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Modelling and Predicting Ecosystem Exposure to Bath Pesticides Discharged from Marine Fish Farm Operations: An Initial Perspective

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Foreword

This series documents the scientific basis for the evaluation of aquatic resources and ecosystems in Canada. As such, it addresses the issues of the day in the time frames required and the documents it contains are not intended as definitive statements on the subjects addressed but rather as progress reports on ongoing investigations.

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ABSTRACT

This document focuses on models in relation to the discharge of chemical active ingredients associated with bath pesticide treatments used in net-pen finfish aquaculture operations. The document includes a brief overview of the context and associated conceptual processes to be modelled, specific modelling challenges, a review of modelling efforts to date, and a description of some simple models. In general, modelling for bath pesticides for discharge and dispersal is in an early stage of development. There have been few modelling efforts and few extensively calibrated or validated models. Furthermore, few models have been incorporated into pesticide management considerations.

Models range in complexity from models that make many simplifying assumptions, such as a constant current, to models that use more realistic representations, for example temporally and spatially varying currents. In general, outputs from models which use non-spatially varying currents may not be representative when displacement distances are greater than 500 m. This is problematic since displacement distances of bath pesticide discharges are often greater than 500 m. Hydrodynamic models are one potential solution; however, their implementation and operation is resource intensive and predictions are imperfect representations of real-world situations. Nevertheless, their use should be considered when predicted displacement distances exceed 500 m.

All models have uncertainties and sensitivities associated with them. In general, models for predicting exposure to bath pesticides have not been extensively explored and quantified, including sensitivities to hydrographic detail and resolution, initial condition specification, and active ingredient behaviour. Predictive models, whether they are forecast or hindcast models, are subject to the validity of the assumptions made about future and past conditions; since these are often not well known, any model output needs to be interpreted cautiously and with appropriate respect for the uncertainties. Calibration and validation of models are challenging due to the difficulties in obtaining spatially and temporally extensive observations associated with discharges from multiple farm sites and multiple treatment scenarios.

Despite the uncertainties, models can be useful for regulatory decision support. Model selection depends on the decision maker’s needs; and the interpretation of model results requires clearly defined decision rules. Specific recommendations on model selection will require further clarification of management needs, more detailed evaluations of model uncertainties and sensitivities, as well as verification and validation of chosen models.

INTRODUCTION

As a result of the Government of Canada wanting to improve its regulation of the use of pesticides and drugs by the Canadian finfish aquaculture industry, the Aquaculture Management Directorate of Fisheries and Oceans Canada (DFO) in conjunction with Environment and Climate Change Canada (ECCC) and Health Canada's Pest Management Regulatory Agency (PMRA) have sought scientific advice on several aspects of chemical use by the industry, the potential for environmental exposure to the chemicals, the potential to estimate or model these exposures and impacts, and the potential for sampling and monitoring the exposures and impacts. This research document contributes to this body of advice.

This paper is an initial scoping of the nature of bath pesticide discharges, a review of published models, and a presentation of some preliminary new models that have been developed to describe and predict the characteristics and dimensions of the discharges and their associated exposure domains. The chemical properties, behaviour, toxicity, and thresholds of pesticides used in marine aquaculture operations have been summarized and reviewed in other documents (Burridge and Holmes 2023; Chang et al. 2022; Hamoutene et al. 2023). The objective of this document is to provide an overview of the approaches and models used to predict the potential exposure domains and environmental impacts associated with pesticides discharged from bath treatments of marine finfish aquaculture. Modelling of in-feed treatments is covered in a separate document (Page et al. 2023).

TREATMENT METHODS

Fish are treated with bath pesticides by immersing them for a pre-determined time period in a water bath containing the pesticide. The baths are of two types: open and closed. Closed baths include a tarped net-pen or a well-boat. Open baths include skirting of net-pens. Although skirting is easier to implement it tends to experience loss of pesticide through the bottom of the skirt and hence more pesticide is used to achieve target bath concentrations (Wells et al. 1990). The skirting approach is not considered in this review; in Canada, it is not a preferred pesticide administration method (Health Canada 2017) and, as far as we know, it is very rarely, if ever, used at the present time.

TARPING

The tarping approach has been observed and described by several authors, for example, Wells et al. (1990), Ernst et al. (2001, 2014), Page et al. (2015), and Beattie and Bridger (2023). Tarping involves raising the bottom weight ring of a net-pen mesh to within 3 to 4 m below the sea surface and surrounding the raised net with a tarpaulin that is impermeable to water flow. A quantity of concentrated bath pesticide is added to this tarped volume by pumping, spraying, or pouring. It is generally assumed that the pesticide is thoroughly dissolved and mixed in the prepared stock solution and subsequently homogeneously mixed throughout the bath volume, although this may not always be the case (Page et al. 2015). The fish are allowed to swim freely in the pesticide bath for a specified period of time. The time varies with the pesticide, the condition and behaviour of the fish, and the oxygen content and temperature of the water within the bath. Usually oxygen is injected into the bath water during the treatment period to help reduce oxygen depletion within the bath volume. At the end of the treatment time the tarp is removed and the net weight ring is dropped to its original depth. As soon as the tarp removal begins, the bath water containing the pesticide begins to be flushed from the net-pen by the ambient water flow. This results in a patch of bath water that moves with, and is diluted by, the water currents and turbulence in the receiving waters.

The above treatment procedure is not precise; it includes uncertainties in the quantities of pesticide added to the bath and in the concentration of the pesticide within the bath. These uncertainties are related in part to the difficulties associated with estimating the volume of water contained within the tarp, preparing an appropriate stock solution of pesticide, and ensuring the pesticide is fully dissolved and mixed throughout the bath volume.

The Treatment Concentrations and Amounts

Bath Volume: The volume of bath water is calculated by assuming a shape of the bath containment system and using estimates of the shape dimensions. In the case of a tarp treatment, the shape is usually assumed to be a cylinder or a coned cylinder and its volume is calculated using the perimeter of the net-pen, the depth to which the net edges were raised and an estimate of the depth in the middle of the raised net. Due to distortions caused by the water currents, the actual shape of the bath containment system rarely matches the assumed shape; these distortions generally increase with current speed and therefore bath tarp treatments are usually conducted at periods of weak current speeds. The surface shape of the net-pen and depth to which the outside edges of the net are raised are relatively well known but the central sagging of the net and the depth of the tarp bottom are less well known; hence the bottom shape and interior depth dimensions of the treatment volume are not well known. The estimate of the volume within the bath should also be adjusted for the volume occupied by the fish and this adjustment has uncertainties concerning the size, shape and number of fish within the bath volume. The estimates of water volume within a tarp are therefore imprecise and have been estimated to vary by a factor of two or more for a typical net-pen (Page et al. 2005). This uncertainty is greater than the uncertainty associated with well-boat bath volumes (described below).

Stock Solution: The stock solution is a concentrate of the pesticide prepared in a limited volume of water that contains the total amount of pesticide to be added to the bath volume. The solution is prepared by estimating the amount of active pesticide ingredient needed to achieve a specific target concentration within the bath volume. The actual amount of active ingredient in the stock solution depends upon how completely the pesticide is dissolved or mixed into the stock volume. The preparation of the pesticide stock solution varies between pesticides and treatments. In the case of tarp bath treatments, the stock solution is mixed manually or mechanically prior to injection into the full bath treatment volume. The vigor and duration of the mixing affects the degree to which the pesticide is dissolved and mixed throughout the mixing medium. The dissolution and mixing are often not complete, hence, the quantity of pesticide injected into the treatment volume may not nor provide the recommended treatment level.

Bath Mixing: Complete mixing of the pesticide throughout the tarp bath is difficult to achieve and the concentration of pesticide within the bath volume is subject to considerable spatial and temporal variation associated throughout the bath volume. The stock pesticide solution can be introduced into the bath volume through one or more perforated hoses stretched across the bath volume, through some kind of dispenser or diffuser placed within the bath volume, or by direct pouring. Mixing of the bath water is assumed to be accomplished by the movement of the fish (Chacon-Torres et al. 1988) and the flow of air or oxygen injected into the treatment water. This does not always result in a rapid and complete mixing of the treatment volume; and empirical observations have indicated that the time to mix the water within the treatment volume is of the same magnitude as the duration of the treatment (Page et al. 2015).

Measurement: In addition to the above uncertainties, it is difficult to obtain a representative measurement of the concentration of pesticide within the bath volume. Water samples are usually taken from the outer perimeter of the bath volume and when the volume is not well mixed the measurements may not be representative of the mean concentration or capture the variance in the concentration throughout the bath volume. This hinders the ability to adjust the concentrations to the desired target values. Measurements of pesticide concentrations in bath volumes prior to release suggest the concentrations within the bath vary considerably. For example, Wells et al. (1990) found the initial concentration in tarp bath volumes varied between treatments by a factor of six with the range being from 0.55 to 3.4 times the target concentration.

Flushing into the Receiving Environment

Once the bath tarp treatment is complete, the bath water is flushed into the ambient receiving waters. The flushing process is highly variable because it depends upon the ambient flow of water through the treated net-pen. This flow varies in relation to several factors including the ambient water velocity, the size of the net-pen mesh, the amount of mesh bio-fouling, the size of the net-pen, and the position of the treated net-pen in relation to adjacent net-pens. Biofouling causes a reduction of the openings of the net-pen mesh, typically measured as percent of net aperture occlusion, which impacts flow through and around cages (Guenther et al. 2010). Measurements of net-pen flushing suggest flushing times can range from a few minutes to a few hours (Page et al. 2015).

Transport and Dispersal within the Receiving Environment

Once the bath water is flushed from the net-pen, it is transported and diluted by the ambient water movements. At distances within several multiples of the farm length scale, the ambient water movements are modified by the presence of the net-pen infrastructure (Wu et al. 2014) and these modifications are seldom well known in any quantitative way. Furthermore, the ambient currents and dispersal processes are constantly changing in space and time and are often not well known.

As the pesticide is transported and dispersed it may also be subject to chemical decay, transformation, and adsorption processes that combine to reduce the concentration below that which elicits toxicity. These considerations are discussed in the Chemical Behaviour section of this report and are important to estimating the potential for toxic consequences.

The combination of the above makes it difficult to estimate the exposure potential associated with the discharge of pesticides from bath tarp treatments. It is difficult to formulate and parameterize the processes in models of exposure, and as a result, models are based on simplifications of the processes. All of the processes and simplifications have significant uncertainties associated with them and these translate into exposure estimates with an unknown degree of uncertainty.

WELL-BOATS

The well-boat treatment method has been described by Page et al. (2015) and Beattie and Bridger (2023). Well-boat treatments involve filling a well, of fixed shape and volume, with ambient sea water. The water within the well is the bath volume and the fish to be treated by the bath pesticide are pumped into the well from a pursed section of a net-pen held adjacent to the well-boat. The fish are allowed to acclimate to the water within the bath for a period of time prior to introduction of the pesticide. A quantity of concentrated bath pesticide is added to a small volume of water contained within a mechanical mixing chamber and mixed for a period of time. The stock solution of pesticide is then pumped into and dispersed throughout the bath volume by the mechanical well recirculation system to give a homogeneous treatment bath (Page et al. 2015). As with tarp treatments, the treatment time varies with the pesticide, the condition and behaviour of the fish and the oxygen content and temperature of the water within the bath. At the end of the treatment time the bath water is flushed from the well into the receiving waters with the water in the well being replaced with ambient water. Once flushing is complete, the fish are maintained within the well for a period of time to allow them to recover from the treatment before being pumped out of the well and back into a net-pen. The well-boat treatment procedure includes fewer uncertainties, is more reproducible, and is more likely to achieve the target treatment level than for tarp treatments.

The Treatment Concentrations and Amounts

Bath Volume: Unlike tarp treatments, the volume of water within the bath is well known and repeatable. The shape and dimensions of the bath are accurately measured and constant. As with tarps the estimate of the volume within the bath should also be adjusted for the volume occupied by the fish and this adjustment has uncertainties in the size, shape and number of fish within the bath volume. Nevertheless, the volume estimates are precise compared to estimates for tarp treatments.

Stock Solution: The stock solution is made in a mechanical mixing chamber. The formulated pesticide is added to the volume of water within the mixing chamber and the mechanical mixing allows the pesticide to become fully dissolved and dispersed throughout mixing volume, so the stock solution is homogeneous. The process allows stock solutions to be made with repeatable concentrations of pesticide.

Bath Mixing: Unlike tarp treatments, the bath water is well-mixed. The mixing is due to the continual recirculation of the bath water and is not dependant on the activity of the fish. Empirical observations have indicated that the time to mix the water within the treatment volume is much less than the duration of the treatment; hence the concentration of pesticide within the bath volume is reasonably homogeneous throughout the bath volume and the treatment time.

Target Concentration: Unlike tarp treatments the target concentration is easier to achieve because the bath volume is known, the pesticide can be fully dissolved in the mixing chamber volume and the bath water is well mixed within a short amount of time.

Measurement: Measurement of the concentration in the bath volume is usually achieved by taking water samples through a hatch in the well. Samples from multiple locations within the interior of the well are difficult to obtain because of the closed nature of the well. However, dye studies have shown that the water within wells is reasonably well mixed, so the hatch samples are likely representative of the concentration of pesticide throughout the bath volume (Page et al. 2015). The ability to monitor the concentration of pesticide within the bath volume allows the pesticide applicators to adjust the concentration to the desired target values.

Release into the Receiving Environment

The release of the bath water, and hence pesticide, into the receiving environment consists of flushing the water from the well and discharging the flushed water into the ambient water.

Flushing: The flushing of the pesticide bath volume from the treatment well is achieved by pumping the water out of the well at a controlled, although sometimes not well known, rate and by pumping ambient water into the well at the same rate. The water within the well at any given time during flushing is therefore a combination of ambient and bath water which is continually mixed by the recirculation pumps. This results in an exponential reduction in the concentration of the pesticide over time within the well (Page et al. 2015) and hence the concentration of the pesticide that is discharged from the well into the receiving environment. The duration of the discharge or the flushing time is typically about 20–30 minutes (Page et al. 2015). During this time the concentration of pesticide in the discharge is not monitored.

Transport and Dispersal in the Receiving Environment

The flushing of the bath water from the well results in the pesticide being pumped through pipes in the hull of the vessel and discharged into the receiving waters from the end of the pipe. This results in an initial jet of bath water that evolves into a plume as the jet merges with the ambient flow. The pesticide within the discharge jet is initially diluted by the jet mixing dynamics and then further diluted by the ambient water turbulence. The trajectory of the jet and subsequent plume is controlled initially by the jet dynamics and then by the ambient water advection. At the end of the discharge period, the plume becomes a patch whose characteristics continue to evolve.

The above factors lead to more rapid dilution than those for tarp treatments and discharge characteristics, e.g., duration, rate, and quantity, from well-boat treatments being less variable. In well-boat treatments the dilution of the pesticide occurs in three phases: initially the pesticide is diluted in the well due to the mixing of ambient and bath waters by the well recirculation pumps; secondly, the already diluted bath water is further diluted in the receiving waters by the entrainment dynamics of the discharge jet; and, finally, the pesticide is diluted by the ambient turbulence in the receiving waters. In this final stage, the characteristics of well-boat discharges are subject to the same sources of variability as tarp discharges.

As the pesticide is transported and dispersed it may also be subject to chemical decay, transformation, and absorption processes that combine to reduce the concentration below that which elicits toxicity. These considerations are discussed in the Chemical Behaviour section of this report and are important to estimating the potential for toxic consequences.

OVERVIEW OF FIELD MEASUREMENTS

Field measurements of the flushing, transport and dispersal of bath pesticides released from bath treatments are essential for the development of accurate prediction capabilities of pesticide dilution rates and exposure domains and the assessment of environmental impacts. Unfortunately, there are relatively few reports documenting the transport and dispersal of bath pesticides and most involve tarp and/or skirt bath treatments (Wells et al. 1990; Dobson and Tack 1991; Ernst et al. 2001, 2014; Corner et al. 2008); a few recent studies involve well-boat discharges (Page et al. 2005; Ernst et al. 2014). Most of the observations have been made in Scottish Lochs (Wells et al.1990; Davies et al. 1991; Dobson and Tack 1991; Turrell 1994) and in the macro-tidal environment of the Bay of Fundy, eastern Canada (Ernst et al. 2001, 2014; Page et al. 2015).

The studies indicate the following:

- Target concentrations of pesticide are more difficult to achieve in tarp and skirt treatments than in well-boat treatments and hence concentrations of pesticide at the time of release are more variable for tarp and skirt treatments than for well-boat treatments.
- The uptake of pesticides during treatment can reduce the concentration of pesticide in the treatment volume.
- Well-boat treatments result in less total pesticide and lower concentrations of pesticide in the receiving environment than tarp treatments and the concentrations in the receiving environment differ from those of tarp treatments by an order of magnitude.
- The discharge patch trajectory and dilution from tarp and skirt treatments follow the water currents in the receiving environment as soon as the skirt or tarp is removed. These trajectories and dilution rates are highly variable; path lengths vary from meters to kilometers and dilution rates vary over several orders of magnitude.

- The trajectory or path and dilution of discharges from a well-boat are initially dominated by the dynamics of the discharge jet and hence their dimensions and direction are more consistent. Once the jet momentum has dissipated, the patch is diluted and transported by the ambient water circulation resulting in more variable path lengths and dilution rates.
- The time and distance after discharge over which a pesticide is detected depends upon the application method, the rates of advection and dispersion in the receiving environment, the concentration of pesticide within the bath volume at the time of discharge, the behaviour of the pesticide, the detection limit of the chemical, and the chemical analytical technique.
- Discharges from tarp and skirt treatments in low current areas do not move away from release points as quickly as in high current areas. This means the distance travelled by the discharged pesticide for a given period of time is less in weak current areas than in strong current areas.
- The distances over which pesticides or their proxies (dye) released from bath treatments have been observed ranged from a few meters to a few kilometers.
- Independent of treatment method, the concentrations of pesticides and their proxies (dye) have been observed to be diluted by one to three orders of magnitude within minutes to hours; dilution occurs more quickly during well-boat treatments than in tarp treatments.

THE MODELLING CONTEXT

Models for predicting the transport and dispersal of pesticides from bath treatments range in complexity (Henderson et al. 2001). At one end of the spectrum are models with many simplifying assumptions that can be implemented relatively easily. At the opposing end of the spectrum, are complex models involving more detailed input and requiring more time and effort to implement. In between, are a range of models of varying complexity and difficulty to implement.

There are multiple purposes for models and the choice of model will depend on the purpose of the model and how the model outputs are going to be used (Henderson et al. 2001). In general models attempt to estimate an exposure profile for an organism or location. The exposure profile may consist of a time series or temporal sequence of chemical concentrations in the immediate proximity of an organism or habitat at a given location.

A screening assessment of exposure and consequence potential may not require as detailed or accurate a model as a scenario in which it has already been determined that detailed, spatially and temporally high resolution and accurate prediction is needed. At this point, it should also be noted that more complex models are not necessarily more accurate; the increased complexity often requires more knowledge by the user, more assumptions and more choices involving modelling specifics such as parameter values, functional relationships and numerical methods. The model will likely need more detailed calibration and validation that is relevant to the specific conditions under consideration before confidence in the outputs is sufficiently high for the model outputs to be deemed useful. Implementation of a model for one region does not necessarily imply an implementation in a new location or new set of circumstances will give similar quality results and be adequate for the new purpose (Henderson et al. 2001). This is true regardless of the complexity of the model. Also, there is no guarantee that outputs from a more complex model will result in a substantially different perspective and hence result in substantially different advice or a substantially different decision. This is particularly true if the choice of screening model was carefully considered. Hence, consideration of the trade-offs between the effort needed to implement different models, the differences in accuracy, the time available to generate model outputs, and the influence of the output on client or target audiences, including their ability and willingness to accept results from models they may not understand or feel comfortable with, are all important considerations in choosing a modelling strategy. Many of these considerations have been identified in the past and are now acknowledged and accepted. Recent regulatory frameworks announced for Scotland by SEPA (Scottish Environment Protection Agency) are requiring more rigor in the choice, calibration and validation of models used for regulating and siting fish farms in Scotland (SEPA 2019a). However, as has been stated by several in the past, this approach may prove to be prohibitive, in terms of cost and labour requirements, for day-to-day management, and run times may be too long for short-term management needs (Gillibrand and Turrell 1999).

In addition to the above general considerations, it should be recognized that estimating the exposure profile of marine pelagic and benthic organisms to chemicals released from fish farming net-pen operations is a challenging task. The transport and dispersive processes around fish farms are generally quite complex, in that they are spatially and temporally variable at the time and space scales of relevance: minutes to hours and meters to kilometers (Wu et al. 2014; Page et al. 2015). The variations are influenced by multiple factors and processes that are not always well understood. Furthermore, the magnitudes of these variations are often not well known for specific farm locations and scenarios. In addition to the mechanics of transport and dispersal, the processes associated with the administration and release of the chemicals are subject to variability between farms, applicators, treatment methods and chemicals. The effort required to sufficiently understand the variation so it can be adequately and quantitatively included in estimates of exposure to chemicals and the subsequent estimates of impact or consequence is considerable. Hence, the development and use of relatively simple models is often a pragmatic necessity and the degree of effort to develop and implement credible detailed models is often underestimated.

The merits of relatively simple models for estimating and predicting the impact of aquaculture on the environment have been promoted for some time (Gowen and Bradbury 1987; Turrell 1994; Silvert and Sowles 1996). The outputs from simple models should be considered, for the most part, as first order estimates of chemical concentrations and/or the zones of exposure and impact (Gillibrand and Turrell 1997). The models idealize the main essence of the situation being modelled by making many simplifying assumptions. As a result, they are quick to run and provide a useful initial triage level of understanding and prediction of exposure and impacts. The models do not provide spatially and temporally precise estimates of exposure and impact and do not provide precise estimates of exposures resulting from specific chemical releases (Gillibrand and Turrell 1997). Often risk assessment processes start with simple and conservative estimates of exposure and impacts and progress to more complex estimates if needed (Metcalfe et al. 2009; SEPA 2019b).

The above discussion of models is based on our own recent experiences and examination of the literature and is in line with earlier sentiments expressed by Henderson et al. (2001). Interestingly, perspectives have not changed significantly over the last twenty years and the general considerations still need to be considered in the development and application of pesticide discharge, transport and dispersion models. The representativeness and credibility of models depends upon the choice of appropriate simplifications for the scenario being modelled, and how extensively the models have been calibrated and validated for the situation of interest (Turrell and Gillibrand 1992). When done well and compared appropriately, the outputs from the simple models should be consistent with outputs from more detailed models. When they incorporate or are combined with appropriate environmental quality standards, they provide useful initial perspectives upon which management actions and future research can be based. It should be noted, however, that care must be taken when using a model to ensure that the conditions in the region of application are consistent with the underlying model assumptions.

GENERIC MODEL COMPONENTS

There are several generic components to exposure models, including but not limited to:

- methods of treatment,
- properties and behaviour of the chemical,
- characteristics of the receiving environment, and
- exposure consequence.

Methods of treatment

The approaches used for treatment have been described in the Treatment Methods section of this document. There are two types of bath treatment used in Canada, tarp treatments and well-boat treatments (Beattie and Bridger 2023), and somewhat different models are required for each treatment approach. The treatment approach defines the initial conditions for the discharge. These conditions define the following characteristics of the discharge:

- size,
- momentum,
- concentration,
- total quantity,
- location,
- time,
- rate, and
- duration.

Size: Bath tarp treatments have an initial size defined by the shape and dimensions of the tarped net pen. For the typical circular net pen, the diameter of the pen is of order tens of meters (28 to 48 m for net pens of circumference 90 and 150 m, respectively) and has an initial depth of approximately 4 m. The initial scale of a well-boat discharge is the diameter of the discharge pipe (~0.5 m).

Momentum: Discharges from tarp treatments have no added momentum associated with them, whereas discharges from well-boats are actively pumped into the receiving environment.

Concentration: The initial concentration of pesticide in the discharge is determined by the target treatment concentration and is similar in tarp and well-boat treatments. The target concentration varies with the pesticide and the water temperature (Beattie and Bridger 2023). The discharge concentrations for tarp treatments can deviate from the target concentration due to uncertainties in the size of the bath treatment volume and due to lack of mixing of the pesticide in the bath (Page et al. 2015). The discharge concentration for both tarp and well-boat treatments can differ from the target concentration due to uptake of the chemical by the fish (Corner et al. 2008), and reaction of the chemical with organics and other substances in the bath water (see the Chemical Properties and Behaviour Section).

