Supplement 1

Model variables and parameters in XLDEPMOD are used as input data in linked MS Excel® worksheets to calculate daily temperature-dependent fish growth, particulate waste production, dispersion and particulate organic carbon (POC) total and net and sedimentation over a specified grow-out period. Equations are written as formatted in Excel worksheets.

Water temperature and fish growth

Growth (g wet weight d^{-1}) is determined by applying a thermal-unit growth coefficient (TGC) ($g^{1/3}$ deg C^{-1} d^{-1}) to an initial smolt weight to achieve a final harvest weight using predicted daily temperatures over the grow-out period (Jobling 2003, Strain & Hargrave 2005, Thorarensen & Farrell 2011). Surface layer (upper 1 to 5 m) water temperatures in 2014 and 2015 from three monitoring stations (22, 23, 24) in Passamaquoddy Bay near the mouth of Bliss Harbour (Robinson 2022) were used to determine surface layer annual maximum (T_{max}) and minimum (T_{min}) temperatures (°C) expressed as a sine wave function for each Julian Day (JD) in one year:

$$((T_{max}+T_{min})/2)-((T_{max}-T_{min})/2)*COS((2*3.14)*((JD-JD_{Tmin})/365)) \qquad (S1)$$

The adjusted TGC combined with cumulative degree days (T_{cum}) is used with initial smolt weight (W_i) to predict wet weight each day throughout the grow-out period (GP) (d) as:

$$((Wi)\text{^}0.333)+(TGC*T_{cum}*1))\text{^}3 \qquad (S2)$$

It is assumed that the stocking date (JDs) is May 1 (JD 120) with harvesting in the summer approximately two years later, typical dates for the industry in SWNB (Chang et al. 2014). In the present study, a TGC coefficient of 0.002368 $g^{1/3}$ deg C^{-1} d^{-1} yielded a harvest weight of 4.90 kg wet weight $fish^{-1}$ after 791 d. JD_s, T_{max}, T_{min} and JD_{Tmin} can be selected for conditions in a specific study area.

Total particulate waste production and sedimentation

Calculated values for temperature-determined daily growth are combined with mass balance coefficients for respiration, fecal production and waste feed to determine feed input required to reach harvest weight over the grow-out period expressed as g POC $fish^{-1}$ d^{-1} based on median values for coefficients from previous studies at Atlantic salmon farms in Canada and Norway (Strain & Hargrave 2005, Wang et al. 2012, 2013). Recent modelling studies have applied values for total fecal matter production (17 to 20% of feed supply) for calculating salmon waste production (Cubillo et al. 2016, Carvajalino-Fernández 2020) similar to those we have assumed. Waste feed loss (1-5% of input) corresponds to values used in DEPOMOD (Cromey & Black 2005). Adoption of automatic feeding technologies for open net-pen salmon aquaculture has reduced loss of waste feed over the past two decades and values <5% have been calculated (Ballester-Moltó et al. 2017a). The amount of waste feed is usually based on industry-reported estimates but higher values (8 to 15%) have been reported and used in mass balance models (Stucchi et al. 2005, Strain & Hargrave 2005). Since model output in our study is compared to results using DEPOMOD we assume that 3% of POC input is lost as waste feed (Table 1), a typical value reported for Atlantic salmon farms in New Brunswick (Stewart 2005) and assumed by Chang et al. (2014). The value can be altered to evaluate the effect on waste output, dispersion and sedimentation.

Biomass on the farm is the initial stocking number corrected for the fraction lost due to mortality (f_{mort}) assumed to be distributed evenly throughout the grow-out period. A mass mortality event can be considered by reducing the number of fish at the time in the growth cycle when it occurs. The total weight of fish on the farm each day is calculated as the number of fish x the daily predicted wet weight fish^{-1}. Since the spreadsheet template is adjusted to run for 791 days a 0 value is added to Eq. S1 for growth and NA for all other mass balance terms if the number of days in the model extends beyond the grow-out period. Fractions of wet weight and POC in feed and fish are used to express feed retained as growth, respired and released as feces and waste feed as g POC fish^{-1} d^{-1}. The economic food conversion ratio (FCR) is the ratio of total wet weight of feed used over the grow-out period to reach harvested wet weight (g fish^{-1}).

