# CLAWS – Chemicals Lice and Waste from Salmon Farms

# 3. Nutrients Model

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### **Executive Summary**

A particle-based nutrients model has been developed for application in salmon farms in semienclosed sea lochs and open sea areas. The nutrients model is part of a suite of particlebased, open-source modules known as CLAWS – Chemicals, Lice and Waste from Salmon Farms [CLAWS, 2022]. Other particle modules in the CLAWS repository include those to describe sea lice bath treatments and particulate waste deposition from finfish farms. The nutrients model calculates the sea area, mean height, volume and flushing time prior to deriving an equilibrium concentration enhancement (ECE) index for soluble nitrogen. A 3D hydrodynamics model based on the Telemac code is used to drive the particle-based flushing time calculation. The hydrodynamics model contains the influence meteorological forcing and of stratification brought about by freshwater inflows and air-water heat transfer. For the Lagrangian particle-tracking the open-source code OpenDrift [OpenDrift, 2022] has been used. Results show that the estimated flushing times are in broad agreement with previously published data.

#### About the Report Authors

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Tom is a chartered professional engineer with over 25 years' experience in applied computational mechanics. After a first degree in Environmental Engineering at the University of Strathclyde, Tom undertook a Ph.D in Vortex Shedding Flowmeter Pulsating Flow Computational Fluid Dynamics (CFD) Studies at the same university. Subsequently, he was awarded a JM Lessels scholarship from the Royal Society of Edinburgh for a one-year post-doctoral position at the Institute de Mécanique des Fluides de Toulouse, France in the field of numerical oceanography. The IMechE presented Tom with the Alfred Rosling Bennett Premium and Charles S Lake Award in 2003 for CFD in applied aerodynamics. In 2013 Tom returned from an EPSRC-funded sabbatical in the USA, where he carried out fundamental research in rarefied gas dynamics at the University of Michigan and the Lawrence Berkeley Laboratory in California. From 1994-2017 he was a Senior Lecturer in the Department of Mechanical and Aerospace Engineering at the University of Strathclyde specialising in heat transfer, fluid mechanics and applied CFD. His work is reported in over 50 refereed journal and conference publications. He is currently a director at the engineering consultancy firm MTS-CFD.

# Dr Vincent Casseau MSc PhD, Engineering Consultant

Vincent is an engineering consultant with background experience in fluid dynamics and computer science. He obtained his Masters engineering degree in Aeronautics and Aerospace at ISAE-ENSMA, Poitiers, France. Following an internship at the European Space Agency, Vincent undertook a Ph.D in high-speed re-entry physics at the University of Strathclyde under the supervision of Dr Tom Scanlon, where he developed an open-source platform to solve hypersonic continuum and rarefied flows that has since been used in 15+ countries. Vincent was a Postdoctoral Fellow at McGill University in Montreal, Canada from

2019-2021, where he co-led the development of a monolithic software system to simulate hypervelocity civilian craft, partnering with Ansys and Lockheed Martin.

# 1 Introduction and motivation

This report has been prepared for the Friends of the Sound of Jura, by engineering consultants MTS-CFD, as part of hydrodynamic modelling services to consider the impact of nutrients emanating from existing and proposed fish farms on the West Coast of Scotland.

Operational fish farms have the potential to affect the marine environment in several ways, via the release of waste in the form of dissolved nutrients, particulate organic matter, pesticides and live parasitic salmon lice.

The report describes the development of a particle-based nutrients model to determine sea area, mean height, volume and flushing time prior to deriving an equilibrium concentration enhancement (ECE) index for soluble nitrogen [GILL, 2002]. The nutrients model is part of a suite of particle-based, open-source modules known as CLAWS – Chemicals, Lice and Waste from Salmon Farms [CLAWS, 2022]. Other particle modules in the CLAWS repository include those to describe sea lice bath treatments and particulate waste deposition from finfish farms.

A 3D hydrodynamics model based on the TELEMAC code [Scanlon, 2022] is used to drive the particle-based flushing time calculation. The hydrodynamics model contains the influence of weather forcing and stratification through the salinity and temperature fields.