Several bath pesticides have been used over the years for finfish aquaculture (Beattie and Bridger 2023). At the time of writing, only three products are registered in Canada for use as bath pesticides by the finfish net-pen aquaculture sector (Health Canada 2016, 2017; Beattie and Bridger 2023). The active ingredients in these products are hydrogen peroxide and azamethiphos. The specific products include Interox® Paramove® 50 (hydrogen peroxide), Aquaparox 50 (hydrogen peroxide), and Salmosan Vet® 50% w/w (azamethiphos) (Beattie and Bridger 2023; Wong et al. 2021). The target concentrations for bath treatments using hydrogen peroxide are 1200–1800 mg a.i. L^{-1} (Solvay Chemicals Inc. 2018; Alpha Chemical Ltd. 2019) and the target concentrations for azamethiphos are 20 g of Salmosan Vet (~10 g of a.i.) for 100m^3 of water for tarp treatments, and 80 to 105 m^3 of water for well-boat treatments (Benchmark Animal Health Ltd. 2018).

Quantity: The total quantity of pesticide discharged is larger for tarp treatments since the bath volume is an order of magnitude larger for a tarp treatment than for a well-boat treatment. For example, a 100 m polar circle cage pursed to a depth of four (4) meters for tarping contains a water volume of approximately 3200 m^3 whereas the volume of water within a well-boat well used in Atlantic Canada is approximately 330 m^3 (Page et al. 2015). These differences will change if well-boats with different sized wells are used.

Location: The location of the discharge is different for every farm site, every cage on the site and every mooring location of the well-boat during its discharge. In eastern Canada the well-boat discharges while moored to a cage, i.e., well-boats typically do not steam away from the farm to a discharge location.

Time: The timing of discharges is unique for each discharge and depends on treatment needs and schedules, as well as weather and oceanographic conditions (Beattie and Bridger 2023).

Rate: The rate of discharge is much greater from well-boat discharges than from tarp discharges. This is because discharges from well-boats are pumped out of the bath volume and thus have an initial added momentum (Page et al. 2015). The discharge rate from a tarp treatment is based on the ambient flow of water through the untarped net pen.

Duration: The duration of discharge varies between treatment methods and ambient conditions. The duration of typical discharge from a well-boat is 20 to 30 minutes whereas the duration of discharge from a tarp treatment can vary from less than ten minutes to about three hours (Page et al. 2015).

Properties and Behaviour of the Chemical

The properties and behaviour of a chemical, in this case a bath pesticide, influence many aspects of both the potential to expose non-target organisms and habitats, and the potential for exposures to result in consequences or impacts. Factors influencing the potential to expose include the chemical's ability to be dissolved in the receiving water and bind to suspended particles, persist in sediments if it is deposited on the seabed, decay, breakdown into other chemical compounds, bioaccumulate, and be excreted or egested after metabolization. The chemical's mode of action encountered by target and non-target organisms will also influence the likelihood of consequences or impacts. In this section we summarize some of the important processes that affect exposure estimates. The details of the chemicals' model of action and toxicity, along with additional information are provided in Burridge and Holmes (2023), Hamoutene et al. (2023), and Wong et al. (2021).

Water/Sediment Partitioning

One important chemical behaviour is its tendency to either remain in the aqueous phase, i.e., seawater, or bind to organic material, e.g., particulates. An indication of this potential is given by a chemical's octanol/water partition coefficient (log K_{ow}) (Hermens et al. 2013). Low values of this coefficient suggest the chemical is highly miscible with water and not likely to bind to organic particulates whereas high values suggest the chemical is likely to bind to organics in the water and sediment and thus not be found dissolved in the water but could still be found bound to small particulates. A log K_{ow} value of less than three is often used as an indication that the compound will not bind significantly to organics (Cole et al. 1999). It should be noted that log K_{ow} values are calculated based on data generated using the pure active ingredient under controlled laboratory conditions (Hermens et al. 2013). The use of the formulated product in the field may result in unexpected behaviours and so the log K_{ow} value may not always be an accurate indication of a chemical's behaviour, for example oxytetracycline (Brooks et al. 2008).

Both of the chemicals registered for use as bath treatments for the treatment of finfish in net-pens for sea lice by the Canadian aquaculture industry, i.e., hydrogen peroxide and azamethiphos, have low octanol/water partition coefficients. Reported log K_{ow} values for hydrogen peroxide and azamethiphos are -1.57 and 1.05, respectively (Munn et al. 2003; Haya et al. 2005; Health Canada 2016, 2017; Burridge and Holmes 2023; Wong et al. 2021). The behaviour suggested by the log K_{ow} for azamethiphos is supported by analyses of water that was collected from a patch of bath water released from a commercial bath treatment; the water was separated into particulate and dissolved fractions by filtration and the analyses indicated that the ratio of azamethiphos found in water relative to particulates was 100:1 (Ernst et al. 2014). Hydrogen peroxide will react with but not bind to dissolved and suspended organic matter (Health Canada 2016).

Since bath pesticides such as those currently registered for use in Canada are highly water soluble, models of exposure to these pesticides can assume they will remain within the water column and can be modelled as passive scalars rather than sinking particles, for example as has been done by Falconer and Hartnett (1993), Gillibrand and Turrell (1999), and Page et al. (2015); however, this assumption needs to be evaluated on a chemical by chemical basis. For chemicals that bind to particulates in the water column due to their high log K_{ow}, models should take this into account, for example as was done by Willis et al. (2005) for cypermethrin.

Decomposition

Another important chemical behaviour is its rate of decomposition in water and the resulting breakdown products. In water, hydrogen peroxide decomposes into water and oxygen (Haya et al. 2005). Estimates of the half-life of hydrogen peroxide in water varies from 50 h to 28 days with the half life depending on multiple factors including temperature, the presence of organics, aeration, agitation and formulation (Munn et al. 2003; Haya et al. 2005; Lyons et al. 2014). For example, 21% and 54% of hydrogen peroxide was reported to have decomposed in sea water after seven days at temperatures of 4 and 15°C, respectively (Haya et al. 2005). The amounts increased to 45% and 67% when the water was aerated or agitated (Haya et al. 2005) and may increase even more under field conditions (Haya et al. 2005). Lyons et al. (2014) monitored the degradation of the Interox® Paramove® 50 formulation of hydrogen peroxide in seawater under laboratory conditions and found the half-life to vary from 14–28 days. As noted by Haya et al. (2005) these laboratory times may be overestimates of the in-situ half-life.

The typically reported decay time for azamethiphos is 8.9 days (Haya et al. 2005; Wong et al. 2021) and the chemical is broken down into four non-toxic products by a combination of hydrolysis, photolysis, and microbial activity (Health Canada 2017; Benchmark Animal Health Ltd. 2019). This decay time is long compared to the time scales (minutes to hours) of turbulent dispersion associated with tarp and well-boat discharges (see section OVERVIEW OF FIELD MEASUREMENTS); hence, for the purposes of modelling exposure to acute concentrations, chemical decay is typically not included in model considerations. However, models of chronic exposures need to include decay rates since these models attempt to estimate exposure profiles over time scales of days, weeks, or longer.

Characteristics of the Receiving Environment

In addition to the above, the exposure of an organism or area to a discharged bath pesticide depends on the characteristics of the receiving environment. These characteristics include, but are perhaps not limited to:

- rates of horizontal and vertical dispersion,
- rates of horizontal and vertical advection,
- water depth,
- water temperature and salinity,
- suspended particulates, and
- light penetration.

Rates of Dispersion: These will impact how quickly the pesticide dilutes and increases in areal extent. Dispersion rates in the ocean increase with the size of the patch (Okubo 1968, 1974). Despite this, many models assume a constant diffusion rate (Falconer and Hartnett 1993; Gillibrand and Turrell 1997,1999; Willis et al. 2005). However, estimates of dispersion rates are highly variable and have a range of at least an order of magnitude (Lewis 1997). They vary with both time and space in relation to spatial variation in local turbulence and shears in the flow field. In the coastal zone, horizontal rates are typically at least an order of magnitude greater than vertical dispersion rates (Lewis 1997). Typical values are approximately 1 $m^2 \cdot s^{-1}$ for horizontal dispersion and 0.01 $m^2 \cdot s^{-1}$ for vertical dispersion (Lewis 1997). For example, Davies et al. (1991) used a Gaussian diffusion model and found a horizontal diffusion rate of 2 $m^2 \cdot s^{-1}$ provided the best fit to their limited observations. Modellers should test the sensitivity of their models to the values of dispersal rates and compare their models to observed dispersal rates. However, this is often not done since observations are expensive and challenging to obtain.

Rates of Advection: The local water current speeds and directions determine where a patch is transported, how long it takes to get there and what path it takes. Currents vary on spatial scales of tens of meters to kilometers and on temporal scales of minutes, hours, months and years. There can be significant changes in the current direction including complete reversal in tidally-dominated regions. Prediction of these currents is important for estimating acute exposures in areas where the currents vary significantly either spatially and/or temporally. High resolution (order ten meters in the horizontal and one meter in the vertical) hydrodynamic models are required to obtain spatially and temporally varying current estimates on these scales. These models must be forced by appropriate spatially and temporally variable offshore boundary water and atmospheric conditions. Furthermore, models should be calibrated and validated using multiple observations of local current and sea level time series, as well as drift trajectories, before they are used to give estimates of discharge transport and dispersal. SEPA has recently indicated that exposure models must meet these requirements (SEPA 2019b).

The fish farm configuration (number, size, shape, and arrangement of cages), the location and proximity of the cage relative to other cages in the farm, the mesh size of nets on the cages and their degree of bio-fouling, also influence the speed and direction of the near-field (within several multiples of the cage array length scale) currents (Gansel et al. 2012a, 2012b; Turner et al. 2015). The details of these influences are extremely difficult to simulate and predict when the cages are stationary, let alone when they are moving and changing shape in response to the forces acting on them. As a consequence, these processes are often unknown for specific discharge scenarios and thus left out of existing exposure models even though they are expected to contribute to a significant degree of uncertainty to near-field patch behaviour and hence estimates of exposure.

Water depth: The local coastline and bathymetry have a strong influence on the near and far-field water circulation (e.g., Bowden 1983) as well as limiting the extent to which a discharge patch can grow horizontally and vertically. In areas with tidal amplitudes that are a significant proportion of the water depth, the changes in water depth over tidal time scales are also needed. Relatively simple models often assume the water depths are constant, both spatially and temporally, whereas the high-resolution hydrodynamic models require high resolution bathymetry to correctly model current speed and direction.

Water Temperature and Salinity: The temperature of the receiving water may influence the behaviour of the discharged pesticide, including its decay rate. In the case of Interox® Paramove® 50, a three-hour laboratory study showed decay rates varied less than three percent over a 15° temperature range (Lyons et al. 2014). Temperature may also influence the sensitivity and response of organisms to exposures. Typically, toxicity increases with temperature though there are exceptions, for example toxicity to pyrethroid decreases with temperature (Delorenzo 2015). Salinity is also likely to have some influence, although its effects are poorly studied. The density of water is a function of temperature and salinity. If the density of the discharge differs significantly from the density of the receiving water, the density difference impacts the advection and dispersion of the discharge, until sufficient mixing occurs to equalize the densities. It is generally assumed that these considerations have only minor influences on exposure estimates and hence models typically assume that the density of discharge is the same as that of the receiving waters. However, the validity of this assumption has not been verified.

Suspended Particulates: Suspended particulates provide surfaces to which discharged chemicals can adsorb or with which they can react. These in turn can change the concentration and behaviour of the discharged pesticide.

The bath pesticides registered in Canada (Paramove® 50, Aquaparox 50 and Salmosan®) have low log K_{ow} coefficients for the active ingredients (hydrogen peroxide and azamethiphos, respectively) and are not expected to bind with suspended organic particulates (Health Canada 2016, 2017). Therefore the concentrations are expected not be affected by settling processes.

Studies have indicated that the presence of dissolved and suspended organics, marine plankton, and bacteria influences the decay of hydrogen peroxide. For natural hydrogen peroxide the rate of decomposition decreased in filtered seawater samples (Petasne and Zika 1997) whereas for Paramove®50, the formulation used for sea lice treatments, the opposite behaviour has been observed (Lyons et al. 2014).

Light Penetration: The decay of some pesticides may be influenced by light (Petasne and Zika 1997; Health Canada 2016, 2017) and for these chemicals the intensity and depth penetration of the relevant light wavelengths may need to be considered. However, sun light intensity rapidly decreases with depth in the ocean and hence photolysis is not expected to be an important decomposition process for the pesticides that are mixed within the surface layer (Petasne and Zika 1997). To our knowledge, models to date have not considered this potential process or have assumed it is included in the bulk estimates of decay rate.

Exposure Consequence: Environmental Quality Standards or Thresholds

The previous sections describe processes and conditions that influence the discharge, transport and dispersal of a discharged pesticide. Another important consideration is the environmental threshold of interest.

Ideally a threshold or environmental quality standard (EQS) defines both a threshold of concentration and threshold of time needed for the toxic response to be triggered. EQS thresholds are usually derived from laboratory studies in which organisms are exposed to a series of temporally constant concentrations for specified periods of time. In situ exposures are, however, complex combinations of temporal variations in concentration resulting in spectra of exposure durations at multiple concentrations. Toxic consequences can be expected when the in situ exposure profile is such that at least one sequence of exposure is characterised by concentrations being above the EQS threshold concentration for the length of time required for toxic response to be triggered. Consequences are more difficult to estimate under the following circumstances: when the exposure profile does not have such a sequence but may be above the EQS concentration for multiple shorter exposures; the exposure profile is not known or cannot be predicted. In these cases, it may not be prudent to conclude that if the EQS sequence does not occur, there will be no consequences. A precautionary approach is to assume that any duration of exposure, no matter how short, may result in the toxic consequence. This approach is consistent with toxicological data that suggests EQS concentration thresholds for acute effects may be independent of exposure duration (Hamoutene et al. 2023).

The main objectives of many models are therefore to:

- estimate the time needed to dilute a discharged pesticide to a concentration below a threshold,
- estimate the exposure area to discharge concentrations that are above the threshold,
- estimate the location(s) exposed by the discharge and particularly the locations exposed to discharge concentrations that exceed the specific thresholds,
- estimate the duration of these exposures,
- use prescribed thresholds and estimated exposures to infer toxic consequences, and
- estimate the amount of pesticide that can be used to ensure that exposures remain below a specified threshold, for example as is done by SEPA (2008)

Reviews of environmental quality thresholds and standards are given by Burridge and Holmes (2023) and Hamoutene et al. (2023).

MODEL VALIDATION

There are several challenges associated with validating a model. The main consideration is whether the model contains the processes, parameterizations, and outputs needed for the required representation. For example, older models may not adequately represent modern treatment methods. Another challenge is the need to compare model results to observations. This step is crucial as it is the only way that model performance can be assessed. Ideally, all models should be adequately validated before being applied (Turrell and Gillibrand 1992; Falconer and Hartnett 1993; Gillibrand and Turrell 1997). Validation should use all applicable data including those from other countries. The amount of validation depends on the purpose of the model. For example, if the purpose of the model is to help develop understanding about model behaviour and stability, calibration and validation using field data may not be necessary. However, if the model outputs are to be used for decision making the model should be validated with field observations that are relevant to the type and area of application.

In general, dispersion studies are conducted with tracers, for example dye or drifters, which result in estimates of dispersion rates, for example (Okubo 1971, 1974; Bowden 1983; Lewis 1997). Most pesticide models assume typical values of these dispersion rates, for example Turrell (1994), Turrell and Gillibrand (1995), and Gillibrand and Turrell (1997). Establishing the validity of this assumption is important as models assume the dispersion of tracers mimics that of pesticides and needs to be done for each pesticide formulation. Few studies have been conducted to verify this assumption (Ernst et al. 2001, 2014; Page et al. 2015). In these studies, fluorescent dye (rhodamine or fluorescein) was mixed with a pesticide (azamethiphos, deltamethrin, or cypermethrin). The mixture was introduced into tarped fish cages. Water samples were collected within and outside the visible dye patch at various points in time after removal of the tarp. Concentrations of pesticide and dye were determined for each water sample and statistically significant relationships were found between the concentrations of pesticide and dye, although the details and universality of these relationships could benefit from more studies.

REVIEW OF EXISTING MODELS

Exposure models associated with aquaculture bath pesticide discharge have focused on estimation of the dilution of the toxic substance, the extent (spatial and temporal domains) of exposure, and the location and duration of exposure. Few models have focused on directly predicting the consequence of the exposure; instead they compare predicted concentrations to empirically derived EQS concentration thresholds.

Models are a representation of reality and estimate processes that are of interest or importance (Turrell and Gillibrand 1992). How well a given model represents a specific situation depends on the assumptions made by the model and if these assumptions are reasonable for the situation in question. Typically, the assumptions used depend on what question the model is trying to address.

The models reviewed in this document consider the dilution and transport of pesticides released by aquaculture bath treatments. The underlying assumption is that the release of pesticides produces a patch containing the treatment pesticide which changes in size, shape, location, and concentration with time. These patch characteristics can be used to determine the following exposure characteristics: spatial extent, location, and duration of exposure. Models usually estimate some subset of these, but more complicated models have the ability to predict all of these characteristics. Model selection should consider what information is required.

Size of Discharge Patch

The size of the discharge patch is the temporally varying spatial area and volume occupied by the patch. It is determined by the characteristics of the discharge type (tarp vs well-boat), chemical decay, dispersion, and advection in the receiving environment. Determination of the size depends on a definition of a concentration threshold that marks the boundary of the patch. This threshold is often assumed to be the acute or chronic EQS concentration.

Shape of Discharge Patch

The shape of the discharge patch is determined by the release method and the environment into which it is released. The shape of the patch is often irregular and undergoes stretching and bending due to the bathymetry, the coastline, and the shear in the local currents.

Location of Discharge Patch

The location of the initial discharge depends on the location of the cage that has been treated or the location of the well-boat when it is discharging. The location of the resulting patch varies in time and depends on the dispersion, chemical decay, and advection processes in the receiving environment.

Concentration Within the Discharge Patch

Concentration of the discharged pesticide decreases with time. The dilution rate is controlled by the dispersion and chemical decay processes operating in the receiving environment. The dilution is usually parameterized as a two or three dimensional dispersion process in which the rate of dispersion is temporally and spatially constant, temporally variable but spatially constant or a function of patch size. The concentration also decreases due to decay; this is usually assumed to be an exponential process that is expressed in terms of either an e-folding time (i.e., the time for the discharged concentration to reduce to e^{-1} (~36%) of its initial concentration) or the half-life (i.e., the time for the concentration to reduce to 50% of the pre-discharge concentration).

Spatial Extent of Exposure

The spatial extent of the exposure is the total area, in units of a length measure squared, exposed throughout the temporal evolution of the patch until the time at which all concentrations within the patch are below a given threshold concentration such as an EQS.

Location of Exposure

The location of exposure is the complete set of all the discharge patch locations from the start of the discharge until the time at which all concentrations within the patch are below a given threshold concentration such as an EQS.

Duration of Exposure

The duration of exposure at a single location is the time that the location is exposed to concentrations above a given threshold.

Models of Discharges from Tarp Treatments

Surprisingly, relatively little literature exists concerning the modelling and prediction of ecosystem or environmental exposures to bath pesticides discharged by finfish aquaculture operations. This is certainly the case in Canada, where only a few modelling efforts have been made (DFO 2013; Page et al. 2015). Here we review existing models in the literature. A list of the reviewed models, their input assumptions and output variables are given in Table 1 and Table 2.

Some of the earliest models were developed in Scotland where, at the time, aquaculture sites were in lochs. The models used loch-specific information such as the volume of the loch and the flushing time. Turrell (1990) developed a model to predict the annual mean concentration from treatments of all farms in a loch system. Gillibrand and Turrell (1997) developed a simple model to calculate the amount of dichlorvos that could be used annually without exceeding the annual mean EQS. These models assume that aquaculture farms occur in Scottish lochs and may not be valid for many of the farms located in Canadian waters because of differences in hydrographic conditions. Furthermore, these models are only of use if regulations restricting the quantity of pesticides used annually are in place.

Another simple model is described by Metcalfe et al. (2009) who calculated the predicted environmental concentrations (PEC) that would occur in the surface waters beyond the treatment area. The PEC is simply the ratio of the mass of the applied pesticide divided by the volume of water over which the dilution occurs. The volume is assumed to be a circle centred on the cage where the treatment occurs and extending some lateral distance beyond the cage in all directions. This distance is set to some pre-determined mixing zone size. Vertically, the mixing zone is extended to the bottom unless a surface mixed-layer depth is known. The model is of use in jurisdictions that have regulations in place specifying that toxic conditions cannot occur outside the mixing zone. Successful application of this model requires local regulations that specify both the extent of the permitted mixing zone and the critical concentration against which the calculated PEC can be compared. This model can help fish-farm operators determine if a given treatment meets regulations and can be used for scenarios involving treatments of multiple cages. This model may only be of limited value to the Canadian situation.

The models described above do not take into account the temporal nature of a patch of pesticide from a treatment, i.e., the patch grows in size due to dispersion and hence decreasing the pesticide concentration, the shape of the patch changes due to local currents and bathymetry, and the location of the patch moves due to local current conditions; and thus cannot provide a detailed spatial and temporal prediction of pesticide exposure characteristics. A simple model that defines an area which, similar to the model of Metcalfe et al. (2009), is a circle centred on the cage (or farm). In this case, the lateral distance beyond the edge of the cage is the distance travelled by the patch before the treatment concentration falls below some critical value. The distance is the product of a representative current speed and the time required for the patch concentration to dilute or decay to the critical level. We will refer to the area predicted by the model as the PEZ (potential exposure zone) model. Although simple to implement, this model takes into account both local current conditions and the decay properties of the treatment pesticide. The PEZ gives a region which encompasses the location of exposure. It should be highlighted that not all regions in the PEZ will be exposed but, if an appropriate current speed is used, all exposed regions will fall within the PEZ. Selection of the appropriate current speed will be discussed further in the section on PEZ Models.

Due to regulatory desires, Scotland spent considerable time and effort during the 1990s developing models for predicting the dispersion of pesticides used in the treatment for sea lice in salmon net-pen facilities (Turrell 1990, 1994; Gillibrand and Turrell 1997, 1999). These models were developed to be management tools. They simulate possible treatment scenarios and determine if resulting concentrations are in excess of adopted EQS and, if so, over how large an area. Over time, more complexities were added to the models but all rely on the same assumptions. When a fish cage is treated using a pesticide, the pesticide is released into the ambient receiving water resulting in a patch of pesticide. The concentrations within the patch are calculated using a two-dimensional Gaussian diffusion equation that includes pesticide decay. The patch is advected in the horizontal dimension using specified local current conditions. The final version of the model (Gillibrand and Turrell 1999) allows for three different types of farm locations (loch, channel or open water) and takes into account the presence of the coastal boundaries in the calculation of the patch concentration. Multiple treatments are permitted and the resulting patches are advected by a tidally varying current. The model allows for spatial and temporal overlap of the discharge patches and calculates the time-varying total concentrations at each location.

SEPA (2008) developed a spreadsheet tool (BathAuto) based on two models for assessing the use of pesticides used in bath treatments for the treatment of sea lice. The first model was a simplified short-term model developed to help assess the potential for acute effects from chemicals that take longer than a single tidal cycle to disperse to non-toxic concentrations. This model was developed for simulations of up to six hours. The patch is assumed to be an ellipse that grows with time. The patch grows in the longitudinal direction at a rate determined by the mean current at the farm site and laterally at a rate determined by a dispersion coefficient. This model is only valid for determining the concentration from a single treatment. Longer simulation times and multiple treatments require the use of the more complex model by Gillibrand and Turrell (1999).

Table 1: Summary of input variables for tarp models.

Model	Current	Bathymetry	Coastline	Dilution	Chemical properties
Patch Diffusion (Turrell 1990)	no	no (mixed surface layer)	no	constant	none
Loch Diffusion (Turrell 1990, 1994)	residual flushing velocity	no (mixed surface layer)	idealized loch	constant	decay
Annual Mean (Turrell 1990)	no	no (mixed surface layer)	idealized loch	no	no
Tracer concentration (Falconer and Hartnett 1993)	2D spatially & temporally varying	spatially varying	realistic representation	constant	decay
Gillibrand and Turrell (1999)	single record, M2 tidal + constant residual	no (mixed surface layer)	idealized domain	constant	decay
Particle Tracking (SAMS 2005; Willis et al. 2005)	single record derived from observations	spatially varying	realistic representation	constant	adhere to sinking organic particles
Metcalfe et al. (2009)	no	single value	no	calculated over fixed area	none
Okubo based (Page et al. 2015)	single record, current meter	single value	no	scale dependent (Okubo)	none
Particle tracking (Page et al. 2015)	spatially & temporally varying	spatially varying	realistic representation	constant	none
PEZ (potential exposure zone)	single speed	single value	no	dilution time to a threshold*	decay time to a threshold*

* The time scale used to calculate the PEZ is the lesser of the dilution time and the decay time.

