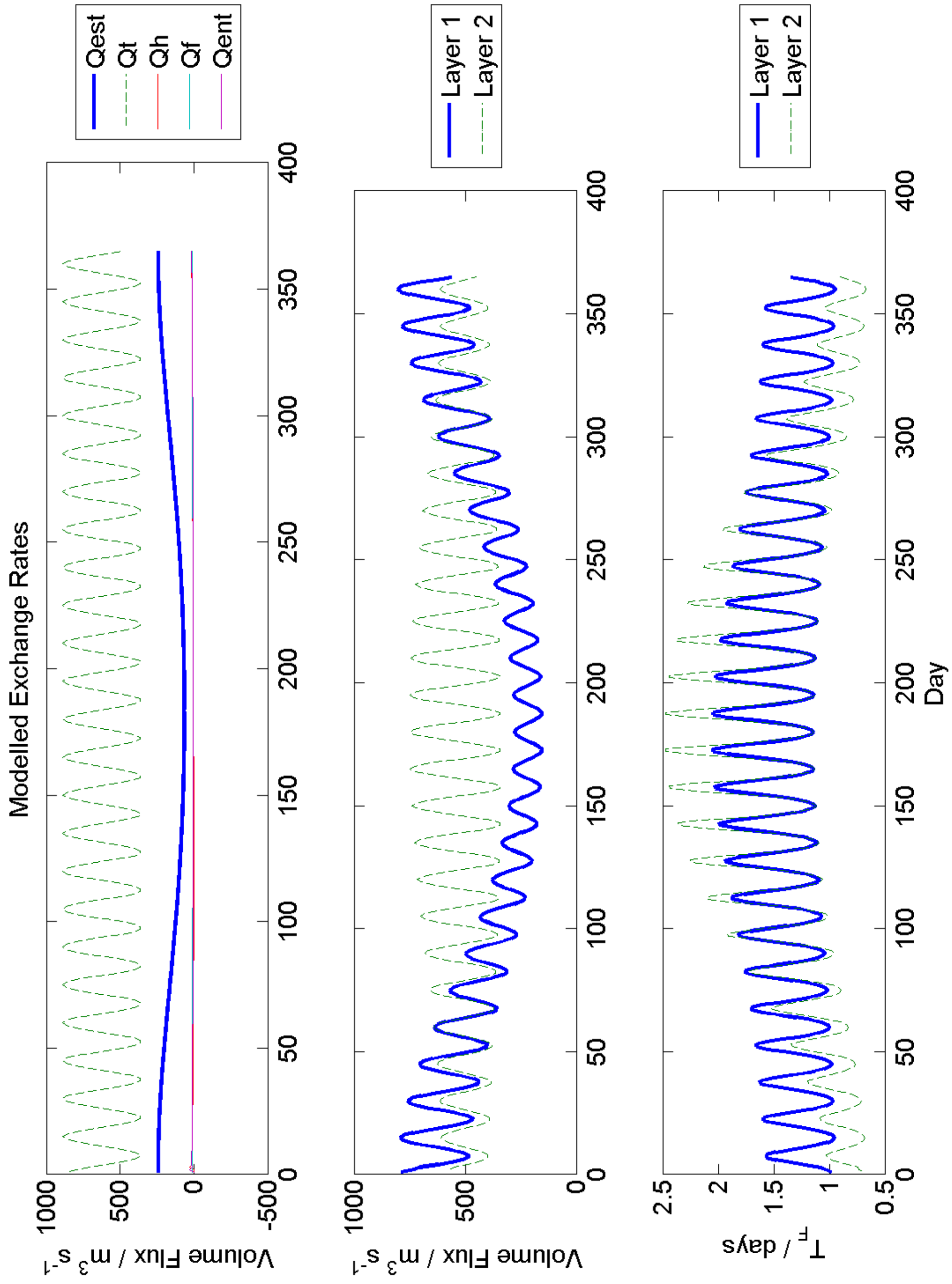

Figure 4. Example results of predicted exchange rates from the diagnostic model for Loch Creran over an annual cycle.

