26th International Congress on Modelling and Simulation, Adelaide, SA, Australia, 30 Nov–4 Dec 2025
mssanz.org.au/modsim2025

Tracking the cure: Finding the right numerical tool for bath treatment dispersion

GL Gunaratne [a], GL Stones [a], LC Bruce [a]

[a] *BMT Commercial Australia, Pvt Ltd, Perth, Australia*
Email: gayan.gunaratne@apac.bmt.org

Abstract: Reasonable prediction of bath treatment dispersion is an essential step in the assessment of environmental risk and demonstration of regulatory compliance in marine aquaculture systems. This study compares two numerical modelling approaches—Lagrangian structured grid (LSG) and Eulerian–Lagrangian flexible grid (ELF)—to evaluate their performance in simulating the dispersion of Azamethiphos under regulatory conditions. Using a calibrated hydrodynamic model and a structured sensitivity analysis, we assessed environmental quality standards (EQS) compliance areas, and maximum allowable concentration (MAC) exceedance footprints, the impact of grid resolution, and particle counts, on predicted concentration fields. Results show that ELF methods produce larger and more conservative dispersion footprints, while LSG offers smoother gradients with lower peak concentrations. Both methods achieved compliance under Scottish EQS criteria, but their sensitivity to configuration parameters highlights the need for careful model selection. This study provides practical guidance for balancing computational efficiency and regulatory robustness in bath treatment modelling.

Keywords: *Azamethiphos, dispersion, modelling, aquaculture, particle tracking, TUFLOW*

1. INTRODUCTION

Bath treatments are widely used in aquaculture to control parasites and maintain fish health (Burridge et al. 2010), but their dispersion and dilution in the marine environment must be accurately predicted to ensure compliance with environmental quality standards (Sævik et al. 2022). Regulatory frameworks typically require that concentrations remain below specified thresholds over defined periods, such as 72 hours (SEPA 2024). Failure to meet these criteria can lead to environmental harm and regulatory non-compliance, making robust dispersion modelling a critical component of environmental impact assessments.

Numerical modelling is the primary tool for predicting the fate and transport of bath treatment chemicals. Two dominant approaches are employed: Eulerian (tracer-based) and Lagrangian (particle tracking-based) methods (BMT 2023a, 2023b, Page et al. 2023). Eulerian models represent concentration as a scalar field on a fixed grid, offering efficient compliance mapping but introducing potential numerical diffusion, particularly in advection-dominated flows (Page et al. 2015). As a result of these factors, regulatory authorities typically do not support the Eulerian-based approach; instead, the Lagrangian method is recommended. Lagrangian models with random walk particle tracking (RWPT) on structured grid (LSG), by contrast, track discrete particles, conserving mass and avoiding numerical diffusion, but they can exhibit reconcentration artifacts, and higher computational demands (Suh 2006, Talbi et al. 2021). Even with higher computational power, the particle number must be restricted because the saving and tracking of the history of every particle requires large amounts of memory and computing time (Suh 2006).

Thus, a combined method that exploits the desirable characteristics of Eulerian and Lagrangian such as Eulerian–Lagrangian approach on flexible (unstructured) grid (ELF), have been developed for coastal dispersion modelling in advection-dominated systems (Suh 2006). In the combined 'ELF' method, the Lagrangian with RWPT was incorporated into the concentration model by projecting the number of particles into a Eulerian control volume. Both methods are sensitive to model configuration choices, including mesh resolution, domain size, dispersion coefficients, and, in the case of Lagrangian models, particle count.

Although Lagrangian structured grid (LSG) methods are widely applied in bath treatment modelling, to the authors' knowledge, the hybrid Eulerian–Lagrangian flexible grid (ELF) approach has not been previously documented in this context. This absence can be attributed to regulatory modelling guidance, which has historically favoured LSG methods, combined with the ELF method's limited regulatory precedent and the perception of increased methodological complexity. Furthermore, no systematic comparison of these methods under controlled conditions relevant to aquaculture compliance assessments has been published to date. This knowledge gap is significant because method selection and parameterisation can materially influence predicted compliance footprints and, consequently, regulatory outcomes. To address this gap, the present study systematically evaluates the sensitivity of predicted bath treatment dispersion to the choice of numerical method and key model configuration parameters. A structured one-factor-at-a-time (OFAT) sensitivity analysis was conducted across both LSG and ELF approaches, examining the influence of individual parameters on spatial and temporal concentration fields, 72-hour EQS compliance areas, and MAC exceedance footprints. The findings provide practical guidance for selecting and configuring models to balance accuracy, computational efficiency, and regulatory robustness.