Previous work on flushing times has been based on yearly estimates of sea loch volumes derived from Admiralty chart data and a maximum tidal range that is assumed to exist continually throughout the year [Edwards, 1986]. This yearly-based approach will produce general guidance on flushing times but it cannot adequately take into account local effects of complex bathymetry (sills), littoral topography, weather forcing, stratification, cumulative effects of nutrients emanating from different water body types such as sea lochs/open sea zones and variations in the tidal range due to the spring/neap tidal cycles throughout the year. The authors [Edwards, 1986] also state that possible errors may exist where bathymetry data is sparse, as in and around many of the sea loch sills.

The work proposed in our new model represents a more sophisticated and realistic approach. We take account of the fact that flushing times, and hence ECE values, will vary according to the time of year due to variations in the spring/neap tide cycles. We propose that an average value of the tidal range during the period of the study should be used as opposed to the maximum and minimum values. Using maximum and minimum values for the tidal range will lead to shorter flushing times and a non-conservative estimate of the ECE index.

# 2 Background data

#### 2.1 Hydrodynamic data

The hydrodynamic data used to determine the flushing times is based on a 3D, non-hydrostatic Telemac model of the West Coast of Scotland, the extent of which is shown in Figure 1. 10 terrain-following vertical sigma layers are applied in the model and it also includes meteorological forcing and stratification due to freshwater inflows and atmosphere-water heat

exchange. Extensive validation and verification tests have been undertaken against physical data and inter-model comparisons with the Scottish Shelf Model (SSM) results [Scanlon, 2022].

# 2.2 Bathymetry data

The bathymetry data for the present study have been collected from a range of different sources including publicly available data sets provided by Marine Scotland for the Scottish Shelf Model [SSM, 2022], digitised Admiralty charts and bathymetry information from the UK's Digimap Ordnance Survey Collection [DOSC, 2022]. The bathymetry used in the model is shown in Figure 2.

#### 2.3 Particle-tracking

For the Lagrangian particle-tracking the open-source software OpenDrift has been used [OpenDrift, 2022].



Figure 1 Telemac hydrodynamic mesh and model extent.



Figure 2 West Coast model bathymetry (m).

#### 3 Methodology

#### 3.1 Shoreline database

The shorelines delineating land and water areas are obtained from the GSHHG (Global Selfconsistent, Hierarchical, High-resolution Geography) database [WESSEL, 1996] [DAGESTAD, 2018] and the highest possible resolution is applied. The shorelines were then constructed using the freely-available BlueKenue software [BLUEKENUE, 2011] with results as shown in Figure 3. The computational mesh used in the Loch Long study is presented in Figure 4.



Figure 3 Shorelines and land drawn in the Loch Long area.



Figure 4 Computational mesh used in the Loch Long area.

# 3.2 Particle seeding in CLAWS

The format JSON (JavaScript Object Notation) [JSON, 2022] is used to select the control and seeding areas for the flushing time calculation. JSON is a lightweight file format storing text as a series of keyword – value pairs and its extension GeoJSON conveniently encodes geographic data structures. The website <a href="http://geojson.io/">http://geojson.io/</a> allows the user to draw a polygon around the geographic area of interest. The example of Loch Long, including its upper basin, and Loch Goil is shown in Figure 5 and the polygon is saved in GeoJSON format.



**Figure 5** Control area *polygon drawn around Loch Long (including its upper basin and Loch Goil) on* <u>http://geojson.io/</u>.

The polygon coordinates are decoded using Python's *json* package and the control area is computed by interrogating the mesh in OpenDrift. Particles are seeded randomly in each of the mesh elements that are fully inside the seeding areas, which in this example is set to be the control area, and the target number of particles per element is a function of the total number of particles to insert and the element to seeding area ratio. The initial locations of the 16,375 seeded particles are shown in blue in Figure 6, though they can't be individually distinguished.



Figure 6 Example of random particle generation within the bounds of a control area in CLAWS.

#### 3.3 Loch area, mean depth, and volume calculations

The control area polygon, P, is passed to OpenDrift and the computational mesh is interrogated to determine whether each of its elements is fully contained within the bounds of the polygon. The loch area is then computed from the list of these elements as:

$$A_{\text{loch}} = \sum_{e \in P} A_e \qquad (1)$$

where the subscript e refers to a mesh element and A is an area.

