

Bath Treatment Dispersion Modelling at Caolas

Dispersion of Azamethiphos at Caolas finfish pen site, Loch Portain, using coupled hydrodynamic-particle tracking modelling in TUFLOW FV





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Executive Summary

This report details the simulation of Azamethiphos dispersion at the Caolas finfish site. Using a calibrated hydrodynamic model (TUFLOW FV) coupled with the Particle Tracking Module (PTM), the dispersion of Azamethiphos was reasonably represented. The model was calibrated with Acoustic Doppler Current Profiler (ADCP) data collected from November 2022 to March 2023, ensuring realistic hydrodynamic conditions. The high-resolution mesh around pen sites and refined bathymetry contributed to the model's accuracy.

Boundary conditions included tidal data from the FES2014 global tide model, regional currents from the HYCOM ocean model, and meteorological data from the ECMWF ERA5 climate model. The General Ocean Turbulence Model (GOTM) simulated vertical mixing, with TUFLOW FV providing a full representation of water levels, velocity, and chemical transport. The calibration process involved comparing model outputs to ADCP data over a 100-day period, achieving 'fit for purpose' accuracy in water levels, velocity magnitude and direction.

Dispersion simulations were conducted to evaluate compliance of proposed bath treatments against the Environmental Quality Standards (EQS) established by the Scottish Environmental Protection Agency (SEPA). Two periods, neap and spring tides, were tested to evaluate dispersion characteristics and treatment impacts. Sensitivity analyses on various parameters ensured robust results, indicating that the bath treatments met SEPA's EQS criteria. Simulated Azamethiphos concentrations were consistently below allowable limits during baseline and sensitivity check simulations. The treatment scenarios were conservative, making the results reliable for regulatory compliance.

Priority Marine Features near the site were evaluated, showing minimal risk from the treatments. The findings underscore the importance of considering multiple factors in chemical dispersion simulations to ensure accurate predictions and environmental protection.



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1 Introduction

1.1 Project Understanding

BMT Ltd (BMT) has been commissioned by Loch Duart Plc (hereafter referred to as Loch Duart) to conduct an assessment of the transport and fate of the bath treatment agent Azamethiphos at the Caolas finfish pen site at Loch Portain, Scotland.

The purpose of this assessment is to support an application for the modification of the permitted quantities of Azamethiphos, following Loch Duart's successful application to increase fish biomass at the site to 1,720 tonnes, with a change in cage layout from the existing fourteen 80 m pens to twelve 100 m circumference pens in a 60 m grid with a net depth of 12 m, arranged in a 2 x 6 grid (TransTech Environmental, 2023a). This site modification has been consented under CAR/L/1002994, and the nearby site Ferramus – FERR1 (CAR/L/1003024) with a biomass of 670 t has now been surrendered. The assessment of bath medicine modelling follows a two-part approach:

- 1. **Hydrodynamic Calibration**: Calibration of the hydrodynamics for the Caolas area.
- 2. **Dispersion Modelling**: Evaluation of the temporal and spatial dispersion footprint of Azamethiphos using particle tracking simulations.

This report details the calibration of the hydrodynamic model near the Caolas farm site, explicitly covering the TUFLOW FV model, model domain specifications, model mesh configurations, bathymetry data, and hydrodynamic model calibration processes. The outputs of the TUFLOW FV model are compared against measured Acoustic Doppler Current Profiler (ADCP) data for validation.

Additionally, this report includes the simulation results of Azamethiphos dispersion under different tidal conditions, specifically spring and neap tides. The dispersion analysis and its compliance with Environmental Quality Standards are performed in alignment with SEPA's prescribed requirements for bath treatment modelling (SEPA, 2024).

1.2 Environmental Quality Standards for Azamethiphos

When Azamethiphos is released into water, it stays in the water until it breaks down into non-toxic derivatives, for which a decay half-life of 5.6 days has been determined (SEPA 2024b). According to SEPA regulatory framework, to ensure safety, two standards are used: one is applied three hours after any discharge, and the other is applied 72 hours after the final discharge in any treatment period. The model was used to assess if proposed treatment scenarios, based on realistic farm operations, complied with Environmental Quality Standards (EQSs) established by SEPA. To assess the 3-hour EQS, a single pen release simulation was modelled and the size of the area where the concentration exceeds 250 ng/L was compared against the allowable mixing zone as calculated using BathAuto. The calculated ellipse area was marked in the plot as a line. After 72 hours, the area exceeding 40 ng/L should not exceed 0.5 km², while the maximum concentration in the domain should not exceed 100 ng/L (maximum allowable concentration - MAC) (Table 1.1).

Table 1.1 Environmental Quality Standards (EQSs) for Azamethiphos (SEPA 2024)

Standards for Azamethiphos Timescale	Standard (ng per litre)	Туре
3 hours	250	EQS
72 hours	40	EQS

Standards for Azamethiphos Timescale	Standard (ng per litre)	Туре
72 hours	100	MAC

1.3 Presentation of Results

Based on the compliance criteria (section 1.2), spatial maps and time series analyses were used to interpret the model outputs as follows:

- Time Series of Areal Extent:
 - 3-hour EQS: The area with Azamethiphos concentrations exceeding 250 ng/L was analysed over time. The maximum extent must remain within the mixing zone ellipse area defined in BathAuto. For this exercise, the ellipse area (mixing zone) calculated by BathAuto is 0.0662 km² (TransTech Environmental, 2023b).
 - 72-hour EQS: The area with Azamethiphos concentrations exceeding 40 ng/L was analysed over time. The maximum extent must not exceed 0.5 km².
- Time Series of Maximum Concentrations:
 - Maximum Azamethiphos concentrations were tracked over the entire simulation period.
- Spatial Maps:
 - Concentration maps of the maximum Azamethiphos concentration in the water column were generated for the 3-hour EQS and 72-hour EQS thresholds.



2 Model Selection

The impact of Azamethiphos is represented through the dispersion of particles carrying dissolved constituents, demonstrating increased dilution from point of treatment. The dispersion of Azamethiphos following treatment was simulated using the 3D hydrodynamic flexible mesh modelling software, TUFLOW FV. The release and dispersion of bath treatment was simulated using the particle tracking module with sufficient resolution at the farm site, as defined by SEPA (SEPA, 2023).

Particle tracking models have been used in prior instances to predict the transport and fate of various discharge constituents in the marine environment to assist with the Environmental Impact Assessment (EIA) process (BMT, 2021 & 2022 and Cooke Aquaculture Scotland, 2021).

Prior to the particle tracking dispersion modelling exercise, the hydrodynamic model was calibrated using measured current and water level data from an ADCP measured from 22/11/2022 to 13/03/2023. Section 3 of this report refers to the calibration of the TUFLOW FV model, which was used for the particle tracking study.

2.1 TUFLOW FV Hydrodynamic Model

TUFLOW FV (https://www.tuflow.com) is a 3D flexible-mesh (finite volume) hydrodynamic model developed and distributed by BMT. It can be used for modelling a diverse array of inland and coastal water bodies and it is able to call a water quality module (WQM) directly via a custom interface. The model accounts for variations in water level, the horizontal salinity distribution and vertical density stratification in response to inflows and surface thermodynamics. The finite volume numerical scheme solves the conservative integral form of the Non-Linear Shallow Water Equations in addition to the advection and transport of scalar constituents such as salinity, temperature, inert tracers and the state variables from the coupled biogeochemical model (TUFLOW, 2020a). The equations are solved in 3D with baroclinic coupling with both salinity and temperature using the UNESCO equation of state. Surface momentum exchange and heat dynamics are solved internally within the model from available meteorological boundary condition data.

2.2 TUFLOW FV - Particle Tracking Module (PTM)

The TUFLOW Particle Tracking Module (PTM) enables the 2D or 3D simulation of discrete Lagrangian particles as they are transported by a flow field and/or other forcing terms (e.g. wind drift). Particle behaviours such as settling, buoyancy, decay, sedimentation and resuspension can all be simulated. This tracking of discrete particles can be used to output particle age and fate, which are often useful metrics for environmental applications that are not easily modelled using the Eulerian scheme. The PTM is invoked through the HD Engine, which controls the overall simulation, supplies the forcing fields to the PTM and handles certain PTM outputs. Additional details about the TUFLOWFV-PTM can be found in the user manual (TUFLOW, 2020b).

2.3 Model Mesh

The TUFLOW FV model domain covers an overall area of 55 km², with an open boundary of approximately 150 km extending along the south-east boundary (Figure 2.1).

The model mesh has been refined as required for this study with reduced resolution offshore and increased resolution around pen sites. As per SEPA recommendations, a horizontal resolution of no greater than 25-30 m was maintained in areas around pen sites, with the target resolution being 20 m to ensure suitable detail is modelled (Figure 2.1). This mesh then gradually reduced in resolution, reaching 350 m at the boundary.



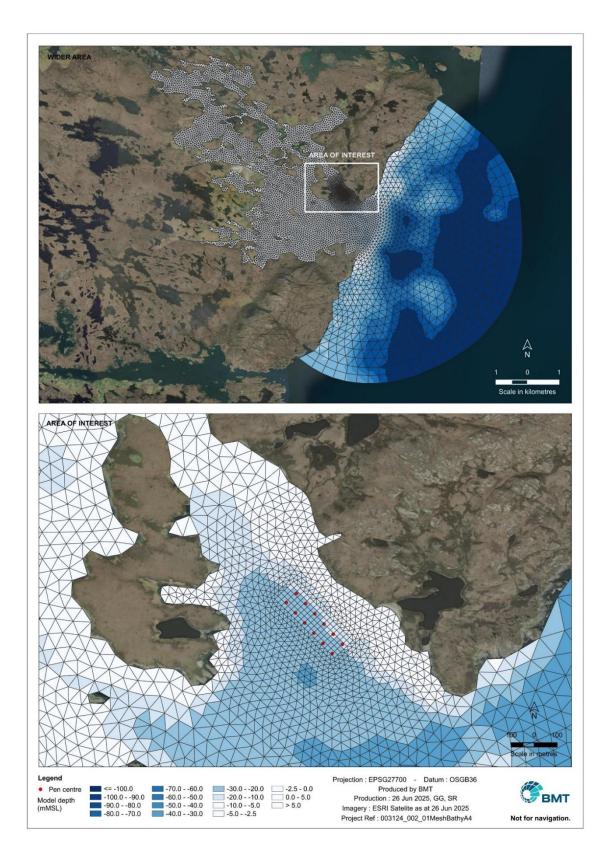


Figure 2.1 Model domain, mesh and bathymetry with pen locations



2.4 Model Bathymetry

A combined bathymetry comprising of multiple sources was used in this study to ensure suitable resolution for current speeds around the area of interest (Figure 2.1). The final bathymetry comprised the following:

- Bathymetry survey data provided by Loch Duart for the farm area (Namara projects, 2011).
- Bathymetric data digitised from Navionics.
- Bathymetric data from General Bathymetric Chart of the Oceans (GEBCO).