1.1. Regulatory context

When Azamethiphos, a bath treatment chemical, 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 2024). For this exercise, bath treatments EQS criteria in Scotland were used because of the ease of use in comparative analysis as they are established guidelines, used in salmon aquaculture. Key compliance criteria are listed in Table 1 with full methods described in SEPA (2024). 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, which is 0.06 km^2 for the selected study site (TransTech Environmental, 2023a). 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 km^2, while the maximum concentration in the domain should not exceed 100 ng/L (maximum allowable concentration - MAC)

Table 1 Environmental Quality Standards (EQSs) for Azamethiphos (SEPA 2024)

Standards for Azamethiphos Timescale	Standard (ng per litre)	Type
3 hours	250	EQS
72 hours	40	EQS
72 hours	100	MAC

1.2. Study site

The modelling study was conducted for a salmon farm located in a semi-exposed Scottish loch. The site comprises 12 net pens, all intended for treatment against salmon lice infestation (TransTech Environmental, 2023b). The surrounding environment features complex morphometry, including shallow mudflats and smaller embayments adjacent to the farm. These characteristics influence local hydrodynamics and, consequently, the dispersion of bath treatment chemicals. The site's semi-exposed nature introduces tidal and wind-driven variability, making it a representative case for sensitivity analysis of numerical methods under realistic operational conditions.

2. HYDRODYNAMIC MODELLING

The hydrodynamic model was calibrated during a previous work using observed water levels and current magnitude/direction from ADCP deployments. TUFLOW FV hydrodynamic model platform (TUFLOW 2020, 2023) was used for the calibration assessment. Calibration achieved skill metrics within accepted thresholds (Table 2). Full hydrodynamic model calibration details, including ADCP data, domain configuration, bathymetry, boundary conditions, and observation datasets and error statistics are provided in BMT (2024) and TransTech Environmental (2023c)**.**

Table 2 Skill metrics for the hydrodynamic calibration

Position	Extraction Depth (m above seabed)	Variable	R	BIAS	MAE	RMSE
–	–	Water level	0.98	0.10 m	0.18 m	0.22 m
Sub-surface	22.35–23.35	Vx	0.34	-0.00 m/s	0.04 m/s	0.05 m/s
Sub-surface	22.35–23.35	Vy	0.13	0.06 m/s	0.06 m/s	0.07 m/s
Near-bottom	17.35–18.35	Vx	0.36	0.01 m/s	0.03 m/s	0.04 m/s
Near-bottom	17.35–18.35	Vy	0.31	0.00 m/s	0.03 m/s	0.05 m/s

Position	Extraction Depth (m above seabed)	Variable	R	BIAS	MAE	RMSE
Near-bed	2.35–3.35	Vx	0.04	0.02 m/s	0.04 m/s	0.05 m/s
Near-bed	2.35–3.35	Vy	0.23	-0.11 m/s	0.11 m/s	0.12 m/s

3. DISPERSION MODELLING

3.1. Simulation periods

To simulate the worst-case condition, the dispersion modelling was conducted using TUFLOW FV (TUFLOW 2020, 2023) flow fields over a period of two weeks centred on a small neap tidal range taken from the calibrated hydrodynamic model simulations (Table 3). These ambient conditions were considered the least dispersive, meaning that under such conditions, Azamethiphos dispersion was least likely to achieve the required EQS. The timing of the last treatment coincided with the neap maxima, reinforcing the selection of this period as the most conservative scenario; for the 3-hour EQS assessment, the single release overlapped with this same neap maxima.

