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Modelling and Predicting Ecosystem Exposure to In-Feed Drugs 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 modelling in relation to the discharge of active ingredients associated with in-feed drugs used in marine net-pen aquaculture farming operations in Canada. The document includes an 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 for potential use.

In general, modelling for in-feed drug discharges and depositions is in an early stage of development. Few models have been developed specifically to predict the benthic deposition of in-feed drugs and these range in complexity. Model results are sensitive to input parameters, including treatment details, hydrographic conditions, drug partitioning specifics, and sinking rates and timing of discharges. Many of these parameters are poorly understood, difficult to measure, and hence, not well quantified. Thus, determining the quantification of uncertainties and sensitivities of model results remain challenging.

Many models for predicting the deposition of organic waste produced by net-pen fish farms have been developed. Although similarities exist between the underlying assumptions of these models and those for in-feed drugs, their adaptation to use for modelling the deposition of in-feed drugs is not necessarily simple or straightforward. Of particular importance is the inclusion of drug partitioning specifics which is necessary in order to correctly model in-feed drug deposition dynamics; simple conversion factors between organic waste deposition and in-feed drug deposition are likely not a suitable approach as the ratio between carbon and drug in the released feces varies with time.

The objectives of modelling must be specified before a model is selected and assessed for its adequacy and sufficiency. Once models have been selected and/or developed, models must be validated before being used. In general, existing models of in-feed drug deposition have not been extensively calibrated or validated. Of the few validations that have been done, the literature suggests that, regardless of complexity, existing models give, at best, an order of magnitude estimate of seabed drug concentrations.

Despite the uncertainties surrounding model precision and validity, models can be useful for regulatory decision support. Model selection depends on the decision maker's objectives. Precision and accuracy of the model cannot be estimated until the chosen model is verified and validated. Existing validation studies indicate that available models are only able to provide order of magnitude estimates of in-feed drug depositions. At this time, simple models may be sufficient for decision support. This sentiment may change as science better characterizes model inputs and processes, and conducts more validation studies.

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 areas of advice include, 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 in-feed drug 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 drugs 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 drugs discharged from in-feed treatments of marine finfish aquaculture net-pens. Modelling of pesticide treatments is covered in a separate document (Page et al. 2023).

BACKGROUND

There are several categories of chemicals used by finfish farming operations, including pesticides, drugs, anti-foulants, disinfectants, pigments, vitamins, and minerals (Falconer and Hartnett 1993; Burridge et al. 2010; Samuelsen et al. 2015; Bloodworth et al. 2019; Rico et al. 2019; Beattie and Bridger 2023; Burridge and Holmes 2023). Finfish contained in open net-pen operations sometimes experience problems associated with pests and pathogens. These problems can result in the use of drugs and pesticides to help manage the pests and pathogens and to treat the symptoms exhibited by the fish. This document focuses on in-feed drugs. Although the drug treatments may not harm the cultured fish, when released, they may harm non-target organisms and may accumulate in the receiving environment (Haya et al. 2005; Rico et al. 2019; Burridge and Holmes 2023; Hamoutene et al. 2023).

There is little to no natural exposure of the marine environment to the drugs used by the aquaculture industry. There are possibly exposures due to other anthropogenic activities, i.e., lobster holding facilities (oxytetracycline may be used to treat gaffkaemia in lobster), coastal municipal waste facilities with only secondary treatment systems, agricultural runoff (ivermectin exposure), and untreated sewage from coastal long term care home septic tanks or hospitals. Any exposure generated by the use of drugs in aquaculture operations may elicit some degree of response by the ecosystem. Changes to the ecosystem due to drug exposure may not be detectable because they may be masked by changes due to other natural and unnatural stressors.

Various entities, including environmental regulators, First Nations, concerned citizens, various stakeholders, and the aquaculture industry, are concerned about the potential for actual or perceived harm to the environment and ecosystem. Regulators are also interested in being able to predict the potential for environmental and ecosystem exposures and the consequences associated with the introduction of drugs into the environment as part of fish farming operational activities. These predictions can be used to help avoid and mitigate any potential exposures and consequences of concern. Results of predictions can also help interpret any observed consequences that may be suggested to have resulted from exposure to an aquaculture-based release of drugs. This document outlines the basic principles and concepts underlying efforts to model exposures associated with in-feed drugs.

IN-FEED TREATMENT METHODS

Drugs can be introduced into fish orally or through injection; most of the drugs administered to fish in net-pens are administered orally as additives to fish feed. The medicated feed is prepared by a feed manufacturer by either mixing the drug with the feed or coating the feed pellets with a solution of the drug. Since the fish may exhibit reduced feeding rates when given medicated feed (Rigos et al. 1999), feeding practices prior to and/or during the treatment regime may be altered in order to increase ingestion and decrease waste of the medicated feed. The medicated feed is delivered in the usual manner. Sometimes the fish are fed the medicated feed for a few days, then no medicated feed for a couple of days, and then fed medicated feed for a few more days. The feeding activity is often monitored on video and can be terminated when feed begins to be detected near the bottom of the net-pens.

The quantities of drug administered are based on estimates of the biomass of fish in a given net-pen at the time of treatment and the target dose (Beattie and Bridger 2023). Typically, the fish are fed medicated feed at a daily rate based on their body weight; for example, the suggested feeding rate for Slice® treatments is 0.5% of fish biomass per day but can vary from 0.25% to 4% (MSD Animal Health 2012). The total quantity of drug per unit mass of feed varies with the drug and feed rate. For example, for a 1% feed rate, the amount of active ingredient (a.i.) per metric tonne of feed can vary from as little as 5 g to 7.5 kg (Table 1). In Canada, drugs are prescribed by a veterinarian who may authorise deviations from the labelled treatment dosage and regime that may impact the treatment duration, the amount of active ingredient in the feed, and total quantity of drug used (Beattie and Bridger 2023).