The accuracy of the model is constrained by limitations of the available bed level data, as only a limited area has been surveyed specifically for this study. Consequently, the complex intertidal zones, both inland of the site and around the bay have been modelled based on the other data available combined with expert judgment.

This primarily implies that the volumes of water reaching and flowing through different areas will vary in accuracy according to the bed level data available. In addition to this, data are lacking for intertidal areas and waterways as well as island topography and surrounding shallow water bathymetry, which would inherently influence the resultant hydrodynamics. Although the bathymetric data available do not fully capture these details in the digital elevation model, the model is able to provide a fit-for-purpose estimate of the hydrodynamics, and general circulation pattens in the area of interest.

2.5 Boundary Conditions

The following meteorological and open tidal boundary conditions have been used for the model:

- Tidal boundary conditions provided by the FES2014 global tide model.
- The model was forced with regional current forcing (residual water level, current magnitude and direction), temperature and salinity profiles at the open boundary derived from the ocean general circulation model, HYCOM (http://hycom.org/). These vary both in space (longitude, latitude and elevation) and time. To capture the sub-daily regional processes, three-hourly HYCOM model datasets were prescribed at the ocean boundary.
- Atmospheric heat fluxes and water column heat dynamics were simulated internally by TUFLOW FV. Boundary condition data including wind, air temperature, long- and short-wave radiation, precipitation and relative humidity were derived from meteorological data extracted from the European Centre for Medium-Range Weather Forecasts (ECMWF) ERA5 climate model (https://www.ecmwf.int/).
- The General Ocean Turbulence Model (GOTM) was coupled with the 3D TUFLOW FV
 hydrodynamic model to simulate the vertical mixing processes in the presence of density
 stratification (http://www.gotm.net/).

There are no gauged freshwater inputs to the area of interest (National River Flow Archive, 2023) and it was assumed freshwater inflows are not significant so none were included as river boundary conditions to the model.



3 Hydrodynamic Calibration

3.1 ADCP Data

The hydrodynamic model was calibrated against data from an ADCP deployed by TransTech Environmental at the seabed close to the farm site from 22/11/2022 to 20/02/2023 (Figure 3.1) (TransTech Environmental, 2023c). The calibration period described in this report covered these 100 days of the deployment period.

The calibration process involved comparing modelled water levels, velocity direction, velocity magnitude and the u and v vector components of the modelled flow to observed ADCP data, adjusting model parameters and bathymetry to achieve a desired level of model fit.

This ADCP data had been processed by TransTech Environmental (2023c) prior to BMT receiving it. BMT were provided with timeseries of speed, direction, and pressure at three depths. These data had been stitched together from three separate ADCP deployments.

The calibration was carried out at three different depths throughout the water column:

- Sub-Surface approx. 22.85 m above the seabed.
- Net-Bottom approx. 17.85 m above the seabed.
- Near-Bed approx. 2.85 m above the seabed.

The pressure sensor data indicated that the ADCP remained undisturbed during the separate deployment periods. Any minor changes in pitch, roll and heading during the 100-day deployment period remained within the ADCP's tolerance for data auto-correction. Further details on the ADCP deployments, GPS calibration and data processing can be found in the hydrographic survey report for the Caolas site (TransTech Environmental, 2023c).

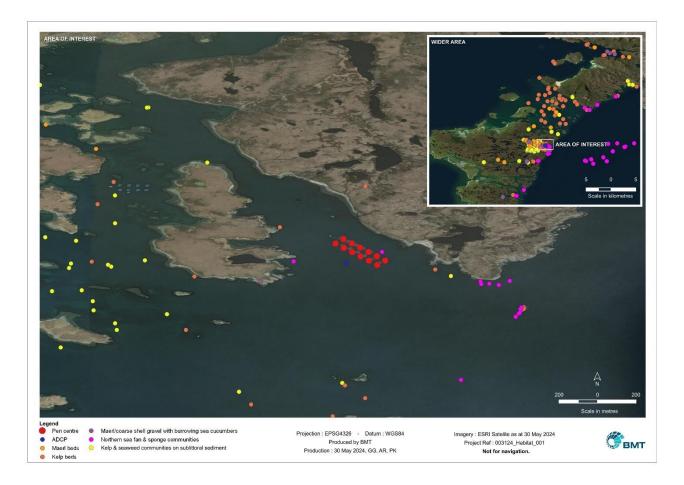


Figure 3.1 Pen centroids with ADCP location and priority marine features (PMFs) nearby

3.2 Model Extraction Depths

To compare the model with the ADCP measurements, timeseries were extracted from the model at three corresponding depths (Table 3.1). The model output was averaged over a depth of 1 m encompassing the depths the ADCP were extracted for over all three deployments.

Table 3.1 Extraction Depths

Position	ADCP depth for each deployment (m above seabed)	Model data extraction depth (m above seabed)
Sub-Surface	22.85,22.86,22.85	22.35-23.35
Net-Bottom	17.85,17.86,17.85	17.35-18.35
Near-Bed	2.86,2.86,2.85	2.35-3.35

3.3 Model performance

Comparisons of modelled against observed data are shown in Figure 3.2 to Figure 3.13 and statistics for R (correlation coefficient), BIAS (mean bias error), MAE (mean absolute error), and RMSE (root mean square error) are included on the plots for comparison. The BIAS has been calculated so that a positive BIAS indicates the model data has higher values than the ADCP data. These statistics were calculated based on an interpolated model timeseries to enable comparable datapoints in the time domain. Statistics have been calculated over the full ADCP deployment period with additional detailed plots included as representative of spring and neap tidal periods.



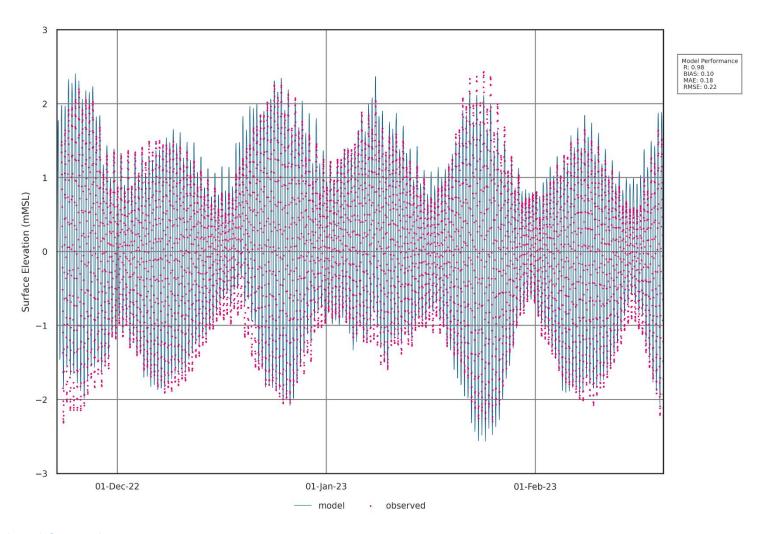
The water level is displayed on each multi-plot figure to allow comparisons within the context of the spring-neap tidal cycle. Although model performance statistics for direction are included it should be noted that the north south directions dominate so small time lags will result in large errors. Statistical measures of model fit on current vector components are a more suitable representation of the model calibration. The direction plots are included to highlight the complexity of the area.

It should be noted that an oceanographic event occurred in the middle of December 2022, this event can be seen in the ADCP data, particularly at the bed where there are southerly flows, whilst at the surface the current direction is consistent. However, this event is not well represented by the model. Other data sources in the surrounding area were analysed, and an event was also observed in the data from the West of Hebrides directional wave buoy, where during this time the wave direction was almost consistently from the north (WaveNet, 2024). This confirms that there was an event occurring during this time that was picked up by both this ADCP and the wave buoy, however the detail and reasons for this event have not been explored here as this is beyond the scope of the study and available data.

Water Level

- The R value is high (0.98), signifying a strong correlation between the model predicted water level and the observed data (Figure 3.2).
- The tidal range predicted by the model is consistent with the observed data and predicts the variations in tidal range between spring and neap tides.
- The MAE for water levels is 0.18 m, slightly above the SEPA guideline of ±0.1 m. However, percentage differences are within limits: 3.1% for neap tides and 10% for spring tides, both meeting SEPA's specified ranges (SEPA, 2019).
- The timing of the high and low water matches well between the ADCP and modelled data. With the timing of both peaks and troughs combined having an MAE of approximately 16 min. The SEPA guidelines are that the absolute error for the phasing should be +/- 15 min (SEPA, 2019). It should be taken into account that the ADCP measured the data every 20 min (TransTech Environmental, 2023c), which is longer than the SEPA recommended error. This MAE is only slightly larger than what is required by the SEPA guidelines (1 min), this should be considered alongside the tidal range which is within the SEPA guidelines.

This model has a water level calibration suitable for the use of modelling the dispersion of bath treatment.



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Figure 3.2 Water Level Comparison



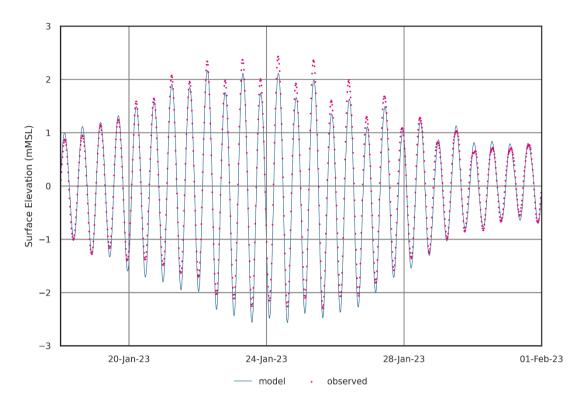


Figure 3.3 Water Level Comparison for a Spring Tide

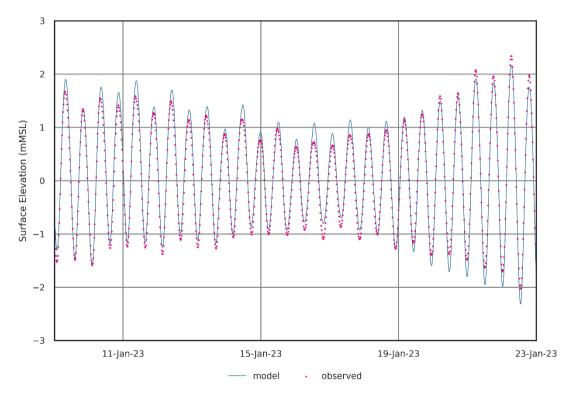


Figure 3.4 Water Level Comparison for a Neap Tide





Sub-Surface

Velocity Magnitude

- The R value is 0.03, indicating a weak correlation between the ADCP and model data.
- The bias for water velocities is minimal at 0.03 m/s. This indicates that the model's predicted velocity magnitudes closely match those measured by the ADCP.
- The MAE is low (0.04 m/s) and sits within the regulatory calibration guideline of 0.1 m/s (SEPA, 2019).
- From the full calibration period timeseries, it can be seen that the model represents the difference in velocity magnitude between the neap and spring tidal cycles, with magnitudes varying in a similar range to the ADCP data.