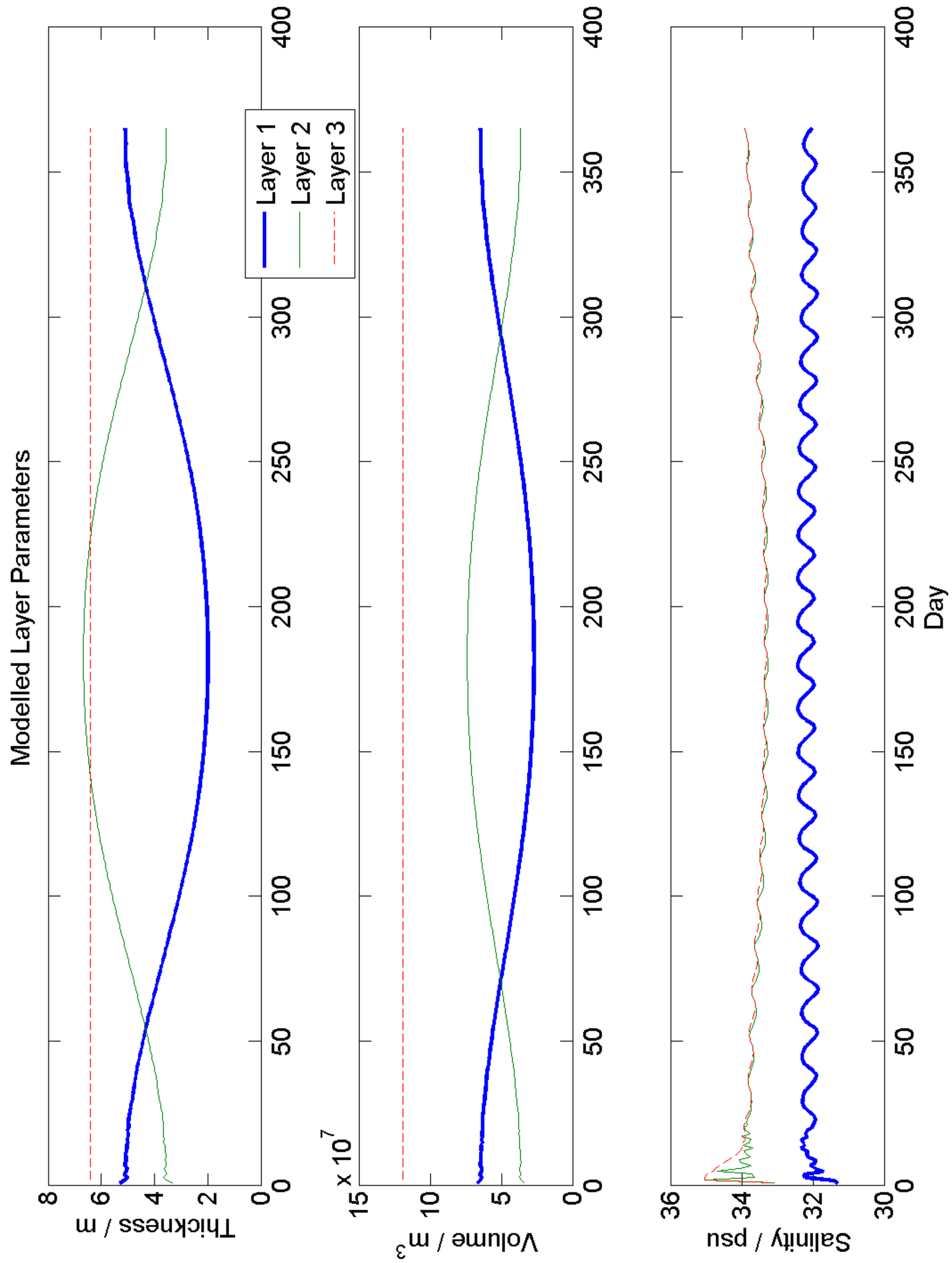

Figure 5. Example results of predicted layer parameter values from the prognostic exchange model for Loch Creran over an annual cycle.