Table 1. Medicating ingredients approved for salmon in Canada (CFIA 2020)

Product	Active Ingredient (a.i.)	Treatment dosage of a.i. ($mg \cdot kg^{-1} \cdot d^{-1}$)	Amount a.i. in feed ($g \cdot kg^{-1}$)*	Treatment regime (d)
Slice® 0.2% Premix (CFIA 2020; MSD Animal Health 2012)	Emamectin Benzoate (0.2%)	50×10^{-3}	5×10^{-3}	7
Aquaflor® 50% Medicated Premix (CFIA 2020)	Florfenicol	10	1	10
Tribrissen™ 40% Powder (CFIA 2020)	Sulfadiazine	25	2.5	7 – 10
	Trimethoprim	5	0.5	
Terramycin-Aqua© Oxytetracycline Dihydrate Medicated Premix (CFIA 2020)	Oxytetracycline hydrochloride	75	7.5	10
Romet® 30 Medicated Premix (CFIA 2020)	Sulfadimethoxine	15	1.5	10
	Ormetoprim	15	1.5	

*Based on 1% feed rate

EXPOSURE PROCESS

After ingestion by the fish, the drug follows several metabolic pathways before any non-metabolised parent drug is finally released into the environment (Figure 1). The total amount of drug released into the environment will depend principally on the amount administered. The details of how and when the active ingredient enters the environment are dependent on how the drug is partitioned between waste feed, egestion, and excretion. The type of discharge in turn affects how far the drugs are transported and how much they are dispersed by the ambient environment.

The pathways of drug discharges start with the administration of medicated feed into a net-pen. Most, but not all, of this feed is ingested by the fish. The portion that is not ingested, i.e., the waste feed, sinks towards the seabed. During the sinking, feed pellets may swell, break up, and/or be consumed by other wild organisms. Of the ingested feed, some of the drug is absorbed by the fish and the remainder is excreted. The absorbed drug is metabolized by physiological processes and eventually the fish egest and excrete the parent drug and its metabolites. The route of the drug within the fish from ingestion to excretion is commonly referred to as pharmacokinetics. Each of the release pathways, i.e., waste feed, egestion (feces), and excretion, results in different exposure zones that may overlap.

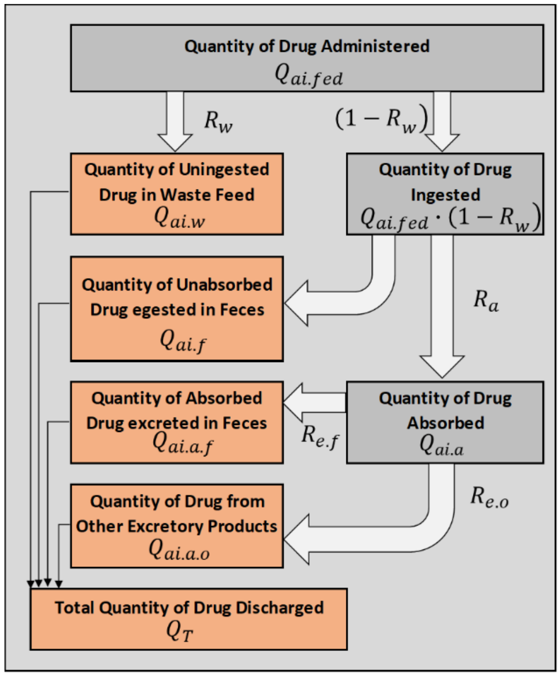


Figure 1. Flow diagram of partitioning pathways.

A major factor determining the size of the benthic exposure zone associated with the in-feed administration of drugs is the sinking rates of waste feed and feces (Chamberlain and Stucchi 2007; Bannister et al. 2016). The zone of exposure associated with waste feed is expected to be the smallest area; waste feed pellets have the greatest sinking rates (Table 2) resulting in the smallest transport distances (Table 3) and the smallest spread of sinking particles (Cromey et al. 2002). The size of this zone will be larger in areas characterised by deeper waters and/or stronger current speeds. During the settling phase, as well as once on the seabed, wild organisms may ingest some of the waste feed and hence influence the concentration and distribution of the drug.

The zone of exposure associated with feces resulting from the ingestion of medicated feed is larger than that associated with waste feed and contains a greater quantity of drug. It is commonly recognized that fecal composition (Tlusty et al. 2000) and sinking rates (Table 2) vary in relation to feed composition, including medication type which can impact digestibility of the feed (Toften and Jobling 1997), fish species and size, fish health, and environmental conditions (Chamberlain and Stucchi 2007; Reid et al. 2009) but there are few measurements that allow quantification of these factors for sinking rates. In general, sinking rates of fecal pellets are less than that of waste feed and greater than that of excretory products. Hence, the duration of time in which drugs are available for transport and dispersal by the receiving water currents is likely longer than for waste feed and less than for excretory products, although fecal slurries may behave more closely to fish excretory products than to sinking fecal pellets. As with waste feed, wild organisms may ingest some of the settling or settled fecal waste and hence influence the concentration and distribution of the drug.

*Table 2. Estimated sinking rates for salmonid feeds and feces. Data are for salmon in seawater, except * indicates trout in freshwater. Ranges are minimum and maximum values (except where indicated). Blank cells ("-") indicate that data were not available. Data for feces prior to 2009 are summarized in Reid et al. (2009).*