A possible cause for some of the weaker statistics, despite a low overall bias and MAE, may be attributed to phase discrepancies in the peak velocities. This can be seen clearly in the spring and neap plots (Figure 3.3 and Figure 3.4). However, although the phasing is misaligned, the magnitude remains similar, and it is this magnitude that will control the speed at which the bath treatment will disperse from the site.

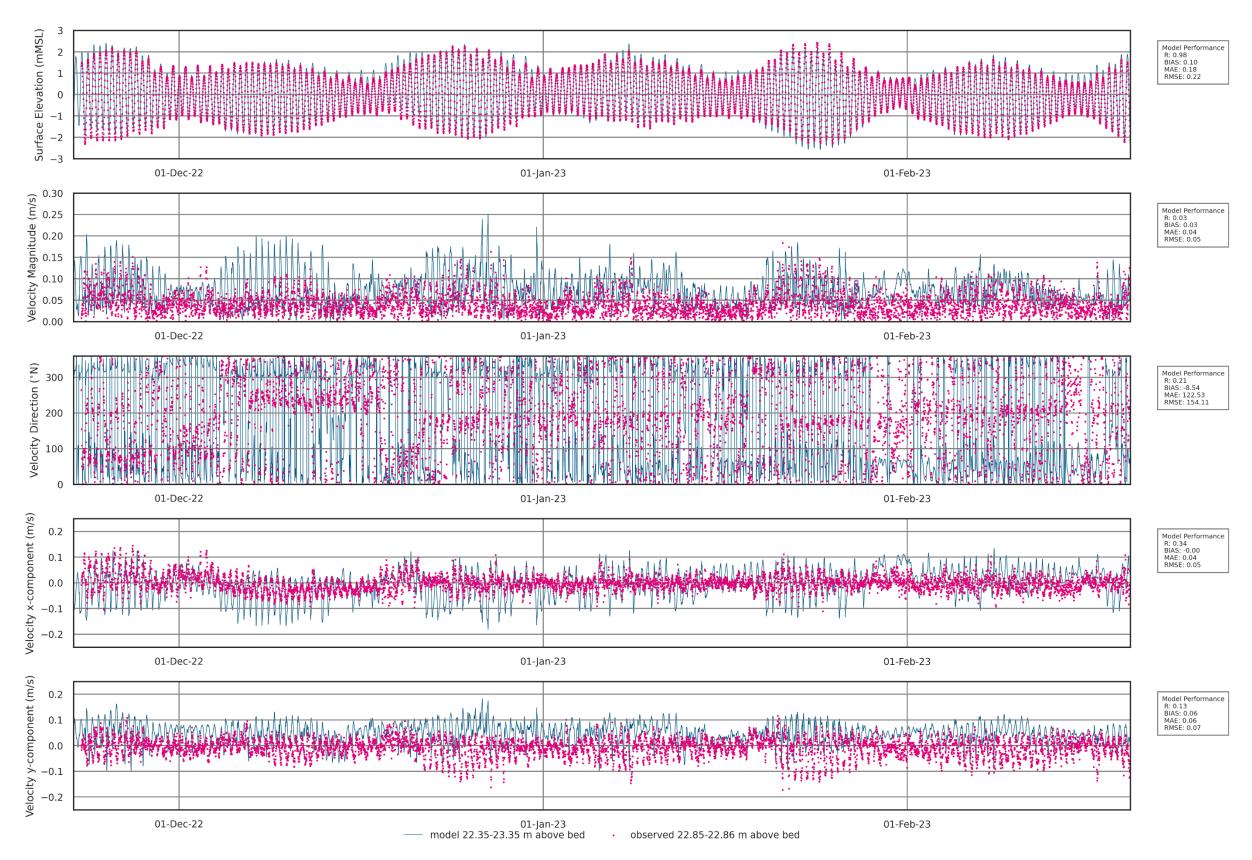
Current Direction

- Analysis of the timeseries reveals that the ADCP data does not follow the expected clear bidirectional current typical of a tidal area, indicating the complexity of the dynamics in the area. In addition, there have been some uncertainties about the ADCP direction highlighted in the notes that accompanied the data (TransTech Environmental, 2023d).
- Particularly during the neap cycles, the velocity magnitudes are low (< 0.5 m/s), making it challenging to get an accurate direction due to minimal water movement.

Vector Velocity Components

- The model velocities follow the same pattern as the ADCP data with smaller velocities during the neap than spring tide, indicating the model reasonably reproduces the difference in tidal cycles. This is expected due to the strong calibration of water levels.
- However, examination of the spring and neap plots reveals that there is a misalignment in the phasing of the velocity. This is likely the cause of the low correlation shown in the statistics.





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Figure 3.5 Velocity magnitude, direction and vector components at the sub-surface



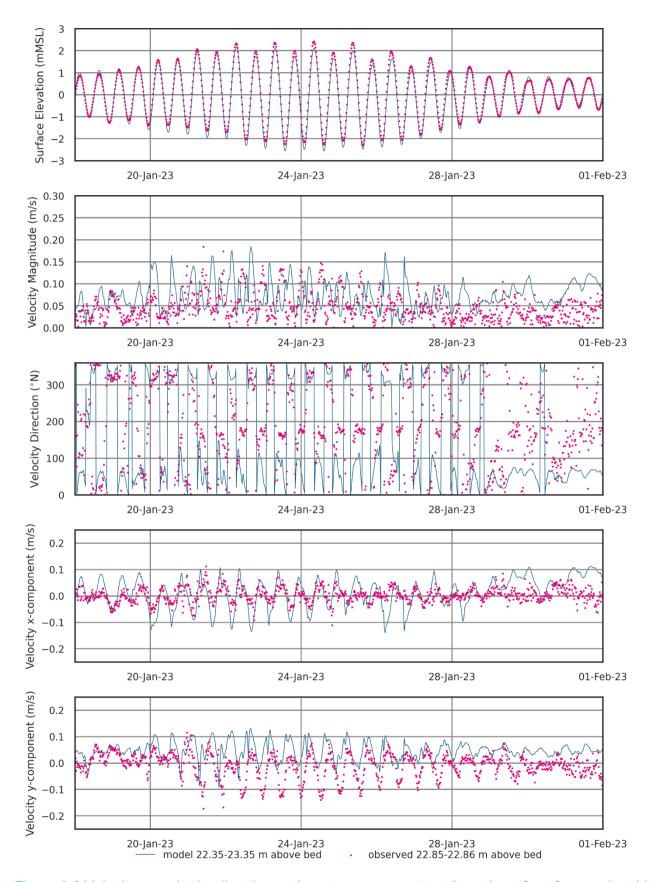


Figure 3.6 Velocity magnitude, direction and vector components at the sub-surface for a spring tide



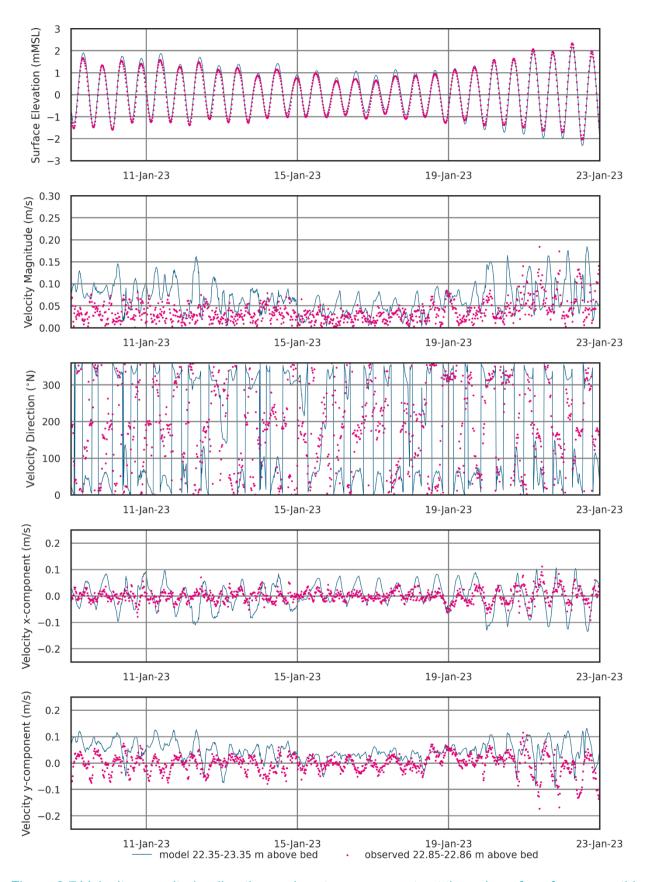


Figure 3.7 Velocity magnitude, direction and vector components at the sub-surface for a neap tide



Net-Bottom

Velocity Magnitude

- An R value of 0.29 indicates that there is only a weak correlation between the ADCP and model data. This is expected as we see this lack of correlation at the other water depths.
- There is a BIAS of 0.02 for water velocities. This indicates that the model is predicting velocity magnitudes that are of a similar magnitude to the ADCP.
- The MAE is low (0.03 m/s) and within the regulatory calibration guideline of 0.1 m/s (SEPA, 2019).
- The full calibration period timeseries shows that the model accurately captures the difference in velocity magnitude between the neap and spring tidal cycles, with magnitudes varying in a similar range to the ADCP data.