BathAuto (SEPA 2008) is a useful model for predicting the temporal evolution of concentrations of pesticides that occur due to a given treatment scenario for a specific farm and, as intended, can be used as a management tool to help design treatment regimes that keep the resulting concentrations below the EQS. The user should keep in mind, however, that there are many simplifying assumptions to the underlying models. The user can specify the type of spatial domain (loch, channel, or straight) which the model represents as idealized domains of rectangular shape. Complicated coastlines or bathymetry are not taken into account. Furthermore, the current does not vary spatially and the patch shape is assumed to be an ellipse. Both of these assumptions result in likely inaccurate representations of the location and shape of the patch as it evolves in time. Thus, these models cannot predict the exact regions that may be exposed; they only predict the level and size of exposure, and the magnitude of the displacement from the source. The accuracy of the predictions varies with the appropriateness and degree of simplification.

Table 2: Summary of output variables for tarp models.

Model	Time	Size	Location	Concentration
Patch Diffusion (Turrell 1990)	temporally varying output	patch size	no	patch concentration
Loch Diffusion (Turrell 1990, 1994)	temporally varying output	patch size	x-y distribution of concentration	patch concentration
Annual Mean (Turrell 1990)	no	no	average over entire loch	annual mean concentration
Tracer concentration model (Falconer and Hartnett 1993)	temporally varying output	patch size	location of patch	patch concentration
Gillibrand and Turrell (1999)	temporally varying output	patch size	location of patch in idealized domain	patch concentration
Metcalfe et al. (2009)	no	no	no	average concentration over area
Particle Tracking (SAMS 2005, Willis et al. 2005)	temporally varying output	patch size	location of patch	patch concentration
Okubo based (Page et al. 2015)	temporally varying output	patch size	location of patch	patch concentration
Particle tracking model (Page et al. 2015)	temporally varying output	patch size	location of patch	patch concentration
PEZ (potential exposure zone)	no	no	potential coverage of patch	no

A variant of the Gillibrand and Turrell (1999) model was adopted by Page et al. (2015). Both models predict temporal evolution of the concentration of the pesticide patch, but Page et al. (2015) use the Okubo relationship (Okubo 1974) to determine the increasing patch size over time. The patch was advected using current velocity data collected in the field. Field observations of a patch location were obtained by mixing dye with pesticide in commercial bath treatments and tracking the evolution of the patch size and position. The model was compared against observations using data collected from multiple single current meter records during and after the pesticide release at various locations in proximity to the farm sites. The comparisons showed that within about one hour of the release, the patch size increased more rapidly than predicted by the Okubo relationship and then subsequently followed the Okubo relationship. The differences between observations and predictions were attributed to the influences of the farm infrastructure which were not taken into account in the model. Furthermore, it was established that the predicted locations of the patch were dependent on the current meter record used to advect it, resulting in predicted locations often differing from the observed locations. This result is important, as most simple models use currents obtained from a single location. The results of Page et al. (2015) indicate that simple models are not reliable predictors of the exact location of a patch of pesticide, but they often give a reasonable estimate of the distance travelled by the pesticide during the first few hours after release. Thus, simple models should not be used to determine the exact trajectory of a pesticide patch. This limitation does not reduce the value of simple models. If properly validated, these models can be used to calculate resulting concentrations from treatments. They can also be used to determine the likely extent of the patch displacement and whether these displacements exceed regulatory mixing zone distances when such regulatory distances exist.

Another approach to predicting the dispersion of a pesticide patch is to use a particle tracking model (SEPA 2013). A particle tracking model was used by Turrell and Gillibrand (1995) to model the dispersion and sinking of cypermethrin. Black et al. (2005) and Willis et al. (2005) also used a particle tracking model to simulate the dispersion of cypermethrin. In these models, the particles were advected using currents estimated from current meters and drifter displacements. The current field was assumed to be spatially homogeneous and coefficients of horizontal diffusion were determined from drifter data. To simulate the settling of cypermethrin Willis et al. (2005) added a vertical settling velocity such that all the particles settled to the bottom within a six-hour period.

There is sometimes the need for more complicated models. However, complicated models require significantly more resources and expertise to develop and operate, and these requirements are often beyond the desires, capacities or abilities of regulatory agencies, industry, stakeholders or researchers. It is often best to develop and use these models after simple models have indicated a more detailed and precise prediction or estimate is needed. SEPA (2019a) recently released new modelling guidelines, an overview of which is given in the appendix, and has adopted the view that a more complicated model is required for licensing the release of pesticides from bath treatments, unless the applicant can demonstrate that SEPA's simple model, BathAuto, is suitable.

SEPA (2013) provides a general overview of modelling coastal discharges. Although the report is not specific to aquaculture and does not describe any particular model in detail, it does provide some insight into the issues that must be considered when developing/choosing a model. These include the duration of the process being modelled, the domain in which the event takes place, the dimensionality required to adequately capture the process and the grid required. Three types of models are identified: hydrodynamic models, water quality models, and particle tracking models. Hydrodynamic models require much effort and time to develop for a given area, but output files can be used to provide current, temperature and salinity fields for both particle tracking models and water quality models.

Perhaps the area in which existing complicated models differ most from simple models is in the use of a hydrodynamic model to provide higher spatial and temporal resolution of the current and hydrographic regime in the vicinity of fish farms. One of the factors that impacts the accuracy of the results of simple models is the hydrodynamic data used in the model. Often currents from a single source and a short time period are used. These data are typically acquired by deploying a current meter at the aquaculture site for about a one-month period. It has been shown that the location of the current meter data used can influence the details of the model results (Chang et al. 2014; Page et al. 2015). Furthermore, currents are typically subject to seasonal changes which are not taken into account if a short record is used.

One advantage of hydrodynamic models is the ability to predict spatial and temporal variability of currents. The first use of a hydrodynamic model in relation to estimation of aquaculture net-pen pesticide treatment was by Falconer and Harnett (1993) who coupled a two-dimensional hydrodynamic model with a concentration model to assess the advection and dispersion of pesticides used by the aquaculture industry in Ireland. Since then, there have been significant developments in both hydrodynamic models and computing power. Modern hydrodynamic models have the ability to include temporal and spatial variation in model boundary forcing, including surface heat flux, barometric pressure, and wind speed from weather models, freshwater discharges from multiple rivers, and open boundary sea level, water velocity, water temperature and water salinity conditions. Models use both structured and unstructured meshes but unstructured meshes are particularly well-suited for modelling the coastal waters in which aquaculture farm sites are often located as they have the ability to resolve complex coastlines and bathymetry and allow for high resolution in the grid discretization in only the needed regions. Faster computers and the ability of models to run in parallel are now allowing models to be run with higher grid resolutions and for longer periods of time. When sufficiently calibrated and validated for the spatial and temporal domain of interest, these improvements allow for more complete prediction of the currents that transport and disperse the drugs and pesticides released from aquaculture fish cages. Recent models used to simulate processes that occur due to the presence of aquaculture cage sites include, but are not limited to: POM (Doglioli et al. 2004), MOHID (Moreno Navas et al. 2011), SUNTANS (Venayagamoorthy et al. 2011), FVCOM (Wu et al. 2014; Foreman et al. 2015; Page et al. 2015), POLCOM (Salama et al. 2013) and MIKE 3 FM (Payandeh et al. 2015).

There are two methods for modelling the transport and dispersal of bath pesticides released from aquaculture sites: 1) conservation equation models; and 2) particle tracking models. Both methods require an underlying hydrodynamic model and can either be coupled (on-line) or decoupled (off-line) with the underlying model.

The first method was used by Falconer and Hartnett (1993). They solved a concentration equation which was coupled with the current fields output by a hydrodynamic model. This method has the advantage of calculating directly the concentration of the released contaminant. It does, however, suffer from a couple of drawbacks. For each different treatment scenario, a re-run of the model is required which can be computationally expensive and require time. This can be resolved by using a separate, or off-line, concentration model, as was done by Wu et al. (1999). Also, as noted by Suh (2006), concentration models can give erroneous results near the release site. Nevertheless, numerically solving the concentration equation has been used successfully in studies involving aquaculture issues such as water quality (Wu et al. 1999), the effects of fish farms on eutrophication using a coupled hydrodynamic, chemical and biological model (Skogen et al. 2009), the effect of cage drag on the tracer patch (Venayagamoorthy et al. 2011), and pollutant load based on residence time (Payandeh et al. 2015). Although we are not aware of any recent studies using the concentration method coupled with a hydrodynamic model for investigating the fate of bath pesticides released from aquaculture farms, there are modern studies that show potential for this approach. For example, POM was coupled with an offline ecotoxicological model to estimate the dispersion of Bisphenol A in Tokyo Bay (Kim et al. 2004).

An alternative approach was adapted by (Page et al. 2015) who implemented the FVCOM hydrodynamic model (Chen et al. 2003, 2006) for the southwest New Brunswick area of Canada and used its output as input into a particle tracking model that estimated the transport and dispersion of pesticides used to treat fish farms for sea lice. The exposure envelope predicted by the model when particles were released at all phases of the tide encompassed the majority of the areas exposed by dye released at specific phases of the tide. This approach avoids the problems of erroneous concentrations near the release site (Suh 2006), allows for independent parameterization of dispersion and thus avoids issues associated with numerical diffusion. As the particle tracking model is a separate module from the hydrodynamic model, once output from the hydrodynamic model is available, it is easy to run multiple scenarios. This reduces the need for computing resources, since the particle tracking model typically requires less computing power and memory than the hydrodynamic model. The disadvantage is that pesticide concentration is not a direct output of the particle tracking model, but needs to be calculated by dividing the model domain into grid elements and calculating the number of particles in each element. Calculated concentrations are sensitive to both the size of the grid elements and the number of particles used. Obtaining accurate results may require using a large number of particles and small grid elements. In addition to the study by Page et al. (2015), particle tracking models have been used to model the dispersion of fish farm organic wastes (Doglioli et al. 2004), disease pathogens (Page et al. 2005; Foreman et al. 2015) and pests such as sea lice from fish farms (Salama et al. 2013). Moreno Navas et al. (2011) also used a particle tracking model to examine the advection of passive tracers from a fish farm and advocated importing results of hydrodynamic models into a GIS system to support aquaculture decision making.

Moreno Navas et al. (2011) suggested importing results of a hydrodynamic model into a GIS system to support aquaculture decision making raises several important considerations. One of the main drawbacks to using the results of hydrodynamic models in decision making is the significant amount of resources required, both in terms of manpower and computing power, to implement, calibrate and validate a model for a given region. Hydrodynamic models cannot be configured and applied quickly. Thus, results of hydrodynamic models can only be used for rapid decision making if they already exist; it is impractical to implement such models on the short timescales (days to months) often required by decision makers. Additionally, even if a hydrodynamic model exists, it must be evaluated before being used as a tool for decision makers. In the validation of their implementation of FVCOM for southwest New Brunswick, Page et al. (2015) found that the model did not always correctly predict the phase of the currents and model results of individual releases of pesticides did not always exhibit the behaviour of the observed dye patch, thus illustrating the importance of model validation. Finally, if output from a hydrodynamic model is required for aquaculture decision making, models implemented specifically for aquaculture purposes will likely be required. Due to the relatively small scales (10 m to 100 m) associated with fish farm exposure modelling, high spatial resolution models in the regions of fish farms will likely be required. Furthermore, the effects of the fish farm infrastructure may need to be incorporated into the model. Fredriksson et al. (2006) measured currents at a fish farm site in Eastport Maine, USA and found that there was a reduction of the near-surface current speeds within the farm site, dependent on the size of the pens' netting and the amount of biofouling present. Model studies have also shown that the presence of fish farms has an impact on the local flow dynamics. A two-dimensional study using the SUNTANS model (Fringer et al. 2006) was conducted by Venayagamoorthy et al. (2011). The behaviour of the plume from a continuous pollutant point source placed inside the cage pen was examined. Simulations without any additional drag due to the presence of the cage and with the addition of cage drag were performed. It was observed that the presence of the cages enhances the spread of the pollutant plume and increases the lateral diffusivities by a factor of 3 to 5 when compared to the case with no cage drag. This increase is consistent with the dye dispersion results obtained by Page et al. (2015). Wu et al. (2014) ran FVCOM in three-dimensions with cage drag added to the momentum equations to examine the impact the presence of a fish farm has on the local currents. Both observations and the model showed that the speed in the surface layer where the fish farm is located is slower than below the farm. Model results also indicated that the presence of the fish farm can significantly change the local current field around the farm site. Comparison between model results and observations shows that predicted tidal current amplitudes and phases are improved when cage friction is included in the model.

In conclusion, hydrodynamic models are powerful tools that have potential for predicting the spatially and temporally varying currents that occur near aquaculture farm sites. The use of hydrodynamic models for predicting the fate of bath pesticides released during farm treatments for pests requires the implementation of additional models for tracking the evolution of the released agent. Two approaches have been used: the solution of a concentration equation and a particle tracking approach. Both methods have been used to investigate aquaculture related issues such as water quality, the effect of cage drag on the flow, disease spread and the dispersion of sea lice. However, other than the studies by Falconer and Hartnett (1993) and Page et al. (2015), we are unaware of the application of such methods for modelling the release of pesticides from fish farms. There are, as discussed in Rico et al. (2019), many models that could be adapted to this application, including water quality models and integrated population and ecosystem models to predict risks to non-target organisms. As emphasized by Rico et al. (2019), these would not only require modification but evaluation for the different agents and environments in which they would be applied.

With regards to the practicality of using hydrodynamic based models for decision making, the time and effort required for the development of these models limit their usefulness for quick decision making. The exception, of course, is if validated hydrodynamic models already exist for the area of interest. In the case of existing models, once validated, the potential additional information provided for regulatory decisions could be great (Henderson et al. 2001). The limited use for rapid decision making does not negate the usefulness of hydrodynamic based models. Such models can have an important role in the decision-making process. Models that have been properly validated can be used to help evaluate the usefulness of more practical simple models. This would need to be done for a set of regions that are representative of the wide range of conditions in which Canadian aquaculture farms are located. Furthermore, hydrodynamic models can help in evaluating the influence of spatial and temporal variations in currents and their implications to impacts, aspects that are particularly important for evaluating far-field effects. Simple models use local current conditions, usually from a single location, that are unlikely to be valid for large distances. In summary, hydrodynamic models and accompanying pesticide transport and diffusion models can be extremely useful, providing that it is recognized that their development requires both time and effort and that field studies are required to validate the model and assess the uncertainty associated with the outputs.

Models of Discharges from Well-boat Treatments

In contrast to tarp treatments, the initial characteristics of the discharge patch are controlled by different dynamics. The discharge of treatment water from a well-boat into the ambient environment is an intrusion of one fluid into another and the merging of this intrusion with ambient flow and concentration fields.

Intrusions of one fluid into another occur frequently due to both natural and man-made processes and have been the subject of much study in the field of fluid mechanics. Intrusions are classified according to their characteristics (Cushman-Roisin 2018) as described in Table 3. Although the discharge of treatment bath water from a well-boat has a finite duration, the discharge period is long enough for a jet to be established, as observed by Page et al. (2015). For this reason, jet dynamics and modelling are reviewed and their applicability to well-boat discharge is discussed.

Table 3: Types of intrusions. Reproduction of Table 9.1 from Cushman-Roisin (2018).

	Continuous injection	Intermittent injection
Momentum only	Jet	Puff
Buoyancy only	Plume	Thermal
Momentum and buoyancy	Buoyant jet or forced plume	Buoyant puff

Jet Models

Background

A jet occurs when a continuous source of fluid (water or air) with an associated momentum exits from a relatively narrow outlet into a larger body of fluid. A familiar example is the discharge of wastewater into a river (Cushman-Roisin 2018). The behaviour of a jet can be divided into three regimes: near-field, intermediate-field, far-field. Near-field dynamics are governed by the discharge configuration, i.e., outlet diameter, discharge rate and the density difference between the jet and the receiving environment. In the near field, typical time scales are of order minutes and length scales are of order tens to hundreds of meters (Zhao et al. 2011). In the far field, the behaviour of the discharged fluid is dominated by the ambient flow conditions. The intermediate-field is the transition zone between the near- and far-fields. When ambient flows are strong, processes in the intermediate-field are often neglected as they are much less significant than processes in the far-field (Zhao et al. 2011). Typically, different models are used in the near- and far-field regimes of jet dynamics, due to the differing scales and processes of importance to the fluid dynamics (Morelissen et al. 2013).

Zhao et al. (2011) provide a good description of the types of models available for the discharge and dispersion of offshore pollution sources and discuss the strengths and limitations of the models. Four major modelling techniques are identified: analytical and empirical solutions, numerical methods for directly solving the advection-diffusion equations, random walk particle tracking models, and jet-type integral methods.

Jet dynamics are governed by a non-linear system of partial differential equations. In order to obtain analytical solutions to the equations, simplifying assumptions, steady-state conditions, must be made. A simple well-boat model which combined the steady-state solutions with an exponentially decreasing discharge concentration has been shown to give a good approximation of the concentration within the major-axis of a well-boat discharge jet (Page et al. 2015).

Empirical solutions are mainly for solutions in the near field. They have the advantage of being easy to apply. The disadvantage is that empirical solutions are for specific configurations and may have limited applicability.

There are many open source and commercial ocean circulation models in active use for many applications. These models numerically solve the equations governing fluid dynamics (i.e., the Navier-Stokes equations, conservation of mass equations and conservation of energy equations) as applied to ocean dynamics. These models use different numerical schemes and their suitability to solve a given problem depends on both a model's features and available expertise to run the model. Most ocean models include the ability to solve the advection-diffusion equation of a general solute or tracer. These models have been shown to be effective for modelling the movement of a patch of tracer (Chen et al. 2008). However, due to the small spatial scales near a jet discharge source, it is not practical to use ocean circulation models to directly compute near-field solutions of a jet. For a well-boat discharge pipe with a 0.5 m diameter, which is typical of well-boats used in Canadian waters, a spatial resolution of approximately 0.25 meters would be required to model a well-boat jet. This resolution would need to be applied over the length scales of a typical jet discharge, 200 m by 500 m, resulting in, for a triangular unstructured mesh, approximately 1,600,000 nodes and 3,200,000 elements, with a time step of approximately 0.01 seconds. To run this model for a two-hour simulation would take over 24 hours while using 1000 cores.

Random walk particle tracking models are an alternative to the direct numerical solution of the concentration equation described above. This Lagrangian method calculates particle positions by advecting each particle using a given current field and an added diffusion which is simulated using the random walk method. Typically, current fields are from an ocean circulation model and vary both spatially and temporally. Concentrations are calculated by dividing the domain into grid cells and computing the number of particles in each cell. One disadvantage of this method is the difficulty of accurately calculating concentrations as the particles disperse. In order for a particle tracking model to be suitable for modelling near-field jet dynamics, the jet momentum must be included in the particle tracking model itself, which is typically not a feature of standard particle tracking models; or the underlying hydrodynamic model used to advect the particles.

Integral jet models are based on the principle that fully developed jets exhibit self-similar solutions that can be approximated to the first-order by Gaussian profiles (Jirka 2004). Inspired by the principle of self-similarity, the integral jet method uses this approximation to specify the jet distribution functions for the axial velocity, density and concentration. Boundary layer theory is used to simplify the governing Navier-Stokes equations (Agrawal and Prasad 2003) and all terms of the governing equations are integrated across the cross-sectional plane (Jirka 2004). Solutions of integral jet models have compared favourably with laboratory experiments (Zhao et al. 2011) but their application to more complex turbulent flows, where it is difficult to assign profile shapes, may be restricted (Agrawal and Prasad 2003).

Modelling Packages

Several modelling packages have been developed for simulating jet dynamics and concentrations of scalars discharged with the momentum jets. For the most part, these packages use the methods mentioned above, i.e., either analytical solutions, empirical solutions, jet integral methods, or some combination of these (Zhao et al. 2011). The better-known packages are Visual Plumes (United States Environmental Protection Agency 2018), CorMix (MixZon Inc 2019), and VisJet (The University of Hong Kong 2017). The models are valid for both jets and plumes. They predict dilution, trajectory, and other properties associated with the discharge. Although the packages described may predict the far-field evolution of the plume, complex coastlines and temporospatial variation of currents are not considered. Thus, their strength lies in the near-field prediction.

Visual Plumes was developed by the United States Environmental Protection Agency (USEPA) and is freely available. Visual Plumes is a suite of models to simulate single and merging submerged plumes in arbitrarily stratified ambient flow. Buoyant surface discharges can also be modelled. The suitable model to use is dependent on the flow category. Although Visual Plumes does not determine which model to use, it has recommendations of which model best suits a given flow category. Models may be run consecutively to allow comparison between the results. Visual Plumes also includes a module to simulate far-field behaviour. It is a Windows-based computer application but does not run beyond Windows XP. Its last release date was August 2001 (United States Environmental Protection Agency 2018). We do not consider it to be useful for simulating well-boat discharges, because it is no longer maintained and it is limited to use with Windows XP.

CorMix is a widely used commercial package. It is a software package designed for the analysis, prediction and design of pollutant discharges with an emphasis on dilution in the initial mixing zone. Although the emphasis is on prediction in the near-field, it predicts the behaviour of the discharge in the far-field. CorMix was developed specifically for the assessment of environmental impacts and for regulatory management. Similar to Visual Plumes, CorMix is a suite of four hydrodynamic simulation models for different flow categories. Unlike Visual Plumes, the user does not specify which model to use, as CorMix has a rule-based system that selects the appropriate model to simulate a given discharge-environment interaction. The development of this rule-based system was motivated by the widespread misapplication of USEPA plume models (Doneker and Jirka 2017).

VisJet is a user-friendly interface to the Lagrangian jet mixing model JETLAG. The computer model JETLAG is described in Lee and Chu (2003) and was developed for environmental impact assessment, outfall design, and post-operation monitoring. VisJet is a predictive flow visualization tool that models the evolution and interaction of multiple buoyant jets discharging at varying angles into an ambient tidal current.

The strength in the described modelling packages is their ability to predict the flow in the near-field. Any far-field predictions do not include the complexity of the ambient coastline and temporospatially varying current fields to which the evolution of the well-boat discharge patch in the far-field is sensitive. For this reason, we do not feel that these models offer stand-alone solutions to the problem of modelling well-boat discharges. Ideally a model should take into account both the complexities of near-field and far-field solutions. The above modelling packages offer a solution for the near-field problem. Hydrodynamic models with either tracer concentration or particle tracking can address the far-field problem. A model that integrates these two types of models is crucial in order to adequately predict the temporal and spatial evolution of a patch discharged from a well-boat.

Integrated Models

As mentioned earlier, the simulation of well-boat discharges requires consideration of both jet and ambient dynamics. The models described above can be categorized into near-field models (empirical and analytic solutions and jet-type integral methods) and far-field models (numerical solutions of the advection-diffusion equations and particle tracking models). Since the near-field and far-field have different dispersion mechanisms (Zhao et al. 2011), a model that incorporates both processes is required in order to properly model the complete evolution of a jet. There are well-developed application specific models used to simulate the discharge of a fluid into the ocean. Zhao et al. (2011) identify two models used by the oil industry to simulate the discharge of produced water: DREAM (Reed and Hetland 2002) and PROTEUS. Although these models may not to be applicable to well-boat discharges, model descriptions are provided here as they illustrate how integrated models work. Both DREAM and PROTEUS are based on the random walk particle tracking approach and both take into account the different dynamics of the near and far fields. The specific implementations of these models, however, differ significantly.

DREAM (Dose-Related Exposure Assessment Model) was developed by SINTEF in Norway. It is a three-dimensional multiple component model which simulates the transport, exposure and dose of pollutants and assesses the environmental impact. The model is based on Lagrangian particle tracking and includes both near-field and far-field components. In the near field, a Lagrangian plume model is used. In the far-field, each particle represents a Gaussian cloud of chemicals. A given cloud is advected using supplied currents. In the horizontal, diffusion is modelled using the empirical relationship given by Okubo (1974). Concentrations are calculated by summing the contributions from each cloud (Reed and Hetland 2002).

