G Models for assessing the use of medicines in bath treatments

Contents

Tables and Figures

G.1 Introduction

Typically, the topical chemical solutions that are used in marine cage fish-farms to treat infestations of parasitic sea-lice are rapidly broken down or bind to particles in the water, making them unavailable to marine life. Therefore, the tools used to assess their potential impact only need to be able to simulate short periods of time.

The dispersive processes that are found around fish-farms are typically complex. To describe and quantify them to simulate the dispersion of treatment chemicals with precision would entail onerous site-specific survey work and numerical modelling. SEPA considers such a strategy to be overly complex for the site-specific assessment of the relatively short-lived aqueous discharges from fish farms.

SEPA has developed the mixing zone approach, as is applied to other marine discharges, for application to solute releases from fish farm sites to enable a rapid assessment of the likely concentrations of chemical residues in the short-term. SEPA has developed a simple model, in which dilution of discharged chemicals is governed by the mean current speed and a dispersion coefficient. The model predicts environmental concentrations that can be compared with quality standards to determine the quantity of medicine that can be licensed for a particular site. This document presents this short-term assessment tool and describes its application.

For some medicines, due to their relative longevity and the use of multiple treatments, a second model is required that simulates the more complex dispersion processes that occur over the longer-term. The results from this assessment are compared with a different standard to determine the quantity of chemical that can be used. This document presents a model that is considered suitable for assessing the fate of chemicals that remain at potentially toxic concentrations in the water column for periods greater than a single tidal cycle.

The two modelling tools share many of the same site configuration and descriptive environmental parameters; indeed, the longer-term model uses the outcome of the short-term model to determine its initial configuration. Accordingly, SEPA has produced a common spreadsheet-based model configuration and automated iteration tool that incorporates the short-term model with a record of the results from the longer-term model. This tool and its application are described in section G.5.

G.2 Environmental Quality Standards

The Environmental Quality Standards (EQS) applied by SEPA to bath treatment chemicals have been determined in response to the toxicity and nature of the compounds. The derivation of these standards is reported elsewhere, but summarised below.

G.2.1 Azamethiphos

Azamethiphos remains in the aqueous phase until it is broken down into non-toxic derivatives, for which a decay half-life of 8.9 days has been determined. As a result, two standards are applied, one at 3 hours after any discharge and the other 3 days after the final discharge in any treatment period, after which periods the quantity of chemical is predicted to have reduced by 1% and 21% respectively. Consequently, decay is not included in the short-term modelling but is in the longer-term.

Table G-1 Standards for azamethiphos

Timescale	Standard	Type
3 hours	250 ng l^{-1}	EQS
72 hours	40 ng l^{-1}	EQS
72 hours	100 ng l^{-1}	MAC

SEPA applies the 72-hour EQS outwith an allowable zone of effect (AZE), in common with the ‘mixing zone’ concept applied to other point-source marine discharges, which for azamethiphos is defined as the lower of: 0.5km^2, or 2% of loch area. Areas for the majority of lochs and voes have been systematically defined in the Sea Loch Catalogue (Edwards and Sharples 1986), failing which, a suitable area for a similarly constrained receiving water should be determined and justified.

The EQS may be exceeded within the AZE, subject to the condition that the peak concentration does not exceed the maximum allowable concentration (MAC).

G.2.2 Cypermethrin

Cypermethrin readily binds to particles and is hence rapidly removed from the aqueous phase under the biologically active conditions prevalent in Scotland's coastal waters. Thereafter it is incorporated into the sea-bed sediment where it is considered to be of insignificant risk to the environment. Consequently, an EQS is applied 6 hours after discharge, setting a maximum concentration whilst in the aqueous phase.

Table G-2 Standard for cypermethrin

Timescale	Standard	Type
6 hours	16 ng l^{-1}	EQS

G.2.3 Deltamethrin

Deltamethrin behaves in a manner analogous to Cypermethrin; consequently, its impact is assessed in the same manner.

Table G-3 Standard for deltamethrin

Timescale	Standard	Type
6 hours	6 ng l^{-1}	EQS

G.3 Short term model

SEPA has developed a simple model, the results from which are primarily governed by the mean current speed at the site and the distance of the farm site from the shore. The model applies the assumptions that the chemical patch is transported longitudinally at the mean current speed, whilst spreading laterally at a rate determined by a dispersion coefficient. The area of the chemical patch is thus a function of the time since release. The volume of the patch is calculated by multiplying the area by an assumed constant depth. Therefore, the mean concentration within the patch at the end of the evaluation period can be calculated by dividing the initial mass released by this volume. Details of the calculations employed are attached at Appendix A.