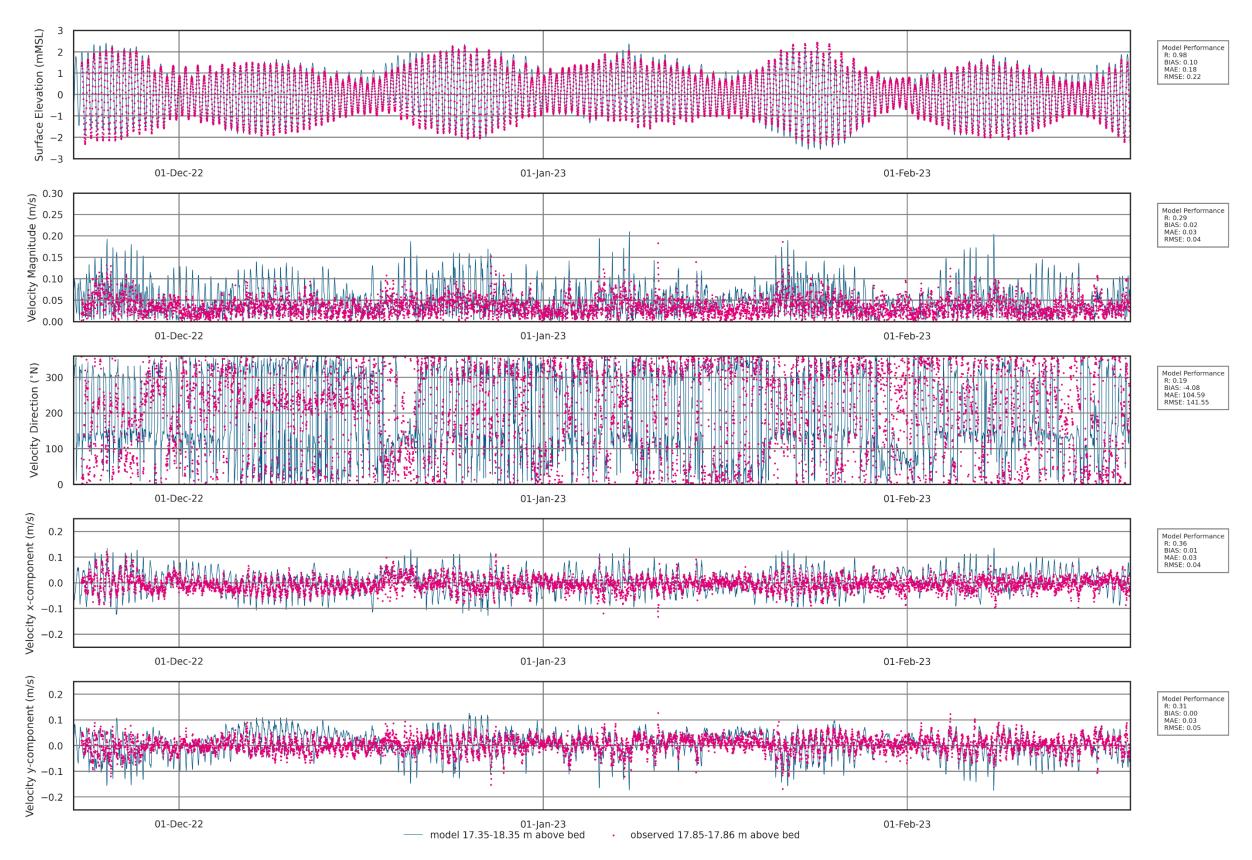
Current Direction

As at the sub-surface and particularly during the neap cycles, the velocity magnitude is very small (< 0.5 m/s), at such low speeds accurate direction measurement is challenging due to minimal water movement.

Vector Velocity Components

- As observed at the sub-surface the model velocities follow the same pattern as the ADCP data with smaller velocities during the neap than spring tide, indicating the model accurately reproduces the difference in tidal cycles. This is expected due to the strong calibration of water levels.
- However, examination of the spring and neap plots reveals that there is a misalignment in the phasing of the velocity. This is likely the cause of the low correlation shown in the statistics.





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Figure 3.8 Velocity magnitude, direction and vector components at the net-bottom



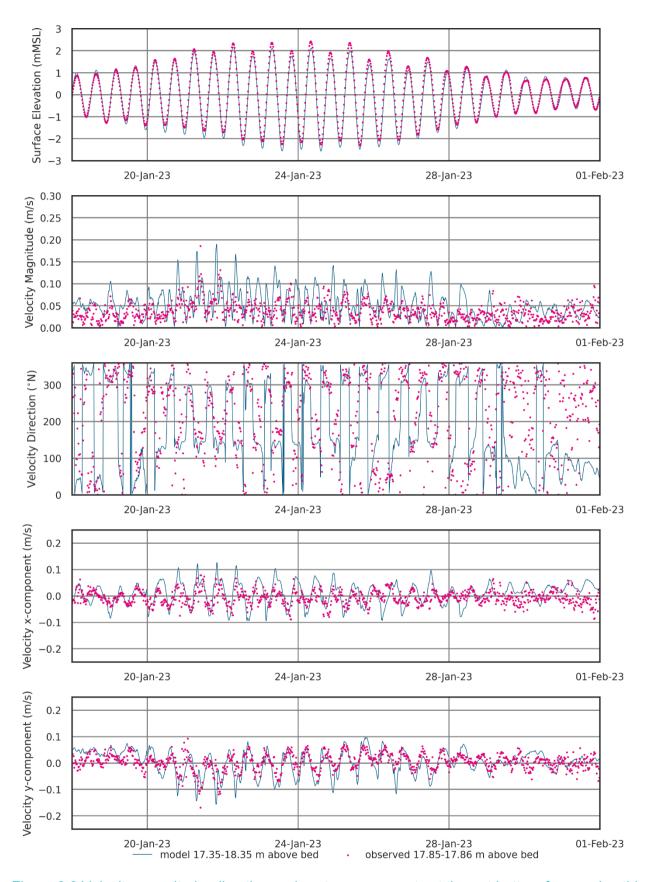


Figure 3.9 Velocity magnitude, direction and vector components at the net-bottom for a spring tide



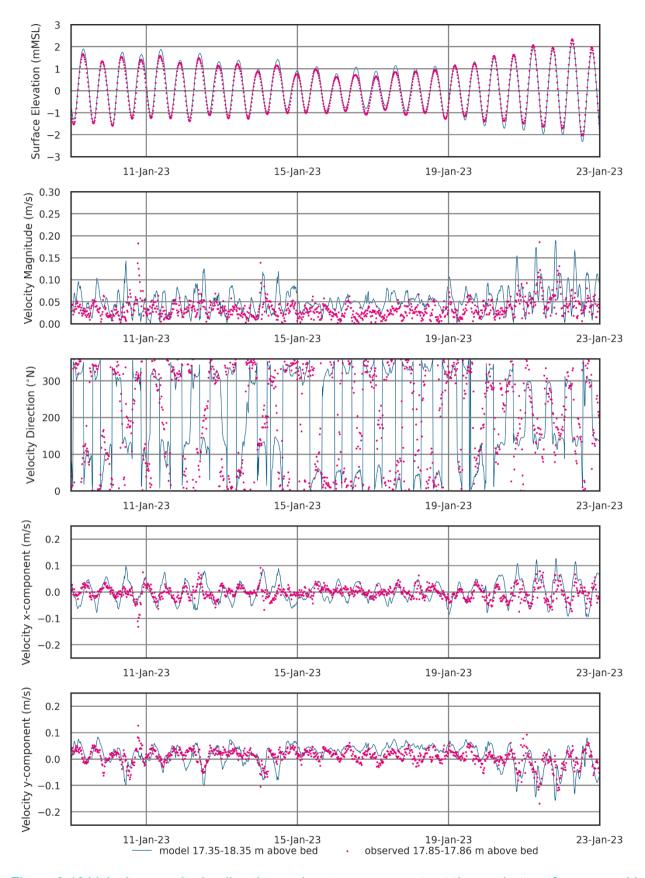


Figure 3.10 Velocity magnitude, direction and vector components at the net-bottom for a neap tide



Near-Bed

Velocity Magnitude

- The calibration at the near-bed is weaker than at the net-bottom or surface.
- The MAE is low (0.07 m/s) and within the regulatory calibration guideline of 0.1 m/s (SEPA, 2019).
- The near-bed shows less distinct differences between spring and neap tidal cycles. However, the model still reflects the differences, particularly in the middle ADCP deployment.

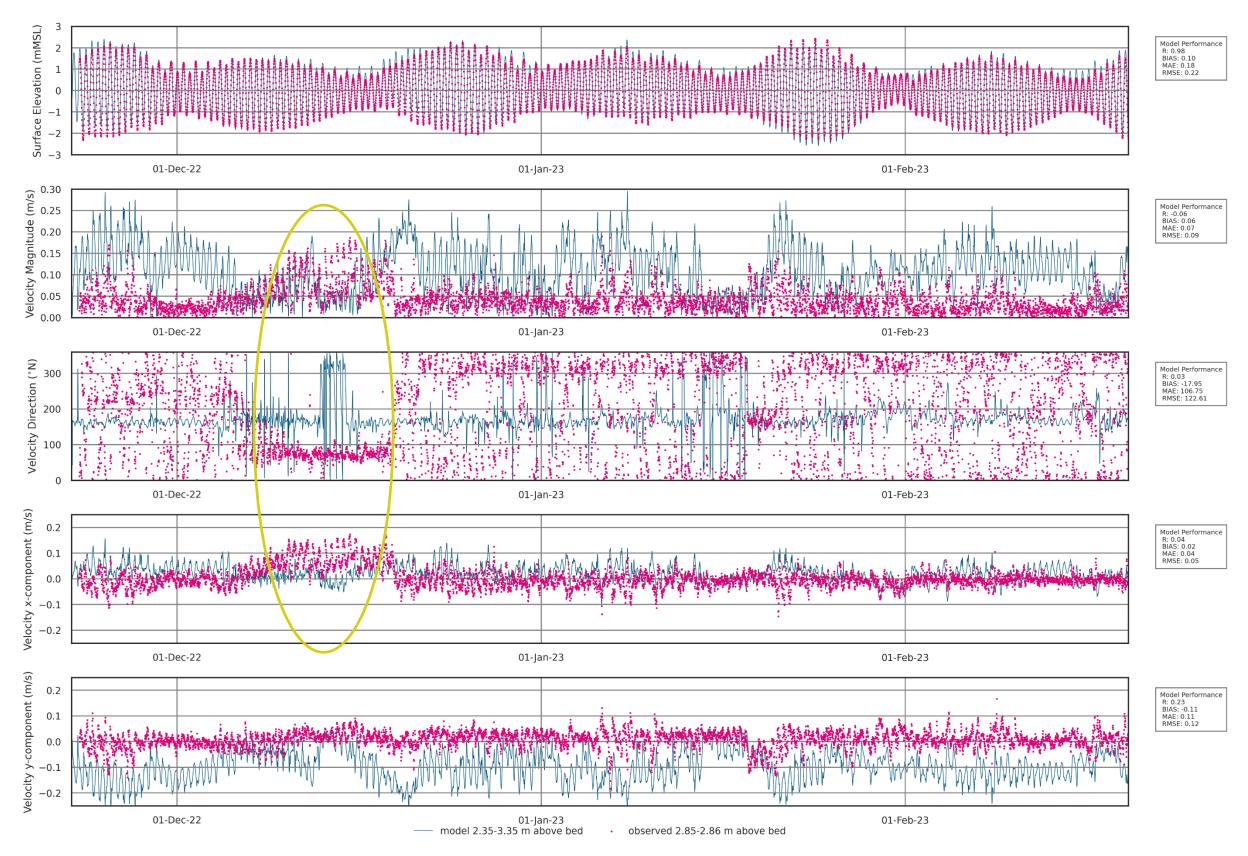
Current Direction

- As at the other depths analysed, and particularly during the neap cycles, the velocity magnitude is very small (< 0.5 m/s), at speeds this low it is hard to get an accurate direction due to minimal water movement.
- It should be noted that there appears to be an unexplained oceanographic event in the middle of December that the model is not able to represent, this can clearly be seen in the ADCP direction at the near-bed. This period is highlighted by a yellow ellipse in Figure 3.11 illustrates this occurrence.

Vector Velocity Components

- As at the other depths analysed, the model velocities follow the same pattern as the ADCP data
 with smaller velocities during the neap than spring tide, indicating the model accurately reproduces
 the difference in tidal cycles. This is expected due to the strong calibration of water levels.
- However, examination of the spring and neap plots reveals that there is a misalignment in the phasing of the velocity. This is likely the cause of the low correlation shown in the statistics.





