The Scottish Salmon Company



NewDepomod Simulation Report

Gometra, Isle of Gometra

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List of Abbreviations

τε	Minimum resuspension modelling used in simulations		
θ	Shields parameter		
2D	Two dimensional simulations along horizontal plane		
3D	Three dimensional simulations along horizontal and vertical plane		
MAE	Mean Absolute error		
CAR	Controlled Activities Regulations		
D ₅₀	Median grain velocity		
D*	Dimensionless grain size		
EmBZ	Emamectin Benzoate (SLICE active ingredient)		
EQS	Environmental Quality Standard		
FVCOM	Hydrodynamic simulation package – Open source		
g/m3/yr	Grams per square metre per year (deposition)		
IQI	Infaunal Quality Index		
ITI	Infaunal Trophic Index		
mCD	Meters below Chart Datum (local)		
MIKE3	Hydrodynamic simulation package developed by DHI consulting		
MZ	Mixing Zone		
NB	Nota Bene: Note Well		
NDM	NewDepomod (simulation software)		
OS	Ordnance Survey		
r ²	R-squared error		
RMSE	Route Mean Squared Error		
SDM	Standard Default Method		
SEPA	Scottish Environmental Protection Agency		
SSC	Scottish Salmon Company		
Т	Tonnes (biomass)		
TAQ	Total Allowable Quantity		
U*	Shear velocity		
WEI	Wave Exposure Index		

Summary

This report was written by The Scottish Salmon Company (SSC) to meet the requirements of the Scottish Environment Protection Agency (SEPA) for updated benthic sampling, under the Controlled Activities Regulations ((CAR) 2011). Updates are according to contemporary guidance (July 2019¹). This report describes the methodology used to model the biomass accepted by SEPA as permissible under CAR consent CAR/L/1102386. Bath treatments were also simulated to review the current licensed quantities,

1 although a variation of the licenced quantities is not proposed. Modern simulation techniques have been used based on 110 days of hydrographic observations and related to observed conditions where available. A summary of the existing licenced quantities and the conclusions from the contemporary modelling is presented in Table 1.1.

Site details				
Site name		Gometra		
Site location		Isle of Gometra		
Site configuration details				
Number of pens		16		
Pen circumference (m)		100		
Net depth (m)		10		
Group layout		8 x 2 pens		
Hydrographic summary				
Sub-surface currents Average speed (m/s)		0.10		
Residual direction (°True)		275		
Pen-bottom currents Average speed (m/s)		0.099		
	Residual direction (°True)	275		
Near-bed currents	Average speed (m/s)	0.087		
	Residual direction (°True)	285		
	Bed residual mean current (m/s)	0.032		
Benthic modelling- Standard default method				
Peak biomass		1,500		
Peak stocking density (kg/r	n³)	11.80		

Table 1.1. Summary of modelling results.

¹ SEPA (2019) AQUACULTURE MODELLING: Regulatory Modelling Guidance for the Aquaculture Sector: July 2019 – Version 1.1

Benthic modelling - Calibrated model		
Peak biomass 1,944		
Proposed peak stocking density (kg/m ³)	15.30	
In-feed treatments		
EmBz (g): MTQ/TAQ	525 / 1,444.6	
Licensed Bath treatment quantities		
Cypermethrin (g)	70.65/ 3 hr	
Deltamethrin (g)	26.5/ 3 hr	
Azamethiphos (g)	318.3 / 24 h	
Re-simulated Bath treatment quantities		
Cypermethrin (g)	71.4/ 3 hr	
Deltamethrin (g)	26.8/ 3 hr	
Azamethiphos (g) 394.2/ 3 hr & 509.1/ 24 h		

Introduction

This modelling report was written by The Scottish Salmon Company (SSC) to describe the application of modern hydrographic data (collected between 2017 and 2018) and updated NewDepomod simulations using the Standard Default Method¹ and bespoke model calibration to predict benthic impacts at the finfish site, Gometra, located north of the Isle of Gometra on west of the Isle of Mull (Figure 2.1). The report outlines four modelling exercises:

- 2
- Standard Default Method (SDM) risk assessment of the current consented tonnage;
- Extensive model calibration process based on SDM model setup against observed benthic conditions;
- Application of the calibrated model to review the appropriate peak biomass at the Gomera site; and
- Application of modern hydrographic datasets to review permissible bath treatment quantities.

The aim of this modelling report is to apply modern simulation techniques to risk assess the hydrographic conditions and the dispersal of farm related discharge at the Gometra site, and review licence conditions. To facilitate this and to increase reliability, model calibration has been performed in collaboration with SEPA, tuning depositional modelling to match observed benthic footprints. SEPA's Modelling Team have reviewed and approved the methodology in advance of this report.



Figure 2.1: Gometra site location

2.1 Context

Each finfish operation site occupies a unique hydrographic context with varying waste input rates and, as a result, the SDM risk assessment approach has been found to approximate the observed benthic Mixing Zone. However, this set of model defaults fails to accurately represent the fate of particle diffusion and associated benthic impact (particularly where synthetic datasets are applied). Subsequently, where appropriate benthic observations exist, it is necessary to modify the

representation of physical processes within the model to better represent the site transport regime and facilitate the prediction of benthic impact as accurately as possible.

At the time of writing, whilst the methodology presented herein has been approved by SEPA, no paradigm for the calibration of a NewDepomod model to observed benthic conditions exists and the literature assessing the performance of the model against observed conditions is limited. SEPA's unpublished SDM remains the most extensive review of model performance and represents a risk assessment approach which has been found to accurately predict compliance (of Mixing Zone area and intensity) based on multiple sites along the Scottish west coast and Archipelago's. The application of this methodology at selected SSC sites, demonstrates approximation of compliance but limited predictive validity on the ultimate fate of waste particles. In addition, simulations hold varying degrees of accuracy observed in the prediction of benthic Infaunal Trophic Index (ITI) and Infaunal Quality Index (IQI) at sites assessed.

Few published model calibration reports are available given the relative infancy of the regulatory framework and the novelty of the NewDepomod package. The majority of these assessments have been performed using external model hydrodynamic forcing, derived from FVCOM or MIKE3, with limited calibration exercises performed based on a single hydrographic time series. In addition, these assessments have anecdotally attempted to calibrate models to the observed Emamectin Benzoate (EmBz) concentrations in localised samples but have had limited success due to; small sample size, uncertain decay properties of EmBz in the environment, and high detection thresholds. Given the novelty of the approach to model calibration undertaken here, the requirement for regulatory review prior to widespread implementation is evident.