The loch mean depth,  $\bar{z}_{loch}$ , is then calculated as an area-weighted average for all elements satisfying the condition  $e \in P$  as:

$$\bar{z}_{\text{loch}} = \frac{1}{A_{\text{loch}}} \sum_{e \in P} \left( \frac{A_e}{n_{\nu_e}} \sum_{\nu_e} z_{\nu_e} \right)$$
(2)

where  $v_e$  is a vertex of element e,  $n_{v_e}$  is the number of vertices of element e, and  $z_{v_e}$  is the depth at the location of vertex  $v_e$ .

The loch volume is defined as the product of the loch area and the loch mean depth.

Using the control area shown in Figures 5 and 6, the loch area and mean depth are found to be 44.5 km<sup>2</sup> and 37.4 m, respectively. There is thus a good agreement with the data obtained by (a) Edwards and Sharples [Edwards, 1986] who estimated the low-water water area and mean depth of Loch Long (including its upper basin and Loch Goil) to be 41.2 km<sup>2</sup> and 40 m, respectively, and (b) PARTRAC [PARTRAC, 2020] who reported values of 44 km<sup>2</sup> and 40 m, respectively (the small area discrepancies may be attributed to the arbitrary location of the loch's mouth).

#### 3.4 Bathymetry plot

The bathymetry data described in section 2.2. is loaded into the TELEMAC hydrodynamics software and later exported in *selafin* format as one of the solution fields. The TELEMAC output *selafin* file is read into OpenDrift and the bathymetry variable stored. It can be interrogated to give the height of the water column at a specific location or for all mesh points, in which case it is shown to produce the contours presented in Figure 7.



Figure 7 Bathymetry profile in the Loch Long area.

#### 3.6 Random initial depth distribution and flushing time calculation

The initial depth of the water particles is set according to a random distribution using local bathymetry information. These particles are subject to water currents and turbulent diffusion effects in the horizontal and vertical directions with diffusion coefficients equal to 0.1 and 0.001 m<sup>2</sup>/s, respectively. Figure 8 shows snapshots of the initial particle distribution and the dispersion after 2 days. Note that the units in these plots are arbitrary and they represent the concentration of particles in a sampling box of surface area 500 m × 500 m and depth extending down to the sea bed.





Figure 8 Snapshots of the initial particle distribution (upper) and the dispersion after 2 days (lower).

The flushing time is defined as the time taken for 63% of the particles to leave the original polygon zone [PARTRAC, 2020], [MONS, 2002]. A time-step sensitivity analysis has been conducted as shown in Figure 9 and a simulation time step of  $\Delta t = 1.25$  min was selected. The flushing time of Loch Long (including its upper basin and Loch Goil) is shown to be approximately 17 days (when extrapolated). This is in contrast to PARTRAC's [PARTRAC, 2020] reported value of 9 days. Differences may be due to the fact that the TELEMAC hydrodynamics were 3D (8 terrain-following sigma layers for the Clyde system model), non-hydrostatic with stratified conditions due to freshwater salinity and temperature effects included in the model. The results also highlight the importance of carrying out a time-step sensitivity analysis for the flushing time calculation.



Figure 9 Time step sensitivity analysis for the number of particles in the control area for neutrally-buoyant particles.

Other scenarios have been explored in Figure 10 to investigate the effects on the flushing time of (a) releasing floating particles (solid black line), (b) releasing neutrally-buoyant particles at sea surface level (solid blue line), and (c) changing the vertical interpolation method of hydrodynamic quantities at the particles positions from *nearest sigma layer* (solid red line) to *linear interpolation* (solid green line).



**Figure 10** Particle number evolution in the control area for other scenarios ( $\Delta t = 10 \text{ min}$ ).

It is seen that the overall flushing times appear moderately sensitive to changes in the vertical interpolation method or initial particle vertical position. However, it is evident that particle vertical diffusion must be included in the model in order to have consistent and realistic values of flushing time. The results also highlight the importance of carrying out particle-number and time-step sensitivity analyses.