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Figure 3.11 Velocity magnitude, direction and vector components at the near-bed. Highlighted by a yellow ellipse is a period of unexplained oceanographic event.

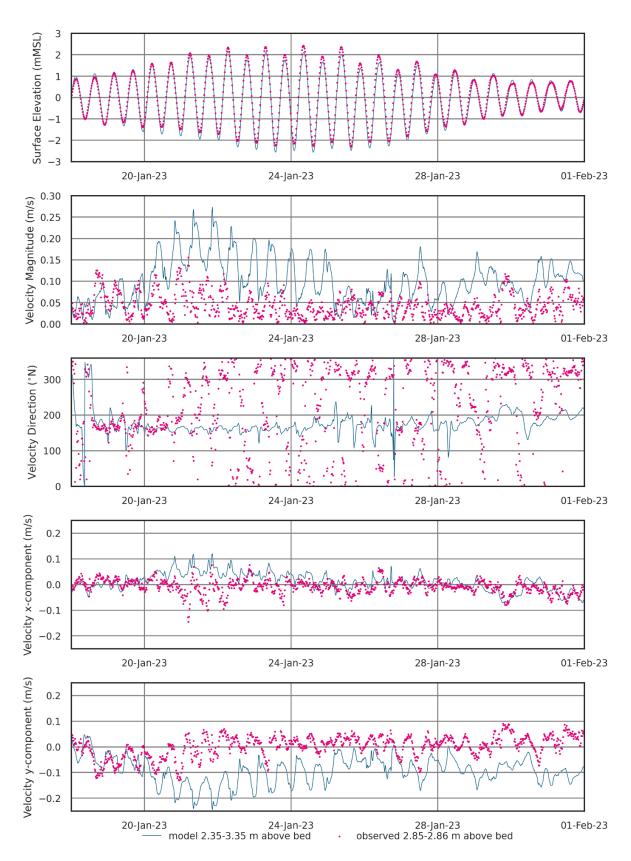


Figure 3.12 Velocity magnitude, direction and vector components at the near-bed for a spring tide

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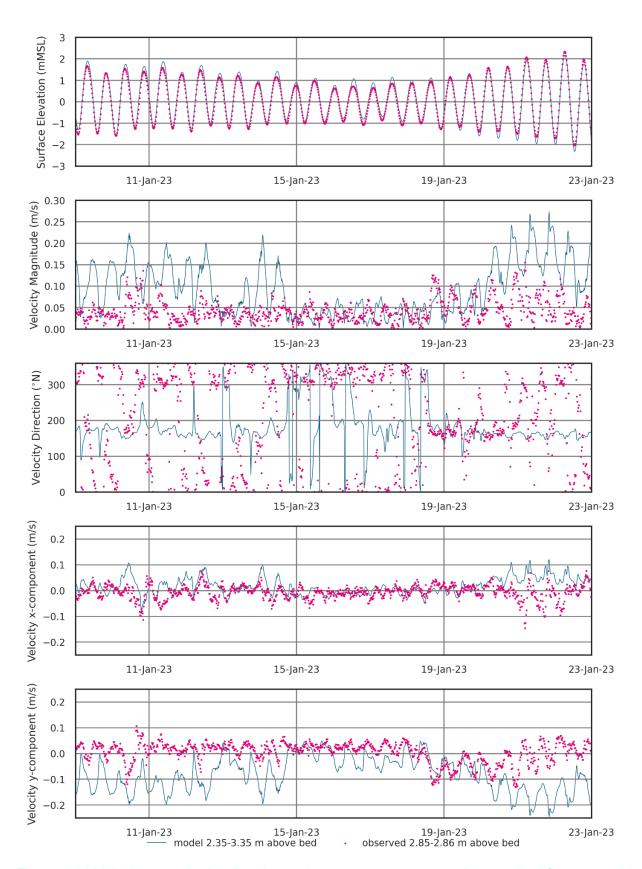


Figure 3.13 Velocity magnitude, direction and vector components at the near-bed for a neap tide

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4 Dispersion Modelling

4.1 Simulation Time Periods

To simulate the worst-case condition, the dispersion modelling was initially conducted using TUFLOW FV flow fields over a period of two weeks centred on a small neap tidal range taken from the calibrated hydrodynamic model simulations. This was assumed to be the least dispersive set of ambient conditions, when Azamethiphos dispersion was least likely to meet the required EQS (See section 1.2). Simulations were also conducted during a two-week period of spring tides for comparison and understanding of upper limit of spread.

The two-week simulation period covered the duration of treatment, a dispersion period for the EQS assessment after 72 hours (long-term assessment as per guidelines) and an extra 24 hours to check for any chance concentration peaks. It has been identified that the medicines used in bath treatments are either rapidly broken down or bind to particles in the water rendering them unavailable to marine life. For this reason, short period simulations have been deemed sufficient to predict any potential impact (SSFL, 2011).

Two particle tracking simulations were carried out for two distinct periods representative of neap and spring tide conditions extracted from the 90-day model calibration period in 2022/2023:

Neap tide model period (Figure 4.1):

The particle tracking model was initiated on 08/12/2022 00:00:00 and ends 08/01/2023 00:00:00. The first treatment was administered at 11/12/2022 17:00:00 and the last treatment at 14/12/2022 23:05:00, corresponding to the smallest maxima of the neap tidal cycle, where the final treatment was released at highwater.

Spring tide model period (Figure 4.2):

The particle tracking model was initiated on 18/11/2022 00:00:00 and ends 18/12/2022 00:00:00. The first treatment was administered at 21/11/2022 12:30:00 and the last treatment at 24/11/2022 18:35:00, corresponding to the highest maxima of the spring tidal cycle, where the final treatment was released at highwater.

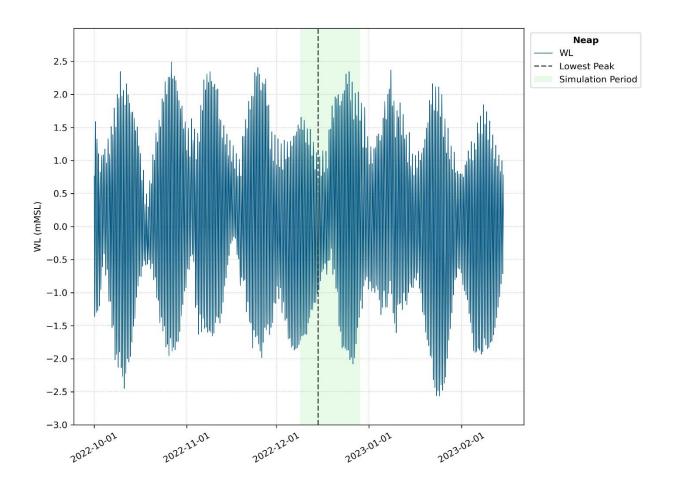


Figure 4.1 Neap simulation period: The smallest neap maxima was on 14/12/2022 23:05:00.

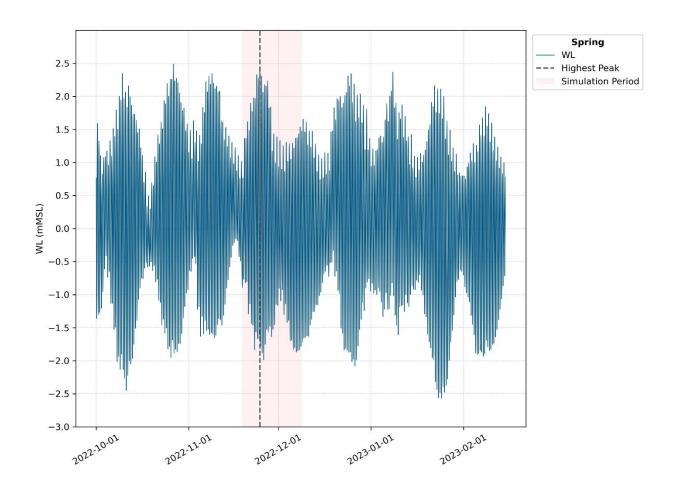


Figure 4.2 Spring simulation period: The highest spring maxima was at 24/11/2022 18:35:00.

4.2 Bath Treatment

Dosage and schedule

The method of bath treatment was simulated by applying 300 g of Azamethiphos to each pen with releases at three times per day with 3 hourly intervals (Pers com. Loch Duart) to represent a realistic daily treatment campaign. A total of 3.6 kg of Azamethiphos was discharged over the four-day period. The order of pens treated in this scenario is shown in Figure 4.3. The treatment schedule was designed with consideration to the time needed for setting up each treatment, moving between pens, and the duration of the treatment.

The Azamethiphos treatment was simulated by releasing particles over 5 minutes within the upper 4 m of the water column. Particle concentrations were calculated using a 25 m x 25 m grid, matching the treatment depth (0–4 m), to simplify calculation and presentation of results. Table 4.1 and Table 4.2 present the simulated particle release times and order for all pens in the farm during both neap and spring tide scenarios.

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Azamethiphos discharge was included as a point source release with specifications of location coordinates of pens, discharge rate, and bath treatment schedule with concentrations or mass of the Azamethiphos as determined by Loch Duart. The 3 hr EQS only considered a single release from pen #10, while the 72 hr EQS and MAC considered all releases.

The simulations used 120 million particles in total, with each pen discharge containing 100,000 numerical particles representing 3 mg of azamethiphos each.



Figure 4.3 Bath treatment order.

Table 4.1 Treatment schedule for the neap tide simulation period.

Day	Date	Time	Pen #
1	11/12/2022	17:00:00	1
1	11/12/2022	20:00:00	3
1	11/12/2022	23:00:00	5
2	12/12/2022	17:00:00	2
2	12/12/2022	20:00:00	4
2	12/12/2022	23:00:00	7

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Day	Date	Time	Pen #
3	13/12/2022	17:00:00	9
3	13/12/2022	20:00:00	6
3	13/12/2022	23:00:00	8
4	14/12/2022	17:00:00	11
4	14/12/2022	20:00:00	12
4*	14/12/2022	23:00:00	10

^{*}Final treatment was based on the smallest maxima for the neap tide.

Table 4.2 Treatment schedule for the spring tide simulation period.

Day	Date	Time	Pen #
1	21/11/2022	12:30:00	1
1	21/11/2022	15:30:00	3
1	21/11/2022	18:30:00	5
2	22/11/2022	12:30:00	2
2	22/11/2022	15:30:00	4
2	22/11/2022	18:30:00	7
3	23/11/2022	12:30:00	9
3	23/11/2022	15:30:00	6
3	23/11/2022	18:30:00	8
4	24/11/2022	12:30:00	11
4	24/11/2022	15:30:00	12
4*	24/11/2022	18:30:00	10

 $[\]ensuremath{^{*}\text{Final}}$ treatment was based on the highest maxima for the spring tide.

Decay Rate

A half-life of 5.6 days was applied to represent Azamethiphos decay (SEPA 2024), this equated to the time required for half of the substance to decay (equivalent to a decay rate of 0.12377 per day).