Particle type	Sinking rate (cm · s^{-1})			Data source
	Mean ± SD	Median	Range of values	
Feed	-	-	9–15	Gowen and Bradbury (1987)
	5.5 ± 1.0 to 15.5 ± 1.3 (SD range: 0.7–2.4)	-	-	Findlay and Watling (1994)
	10	-	-	Panchang et al. (1997)
	8	7	2–12	Elberizon and Kelly (1998)*
	5.15 ± 0.31 to 14.91 ± 0.91 (SD range: 0.25–1.80)	-	-	Chen et al. (1999a)
	10.8 ± 2.7 (overall mean)	-	~6 to ~17 (dataset means)	Cromey et al. (2002)
	10.5 ± 1.36 to 20.1 ± 0.81 (SD range: 0.81–2.79)	-	-	Sutherland et al. (2006)
	8.67 ± 2.12 and 9.87 ± 1.30	7.6–10.9	3.9–12.4	Moccia et al. (2007)*
	5.5 ± 1.7 to 10.3 ± 1.0 (SD range: 0.9–2.1)	-	-	Moccia and Bevan (2010)*
	5.6 ± 1.0 to 17.0 ± 2.9 (SD range: 0.5–2.9)	-	-	Skøien et al. (2016)
Feces	2.0	-	-	Findlay and Watling (1994)
	3.2	-	70% within 2–4	Panchang et al. (1997)
	2.9 ± 1.0 (>2000 μm fraction); 1.5 ± 1.0 (>500 μm fraction)	3.1 1.4	-	Elberizon and Kelly (1998)*
	5.3 ± 0.8 to 6.6 ± 1.3 (SD range: 0.8–2.0)	-	-	Chen et al. (1999b)

Particle type	Sinking rate ($cm \cdot s^{-1}$)			Data source
	Mean ± SD	Median	Range of values	
	-	0.7	-	Wong and Piedrahita (2000)*
	3.2 ± 1.1	-	1.5–6.3	Cromey et al. (2002)
	5.1 ± 1.1 to 6.4 ± 1.4 (SD range: 0.8–1.4)	-	3.7–9.2	Chen et al. (2003)
	2.7–3.9	-	-	Ogunkoya et al. (2006)*
	5.2	4.4–5.8	2.8–8.1	Moccia et al. (2007)*
	3.97 ± 0.20 to 7.58 ± 0.48 (SD range: 0.09–0.48)	-	50% mass >5.9	Moccia and Bevan (2010)*
	-	-	58–78% mass 5 – 10; 8.5–10% mass ≤1	Bannister et al. (2016)

Table 3. Estimated displacement distances (rounded to the nearest meter) for salmon feed and feces. The particle types indicate the range of sinking speeds illustrative of feed (5 – 15 cm·s^{-1}) and feces (1 – 10 cm·s^{-1}).

Particle Type	Sinking Speed (cm·s^{-1})	Water Depth (m)	Sinking Time (min)	Water velocity (cm·s^{-1}) 5	10	15	20	40	80
Feces	1	**10**	17	50	100	150	200	400	800
		25	42	125	250	375	500	1000	2000
		50	83	250	500	750	1000	2000	4000
		100	167	500	1000	1500	2000	4000	8000
		200	333	1000	2000	3000	4000	8000	16000
Feces, Feed	5	**10**	3	10	20	30	40	80	160
		25	8	25	50	75	100	200	400
		50	17	50	100	150	200	400	800
		100	33	100	200	300	400	800	1600
		200	67	200	400	600	800	1600	3200
Feces, Feed	10	**10**	2	5	10	15	20	40	80
		25	4	13	25	38	50	100	200
		50	8	25	50	75	100	200	400
		100	17	50	100	150	200	400	800
		200	33	100	200	300	400	800	1600
Feed	15	**10**	1	3	7	10	13	27	53
		25	3	8	17	25	33	67	133
		50	6	17	33	50	67	133	267
		100	11	33	67	100	133	267	533
		200	22	67	133	200	267	533	1067

The largest zone of exposure is that associated with the non-sinking excretory products from the fish since these remain in the water column for lengths of time that are usually much longer than the time for waste feed and feces to sink to the bottom. These excretory products are therefore transported the largest distance from the release point. The exposure domain resulting from this pathway is to a large extent a pelagic zone of exposure.

Models of exposure zones should reflect the different pathways of release and behaviours of the released products, i.e., sinking or non-sinking products. Typically, benthic exposure models do not include leaching. However, leaching of the drug into the water column may be significant: resulting in a pelagic exposure (Rigos et al. 1999; Fais et al. 2017; Barreto et al. 2018), and a reduction in the level of the benthic exposure zone. Factors which could influence leaching include the feed type, chemical properties of the drug, method of incorporation of drug into the feed (Duis et al. 1995; Rigos et al.1999), environmental conditions, and sinking time.

THE MODELLING CONTEXT

CONCEPTUAL COMPONENTS

The objective of drug exposure models is to estimate the scale (area, length, width), location, concentration, and persistence of a drug in the environment. Models of the exposure to released drugs include four fundamental components:

1. an estimate of the partitioning (i.e., proportions of waste feed and feces, sinking rates, and release times) and loading (i.e., total amount of drug active ingredient associated with each partition that is discharged),
2. the transport, dispersal, and deposition of the active ingredient that is released from each of the above partitions,
3. the post-deposit persistence of the deposition, and
4. the consequences stemming from the exposure.

These components have been recognized since the beginning of exposure modelling and have been reiterated by many authors (Findlay and Watling 1994; Gowen et al. 1994; Silvert 1994).

The specific size, location, and intensity of exposure varies in relation to many factors, including release location, release time, hydrography, water depths, drug type, drug delivery approach, health status of the fish, fish size and stocking density, post-deposit persistence including resuspension and chemical decay, and farm arrangement. The details of exposure domains associated with drug delivery are therefore expected to be site and treatment specific. How well resolved the exposure estimates need to be depends on the objective(s) for which the estimates are being made.

All of these factors contribute to the estimation of the scale and intensity of environmental exposure to released drugs. Many of the factors are poorly understood and poorly quantified and most are subject to considerable spatial and temporal variations. Several of these factors are described in more detail below. Whether all factors and pathways need to be considered for each chemical and site will depend on the specific characteristics of the chemical, the site, and the management objectives including the Environmental Quality Standard (EQS). Hence, estimation of exposure domains should include an initial scoping of the magnitude of potential exposure which should then be considered by management and decision makers in an effort to determine whether more precise exposure profiles are desired or required.