Table 3 Model simulation period

Tide Type	Model Start	Model End	First Treatment	Last Treatment	Tidal Cycle Characteristics
Neap Tide	08/12/2022 00:00:00	08/01/2023 00:00:00	11/12/2022 17:00:00	14/12/2022 23:05:00	Smallest maxima of the neap tidal cycle, final treatment at highwater

3.1.1. 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 to represent a realistic daily treatment campaign (Pers com. Loch Duart). A total of 3.6 kg of Azamethiphos was discharged over the four-day period. 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 (uniformly distributed across this 4 m depth). 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.

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 a pen. 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.

3.2. Sensitivity analysis

A structured one-factor-at-a-time (OFAT) sensitivity analysis was undertaken to quantify the influence of individual configuration parameters on predicted bath treatment dispersion. This flowchart summarises the

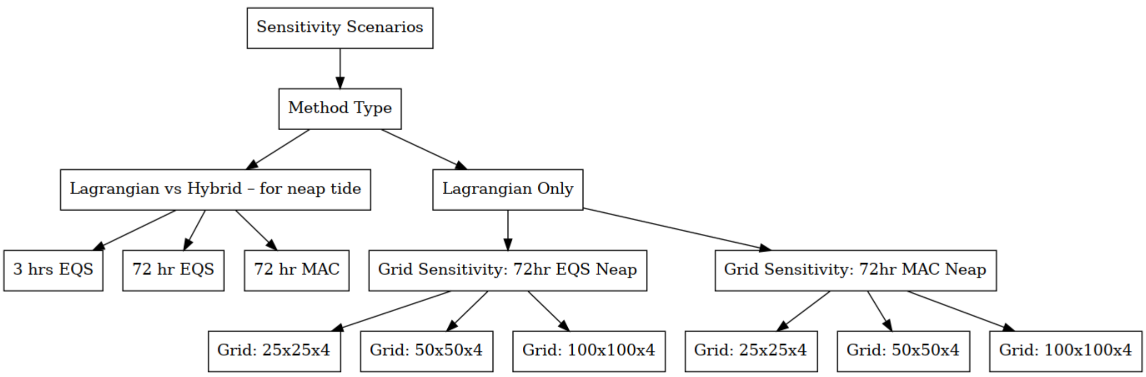

Figure 1 Flow chart for structured one-factor-at-a-time (OFAT) sensitivity scenarios

structured sensitivity scenarios undertaken to compare Lagrangian (LSG) and Lagrangian-Eulerian hybrid (ELF) methods for bath treatment dispersion modelling (Figure 1).

Scenarios were organised by method type, simulation duration (3hr or 72hr), and metric (EQS or MAC) for the neap tidal period. Additional grid resolution and particle count tests were conducted for LSG configurations to evaluate spatial discretisation effects. To assess numerical convergence and artefact resolution in Lagrangian simulations, a particle count sensitivity analysis was conducted using three configurations: 1.2 million particles (high-resolution), 120,000 particles (intermediate resolution), and 36,000 particles (low-resolution). These simulations were evaluated to determine the minimum particle count required to produce stable and realistic concentration fields, particularly within re-circulation zones where numerical noise is more pronounced. In this context, numerical noise refers to spurious fluctuations in concentration values that arise from insufficient particle density rather than representing true physical variability. Additionally, grid resolution sensitivity was examined using three spatial discretisations: 25 × 25 × 4 m, 50 × 50 × 4 m, and 100 × 100 × 4 m. The vertical grid depth of 4 m was selected to align with the bath treatment release depth, ensuring compatibility between particle injection and hydrodynamic representation. These tests support the selection of optimal resolution parameters for robust and computationally efficient dispersion modelling.

4. RESULTS

4.1. LSG vs ELF – Neap tide 3hr EQS, 72 hr EQS and 72 hr MAC

Error! Reference source not found. (top) shows 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 tide. The size of the chemical plume following a single treatment remained well below the calculated near-field mixing zone after 3 hours for both LSG (structured) and ELF (unstructured) methods. The near-field footprint was more than ten times larger for the ELF method. Throughout the neap tide period, the area with concentrations exceeding 250 ng/L stayed below the EQS threshold, indicating no breach of the EQS threshold.