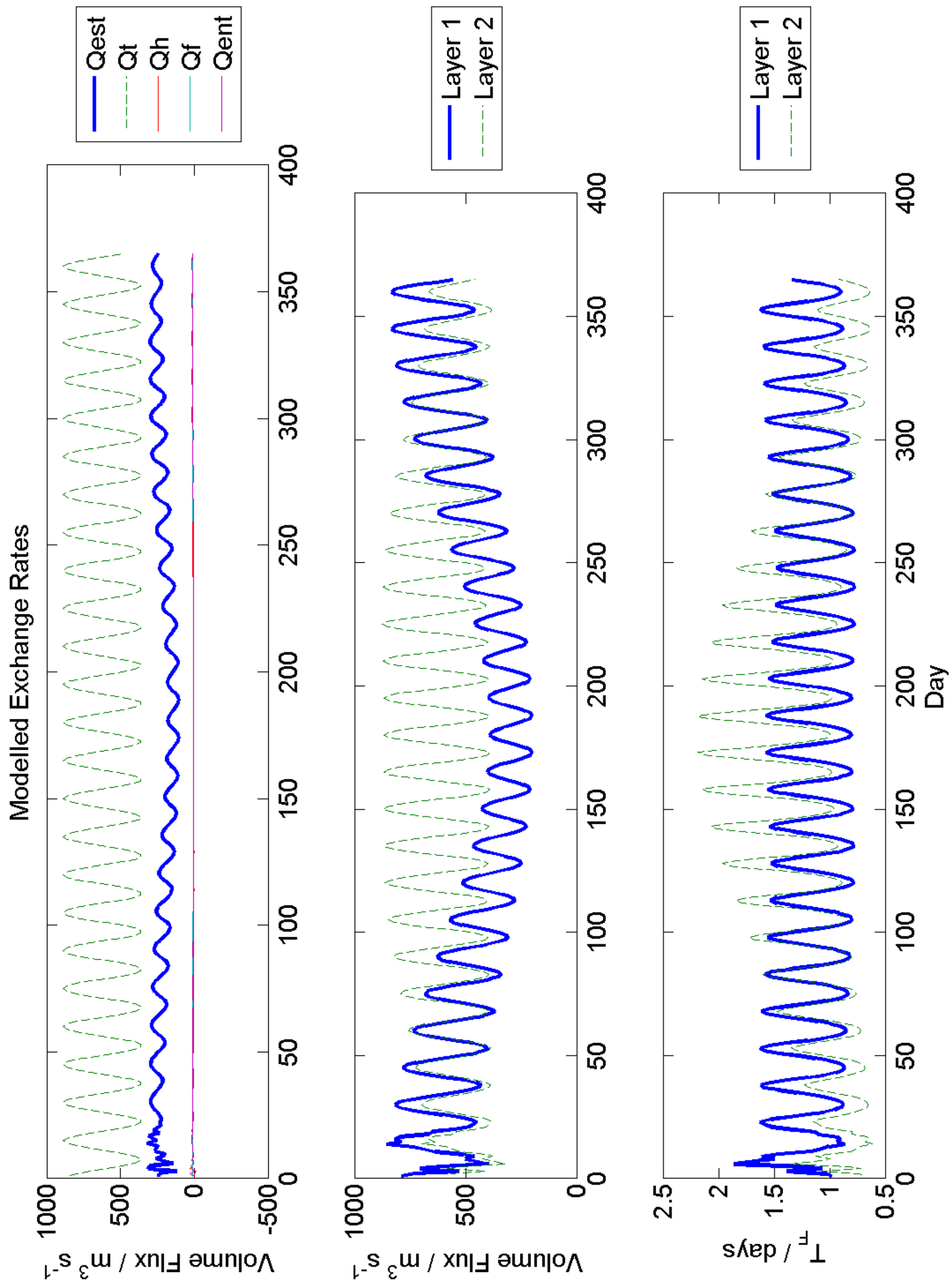

Figure 6. Example results of predicted exchange rates from the prognostic model for Loch Creran over an annual cycle.