2.2 Modelling context

Historically the biomass at this site has been assessed using AutoDepomod, informed by a 15-day hydrographic dataset, a dataset length which is no longer accepted by SEPA. This was supplemented by simulations of bath treatments in BathAuto V5, using the same hydrographic 15-day dataset.

The SDM simulations presented in this report are the initial iteration of simulations undertaken representing this site within NewDepomod and so default parameters derived from SEPA's Guidance released in 2019¹ and revised in June 2021² are applied. The SDM modelling presented here applies a modern, stitched 90-day hydrographic dataset and is required to risk assess the current biomass and review model performance.

The application of the SDM facilitated the review of model performance, prior to calibration and informed the modification of processes governing dispersion in the calibration process, enabling the accurate prediction of processes.

BathAuto simulations of the dispersal were also modernised with the contemporary 90-day dataset, which are more representative of hydrographic conditions at the site.

2.3 Calibration framework

The calibration framework presented here adopts a three-stage process to modify NewDepomod model function and relate this directly to observed, site-specific IQI benthic observations. These stages are outlined below and are illustrated in greater detail in later sections.

Step 1: Model tuning

² SEPA (2021) NewDepomod Draft Guidance_Draft_20210625_final3

This step involves the modification of model behaviour to replicate inferred deposition rates from a given sampling exercise. This is undertaken with specific reference to the role of observed hydrographic data, given model parameters and their relation to observed benthic impact. Model tuning here is achieved through an iterative process, modifying assumptions employed (through parameter selection) to better represent the dispersion of waste solids at the site. This step is therefore concerned with refining the representation of *particle behaviour* within the modelling framework.

This step was significantly modified following discussion with SEPA, with previous iterations using established conversion rates from deposition to ITI and from ITI to IQI. The method proposed here has greater relevance to the existing SEPA risk assessment framework.

NB: The model calibration exercise is considered an approximation of relative benthic deposition rates, replicating patterns in deposition rather than an accurate representation of deposition rates. This approximation is attributed to uncertainties surrounding the conversion rate between IQI and deposition. Any inaccuracies in deposition rates will be mitigated by modification of the nominal IQI conversion used by the scaling of outputs (Step 2).

Step 2: Model scaling

A direct, universal conversion of deposition (in g/m²/yr) to IQI has not been established as it is based on benthic community which is known to be sensitive to a myriad of extraneous variables, not represented within the NewDepomod framework. It was therefore necessary to derive a site-specific conversion based on the calibrated model (established in Step 1) and observed IQI scores. Thus, a representation of the *ecological community's response* to deposition at the site is integrated into the model framework.

Step 3: Model validation/verification

To define model skill, it was necessary to assess the *model performance* against independent observations, not included in the model calibration process. As no additional IQI scores exist at the majority of sites undergoing initial calibration, historic ITI observations can be used, assessing model function. IQI scores should be used where available as these allow calibration of the full calibrated framework. This step constitutes a review of model performance with specific reference to the data available at the time and allows the temporal validity of the modelling to be reviewed.

2.4 Site context

Gometra is situated north of an island shoreline within the Inner Hebrides, influenced by a semi-diurnal, macrotidal tidal regime with a mean spring range of 3.8 m. The site is considered exposed to significant sea swell to the west where an open fetch exists to Tiree and Coll, from where waves generated in the Minch and Malin sea area can propagate and impact the site. The wave regime at the site is thus governed by non-local swell waves with a small influence of local frictional waves. The site is considered well mixed and flushed by tidal and wave related currents with limited freshwater influence. The site sits 250 m north of the Gometra shoreline and in water depths between -18 and -25 mCD.

2.5 Site details

The site currently has planning permission for 16 x 100 m circular pens, in one group arranged in an eight by two formation, a 50 m grid, and with a net depth of 10 m. The SEPA consented biomass on site is currently 1,500 T. Further details of the site are provided in Table 2.1.

Table 2.1. Summary of Gometra site information.

Site Details			
Group Location	136,282 E 742,459 N		
Number of Pens	16		
Pen Circumference (m)	100		
Grid Matrix (m)	50 x 50		
Net Depth (m)	10		
Configuration	8 x 2		
Orientation (°)	090		
Distance from shore (m)	250-300		
Depth at Site (m)	18 - 25		

2.6 Site exposure

The site at Gometra has a wave exposure index of between 2.89 and 2.95 as derived from the Marine Scotland Wave Exposure Index (WEI)³ and so is considered an exposed site. As a result, the average mixing zone intensity threshold here is extended under SEPA's Standard Default approach from 2,000 g/m²/yr to 4,000 g/m²/yr.

2.7 Report layout

The aim of the sections within this report are outlined below along with the content presented in each section:

- Section 3: Outlines model setup and reviews hydrographic forcing and bottom boundary datasets.
- Section 4: Outline model performance using the SDM and discuss the skill of this default model in the replication of observed benthic conditions in the four transect IQI sampling regime.
- Section 5: Unpack the observations of model performance outlined in Section 4 and establish the aim of the calibration exercise (increase resuspension, curtail diffusion, maximise consolidation, etc.). Following this the process of calibration will be outlined.
- Section 6: Outline the proposed application of a calibrated model to define the carrying capacity of the site based on the calibrated model.
- Section 7: Outlines the re-simulation of the licenced quantities of Bath treatments in BathAuto V5 using modern hydrographic data.
- Section 8: Concludes and summarises the modelling undertaken, presenting recommended revisions to the existing CAR license.

³ MarineScotland (2020) MAPS NMPI, part of Scotland's environment. [Accessed online 28/02/2020: <u>https://marinescotland.atkinsgeospatial.com/nmpi/default.aspx?layers=780</u>]

Model setup

To identify model skill, the site was simulated using SEPA's SDM to risk assess the current consented biomass at the site and the role of three different hydrographic datasets in the replication of observed conditions. The model setup from this risk assessment approach and its results are outlined in the sections below.