During feeding, the medicated feed sinks through the water in the net-pen where, ideally, most of it is consumed by the farmed fish. The unconsumed feed falls through the net-pen mesh as waste feed and continues to sink to the seabed. The consumed feed is processed by the fish with some proportion of the drug being absorbed into the fish and the un-absorbed portion being released into the environment in the feces. Some of the waste feed may be eaten by wild organisms (Dempster et al. 2009). The details of the absorbed portion of the drug are dependant on the particular drug being used. The drug can deplete (Horsberg 2003; Lam et al. 2020) and/or transform within the fish (Horsberg et al. 1996; Kim-Kang et al. 2004) and be expelled as the parent compound or metabolites into the environment. The absorbed portion will be discharged from the fish; exact proportions of how the absorbed medication is egested or excreted is poorly characterized and drug dependant. These concepts are discussed in more detail in the following sections.

Partitioning of Active Ingredient

A partitioning represents the pathways of entry into the environment that an active ingredient would typically follow. Partitionings are best envisioned as a flow chart where branches indicate how much of a substance at one stage passes to subsequent stages (Figure 1). The purpose is to determine how each proportion of a substance in a given pathway is discharged into the environment. The partitions discharged into the environment are waste feed, feces (egestion), and urine (excretion); another includes transfer to the environment across the gills. The partitions do not include transformation to metabolites and loss of active ingredient due to mortality and/or harvesting.

The discharge associated with each partitioning pathway depends on specification of partitioning coefficients, i.e., the proportions of drug absorbed, egested, and excreted. The amount of drug in each discharge pathway is determined through a series of calculations corresponding to the steps in the partitioning diagram (Figure 1). First, the amount of drug fed to the fish, $Q_{ai.fed}$, is calculated by

$$Q_{ai.fed} = B \cdot F_{rate} \cdot C_{ai} \, , \tag{1}$$

where

> B is the biomass of fish in the net-pen,
>
> F_{rate} is the feeding rate expressed in the fraction of fish biomass per day, and
>
> C_{ai} is the concentration of active ingredient in the feed expressed as the mass of active ingredient (a.i.) per unit mass of medicated feed.

The amount of drug released as waste feed, $Q_{ai.w}$, is given by

$$Q_{ai.w} = Q_{ai.fed} \cdot R_w \, , \tag{2}$$

where R_w is the wastage rate of feed expressed as the ratio of feed that is not eaten.

The amount of drug immediately released in the feces (i.e., not digested), $Q_{ai.f}$, is given by

$$Q_{ai.f} = Q_{ai.fed} \cdot (1 - R_w) \cdot (1 - R_a), \tag{3}$$

where R_a is the absorption rate of drug expressed as the fraction of ingested drug that is absorbed through the digestive tract into the fish.

Finally, the amount of drug absorbed by the fish, $Q_{ai.a}$, is given by

$$Q_{ai.a} = Q_{ai.fed} \cdot (1 - R_w) \cdot R_a. \tag{4}$$

The absorbed quantity is released slowly over time in the bile, $Q_{ai.a.f}$, (which is excreted via the feces) and other excretory products, i.e., urine, mucus, and transfer across the gills, $Q_{ai.a.o}$:

$$Q_{ai.a.f} = Q_{ai.a} \cdot R_{e.f} \tag{5}$$

and

$$Q_{ai.a.o} = Q_{ai.a} \cdot R_{e.o} \tag{6}$$

where $R_{e.f}$ and $R_{e.o}$ are the proportions of the absorbed drug released in the feces and other excretory products, respectively. If the drug accumulates in the fish, $R_{e.f} + R_{e.o} < 1$. Furthermore, the partition between $Q_{ai.a.f}$ and $Q_{ai.a.o}$ varies among drugs and, for many drugs, it is assumed that all of the drug is excreted via the feces, i.e., $R_{e.o} = 0$. The total amount of drug that is released into the environment, Q_T, is the sum of the individual discharges (Figure 1). In the above equations, values of the partitioning coefficients, R_w, R_a, $R_{e.f}$, and $R_{e.o}$, are dependent on multiple factors including: the drug, fish species, health status of the fish, drug metabolic pathway, and water temperature. Unfortunately, these factors can be variable and are generally sparsely studied and model predictions are sensitive to the parameter values.

All of the above discharges occur over varying time scales. The release of waste feed occurs during feeding and the subsequent sinking time resulting in a total time scale of minutes to hours depending on the water depth. Typically, medicated feeds are administered to net-pens once per day (Beattie and Bridger 2023). The release of feces is more complicated. Studies have shown that defecation in salmonids can occur from 6 – 48 h after feeding, and is affected by many factors, including water temperature, fish size, type of feed, and the time since the last feeding; and there can be considerable variability among individual fish (Grove et al. 1978; Storebakken et al. 1999; Aas et al. 2017; Aas et al. 2020) and, perhaps, among fish populations. It has also been observed that feeding can stimulate defecation (Chen et al. 2003). The details of fecal discharges, i.e., whether feces are released continuously or in pulses, are unknown and can impact the distribution of the fecal matter on the seabed. These studies imply the release time of the fecal egestion of the un-absorbed drug happens over time scales of hours to days and lags the feeding discharge. The absorbed drug will be released more slowly over time, with time scales ranging from days to months; the details of the discharge time-dependence depend on the drug being administered as well as the factors influencing the un-absorbed fecal egestion. For example, emamectin benzoate is released primarily through the feces (Sevatdal et al. 2005) with an estimated excretion half-life, t_e, of 36 days (SEPA 2005). Once the drug has been released into the environment, it decays exponentially with an associated half-life, t_d.

The values of the partitioning coefficients dictate the deposition locations of drug discharges. This has been illustrated by Chamberlain and Stucchi (2007) in the context of carbon. They used DEPOMOD (Cromey et al. 2002) to simulate the deposition of feed and fecal releases and showed that the relative contributions of each to the total bottom deposition changed with distance from the release site; near-field deposition was dominated by the relatively fast sinking waste feed releases and the far-field deposition was dominated by the relatively slow sinking fecal releases. In the scenarios they modelled, deposition within ~60 m of the release location consisted of 50 – 80 % waste feed whereas >100 m from the release location the deposition consisted of more than 90% fecal waste (Chamberlain and Stucchi 2007). The area between 60 and 100 m was a transition zone in which the dominance of contributions from waste feed and fecal egestion switched. The same concept applies to drugs, but the specific distributions will differ as the partitioning coefficients for a drug differ from that of carbon. For the partitioning diagram shown in Figure 1, illustrative parameter values for a low absorption drug, a high absorption drug, and, for comparison, carbon are given in Table 4.