PROTEUS was developed in the UK by BMT to support environmental risk assessments of discharges of produced water and drilling wastes. PROTEUS is built on a set of modules which specialize in specific environmental processes. Included is the prediction of jet/plume turbulent dispersion (Sabeur and Tyler 2004). The module represents matter as an ensemble of fundamental particles. Within a particle tracking model, ambient hydrodynamic turbulence is used to advect and disperse particles. An extended random walk method has been implemented to model turbulent diffusion (Zhao et al. 2011). The particles undergo three stages of turbulence: initial momentum dominated jet-like motion; momentum loss and buoyancy dominated plume-like motion; and ambient turbulent dispersion plume-like motion (Sabeur et al. 2000). The three stages of turbulence model the near, medium and far fields.

Both DREAM and PROTEUS models have been widely used in Europe (Zhao et al. 2011). Both models include the different dynamics found in the near- and far-fields of a discharged plume and were developed specifically for the application of the discharge of produced water. Although they may be useful for modelling well-boat discharges, further investigation is required to determine their suitability.

Morelissen et al. (2013) describe an approach with a broader range of applicability. Separate models are used for the near- and far-fields: the commercial near-field jet model CORMIX (Doneker and Jirka 2017) and the open-source ocean circulation model Delft3D-Flow (Deltares 2014). These models are coupled into a single system which handles the boundary interaction between the two solutions. A similar, yet simpler, strategy was adopted by Inan (2019) for modelling the dilution of a pollutant from a sea outfall system. A two-step approach was used. First pollution concentrations in the near-field were predicted by CORMIX. Second, HYDROTAM-3D, a 3D hydrodynamic model with a pollution transport module, was initialized with the near-field pollution concentrations and used to determine the far-field solution. The commercial hydrodynamic model MIKE 3 Flow Model FM (DHI 2017) has integrated a near-field integral jet model directly into the far field hydrodynamic model. This allows the near- and far-field solutions to be calculated simultaneously. JetLag, the underlying model to the VisJet package described above, has also been coupled with a three-dimensional shallow water circulation model to predict the mixing and transport in the intermediate-field (Choi and Lee 2007; Choi et al. 2016).

Application to Well-Boats

To our knowledge, the only efforts made to model the discharge of pesticides from a well-boat were those of Page et al. (2015). Two models were examined. It was observed that near the discharge orifice, the resulting plume of dye behaved like a steady-state jet into a quiescent fluid. A modification of the steady-state jet solution was proposed where the centre-line concentration decayed exponentially as the dye in the well-boat was diluted during the discharge period. Comparison with limited field work indicated that this is a reasonable first approximation. It should be noted, however, that this model is only valid in the near-field. Another approach was investigated where results of an FVCOM model were used to drive a particle tracking model. As near-field jet dynamics were not included in this model, the initial dispersion of the dye patch was underestimated. Also, details of the observed patch were not always well reproduced. The authors did not view this as a comment on the lack of suitability of the approach, but of the need to refine the underlying hydrodynamic model. In particular, the effects of the fish farm infrastructure need to be included, especially in the cases where the well-boat discharge interacts with the fish farm. Additionally, higher resolution near the fish farm is required to better resolve local flow conditions. The work of Page et al. (2015) illustrated the complexity of modelling discharges from well-boats and the requirements of a suitable model that accounts for all the processes involved and links near- and far-field solutions.

Even if an appropriate model is developed for well-boat discharges, i.e., a model that includes jet discharge dynamics merged with ambient transport and dispersal processes, accurately modelling well-boat discharges is challenging. There are several unknown variables which impact the fate of a discharge from a well-boat. With regards to the discharges themselves, the exact discharge rate is often unknown and can vary not only between well-boats, but between discharges of a given boat (Page et al. 2015). Furthermore, the times and locations of the discharges vary and are unpredictable. Farms are treated on an as needed basis and there is no way of knowing a priori the flow conditions at the time of discharge. Furthermore, at the time of writing, well-boat discharges in the southwest New Brunswick region of Canada occur adjacent to the treated fish cage. Discharges occur on either side of the well-boat, typically one in the direction away from the cage and one into the cage itself. The presence of the fish cages and the supporting infrastructure impacts the local flow conditions and can significantly slow down the dispersion of the treatment pesticide. These challenges raise the important question of the feasibility of accurately modelling the temporal and spatial evolution of a well-boat discharge.

NEW MODELS FOR POTENTIAL PRACTICAL APPLICATION

Tarps

Okubo Based Models

A relatively simple model of the transport and dispersal of pesticides discharged from tarp treatments was described by Page et al. (2015). The model assumes the size of the discharge patch increases with time according to the relationship initially suggested by Okubo (1968, 1971). The horizontal location of the patch changes with time based on a prescribed current speed and the vertical extent increases with time, based on a constant rate of vertical dispersion.

The initial shape of a discharge from a tarped cage treatment is the shape of the cage. The shape changes over time; it becomes wider, elongated and curved, with the long axis of the patch aligned with the direction of the prevailing current. As the shape evolves it may be thought of as a meandering patch. Okubo (1968, 1971) and others (e.g., Lawrence et al. 1995) showed that when the relative spatial distribution of concentration of dye in a freely evolving patch was transformed into a radially symmetric Gaussian distribution, the variance of the distribution increased with time in a non-linear way. Page et al. (2015) showed that the evolving size of discharges from tarp treatments was consistent with this relationship and that the relationship was a conservative representation, i.e., it sometimes underestimated the size of dye and pesticide released from tarped net-pens.

The Gaussian radial model describing the temporal evolution of the radial distribution of the concentration is (Okubo 1968)

$$C(t,r) = C_{\max}(t)e^{-r^2/\sigma_{rc}^2(t)} \tag{1}$$

in which

$C(t,r)$ is the concentration of the substance at time t and radius r,

$C_{\max}(t)$ is the maximum concentration of the substance at time t,

r is the radial distance from the centre of the patch, and

$\sigma_{rc}(t)$ is the time dependent standard deviation of the equivalent radial distances.

$C_{\max}(t)$ is defined as (Okubo 1968)

$$C_{\max}(t) = \frac{M/H(t)}{\pi\sigma_{rc}^2(t)} = \frac{M}{\pi\sigma_{rc}^2(t)H(t)} \tag{2}$$

where

M is the total mass or quantity of substance within the patch,

$H_{\text{mix}}(t)$ is the depth to which the substance is distributed at time t.

By examining data from dye dispersal studies, Okubo (1968, 1971) showed that the following functional dependence is appropriate.

$$\sigma_{rc}^2(t) = \alpha t^{\beta} \tag{3}$$

Expressing the variance and time in units of cm^2 and seconds, respectively, Okubo (1968) initially estimated the values of $\alpha = 0.0108$ and $\beta = 2.34$ by visually fitting the compiled data. These values were confirmed in Okubo (1971) and updated to $\alpha = 5.6 \cdot 10^{-6}$ and $\beta = 2.22$ by Lawrence et al. (1995) using more data and a regression analysis. The values from Lawrence et al. (1995) have been used in the calculations presented in this document.

Okubo (1968, 1971) also defined the effective diameter D_e of a patch as $D_e = 3\sigma_{rc}$, the diameter within which 95% of the dispersing substance occurs when the distribution is a radial Gaussian distribution. The corresponding radius is $R_e = D_e/2 = 1.5\sigma_{rc}$.

The discharge from a tarp begins as a patch with the diameter of the tarped cage. The standard deviation associated with the initial patch size can therefore be estimated as

$$\sigma_{rc}(t=0) = D_{net}/3 \text{ or } \sigma_{rc} = R_{net}/1.5 \tag{4}$$

in which D_{net} and R_{net} are, respectively, the net-pen diameter and radius. This initial standard deviation can be substituted into the Okubo power relationship, given by (5), to calculate an equivalent time that corresponds to the initial variance, i.e.,

$$t_0 = \sqrt[\beta]{\frac{\sigma_{rc}^2(t=0)}{\alpha}} = \left(\frac{\sigma_{rc}^2(t)}{\alpha}\right)^{1/\beta}. \tag{5}$$

The increase in variance with time after discharge (t) can then be calculated as

$$\sigma_{rc}^2(t) = \alpha(t_0 + t)^{\beta}. \tag{6}$$

This allows the increase in the patch diameter to be calculated as

$$D_e(t) = 3\sigma_{rc} = 3\sqrt{\sigma_{rc}^2(t)}, \tag{7}$$

the increase in the area occupied by the patch to be calculated as

$$A_e = \pi\left(\frac{D_e(t)}{2}\right)^2, \tag{8}$$

and the average concentration within the patch to be calculated as

$$C_{\text{avg}} = \frac{M}{A_e\, H_{\text{mix}}(t)}. \quad (9)$$

In the present analyses we have assumed

$$H_{\text{mix}}(t) = \begin{cases} H_{\text{net}} + \sqrt{K_z t}, & H_{\text{mix}}(t) < H_{\text{max}} \\ H_{\text{max}}, & H_{\text{mix}}(t) \geq H_{\text{max}} \end{cases} \quad (10)$$

where H_{max} is the maximum depth to which the patch can mix and K_z is the vertical coefficient of diffusivity. For a given time, the radius, r_{EQS}, at which the concentration is equal to the environmental quality standard (EQS) threshold, C_{EQS}, is given by equating the concentration, given by (1), to the EQS concentration value and solving for the radius.

$$r_{\text{EQS}}(t) = \sqrt{-\sigma_{rc}^2(t) \ln\left[\frac{C_{\text{EQS}}}{C_{\text{max}}(t)}\right]} \quad (11)$$

The calculated circular patch dimensions using the Okubo relationship with the Lawrence et al. (1995) values is shown in Figure 1 for an initial cage size of 120 m in circumference (38.2 m in diameter). The figure shows that the equivalent diameter and area covered by the discharged pesticide increase with time. Figure 1 (top panel) also illustrates that although the patch size increases indefinitely (blue line), the size of the toxic patch (dashed line) can be considered to become zero when the average concentration C_{avg} reaches the defined concentration threshold.

Figure 2 shows a planar view of the area of the equivalent circular patch increasing with time, a cross section through the patch illustrating how the patch widens as the average concentration decreases and the change in vertical extent of the patch with time. Figure 3 focuses on the temporal decrease in the average concentration within the patch and indicates when the average concentration drops below the specified EQS concentration. The decrease in the average concentration is exponential with time, so that the concentration is reduced by a factor of ten (one order of magnitude) after ~0.5 h, by a factor of 100 (two orders of magnitude) after ~2 h and by a factor of 1000 (three orders of magnitude) after ~6.5 h (Figure 3). In the figures referred to in the above and following paragraphs a dose of 100 µg·L^{-1}, and an EQS concentration (C_{EQS}) of 1 µg·L^{-1} and the vertical extent of the discharge patch has been assumed to increase with time from an initial tarp depth of 4 m to a maximum of 20 m using a vertical coefficient of diffusivity of $K_z = 0.01$ m^2·s^{-1} (Figure 2). The time for the average concentration to decrease from the assumed treatment dose of 100 µg·L^{-1} to the specified EQS concentration of 1 µg·L^{-1} is estimated as 2.3 h (Figure 3).

The exposure duration at any given location depends on the distance from the source, the size of the patch when it reaches the location, and the time it takes for the patch to travel across the location (which is dependent on the patch size and the current speed). The duration of the exposure can be estimated as the diameter of the discharge patch at the time it reaches the location, divided by the speed of the current advecting the patch. The exposure time estimate increases with elapsed time since the initiation of discharge, because the patch size gets larger with time. Also, since the current speed determines the time required for a patch to travel across a given location, the exposure time decreases as the current speed increases (Figure 4). For a uni-directional constant current speed, the exposure durations increase with distance from the discharge, since the patch grows and moves away from the discharge simultaneously.

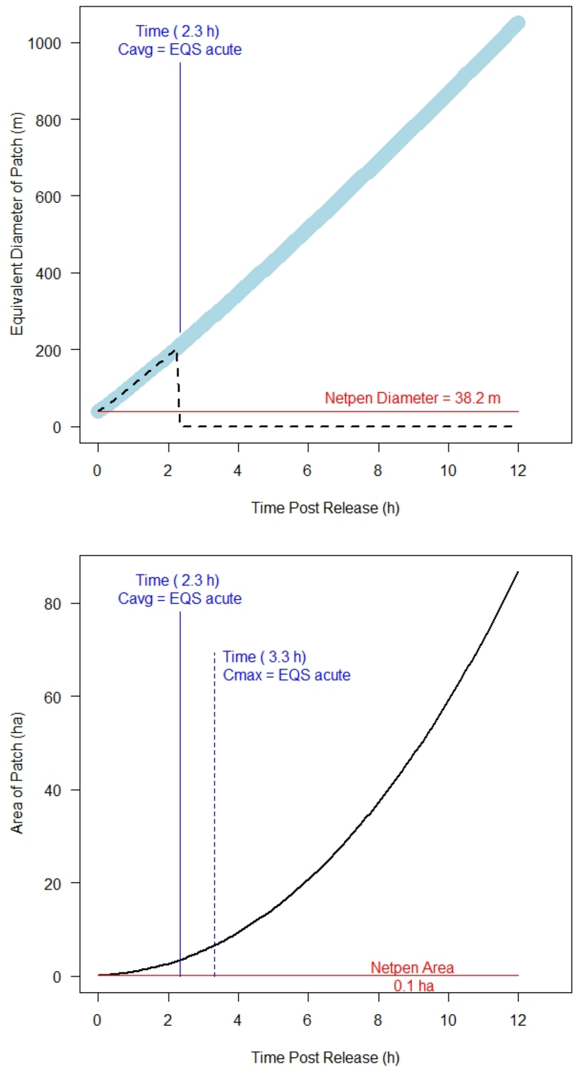

Figure 1. The increase in the equivalent diameter (top panel) and equivalent area (bottom panel) of a dispersing pesticide patch released from a tarp treatment as represented by the Okubo empirical relationship using parameter values derived by Lawrence et al. (1995). The size of the patch that has an average concentration that is greater than a defined EQS concentration is shown as a dashed line in top panel. Model results were obtained using a treatment dose of 100 µg·L^{-1}, an EQS concentration of 1 µg·L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of $K_z =$ 0.01 m^2·s^{-1}.

The distance travelled by the patch is the product of velocity and time; hence as the current speed increases, the distance travelled by the centre of the patch over a given time since discharge increases (Figure 5). The distance travelled varies from zero to several kilometers. The maximum distances travelled during the time for the average concentration to decrease to the EQS concentration are greater than ~4 km assuming current speeds of 0.5 m·s^{-1} or more.

These calculations assume a constant current velocity, a circular patch, and the size of the patch does not change over the exposure time scale. These assumptions are unlikely to be true for time periods that are larger than an hour. In areas with tidal currents, the speed will change throughout the tidal cycle and the direction will reverse at the transition from ebbing to flooding. However, the estimated exposure durations are generally less than a few hours and if the current speed is considered to be a time averaged speed, the exposure duration estimates are useful first order approximations.

Whether the exposure times are enough to result in toxicity depends on the duration of time associated with the EQS concentration. In Figure 4, two EQS exposure times are shown for comparison. When an EQS exposure time of 0 h is assumed, the discharge patch is toxic until the average concentration decreases to the EQS concentration, i.e., toxic throughout the dilution time. When an EQS exposure time of 3 h is assumed, the discharge patch is not toxic. The treatment durations, which are toxic to the target organisms, are about 30 min. It is not unreasonable to assume that the treatment durations are also toxic to non-target organisms. The most appropriate EQS duration is probably somewhere between 0 and 3 h, but without additional information, an exposure duration of 0 h is a precautionary assumption.

The estimates generated by the above simple model are sensitive to several assumptions, including the pesticide treatment concentration, the size of the net-pen, the rate of vertical mixing, the choice of EQS concentration and exposure duration, and the constant water speed. With the assumptions used here the model suggests patches of some pesticides may travel a few kilometers from a treatment site before they are diluted to non-toxic concentrations. The estimates can be customized to specific sites by choosing parameter values most appropriate for the site and they can be bounded by choosing relatively low and high input values appropriate to each specific treatment scenario. In general, the estimates are thought to be precautionary, as they likely underestimate dilution and overestimate exposure durations and distances. The model also predicts that for some values of non-zero current speeds and non-zero EQS exposure durations, exposures near the discharge location will not be toxic since exposure times near the discharge location will be short. We have not conducted an extensive study on the relationship between the EQS exposure duration, ambient current speed, and toxic exposure. However, empirical evidence indicates the pesticide patch does not quickly separate from the treatment cage and hence exposure times near the cage are likely longer than estimated by the simple model.

The Okubo model provides an additional perspective that takes into consideration the radial distribution of the concentrations. In this model the concentration has a maximum at the centre of the pesticide distribution, i.e., where the radius equals zero ($r = 0$). As the pesticide disperses the width of the patch increases as before, i.e., as described by the Okubo relationship. The concentrations in the middle portions of the patch decrease with time and radius. The concentrations on the outer portions of the distribution initially increase with time and then decrease (Figure 6).

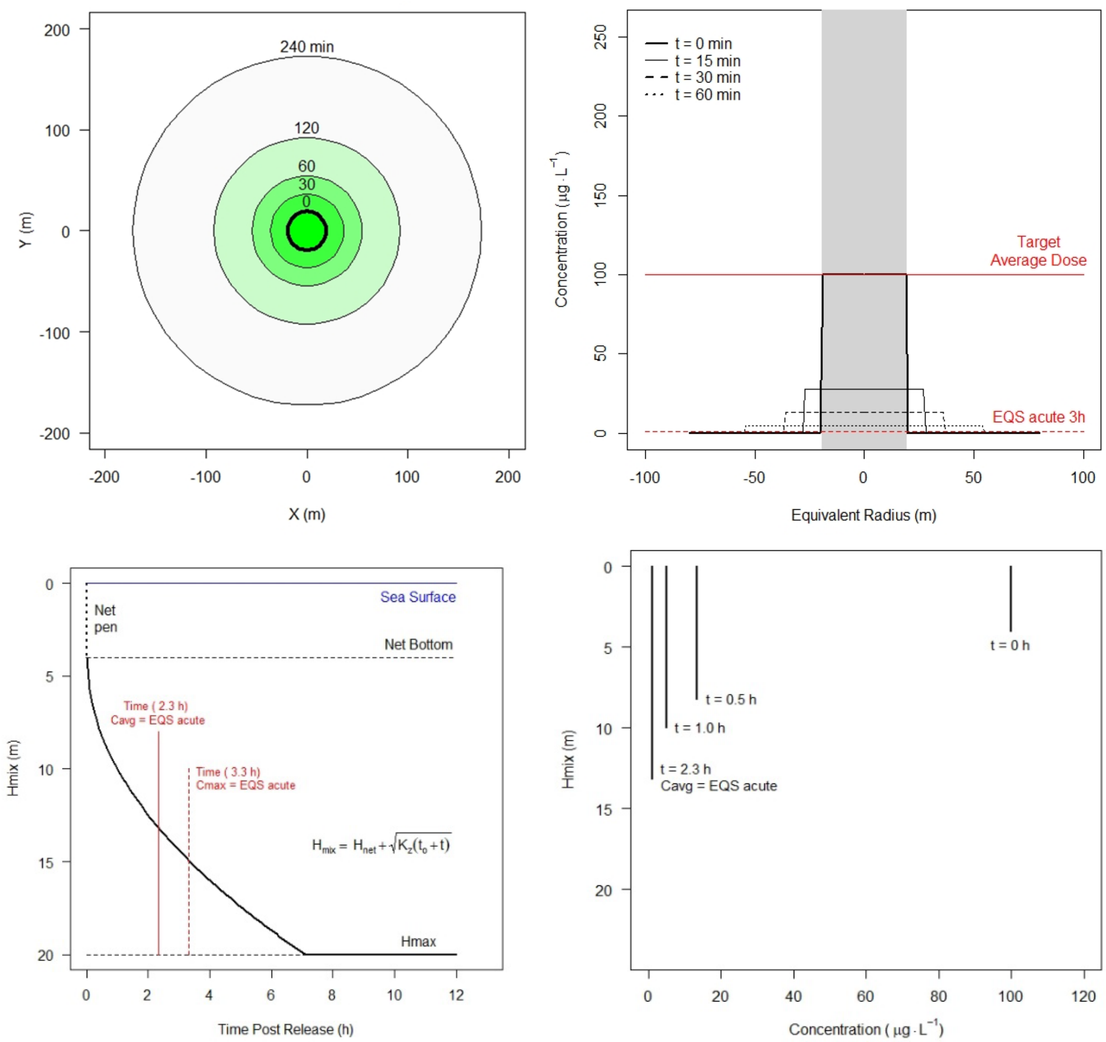

Figure 2. Illustration of the increase in the horizontal size of a circular Okubo patch with time (top left panel), the decrease in the average concentration as the patch width increases (top right panel) and the increase in the temporal increase in the depth over which the discharged pesticide is distributed (lower panels). Model results were obtained using a treatment dose of 100 µg$\cdot$L^{-1}, an EQS concentration of 1 µg$\cdot$L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of K_z =0.01 m$^2\cdot$s^{-1}. The grey shading indicates the relative location of the cage diameter for a stationary patch.

Similar to the average concentration perspective, the maximum concentration decreases exponentially with time. In the illustrated example, the time for the maximum concentration (100 µg$\cdot$L^{-1}) to below an EQS value of 1 µg$\cdot$L^{-1} (i.e., a two order of magnitude drop in concentration) is longer than the time for the average concentration to drop below the same value (Figure 7). Although the dilution times differ, they are both of similar magnitude. The maximum dilution time estimate (3.3 h) can perhaps be considered an upper bound on the exposure duration and the average dilution time (2.3 h) a lower bound. Both estimates are conservative since they may underestimate the initial rate of dilution (Page et al. 2015); the initial rate can be, but is not always, greater than that predicted by the Okubo relationship because the Okubo relationship does not include the influence of the cage array drag on dispersal. For the dosage and cage size illustrated here a reasonable working estimate of the dilution time may be 3 h.

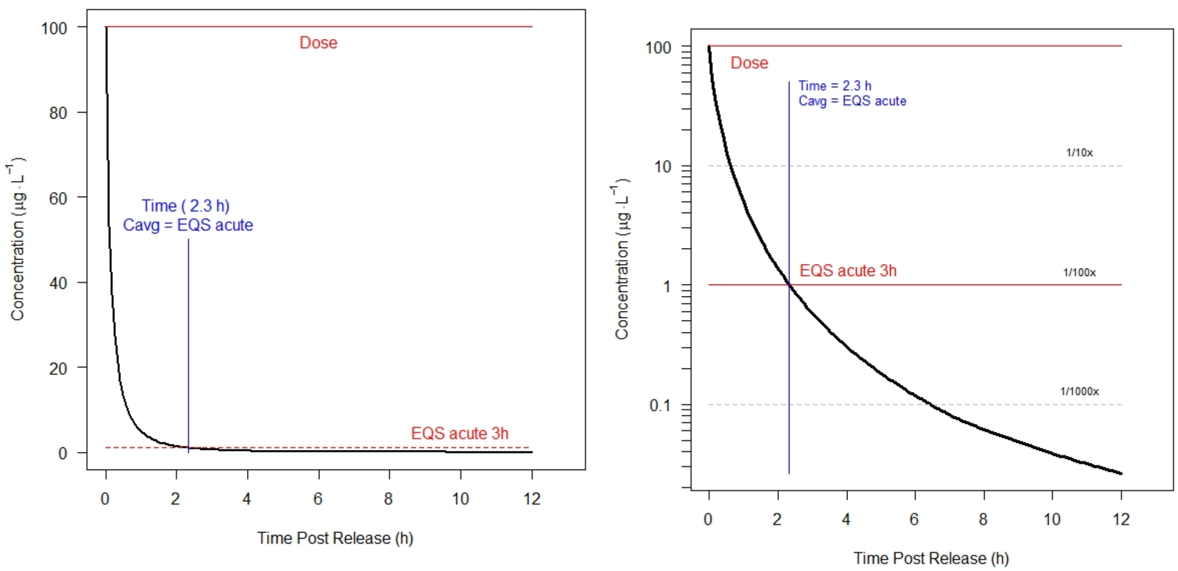

Figure 3. The average concentration of pesticide as a function of time as estimated by the Okubo based model described in the text. The left panel shows concentration on a linear scale and the right panel shows the same concentration on a logarithmic scale. The EQS concentration (horizontal red lines), and the times to dilute to the EQS concentration (vertical blue lines) are shown for illustrative purposes. Model results were obtained using a treatment dose of 100 µg·L^{-1}, an EQS concentration of 1 µg·L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of K_z =0.01 m^2·s^{-1}.