3 **3.1** Model hydrodynamics

Modelling was undertaken using data collected by SSC spanning three data collection exercises, consisting of one 23-day deployment in August 2017, a 49-day deployment in October 2017 and a final deployment of 38-days in January 2018. This cumulative 110-day record was stitched to create a seamless 93-daytime-period in 20-minute timesteps (with data lost through tidal phase stitching). This data was trimmed to represent 90-days of hydrographic data, as per SEPA recommendations. The data collected is discussed in greater detail in following sections and a summary of observed data from the three bins used can be seen in Table 3.1.

Location	Average velocity (m/s)	Residual direction (°)	Average depth (m)	Average residual magnitude (m/s)
Near-bed	0.087	285	32.74	0.032
Pen bottom	0.099	275	11.67	0.060
Sub- surface	0.100	275	6.53	0.058

Table 3.1: 90-day observed dataset summary data.

Residual currents at the bed were estimated to be 36.7% of the total current residual. This is above SEPA's guidance threshold for the application of residual currents on hydrographic datasets with greater than 35% of the observed net transport residual. Subsequently, the application of "De-trended" hydrography was required in NewDepomod simulations. Simulations using a full, observed tidal sequence were also undertaken and are presented below for reference and an assessment of sensitivity.

Full-tide

The observed velocity profiles, from the final deployment, can be seen in Figure 3.1 with the average time series shown in Figure 3.2. The velocity profiles demonstrate little vertical shear throughout the water column with only a slight decrease in the 25th, 50th and 75th percentile velocities with depth. This trend in velocity is anticipated to follow a log profile according to the *Logarithmic* or *Power law* induced by friction at the seabed. Here, we see a secondary current between -25 m and -40 m depth, possibly associated with shoreline related currents (up/downwelling, topography jets, etc), hinting at some vertical stratification at the site. Below this signature, the velocity profile is governed by the power law close to the bed, displayed as a steep friction induced tail.

Figure 3.1: Sampled velocity profile for the final, 38-day Gometra deployment

The velocities in the three directional bins used in modelling can be seen in Table 3.1. There is limited difference in the mean velocity magnitude in the upper two bins selected. The bed speed is observed to be lower by 0.013 m/s. A fingerprint of a low to moderate energy storm is evident between timesteps 3,000 and 5,000 eliciting high surface velocities which have propagated to the bed. The observed data does show an evident spring/neap cycle in the velocities with periods of low velocities observed bi-weekly. These observed conditions are considered representative of the conditions observed at the site although the lack of extreme events means this dataset cannot be considered statistically representative. The stitched dataset is considered appropriate for application within the NewDepomod simulations and extrapolation to a representative 365 hydrographic regime.

Table 3.2 illustrates the directional frequency and magnitude of the observed conditions in each of the three depth "bins" used in the modelling. These roses illustrate a strong bi-modal flow corresponding

to the tidal phases and the shoreline orientation at the site. Westward flows are considered dominant, occurring the majority of the time. The directional roses show little directional shear in the water column, beyond a slight increase in northward vectors, yielding a north-eastward dominance in the bed flow regime. Eastward currents are seen to occur much less frequently, yielding the westerly flows highly dominant.

The peak bed-speed is in excess of 0.33 m/s and the dataset exceeds an inferred critical resuspension threshold of 0.085 m/s, 45% of the time. As a result, few sediments are consolidated within the bed model and sediments are readily re-suspended and dispersed throughout a wide area of the seabed.

De-trended Tide

A "De-trended" velocity profile was applied to derive the benthic impact of the Gometra farm, as per the Standard Default Method. The dataset was derived as per SEPA requirements: residual values for U and V (derived from harmonic reconstruction) were subtracted from the observed U and V vectors at the bed for each timestep. The observed current vectors in the remaining upper bins were unedited. Figure 3.3 shows the variation between the observed and De-trended vector sets in the near-bed bin, and the modification along the residual current vector.

It should be noted that this "De-trended" dataset retains the signature of significant events in the hydrographic dataset but shifts the distribution of U and V vectors to a different median value (maintaining distribution shape), modifying the velocity magnitude. It also differs from a traditional astronomic tidal condition. The velocity distribution and rose plot for the De-trended near-bed can be seen in **Figure 3.4**. These plots display the De-trended dataset has a greater frequency of velocities below 0.1 m/s with a low occurrence of bed speeds between 0.1 m/s and 0.2 m/s. The removal of the significant residual current (0.032 m/s) elicits a more symmetrical bed rose, increasing the occurrence and magnitude of south-south-eastward currents.

Figure 3.4: Velocity distribution plots for the bed from observed and De-trended datasets (left) and the Detrended bed rose, derived from the 90-day observed dataset (right).

3.2 Model bathymetry

Model bathymetry was available for the site at Gometra, generated from Admiralty chart data and an OS shoreline. Due to the ambiguity in the depths in the vicinity of the site, a uniform bathymetry was applied based on the recorded depth of the current meter data. This depth was -35.21 m, relative to chart datum. This was cross-checked against historic benthic sample depths and found to be an appropriate approximation for application in the modelling.

Figure 3.5: Available bathymetry in the vicinity of the site

3.3 SDM pen inputs

Standard feed rates were used as per the SEPA SDM. These rates were related directly to the consented biomass (1,500 T). For the SDM runs presented here, peak biomass feed rates were 7 kg t⁻¹ d⁻¹ for 365 days. Default feed and faeces rates were input corresponding to the consented biomass of the site. As per the SDM outlined by SEPA, feed rates associated with peak biomass were input for 365 days with a 3% wastage rate.

3.4 SDM NewDepomod configuration

All model parameters not specified within this document were specified according to SEPA SDM for both solid dispersal and in-feed treatments. It is intended that, when more appropriate benthic sampling is required, the modelling be updated and tuned to these simulations, increasing confidence in model outputs and quantifying predictive validity.

3.5 In-feed treatments

As this report is intended to facilitate an accurate description of the dispersal of feed and faeces, no simulations of any In-feed treatments were undertaken

SDM simulated impact

Model outputs for observed hydrographic dataset are presented below. This assessment is reviewed against criteria outlined by SEPA, based on a Mixing Zone (area encompassed from 100 m radius from pen edge), 151,640 m² and average depositional intensity within the Mixing Zone of less than 4,000 g/m²/yr. In addition, sensitivity tests are presented with the model forced by either the observed flowmetry or the Astronomic. It is intended that these assessments give a better understanding of the hydrographic regime and model function (respectively).