The statistical model in Stucchi et al. (2005) is used to calculate transport distances for deposition of different types of waste particles. It was assumed in that study that the largest mass fraction of feces (0.7) had a settling velocity of 3 cm s^{-1} with smaller fractions (0.15) at 2 and 4 cm s^{-1} representing a normal distribution (mean ± σ) of 3.2 ± 1.1 cm s^{-1} from observations in Cromey et al. (2002a). Bannister et al. (2016) observed that approximately 85% of fecal material released by three size classes of salmon held under *in situ* conditions settled with rates between 5 and 10 cm s^{-1} with lower amounts between 1 and 5 (6%) and <1 cm s^{-1} (9%). We apply the results from Bannister et al. (2016) as summarized in Carvajalino-Fernández (2020) to assume mass fractions of 0.66 for large fecal pellets (range of w of 5 to 10 cm s^{-1}. mean = 7.5 cm s^{-1}), 0.25 for small fecal pellets (range of w of 1 to 5 cm s^{-1}, mean = 3.0 cm s^{-1}) and the remaining fraction (0.09) as flocculated fine fecal matter with w = 0.5 cm s^{-1} corresponding to the minimum velocity category (w <1 cm s^{-1}) for fragmented feces. Total POC waste discharge from the farm (kg POC farm^{-1} d^{-1}) is the daily total amount released fish^{-1} x the number of fish corrected for mortality. Maximum (worst-case) and average discharge for the grow-out period are calculated from the daily rates of waste release, but the total for any specified time interval during the grow-out period can also be determined.

Waste dispersion

Horizontal displacement distances (m) are calculated for all waste types categorized by their mass fraction and settling rates to reach the bottom for the depth-averaged velocity field (Stucchi et al. 2005). The dispersion from the center of a single net-pen is described by two probability density functions as normal (Gaussian) distributions. If bottom depth is assumed to be uniform and all waste particles exit the bottom of a cage, transport distances (m) for deposition in x and y directions are determined by the vertical fall distance (the difference between mean tide LW (Z_m) and net-pen side wall depth (NP_Z)), under-pen depth (m), particle settling velocity (w_{pt}) (cm s^{-1}) and standard deviations (σ) for currents in the E-W (u) and N-S (v) directions as:

$$x = ((Z_m - NP_Z)/(w_{pt}/100))*\sigma_u/100 \tag{S3}$$

and

$$y = ((Z_m - NP_Z)/(w_{pt}/100))*\sigma_v/100 \tag{S4}$$

Unlike DEPOMOD that requires known values for feed input to separate cages, we assume that salmon biomass is equally distributed among all net-pens to determine deposition at x, y distances (m) from the center (0, 0) cage position of the two distributions. The mean (μ) and standard deviation (σ) for currents in u (EW) and v (NS) directions where b_1 (μ_u cm s^{-1}) and

$c_1(\sigma_u)$ and b_2 (μ_v cm s^{-1}) and c_2 (σ_v) determine the amount of each waste type deposited (g POC m^{-2} d^{-1}) at x, y distances from a single cage as:

$$a*(1/(c_1*SQRT(2*PI())))*EXP(-0.5*((x-b_1)/c_1)^{\wedge}2)*(1/(c_2*SQRT(2*PI()))) *EXP(-0.5*((y-b_2)/c_2)^{\wedge}2) \quad (S5)$$

Maximum sedimentation (g POC d^{-1}) for each waste type (a) based on the combined Gaussian functions occurs at the center (0, 0) position of a single net-pen. To convert the point source to an integrated value for the net-pen bottom area the sum of g POC d^{-1} flux for all waste types in each cell within the bottom area of the net-pen is divided by the number of cells equivalent to the net-pen area. This would be the deposition rate if a net-pen was resting on the bottom. As depth increases horizontal transport results in higher deposition rates outside of the area directly under the cage and the maximum rate at the center of a net-pen decreases. The advective component that displaces a depositional footprint in the direction of the mean current represented by the mean currents (μ_{EW} and μ_{NS}) was not considered by Stucchi et al. (2005) since residual flow at the farm site where the statistical model was applied was small relative to the standard deviations of directional currents. Since our model is intended for general application we have included μ_u and μ_v in the dispersion calculation (parameters b_1 and c_1) (S5).