Table 4. For the partitioning diagram shown in Figure 1, parameter values illustrative of a low absorption drug and a high absorption drug, as well as those used for emamectin benzoate in the partitioning model described in the Partitioning section. For comparison, values for carbon are also given. The amount of drug administered, $Q_{ai.fed}$, is not necessarily representative of actual values.

Scenario	R_w	R_a	$R_{e.f}$	$R_{e.o}$	$Q_{ai.fed}$ (g)	$Q_{ai.w}$ (g)	$Q_{ai.fed} \cdot (1 - R_w)$ (g)	$Q_{ai.f}$ (g)	$Q_{ai.a}$ (g)	$Q_{ai.a.f}$ (g)	$Q_{ai.a.o}$ (g)
Drugs											
Low absorption	0.05	0.20	1.0	0.0	9.947	0.497	9.450	7.560	1.890	1.890	0.0
High Absorption	0.05	0.80	1.0	0.0	9.947	0.497	9.450	1.890	7.560	7.560	0.0
Emamectin benzoate	0.05	0.90	1.0	0.0	7.957	0.398	7.560	0.756	6.804	6.804	0.0
Carbon											
Carbon	0.05	0.85	0.0	0.0	99 500	5 000	94 500	14 200	80 000	0.0	0.0

Previous research has shown that a major factor influencing the intensity of exposure is the amount of medicated feed that is not eaten by the fish, i.e., waste feed (Cromey and Black 2005). Rates of feed ingestion and wastage are difficult to measure (Gowen et al. 1994) and are not well known and hence specifications of these parameters are based on approximate estimates and informed assumptions (Cromey and Black 2005). Chamberlain and Stucchi (2007) summarized the literature on feed wastage rates and commented that few quantifications of this parameter exist. Early estimates of the uningested proportion of food fed to the fish range from 1 to 40%, with 5 to 15% being reported the most often (Findlay and Watling 1994; Chen et al. 1999 and references therein). Finlay and Watling (1994) estimated 11% wastage for one farm and 5% for another in Maine; however, they noted that 5% or less was likely typical in Maine at the time of their study. Gowen and Bradbury (1987) suggested that 80% of the provided non-medicated feed was consumed and that 20% was wasted; however, this estimate was likely for moist feed, which is rarely used now. Improvements to feed formulations over the years, automated feeding systems, and incorporation of in-situ monitoring equipment such as camera systems near the bottom of each net-pen have reduced the amount of wasted feed. Current assumptions are that 95% or more of the provided non-medicated feed is usually consumed. For example, in the early 2000s, the industry in British Columbia, Canada assumed their wastage rates were 5% or less (Chamberlain and Stucchi 2007). The Scottish Environment Protection Agency (SEPA) recommends using a food wastage rate of 3% for modelling discharges of organic solids and in-feed medicines from fish farms (SEPA 2019). A food wastage rate of 3% is commonly used for regulatory purpose, for example by Scotland (SEPA 2019) and Canada (Government of Canada 2014), and in research studies (Corner et al. 2006; Chang et al. 2012; Keeley et al. 2013), whereas estimated values can range from less than 1% (Cairney and Morrisey 2011) to 5% or more (Brooks and Mahnken 2003; Chamberlain and Stucchi 2007; Gjøsæter et al. 2008, as cited in Skøien et al. 2016; Riera et al. 2017). With respect to medicated feed, wastage rates are largely unknown; they are usually assumed to be similar to those for non-medicated feed though in practice may differ.

Changes in deposition quantities and rates are expected to be proportional to the change in feed wastage; i.e., a 150% increase in feed wastage rate results in 150% change in the deposition quantity and rate and a reduction in wastage rate of 50% results in a 50% reduction in the deposition quantity and rate. This was the finding of Chamberlain and Stucchi (2007) who examined the sensitivity of DEPOMOD predictions to changes in feed wastage rates. They compared deposition rates predicted using feed wastage rates of 5%, 10% and 15%. The predicted rates of deposition with the 5% and 15% feed wastage rates were 0.5 and 1.5 times that of the 10% feed wastage rate, respectively.

Of the feed and medication that is consumed, only a fraction of the drug active ingredient (a.i.) is absorbed into the fish. The remaining amount of a.i. is egested in the feces. The absorbed fraction is excreted via the feces either in the original form or as metabolites. Absorption coefficients of ingested drugs range from approximately 10 – 20 % on the low end to approximately 80 – 90 % on the high end (Kemper 2008) and depend on the specific dynamic action (associated with diet type, meal size, water temperature, available dissolved oxygen, and size or species of fish), see Beattie and Bridger (2023) and references within. Excretion products and rates also vary among drugs and the specific dynamic action. Table 4 gives examples the partitioning of active ingredients for a highly absorbed drug and a weakly absorbed drug.

In summary, the quantity of drug deposited on the seabed as a result of each discharge pathway depends on several parameters; furthermore, the actual values of these parameters are not well known and are likely not constant. Therefore, deposition predictions are sensitive to the assumptions made in selecting parameter values. Using the low absorption partitioning coefficients given in Table 4, three overlapping deposition zones would be expected. One near-field zone dominated by waste feed, a mid-field zone dominated by feces, and a far-field zone dominated by urine excretion. The distances associated with the near-field zone will depend on sinking rates of waste feed. The mid-field will depend on the sinking rates for feces. The far-field will consist of flocculated and resuspended discharged. The total predicted area of impact will depend on the current velocities as well as the EQS of the released drug. A better understanding of the sinking rates will be important to accurately predict these zones.