4.1 De-trended ride

4

The De-trended model output was identified as the appropriate hydrographic dataset to apply to the site at Gometra (due to the high percentage of residual currents at the bed). This dataset was used to simulate the licenced biomass (1,500 T). The modelling produced an average Mixing Zone area of 67.60% of the permissible area with an average depositional intensity within the Mixing Zone of 701 g/m²/yr, well below the 4,000 g/m²/yr threshold. The modelling of the site according to SEPA's Standard Default Method demonstrates the simulated biomass at the Gometra site is appropriate for consent under SEPA's Standard Default Method in NewDepomod.

Figure 4.1: De-trended tide simulation outputs.

The De-trended dataset produces a dispersal plume focused around the pens with dominant east/west dispersion. The persistence of low current speeds within the dataset, with moderate levels of resuspension, indicates there will be high levels of deposition under the pens. It is expected that these sediments are resuspended for short periods of time and re-deposited shortly after under, or close to, the cage group. The application of a uniform bathymetry here is likely to have a significant impact on the modelled destination of sediments. The steeply sloping shoreline is likely to cause increased

distribution downslope, depositing sediments northward. In lieu of calibration this Standard Default Method applied in NewDepomod is considered the best estimation of the impact of the proposed Gometra site on benthic Infaunal Quality Index.

4.2 Model sensitivity

The sensitivity of these modelling outputs to the hydrography applied was reviewed to determine the role of the application of the De-trended dataset in forcing the model. These sensitivity tests were undertaken using the observed tide (full tide) and a reconstructed astronomic series and are presented below.

Full-tide

The Full-tide model output simulating the licenced biomass (1,500 T) is seen to produce a peak deposition of 136.8 g/m²/yr. As this does not breach the 250 g/m²/yr Mixing Zone threshold, the simulated Mixing Zone area and depositional intensity are reported as zero. A visual representation of the dispersal of waste sediments can be seen in Figure 4.2. The modelling of the site using the observed hydrographic dataset demonstrates the site satisfies SEPA's risk assessment approach.

Figure 4.2: Full-tide simulation outputs.

The high percentage (45 %) of time when bed speed is in excess of a critical resuspension threshold of circa. 0.085 m/s results in high degrees of resuspension. The simulation shows a westerly drift of resuspended sediments. These sediments are dispersed throughout a wide area with a high proportion of sediments exported from the domain. The high current speeds of this dataset cause minimal consolidation within the simulation resulting in wide scale dispersal.

4.3 Validation of SDM runs

The observed benthic IQI scores of samples taken at the site on 26/02/2020, are displayed in Figure 4.3 and presents 30 grab samples along four transects in the vicinity of the site. As the westerly transect did not encapsulate the Mixing Zone, interpolation was necessary to define the 0.64 IQI crossing threshold via a polynomial regression producing an intercept at circa. 380 m along this transect. This resulted in a Mixing Zone area ranging from 89.1% or 81.4% of the permissible⁴, depending on the method of interpolation applied with 84% considered the observed Mixing Zone. This is considered conservative, with a linear regression producing an intercept of 225.4 m, highlighting the uncertainty in the definition of a precise Mixing Zone area in this context.

Figure 4.3: Benthic sampling IQI scores from 26/02/2020 with SDM Mixing Zone

De-trended tide

The model outputs derived from the De-trended simulations were used to inform the benthic sampling exercise undertaken in 2020 and are displayed in Figure 4.3. The simulated Mixing Zone does not hold relevance to the observed conditions along all transects, omitting the elevated level of impact observed along the westerly transect, and overpredicting the benthic impact along the northerly and easterly transect. The De-trended dataset omits the westerly dispersion of feed and faeces observed in the 2020 sampling exercise and in all preceding ITI samples at the site. Given that the sampling does not corroborate the impact predicted by the De-trended SDM simulations, this simulation was not considered appropriate for application in model calibration.

Astronomic tide

The astronomic harmonic constituents were also used to drive model simulations. This identified better representation of the westerly component of the simulation with high levels of deposition simulated

⁴ Benthic Solutions (2020) Summary Assessment of Ecological Quality Status and Mixing Zone Compared to the Depositional Zone Regulation (DZR).

below the northwest cage group. The application of this dataset in calibrated simulations is however not considered appropriate given the extensive stitching used, and so was excluded from latter stages of calibration.

Figure 4.4: Astronomic tide simulations

Observed tide simulations

The observed dataset is considered the most appropriate basis for model calibration as this represents the westerly transport observed in benthic samples. The SDM model setup however simulates excessive resuspension of particles, preventing consolidation in bed material beneath the pen array. As a result, the modelling does not produce a Mixing Zone. Model calibration using this dataset will therefore focus on decreasing sediment mobility in the resuspension phase, replicating the retention of particles within the bed.

Model Calibration

The model outputs elicited from the SDM method hold limited relevance to the observed conditions and the pattern of waste solid dispersal inferred. Therefore, model calibration is required to attain predictive validity from the modelling framework. However, as discussed in Section 2, at the time of writing no established methodology has been defined to calibrate NewDepomod simulations against benthic observations. This section illustrates the three-step model calibration framework outlined in Section 2.3, modifying the SDM, presented in Sections 3 and 4 to improve model relevance to observed conditions.

5

5.1 Model Setup

Model bathymetry

Model bathymetry remains unchanged from the SDM. Sensitivity tests were undertaken to determine the impact of sampled bathymetry on the modelled fate of particles, but this was found to be of limited relevance to observed conditions, with minimal deposition below the pens. This is attributed largely to the horizontal extrapolation of hydrographic data within the domain and ambiguity surrounding the interaction between variable bathymetry and resuspension processes. Therefore, a uniform bathymetry was applied, based on the depth of the current meter providing congruence with the SDM.

Model flowmetry

The observed flowmetry was stitched from three separate hydrographic deployments between 2017 and 2018. The full, observed tidal dataset was used as the basis for simulations as this holds the most relevance to the conditions observed at the site, as discussed in Section 4.3. It is acknowledged that the 90-day hydrographic dataset is not representative of the conditions of the 365 days simulated and the calibration performed is subsequently limited.

Model feed inputs

The modelling was based on the recorded feed administered in the 365 days preceding the sampling exercise on the 26/02/2020 as displayed in Figure 5.1. Standard feed wastage (3%) and feed to faeces conversion was applied to modelling and the resultant effluent mass was applied evenly between pens.