4.3 Particle Diffusivity

In TUFLOW-FV, the 'constant' horizontal dispersion model utilises a fixed diffusion coefficient to simulate the horizontal mixing and transport of scalar quantities, such as temperature or concentration, due to turbulence and mixing processes. This model is based on Gaussian random walk component that applies constant diffusivity, aiding in the accurate representation of how these quantities are spread and mixed horizontally within the fluid (TUFLOW 2020b).

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Horizontal scalar diffusivity is generally calibrated based on field observations or laboratory experiments to accurately represent the true horizontal diffusion characteristics of the modelled fluid. However, SEPA (2023) advised that, given the high dispersion characteristics at the site, calibration of the marine model using dye or drogue data was not required for this site. Accordingly, this study adopted a global horizontal diffusivity value of 0.1 m²/s, and vertical diffusivity of 0.001 m²/s as recommended by SEPA.

Typical values for horizontal dispersion coefficients measured using dye patch studies in coastal waters vary considerably, ranging from 0.004 to 2.17 m²/s (Anderson Marine Surveys, 2023; Elliott et al., 1997; Morales et al., 1997). Sensitivity analyses were performed following SEPA's marine modelling guidelines to verify the compliance criteria within a range of parameters.

4.4 Sensitivity Analysis

A sensitivity analysis was undertaken to ensure that the model parameter values chosen did not have a significant effect on the overall result of the compliance assessment. The sensitivity analysis was performed on the neap tide, as this is the theoretical worst-case simulation. Time-series of allowable zone of effects (AZE) plotted against the 72 hr EQS (area with a concentration greater than 40 ng/L should be less than 0.5 km²), for the full treatment regime, were used for assessment comparisons.

Sensitivity checks were undertaken for following scenarios:

- Horizontal Diffusivity three scenarios with constant diffusivity values:
 - Base case: SEPA recommended dispersion parameter of 0.1 m²/s.
 - Low diffusivity: Fixed at 0.004 m²/s.
 - High diffusivity: Fixed at 0.8 m²/s.
- Vertical Diffusivity two scenarios with constant diffusivity values:
 - Base case: SEPA recommended dispersion parameter of 0.001 m²/s.
 - High diffusivity: Fixed at 1.0 m²/s.
- Time of Release: The sensitivity of the results to the timing of bath treatment releases was assessed by varying the release time by ±6 hours to account for different phases of the tidal cycle.
- Grid Size: The sensitivity of the structured grid resolution was evaluated through increasing the cell area from the base case of 25m x 25m to both 50m x 50m and 100m x 100m.
- Particle Count: Sensitivity to the number of released particles was evaluated by reducing the baseline value of 1.2 million particles to 120,000 and 36,000 particles, respectively.

5 Results

5.1 Presentation of Results

Based on the compliance criteria (Section 1.2), time series analyses and spatial maps were used to interpret the model outputs as follows:

- Time Series of Areal Extent: 3-hour EQS and 72-hour EQS
- Time Series of Maximum Allowable Concentrations (MAC)
- Spatial Distribution

5.2 Time Series of Areal Extent – 3-hour EQS

To assess the short-term compliance for Azamethiphos, a single tarpaulin release of a 3-hour mass (300 g) was modelled. Figure 5.1 and Figure 5.2 show the area covered by the plume that exceeds a concentration of 250 ng/L within the top 4 m of the water column following the initial release (at 0 hours on the x-axis), for the neap and spring tides, respectively. In both cases, the size of the chemical plume after a single treatment is well below the calculated ellipse area after 3 hours.

During the neap tide simulation, the particle plume area never exceeded 0.005 km², while during the spring tide, it never exceeded 0.004 km². Throughout the neap tide period, the area greater than 250 ng/L remained below the EQS area, indicating no breach of the EQS threshold.

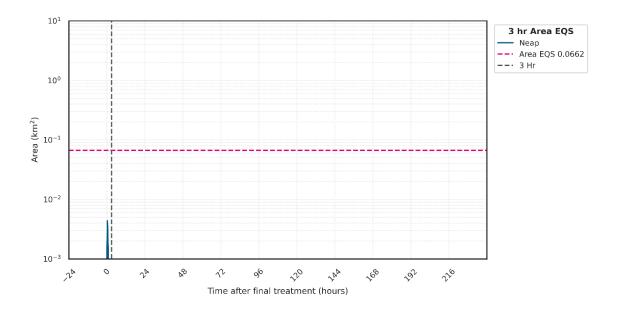


Figure 5.1 Neap tide area exceeding 3 hr EQS value (250 ng/L).

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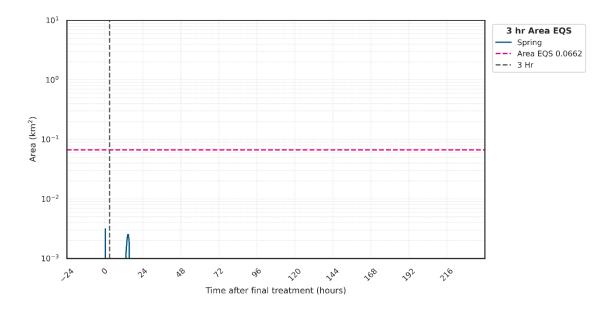


Figure 5.2 Spring tide area exceeding 3 hr EQS value (250 ng/L).

5.3 Time Series of Areal Extent – 72-hour EQS

The area of the Azamethiphos plume exceeding a concentration of 40 ng/L (72-hour EQS) within the top 4 m of the water column is plotted in Figure 5.3 and Figure 5.4. For both the neap and the spring conditions, the area greater than 40 ng/L never exceeded $0.5 \, \mathrm{km}^2$.

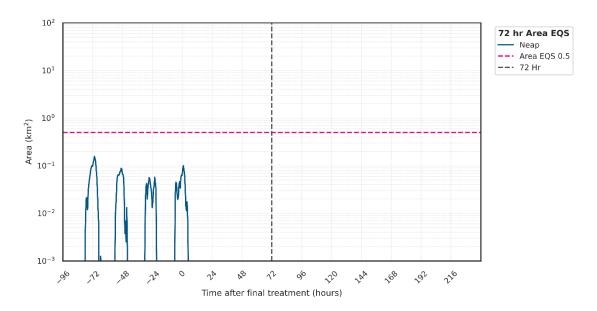


Figure 5.3 Neap tide area exceeding 72 hr EQS value (40 ng/L).

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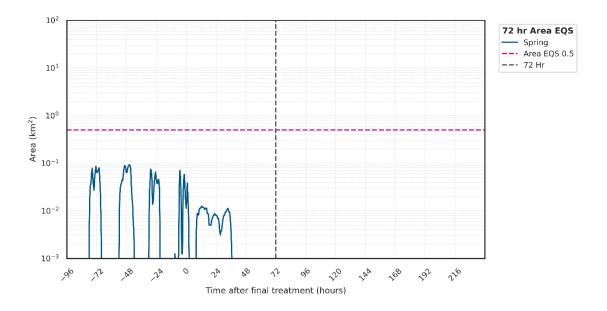


Figure 5.4 Spring tide area exceeding 72 hr EQS value (40 ng/L).

5.4 Maximum Allowable Concentration (MAC) - 72 hr

To assess the long-term risks from Azamethiphos, the full treatment regime is modelled. This simulated an individual treatment mass of 300 g, resulting in a maximum 24 hr treatment mass of 900 g, and a total treatment regime of 3.6 kg over 4 days. The maximum concentration within the whole water column for the neap and spring tide cycles are plotted in Figure 5.5 and Figure 5.6 respectively.

The individual pen treatments are recognisable by the sharp peaks in maximum chemical concentrations. The Azamethiphos mass is introduced rapidly into the model domain creating a steep increase; following this, decay and dispersion causes a rapid decrease in peak concentrations. Under both neap and spring tide conditions, the concentration at the site 72 hours after the final treatment remained well below the 100 ng/L EQS. The spring tide scenario showed a slightly lower MAC at the 72-hour mark. Following the final treatment, a general decline in maximum concentration was observed for both tidal conditions.

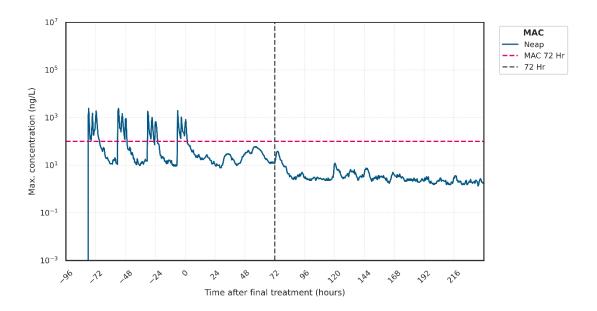


Figure 5.5 Maximum concentration of Azamethiphos during neap tide release.

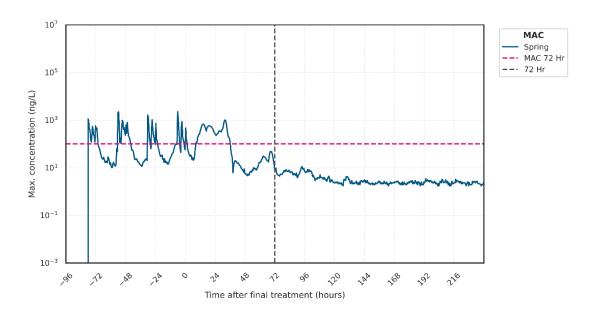


Figure 5.6 Maximum concentration of Azamethiphos during spring tide release.

5.5 Spatial Distribution

Figure 5.7 and Figure 5.8 show the spatial distribution of Azamethiphos (average concentrations in the top 4 m) during neap and spring tides, respectively. At the 3-hour mark, the discharge from a single pen resulted in no concentrations above the EQS value (250 ng/L) in each of the neap and spring tide conditions.

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Bath Treatment Dispersion Modelling at Caolas



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The spring tide release scenario shows coverage below the EQS value to the western side of the farm, however the maximum concentration observed within this plume (230 ng/L) was still below the EQS threshold (250 ng/L). During neap tide conditions, coverage to the region southeast of the farm was significantly lower than the EQS value. By the 72-hour mark, the bath treatment plumes had dispersed, falling below the EQS threshold (40 ng/L) for both neap and spring tides. This indicates that the dispersion and dilution processes have effectively mitigated any potential adverse impacts, leading to concentrations that comply with the EQS value.