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 **Error! Reference source not found.** (middle). For both LSG (structured) and ELF (unstructured) and the area greater than 40 ng/L never exceeded 0.5 km² however for the ELF method it exceeded but nothing exceeded after 72 hrs from the final treatment.

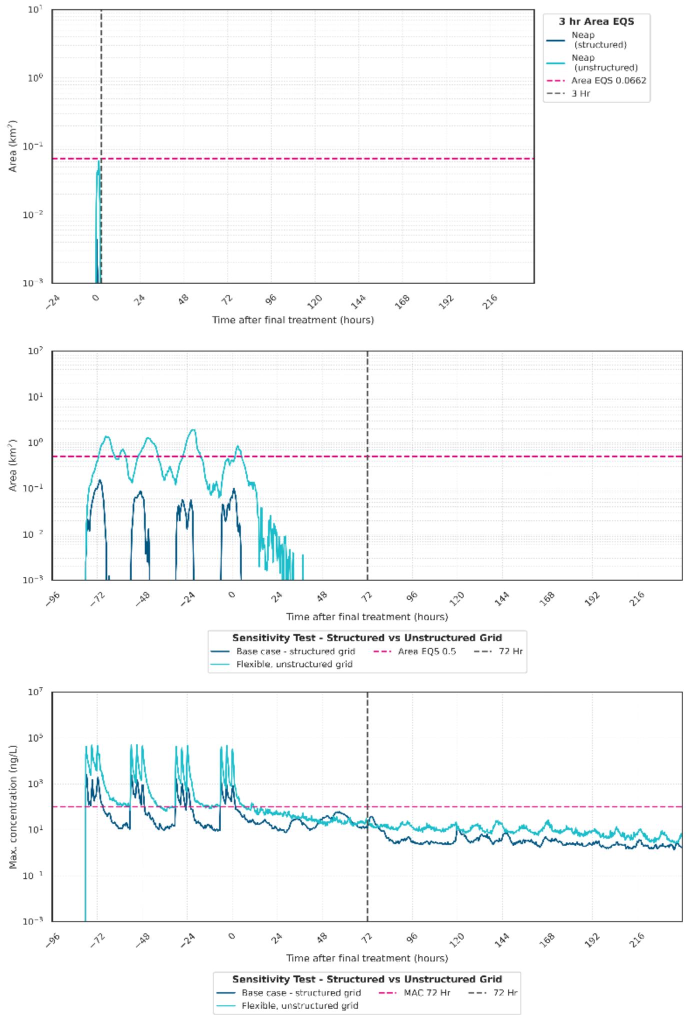

Figure 2 LSG Vs ELF comparison during Neap tide; 3hr EQS (top), 72 hr EQS (middle) and 72 hr MAC (bottom)

The full treatment regime was simulated to evaluate compliance with the 72-hour MAC criterion. Each individual pen treatment involved the release of 300 g of Azamethiphos, resulting in a maximum daily discharge of 900 g and a cumulative release of 3.6 kg over a four-day period. The resulting maximum concentrations within the entire water column during the neap tide cycle are presented in **Error! Reference source not found.** (bottom) for both the LSG (structured) and ELF (unstructured) methods. Distinct peaks in concentration correspond to individual pen treatments, reflecting the rapid introduction of chemical mass into the model domain. These peaks were followed by a sharp decline due to dispersion and first-order decay processes. At 72 hours post-final treatment, concentrations across the domain remained well below the 100 ng/L MAC threshold. Notably, the ELF method, which employs a flexible unstructured grid, produced peak concentrations nearly an order of magnitude higher than those predicted by the LSG approach, highlighting the conservative nature of the ELF hybrid method in representing far-field exposure.

4.2. 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 and MAC (Figure 3**Error! Reference source not found.**) results indicate that the base case was the most conservative, with increased cell areas acting to dilute simulated concentrations. All three cases met the EQS and MAC threshold values, achieving compliance.