Post-depositional loss and net waste sedimentation

Net waste sedimentation is calculated from predicted values of total waste deposition for each waste type by applying fractional losses to account for removal of total waste released from net-pens by reuspension, decomposition and consumption by wild populations of fish and invertebrates. The default parameterization in the original DEPOMOD model assumed that resuspension of deposited waste only occurs when currents exceed 9.5 cm s^{-1} and resuspended material is re-deposited if currents fall below this threshold (Cromey et al. 2002b, Cromey & Black 2005). This can be varied indirectly by altering the critical erosion stress and other bed model parameters as in NewDEPOMOD (SAMS 2019), but using the fixed value has been found to result in predicted sedimentation rates that are low relative to observations (Cromey & Black 2005, Stucchi et al. 2005, Sutherland et al. 2006, Chamberlain & Stucchi 2007, Chang et al. 2014, Keeley 2013). Thresholds for waste feed and fecal pellet resuspension have also been shown to change with sediment type (Sutherland et al. 2006, Black et al. 2016, Law et al. 2016). Bottom substrates (B_{sub}) in our study are qualitatively classified as (1) mud/sand (>50% mud), (2) sand/mud (>50% sand) or (3) gravel allowing application of substrate-specific erosional thresholds (vr_{sub}) for these categories. Since surface sediments in Bliss Harbour are predominantly mud (>70% <63 μm) (Wu et al. 2014), a substrate category of 1 is applied.

Data in Sutherland et al. (2006) and Law et al. (2016) are used to select current velocities above which feed and large fecal pellets begin to roll or saltate on mud, sand and gravel (15, 22.5 and 35 cm s^{-1}, respectively). The critical erosion threshold used in DEPOMOD (9.5 cm s^{-1}) is applied for fecal pellets irrespective of substrate type. A lower threshold of 5 cm s^{-1} (approximately 0.01 Pa) was observed to resuspend flocculent material on surface sediments near salmon cages in SWNB (Law et al. 2016) and we apply this threshold for disaggregated (non-fecal pellet) waste particles on all substrate types. Production for each waste type is reduced by this fraction to yield a value for net sedimentation. Once particles are resuspended it is assumed that they are advected and deposited outside of the modelled area.

Additional losses to total waste produced are due to solubilisation (leaching) and decomposition. Strain & Hargrave (2005) and Wang et al. (2012, 2013) calculated or assumed that 50% of feed and feces would be lost relatively quickly (within 5 days) after settling by these processes. Stewart & Grant (2002) observed that feed particles degraded in <5 d depending on pellet size and water flow speed. The disaggregated nature, lower density and slower settling rate of flocculated fecal matter may make this waste type more labile and rapidly decomposed than intact fecal or waste feed pellets. We did not apply differential loss rates and total release of all four waste types was corrected by a single factor ($f_{decomp} = 0.1\ d^{-1}$) to account for losses due to solubilisation and decomposition.

Populations of wild fish and invertebrates aggregated around finfish cages can consume waste feed as it exits net-pen side walls (Dempster et al. 2002, Callier et al. 2017, Uglem et al. 2014, Ballester-Moltó et al. 2017b) or after being deposited (White et al. 2017a, b). Almost all (>90%) feed pellets were consumed shortly after reaching the bottom around finfish farms in the Macronesian archipelago in the NE Atlantic Ocean (Riera et al. 2017) while a smaller proportion (~17%) was estimated to be consumed as it exited cage side walls by open-pen cultured seabream (Ballester-Moltó et al. 2017b). Consumption of waste feed by wild populations of fish and invertebrates has been observed at many salmon aquaculture sites but the magnitude for any given farm is unknown. We reduced waste feed deposition rates (f_{cons}) by a constant rate ($0.5\ d^{-1}$) to account for this loss assuming that equal fractions are consumed from net-pen side-walls and by bottom feeding fish and invertebrates.