Sinking Rates of Feed and Feces

Exposure model outputs are very sensitive to the assumptions made in relation to the sinking rates of feed and feces (Magill et al. 2006; Reid et al. 2009); hence accurate predictions of exposure domains require accurate characterization of particle sinking rates (Magill et al. 2006). Unfortunately, it is difficult to characterize these sinking rates; although several efforts have been made (Table 2) but the number of measurements continues to be relatively small (Magill et al. 2006; Reid et al. 2009).

Fish Feed

Fish feed pellets are manufactured to be of a consistent size, shape, and composition for each particular pellet type. Sinking rates for particular pellet types are generally considered to be normally distributed (Chen et al. 1999a; Cromey et al. 2002; Skøien et al. 2016). Measured mean sinking rates of salmonid feed pellets range from 5 to 20 $cm \cdot s^{-1}$, with standard deviations varying from 0.25 to 2.9 $cm \cdot s^{-1}$ (Table 2). Standard deviations increased with mean sinking rates (Chen et al. 1999a; Skøien et al. 2016); however, this was not the case in the Sutherland et al. (2006) study.

Mean sinking rate increases with pellet size (i.e., diameter) (Chen et al. 1999a; Cromey et al. 2002; Sutherland et al. 2006; Skøien et al. 2016). However, Elberizon, and Kelly (1998) and Findlay and Watling (1994) reported that feed pellet size was not a good predictor of the sinking rate, although both studies found a general trend of increasing sinking rates with increasing pellet size; in both studies, differences in pellet shapes and/or manufacturers of the tested pellets may have been factors. Feed pellets fed to larger fish are larger, and therefore will likely sink faster than smaller pellets fed to smaller fish. Feed pellets for pre-market fish sink about twice as fast as those for smolts.

Feed pellet sinking rates are higher for higher density feed pellets of the same size (Skøien et al. 2016), as would be expected. The density, and hence sinking rates, of feed pellets may be affected by their composition. Ogunkoya et al. (2006) found that pellets incorporating soybean meal and an enzyme cocktail fell at slower rates than feed pellets without these supplements. Chen et al. (1999a) compared standard (20 – 24 % oil) and high energy (28 – 30 % oil) pellets of the same sizes from two different feed manufacturers, Ewos and Trouw. For Ewos 6 mm pellets, the sinking rates were similar in the two formulations, but for Ewos 10 mm pellets, sinking rates were higher for standard pellets, while for Trouw 6 mm pellets, sinking rates were higher for high energy pellets.

Water temperature and salinity may also affect feed sinking rates. Chen et al. (1999a) found faster sinking rates at 10°C vs. 20°C for most of the pellet types tested (contrary to expectations, since water is denser at 10°C than at 20°C); while Elberizon and Kelly (1998) found some increase in sinking rates with increasing temperatures (2, 10, and 13°C), but the differences were not statistically significant. The Chen et al. (1999a) study also found that sinking rates were significantly higher at a salinity of 20 psu than at 33 psu, as would be expected, since higher salinity seawater has a higher density.

Although feed pellets absorb water with time when they are immersed, sinking rates were found to be the same, at least for initial immersion times of up to 15 min in the Chen et al. (1999a) study. After this, the sinking rates probably decrease as the pellet density approaches the water density. Feed sinking times range from about a minute to up to an hour (Table 3). The data provided in Stewart and Grant (2002) indicate that the changes in mass are small on these time scales and hence the assumption of a constant sinking rate for a given feed particle is reasonable.

The measurements of sinking rates for feed pellets may not be representative of what exits a fish net-pen since feed pellets may be broken and disaggregated by fish feeding activity, fish movements, and water currents as they fall through water within the fish net-pen; this may lead to a bias in the assumptions of feed pellet sinking rates toward the larger, faster sinking, intact pellets. To our knowledge, there is no information available to quantify most of these processes. Some data have been reported on the friability of pellets. Chen et al. (1999a) found that friability was greater in larger pellets (for pellets 2 – 14 mm in diameter). Khater et al. (2014) also found that larger pellets were less durable than smaller pellets in a study of Egyptian fish feeds (1 – 3 mm diameter pellets). However, Stewart, and Grant (2002) found that smaller (6.5 mm diameter) salmon feed pellets eroded faster in a flume tank than larger pellets (12 mm diameter). The Khater et al. (2014) also found that pellet durability decreased as the protein level increased.

Fish Feces

Fish feces have multiple characteristics (size, shape, and density) and are commonly categorized as either pellets, mucus strings, or slurries. The relative proportion of these is likely to vary, has not been well quantified, and pellets may not constitute the majority of fecal production (Findlay and Watling 1994). Furthermore a proportion of well formed feces pellets will likely be broken down and disaggregated into smaller particles by fish motion, water turbulence, and contact with net mesh during their descent through the net-pen (Gowen and Bradbury 1987; Findlay and Watling 1994; Magill et al. 2006; Reid et al. 2009). The characteristics may further change due to disaggregation during the sinking time to the bottom. Sinking rates of fish feces are dependent on the feces' type. Measuring the sinking rates of fish feces is more difficult than for fish feed; the feces must be collected from the digestive track of fish, from nets, or traps deployed in-situ within or beneath fish tanks, net-pens, or beneath fish farms.