Model parameters

Only parameters specified in the subsequent Section 5.2 were modified through the calibration process. The remaining model parameters are based on default values specified in the SDM.

IQI to deposition conversion:

No direct conversion from simulated deposition to IQI exists and empirical research on this conversion within an aquaculture context is in its infancy. However, to perform a comparison of model behaviour with observed IQI, it was necessary to approximate the benthic deposition rate from the IQI scores. To define the existing relationship between simulated deposition and IQI, the SDM outputs for the site were reviewed. The simulated deposition for simulations using both Full Tide and De-trended datasets can be seen in Figure 5.2.

Figure 5.2: Standard Default Method Vs. 2020 observations

Figure 5.2 demonstrates the poor skill of the SDM model settings in accurately predicting the variability observed in 2020 benthic IQI scores, producing r^2 values of 0.133 and 0.046 for Full tide and De-trended simulations (respectively). These low r^2 values demonstrate the model describes little of the relationship between IQI and deposition and as a result, the SDM should not be used to define the depositional footprint at this site.

To facilitate model tuning an initial exponential conversion formula was defined based on the relationship between three IQI scores and simulated deposition, outlined in Table 5.1. This initial equation form and associated constants represent a coarse, non-empirical representation of the complex relationship between the two variables and provides a vital basis for the comparison between deposition and IQI, facilitating the initial step of calibration: Model Tuning.

IQI score	Deposition	Source	
	(g/m²/year)		
0.88	0.001	Highest IQI score	
0.64	250	Standard SEPA guidance	
0.18	2,298	Lowest IQI score & NDM max simulated deposition at sample point	

Table 5.1: IQI and inferred deposition rates

The accuracy or predictive validity of this conversion is not highly important as the purpose of Step 2: Model scaling (outlined in Section 2.3) is to review and revise this equation (both form and constants), following model tuning to better define the relationship between simulated deposition and IQI scores at this site specifically. Should an empirical relationship between IQI and deposition be defined or as the relationship becomes better understood, a revised relationship can be defined as the starting point for model tuning.

5.2 Modified parameters

As presented above, the model applying the observed hydrographic dataset does not represent observed behaviour and dispersion, therefore it was necessary to vary model function and the representation of select physical processes. These modified parameters can be divided into two groups:

- 1. Modify baseline model resuspension and adjust the representation of model physics to better represent inferred transport processes at the site.
- 2. Iterate select *Tuning parameters* to identify which model function replicates (as close as possible) the observed conditions. These model parameters were selected due to uncertainty surrounding default values and parameter transience.

The parameters selected and modified in the calibration exercise here are not considered prescriptive and additional model parameters (such as hydraulic roughness) should be considered in subsequent model calibration exercises. Although these modified parameters provide a good basis to increase intensity below the cage group, they are not suitable for calibration exercises where calibration exercises are required to decrease intensity. Therefore, each model calibration exercise should use a bespoke and ad-hoc approach, modifying the least number of parameters possible, within the limits of uncertainty where possible and, where this is not possible, within the limits of physics.

Baseline model function

Several parameters were modified to increase the retention of sediments in the bed layer to better replicate the high IQI scores beneath the pens. The sensitivity of the modelling to each of these parameters was reviewed and the model was identified as not highly sensitive to the variation of these values in isolation. It is expected that the variation in these parameters will exacerbate the influence of the calibration parameters τ_E and bed critical resuspension threshold, this is discussed later in the report.

Parameter	Sensitivity	Default	Applied	Rationale
		value	value	
Bed particle	Moderate	0.0016	0.0024	Reduce role of random process in
release per area				resuspension phase
Friction velocity	Moderate	Law of	Clauser	NewDepomod documentation default
regime		the Wall	Chart	(increase bed retention in this instance)
Bed particle release position	Moderate	Centre	Random	Better representation of turbulence processes to be integrated with the varying release height condition
Consolidation time – Feed	Low	0 days	2 days	Modify bed retention
Consolidation time – Faeces	Low	0 days	2 days	Modify bed retention

Table 5.2: Calibration parameters modified in calibration processes.

Tuning parameters

To better identify the appropriate simulation parameters to be applied, three additional parameters were varied between conditions as displayed in Table 5.3. These iterations resulted in a total of 36 calibration runs. To control for lagrangian particle diffusion, five replicate simulations were undertaken for each setup with values averaged at the same location from where historic samples were taken. In total, 180 formal model calibration runs were undertaken. The rationale presented for the selection of these parameters is briefly outlined below. However, it should be noted that additional, unreported variation of the three specified calibration parameters was performed along with the assessment of additional parameters. The calibration presented here is the best performing model setup identified from an assessment reviewing over 100 model setups.

Parameter	Default value	Condition 1	Condition 2	Condition 3
Bed model release height (m)	0.0	0.0	0.05	0.1
τ _ε -Critical minimum (m/s)	0.02	0.09	0.105	-
Dispersion coefficient – suspension &	0.1	0.1	0.085	0.075
resuspension, X & Y (m)				

Table 5.3: Model parameters iterated in model tuning process.

The bed model release height parameter, under the default value does not replicate physical processes correctly, duplicating the representation of bed model layering. When the release height is set to 0.00 m, the normal distribution of vertical diffusive process results in 50% of resuspended particles returning to the bed immediately, with circa. 50% of the sediments released into the water column. Thus, mitigating the impact of bed model layering, mitigating the role of resuspension, significantly reduces particles available for transport. The influence of the modification of this parameter is exacerbated by the variation in bed model release position (discussed above) and is expected to better simulate resuspension, allowing better representation of a mobile sediment layer directly above the seabed.

The τ_{E} -Critical minimum threshold applied for calibration deviates significantly from the default value of 0.02 m/s. This is considered appropriate given that the "Bed Cell" measurement is an average velocity from an observed bin between 2.5 and 3.5 m above the seabed. In addition, the Shields parameter (θ) at the bed for unconsolidated sediment is required to be greater than 0.55 for resuspension to occur, Figure 5.3, requiring a shear velocity (u_*) at the boundary layer in excess of 0.70 m/s for non-cohesive feed particles ($D_{50} > 0.009$ m) and 0.037 m/s for non-cohesive feces particle ($D_{50} > 0.005$ m). This value is higher if the sediments are considered cohesive. Given that the velocity profile follows a log shape, and the behavior of the feces is likely to be cohesive, these critical resuspension velocities are expected to be low estimates. Subsequently, the high values of τ_{ε} used in the calibrated model is considered appropriate. This is also corroborated by research undertaken by Van Rijn⁵ which found that for velocities below 0.1 m/s a minimal bed load transport (0.0013 kg/s/m) is observed in coastal transport regimes with wave influence. In addition, work undertaken recently has identified τ_{ε} values as high as 0.12 m/s in Scottish sites⁶.