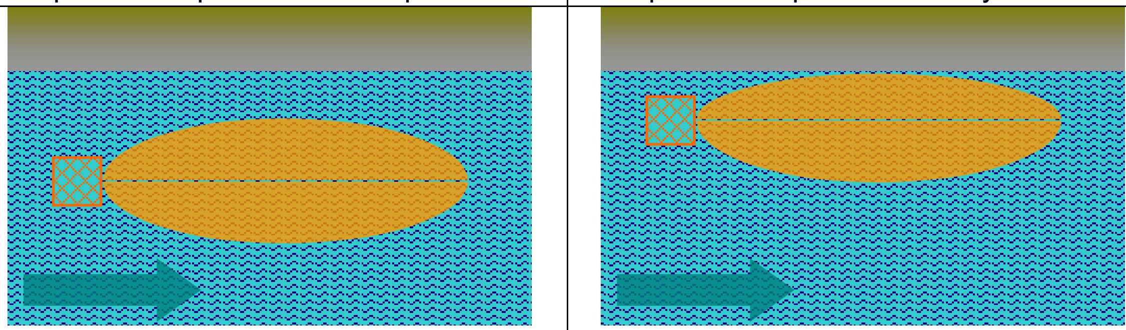
There are several simplifying assumptions in the modelling approach that must be highlighted:

- The model assumes material is transported by a unidirectional mean current speed. This is a gross simplification at most locations. The model is not valid for periods extending beyond a single flood or ebb, i.e. it should only be used for periods no longer than 6 hours.
- The model includes dispersion in the lateral direction; dispersion is assumed to be negligible relative to advection in the longitudinal direction.
- Lateral dispersion is assumed to be proportional to the square root of the time elapsed since discharge.
- Calculation of mean concentration within the patch assumes homogenous concentration, whereas the derivation of patch width assumes that the actual concentrations within the patch are normally distributed. With increasing time, the variation in patch size will depart from proportionality and the concentrations will similarly depart from a normal distribution. Consequently, the model becomes less valid over time.
- The model assumes mixing to a depth of up to the lesser of 10m, or half the average depth, to account for the effects of vertical and lateral current shear and turbulence.

- During the simulation, if the patch impinges on the shore boundary due to lateral dispersion (see Figure G-1:A), one half of the patch ellipse is reduced to the distance to the shore (see Figure G-1:B).

Figure G-1 Comparison of ellipse areas with and without shore limitation

A: expansion of patch due to dispersion | B: expansion of patch limited by shore



KEY: land: sea: current: cage group: patch:

G.3.1 Data requirements

The model requires little in the way of input data although other site-specific information may assist in interpretation of the results. The key data requiring specification are as follows:

- Mean current speed: the longitudinal dimension of the mixing zone is a function of mean current speed and time. The mean current speed is calculated from measurements of current velocity at the site made in accordance with SEPA guidelines. Detailed specification for the collection of this data is given in Attachment VIII.
- Cage volume during treatment, i.e. cage area and shallowing depth, is required to assess the number of cages that may be treated in any 3 hour period.
- Distance to shore: this is required so that the model can simulate restriction of the spread of the patch by the shore.
- Available depth of water: the mixing depth is assumed to extend to the lesser of 10m or half the depth of the receiving water - see notes under BathAuto, G.5.1.3 .

G.3.2 Example assessment of cypermethrin against the 6 hour EQS

Cypermethrin standards derived from toxicity assessments of this chemical are given in Table G-2. These are applied at 6 hours after the release of the chemical from the treated cage(s).

Table G-1 illustrates examples of the short-term model being applied. In this instance, the cages are assumed to be 25 m square cages, shallowed to a depth of 3 m and treated with a concentration of 5000 ngl^{-1} of cypermethrin. The various current and distance to shore scenarios are evaluated against the 6hr EQS of 16 ngl^{-1}.