Unlike the results using the average concentration, the results using a radial distribution in the concentration show that the width of the portion of the discharge that has concentrations greater than a specified EQS concentration initially increases to a maximum and then decreases to zero (Figure 6 and Figure 8). This occurs because the concentrations within the shoulders of the patch are initially below the EQS concentration but as the patch spreads, the concentrations in the shoulders increase and the size of the patch with concentrations above the EQS concentration increases. As the spreading continues the shoulder concentrations drop below the EQS concentration and the patch size decreases until the peak concentration drops below the EQS concentration. This behaviour is dependent the value of the EQS concentration and the initial patch size.

Assuming a radial distribution in concentration, the durations of exposure at a given location to a concentration greater than a specified EQS concentration (Figure 9) can be considerably less than those estimated by assuming an average patch concentration (Figure 4). The patch radii at which the concentration equals the EQS concentration can be used to estimate the exposure time. For current speeds ranging from 0.05 to 1 m·s^{-1} the duration of exposure at a given location is less than 1 h (Figure 9). Whether these exposure durations are sufficient to cause toxic effects depends on the exposure durations associated with the EQS concentration. As with the average concentration perspective, patches are considered toxic/non-toxic when EQS exposure times are assumed to be 0/3 h, respectively.

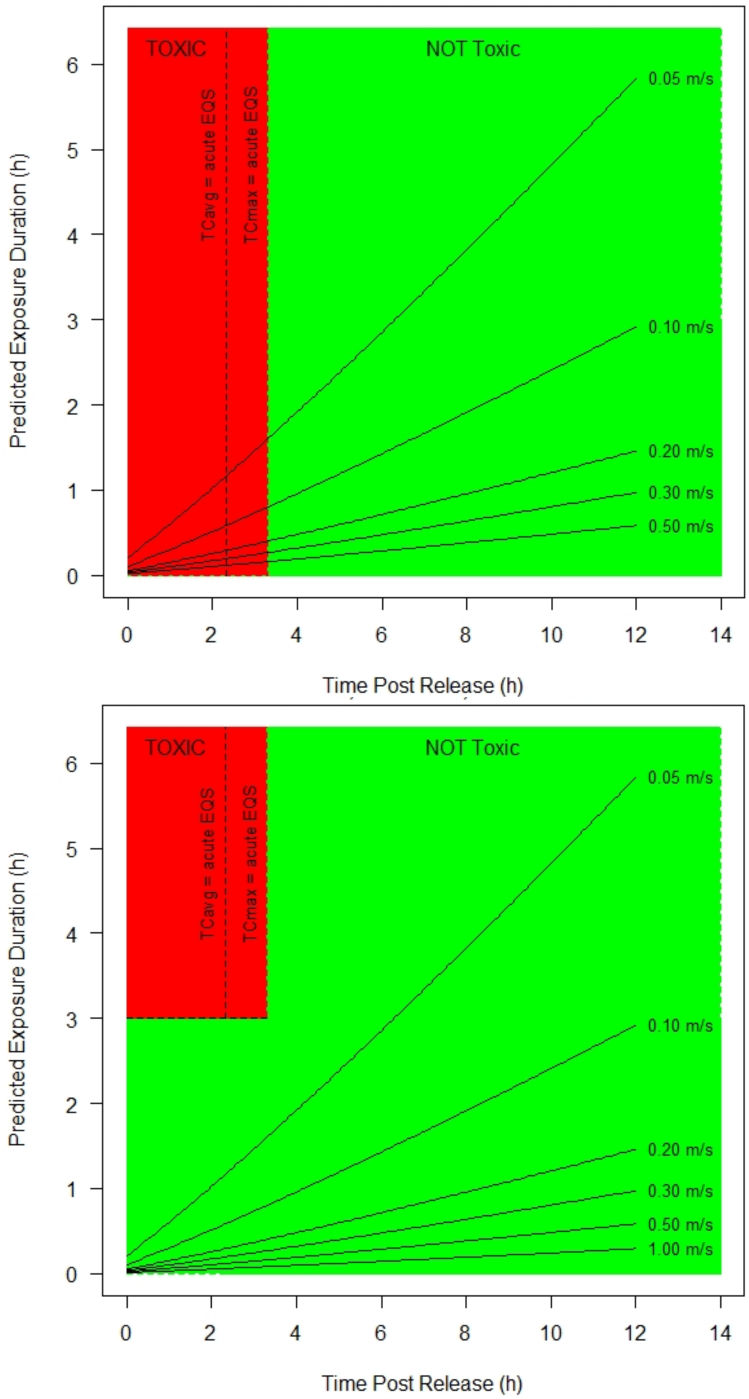

Figure 4. Exposure time as a function of constant water velocity and time elapsed after the start of discharge. Red indicates toxicity based on the exposure time associated with the EQS and green indicates non-toxic. In the upper panel, the EQS exposure time is assumed to be 0 hours; in the bottom panel, the EQS exposure time is assumed to be 3 hours. Model results were obtained using a treatment dose of 100 $\mu g \cdot L^{-1}$, an EQS concentration of 1 $\mu g \cdot L^{-1}$, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of K_z =0.01 $m^2 \cdot s^{-1}$.

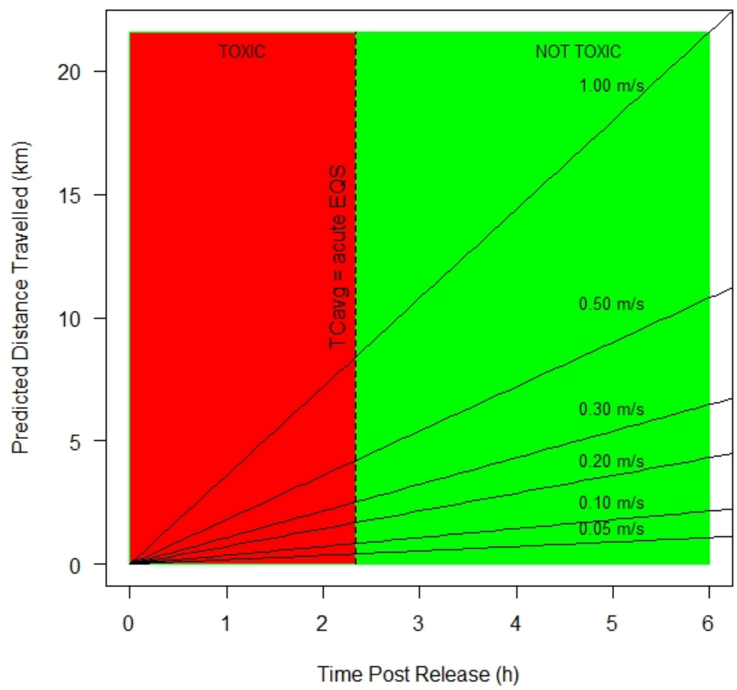

Figure 5. Distance travelled from the discharge location as a function of water velocity and time elapsed since the start of discharge. Model results were obtained using a treatment dose of 100 µg·L^{-1}, an EQS concentration of 1 µg·L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of K_z =0.01 m^2·s^{-1}.

Both of the above approaches indicate that a location is exposed to the discharge patch for only a subset of the dilution time, i.e., the time between discharge and dilution to the EQS concentration. Estimates of the duration of the exposure vary with the selected concentration model, distance from the discharge, and ambient current speed. It is important to note that for both models, extrapolating implications of toxic consequences depends on the duration of assumed exposure time required to generate the toxicity.

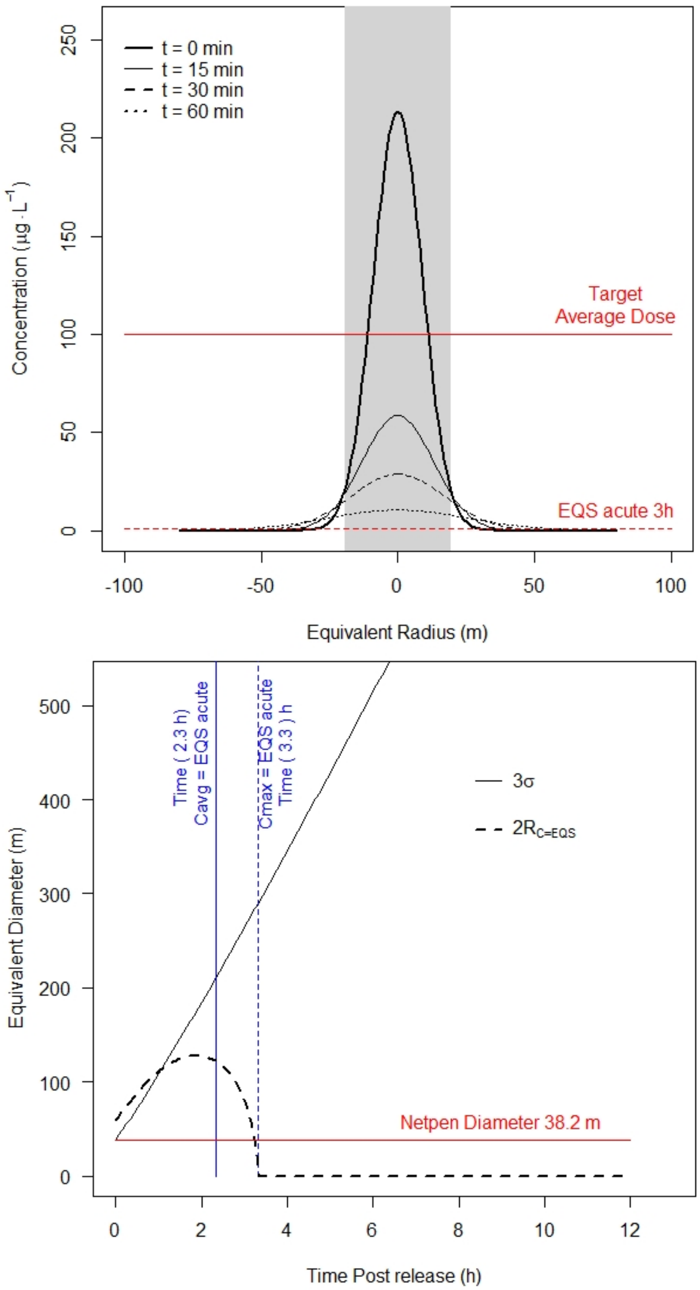

Figure 6. The top panel shows the concentration of pesticide as a function of radius and time as estimated by the Okubo based model when a Gaussian radial distribution of concentration is assumed. The lower panel shows how the equivalent diameter of the dispersing pesticide patch increases with time under the average concentration model with no EQS limitation (solid line) and the diameter of the patch based on a Gaussian radial distribution of concentration that has concentrations greater than the EQS concentration (dashed line). The diameter of the net-pen is shown (horizontal red line) along with the times for the average and maximum concentrations to dilute to the EQS concentration (vertical blue lines). The initial distribution is defined so that 95% of the total quantity of pesticide is within the diameter the fish cage i.e., within a diameter (radius) of three (one and a half) standard deviations of the normal distribution. Model results were obtained using a treatment dose of 100 µg·L^{-1}, an EQS concentration of 1 µg·L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of K_z =0.01 m^2·s^{-1}. The grey shading indicates the relative location of the cage diameter for a stationary patch.

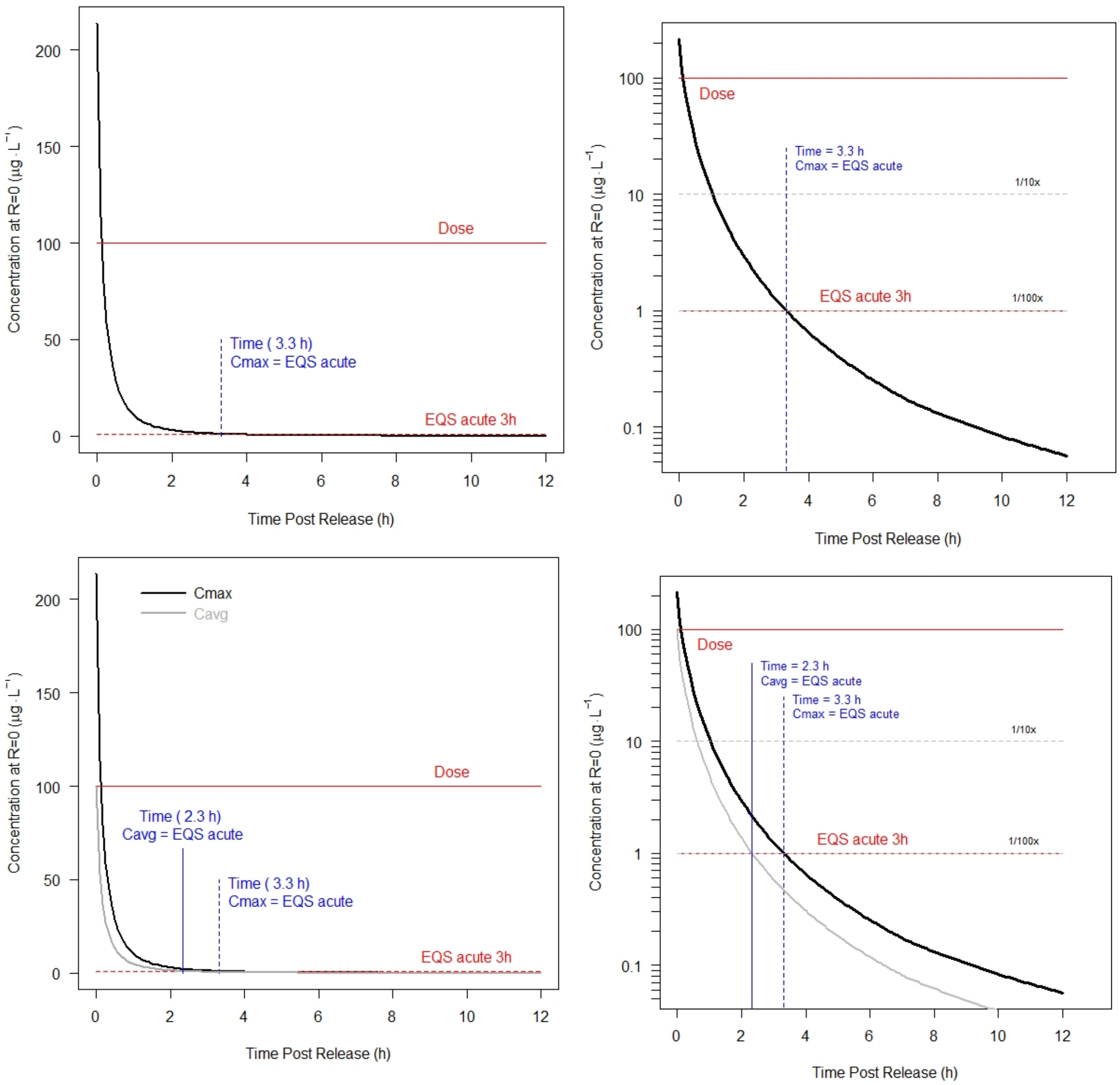

Figure 7. The decrease in the concentration of pesticide with increasing time since discharge. The top panels show the decrease in maximum concentration as estimated by the Okubo based model when a Gaussian radial distribution of concentration is assumed. The lower panels show both the decrease in the maximum and average concentrations. The left panels show the maximum concentrations on a linear scale and the right panels show the same concentration on a logarithmic scale. EQS concentration (horizontal red line), and the time to dilute to the EQS (vertical blue line) are shown for illustrative purposes. The initial distribution is defined so that 95% of the total quantity of pesticide is within the diameter of the fish cage i.e., within a diameter (radius) of three (one and a half) standard deviations of the normal distribution. Model results were obtained using a treatment dose of 100 µg·L^{-1}, an EQS concentration of 1 µg·L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of K_z =0.01·m^2·s^{-1}.

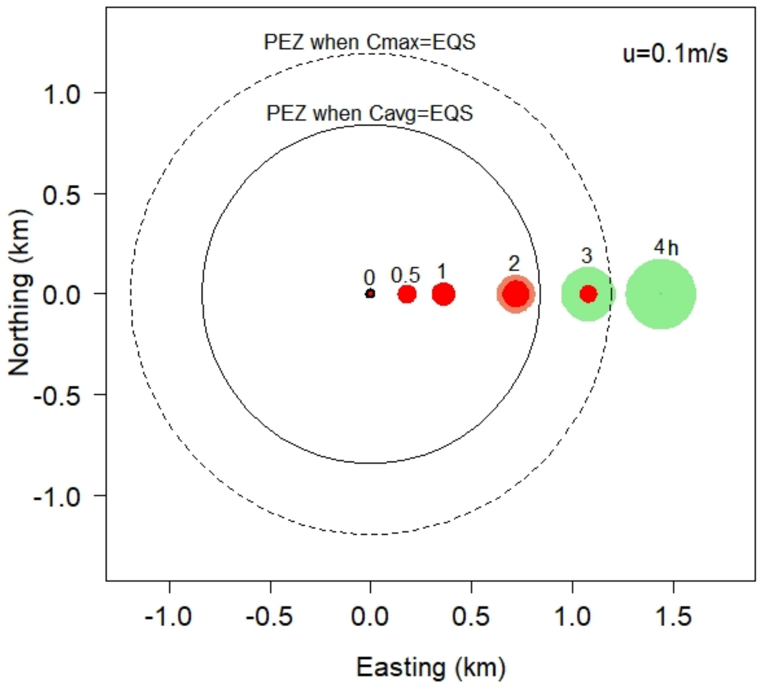

Figure 8. An illustration of how the patch sizes, with the patch variance based on the Okubo relationship (see equation (7)) and the patch size based on the EQS concentration value (see equation (11)), change with time and distance from the discharge location. The coloured circles represent the patches. Dark red indicates the concentration, based on the Gaussian distribution, is above the EQS concentration, light red indicates the average concentration is above the EQS concentration, and green indicates the concentration is below the EQS concentration. Note that at 0.5 h and 1 h post release, the concentration in the entire patch is above the EQS concentration for both the Gaussian distribution and the average concentration models. The total patch size is defined by the Okubo diameter (3 sigma). For a given patch, the maximum concentration occurs at its centre. For comparison, PEZ are shown using the time required for the average concentration (solid black circle) and the maximum concentration (dashed black circle) to reach the EQS concentration. Model results were obtained using a treatment dose of 100 μg·L^{-1}, an EQS concentration of 1 μg·L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of $K_z = 0.01$ m^2·s^{-1}.

In summary, the estimate of extent and duration of exposure depends on the choice of concentration model, EQS concentration, and exposure time for toxicity to occur. The basic Okubo relationship assumes the patch length scale is the radius of a patch with an area equivalent to the area within the irregular shape of a real patch and that the radius is defined as 1.5 times the standard deviation of the radial distance-weighted concentration. In the simple model described above the total quantity of pesticide discharge is assumed to be contained within the Okubo radius and uniformly distributed. In reality, however, concentrations vary within the patch and this radius does not usually correspond to the radius at which the concentration equals the EQS concentration. As a consequence, for the radially distributed concentration, the size of the toxic patch varies with the assumed EQS concentration; when the EQS concentration occurs at a radius less (greater) than the Okubo radius the exposure area is smaller (larger) and the exposure times are shorter (larger) than those in the uniformly distributed concentration Okubo model. However, both models suggest exposures to pesticide concentrations above an EQS value for stationary organisms may be on the order of tens of minutes to a few hours. Whether this translates into expected toxic consequences depends on the assumption of exposure duration needed to generate the effects. A precautionary assumption is that any exposure time to EQS concentrations is enough to generate toxic consequences. Although the distance travelled by the toxic patch varies with current speed, the distances travelled for current speeds typical of fish farming areas are of order kilometers and the areal extent of the patch will vary as it travels this distance. The average Okubo model may overestimate the size of the patch at the extreme distances and the Gaussian Okubo model may underestimate the size. Therefore it may be reasonable to conclude that the size of the toxic portion of the discharge patches at the extreme distances is in the order of thousands to tens of thousands of square meters.

The above describes the application and further development of Page et al.'s (2015) Okubo based model. The models give insight into the behaviour of a released treatment patch, the sensitivity of exposure time to how concentration is distributed within the patch, and the importance of good experimental data to select appropriate EQS concentrations and time durations. Although the models can be used to provide upper and lower bounds for the total exposure area, in the simple form presented here, they do not provide information about expected exposure locations. Below we examine some models that provide information about the exposed locations.

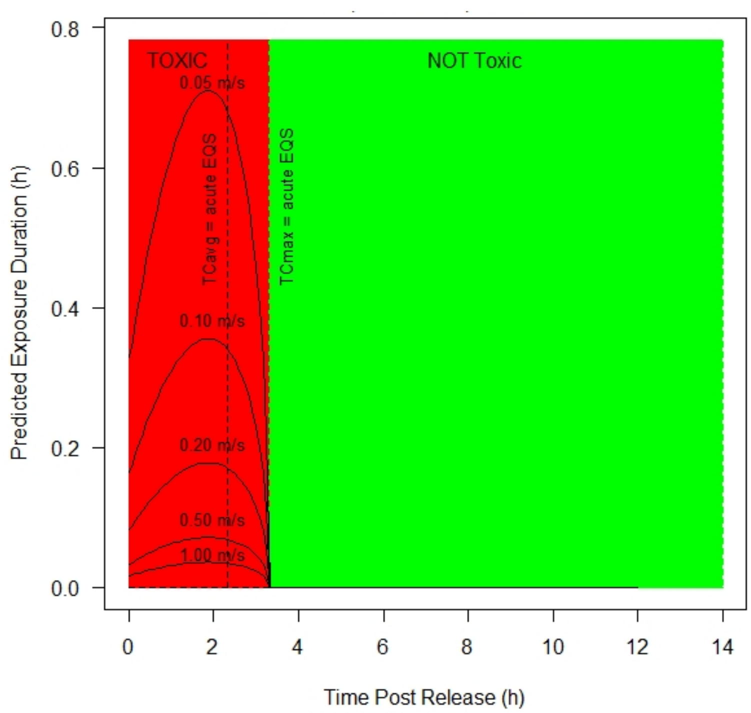

Figure 9. Exposure time to concentrations above the EQS concentration associated with the assumption of a Gaussian distribution of concentration within the discharged bath water as a function of constant water velocity and time elapsed after the start of discharge Model results were obtained using a treatment dose of 100 μg·L^{-1}, an EQS concentration of 1 μg·L^{-1}, an initial depth of 4 m, a maximum depth of 20 m, and a vertical coefficient of diffusivity of K_z =0.01 m^2·s^{-1}.

Potential Exposure Zone Models

The potential exposure zone (PEZ) model, described in section Models of Discharges from Tarp Treatments, is a simple model that defines the potential exposure zone as a circle centred on the release of the pesticide discharge with a radius determined by the time required for the patch to dilute to some threshold value. When applying PEZ to determine regions of potential exposure to toxic chemicals, care is required in the selection of the current speed, as discussed below and shown in Figure 10, which was generated using near-surface currents from an ADCP at an anonymous location and a dilution time of 2 h (assuming, for azamethiphos, a treatment concentration of 100 $\mu g \cdot L^{-1}$ and a threshold of 1 $\mu g \cdot L^{-1}$).

The PEZ approach takes into account several of the important features of a discharge patch: the length of time of concern (e.g., dilution time) and the potential location of exposure. It should be emphasized, however, that since directionality of the current is ignored, that all exposed areas should lie within the PEZ but not all areas within the PEZ will be exposed. Furthermore, the PEZ does not predict exposure concentrations or duration. Nevertheless, it is useful as a first step in a triage approach; if there is nothing of concern in the region, there is no need to look further.