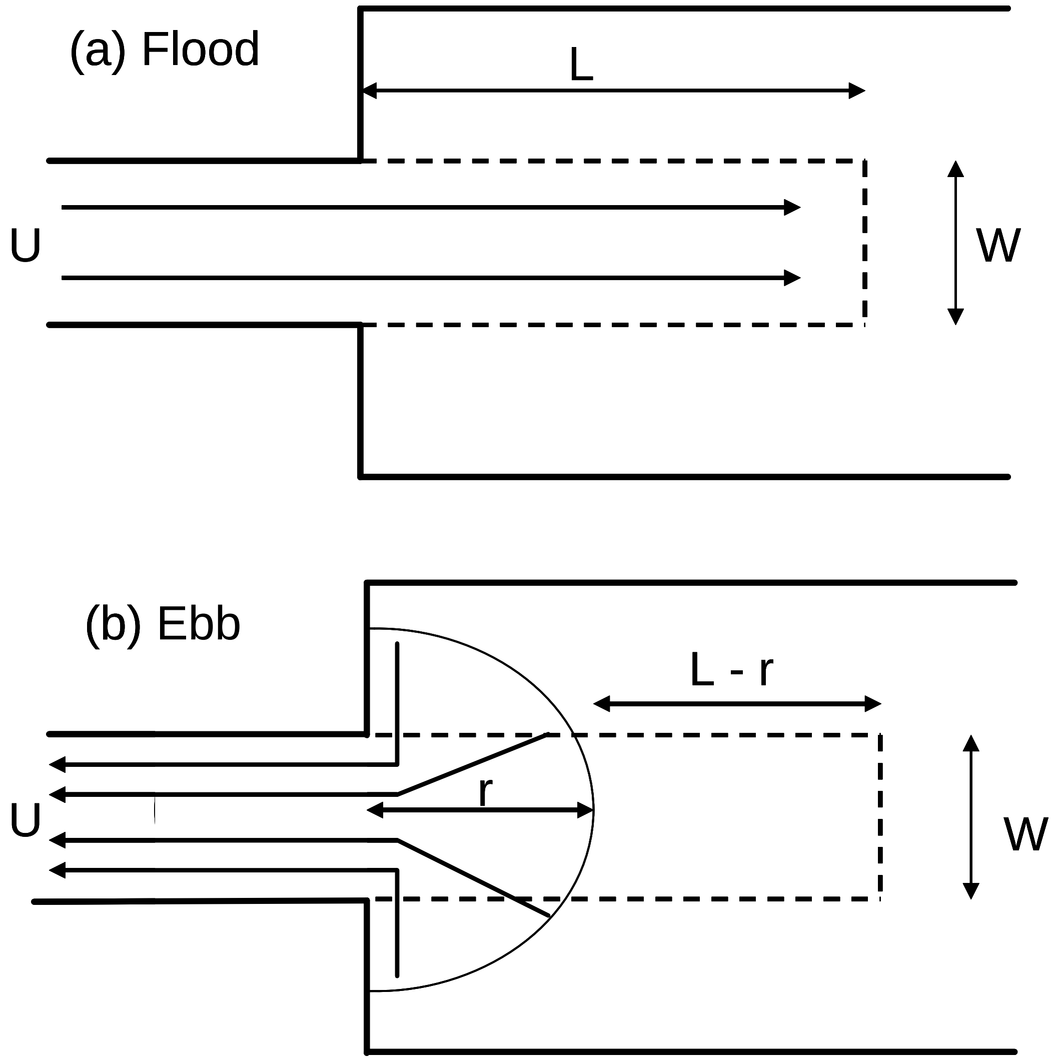

Figure 7. Schematic of the conceptual model for tidal exchange mixing efficiency. During flood tide (a), the tidal flow passing through a narrow channel can form a jet which intrudes into the widening basin over a length scale L. During the ebb (b), the basin water within a distance r is drawn through the entrance channel, leaving a portion of jet water from the previous flood in the basin. This volume is the effective flushing volume. Adapted from Wells and van Heijst (2003).

Appendix A: Governing Equations

Surface Layer Depth

$$h_1 = \frac{N}{2Q_f M} + \varphi\left(\frac{Q_f^2}{MB_m^2}\right)^{1/3} \qquad (A1)$$

where

$$N = ce.Uw^3.A_f$$

$$M = g\beta S_2$$

Surface Layer Salinity

$$S_1 = \frac{S_2 N}{N + 2\varphi\left[Q_f^5\left(\frac{M}{B_m}\right)^2\right]^{1/3}} \qquad (A2)$$

Continuity

$$\frac{\partial h_1}{\partial t} - \frac{1}{A}(Q_h - Q_{ent}) = 0 \qquad (A3a)$$

$$\frac{\partial h_2}{\partial t} + \frac{1}{A}(Q_h - Q_{ent}) = 0 \qquad (A3b)$$

Scalar Conservation

$$V_j \frac{\partial \phi_j}{\partial t} + \nabla(Q_j \phi_j) - V_j K.\nabla^2 \phi_j = 0 \qquad (A4)$$

where h_1, h_2 are the surface and intermediate layer depths (m), U_w^3 is the wind speed (m s^{-1}), A_f is the surface area of the fjord (m^2), S_1 and S_2 are the surface and intermediate layer salinities (psu), g is the acceleration due to gravity (m s^{-2}), β is the salt contraction coefficient (psu^{-1}), Q_f is the river discharge (m^3 s^{-1}), B_m is the width of the entrance sill, or the mouth, of the fjord (m), ce and φ are constants (see Appendix C), A is the horizontal area of the fjord at the base of the surface layer (m^2), Q_h is the vertical flux due to interface displacement ($m^3 s^{-1}$), and Q_{ent} is the vertical flux due to entrainment from the surface to the intermediate layer ($m^3 s^{-1}$).