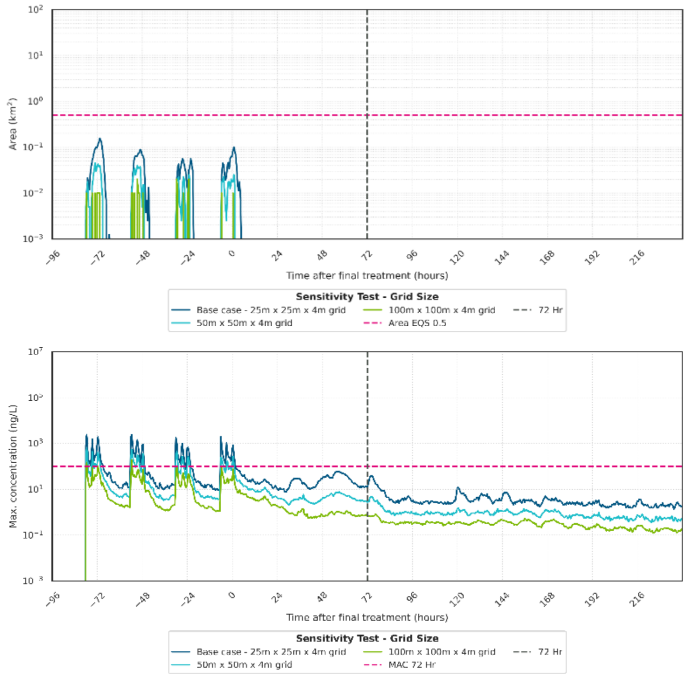

Figure 3 Sensitivity analysis comparing different grid sizes under 72hr EQS (top) and 72 hr MAC (bottom) for LSG neap tide conditions

4.3. 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 in LSG approach. The EQS (Figure 4) indicated general alignment between the three cases, with the lowest particle count appearing most conservative. Likewise, the MAC results indicated higher observed concentrations with lower particle counts, although all three cases achieve compliance. While lower particle counts tended to produce more conservative estimates, a higher number of particles was necessary to adequately resolve spatial and temporal variations in concentration, as evidenced by the smoother concentration gradients in the base case.

5. DISCUSSION

5.1. LSG vs ELF – Neap tide 3hr EQS, 72 hr EQS and 72 hr MAC

The comparative analysis of LSG and ELF modelling approaches revealed significant differences in predicted dispersion footprints, particularly under low-dispersion neap tide conditions. The ELF method consistently produced larger plume areas and higher peak concentrations, suggesting a more conservative representation of chemical transport. This aligns with findings from Suh (2006), who noted that hybrid methods can amplify concentration estimates due to particle-to-grid projection effects. Conversely, the LSG approach demonstrated smoother concentration gradients and lower peak values consistent with its mass-conserving formulation and reduced susceptibility to numerical diffusion. This observation aligns with Talbi et al. (2021), who reported similar performance characteristics in Lagrangian RWPT dispersion modelling.

Importantly, this study simulated the dispersion of a dissolved chemical (Azamethiphos) using particle-based techniques. While this introduced conceptual limitations, since particles do not physically dissolve or diffuse, the random walk and decay algorithms embedded in both LSG and ELF frameworks allowed for an effective approximation of solute behaviour. This hybridisation of particle tracking for dissolved substances is increasingly common in environmental modelling, but it requires careful interpretation of results, especially when assessing concentration thresholds.

The 3-hour and 72-hour EQS thresholds were primarily designed to assess near-field impacts, where concentrations were highest shortly after release and within close proximity to the source. These metrics were sensitive to local hydrodynamics and model resolution, making them useful for evaluating immediate compliance risks. In contrast, the 72-hour MAC criterion reflected far-field exposure, capturing the cumulative effects of dispersion and decay over time and space. In this study, both LSG and ELF methods demonstrated compliance across all metrics; however, their behaviour diverged under different spatial and temporal scales. ELF may produce higher near-field concentration estimates due to its conservative particle-to-grid projection approach, while LSG tends to yield smoother and more stable concentration fields that may better reflect far-field dilution. However, in the absence of measured data for validation, it is not possible to determine whether these differences represent overestimation, underestimation, or accurate predictions. This distinction plays a crucial role in determining the appropriate modelling approach, depending on whether the regulatory emphasis is on acute, localised exposure or on broader, long-term environmental risk.