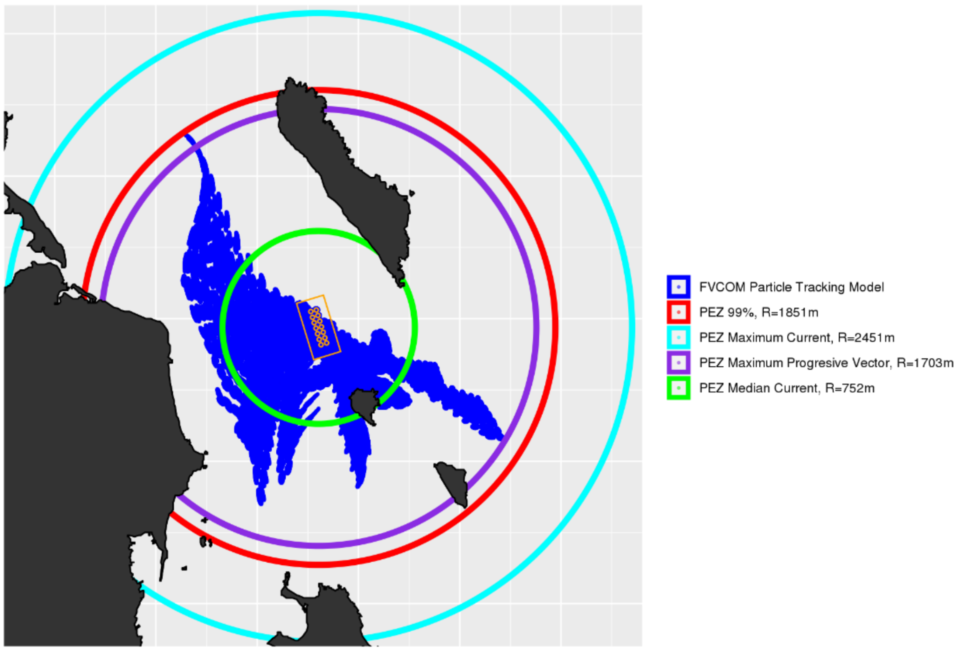

Figure 10. Estimated exposure zones for a pesticide released from an anonymous farm site (shown in orange) using the PEZ model with different current speeds. The PEZ were calculated using near-surface currents from an anonymous ADCP and a dilution time of 2 hours. In this example, the radius of the PEZ includes the displacement distance and the distance from the centre of the cage array to the furthers cage edge. The exposure zone for a particle tracking model forced with output from a hydrodynamic model (FVCOM) is also shown.

As with the Okubo models, the PEZ model assumes the current is spatially and temporally constant with a suitable magnitude. This approach is perhaps the simplest and, when the current speed is set to the estimated maximum current in the local area, is cautionary. However, due to the temporal variation in the current speed, the maximum speed may not be persistent for the duration of the dilution period. The estimate of distance travelled using this approach gives an indication of the scale of transport. This should encourage advisers and managers to question whether it is reasonable to assume the currents are spatially and temporally homogeneous over this length scale, and whether potential exposures to sensitive organisms within this length scale are of sufficient concern. If this is the case, then higher resolution information on currents is required so that exposure risks can be re-evaluated, and the consequences reconsidered.

Examples of some simple calculations are given below. The frequency distributions of water speed for a specific current record are shown in Figure 11 (top panel). In this example the frequency of current speeds is right skewed (i.e., the tail is extended on the right), the mean speed is 8.9 $cm \cdot s^{-1}$, the median speed is 8.3 $cm \cdot s^{-1}$, the maximum speed is 31.9 $cm \cdot s^{-1}$ and 99% of the current speeds are less than or equal to 23.8 $cm \cdot s^{-1}$. The frequency distribution of the horizontal distance travelled, the displacement distance, over a 2-h period assuming the current is spatially and temporally constant is also shown in Figure 11 (middle panel). Like the current speeds, the displacement distances are right skewed. The mean displacement is 644 m, the median displacement is 598 m, the maximum displacement is 2297 m, and 99% of the displacements are less than or equal to 1697 m. The displacement distance associated with the maximum speed is likely to differ from the actual distances travelled because of temporal and spatial variations in the current speed. An estimate of the displacement frequency distribution, calculated as the sum of the individual displacements associated with each current speed measurement and the duration of time between these measurements for the dilution time period and for releases beginning at each of the current measurements, takes into consideration temporal variation in the current speed. These progressive displacements are shown in Figure 11 (bottom panel) and are less than those based on the constant current scenarios when the maximum, 99th percentile, and mean values are considered. The progressive displacement distances are less skewed due to the averaging of the current speeds. The mean progressive displacement is still 644 m, the median displacement is 599 m, the maximum displacement is 1549 m and 99% of the displacements are less than or equal to 1341 m. In all cases the maximum distances are in the order of kilometers and 50% of the displacement distances are greater than 0.6 km. These statistics will vary with location and current meter record.

The PEZs based on the above statistics are shown in Figure 10. It is evident that the size of the PEZ is sensitive to the speed used to estimate the displacement distance. Since it is difficult to pre-determine the spatial variation in the current, it is uncertain whether the displacement estimates are greater than or less than the actual values. One way of incorporating spatial variation into estimates of pesticide transport is to use estimates of the spatially and temporally varying currents generated by a well-calibrated and evaluated circulation model. This is illustrated using preliminary results of an FVCOM model developed for the region to estimate the exposure area using a particle tracking model. Particles were released from the farm site at hourly intervals over a tidal cycle, kept at the surface, and tracked for the dilution time. The estimated exposure zone is shown in Figure 10. Although not calculated here, the results of a particle tracking model can be used to estimate the temporal variation of a patch's location, size and the concentration within. The reader should be aware that, although the prediction based on the particle tracking results is more precise than for the PEZ, its accuracy is uncertain.

At this location, comparison between the computed PEZ and the exposure area predicted by the particle tracking model suggests that the 99th percentile cut-off of the current speed gives a good estimate for the PEZ. There are, however, factors that are not taken into account which could impact both results. The current speeds for the PEZ are taken from an approximately month-long current meter record. Thus seasonal variations are not taken into account. The particle tracking results are based on currents from an even shorter time frame of less than a day. Without proper model validation and particle tracking runs based on longer periods, if the PEZ approach is used, then it would be prudent to adopt a cautionary approach and use the maximum current speed.

The above results suggest that, if organisms, habitats, and human activities that are sensitive and vulnerable to the pesticide and exist within a few kilometers of the discharge location, refined estimates of exposure should be made. These estimates should take into consideration the duration of potential exposures as well as spatial and temporal variations in the current within a few kilometers of the current meter location. In the absence of more detailed information, the maximum current is perhaps the most appropriate and most precautionary value to use in the estimation of exposure potential to bath pesticides. The exposure distances will also vary with changes in the dilution and/or decay rates which are associated with uncertainties in pesticide dilution rates and exposure thresholds.

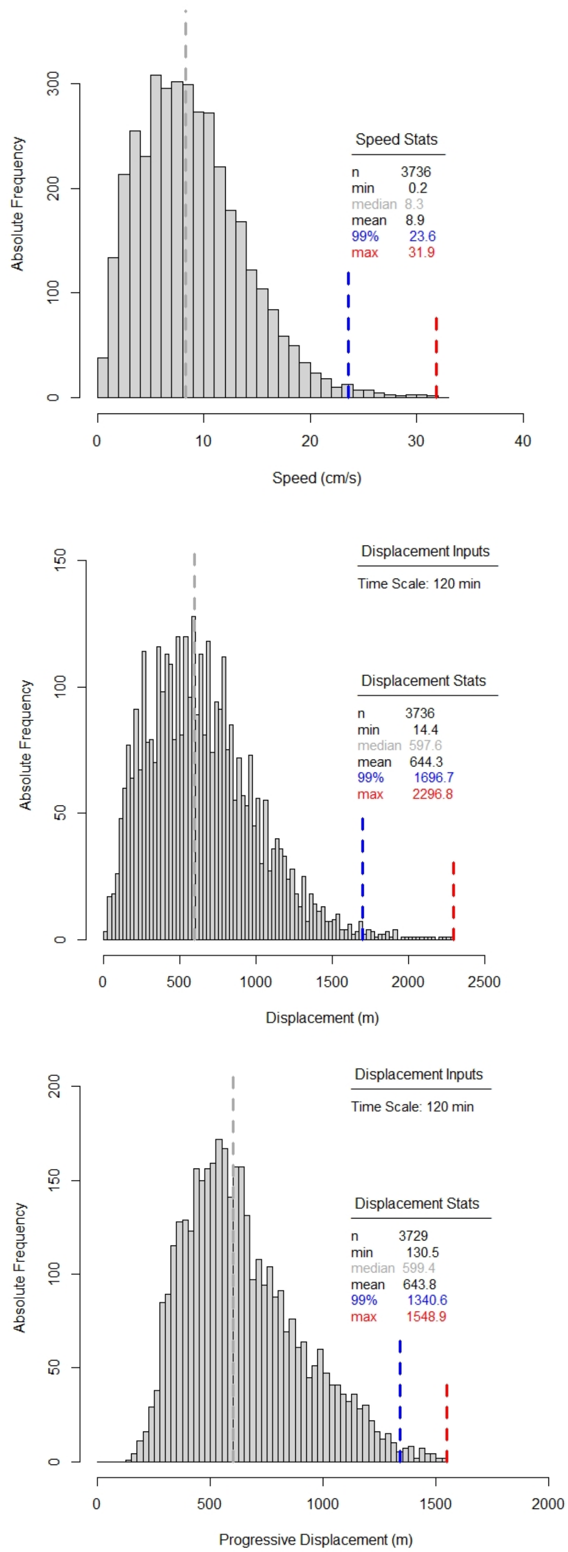

Figure 11. Density distribution of current speeds (top), displacement based on a dilution time of 2 h (middle), and progressive vector displacement using current speed and a dilution time of 2 h (bottom). All figures were produced using near-surface current meter data for an anonymous fish farm site.

Well-boats

Recognizing the challenges of modelling the temporal and spatial evolution of a well-boat discharge, we explore four simple models which may be of use to management, regulators and operators. The models use a combination of the near-field solution for a turbulent jet into a quiescent fluid and the Okubo (1974) dispersion formulation with updated values from Lawrence et al. (1995). A jet is fully turbulent if its Reynolds number (Re), based on the discharge velocity, outlet dimension, and fluid kinematic viscosity, is greater than approximately 10^3 (Jirka 2004). To calculate the approximate Reynolds number for a well-boat discharge, we use a discharge rate of Q=1000 $m^3 \cdot h^{-1}$, a discharge pipe diameter of d = 0.5 m (Page et al. 2015), and a kinematic viscosity ν=13.51×10^{-7} $m^2 \cdot s^{-1}$ for water with a salinity of 30 $g \cdot kg^{-1}$ and temperature of 10°C (Nayar et al. 2016) which gives Re=$Ud/\nu \approx 5.2 \times 10^5$, confirming the validity of the turbulent assumption. The turbulent assumption is likely to be true for all well-boat discharges but should be verified for individual well-boat parameters.

Page et al. (2015) discussed the application of the steady-state solution for a horizontal round turbulent jet being discharged from a well-boat into an unbounded stagnant environment. Here we describe details of the steady-state horizontal round turbulent jet model described by Lee and Chu (2003) which are similar to the jet dynamics used by Page et al. (2015). It is known that jets discharged into a quiescent fluid display a conical shape with the jet radius given by

$$R = \beta x, \qquad (12)$$

where x is the distance along the centre-line of the jet and R is the jet radius. By convention, the jet radius is defined as the radial distance where the x-component of the velocity is equal to $u_{\max}/e$, where $u_{\max}$ is the velocity along the jet centreline. If the jet contains a dissolved substance, the width of the concentration profile (R_c) is usually wider and can be written as

$$R_c = \lambda \beta x. \qquad (13)$$

The constants β and λ are determined experimentally and we use the values 0.114 and 1.2 respectively, as suggested by Lee and Chu (2003). Velocity and concentration profiles are self-similar. At any given distance along the jet centre-line, they can be approximated by Gaussian profiles:

$$u(x,r) = u_{\max} \exp\left(-\frac{r^2}{(\beta\, x)^2}\right), \qquad (14)$$

and

$$C(x,r) = C_{\max} \exp\left(-\frac{r^2}{(\lambda\beta\, x)^2}\right), \qquad (15)$$

where r is the radial distance from the centreline and $C_{\max}$ is the concentration along the jet centreline. For a round jet, $u_{\max}$ and $C_{\max}$ are inversely proportional to the distance downstream

$$u_{\max} = \frac{6.2\, d}{x}\, U; \;\; C_{\max} = \frac{5.26\, d}{x}\, C. \qquad (16)$$

In (16), d is the pipe diameter, U is the discharge speed, and C is the concentration of the discharged water. The discharge speed can be calculated from the discharge rate, Q, and the pipe diameter

$$U = \frac{4Q}{\pi d^2}. \tag{17}$$

A schematic of a jet discharging into a fluid at rest is given in Figure 2.4 of Lee and Chu (2003). It should be noted that laboratory observations show it takes about 10 pipe diameters downstream from the outlet for the steady state solution to become valid (Fischer et al. 1979). For well-boats this distance is approximately 5 m assuming a diameter of 0.5 m for the discharge pipe. In the models described here, we ignore this initial zone of establishment and assume the conical shape is established immediately at the discharge location of the jet.

Since we are interested in the jet containing the dissolved pesticide, we use (13) to define the radius of the jet. However, the radii defined in equation (13) is for the distance where the concentration is $1/e$ the value at the centre-line. Following Cushman-Roisin (2018), we wish to define the distance (from $r = -R$ to $r = R$) over which the distribution (15) covers 95% of the total quantity of pesticide. This results in a radius R of

$$R_c = \alpha x + \frac{d}{2}, \tag{18}$$

where $\alpha = \sqrt{2}\lambda\beta$ and the virtual origin, as discussed in Cushman-Roisin (2018), is taken into account (see Figure 12).

During a well-boat discharge, the concentration of the treatment pesticide is continuously diluted. Page et al. (2015) have shown that the concentration at a time t of the discharge, $C(t)$, can be approximated by

$$C(t) = C_0 \, exp\left(-\frac{Qt}{V}\right), \tag{19}$$

where C_0 is the initial concentration, Q is the discharge rate, and V is the volume of the well. Page et al. (2015) proposed that the concentration in a well-boat discharge jet can be approximated by substituting (19) into (16). The concentration equation (15) can then be written as

$$c(x, r, t) = \frac{5.26\, d}{x} \, C_0 \, exp\left(-\frac{Qt}{V}\right) \, \exp\left(-\frac{r^2}{(\lambda\beta x)^2}\right). \tag{20}$$

Equations (16), (17), (18), and (19) will be used in the models below. These models are implemented numerically using discrete time steps. For comparison purposes, the models are run for the time of the field observations with a time step of one second. The value of the time step was chosen arbitrarily and has not been assessed to determine the optimal value. Descriptions of the parameters used in these models are given in Table 4.

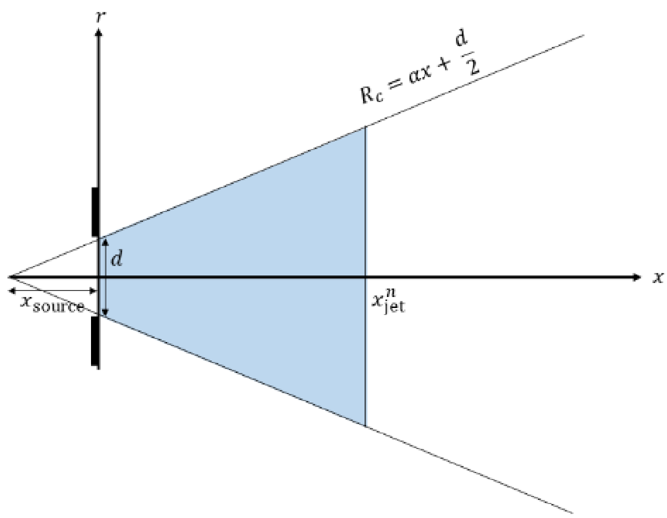

Figure 12. Schematic of plan view of round jet. The shaded area indicates the region used to determine the area of a steady state jet for $x = x_{jet}^{n}$.

Table 4. Description of model parameters. Note that not all parameters are used in all models.

Parameter	Units	Description	Model
d	m	Diameter of discharge pipe	Used in models 2, 3, and 4
Q	$m^3 \cdot h^{-1}$	Discharge rate	Used in models 1, 2, 3, and 4
C_0	$\mu g \cdot L^{-1}$	Initial concentration	Used in models 1, 2, 3, and 4
C_{EQS}	$\mu g \cdot L^{-1}$	EQS concentration	Used in models 1, 2, 3, and 4
V	m^3	Volume of well	Used in models 1, 2, 3, and 4
Δt	s	Model time step for numerical integration	Used in models 1, 2, 3, and 4
U_a	$m \cdot s^{-1}$	Ambient current speed	Used in models 3 and 4
t_{jet}	s	Duration of discharge	Used in models 1, 2, 3, and 4
t_{max}	s	Duration of simulation	Used in models 1, 2, 3, and 4
h_{mix}	m	Constant mixing depth	Used in model 1
K_z	$m^2 \cdot s^{-1}$	Vertical coefficient of diffusion	Used in models 1, 2, 3, and 4
H_{max}	m	Maximum depth to which substance can mix	Used in models 1, 2, 3, and 4

Description of Models

1. O*kubo Model*: This model ignores the jet dynamics and assumes that the patch grows horizontally according to the Okubo relationship. To obtain the patch size at any given time, the area is first determined from the patch's volume and depth from the previous time step, $A = V/D$, where A, V, and D are the patch's area, volume and depth, respectively. The patch area grows according to the Okubo formulation with parameters defined by Lawrence et al. (1995). In the vertical direction, it grows according to the following relationship:

$$D = \max\left(D_0 + \sqrt{K_z t}\, , H_{\max}\right), \qquad (21)$$

   where $D_0 = h_{\text{mix}}$ is the initial depth of the patch, K_z is the vertical coefficient of diffusion, and $H_{\max}$ is the maximum depth to which a substance can mix. In addition, if the well-boat is discharging, a volume of fluid equal to the amount discharged since the previous time step, $Q \cdot \Delta t$, is added to the volume to give the total volume discharged to this point in time. Similarly, $Q \cdot \Delta t/D$is added to the horizontal area.
2. *Jet Model:* This model uses the steady-state jet solution described by Cushman-Roisin (2018) and discussed in Page et al. (2015) for well-boat discharges. The model assumes that the entirety of the discharged fluid goes into a conical-shaped jet. The length of the jet is calculated numerically using equation (16):

$$x_{\text{jet}}^{n} = x_{\text{jet}}^{n-1} + \Delta t \, \frac{6.2d}{x_{\text{jet}}^{n-1}} \, U, \qquad (22)$$

   where x_{jet}^{n} is the length of the jet at time step n. During the discharge period, the surface area of the jet is assumed to be a section of a triangle (see Figure 12), given by

$$A^{n} = R_c \left(x_{\text{jet}}^{n} + x_{\text{source}}\right) - \frac{d}{2} x_{\text{source}}\, , \qquad (23)$$

   where $x_{\text{source}} = d/(2\alpha)$ and R_c is evaluated at x_{jet}^{n} using equation (18). The jet is assumed to be discharged horizontally at the surface and so the volume of the jet is assumed to be half of the cone segment at a given time:

$$V^{n} = \frac{\pi}{6}\left[R_c^2 \left(x_{\text{jet}}^{n} + x_{\text{source}}\right) - \left(\frac{d}{2}\right)^2 x_{\text{source}}\right]. \qquad (24)$$

   If the jet radius R_c exceeds the maximum mixing depth $H_{\max}$, the segment of the cone that exceeds the mixing depth is removed from the volume. Once the well-boat discharge has finished, i.e., $t > t_{\text{jet}}$, the resulting patch continues to grow in the horizontal direction using Okubo's relationship for the horizontal diffusion coefficient, and vertically using equation (21) where the initial depth D_0 is calculated using the patch's volume and surface area at the end of the discharge period.
3. *Puff Model*: The steady-state jet solution described by equations (12) to (16) is only valid in the near-field where jet-dynamics are dominated by the discharge configuration. It is not valid when the dynamics of the receiving waters dominate the behaviour. A refinement to the above is to define a transition point between a near-field solution (the jet model described above) and a far-field solution (patch growth according to the Okubo relationship). We define the transition point as the distance along the jet centre-line where the centre-line jet velocity, given by (16), is equal to the ambient current speed,

U_a. Thus the patch has two components: a portion that grows according to jet-dynamics and a portion that grows according to the Okubo relationship. At each time step, two processes occur. First, if non-zero in size, the ‘Okubo’ portion of the patch grows horizontally and vertically as described in the Okubo model above. Next, the length of the jet is calculated using (22) and the area and volume of the jet are calculated using (23) and (24). The speed along the centre-line at the head of the jet is calculated by setting $x = x_{\mathrm{jet}}^{n}$ in (16). If this speed is equal to the ambient speed, which is assumed to be constant, then the entire jet portion of the patch is incorporated into the Okubo portion. At the next time step, the jet restarts its growth until it once again reaches the transition point at which time, the entire jet is merged with the existing Okubo portion of the patch. When this occurs, the area and volume of the jet patch are added to the area and volume of the Okubo patch, respectively, and the new depth of the Okubo patch is calculated from the resulting area and volume. This model can be viewed as a series of puffs that grow according to jet dynamics and are sequentially incorporated into a patch that grows with Okubo. This continues until the end of the discharge period at which point any remaining jet solution is merged with the Okubo patch and the patch continues to grow according to the Okubo relationship.

4. *Jet-Okubo Model*: The above puff model can be further refined by assuming a continuous transition between the near-field and far-field solutions. As in the puff model, the patch is composed of two portions: one that grows horizontally and vertically as described in the above Okubo model, and one that grows according to jet dynamics. The jet portion initially grows according to the steady-state solution until the jet centre-line speed equals the ambient current speed. At this point, instead of incorporating the entire jet portion into a patch that grows according to Okubo, only the portion that flows out of the end of the jet during the next time step is incorporated into the Okubo patch. The change in area to the Okubo patch due to fluid flowing in from the jet, dA, is given by

$$dA = R_c(x^* + \Delta t\, u^*)(x^* + \Delta t\, u^* + x_{\mathrm{source}}) - R_c(x^*)(x^* + x_{\mathrm{source}}), \qquad (25)$$

where $x^*$and $u^*$are the location along the centre-line and the centre-line velocity, respectively, at the transition point between the modelled near-field and far-field. Theoretically, u^* is equal to the ambient current speed but in practice may differ slightly from this value due to numerical discretization. The change in volume, dV, of the Okubo patch is calculated in a similar manner using the equation for the volume of a cone.

The total patch area is the sum of the jet area and the Okubo patch. Once the jet reaches its ‘terminal’ size, it remains constant until the end of the discharge, while the far-field portion grows due to both the ejection of fluid from the jet and horizontal diffusion using the Okubo relationship. At the end of the discharge period, the jet portion shrinks starting at the discharge location until it has all been incorporated into the Okubo patch. In the model, the patch growth is calculated using the following sequence: 1) if non-zero, growth of the Okubo portion is calculated; 2) growth of the jet portion is calculated; and, 3) if the jet is flowing into the Okubo portion then dA and dV are added to the area and volume of the Okubo portion, respectively, and a new depth of this portion of the patch is calculated from the resulting new values.

For all of the above models, the total mass of pesticide in the patch at a given time step is given by

$$M^n = M^{n-1} + \Delta t\; Q\; C(t), \qquad (26)$$

where $C(t)$ is defined by (19). The average concentration in the patch at a given time is simply the total mass of pesticide in the patch divided by the volume of the patch. The models determine at what time the average concentration falls below the EQS value.

The models described above are simple models that make many assumptions and neglect many parameters. Some of the more important aspects are highlighted below:

- None of the simple models take location into account.
- The Okubo model assumes an initial mixing depth, h_{mix}, which must be provided by the user. It is up to the user to determine a suitable value. Results may be sensitive to this value.
- For the Okubo portion of the model, growth in the vertical direction is governed by the vertical coefficient of diffusion, K_z. This parameter must be determined empirically and supplied by the use.
- In all models, vertical mixing is bounded by a maximum depth to which mixing can occur, H_{max}. This parameter must be determined empirically and supplied by the user.
- The jet-dynamics used in these models are for a steady-state round jet discharging into an unbounded environment with no flow.
  - For the well-boat discharge model, it is assumed that the jet discharges horizontally at the surface. To account for this the jet is sliced in half by the water surface and only the portion below water is considered.
  - For well-boat discharges the receiving waters have both spatial and temporally changing flow dynamics. For the model, the ambient current speed is assumed to be constant and is used to determine the size of the jet.
  - Neither of these assumptions adequately take into account the complicated nature of a surface jet into a non-steady ambient flow.
- The assumption that the well-boat jet is discharging horizontally near the sea surface which may not be representative of the discharge configuration of all well-boats.
- The jet model, used in the jet, puff and jet-Okubo models, assume that the jet instantaneously establishes the steady-state profile, ignoring the initial zone of establishment. Also, the intermediate-field, which transitions between the near-field, here the steady-state jet model, and the far-field, here the Okubo model, is not taken into account.
- Transition from the near-field solution to the far-field solution in the puff and jet-Okubo models occur when the centre-line jet velocity is the same as the ambient current speed. The direction of the ambient current speed is not taken into account and can have a significant impact on the growth of a discharge patch.