⁵ Van Rijn, L., (2007). Unified View of Sediment Transport by Currents and Waves. I: Initiation of Motion, Bed Roughness, and Bed-Load Transport. *J. Hydraul. Eng.* 2007.133:649-667.

⁶ Adams, T. P., Black, K., Black, K., Carpenter, T., Hughes, A., Reinardy, H. C., & Weeks, R. J. (2020). Parameterising resuspension in aquaculture waste deposition modelling. *Aquaculture Environment Interactions*, *12*, 401-415.

Figure 5.3: Van Rijn (2020)⁷ θ* vs. D*. For ease, θ* can be translated as velocity. (top) and Van Rijn (2007)⁵; Observed bed load transport with average velocity (bottom)

The modification of the dispersion coefficient is a standard methodology for the calibration of particle tracking simulations. It is specifically relevant to the scales of diffusion and sub-cell scale variation in the model domain. Given that no variation in horizontal shear is represented within this framework, this was considered a key tuning parameter.

5.3 Model tuning

The two model setups displayed below were identified as the best iterations of the 180 tuning runs undertaken with Setup 12 generating the best r^2 score and Setup 25 generating the best *RMSE (Route Mean Squared Error*) score. Table 5.4 displays the parameters applied, while Figure 5.4 illustrates model performance against inferred deposition (from IQI). The magnitude of dispersion was significantly greater than that simulated by Setup 25. However, both significantly underestimate the inferred deposition, where inferred deposition is greater than 1,200 g/m²/year.

Table 5.4. Selected model tuning setups			
Parameter	Setup 12	Setup 25	
Bed model release height (m)	0.100 m	0.100 m	
τ _ε -Critical minimum (m/s)	0.105 m/s	0.090 m/s	
Dispersion coefficient – suspension & resuspension, X & Y (m)	0.100 m	0.085 m	

⁷ Van Rijn, L., (2020). Simple General Formulae for Sand Transport in Rivers, Estuaries and Coastal Waters. [Available online, Accessed 22/10/2020:

Figure 5.4: Inferred deposition and simulated deposition for best performing setup

As the final model iteration is anticipated to infer Mixing Zone area, IQI scores less than 0.3 are excluded from the analysis as uncertainties in the IQI to deposition conversion caused increased uncertainty in the simulations. In addition, this relationship between measured benthic habitats and intense farm deposition (>2,700 g/m²/year) is known to be non-linear in nature, highly complex and community specific. Subsequently, significant extraneous variables become dominant in this phase. Consequently, as these high scores are not considered appropriate for the identification of Mixing Zone area, it is not considered appropriate to describe benthic IQI solely by deposition and so these values were excluded from this analysis.

Table 5.5 displays the performance statistics of the two chosen model setups. These iterations were selected for superior $r^2 \& RMSE$ scores (setup 12 and setup 25) which are illustrated in Table 5.5. It is anticipated that the influence of this conversion method will be severely mitigated with the application of a bespoke IQI to deposition score in Step 2. Therefore, the true measure of performance will be evident following stage two of model calibration.

Ctatistic	Setup 12	Setup 25
Statistic	IQI > 0.3	IQI > 0.3
Bias (g)	901.8	698.6
RMSE (g/m ² /year)	1463.0	1,136
MAE (g/m²/year)	696.3	555.8
r ²	0.999789	0.989459

Table 5.5: Performance statistics of chosen model setups for IQI samples greater than 0.3

5.4 Model scaling

The relationship between the modelled deposition and the observed IQI was defined using several equation forms for the chosen model setups presented in Section 5.3. Run 25 was identified as having superior r^2 and *RMSE* values for each equation form and so this was selected to identify a bespoke conversion equation defining the relationship between simulated deposition and observed IQI from the

tuned model. The performance statistics of the best performing hybrid approach (using the chosen model setup, and the deposition: IQI conversion) for all locations are displayed in Table 5.6.

Equation fo	orm:	Cubic	Quadratic	Log	Exponent	Power	Linear
For IQI	Bias	-0.005	0.000	0.000	-0.020	-0.013	0.000
scores	r ²	0.723	0.689	0.688	0.679	0.615	0.610
less than	RMSE	0.120	0.127	0.128	0.132	0.150	0.143
0.3	MAE	0.087	0.095	0.097	0.101	0.113	0.119
Resultant	IQI =						
0.64		161	193	92	126	72	200
(g/m²/yed	nr)						

 Table 5.6: Derived conversion equation forms and error statistics for Deposition – IQI conversion using model

 setur 25

As outlined above, the Cubic, Quadratic, Exponent and Linear equations all produce r^2 values greater than 0.65, describing the relationship between the two variables well. Quadratic and Linear equation forms produce similarly low RMSE and MAE values. Through this measure, the Cubic equation has been identified as the most accurate equation, however, the quadratic equation was more accurate for IQI scores between 0.59 and 0.7, producing an *RMSE* value of 0.0605 and an r^2 value of 0.9058. This Quadratic equation was identified as the most appropriate equation. The performance of the tuned NewDepomod model against observations is illustrated in Figure 5.5 with the quadratic curve also displayed. The curve shows close replication of the simulated trend between modelled deposition and IQI. The final equation is available in Equation 1.

The Exponential equation format was found to have a superior RMSE between 0.59 and 0.7, however, the equation form was highly volatile in the vicinity of IQI scores of 0.64, with a deposition of 15 $g/m^2/year$ giving an IQI score of 0.65. given the random variability in NewDepomod model runs, this was considered too sensitive for meaningful application of the model and so the Exponential equation was not used.