Waste deposition matrices

Calculations using Eq. S5 for each waste type are summed in four separate worksheets in cells in two 2-dimensional x-y matrices for a single net-pen and a multi-cage array to describe total and net sedimentation as maximum (worst-case) and average values (kg farm^{-1} d^{-1}) for the grow-out period. We assume that net-pens are circular, the most common design for salmon farms in SWNB. The maximum distance from the net-pen center to the model boundary (D) (m) is used to create a square matrix (200 x 200 cells) around the center (0, 0) x, y position in each matrix. Since the number of cells in the model is fixed, D determines cell dimensions. The value in Input Data is adjusted to ensure that the total waste released is accounted for by deposition within the model boundary (discussed below).

Net-pen diameter and spacing between cages and rows are used to locate the center point of each cage in a cell in the x, y array system of the multi-pen matrix. Since we assume that salmon biomass is equally distributed among all net-pens, calculations for a single net-pen are scaled to the multi-pen array using cage number (NP_n) and diameter (m) (NP_d), number along one row of the length of the array (NP_{nl}), across the array width (NP_{nw}) and distances (m) between adjacent net-pens along (NP_{dl}) and across (NP_{dw}) rows. The model allows up to 24 net-pens (a maximum for most farms in SWNB) arranged in any number of rows up to this number. If "Y" is indicated for customized cage positioning in Input Data, the x position (D_x) (m) for that numbered net-pen is D_x. If customized position are not used ("N") the x position is determined by:

$$\mathrm{IF}(NP_n=\text{"Y"},D_x,\mathrm{IF}(NP_{nw}=1,1*(NP_{nl}/2),\mathrm{IF}(NP_{nw}=2,1*(NP_{nl}/2),\mathrm{IF}(NP_{nw}=3,1*(NP_{nl}/2),\mathrm{IF}(NP_{nw}=4,1*(NP_{nl}/2),\text{"NA"}))))+\mathrm{IF}(\mathrm{MOD}(NP_{nl},2)=0,0,-NP_{dl}/2)) \qquad \text{(S6)}$$

and the non-customized *y* position is:

=IF(NP_n=”Y”,NP_{nw},IF(NP_{nw}=1,0,IF(NP_{dw}=2,-1*(NP_{nw}/2),IF(NP_{nw}=3,0,IF(NP_{nw}=4,-1 *(NP_{dw}/2),”NA”))))) (S7)

Rows of cages can be oriented relative to the direction of the major current by the angle (NP_a) (0 to 180°) in Input Data to indicate rotation of the long axis of the array relative to north (0 perpendicular, 90 parallel). The spacing remains as specified by distances (m) along (NP_{nl}) and across (NP_{da}) the array and changes in orientation do not affect waste deposition matrix values for a single net-pen. The values for cells in the singe cage matrix appear in the multi-pen array matrix in adjusted positions reflecting the angle of rotation. Individual net-pen center positions using D_x and D_y from the x-y array system are expressed as rotated $D_{x'}$ and $D_{y'}$ distances (m) from the matrix center (0, 0) in E-W (x) and N-S (y) directions as:

=IF(NP_n=”Y”,ROUND(D_x*COS(N_a*PI()/180)-D_y*SIN(D_x*PI()/180),2),10000) (S8)

An input of “N” rather than “Y” indicates that no cage is present and the formula returns a distance (10000) outside the maximum matrix boundary in the E-W direction. Similarly, the rotated E-W (x) position is:

=IF(NP_n=”Y”,ROUND(D_y*COS(NP_a*PI()/180)+D_x*SIN(NP_a*PI()/180),2),10000) (S9)

A final step to calculate cage center positions within the rotated array is to convert x and y distances (m) relative to the centre (0, 0) position in the cell matrix. As explained below contouring for ranges of waste deposition within the two-dimensional matrix requires that positions be expressed in numbers of cells. The offset value (number of whole cells) in the x direction (D_{xcn}) and y direction (D_{ycn}) for each net-pen is:

=ROUND(+$D_{x'}$/(D*2/100),0) (S10)

=ROUND($Dy_{'}$/(D*2/100),0) (S11)