Test Cases

All four of the above described simple models were run using input corresponding to the field experiments performed by Page et al. (2015) which are shown in Figure 13. All model runs use a discharge pipe diameter of 0.5 m, $K_z = 0.01$ m^2·s^{-1}, and $H_{\text{max}} = 20$ m. Since the exact discharge rate was unknown, each scenario was run using 1000 m^3·h^{-1} and 3000 m^3·h^{-1}. During the field study, bottom mounted current meters were deployed near the well-boat discharge site. The ambient current at the time of discharge was set to the vertically averaged value from these data during the time of discharge. Although surface values are preferable, one of the current meter records had large data gaps near the surface and so, for consistency, vertically averaged values were used for all cases. Comparisons of the predicted patch areas are shown in Figure 14 and are discussed below.

Case 1: The well-boat discharge took place on August 5th, 2011 between 13:11 and 14:06 UTC, giving a discharge time of 55 min. The boat was tethered to the cage being treated and the treatment water was discharged on the side away from the cage. The discharge patch was deflected by the current and grew roughly in a direction perpendicular to the discharge direction. The evolution of the patch was not significantly influenced by the presence of the fish cages. Outlines of dye patches are shown in Figure 13a which also gives the time evolution of the patch sizes. The time of each observation was taken as the mid-point between the start and end times associated with each patch delineation. The simulation was run until the last observed time of 14:33 UTC for a total simulation time of 82 min. Comparison of the observed temporal evolution of the patch area with the predicted areas are shown in the top row of Figure 14. All of the models underestimate the size of the discharge patch; the puff model gives the smallest underestimate.

Case 2: The well-boat discharge took place on August 5th, 2011 starting at 15:06 UTC. Note that the end of the discharge period is not given in Page et al. (2015). This well-boat discharge was at the same location as in Case 1 but with the discharge being on the other side of the boat directly into the net-pen fish cage. Since time at which discharging ended was not given, the model used 15:55 UTC as the patch appears to start to detach from the well-boat at this time, giving an assumed discharge time of 49 min. The simulation was run until the last observed time of 16:03:30 UTC for a total simulation time of 57.5 min. Outlines of dye patches are shown in Figure 13b which also gives the time evolution of the patch sizes. Comparison of the observed temporal evolution of the patch area with the predicted areas are shown in the middle row of Figure 14. In this case, both the puff model and the jet-Okubo model quickly overestimate the size of the discharge patch. Since the jet is discharged directly into the fish cage, the dynamics are more complicated and it is not clear what mechanisms dominate the flow. It is unexpected that the jet model with Q=3000 $m^3 \cdot h^{-1}$ gives the best results and we do not recommend that any conclusions should be drawn from this as there is little data with which to validate the models.

Case 3: The well-boat discharge took place on November 17th, 2011 between 14:37 and 14:59 UTC. The boat was tethered to the cage being treated and the discharge was from the side away from the cage. The discharge patch initially flowed away from the boat but was quickly diverted by the ambient current back towards the fish cages. This impacted the growth of the discharge patch and also hindered the field workers' ability to outline the patch edge. Collected outlines of dye patches are shown in Figure 13c which also gives the time evolution of the patch sizes. Comparison of the observed temporal evolution of the patch area with the predicted areas are shown in the bottom row of Figure 14. The simulation was run until the last observed time which was 15:37 UTC for a total simulation time of 60 min. This case has a relatively short discharge period of 22 min, compared to 55 and 49 min for Cases 1 and 2, respectively. The short discharge period results in the jet centre-line speed never reaching the ambient speed during the discharge period when the discharge rate is 3000 $m^3 \cdot h^{-1}$ and thus the results of the jet and puff models are identical.

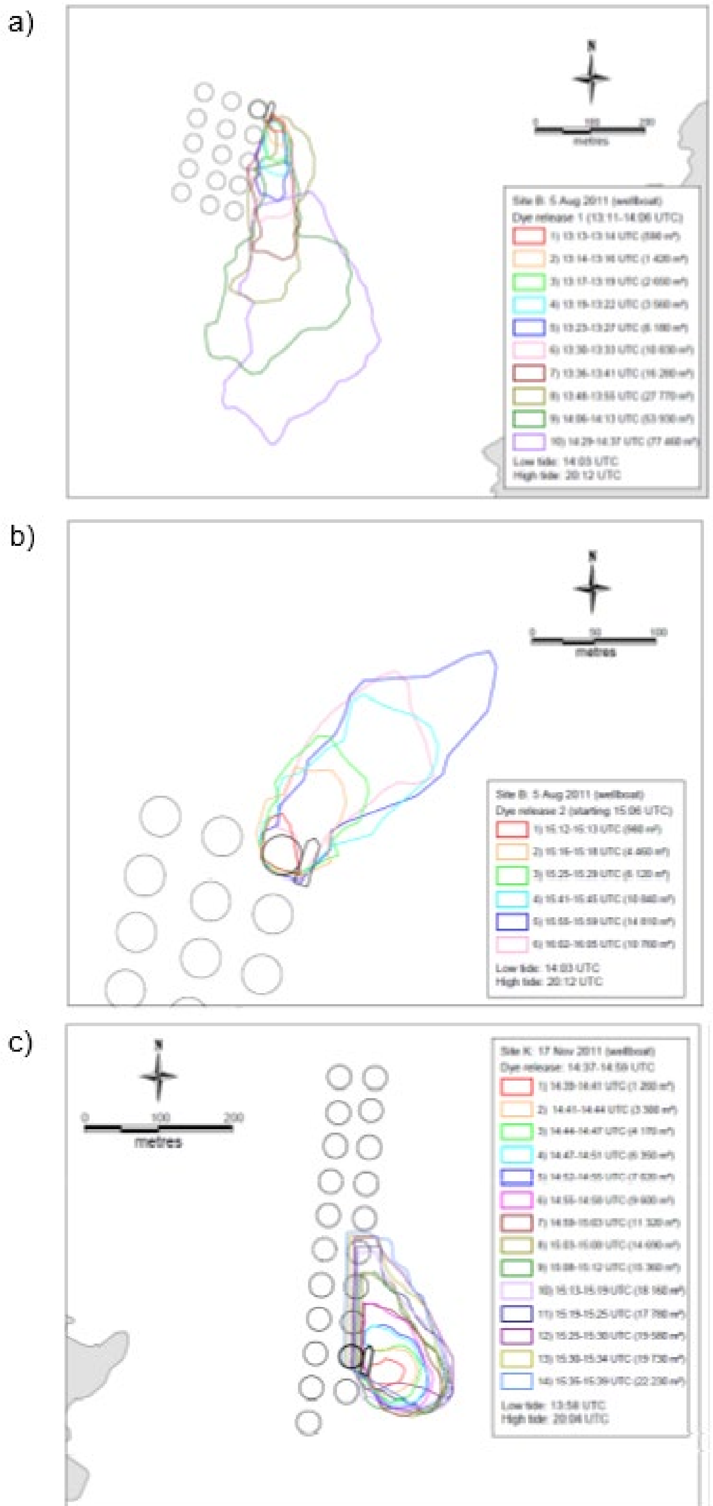

Figure 13. Field results used for well-boat model test cases: a) case 1: Figure 67 from Page et al. (2015); b) case 2: Figure 68 from Page et al. (2015); c) case 3: Figure 69 from Page et al. (2015). The coloured polygons indicate the outline of the dye patches. The black polygon indicates the location of the well-boat at the time of release.

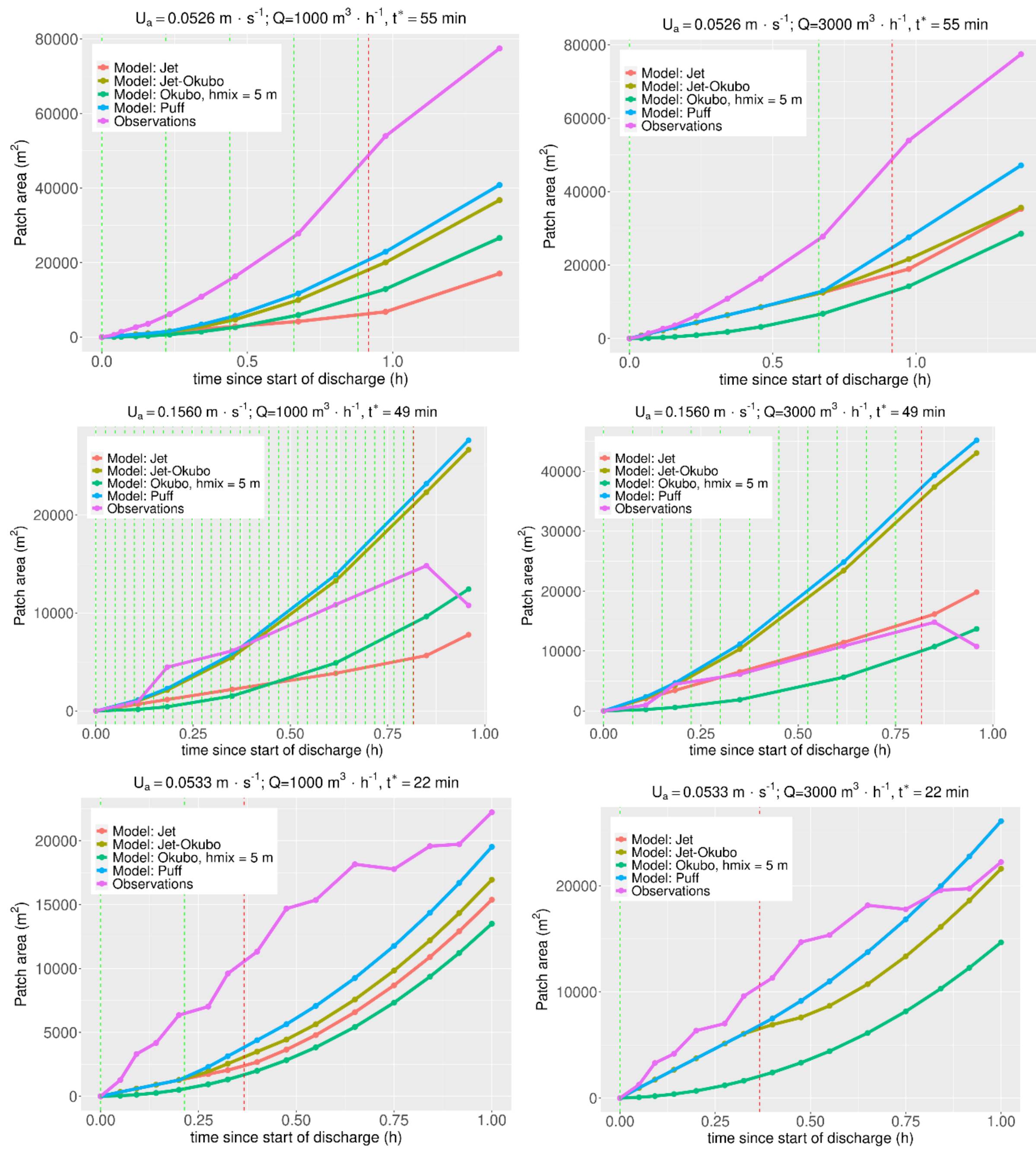

Figure 14. Comparison of the predicted patch areas from the proposed simple models and the observations from Page et al. (2015) for cases 1 (top row), 2 (middle row), and 3 (bottom row). For all model runs, the pipe diameter, d, is set to 0.5 m, the horizontal coefficient of diffusivity, K_z, is 0.01 $m^2 \cdot s^{-1}$, the initial concentration within the well-boat is 100 $\mu g \cdot L^{-1}$, the well-boat volume is 330 m^3. U_a is the speed of the receiving waters and t^* is the discharge time. Models were run using two discharge rates: $Q =$ 1000 $m^3 \cdot h^{-1}$ (left column) and $Q =$ 3000 $m^3 \cdot h^{-1}$ (right column). The green vertical lines are the times when the jet is converted to an Okubo patch in the Puff model. The red vertical lines indicate the end of the well-boat discharge.

Discussion of Results

It is difficult to draw any conclusions from the model results based on the limited field data. For all model runs, the Okubo model underestimates the observed size of the discharge patch. Results from the other models depend on the ambient current speed, discharge rate and discharge period. Furthermore, the varying conditions under which the treatment water was discharged during the field study had a large impact on the behaviour of the discharge patch. Based on the limited field observations, when the treatment water is discharged away from the cage and the ambient currents are also in a direction away from the cage, as in Case 1, the puff model or the jet-Okubo model are the most appropriate. When the treatment water is discharged directly into a fish-cage, as in Case 2, the Okubo model is likely a better choice as it appears that the presence of the cage damps the jet dynamics. When the treatment water is discharged away from the cage array and then deflected back into the cages by the ambient current, the puff model or the jet-Okubo model gave the best agreement. However, for Case 1, where the discharge patch does not interact with the cage array, all the models underestimate the area of the patch. Since the cage array impedes the growth of the patch in Case 3, the model results are more in-line with the observations.

The results discussed above indicate that the simple models put forth here do not provide accurate estimates of the discharge patch area. However, it should be noted that model results all have the correct order of magnitude which is perhaps the best that can be achieved for such simple models. We believe that these models can be of value in predicting the concentrations and the time required to reach a specified EQS value. The above models were all run with an initial concentration within the well-boat of 100 $\mu g \cdot L^{-1}$, a well-boat volume of 330 m^3 (Page et al. 2015), and an EQS concentration of 0.1 $\mu g \cdot L^{-1}$. Predicted concentrations are shown in Figure 15. All concentration profiles have similar behaviour with the concentration reaching a peak after the first-time step and then decaying as the patch size continues to grow and the well-boat concentration is diluted. The Okubo model gives the highest concentrations, which is expected as it consistently predicts the smallest area. When the discharge rates are 1000 and 3000 $m^3 \cdot s^{-1}$, the maximum average concentrations are 99.92 and 99.75 $\mu g \cdot L^{-1}$, respectively. The initial concentrations for the jet, puff, and jet-Okubo models are identical since, at the beginning of the simulation, the models are all based on the jet behaviour. When the discharge rates are 1000 and 3000 $m^3 \cdot s^{-1}$, the maximum average concentrations are 80.12 and 25.31 $\mu g \cdot L^{-1}$, respectively. If the discharge speed is slower than the ambient current speed, the puff and jet-Okubo model would give the same results as the Okubo model as there would be no jet portion to the models. The times that it takes the concentration to reach the EQS concentration are given in Table 5. The higher discharge rate reaches the EQS concentration more quickly than the lower discharge rate regardless of the model. The Okubo model takes the longest to reach the EQS concentration, for all cases. The times to reach the EQS concentration, for the other models, depend on the ambient current speed, the discharge rate and the length of the discharge time. A conservative estimate would be to use the time to reach the EQS concentration as determined by the Okubo model, since it is likely a longer time than in practice since the Okubo model consistently underestimates the patch size. Unfortunately, there is not sufficient field data to validate the volume of the discharge patch, which directly influences the predicted concentrations. Also, further study to determine the relationship between the discharge rate and the time required to reach the EQS concentration is required. It should be noted that the models estimate the average concentration and do not estimate the maximum concentration.

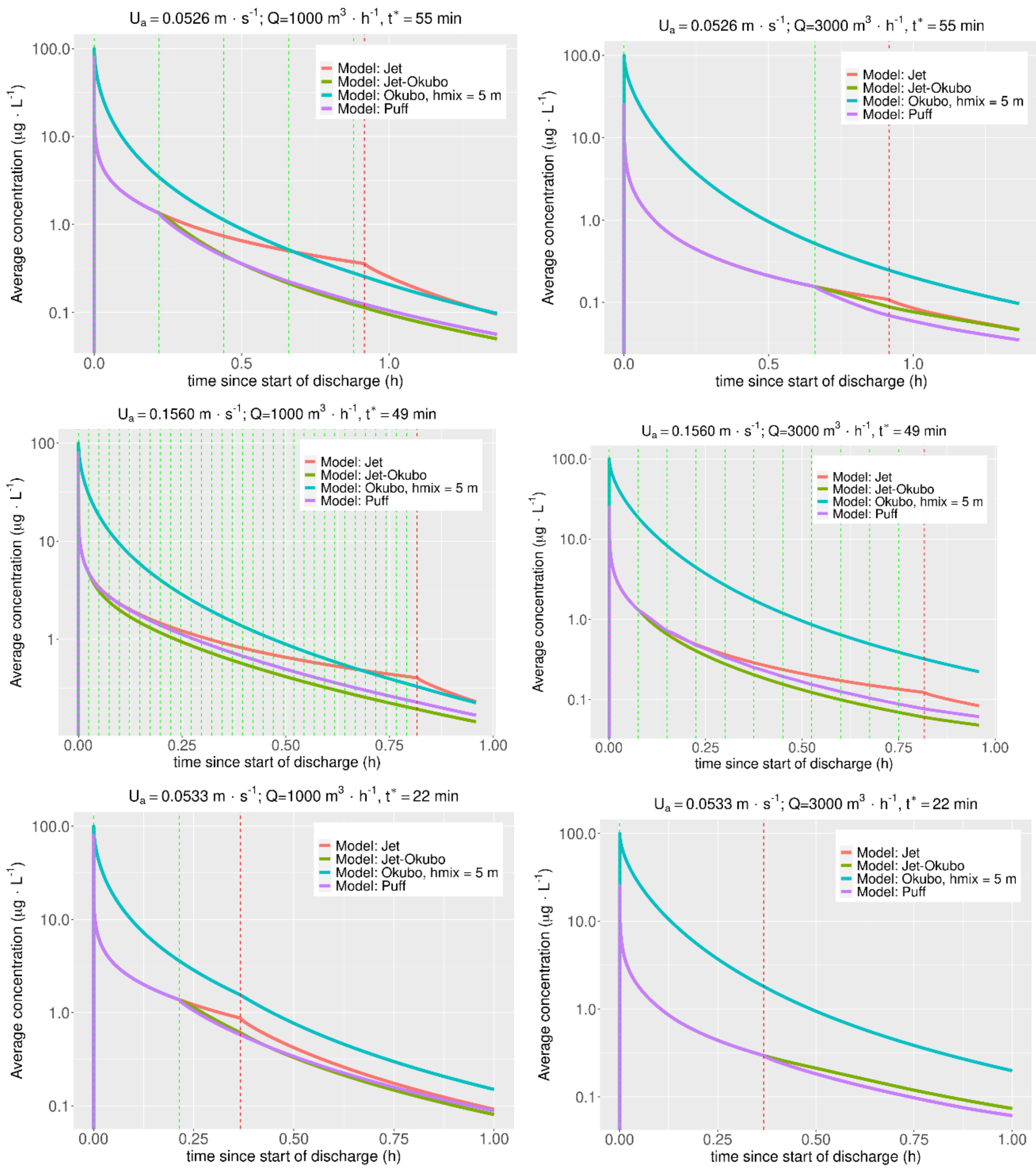

Figure 15. Comparison of the predicted concentrations from proposed simple models using parameters from field observations of Page et al. (2015) for cases 1 (top row), 2 (middle row), and 3 (bottom row). Note that concentrations are plotted using a log scale. For all model runs, the pipe diameter, d, is set to 0.5 m, the horizontal coefficient of diffusivity, K_z, is 0.01 m^2·s^{-1}, the initial concentration within the well-boat is 100 μg·L^{-1}, the well-boat volume is 330 m^3. U_a is the speed of the receiving water and t^* is the discharge time. Models were run using two discharge rates: Q = 1000 m^3·h^{-1} (left column) and Q = 3000 m^3·h^{-1} (right column). The green vertical lines are the times when the jet is converted to an Okubo patch in the Puff model. The red vertical lines indicate the end of the well-boat discharge.

Table 5. Time (rounded to nearest minute) to reach an EQS concentration of 0.1 $\mu g \cdot L^{-1}$ assuming an initial concentration within the well-boat of 100 $\mu g \cdot L^{-1}$ and a well-boat volume of 330 m^3.

		Case 1		Case 2		Case 3	
	Discharge rate ($m^3 \cdot h^{-1}$)	1000	3000	1000	3000	1000	3000
Model	Okubo	81	81	*	*	*	*
	Jet	81	56	*	53	58	44
	Puff	62	47	*	42	57	44
	Jet-Okubo	58	52	*	36	54	50

*the concentration did not go below the EQS threshold during the simulation time.

Since the simple models described above are sensitive to input parameters, we examine the effects of discharge rate and ambient current speed on the results of the jet-Okubo model for Case 1. This case was chosen as it has the simplest discharge configuration: away from the cage array into a current that does not deflect the discharge patch back into the cages. We have run the jet-Okubo model with discharge rates of $Q = 1000$ and 3000 $m^3 \cdot h^{-1}$ into a receiving ambient current of 0.01 and 1 $m \cdot s^{-1}$. These conditions represent low and high discharge rates, and weak and strong current speeds. The predicted patch area, depth, volume, and average concentration of the treatment chemical are shown in Figure 16.

Figure 16a shows a larger discharge rate yielding larger areas. For a given pipe diameter, here assumed to be 0.5 m in all cases, the centre-line velocity at a given location along the jet centre-line is proportional to the discharge rate, see equation (16) and (17). Furthermore, from equation (22) we have

$$\frac{dx_{\text{jet}}}{\Delta t} = \frac{6.2d\ U}{x_{\text{jet}}}. \qquad (27)$$

Assuming $x_{\text{jet}} = 0$ at $t = 0$, the solution to (27) gives

$$x_{\text{jet}} = \sqrt{12.4\ d\ U\ t}\,. \qquad (28)$$

Hence, when all other parameters are equal, the jet portion of the patch is larger for higher discharge rates. It is observed that, as the ambient current speed increases, the patch size increases. When a larger ambient current speed is specified, the jet portion of the patch is smaller since the centre-line jet velocity will reach the ambient current speed sooner. This result implies that the area of the Okubo portion of the patch grows more quickly than the jet portion. This also sheds some potential light onto the differences in predicted areas for the $Q = 1000$ $m^3 \cdot h^{-1}$, $U_a = 0.1$ $m \cdot s^{-1}$ (run 5c) and $Q = 3000$ $m^3 \cdot h^{-1}$, $U_a = 0.01$ $m \cdot s^{-1}$ (run 5b) simulations. Initially, the jet for run 5b will grow faster than that for run 5c as the discharge rate is higher. However, since the ambient current speed is higher for run 5c, the centre-line jet velocity will reach the ambient current speed sooner (Table 6) and so the Okubo patch begins its growth sooner and the total size of the patch overtakes that of run 5b, as seen in Figure 16a.

Results for predicted patch depths are shown in Figure 16b. Since the patch initially only has a jet portion whose growth depends on the discharge rate, the initial deepening of the patch is the same for runs with the same discharge rate (5a & 5c and 5b & 5d). The jet portion of the patch stops growing at t', the time at which the centre-line jet speed equals the ambient current speed and is given by

$$t' = \frac{12.4\ Q}{U_a^2\ \pi\ d} \tag{29}$$

(see Table 6). Thus, for the same discharge rate, the Okubo portion of the patch starts to grow sooner for larger ambient current speeds. The depth of this portion of the patch is governed by equation (21) and dependent on the initial depth D_0 which is determined by the size of the jet portion when the transition occurs. Thus, the longer the jet grows, the deeper the initial depth (until the maximum depth of h_{mix} is attained). From equation (18), the length of the jet at which the maximum depth is given by $x_{\mathrm{jet}} = (2H_{\mathrm{mix}} - d)/2\alpha$ which is approximately 102 m for the values used here. Substituting this value into (28), the time at which the maximum depth is achieved in the jet portion of the model is given by

$$t = \frac{\pi d}{49.6\ Q}\left(\frac{2H_{\mathrm{mix}} - d}{2\alpha}\right)^2 \tag{30}$$

Which is approximately 20 and 7 min for discharge values of 1000 and 3000 $m^3 \cdot h^{-1}$, respectively. Comparing these values with t' in Table 6, we see that runs 5a, b and d reach their maximum depths in the jet portion (note that since the volume of the jet is a portion of a cone, the average depth in the jet never reaches the maximum). The modelled depth value is a combination of the above factors: how soon the centre-line jet velocity reaches the ambient current and how deep the jet grows before discharging into the Okubo patch.

Predicted volumes are shown in Figure 16c. The patch volume is the product of the patch area and the average depth and is determined by the behaviour of these two variables. It is clear that the runs with the extreme values (5a & 5d) have a similar behaviour as the patch area. Predicted volumes from the other two runs fall in between these two extremes.

Predicted concentrations are shown in Figure 16d. As with the previous simulations, the concentrations reach a peak in their first time steps to a value that is dependent on their discharge rate (Table 6). After that they decay quickly. EQS values are reached more quickly with stronger discharge rates and stronger ambient currents.