Figure 5.5: Modelled deposition vs observed IQI scores

Equation 1:		$v = bx^2 + cx + d$	
Parameter	b	С	d
Constant	0.0000001611	-0.0005898563	0.7478982807

Subsequently, the proposed model setup with the best performing simulated deposition to IQI score results in an IQI = 0.64 equivalent deposition of 193 g/m²/year, the amended Mixing Zone threshold for calibrated simulations.

Model relevance

The modelling is primarily intended to assess compliance of existing sites, based on the area encompassed by the IQI = 0.64 contour. Therefore, the modelling is considered to accurately identify the impacted area based on the feed input, producing an RMSE IQI score of 0.02 for the seven observed IQI values between 0.59 and 0.7.

The modelling performed is, however, a significant simplification of the processes impacting benthic IQI scores with other processes, not represented within the modelling. Some uncertainties surrounding the simulations are outlined below:

- Hydrographic climate is not statistically representative and does not explicitly leave any representation of extreme events. This has an undefined relevance to annual conditions given the lack of statistical review.
- IQI is an ecological parameter and is highly dependent on the benthic community present beneath the site. Its variation is impacted by variation in salinity, temperature, nutrient availability and other factors not included in the modelling.

The impact of these simplifications is demonstrated in Figure 5.6 where the simulated to observed IQI scores are plotted along with the prevalence of Type I (false positive) and Type II (false negative) errors based on the IQI=0.64 threshold. Five samples are wrongly predicted with, two Type I errors and three Type II errors. Type II errors are of primary concern for the application of the modelling as they incorrectly predict compliance when it was not observed. These can be largely attributed to extraneous physical or ecological processes not represented in the model framework and are discussed in detail in a later section. The modelling does however successfully predict the scores lower than the 0.64 contour in 12 samples and the correct prediction of compliance in 13 samples. Based on these samples, used in the model calibration exercise, the final setup can be considered to have a 76.7% accuracy rate. However, for a more robust assessment of model accuracy, independent samples should be used when these become available.

Figure 5.6: Simulated IQI to Observed IQI Q-Q plot demonstrating error type

Calibrated simulations

The calibrated model described in Section 5 provides the basis for prediction, incorporating the quantified skill of the composite calibration method to identify future compliance based on farmed tonnage.

6.1 Default feed rates

⁶ To assess the ability of the model to predict contemporary compliance, standard feed rates (as defined by the SDM) were applied on the current consented biomass (1,500 T), applying a constant feed rate of 7 kg/t/day over the model period. The modelling was assessed based on the predicted Mixing Zone area (193 g/m²/year) and the average intensity. Results can be seen in Table 6.1.

Iteration	Mixing Zone	Average deposition
	(% permitted)	(g/m²/year)
1	81.61%	768.1
2	84.08%	736.1
3	85.32%	740.8
4	76.25%	838.1
5	80.37%	815.3
μ	81.53%	779.7

Table 6.1: Model output using default input parameters for consented biomass

The model outputs demonstrate good comparison with the conservative estimation of the observed Mixing Zone, accurately approximating the 84% Mixing Zone estimated from 2019 sampling⁴. Given the large number of confounding variables, not represented within the model framework, this model calibration is considered an accurate representation of farm deposition and the subsequent benthic environment, as assessed by IQI.

6.2 Scoping iterations

The calibrated model and the contemporary farm layout has been iterated to generate the maximum permissible Mixing Zone using standard feed rates. Modelling was iterated to the previous peak biomass at the site (2,000 T) with five simulations undertaken for each tonnage and results are presented in Figure 6.1. A linear trendline was fitted to the data and used to identify the peak farm biomass based on a Mixing Zone threshold of 100 %. The equations are displayed below and indicates a peak biomass of 1,944.9 T will satisfy Mixing Zone requirements while producing an average deposition of 1,472.6 $g/m^2/year$.

Figure 6.1: Scoping iterations for changes to biomass

Equation 2:		y = mx + c	
Parameter	m	C	r ²
Constant: Mixing Zone	0.0002572	0.4996671	0.975
Constant: Average deposition	1.5172457	-1478.3700952	0.990

Although the pen layout can be considered part of the model calibration, the calibration undertaken has focused on the physics surrounding the resuspension of bed material. Farm layout is considered completely independent from this calibration and the iteration of pen inputs has been simplified where possible. It is intended that this disconnect from farm layout and model geometry will facilitate the free variation of pen layout in future iterations of potential farm compliance.

6.3 Model limitations

Whilst the relevance of the modelling displayed to observed conditions has been established, the modelling remains a simplification of the physical processes at the site and approximation of the impact of farm deposition on benthic IQI.

- The modelling was undertaken with specific reference to the conditions in the 365 days preceding the sampling in 2020. It subsequently does not include representations of antecedent conditions at the bed, caused by previous farm operation at a higher biomass.
- Waste feed and faeces have been distributed evenly across the pen areas. Historically there has been variation in the amount of feed administered between the pen areas. This is likely to have influenced benthic impact, particularly at pen edge. As no clear pattern in pen feed rates exists, the even distribution of feed and faeces however is considered a more robust and conservative approach.
- The hydrographic forcing of the modelling is the best available and the application of observed conditions gives a relevance not possible through the application of simulated hydrographic

vectors. However, care must be taken as the 90-day hydrographic regime is not considered statistically robust and representative of the spatial and temporal variation at the site.

6.4 Model Conservatism

Due to the relative simplicity of NewDepomod model physics and the reality of interactions between farm waste and benthic IQI, conservative assumptions were employed where possible. Select assumptions are presented below and it is intended that this approach reduce the risk of non-compliance at the farm;

• The simulation using standard feed rates (7 kg/t/day) is highly conservative given that historic feed rates at the site are significantly lower, as displayed in Table 6.2. The average feed rate for the 365 days preceding peak biomass for the four periods assessed is 4.359 kg/t/day.

Period	Average feed rates (kg/T/day)			
15/01/2013 - 15/01/2014	3.052			
20/01/2015 – 20/01/2016	3.795			
22/02/2017 – 22/02/2018	5.990			
27/02/2019 – 27/02/2020	4.598			

Table 6.2: Historic feed to biomass rates

- The most accurate conversion equation between simulated deposition and IQI (linear form) was not selected for application in favour of an alternative equation which produces a lower Mixing Zone simulation threshold.
- The modelling assumes uniform dispersion of feed and faeces from each pen group. This is not a robust assumption as in the period between 2019 and 2020, the two pens on the west and the two pens on the east, receiving feed rates in excess of the mean. It is likely that this feed-rate, not replicated in modelling, will have influenced the IQI values collected at these transects. The model has been calibrated using low rates of waste and the associated IQI scores, therefore it is likely that the model will overestimate impact of feed administered at the edge pens in this case.