Each cell in the multi-cage depositional matrix for total and net waste sedimentation first establishes if a cage exists (“Y”) at that x, y position in the single cage matrix. 0 is posted if no cage is present (“N”). If a net-pen is present then summed INDIRECT statements are used to address cells in rows and columns in the single cage matrix adjusted for cell offsets to sum values in rows (cell) and columns (cell) in the array matrix to the maximum number of 24 cage positions:

=(IF(NP_n=”Y”,INDIRECT(ADDRESS(ROW(cell)+D_{ycn}, COLUMN(cell)-D_{xcn})),0)) + IF(NP_{n+1}=”Y”,INDIRECT(ADDRESS(ROW+1(cell)+D_{ycn}, COLUMN+1(cell)-D_{xcn})),0)) +IF(NP_{n+23}=”Y”,INDIRECT(ADDRESS(ROW+23(cell)+D_{ycn}, COLUMN+23(cell)-D_{xcn})),0))+CS_{ref} (S12)

If background sedimentation (POC m^{-2} d^{-1}) is known the value in Input Data ($CS_{ref,}$) is added to the sum of all waste type deposited in each cell of the multi-cage array matrix in S12.

Multi-pen array deposition contours

Results illustrating the spatial distribution of waste sedimentation in each multi-cage deposition matrix are displayed in coloured contour plots for grow-out period maximum total and net sedimentation and grow-out period average total sedimentation. It is possible to illustrate contours for a specific date by manually selecting depositional data for that one day. Conditional formatting is used to show spatial patterns of sedimentation within the selected model boundary area. The x-y scale of E-W and N-S axes in each square plot is determined by distance D (m) from the 0, 0 position assigned in Input Data. A standard colour scheme is used to show white in cells <0.3 g POC m^{-2} d^{-1}, the assumed background sedimentation in Bliss Harbour (Hargrave 1994), with blue, dark or light green, yellow, orange and red for six ranges of sedimentation (0.3-1, 1-2, 2-5, 5-7.5, 7.5-10, >10 g POC m^{-2} d^{-1}). The intervals can be altered but the range represents gradients in POC waste sedimentation in previous studies associated with marked changes in sediment geochemical and benthic macrofauna community variables (Holmer et al. 2005, Chamberlain & Stucchi 2007, Hargrave 2010, Chang et al. 2014, Keeley et al. 2013).

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Supplement 2

A model output summary from XLDEPMOD for data in Figs. 5 A, B and Table 3 for maximum and average total waste release and total and net sedimentation from Atlantic salmon at Farm A in Bliss Harbour, Bay of Fundy (Fig. 1) using input data from Table 1.

Economical food conversion ratio (FCR)	1.09

	Maximum	*Average discharge*
Total particulate waste released (g POC fish^{-1} d^{-1})	2.07	0.69
Total sedimentation (kg POC farm^{-1} d^{-1})	588.0	211.4
Net sedimentation (kg POC farm^{-1} d^{-1})	416.6	149.8

Waste Assimilation Coefficient (AC) (ratio of net to total sedimentation)	0.708
Maximum distance from net-pen array center (model boundary) (m)	300
Fraction of waste discharged accounted for by deposition in the model area	1.00

Mean sedimentation integrated over the net-pen bottom area	*Maximum*		*Average*	
	Total	Net	Total	Net
g POC m^{-2} d^{-1}	45.0	30.9	16.2	11.1

Ranges of waste sedimentation g POC m^{-2} d^{-1}	*Contour interval areas (ha)*			
0.3-1	0.73	0.71	0.86	0.86
1-2	0.49	0.48	0.68	0.59
2-5	0.70	0.82	0.83	0.89
5-7.5	0.36	0.31	0.36	0.36
7.5-10	0.28	0.35	0.22	0.29
>10	1.61	1.26	0.65	0.36
	Total contour areas (ha)			
>0.3	4.18	3.93	3.59	3.34
>1	3.44	3.23	2.73	2.48
>2	2.95	2.74	2.05	1.89
>5	2.25	1.92	1.22	1.01
>10	1.61	1.26	0.68	0.36