Table 6. Results of jet-Okubo model run for Case 1 assuming an initial concentration within the well-boat of 100 $\mu g \cdot L^{-1}$, a well-boat volume of 330 m^3, and an EQS concentration of 0.1 $\mu g \cdot L^{-1}$. C_{avg} is the predicted average concentration within the predicted patch and t' is the time at which the centre-line jet speed equals the ambient current speed. The model was run for idealized cases with $Q = 1000$ and 3000 $m^3 \cdot h^{-1}$ and $U_a = 0.01$ and 0.1 $m \cdot s^{-1}$. All other parameters are the same as for Case 1.

Run	U_a ($m \cdot s^{-1}$)	Q ($m^3 \cdot h^{-1}$)	t' (min)	x at max jet size (m)	max[C_{avg}] ($\mu g \cdot L^{-1}$)	t_{eqs} (min)
5a	0.01	1000	365^{+}	170.188^{++}	80.12	+
5b	0.01	3000	1096^{+}	294.764^{++}	25.32	60
5c	0.10	1000	4	43.877	80.12	63
5d	0.10	3000	11	131.637	25.32	35

$^{+}$the centre-line jet velocity did not reach the ambient current speed during the discharge.

$^{++}$length of jet at end of discharge period.

+the concentration did not go below the EQS threshold during the simulation time.

As mentioned above, the practical application of these simple well-boat models is in the prediction of average concentration. Since the models tend to underestimate the predicted area of the discharge patch, the average concentration is likely overestimated which is in line with a precautionary approach. For the anonymous farm described in the previous section on Tarp treatments (Figure 11), we predict the time required to reach an EQS concentration of 1 $\mu g \cdot L^{-1}$ based on an initial concentration of 100 $\mu g \cdot L^{-1}$. Using the median current speed of 8.3 $cm \cdot s^{-1}$ (Figure 11) as the ambient current speed, predicted times to reach the EQS concentration are given in Table 7. We note that the longest predicted time to reach the EQS concentration is about one tenth of that used for tarps based on Figure 15 and Figure 16 and assuming an EQS concentration of 1 $\mu g \cdot L^{-1}$ which is consistent with that used in Section Tarps. For many situations, particularly if the evolution of the well-boat discharge patch does not interact with the fish-farm infrastructure, the time to dilute to the EQS concentration is often much less. It should be emphasized that the conclusions discussed here are based on a single well-boat configuration. The models should be assessed for use with modern well-boat characteristics and discharge protocols which include larger well sizes and varying discharge configurations and rates.

Table 7. Time (rounded to nearest minute) to reach an EQS concentration of 1 μg·L^{-1} using an initial concentration of 100 μg·L^{-1}. For all model runs, the pipe diameter, d, is set to 0.5 m, the horizontal coefficient of diffusivity, K_z, is 0.01 m^2·s^{-1}, the initial concentration within the well-boat is 100 μg·L^{-1}, the well-boat volume is 330 m^3, and the speed of the receiving waters, U_a, is 8.3 cm·s^{-1}.

Model	Q= 1000 m^3·h^{-1}	Q= 3000 m^3·h^{-1}
Okubo	28	29
Jet	19	6
Puff	13	6
Jet-Okubo	13	6

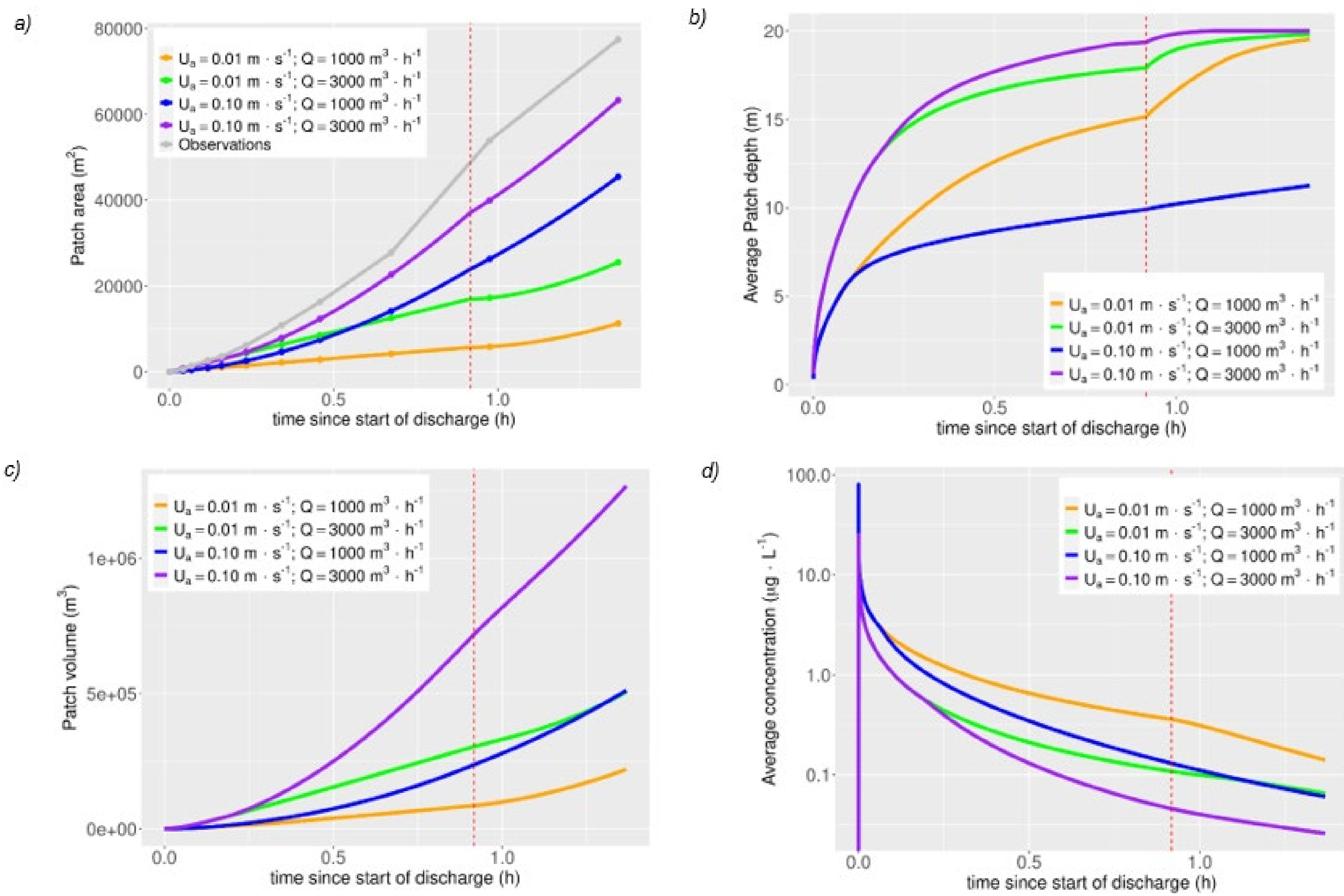

Figure 16. Results of jet-Okubo model: a) patch area, b) patch depth, c) patch volume, and d) average concentration of treatment pesticide in patch (log scale). The model was run for idealized cases with $Q = 1000$ and 3000 m^3·h^{-1} and $U_a = 0.01$ and 0.1 m·s^{-1}. All other parameters are the same as for Case 1.

PREDICTING THE IMPACT OF EXPOSURE TO PESTICIDES

As indicated in Section Exposure Consequence: Environmental Quality Standards or Thresholds of this document, the impact of predicted exposures is not explicitly modelled; it is inferred that toxic consequences occur when exposure concentrations are greater than impact thresholds or when both exposure concentrations and exposure durations are greater than the thresholds.

APPLICABILITY OF EXPOSURE MODELS TO THE CANADIAN SITUATION

Net-pen fish farming in Canada is conducted in multiple regions of the country and overseen by several provincial and Federal departments. Each region has unique oceanographic challenges, environmental considerations, and cultural views as well as variations in regulations. While there are commonalities between regions, the particulars of the differences may alter model suitability when considered against the priorities of a region.

The majority of the models discussed in Section NEW MODELS FOR POTENTIAL PRACTICAL APPLICATION can be applied using minimal site-specific information. The PEZ model only requires a current speed and a dilution or decay time and therefore can be applied to many different locations. In contrast, the Gillibrand and Turrell (1997) model was developed to simulate possible treatment scenarios in a Scottish loch system and as such it may not be applicable to other hydrographic situations. The models reviewed in this document have been designed to answer a range of questions, and deciding which model best answers a specific question is not always a straightforward exercise.

There are many models available, each possessing a range of strengths and weaknesses. When considering the models in the context of the varied hydrographic conditions, species, and climates experienced in Canada it becomes clear there is not a “one size fits all” solution.

Ultimately, the applicability of a model depends on the priorities in a region. A region that requires a detailed prediction of exposure, might consider a full hydrodynamic model. Although hydrodynamic models can provide very detailed information, implementing such a model in a new area can be time consuming and expensive. As a result, hydrodynamic based models would be a poor choice where expediency or cost are important factors. In such cases, a simpler model, such as the PEZ model, may be a more suitable choice. The PEZ model can be rapidly used and requires few inputs; however, it provides coarse rather than detailed information.

DISCUSSION

Modelling the discharge of pesticides used in bath treatments for sea lice by the aquaculture industry is a challenging task. We have reviewed a range of models from the literature and have explored some new simple models. Other than BathAuto (SEPA 2008), which was developed specifically for licensing of pesticide discharges in Scotland, and the PEZ model, which is under development and being used for siting within DFO, we know of no other models that have been developed for regulatory purposes. There are several key points that must be considered when selecting a model for regulatory use. Some of these are the purpose of running the model and the question being addressed; the time frame in which a response is required; available expertise for running the model; existing hydrodynamic models and their suitability near the areas of interest. Of these considerations, the first is the most important; in order to select an appropriate model, one needs to know the question that is being addressed and the type of answer (in terms of model output) that is required.

Models range in complexity. Simple models are generally easier and more cost efficient to implement and can give useful information depending on how well underlying model assumptions apply to the situation. Simple models can be used to help understand the variables that influence the exposure and to explore sensitivities to inputs. Many simple models can give order of magnitude estimates of dilution, exposure durations, and exposure areas. For these reasons, our view is similar to that of Henderson et al. (2001), i.e., that simple models can have an important role in regulatory decision making and should be used if appropriate for a given situation.

Several simple models have been put forth and explored here: a refinement of the Okubo based model developed by Page et al. (2015), the PEZ model, and several simple well-boat discharge models which merge the initial jet discharge into a background Okubo-type dispersion. The Okubo diffusion model is an empirical relationship based on field measurements. It has advantages over Fickian diffusion, used in earlier Scottish models. When Fickian diffusion is used, the coefficient of diffusivity must be specified. Furthermore, Fickian diffusion does not take into account that the coefficient of diffusivity increases with the patch size and so will underestimate the growth of the discharge patch.

Simulations of the simple models investigated here produced some useful information. Results of all models were sensitive to input variables such as ambient current speed and well-boat discharge rate, and this sensitivity should be explored further. The Okubo based model results indicate that proper definition of EQS concentrations and time frames are required to properly interpret results. The well-boat models indicate that the time required to dilute to a specified environmental threshold is much smaller than for tarp treatments. The model results should be viewed, however, as preliminary and further investigation and development of these models is recommended. Also, the available field observations for model validation are limited, especially for well-boat discharges, therefore further studies are recommended, since they are required to advance the precision and utility of the models.

Although we promote the use of simple models, this does not negate the value of more complex models, including hydrodynamic models, for regulatory use. There are several situations in which simple models are not adequate. A limitation of many simple models is that spatial and temporal variations of the ambient current fields are not taken into account. Thus, when large displacements are predicted, the uncertainty in the predicted trajectories increases; in such situations, spatial and temporal variabilities of water currents should be taken into account. The predicted displacement value which determines if a simple or hydrodynamic based model should be used has not been investigated here, but we suggest the following guidelines based on experience:

- If the predicted displacement distance based on a single current record is less than 500 m then results of a simple model may be practical and sufficient because data from a single current record may be relatively representative of the spatial and temporal variations in the current.
- If the predicted displacement distance based on a single current record is greater than 500 m then results of a simple model may not be sufficient because data from a single current record may not be representative of the spatial and temporal variations in the current. Hydrodynamic modelling should be considered in order to estimate the spatial and temporal variabilities in the current and the associated displacements.

Hydrodynamic models have other uses including providing an understanding of the general circulation of the area. This is particularly important for understanding the trajectories of bath pesticide discharges as these tend to travel long distances. Also, hydrodynamic based models can be useful for examining the impacts of simultaneous treatments at multiple farms as well as cumulative effects. Finally, a sufficiently validated model that includes spatial and temporal resolution of currents should be considered when management desires a more precise and accurate prediction.

Although hydrodynamic models provide a route to estimating spatial and temporal variations in the ambient water currents, it should be kept in mind that the development of hydrodynamic models is resource intensive, including the computer and human resources required to set up and run the models. Furthermore, although hydrodynamic models can produce precise solutions, validation against field observation is required to determine and refine the accuracy of these solutions. As the scale of displacement distances is of the order of kilometers, field measurements at multiple locations are required, including measurements of sea level, currents, temperature, and salinity. Predicted exposure zones from hydrodynamic based models should take into consideration the model accuracy and precision and should not be interpreted as the exact representation of the real-world situation.

Setting appropriate EQS concentrations and exposure times is important in order to properly interpret model results. Furthermore, EQS concentrations and exposure times play a role in model selection. To illustrate this point, we look at how siting applications are handled by DFO in Canada and by SEPA in Scotland.

DFO has recently used the PEZ model in siting applications. It is a simple model that produces a circle centred on the cage array. The radius of the circle is determined by an appropriately selected current speed and the time required for pesticide treatment concentrations to dilute to a given environmental threshold concentration. Although DFO has not officially adopted EQS values, the selected threshold value is an equivalent concept. The PEZ model is the first step in a triage approach. It is quickly and easily implemented and provides an order of magnitude estimate, since the predicted area encompasses all exposed areas, but not all areas within the PEZ will be exposed. It is a powerful tool, however, as it gives regulators bounds in which to look for ecologically sensitive areas or potentially negative overlaps. If there are any concerns, a more precise and accurate model, including any required time and resources to implement such a model, can be considered if desired.

SEPA has recently revised its environmental standards (SEPA 2019c). For azamethiphos, there are three standards: 3, 24, and 72 h concentrations. Both the 3 and 24 h concentrations are applied after each individual discharge and pose a maximum allowable concentration after these times. The longer-term standard is applied 72 h after the last discharge in a treatment period and is the concentration that cannot be exceeded over an area greater than 0.5 km^2. It must be demonstrated by the applicants that a proposed farm site is likely to conform to the relevant environmental standards (see the Appendix for a description of SEPA’s new modelling guidelines). Furthermore, SEPA may refuse to grant permission to discharge bath pesticides if “an insufficiently diluted plume is likely to interact with, and pose a risk to the conservation status of, protected species or habitats; or adversely affect the interests of other users of the marine environment” (SEPA 2019c). The site applicant is expected to demonstrate that these criteria are met using modelling; SEPA considers hydrodynamic modelling to be the default.

The above illustrates two ways that environmental standards can be interpreted and applied, and two approaches to modelling. For finfish aquaculture siting advice in Atlantic Canada, DFO has adopted a simple approach that is easy to implement. The philosophy is to examine what may be exposed during the time period over which pesticide concentrations are above a given threshold. If there is nothing of concern in the predicted area, then there is no need to apply a more complex model. SEPA’s approach is at the other end of the spectrum. The expectation is that complex models will be used to predict the spatial and temporal evolution of pesticide discharges and model results will be used to demonstrate that environmental standards are likely to be met and areas of concern unlikely to be exposed to insufficiently diluted pesticides. It is the role of regulators to set appropriate EQS concentrations and exposure times, as well as indicating how these standards are to be applied. With this information in hand, selection of appropriate models can be made.

SUMMARY AND CONCLUSIONS

- The transport and dispersive processes around fish farms are generally complex in that they are spatially and temporally variable. Few observations on pesticide transport and dispersal exist, so it is difficult to assess the accuracy of most exposure models. Although Scotland and DFO have conducted several dye studies related to both tarp and well-boat treatments, a significantly larger sample size is needed to provide better evaluations of models.
- The underlying assumption of most models is that the release of pesticides produces a patch containing the treatment pesticide, and that the patch grows and moves with time. Discharge patches are characterized by their size, shape, location, and concentration within the patch.
- Models rely on simplifying assumptions to make the problem tractable. There are models of varying complexity which predict one or more characteristics of a pesticide discharge patch.
- How well a given model represents a specific situation depends on the assumptions made by the model and whether these assumptions are reasonable for the situation in question.
- The choice of models depends to a large degree on the management objectives.
- There are no existing tarp and well-boat discharge models that are extensively calibrated and validated. Some models have been compared to limited sets of observations from a limited number of locations and times.
- Relatively few models have been developed and applied to pesticide management to date: BathAuto (SEPA 2008) was developed specifically for licensing of pesticide discharges in Scotland; the potential exposure zone (PEZ) model is under development and being used for providing advice on siting within DFO.
- Some simple models have been explored here: a refinement of the Okubo based model developed by Page et al. (2015), the PEZ model, and several simple well-boat discharge models which merge the initial jet discharge into a background Okubo-type dispersion. These models are all preliminary and require further investigation and development.
- The simple models examined here assumed that the pesticide dilution time is much longer than its decay time and so the decay time was neglected.
- The simple models considered here indicate that predicted exposure area, concentration, and location of the discharge patch depend on the ambient current speed and the choice of environmental exposure concentration and its associated exposure time. Defining appropriate environmental quality standards is important for proper interpretation of model output.
- Results from the Okubo based model suggest that the choice of environmental exposure concentration and its associated exposure time can change the implications of the model output from one of predicted impact to one of no impact. The assumption that any exposure time above a regulatory threshold concentration is undesirable is a prudent and precautionary assumption.

- Results from the simple well-boat models suggest that the time required for azamethiphos treatment water discharged from a well-boat to dilute to below toxic concentrations is about one tenth of that used for tarps in the PEZ model. If well-boat treatments are used, the PEZ can be calculated with a shorter dilution time, resulting in a smaller displacement and hence a smaller area of potential exposure.
- Results from the simple well-boat models indicate that dilution below threshold concentration is reached more quickly with higher discharge rates and stronger ambient currents.
- Results of simple models should be viewed as order of magnitude estimates.
- Both the tarp and well-boat models estimate dilution times and give first order estimates of potential exposure domains associated with the discharges of bath pesticides.
- The outputs from models are sensitive to input assumptions and their outputs should not be over interpreted.
- The models make many assumptions. Uncertainties associated with these assumptions should be better understood and quantified.
- The simple well-boat models explored here were for the well-boat configuration and operations associated with the data described in Page et al. (2015). Presented results may not be applicable to different well-boat configurations and operations.
- Simple models are useful to help develop an understanding of the factors and processes influencing exposures.
- Simple models are easily and quickly implemented and are perhaps best suited to give initial precautionary estimates of exposure potential.
- Hydrodynamic models can provide spatially and temporally varying estimates of the ambient current fields.
- Results from hydrodynamic models are imperfect representations of reality and have uncertain accuracies and thus must be interpreted from this perspective.
- Hydrodynamic models do not yet robustly incorporate the influences of cages on the near-field circulation.
- It is best to consider the use hydrodynamic based models after simple models have indicated a more detailed and precise prediction or estimate is needed.
- Both simple and hydrodynamic based models indicate that pesticides can travel hundreds to thousands of meters.
- The uncertainty in the predicted displacement distance varies with model selection and increases with distance from the discharge source. Further investigation is required to better determine the criteria for model selection. However, the following preliminary guidelines are suggested:
  - Less than 500 m: a simple model can be used.
  - Greater than 500 m: a hydrodynamic model should be considered.

KNOWLEDGE GAPS

- Observations concerning the transport and dispersal of pesticides released from net-pens and well-boats are sparse.

- Observations of water current, temperature, salinity, sea level, and waves from multiple locations and times within hundreds of meters to a few kilometers of fish farms are sparse in many locations.
- The sensitivity of estimates of pesticide dilution and displacement to uncertainties in hydrodynamic models is not well characterized.
- High resolution calibrated and evaluated hydrodynamic models do not exist for all areas of Canada where finfish aquaculture takes place.
- There is uncertainty in the extent to which fish uptake the pesticides while they are in a treatment bath.
- The sensitivity of the horizontal displacement estimates of discharged pesticides to the vertical variations in water currents and turbulence is not well known.
- The initial concentrations of pesticides in the bath water are not well known, especially for tarp treatments.
- Few studies have been conducted to test the assumption that the dispersion rate of tracers (i.e., dye and drifters) accurately represents that of pesticides.
- There is limited readily available knowledge concerning well-boat characteristics and operations of relevance to pesticide discharge modelling.

RECOMMENDATIONS

- Fill the knowledge gaps identified above.
- Discussions between science, environmental managers, and the aquaculture industry should be held to:
  - better define the objectives of aquaculture discharge modelling,
  - improve the understanding of modelling capabilities, sensitivities and accuracies,
  - identify models that are suitable for management purposes, and
  - define evaluation criteria and procedures for models.
- Models should be evaluated and validated before they are widely adopted for use in regulatory considerations, including a post-deposit monitoring program.
- More studies quantifying the relationships between dyes and pesticides should be undertaken. These relationships should be verified for all pesticides being considered for use.
- Input data to models used for regulatory purposes should be assessed and accepted before the data are used.
- Models should be evaluated for use in all regions of Canada in which finfish net-pen aquaculture takes place.
- Models need to be further developed and customized for the specific pesticides and treatment scenarios that are approved for use in Canada.
- Collect more data on bath pesticide discharges.
- Models, including the simple Okubo model, well-boat models, and hydrodynamic based models, should be further refined and evaluated.

- Based on experience, the following preliminary approach is recommended for model selection.
  - When the displacement predicted using a single current record is less than 500 m, a simple model can be used.
  - When the displacement predicted using a single current record is greater than 500 m, a hydrodynamic based model should be considered.
  - Recognizing the uncertainty associated with the 500 m threshold recommended above, data should be collected and analysed to verify this threshold.
- Many of the models reviewed show potential but their adoption for regulatory use should take into account the evolving nature of model development and uncertainties associated with model outputs.

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APPENDIX – SEPA GUIDELINES

In June 2019, the Scottish Environment Protection Agency (SEPA) released new guidelines for modelling requirements for aquaculture site applications (SEPA 2019b). These new guidelines are less prescriptive than previous guidelines. The new guidelines include modelling the impact of both in-feed drugs and bath pesticides. Here we review the general modelling guidelines and those specific to bath pesticides.

Within the context of both in-feed drugs and bath pesticides, the purpose of modelling is to show that a proposed farm site is likely to conform to the relevant environmental standards. SEPA assumes that a proposed discharge is harmful and puts the responsibility onto the applicant to demonstrate environmental sustainability. For bath pesticide treatments, it is essential that the model reflects treatment practices and represent worst case scenarios. If there is uncertainty in the treatment practice, a range of scenarios representing the range of plausible treatment scenarios should be modelled.

SEPA considers hydrodynamic modelling to be the default and will be required for most applications. BathAuto, a suite of simple models previously used by SEPA, can be used for cases that are considered low risk, but it is the applicants' responsibility to demonstrate why the requirements for hydrodynamic modelling do not apply to their application.

SEPA recommends that hydrodynamic models developed for application to aquaculture have a horizontal resolution of no more than 25–30 m in areas around farm sites and other areas that may be at risk. Validation data must be collected in locations and at times that are relevant to the questions being addressed by the modelling. For modelling bath treatments, either particle tracking or a water quality module can be used. It is recommended that the modelled dispersion be validated against field studies, for example dye tracer or drifter studies.

Models can provide estimates of environmental impacts when empirical data are not available, but cannot replace monitoring surveys that can provide a more accurate picture of impacts. A model that is validated is preferred to one that is not, but non-validated models can be useful to identify risks with the emphasis on producing conclusions that are safe, rather than accurate. When the perceived impacts are great, a higher level of confidence in model output is required.

SEPA's modelling principles and practices include the recognition that all models use simplifying assumptions which can limit how well the actual system is represented. Furthermore, multiple models may be required to address issues at all the relevant scales. Finally, SEPA recognizes that there may be circumstances where the models cannot provide an adequate prediction of the impact on receiving waters, in which case a subjective judgement may be required.