5.2. Grid Size

Grid resolution had a measurable impact on concentration estimates. Increasing cell size from 25 m × 25 m to 100 m × 100 m diluted concentration fields, with all configurations remaining below EQS and MAC thresholds. The base case (25 m × 25 m) was the most conservative, capturing finer-scale gradients and potential hotspots. These findings align with Page et al. (2015), who emphasised the importance of high-resolution grids in advection-dominated systems. While coarser grids reduce computational demand, they risk underestimating localised exceedances, particularly in complex bathymetric environments. Therefore, grid resolution should be selected based on the regulatory context and the spatial scale of interest.

5.3. Particle Count

Particle count sensitivity analysis showed that lower particle numbers tend to produce more conservative concentration estimates, but at the cost of increased numerical noise and reduced spatial fidelity. The base case with 1.2 million particles provided the smoothest and potentially more realistic concentration fields, especially in recirculation zones. These findings support Suh (2006), who noted that adequate particle resolution is essential for capturing transport dynamics without introducing artefacts. While higher particle counts improve model fidelity, they also increase computational load. Thus, modellers must balance resolution with efficiency, particularly when conducting multi-scenario assessments or real-time operational modelling.

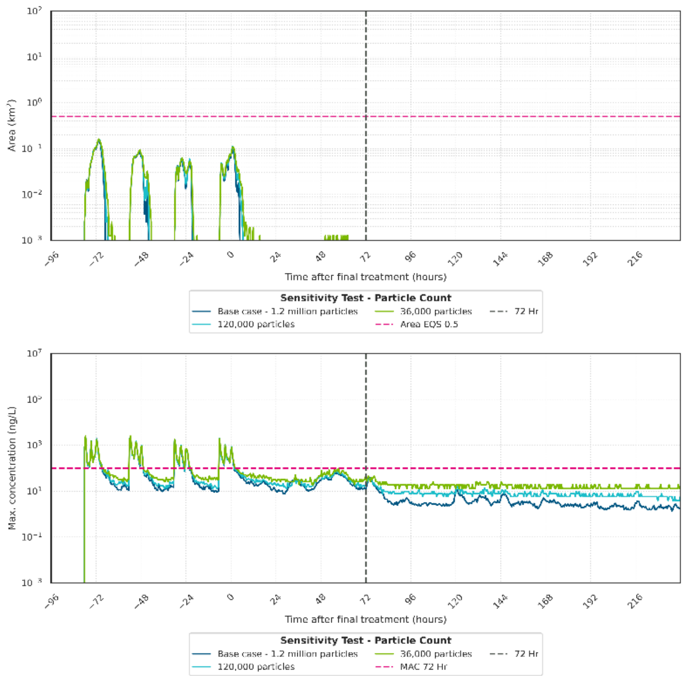

Figure 4 Sensitivity analysis comparing different particle counts under 72hr EQS (top) and 72 hr MAC (bottom) for LSG neap tide conditions

6. CONCLUSION

This study presents a systematic comparison of Lagrangian structured grid (LSG) and Eulerian–Lagrangian flexible grid (ELF) approaches for modelling bath treatment dispersion under realistic aquaculture conditions. By evaluating the influence of grid resolution, particle count, and numerical method on compliance with EQS and MAC thresholds, the analysis provided practical guidance for selecting and configuring models to meet regulatory requirements.

The use of particle-based techniques to simulate the behaviour of dissolved substances introduced conceptual limitations, as particles do not physically dissolve. However, the incorporation of random walk and decay algorithms enabled a reasonable approximation of solute transport, making these methods viable for environmental modelling applications.

Sensitivity analyses revealed that larger grid cells may dilute concentration estimates and underestimate risk, while lower particle counts can introduce numerical noise and exaggerate peak concentrations. These findings reinforce the importance of high-resolution modelling in compliance-critical scenarios, as supported by Page et al. (2015) and SEPA (2024).