Bath treatment simulations

7

Bath treatments were previously undertaken using a 15-day dataset collected in August 2011. This dataset was used to force BathAuto v5 simulations to derive permissible bath treatment quantities. These quantities were licenced by SEPA and presented in Table 7.1:. The modern hydrographic dataset, outlined in Section 3.1 is over seven times longer than the dataset collected in 2011, collected with equipment of superior accuracy and processed using modern techniques. This longer dataset is therefore considered more accurate and more descriptive of the hydrographic regime at the site, superseding historic assessments using Bath Auto.

The parameters of the modern, 110-day hydrographic dataset were input into BathAuto and simulated. The parameters used are presented in Table 7.1. The modelling resulted in an uplift of over 200% for all licenced treatment quantities as displayed in Table 7.2.

Table 7.1. Dath treatment iterations (g)				
	Cypermethrin	Deltamethrin	Azamethiphos 3h	Azamethiphos 24h
Existing	70.65	26.5	-	318.3
Simulated	71.4	26.8	394.2	509.1

Table 7.1:Bath treatment iterations (g)

It is well established that the BathAuto simulation package is a conservative risk assessment method and is understood to produce quantities significantly less than modern hydrodynamic methods. The results presented in Table 7.1 represent the potential for the significant uplift of all bath treatment licenced quantities by over 200% based on this simulation method, applying a more comprehensive dataset. Whilst this demonstrates the extra capacity in bath treatment quantities beyond the current licenced quantities, it is not SSC's intention to review the licenced bath treatment quantities at this time.

Table 7.2: BathAuto – Key parameters

	Variable	Parameter
	Loch/Strait/Open water	Open Water
	Loch area (km ²)	-
	Loch length (km)	-
Waterbody characteristics	Distance to head (km)	-
	Distance to shore (km)	0.3
	Width of Strait	-
	Average water depth (m)	25
Pen & stocking info	Number of pens	16
	Pen shape	Round
	Diameter/Width (m)	31.8
	Working depth (m)	10

	Variable	Parameter
	Stocking density (kg/m ³)	18.1
	No. of pens possible to treat in three hours	1
Treatment info	Initial Treatment Depth (m)	4
	Treatment Depth Reduction Increment (m)	0.1
Hydrographic data	Mean current speed (m/s)	0.100
	Residual Parallel Component U (m/s)	0.056
	Residual Normal Component V (m/s)	0.014
	Tidal Amplitude Parallel Component U (m/s)	0.131
	Tidal Amplitude Normal Component V (m/s)	0.062

Conclusion

The release of organic matter (waste feed and faeces) has been simulated using 90-days of hydrographic data with relevance to observed benthic conditions using a bespoke, calibrated NewDepomod model setup. These simulations are aimed at updating simulations previously undertaken in AutoDepomod for use in an updated modelling framework. BathAuto simulations have also been updated, reviewing licenced quantities of bath treatments. Details of the model outputs have been presented and discussed within the document. Conclusions drawn from the simulations are outlined below.

8.1 Sediment dispersal

8

The SDM model simulations undertaken using NewDepomod and the current consented biomass at Gometra (1,500T) apply a modified hydrographic dataset which illustrates small scales of localised dispersal with the majority of sediments remaining within the domain. The De-trended simulations show a high percentage of deposited sediments remains on or close to the farm footprint with a moderate degree of dispersal around the farm. This modelling exercise outlines that the current biomass at the site satisfies both the Mixing Zone requirements, with 66.8% of the permissible area, and the depositional intensity with an average depositional intensity of 912.19 g/m²/yr within the Mixing Zone.

Calibrated simulations

The calibration methodology described in Sections 5 and 6 outline a modelling exercise that accurately predicts the observed benthic IQI score at the Gometra site. Whilst this modelling exercise contains uncertainty, this has been severely mitigated by the conservative application of 161% of the historic feed rate and other variables outlined in Section 6.4.

The calibrated NewDepomod model has been reviewed and applied to identify the peak "carrying capacity" of the farm using an iterative process of biomass variation. This "carrying capacity" (1,944.9 T) is considered a conservative estimation of the peak biomass at the site and is consistent with long term performance at the site (with an original peak biomass of 2,000T and a current peak biomass of 1,500T).

The methodology presented is considered a robust model calibration process, tuning the model to successfully predict benthic IQI scores and allowing approximation of benthic IQI sample scores and subsequent site pass/fail. The parameters selected for variation have been tailored to facilitate the accurate depiction of benthic impact following a methodology approved by SEPA and, where possible, integrating conservative parameters giving greater confidence in model output and proposed compliance. The calibration presented here is considered an appropriate consistent methodology for the accurate application of a NewDepomod model, based on the SDM and the resultant biomass of 1944.9 T considered an appropriate tonnage for licensing.

Table 8.1 outlines the model outputs for 1,944T using the Standard Default Method (SDM) and the calibrated method outlined in this report is presented below.

Table 8.1. Model Output							
1,944 T	SDM		Calibrated				
	Mixing zone (%)	Average intensity (g/m²/yr)	Mixing zone (%)	Average intensity (g/m²/yr)			
1	81.20%	1,468.50	94.39%	1,525.90			

Table 8.1: Model Output

2	82.02%	1,401.70	105.93%	1,346.30
3	84.49%	1,315.40	100.98%	1,431.20
4	84.08%	1,394.40	104.28%	1,369.00
5	83.26%	1,372.90	103.04%	1,358.80
μ	83.01%	1,390.58	101.72%	1,406.24

NB: In addition to the bespoke model setup for calibrated runs, the Mixing Zone area was assessed against the modified Mixing Zone contour.

8.2 In feed treatment

In feed treatment quantities were not reviewed in this exercise.

8.3 Bath treatments

The permissible quantities of bath treatment medicines have been reviewed using a more comprehensive hydrographic dataset, generated from 110 days of hydrographic data. The updated modelling outlines potential for a significant increase to bath treatment quantities when assessed using BathAuto. However, SSC do not wish to seek a review of the licenced bath treatments at this time.