From these results it can be seen that under more dispersive conditions, e.g. with a mean current speed of 0.1 ms^{-1}, a greater quantity of Cypermethrin may be used. For sites with intermediate dispersion, e.g. mean current speed 0.05 ms^{-1}, the results are likely to depend on local factors, e.g. cage size, proximity to the shore, and are very sensitive to the input parameters. These observations regarding the response of the model to its control parameters, and the resultant implications for the licensed discharge quantities of chemicals, apply equally to Azamethiphos.

Table G-4 Short term model result for cypermethrin treatment

Current velocity [ms^{-1}]	Distance to shore [m]	Patch length [m]	Patch width [m]	Concentration after a single treatment [ngl^{-1}]	Number of treatments	Mass permitted in any 3 hour period [kg]
0.15	200	3240	262	1.4	11.4	0.107
0.15	50	3240	181	1.6	9.9	0.093
0.1	200	2160	262	2.1	7.6	0.071
0.1	50	2160	181	2.4	6.6	0.062
0.05	200	1080	262	4.2	3.8	0.036
0.05	50	1080	181	4.8	3.3	0.031
0.03	200	648	262	7.0	2.3	0.021
0.03	50	648	181	8.1	2.0	0.019

Note: these values are indicative of the EQS-compliant discharge quantities that a 25m wide square cage, 3m deep would achieve under the specified current speed and distance to shore circumstances.

G.4 Longer term (MLA) dispersion model

G.4.1 Description

Modellers at the Fisheries Research Services' Marine Laboratory, Aberdeen (MLA), have developed a dispersion model that estimates the impact of fish farm treatment chemicals resulting from multiple releases made during a treatment episode (Gillibrand & Turrell, 1999).

The model simulates the dispersing plumes from each discrete bath treatment of a number of cages, and predicts the path and concentration of these plumes throughout the period under assessment, during which time concentration reduces according to a specified decay rate. Within the confines of the model domain, each patch is advected by both tidal and residual currents, and horizontally dispersed at a rate parameterised by a dispersion coefficient. Vertical mixing is restricted to a specified depth.

The model determines the peak concentration at each time step, and calculates the total area wherein a specified concentration is exceeded.

The model continues its calculations until a specified time after the last treatment. The model produces time-series files of peak concentration and total area exceeding the specified concentration. It outputs the final values of these parameters to a display window.

In its simplest form, the model domain is a rectangle with length determined from the tidal amplitude, the period of assessment, and the residual current, such that advection due to residual and tidal current flow will not carry any patch of discharged chemical beyond the modelled area. The width of the model domain is explicitly specified by the user, except in the case of 'open water' sites, where the model applies a default width of 5km.

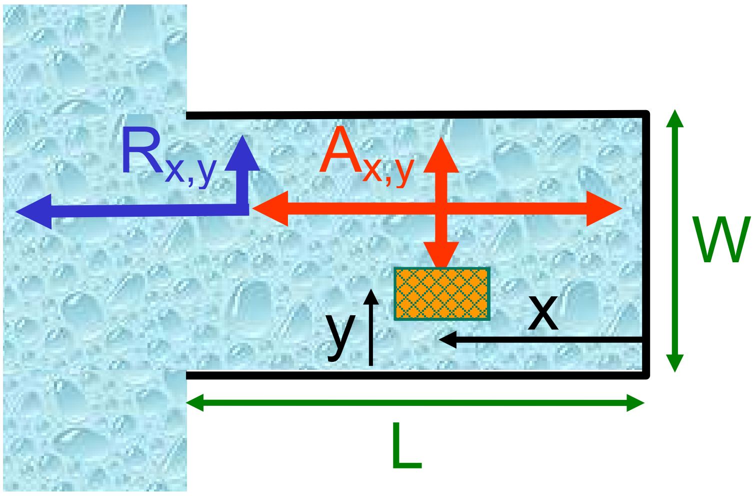
The modelled area may be defined as having one, two, or three, closed boundaries, from which patches are reflected, that correspond to three topographic categories:

- open or coastal waters;
- a strait;
- a sea loch or voe.

For a sea loch, or voe, the area and length of the inlet is specified and the resulting rectangle is bounded by three coastal 'closed' boundaries and one 'open' boundary. Whilst in this inlet, the patches are reflected from these boundaries as they expand and as they are transported by the oscillating tidal current and the unidirectional residual current. Once beyond the confines of the inlet, no restriction is placed upon the patches' movement or growth. A schematic diagrams of the model domains are shown in Figure G-2.