In general, measurements are based mainly on well formed fecal pellets (Magill et al. 2006). Measured sinking rates for fish feces are generally lower and more variable than for fish feed; may not be normally distributed and instead are positively (or right) skewed; increase with pellet size; and may or may not depend on fish size (Chen et al. 2003; Magill et al. 2006; Moccia et al. 2007; Moccia and Bevan 2010; Bannister et al. 2016). Measured mean sinking rates of well-formed salmon feces range from 1.5 to 7.58 $cm \cdot s^{-1}$, with standard deviations varying from 0.09 to 2.0 $cm \cdot s^{-1}$ (Table 2). Hence sinking rates for fecal pellet vary by approximately 10 $cm \cdot s^{-1}$ with most measured values between 2 and 10 $cm \cdot s^{-1}$ (Reid et al. 2009; Bannister et al. 2016). The above measurements do not apply to fecal mucus strings and slurries; these have much lower sinking rates and behave more like passive particles. Thus, using the previously reported fecal sinking rates may not produce the full spectrum of dispersion and spread of the release substance. The relative importance of fecal mucus strings remains uncertain as results from studies are inconclusive. Elberizon and Kelly (1998) determined that 40% of salmon smolt fecal particles collected had a length scale less than 0.5 mm; the sinking rates of these particles were not measured but can be assumed to be slow (Elberizon and Kelly 1998). Bannister et al. (2016) found that over 58% of the mass fraction of collected Atlantic salmon fecal material settled at velocities greater than 5 $cm \cdot s^{-1}$ but the mass and sinking rates of particles with length scales less than 0.5 mm were not measured. Moccia and Bevan (2010) found that more than 75% of the collected rainbow trout fecal mass settled at velocities greater than 5 $cm \cdot s^{-1}$ but the minimum particle size was not given.

Flocculants

The smaller feed dust and fecal particles i.e., those with length scales < 1 cm, are perhaps likely to form flocs (Magill et al. 2006). These may sink at rates of < 0.1 $cm \cdot s^{-1}$ (Magill et al. 2006), will take longer to settle out and will be displaced horizontally by the currents for longer distances than feed or fecal pellets. The intensity of the deposition associated with flocs will be low since only a small proportion of the administered active ingredient will be released as fines. However, although the intensity may be low, the potential for toxicity needs to consider the relevant EQS since a low intensity deposition coupled with a highly toxic drug may produce a toxic deposition.

Implications to Models

Models of the deposition of releases from fish farms must adequately represent and parameterize the processes controlling the deposition (Chamberlain and Stucchi 2007). The models are sensitive to the assumptions made concerning sinking rates of feed and feces (Magill et al. 2006; Reid et al. 2009; Bannister et al. 2016) and to the assumptions concerning the mass distribution of sinking rates, i.e., the proportion of fecal production associated with feces of specific sizes and sinking rates.

Given the uncertainties associated with feed and fecal sinking rates and the lack of quantifications of fecal production by sinking rate, model estimates of exposure should be interpreted cautiously and as being biased toward the well-formed feed and fecal pellets. Some authors have suggested that it may not be reasonable to accurately model the transport, dispersion, spread, and deposition of fish feces from the well defined particle sinking rate perspective because of the degree of uncertainty (Findlay and Watling 1994; Silvert 1994). At a minimum, estimates of exposure domain and intensity should include sensitivity analyses and statements of uncertainty associated with the assumptions made about sinking rates. Perhaps the most robust estimates at present are those associated with the upper and lower limits of sinking rates since these are less sensitive to assumptions about sinking rate distribution. These limit estimates, however, do not indicate details of the extent and intensity of exposure within the limits. Determinations of the potential importance of estimating the exposure domains and intensities associated with the poorly characterized portions of the particle settling spectrum would be useful, so more informed perspectives can be made concerning the importance of this aspect to decision making.

The sinking rate combined with water depth determines the time needed for a particle to sink to the bottom. The horizontal distance a particle will be transported can be estimated using this sinking time and the velocity of the horizontal water current. As a result of the variability in the sinking rates, for a given water depth and horizontal water velocity, there is a wide range of predicted displacement distances. For example, using the range of sinking values in Table 3, a depth of 25 m and a water velocity of 20 $cm \cdot s^{-1}$, the estimated maximum and minimum distances travelled by a waste feed pellet and a fecal particle may differ by factors of 3 (i.e., 33 – 100 m) and 10 (i.e., 50 – 500 m), respectively. The variation in sinking rates influences the spread around the mean travel distances. For a typical range of depths and water velocities the displacement distances can range from a few meters in shallow water to a few tens of kilometers in deep waters (Table 3). The absolute bias will be greater for farms located in areas with higher ambient current speeds and greater water depths, and the bias may be greater for estimates of fecal exposure than for feed exposure. Estimates of exposure based on the assumption of mean sinking velocities result in estimates of exposure that differ from those based on distributions of sinking velocities (Magill et al. 2006).

In the absence of measurements, some authors have used the Stokes' law to estimate feed and feces sinking rates (Cubillo et al. 2016). However, the Stokes' law is generally recognized as being a poor indicator of fish feed and fecal sinking rates; the Reynolds number is inappropriate for Stokes' law and the sinking rates of fish feed (Chen et al. 1999a) are for the most part too large (i.e., sinking rates >~1 $cm \cdot s^{-1}$) for Stokes' law to apply (Chen et al. 2003).

The simplest and earliest models assume single particle sinking rates for feed pellets and feces. Later models assume a distribution of sinking rates. The most common distribution assumption for both waste feed and fecal particulates is a normal distribution with a specified mean and standard deviation of the sinking rate that are constant for all fish sizes and over time. The assumption of a normal distribution may be reasonable for feed pellets but empirical evidence is beginning to indicate that a right skewed distribution may be more appropriate for fish feces (Fish Feces Section), i.e., that measured sinking rate distributions tend toward faster sinking rates and that this distribution is independent of fish size. For a given mean and standard deviation, models assuming a single value or normal distribution of fecal sinking rates may inaccurately estimate the rate of deposition relative to models using non-normal distributions (Bannister et al. 2016).

The variations in the size, density, and sinking velocity of feed pellets and feces may result in horizontal scattering of the waste even in the absence of water turbulence and horizontal currents due to some horizontal motion induced by the particle shapes as they settle through the water. One study has demonstrated this effect for fish feed pellets (Skøien et al. 2016) but similar studies have not been conducted for fish feces. The induced dispersion is small and not likely to be of major practical importance in most in-situ situations because horizontal currents and turbulence are seldom zero in fish farming areas.