# 4 Case study: Loch Melfort and Shuna Sound

#### 4.1 Choice of location

This example was chosen as it represents the combination of a semi-enclosed sea loch (Loch Melfort) connected to an area of open sea (Shuna Sound). The case study highlights how effectively the new model can assess the cumulative effects of nutrients emanating from several farms connected by different water body types (sea loch and open sea).

Figure 11 shows the area of interest including 2 salmon farms in Loch Melfort and 5 farms in the Sound of Shuna. The total biomass from the 7 farms in the system was set to be 10,395 tonnes [AQUA, 2022].



Figure 11 Case study area: Loch Melfort and Shuna Sound. Active salmon farms are highlighted in red. Shellfish zones in green. [AQUA, 2022].

# 4.2 Setting the flushing time area

The area selected for the flushing time is set using the open standard geospatial data interchange format GeoJSON [JSON, 2022], as described in section 3.1. A polygon is drawn around the appropriate area selected for the flushing time as shown in Figure 12 and the resulting file is saved as *shuna.json*.



**Figure 12** Polygon selection for setting the flushing zone area. This includes Loch Melfort and the open sea area in the Shuna Sound.

# 4.3 Setting up the case

# 4.3.1 Using the pre-processing script to calculate the sea area, mean depth, volume and tidal range

As discussed in section 1, using the maximum and minimum values for the tidal range over a year will lead to an under-estimation of the flushing time, i.e., a shorter flushing time. It is more appropriate to use the average tidal range over the period of the study concerned. In this instance the study period is from the 1<sup>st</sup>-16<sup>th</sup> May 2011 and this covers part of the period of the hydrodynamics.

In order to calculate the sea area, mean depth and tidal range, the pre-processing script *pre.py* is run with the results shown in Figures 13-15. The user then inputs these values into the *setup.py* script.



**Figure 13** Tidal range (m) graph in Loch Melfort – Shuna Sound from 1<sup>st</sup>-16<sup>th</sup> May 2011.



**Figure 14** Sea water elevation (*m*) graph in Loch Melfort – Shuna Sound from 1<sup>st</sup>-16<sup>th</sup> May 2011.

The user now writes the value of mean tidal range of 1.527 m into the Python script *setup.py*. In addition, the user will specify other parameters such as the domain extent in lon/lat coordinates and total farm biomass in the *setup.py* script.



**Figure 15** Example output for the pre-processor script pre.py to calculate the zone's area and mean depth in Loch Melfort – Shuna Sound.

#### 4.4 Results

Following the running of the Python scripts *run.py* and *post.py* the results shown below are obtained. Figure 16 shows snapshots of the initial stages of the dispersion patterns of the 39,995 particles used in the flushing time study. The Loch/open sea system is seen to flush mainly to the south, with exiting particles then heading northwards in tidal pulses. Note that the units in these plots are arbitrary for this flushing time study and they represent the concentration of particles in a sampling box of surface area 80 m × 80 m and depth extending down to the sea bed. The concentration plots are also normalised using the maximum initial concentration. The calculation time was ~7 hours on a single core of an Intel i7-7820HK CPU @ 2.90 GHz.





Figure 16 Snapshots of the dispersion of particles from Loch Melfort – Shuna Sound.

The flushing time, defined previously as the time taken for 63% of the particles to leave the original polygon zone [PARTRAC, 2020], [MONS, 2002], was calculated to be 15.45 days as shown in Figure 17. Note that the estimate of flushing time for Loch Melfort alone by Edwards and Sharples was 9 days [Edwards, 1986].



Figure 17 Flushing time calculation for the Shuna-Melfort system.

The ECE calculation output is shown in Figure 18.

```
Loch's flushing time (day) = 15.45
Existing biomass - particulate simulation:
Salmon Farm's ECE (kg/m^3) = 2.580841e-05
Salmon Farm's ECE (ug/L) = 25.808411
Salmon Farm's ECE (umol/L) = 1.843458
Salmon Farm's nutrient enhancement index = 3
```

Figure 18 ECE calculation output based on [GILL, 2002].