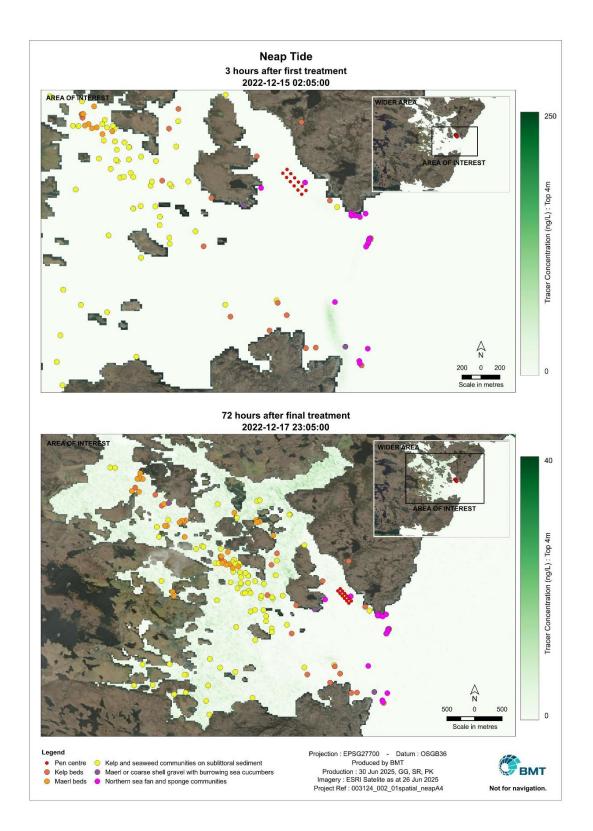


Figure 5.7 Spatial Azamethiphos distribution for tarpaulin release during neap tides, 3 hr after the initial 3-hour mass release (top) and 72 hr after the last treatment event (bottom).

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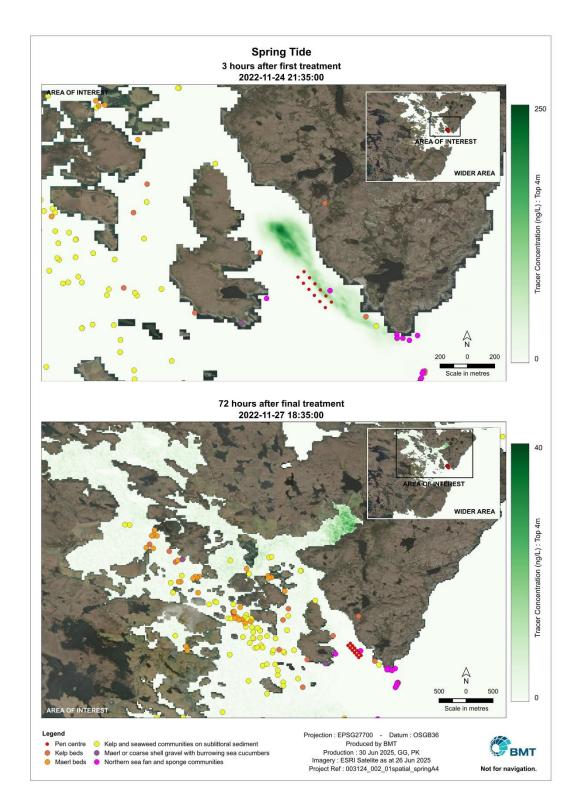


Figure 5.8 Spatial Azamethiphos distribution for tarpaulin release during spring tides, 3 hr after the initial 3-hour mass release (top) and 72 hr after the last treatment event (bottom).



5.6 Priority Marine Features

The model estimated Azamethiphos concentrations at all PMF sites within the model boundary, including sites nearest to the farm, to be below the 72-hour MAC threshold of 100 ng/L. The timeseries of maximum Azamethiphos concentration in the water column were plotted for the seven PMF sites closest to the farm for each of the spring and neap tide conditions (Figure 5.9 and Figure 5.10). The seven PMFs site details are as follows:

- Kelp beds #47610 approximately 1.0 km north-west from the farm
- Kelp beds #82166 approximately 320 m north-west from the farm
- Kelp beds #82176 approximately 25 m from the pen#11
- Kelp beds #97590 approximately 260 m east from the farm
- Maerl beds #46914 approximately 514 m west from the farm.
- Northern sea fan and sponge #21146 approximately 250 m west from the farm.
- Northern sea fan and sponge #212334 approximately 1.1 km south from the farm.

After 72 hrs from the final treatments all sites showed near zero concentrations. Note that plots for sites further from the farm were not included in the report however can be supplied upon request.



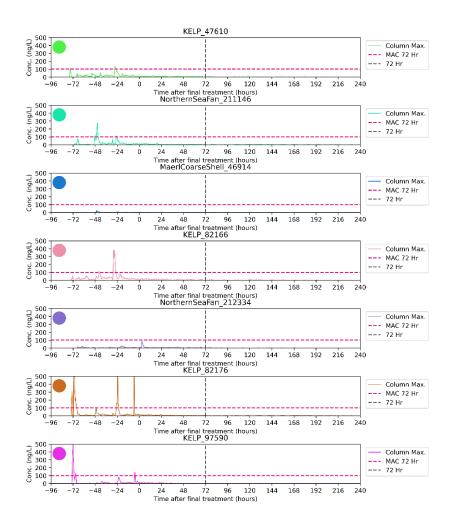




Figure 5.9 Left Panel – Maximum azamethiphos concentration in the water column at the seven closest PMF sites released during neap tide; Right Panel – locations of the selected 'near-by' PMF sites



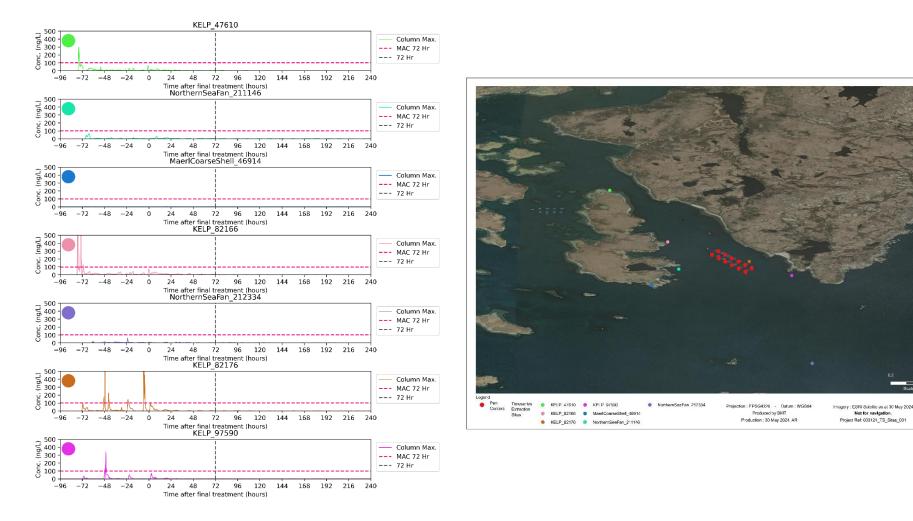


Figure 5.10 Left Panel – Maximum azamethiphos concentration in the water column at the seven closest PMF sites released during spring tide; Right Panel – locations of the selected 'near-by' PMF sites

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5.7 Sensitivity Analysis

A sensitivity analysis was performed to verify that the selected model parameter values do not significantly influence the overall outcomes of the compliance assessment. The sensitivity analysis was performed on the neap tide, as this is the theoretical worst-case simulation. Timeseries 72 hr MAC (maximum allowable concentration – 100 ng/L) and of AZE (allowable zone of effects) plotted with the 72 hr EQS (area with a concentration greater than 40 ng/L should be less than 0.5 km²) are used for comparisons.

5.7.1 Horizontal Diffusivity

Sensitivity testing was conducted on two additional horizontal dispersion parameter values alongside the base case. The EQS results (Figure 5.11) indicate that the line plots for diffusivity value of 0.8 m²/s closely aligns with the base case of 0.1 m²/s, demonstrating minimal sensitivity in terms of area exceedance. The plot line corresponding to 0.004 m²/s deviates from the base case following dosages, indicating that there is a delay in achieving dilution in comparison to the base case. Despite these differences, all tested diffusivity values remained within the Environmental Quality Standard (EQS) threshold limits.

Similarly, the MAC results (Figure 5.12) indicate that the low dispersion value case results in higher observed concentrations than the base case and high dispersion value case. The base case and high dispersion value case consistently remain below the MAC threshold and are compliant. In contrast, the low dispersion value case exceeds the threshold once, approximately 120 hours after the final dose. It is noted that this low dispersion value $(0.004 \text{ m}^2/\text{s})$ is far below the SEPA recommended value $(0.1 \text{ m}^2/\text{s})$.

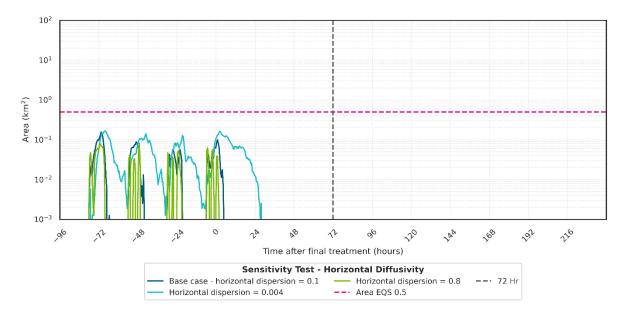


Figure 5.11 Timeseries of area exceeding 40 ng/L Azamethiphos concentration, from water column maximum, comparing a range of horizontal scalar diffusivity values.

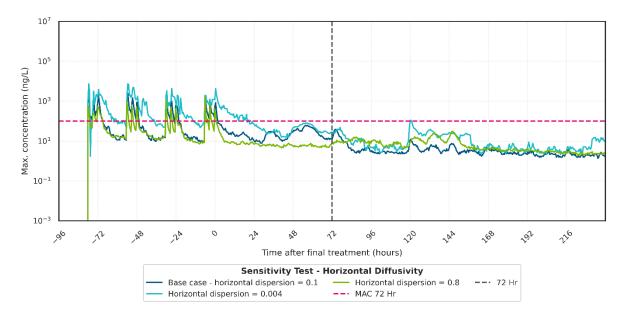


Figure 5.12 Timeseries of maximum Azamethiphos concentration in water column, comparing a range of horizontal scalar diffusivity values.

5.7.2 Vertical Scalar Diffusivity

Sensitivity testing was conducted for an additional dispersion parameter value (1.0 m²/s) alongside the base case (0.001 m²/s). The EQS results (Figure 5.13) show strong alignment of the two constant values, with both remaining well below the EQS limits. Likewise, the MAC results (Figure 5.14) indicate strong agreement of the two cases, which both achieving compliance according to the MAC threshold value.

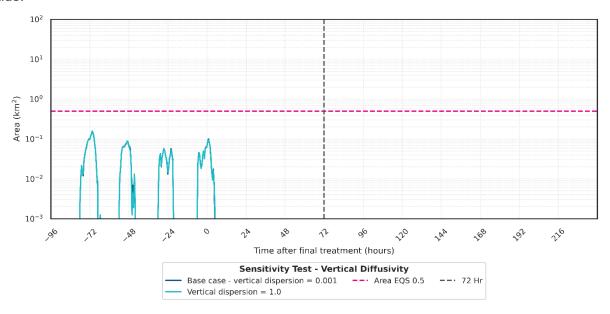


Figure 5.13 Timeseries of area exceeding 40 ng/L Azamethiphos concentration, from water column maximum, comparing vertical scalar diffusivity values.