In Eqn A4, ϕ_j is the value of a scalar property in layer j, where j = 1, 2, 3 for surface, intermediate and bottom layers respectively, V_j is the volume of layer j, $\nabla(Q_j\phi_j)$ represents the net flux of ϕ due to exchange processes, and K denotes turbulent diffusion ($m^2 s^{-1}$).

The net flux of ϕ in each layer is described by:

$$\nabla(Q_1\phi_1) = Q_{est}(\phi_2 - \phi_1) + Q_f(\phi_f - \phi_1) + Q_h(\phi_2 - \phi_1) - Q_{ent}\phi_1 + \left(\frac{V_1}{V_1 + V_2}\right)\left[(Q_t + Q_i)(\phi_0 - \phi_1)\right]$$

$$\nabla(Q_2\phi_2) = Q_{est}(\phi_0 - \phi_2) + Q_h(\phi_1 - \phi_2) + Q_{ent}\phi_1 + \left(\frac{V_2}{V_1 + V_2}\right)\left[(Q_t + Q_i)(\phi_0 - \phi_2)\right]$$

(A5)

where

$$Q_{est} = Q_f.S_1 / (S_2 - S_1) \qquad \text{(A6)}$$

is the estuarine circulation transport, ϕ_0 is the oceanic boundary value of ϕ, and ϕ_f is the value of ϕ in freshwater.

The tidal exchange is given by

$$Q_t = 2\varepsilon a_0 A_f/T \qquad \text{(A7)}$$

where a0 is the amplitude of the semi-diurnal tide (m), ε is the exchange efficiency constant and T is the period of the semi-diurnal (M_2) tide (s).

The exchange due to the intermediary circulation is given by

$$Q_i = \gamma\,(gB_mH_tA_f\Delta M / \rho)^{1/2} \quad \text{or} \quad Q_i = (1/6)B_mH_t(2g\Delta M / \rho)^{1/2} \qquad \text{(A8a,b)}$$

Where H_t is the sill depth, γ is a constant, ρ is the water density, and ΔM is the standard deviation of the weight, M, of the water column outside the fjord from the surface down to sill depth. This variability in the external density profile external drives the intermediary circulation. Eqn 8a is used if the ratio between the surface area of the fjord and the vertical cross-sectional area of the mouth is less than 10^4 i.e. if $A_f/A_m < 10^4$. If $A_f/A_m > 10^4$, then Eqn 8b is used (Stigebrandt, 2001).

In the version of the model presented here, in Eqn A4 K = (K_x, K_y, K_z), with $K_x = K_y = 0$. Only vertical diffusion between the intermediate and bottom water is included.

Appendix B: Module Descriptions

ACExR — This is the main routine. Calls all other modules and outputs the exchange rate data contained in variable E, and the layer parameters contained in Param:

Input: Lochname
Output: E, Param
Usage: [E, Param] = ACExR(Lochname)

ReadCatalogue — Input physical data from the sea loch database (based on the Edwards and Sharples, 1986) catalogue, for the whole loch and for each basin.

Input: Lochname
Output: LochData, SillData

Hypsography — Derives a hypsographic function and associated variables from the topography data contained in the sea loch database. The initial version assumes an inverted pyramid shape for the loch, with volume, surface area and mean depth matching the real data.

Input: LochData
Output: Hypso

ReadForcing — Reads boundary data e.g. daily wind, river flow and external salinity and density profiles. This version currently implements sinusoidally-varying time series of river flow and wind forcing over an annual cycle (January – December).

Input: LochData
Output: Bdata

Initialise — Calculates parameters derived from topography, defines constants, and initialises system parameters e.g. Param.H, Param.V, Param.S, Param.rho

Input: LochData, SillData, Hypso, Bdata
Output: Param, Const

CalcE — This is where the main calculations of exchange rates are performed. The values of E and Param are returned to ACExR at the end of this routine. Calls the following modules: Eficiency, Entrain, Kz23.