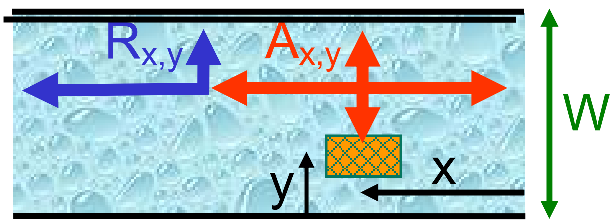
Figure G-2 Schematic diagrams of MLA model domains

a loch

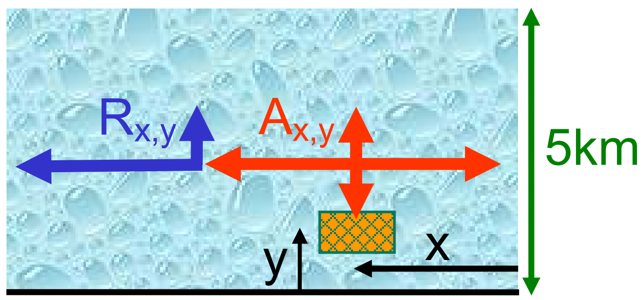


KEY:		Cage group				Closed model boundary	
	L :	Length of loch	**x** :	Distance from cage group to head of loch	**$A_{x,y}$** :	Amplitude of tidal current speed	
	W :	Width of constrained receiving water	**y** :	Distance from cage group to shore	**$R_{x,y}$** :	Residual current speed	

a strait



an open water site



A strait has two opposing closed boundaries for which separation, or width of the strait, is defined; the remaining two boundaries remain open.

At an open water site, only one closed boundary is defined. Open water should be specified where the nearest opposite shoreline is more than 5km distant.

The tidal and residual currents are defined as vector components relative to the model domain's native axes. Figure G-2 illustrates the orientation of the longitudinal (x) and transverse (y) coordinate system; these are arbitrary, the positive longitudinal current direction being defined relative to the 'head' of the loch. From this, it follows that for the 'strait' and 'open' model domains, which do not have transverse closed boundaries, the positive longitudinal direction is in the direction of the current residual.

The model requires definition of a scenario via an input data file, an example of which may be found in Appendix B. This includes site-specific topographic and hydrodynamic parameters and allows the particulars of a treatment programme to be specified, i.e. total area of cage group, number of cages, depth of cages during treatment, number of discrete treatments and interval between treatments.

G.4.2 Data requirements

The dimensions of the system require definition; for lochs, the area and length of the receiving water must be established. In the case of a strait, a representative width scale must be defined. The cage group is positioned within the model domain by specification of distance from the shore and 'distance from head' of a sea loch. For 'strait' and 'open' models this parameter represents a distance to the upstream open boundary, where 'upstream' is the opposite direction to the residual flow, for which a value greater than the tidal excursion is required to prevent loss of chemical through the open boundary.

The Sea Lochs Catalogue of Edwards and Sharples (1986) is a useful reference that defines all of the aforementioned dimensional parameters for the water bodies it embraces. However, there will be cases when this is not appropriate and relevant data will need to be determined by other means.

The model has the capability to determine residual flow from the loch length and a flushing time; this feature is not usually employed, as site-specific data describing the local flow-field is required for all applications to discharge controlled substances from marine caged fish-farms. However, where the current residual is towards the head of the loch the model has the facility to determine a residual towards the mouth – refer to Appendix D for more information.

G.5 SEPA's automated bath treatment assessment tool: BathAuto

SEPA has developed a modelling tool (BathAuto) that integrates the short-term model with an iterating procedure that automatically configures, executes, and examines the results of the MLA model. This tool is built within a MS-Excel spreadsheet that prompts for the required input data, and records the outcome of each model iteration. The tool includes only the minimum of error checking; it is left to the user to ensure that valid parameter values are supplied.

G.5.1 Configuration

BathAuto's 'Site_Input data' sheet invites the user to specify the configuration information required for both models. Sources of the required data are summarised in Table G-6; specific 'troublesome' parameters are discussed below.