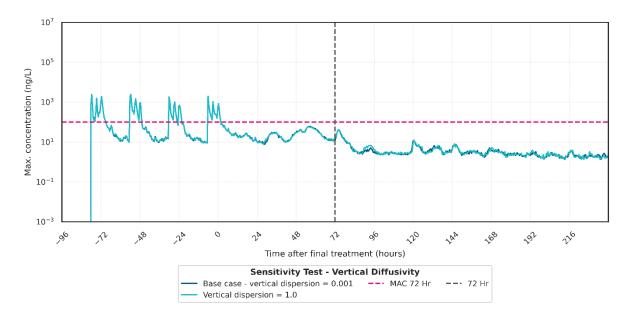


Figure 5.14 Timeseries of maximum Azamethiphos concentration in water column, comparing vertical scalar diffusivity values.

5.7.3 Time of Release

Varying the time of release by +/- 6 hours was included to ensure a range of bath treatment release times relating to tidal cycles were tested for sensitivity in results. Each of the results for EQS (Figure 5.15) and MAC (Figure 5.16) indicate similarity in magnitudes amongst the three cases, with the base case exhibiting slightly higher peaks. Small variations are observable between the shapes of the lines, however all three cases achieve compliance, remaining below the EQS and MAC threshold values.

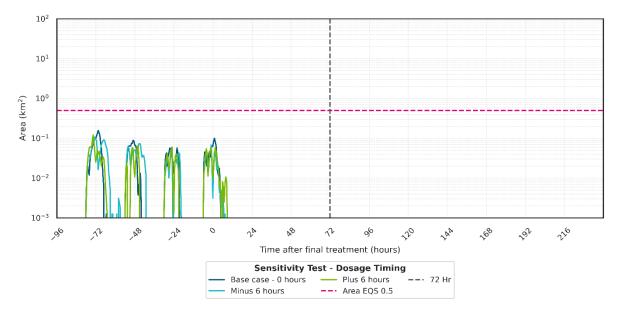


Figure 5.15 Timeseries of area exceeding 40 ng/L Azamethiphos concentration, from water column maximum, comparing various dosage timings.

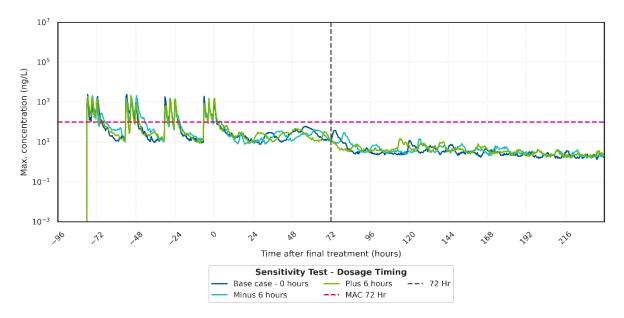


Figure 5.16 Timeseries of maximum Azamethiphos concentration in water column, comparing various dosage timings.

5.7.4 Grid Size

The cell area within the structured grid was increased from the base case (25 m x 25 m) to each of 50 m x 50 m and 100 m x 100 m to investigate sensitivity. Both the EQS (Figure 5.17) and MAC (Figure 5.18) results indicate that the base case is the most conservative, with increased cell area appearing to dilute observed concentrations. All three cases are below EQS and MAC threshold values, achieving compliance.

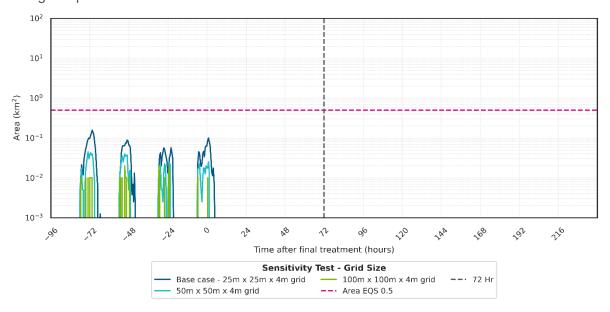


Figure 5.17 Timeseries of area exceeding 40 ng/L Azamethiphos concentration, from water column maximum, comparing various grid sizes.

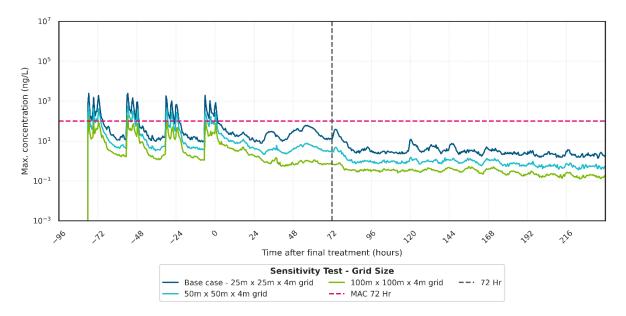


Figure 5.18 Timeseries of maximum Azamethiphos concentration in water column, comparing various grid sizes.

5.7.5 Particle Count

To investigate the sensitivity of total particle count, the number of particles was decreased from the base case (1.2 million) to two different cases of 120,000 particles and 36,000 particles. The EQS (Figure 5.19) indicate general alignment between the three cases, with the lowest particle count appearing most conservative. Likewise, the MAC results (Figure 5.20) indicate higher observed concentrations with lower particle counts, although all three cases achieve compliance.

While lower particle counts tend to produce more conservative estimates, a higher number of particles is necessary to adequately resolve spatial and temporal variations in concentration, as evidenced by the smoother concentration gradients in the base case. Nonetheless, increasing the particle count introduces greater computational demand. Therefore, selecting an appropriate particle number requires balancing sufficient spatial resolution with computational efficiency.

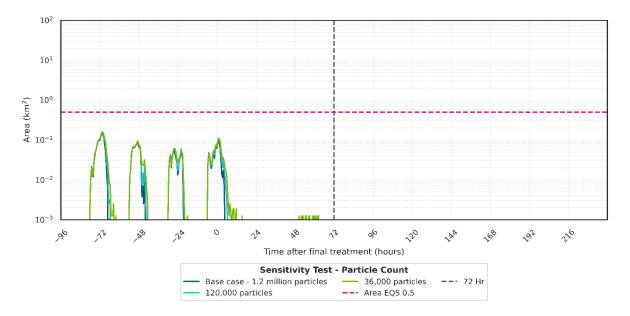


Figure 5.19 Timeseries of area exceeding 40 ng/L Azamethiphos concentration, from water column maximum, comparing various particle counts.

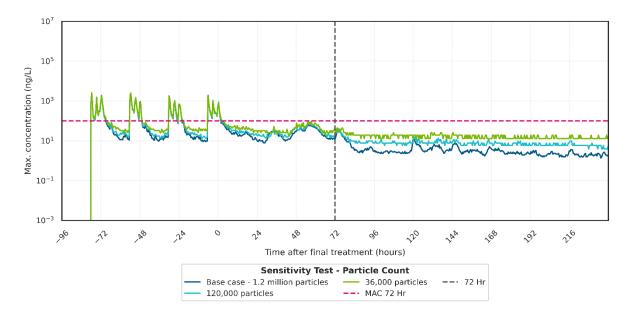


Figure 5.20 Timeseries of maximum Azamethiphos concentration in water column, comparing various particle counts.

6 Summary and Conclusions

6.1 Hydrodynamic Calibration

- This model demonstrates good calibration of water levels, effectively representing the differences between spring and neap tidal cycles.
- This model represents the velocity magnitude reasonably well, with the MAE consistently below 0.1 m/s, which is the SEPA guideline (SEPA, 2019). This magnitude is a critical factor in determining the dispersion rate of the bath treatment from the site, and its impact on priority marine features.
- The direction calibration is weaker, likely due to limitations in the bathymetry data. It should also be
 noted that there are uncertainties surrounding the ADCP directions. As well as this, the complexity
 of the area, the lack of strong bi-directional flow and low speeds further complicate modelling due to
 the numerous interacting factors.
- This study identifies challenges in the model calibration process and acknowledges that some model performance statistics are marginally within SEPA criteria. The model represents the best 'fit for purpose' calibration based on the data available at the time.

6.2 Dispersion Modelling

- This technical report outlines the simulation of bath treatment chemical 'Azamethiphos' at the Caolas finfish site, with a focus on addressing concerns related to Priority Marine Features (PMFs) as raised by SEPA in their 2023 screening modelling and risk identification report (SEPA 2023).
- The application of a calibrated hydrodynamic model allowed for the simulation of bath treatments at the site.
- The Lagrangian based particle tracking model was used to assess environmental compliance during the use of Azamethiphos as a bath treatment chemical. Particle releases were designed to replicate realistic treatment regimes, with three treatments per day at a 3-hour interval. To represent a worstcase scenario, neighbouring pens were consecutively treated with 300 g of Azamethiphos per treatment (daily total 900 g) over four consecutive days, with the final pen treated on day four. The total amount of Azamethiphos discharged over the four-day period was 3.6 kg.
- The simulations were conducted for release during neap and spring tides, while varying diffusion coefficients and time of release start time to assess the sensitivity of the outcomes to key model parameters.
- Based on the model results, it was concluded that the proposed treatment scenarios, involving 300 g per pen with up to three pens treated per day (daily total 900 g), were predicted to consistently meet all EQS as prescribed by SEPA. The maximum concentration observed during the baseline simulations, 72 hours after the final treatment, was found to be less than 11 ng/L, well below the allowable limit. Additionally, predicted AZEs for EQS of 40 ng/L were zero for both spring and neap tide conditions within 72 hours of the final treatment.
- The sensitivity tests performed on horizontal diffusivity, vertical diffusivity, starting times, grid
 resolution and particle count for EQS consistently indicated that the predicted chemical
 concentrations are likely to meet the EQS criteria.



- During spring tides, a slightly greater chemical dispersion was observed compared to neap tides.
 However, predicted concentrations showed a significantly faster rate of decrease during spring tides
 as opposed to neap tides. In both neap and spring scenarios, the predicted chemical levels
 consistently met the EQS criteria.
- As part of the analysis of dispersion model simulations, the impact of bath treatments on Priority
 Marine Features (PMFs) in the wider area around the farm was investigated. The concentration
 levels of Azamethiphos were assessed during and after treatments, and it was found that they never
 exceeded the permissible limit. Additionally, the concentration values remained below 40 ng/L at the
 72-hr mark from the final treatment at all PMFs located near the farm.
- The TUFLOW FV coupled hydrodynamic and particle tracking model used in this study was applied
 to demonstrate that the proposed use of bath treatments with Azamethiphos at the Caolas site is
 likely to comply with SEPA EQS. Additionally, the potential risks to PMFs in the vicinity of the farm
 sites were assessed to be minimal.

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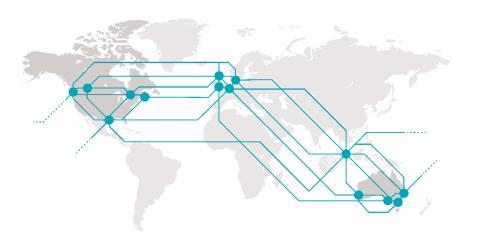
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