Input: LochData, SillData, Hypso, Bdata, Param, Const
Output: E, Param

Efficiency — Calculates the efficiency of tidal exchange based on the jet-sink model of estuarine exchange presented by Wells & van Heijst (2003) and earlier by Stommel & Farmer (1952).

Input: LochData, SillData, Param, Const
Output: eps

Entrain — Calculates the entrainment of water from the surface layer into the intermediate layer caused by the velocity shear between tidal and estuarine circulation.

Input: LochData, SillData, Bdata, Hypso, Param, Const, E
Output: Ent12

Kz23 Calculates the vertical diffusive exchange between intermediate and bottom layers.

Input: LochData, SillData, Param, Const, Hypso, E

Output: E, Param

Appendix C: Description of Key Variables

Lochname	String, Name of loch to be modeled.	
LochData	Contains data from the sea loch catalogue for the whole loch system. Sub-variables include:	
	.Len	Length of loch
	.Range	Tidal range
	.Hmax	Maximum depth of loch
	.HWarea	High Water surface area
	.LWarea	Low water surface area
	.Area2m	Horizontal area at 2 m depth
	.Area5m	Horizontal area at 5 m depth
	.Area10m	Horizontal area at 10 m depth
	.Vol	LW volume of loch
	.Wshed	Watershed
	.Rain	Annual rainfall
	.Qf	River discharge
	.Hmean	Mean depth of loch
	.Nsill	Number of sills
SillData	Contains data from the sea loch catalogue for each basin. Sub variables include:	
	.Len	Length of sill
	.HWwid	Width of sill at High Water
	.LWwid	Width of sill at Low Water
	.Hmax	Maximum depth of sill
	.Hmean	Mean depth of sill
	.Xarea	Cross-sectional area of sill
	.HWuparea	Upstream area at Hoigh Water
	.LWuparea	Upstream area at Low Water
	.Current	Mean current speed across sill
	.Hbasin	Depth of upstream basin
Hypso	Contains hypsographic function data i.e. depth, area, cumulative vertical cross-sectional area. Sub-variables include:	
	.z	depth of horizontal layers (m)
	.A	Horizontal planar area of layers at depth z (m^2)
	.xarea	cumulative vertical cross-sectional area (m^2)
	.vol	cumulative volume of layers (m^3)
Bdata	Contains boundary forcing data e.g. daily wind, river flow, external salinity and density profiles. Sub-variables include:	
	.Qf	Daily river discharge
	.Uw	Daily wind speed
	.S-ext	External salinity profile

	.rho_ext	External density profile
	.sigmarho	Standard deviation of external density profile
	.deltaM	Variability of external water column weight
	.a0	Amplitude of M_2+S_2 tide
	.phi	Contribution of semi-diurnal tide to total tide

Const — Contains constants from the FjordEnv model. Includes:

.ce	ce = 2.5 x 10^{-9}
.cw	cw = 2
.beta	β = 0.0008
.phi	φ = 1.5
.gamma	γ= 17 x 10^{-4}
.g	gravitational acceleration (m s^{-2})
.kappa	von karmen constant
.deltaT	time step (s)
.Tperiod	period of semi-diurnal (M_2) tide (s)
.Cd	drag coefficient

Param — Contains parameter values derived from input data, including layer depths, salinities and volumes. Sub-variables include:

.H	Thickness of layers 1, 2, 3 (m)
.V	Volumes of layers 1, 2, 3 (m^3)
.S	Salinities of layers 1, 2, 3 (psu)
.rho	Densities of layers 1, 2, 3 (kg m^{-3})
.Bm	Width of entrance of loch or of entrance sill (m)
.Af	Surface area of loch at MSL (m^2)
.M	Parameter M from FjordEnv model
.N	Parameter N from FjordEnv model
.Ndays	Length of simulation (days)

E — Contains output data of exchange rates and diffusive fluxes. Sub-variables include:

.Qf	Volume flux due to freshwater input (m^3 s^{-1})
.eps	Efficiency of tidal exchange (0 – 1)
.Qt	Volume flux due to tidal exchange (m^3 s^{-1})
.Qh	Volume flux due to interface displacement (m^3 s^{-1})
.Qent	Volume flux due to entrainment (m^3 s^{-1})
.Qest	Volume flux due to estuarine circulation (m^3 s^{-1})
.Qi	Volume flux due to intermediary circulation (m^3 s^{-1})
.Kz	Vertical diffusivity between layers 2 and 3 (m^2 s^{-1})

Appendix D: Module Call Sequence