The data entered in the 'Site_Input data' sheet are formatted for use by 'opendisp.exe' in the 'input.dat' sheets of the BathAuto workbook; these are updated as each new treatment scenario is examined, and exported to a text file prior to each model run.

G.5.1.1 Type of receiving water

The three types of model domain are differentiated by the number of closed boundaries. A 'loch' model, with three closed boundaries, may be configured such that no plumes reach the boundaries during the simulation-period. This is the case where the longitudinal tidal excursion is less than the distance of the cage group from the head and the combined transverse lateral tidal excursion and residual advection is less than the distance to the opposite shore; this will produce the same results as an 'open water' model.

With the foregoing in mind, the user should select the type of receiving water based on a consideration of the real constraints on the chemical patches' development, and of their advection by the tidal and residual currents.

G.5.1.2 Distance to head

In the case of a 'loch' the 'distance to head' is to the transverse closed boundary; for 'strait' and 'open' configurations, with open transverse boundaries, this parameter can be used to ensure that patches do not leave the model domain by setting it to a value greater than the tidal excursion.

G.5.1.3 Average water depth

Vertical mixing is assumed to be constrained by stratification to maximum depth of 10m. Where the available depth of water is less than 20m, BathAuto reduces the depth of the mixed layer to half the average water depth.

The time taken for full vertical mixing to a depth of 10m can be estimated to take about 3 hours, applying a vertical dispersion coefficient of 0.001m^2/s; consequently, the ‘average depth of water’ applies to the area in which a patch might find itself after 3 hours. This is typically some way distant from the farm site, and consideration should be given to charted depths, the tidal excursion, and the residual drift.

The latter values are calculated within BathAuto for a period of 72 hours, and displayed on the ‘Site_input data’ sheet. The MLA model simulates multiple releases, potentially over a number of days; consequently, some patches will be advected for periods in excess of 72 hours.

Table G-5 Compound-specific parameters for azamethiphos

Dose rate :	100 µgl^{-1}		
Decay half-life :	8.9 days		
Test parameters :	AZE contour	=	0.04µg/l
	EQS period	=	72 hours
	Area of patch exceeding 0.04µg/l	=	the lower of: 2% of loch area, or 0.5km^2

G.5.2 First use

Upon first use of BathAuto (version 4), the user is prompted to navigate through their local file system, to the location of the MLA model executable, ‘opendisp.exe’. BathAuto stores the details of the path in the Windows registry; as long as the executable is not moved or deleted, the user should not be required to locate it again. Therefore, it is prudent to place ‘opendisp.exe’ somewhere secure, such as under ‘Program Files’, typically on the primary hard-drive (usually C:\).

Table G-6 Summary of sources of model input parameters

Spatial configuration of model domain	
Type of receiving water	Determined by modeller
Loch area	Sea loch catalogue or map/chart
Loch length	Sea loch catalogue or map/chart
Width of strait	Map or chart – a representative value
Average water depth	Chart and site survey
Depth of mixed layer	Calculated by BathAuto
Distance from shore	Distance to the nearest closed longitudinal boundary
Distance to head	Map or chart
Flow field	
Longitudinal tidal current speed amplitude Transverse tidal current speed amplitude Longitudinal residual current speed Transverse residual current speed	Site-specific longitudinal and lateral components of residual velocities and tidal amplitudes are determined as detailed in Attachment VIII.
Flushing time	Refer to Appendix D
Diffusion coefficient	Model default (0.1 m^2/s)
Cage group configuration	
Number of cages	Farm operator
Cage dimensions	Farm operator
Total cage area	Calculated by BathAuto from cage dimensions.
Cage depth	Farm operator
Cage reduction increment	Determined by modeller
Treatment configuration	
Dose rate	Model default
Total number of treatments	Calculated by BathAuto
Treatments per day	Calculated by BathAuto
Interval between treatments	Calculated by BathAuto
Assessment parameters	
Duration of model run	Model default (84h)
Concentration thresholds	Model default

G.5.3 Operation

A compliant treatment scenario is obtained by iterative adjustment of the cages per treatment, number of treatments, number of treatments per day, treatment intervals, and cage depths.

The first model run is configured to simulate the treatment scenario predicted as EQS-compliant by the short-term model, described in section G.2.3, which is the maximum quantity of medicine that can be used in any three hour period. The results of the longer-term model are examined for the period after 72 hours have elapsed since the last treatment. A compliant treatment scenario determines the maximum quantity of chemical that may be discharged in any 24 hour period.