The ECE output has been checked with the following hand calculation:

Shuna-Melfort system:

 $Vol = 821.54 \text{ Mm}^3$ 

Tidal range = 1.527 m

Flushing time = 15.45 days

Yearly flushing rate =  $(365/15.45) \times 821.54 \times 10^6 = 19,408 \text{ Mm}^3/\text{yr}$ 

Q = 19,408 flushing rate Mm<sup>3</sup>/yr

S = 48.2 kgN/biomass tonnage per year

M = 10,395 Biomass tonnage per year (total for all farms in the Shuna-Melfort system)

ECE = S × M/Q = (48.2 × 10,395)/19,408 = 25.81 µg/L

 $ECE = 1.84 \ \mu mol/L$ 

ECE index = 3, as defined in Table 1 [GILL, 2002]

 Table 1 – Equilibrium Concentration Enhancement (ECE) Index

Nutrient Concentration Level (µmol/L)	ECE Index
>10	5
3-10	4
1-3	3
0.3-1	2
<0.3	1
0	0

The Python script for *hydrodynamics* can also be used to produce outputs for fields such as the mesh, velocity, salinity, temperature from the hydrodynamics data and local bathymetry plots can be made with the sea bed elevation and two salinity plots shown as examples in Figures 19-21.



Figure 19 Example of mesh output using the post-processing Python script



Figure 20 Example of bathymetry output using the post-processing Python script.



Figure 21 Snapshot of surface salinity in the Shuna-Melfort system.

# 5 Case study: Loch Alsh, Loch Duich, Loch Hourn and Loch Nevis

# 5.1 Choice of location

This example was chosen as it represents the combination of four sea lochs located in relatively close proximity, each of which contains salmon aquaculture activity. The case study highlights how the nutrients model can be set-up as a system of *multi-zones* and how effectively the model can assess the cumulative effects of nutrients emanating from several farms connected by different water body types (sea lochs and inter-connected water ways).

Figure 22 shows the area of interest including the 4 sea lochs and 7 salmon farms in the system. The total biomass from the 7 farms in the area was set to be 6,892 tonnes [AQUA, 2022] as described in Table 2.



Figure 22 Location of 4 lochs and 7 salmon farms.

FARM	Biomass May 2019 (tonnes)
Nevis A - Earnsaig	1278
Nevis B - Stoull	933
Nevis C - Ardintigh	922
Loch Hourn	2800 (proposed)
Duich	318
Ardintoul	302
Sron	339
TOTAL =	6892

**Table 2** Biomasses for salmon farms in the nutrient model calculation.

#### 5.2 Reducing the size of the hydrodynamics data set

The 3D Telemac hydrodynamics model consists of a large data set of flow variables with a file size of 36 Gb. It would be beneficial in terms of disk storage and compute time for the nutrient model if the hydrodynamic data set could be reduced in size to one focusing on the 4 sea lochs in the system. A Python script has been created to achieve this reduction and the file size for the hydrodynamics is reduced substantially from 36 Gb to 2.6 Gb. Figures 23-25 show the original model mesh (36 Gb, blue) and the cropped model (2.6 Gb, red) that is used for the nutrient flushing time calculation.



**Figure 23** Original Telemac 3D hydrodynamics mesh (36 Gb, blue) and reduced size model (2.6 Gb, red).



**Figure 24** Zoomed view of original Telemac 3D hydrodynamics mesh (36 Gb, blue) and reduced size model (2.6 Gb, red).



Figure 25 Final reduced size hydrodynamics model mesh.

# 5.3 Flushing time and ECE calculation

Figures 26-28 show the location of the particle-seeding *json* zones, the sea water elevation and tidal range for Loch Hourn. The initial particle distribution and flushing time plots for the Alsh-Duich-Hourn-Nevis system are shown in Figures 29-33. 60,000 particles were used in the study. Although the weak-flushing loch Nevis has yet to reach the 37% particle threshold, the flushing time for the combined system of the 4 lochs is 15.87 days and it is this value that is used in the ECE calculation.



**Figure 26** Polygon selection for seeding the 3 flushing zone areas in Loch Alsh-Duich, Loch Hourn and Loch Nevis.



**Figure 27** Sea water elevation (*m*) graph in Loch Hourn from 1<sup>st</sup>-20<sup>th</sup> May 2018. Similar results were found for Loch Alsh and Loch Nevis.