By addressing the lack of published comparisons between LSG and ELF methods in aquaculture contexts, this study offers actionable insights for environmental consultants, regulators, and farm operators. The results support informed method selection based on modelling objectives whether for conservative screening, hotspot identification, or operational planning and contribute to more transparent, defensible, and effective environmental impact assessments.

ACKNOWLEDGMENTS

This research was supported by funding from the BMT Innovation Hub. We extend our gratitude to Naomi Dempsey and the team at Loch Duart Salmon Company for their invaluable contributions, particularly in providing site-specific data and operational insights that informed the modelling scenarios. We would also like to thank Ian Teakle and Alex Waterhouse for their valuable technical advice, which greatly assisted in refining our modelling approach and interpretation of results.

REFERENCES

BMT (2024) Calibration of TUFLOW FV model with ADCP data at Caolas for Loch Duart Technical Report prepared for Loch Duart Pvt Ltd (Unpublished data)

BMT (2023a) Bath Treatment Dispersion Modelling at Reintraid; Dispersion modelling for Azamethiphos bath treatment consent limits for Reintraid farm site at Loch a' Chairn Bháin, Scotland. Technical Report prepared for Loch Duart Pvt Ltd

BMT (2023b) Bath Treatment Dispersion Modelling; Dispersion modelling for Azamethiphos bath treatment consent limits for Oldany farm site, northwest Scotland. Technical Report prepared for Loch Duart Pvt Ltd

Burridge L, Weis JS, Cabello F, Pizarro J and Bostick K (2010) Chemical use in salmon aquaculture: A review of current practices and possible environmental effects. In Aquaculture (Vol. 306, Issues 1–4, pp. 7–23). https://doi.org/10.1016/j.aquaculture.2010.05.020

Page FH, Losier R, Haigh S, Bakker J, Chang BD, Mccurdy P, Beattie M, Haughn K, Thorpe B, Fife J, Scouten S, Greenberg D, Ernst W, Wong D, & Bartlett G (2015) Canadian Science Advisory Secretariat (CSAS) Transport and dispersal of sea lice bath therapeutants from salmon farm net-pens and well-boats. http://www.dfo-mpo.gc.ca/csas-sccs/

Page FH, Haigh SP, O'Flaherty-Sproul MPA, Wong DKH, & Chang BD (2023) Modelling and predicting ecosystem exposure to bath pesticides discharged from marine fish farm operations: an initial perspective. Canadian Science Advisory Secretariat (CSAS).

Sævik PN, Agnalt AL, Samuelsen OB, & Myksvoll M (2022) Modelling chemical releases from fish farms: Impact zones, dissolution time, and exposure probability. ICES Journal of Marine Science, 79(1), 22–33. https://doi.org/10.1093/icesjms/fsab224

Scottish Environmental Protection Agency (SEPA) (2024) Marine Modelling Guidance for Aquaculture Applications.

Suh SW (2006) A hybrid approach to particle tracking and Eulerian-Lagrangian models in the simulation of coastal dispersion. Environmental Modelling and Software, 21(2), 234–242. https://doi.org/10.1016/j.envsoft.2004.04.015

Talbi H, Chaabelasri E, Jeyar M, & Salhi N (2021) Random Walk Particle Tracking for Convection-diffusion Dominated Problems in Shallow Water Flows. Journal of Applied and Computational Mechanics, 7(2), 486–495. https://doi.org/10.22055/jacm.2020.35154.2579

TransTech Environmental (2023a) NewDEPOMOD & BathAuto MODELLING - Method Statement for Caolas Loch Portain Finfish Pen Site, Loch Portain, North Uist.

TransTech Environmental (2023b) Bath Treatment Modelling Report, Caolas Finfish Pen Site, Loch Portain, North Uist, Annex A.

TransTech Environmental (2023c) Caolas Dec 2022-Feb 2023 ADCP Deployment, Unpublished field notes

TUFLOW (2020) TUFLOW FV Flexible Mesh Modelling, User Manual: Build 2020.02. https://www.tuflow.com.

TUFLOW (2023) TUFLOW FV Flexible Mesh Modelling; Science Manual, Build 2023.0.