The order in which the treatment parameters are reconfigured is:

1. number of treatments per day,
2. treatment interval,
3. number of treatments (and corresponding number of cages per treatment), and
4. cage depth.

BathAuto automates this reconfiguration process; initially, it determines all of the viable treatment scenarios, from maximum cages per treatment, maximum treatments per day, minimum interval between treatments to a single cage per day. Should all of these fail to achieve the EQS, the treatment depth of the cage is iteratively reduced by a user-defined interval.

The MLA model executable produces three output files, described below:

- PATCH.OUT – this file is updated with time (in days), peak concentration, the area exceeding the EQS threshold, and the total mass of chemical, at the end of each model time-step
- AREAS.OUT – this file is produced at the end of the model run; it reports the threshold concentration subdivided into ten equal increments, and the area of the model domain over which each of these is exceeded.
- RESULTS.OUT – this file is produced at the end of the model run; it summarises the configuration, and the results of the tests against the specified EQS.

The final two files present the state of the model at the end of its run, i.e. 84 hours after the final treatment; care should be taken when comparing these to the results used by BathAuto, as it extracts the peak values between 72 and 84 hours after the final treatment. These are compared with the test values, as per Table G-5, and compliance is determined.

G.5.4 Limitations

The MLA model uses a calculation of the total mass of chemical required to treat the cage group and the user-defined number of treatments to determine the mass of chemical released in any single treatment episode; therefore, all treatments result in the release of an equal mass of chemical. This presents a problem if the number of cages happens to be a prime, i.e. 3, 5, 7, 11, 13, 17, 19, 23, &c., in that the iterative routine will only examine treatment scenarios where all the cages are treated at once, or where they are treated individually. For instance, a group of 7 cages will not be treated as two groups of 3 cages followed by a single cage, or as three groups of 2 cages again followed by a single cage.

To maximise the compliant quantity of chemical, the user should test the impact of using a higher number of cages; in the example above, of a 7 cage group, cage numbers of 8, 9, 10, and possibly even 12 may yield a greater compliant chemical amount, under the same environmental model configuration.

G.5.5 Testing scenarios

BathAuto is equipped with a facility to aid testing the performance of different cage group configurations; it is assumed that the environmental configuration will remain constant, i.e. model domain and flow conditions, whilst cage numbers size and position may be varied. After BathAuto has successfully iterated to a conclusion, the 'Run Log' sheet may be copied. The cage configuration details can then be locked such that they no longer automatically update when the values in the 'Site_Input data' sheet are changed. There is space for adding notes regarding the configuration or outcome.

G.6 Discussion

The modelling has been described and applied for chemical residues resulting from the bath treatment of marine cage fish farms.

The short-term model indicates that local concentrations of chemical residues around a marine cage fish farm are likely to fall within the appropriate standard at all dispersive sites and some intermediate sites. At some sites the standard is likely to be breached, precluding the use of these treatments at these sites. Each application will need to be assessed individually as the model is sensitive to details such as volume of cages treated and proximity to the shoreline. The long-term model is only used to control chemical residue for substances that are still present in potentially toxic dissolved concentrations after 72 hours.

SEPA believes that application of the short term and long term models described will protect the receiving environment adequately from an unacceptable toxicity impact of chemical residues. Local hydrographic data and position information for the cages are required to apply these models

G.7 References

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Edwards, A and Sharples, F 1986. Scottish Sea Lochs: a catalogue. Scottish Marine Biological Association / Nature Conservancy Council.

Gillibrand, P A and Turrel, W R 1999. A management model to predict the dispersion of soluble pesticides from marine fish farms. Marine Laboratory, Aberdeen Report 2/99 SOAEFD

SEPA, 1997. Mixing zone model for fish farm treatment chemicals. DRAFT 23-Jan-97, SEPA West Document 218njb01

Turrell, W R and Gillibrand, P A 1992. Assessing the environmental affect of new and existing fish farms in Scottish sea lochs. Fisheries Research Services Report 3/92.