**Figure 28** Tidal range (m) graph in Loch Hourn from 1<sup>st</sup>-20<sup>th</sup> May 2018. Similar results were found for Loch Alsh and Loch Nevis.



**Figure 29** Initial seeding zones for lochs Alsh-Duich, Hourn and Nevis. There are a total of 3 seeding zones, each containing 20,000 particles.



Figure 30 Flushing time plot for Loch Nevis.



Figure 31 Flushing time plot for Loch Hourn.



Figure 32 Flushing time plot for Loch system Alsh-Duich.



Figure 33 Flushing time plot: all seeding areas combined.

# ECE Calculation across the combined 4-loch system:

Total Volume = 4728.04 Mm<sup>3</sup>

Tidal range = 2.862 m

Flushing time (all seeding areas combined) = 15.87 days

Yearly flushing rate =  $(365/15.87) \times 4728.04 \times 10^6 = 10,874 \text{ Mm}^3/\text{yr}$ 

Q = 10,874 flushing rate Mm<sup>3</sup>/yr

S = 48.2 kgN/biomass tonnage per year

M = 6,892 Biomass tonnage per year (total for all farms in the Alsh-Duich-Hourn-Nevis system)

ECE = S × M/Q = (48.2 × 6,892)/10,874 = 30.55 µg/L

 $ECE = 2.182 \ \mu mol/L$ 

ECE index = 3, as defined in Table 1 [GILL, 2002]

Figures 34 to 36 show snapshots the particle concentrations from each loch system with time. Note that these dye concentration plots represent the instantaneous number of particles (*number / m*<sup>3</sup>) existing in a sampling box of horizontal surface area 60 m × 60 m and depth extending to the sea floor. These plots are for indicative purposes only. The actual particle numbers are used in the calculation of the flushing time. Finally, a plot of bathymetry and two example snapshots of surface salinity (*PSU*) and *y*-direction velocity (*m*/s) are shown in Figures 37, 38 and 39, respectively.

The results highlight the effectiveness of the CLAWS-Nutrients model in being able to consider multiple, interconnected sea loch systems in a combined-zone nutrient ECE calculation.





**Figure 34** Snapshots of particle number concentrations (number/ $m^3$ ) from Lochs Alsh-Duich at time t = 0 (upper) and t = 52 hours (lower).





**Figure 35** Snapshots of particle number concentrations (number/ $m^3$ ) from Loch Hourn at time t = 0 (upper) and t = 52 hours (lower).





**Figure 36** Snapshots of particle number concentrations (number/ $m^3$ ) from Loch Nevis at time t = 0 (upper) and t = 52 hours (lower).



Figure 37 Bathymetry contours across the Loch Alsh-Duich-Hourn-Nevis system.



Figure 38 Snapshot of surface salinity (PSU) contours across the Loch Alsh-Duich-Hourn-Nevis system.



**Figure 39** Snapshot of y-velocity contours (m/s) across the Loch Alsh-Duich-Hourn-Nevis system.

# 6. Conclusions

A particle-based nutrients model has been developed for application in salmon farms in semienclosed sea lochs and open sea areas. The nutrients model is part of a suite of particlebased, open-source modules known as CLAWS – Chemicals, Lice and Waste from Salmon Farms [CLAWS, 2022]. Other particle-based modules in the CLAWS repository include those to describe sea lice bath treatments and particulate waste deposition from finfish farms. The nutrients model calculates the sea area, mean height, volume and flushing time prior to deriving an equilibrium concentration enhancement (ECE) index for soluble nitrogen. The model is capable of handling multiple zones of interconnected sea areas in a combined ECE calculation. A 3D hydrodynamics model based on the Telemac code has been used to drive the particle-based flushing time calculation. The hydrodynamics model contains the influence of meteorological forcing and stratification brought about by freshwater inflows and atmosphere-water heat exchange. For the Lagrangian particle-tracking the open-source code OpenDrift [OpenDrift, 2022] has been used. Results show that the calculated flushing times are in general agreement with previously published data and that particle number and timestep sensitivity studies should be carried out as part of the modelling process.

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