Turrel, WR 1994. Simulating the dispersion of azamethiphos in the marine environment. Fisheries Research Service Report 9/94 SOAEFD

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Appendix A Short-term dispersion model for intermittent aqueous discharges

parameter	*description*	*notes*
Input data		
u $[ms^{-1}]$	near surface mean current speed	obtained in accordance with Attachment VIII
t [s]	duration of dispersion	for a 3 hour assessment, **t = 10,800s**; for a 6 hour assessment, **t = 21,600**s
s [m]	minimum distance from the cages to the shore	obtained from site survey data
z [m]	depth of the mixing zone	the smaller of 10m or half the total depth
v $[m^3]$	cage volume	
c $[ngl^{-1}]$	treatment concentration	$5mgl^{-1}$ [cypermethrin], 100 μgl^{-1} [azamethiphos]
D $[m^2s^{-1}]$	dispersion coefficient	assumed to be $0.1m^2s^{-1}$, unless site-specific data is available
X $[ngl^{-1}]$	3 or 6 hour EQS	See Table G-1, Table G-2, and Table G-3
Calculations		
L [m]	half-length of the mixing zone	**L = 0·5.u.t**
w [m]	half-width of the mixing zone	$\mathbf{w = 0{\cdot}5.4(2.D.t)^{1/2}}$
A $[m^2]$	area of mixing zone ellipse, where **s** ≥ **w** $\mathbf{A = \pi.L.w}$ where **s** < **w** $\mathbf{A = \pi.L.w-(L.w.ACOS((w-s)/w) - L.(w-s).\sqrt{(1-((w-s)/w)^2)})}$	
V $[m^3]$	volume of the mixing zone	**V = A.z**
M [g]	maximum mass of the chemical that would result in the mean concentration in the mixing zone volume, **V**, being equal to the EQS, **X**	**M = X.V ÷ 1,000,000**. this mass is the quantity reported for recommendation as a consent limit.
m [g]	mass required to treat a single cage	**m = v.c ÷ 1,000,000**
N	number of cages that may be treated in a 3 hour period	**N = M/m** this is the size of the initial treatment group used in the longer-term model assessment.

Appendix B Example MLA model input file

example value	*description of parameter*	*notes*
LOCH	*Site name*	
10	*Mixed Layer Depth (m)*	
0.1	*Diffusion Coefficient (m^2/s)*	
L	***L**och, **S**trait or **O**pen water*	*(1)*
17.4	*Length (km) - Loch only*	*(2,6,7)*
26.7	*Area (km^2) - Loch only*	*(2,6,7)*
999999	*Flushing time (days) - Loch only – not used by SEPA*	*(6,7)*
0.008	*Longitudinal residual velocity (m/s)*	*(3)*
0.000	*Lateral residual velocity (m/s)*	
0.052	*Tidal current amplitude U (m/s)*	
0.003	*Tidal current amplitude V (m/s)*	
0	*Tidal current phase (degrees)*	*(8)*
40	*Number of cages to be treated*	
999999	*Annual production*	*(9)*
8930	*Total cage area (m^2)*	
5	*Distance from head of system*	*(10)*
0.5	*Lateral distance of cage from shore (km)*	*(4)*
3	*Cage depth during treatment (m)*	
AZAMETHIPHOS	*Name of medicine*	
100	*Treatment concentration (µg/l)*	
8.9	*Chemical half-life (days)*	*(5)*
20	*Number of separate treatment events*	
4	*Number of treatments per day*	
3	*Interval between treatments (hours)*	
0.04	*EQS (µg/l)*	
0.04	*Concentration of contour enclosing patch area (µg/l)*	
84	*Time after which the standard is applied (hours)*	*(11)*

NOTES

IMPORTANT: ensure that none of the data fields include commas or other punctuation, as these are interpreted as field delimiters by the model code.

1. Specify 'L' for loch, 'S' for strait or 'O' for open water
2. Length is length of loch. Length of model grid is determined by residual velocity. Area is area of loch.
3. If residual velocity is negative, e.g. -1, it is calculated from the length (L) and flushing time (T) by U=L/T (Sea loch only)
4. Distance of cage group from nearest longitudinal closed boundary
5. Chemical half-life in days. A negative value (NOT zero) means decay is not simulated
6. For a Strait, remove length, area, and flushing time. Replace with width (km)
7. For Open water, remove length, area, and flushing time. Width defaults to 5 km
8. Tidal current phase - if zero, simulation starts at high water
9. Not used by the model – '999999' is a dummy value.
10. This value is used in Straits or Open waters to represent distance from the upstream open boundary; should be set to value greater than the tidal excursion
11. Extended beyond the EQS period (72hrs) by a tidal cycle to catch any relict oscillations in concentration

Appendix C Result from long term model for azamethiphos in a strait

Sound of Mull (S)

TREATMENT SIMULATION MODEL

MEDICINE PATCH DETAILS AFTER 72 HOURS

Azamethiphos

72 HOUR EQS = 0.0410 UG/L

EXCEEDENCE AREA SPECIFIED USING .041 UG/L

GRID LENGTH = 49.000 KM

GRID WIDTH = 3.000 KM

GRID RESOLUTION: DX = 300 M, DY = 100 M

MIXED LAYER DEPTH = 10.0 M

RESIDUAL VELOCITY U = 0.080 M/S

RESIDUAL VELOCITY V = 0.013 M/S

TIDAL VELOCITY AMPLITUDE U = 0.270 M/S

TIDAL VELOCITY AMPLITUDE V = 0.080 M/S

TIDAL PHASE = 0.0 DEGREES

DIFFUSION COEFFICIENT = 0.10 M^2/S

FARM LOCATED 1.0 KM FROM HEAD

FARM LOCATED 0.5 KM OFFSHORE

NUMBER OF CAGES = 12

ANNUAL PRODUCTION = 1 TONNES

TOTAL CAGE AREA = 9549.00 M^2

CAGE DEPTH DURING TREATMENT = 3.0 M

TREATED CAGE VOLUME = 28647.00 M^3

TREATMENT CONCENTRATION = 100.0 UG/L

MASS OF MEDICINE USED = 2.865 KG

FARM TREATED OVER 3.250 DAYS

3 TREATMENTS DAILY, AT 3 HOUR INTERVALS

CHEMICAL HALF-LIFE = 8.90 DAYS

PATCH 1: X = 44.644 KM, Y = 2.359 KM

PATCH 2: X = 41.515 KM, Y = 2.359 KM

PATCH 3: X = 40.332 KM, Y = 2.359 KM

PATCH 4: X = 37.765 KM, Y = 2.359 KM

PATCH 5: X = 35.422 KM, Y = 2.359 KM

PATCH 6: X = 33.196 KM, Y = 2.359 KM

PATCH 7: X = 30.546 KM, Y = 2.359 KM

PATCH 8: X = 29.251 KM, Y = 2.359 KM

PATCH 9: X = 26.049 KM, Y = 2.359 KM

PATCH 10: X = 23.041 KM, Y = 2.359 KM

PATCH 11: X = 22.872 KM, Y = 2.359 KM

PATCH 12: X = 19.468 KM, Y = 2.359 KM

MAXIMUM CONCENTRATION AFTER 72 HOURS = 0.100 UG/L

AREA WHERE CONCENTRATIONS EXCEED 0.0410 UG/L = 0.510 KM^2

Appendix D Flushing time

In instances where the hydrographic data collected at the fish-farm site suggests that the residual current is towards the head of a loch, i.e. is negative with respect to the MLA model domain, a positive residual velocity can be estimated by the model, from the length of a system and a flushing time. For many sea lochs, flushing time estimates are available from the Sea Loch Catalogue (Edwards and Sharples, 1986).

The flushing time ($\mathbf{T_f}$) can be estimated from:

the tidal period (**P**, 12.42 hours),

the volume of the system at low tide ($\mathbf{V_L}$),

the mean tidal range (**R**), and

the mean of the high and low water areas ($\mathbf{A_{HL}} = (\mathbf{A_H} + \mathbf{A_L})*0.5$), such that:

$$T_f = \frac{PV_L}{RA_{HL}} \text{ (hours)}$$

The flushing time of the whole system may be applied to individual basins in sea lochs.

An equivalent calculation is given in the Sea Loch Catalogue, whereby $\mathbf{T_f}$ is estimated from:

the volume of the system at low tide ($\mathbf{V_L}$),

the spring tidal range ($\mathbf{R_S}$), and

the high and low water areas ($\mathbf{A_H}$ and $\mathbf{A_L}$), such that:

$$T_f = \frac{1.035V_L}{0.7R_S\left(A_H + A_L\right)} \text{ (days)}$$

(Edwards and Sharples, 1986)