Taking horizontal advection and background turbulence into consideration, the estimated exposure outputs from transport and dispersal models can vary significantly when using the same hydrodynamics but different sinking rate distributions. Many modelling efforts using a normal distribution for salmon feces have assumed a mean of 3.2 $cm \cdot s^{-1}$ and a standard deviation of 1.1 $cm \cdot s^{-1}$. This specification was used by Cromey et al. (2002) in the DEPOMOD model and other modelling efforts have often adopted these values. This assumption may either underestimate (Moccia et al. 2007; Moccia and Bevan 2010; Bannister et al. 2016) or overestimate (Elberizon and Kelly 1998) the fecal sinking rates resulting in inaccurate estimates of the extent and intensity of the deposition areas.

The degree of inaccuracy depends on the exact specifications of the distributions. Unfortunately, the distribution of in-situ fecal sinking or sinking rates is seldom known, is likely to vary between feed types and fish health status, and is likely evolving as fish diets and fish growth efficiencies change. Use of minimum and maximum sinking rates appropriate to each site provide bounding limits on model outputs.

When using ranges of sinking rates for salmon feed and feces, water depths, and horizontal current speeds, the distances estimated for sinking feed and feces can range over several orders of magnitude, from less than 10 m to over 10 km (Table 3). The range for a specific site is likely to be smaller, since local water depth and current speed are not likely to cover the full range of possibilities. For example, the horizontal displacement ranges from 50 to 1000 m for a farm located in a water depth of 50 m and subject to a water current of 0.1 $m \cdot s^{-1}$. The difference between using central tendency values of the parameters and the extreme values is less; with the estimate using the central tendency values overestimating the minimum distance travelled and underestimating the maximum distance travelled. When a frequency distribution of sinking rates is used, the predicted distances are sensitive to the choice of the distribution. For example, in a comparison of estimated distances travelled by feces using a measured frequency distribution of fecal sinking rates and a normal distribution of sinking rates with a mean and a standard deviation of 3.2 and 1.1 $cm \cdot s^{-1}$, respectively, resulted in different spatial distributions of the deposits both close to and far from the release point (Bannister et al. 2016).

In summary, sinking rates of in-situ particles released from net-pen fish farming are not and will not be precisely known for most situations; they may only be known to within an order of magnitude. This situation is likely to persist for some time because of the difficulties in measuring in-situ sinking rates and in the impracticality of characterizing these rates for many different husbandry and oceanographic conditions under which net-pen fish farming occurs. Because of the uncertainties, models will need to make assumptions about the sinking rate distributions and their parameter values. A conservative first order approach that uses lower and upper bounds of parameters such as sinking rates, water depths, and water velocities provides lower and upper bounds on exposure extents and intensities that may be useful to decision makers.

Characteristics of the Receiving Environment

Once a substance is released there are many aspects of the receiving environment that can influence the deposition. Discussed in this section are the three of largest consequence: water depth, advection, and dispersion. Water depth is the distance from the water surface to the seabed and changes spatially and temporally. Advection is the physical transport due to the movement of the water. Dispersion occurs when water containing a substance mixes with water that does not contain a substance; this both spreads the substance out and reduces the concentration (dilution).

The primary outputs of interest are the distribution and concentration of released substances on the seabed relative to the origin of release. To calculate the final locations of the discharged substances, individual trajectories of representative particles are typically calculated. The calculation of these trajectories uses the water currents (advection), sinking speeds, water depths, and dispersion. The location and spread of the released substances on the seabed are determined from the endpoints of these trajectories.

For in-feed drug treatments, the number of releases is relatively small (order 1 – 10 per net-pen) and for each release the patch of released feed or feces is translocated by the current during the time when these particles are sinking toward the bottom and diluted by dispersion processes taking place during its trajectory. The advection processes are very important in determining the location of deposition. Both advection and the dispersal processes determine the spreading, dilution, and hence the concentration, of the discharged drug on the seabed. Therefore, the cumulative distribution of the drug on the seabed is dependent on the details of the hydrodynamics that occur during the multiple feedings of a complete treatment. The specifics involving all fish net-pens receiving treatment and co-located within the farm must also be considered when calculating the cumulative distribution of drugs on the seabed.

Water Depth

Most early models assumed a constant depth even though it is well known that water depths can be highly variable in the vicinity of a fish farm and within the transport and spread area associated with a site. Although some enhanced models include spatial variation in water depth, most do not include the effect of this variation on water currents.

Only four dimensional hydrographic water circulation models have the potential to include spatial variations in water depth and water velocity on the scales of relevance to the transport and spread of drugs from fish farms; for this potential to be reached the models must have vertical and horizontal resolutions of order 1 and 10 m, respectively, and temporal resolutions of minutes. To achieve these resolutions requires considerable resources (time, computing power, skilled modellers, and multiple years of time); these resources are generally not available for application to most farm sites. Therefore, simpler models must still be relied on for most fish farming considerations.

Advection

Horizontal water currents in the general vicinity of net-pen fish farms usually range from 0 to less than 100 $cm \cdot s^{-1}$; average current speeds are usually less than 50 $cm \cdot s^{-1}$ with typical mean currents being in the range of 5 to 25 $cm \cdot s^{-1}$. Maximum current speeds are usually within a factor of 5 of the mean current speed.

The presence of net-pens and net-pen arrays has a significant effect on current speeds and directions downstream of the net-pens at depths similar to the depths occupied by the nets (Helsley and Kim 2005). The effects persist for distances of up to 10 times the diameter of the net-pen (Helsley and Kim 2005). For example, if a net-pen has a diameter of 30 m, its presence affects the water current speed for distances of up to 300 m downstream of the net-pen. If the length scale of a net-pen array perpendicular to the flow is 200 m, the water current speed and direction are affected for distances of up to 2000 m downstream of the farm. Most models of the transport of releases from fish farms do not take into consideration the influence of the net-pens which can be significant. Adding the effect of net-pens to the hydrodynamic model FVCOM resulted in changes to the velocities within, around, and under the fish farm (Wu et al. 2014) which could change the advection and hence deposition in the area around the net-pens.

Vertical water velocities are typically assumed to be small and not included in models estimating the exposure to aquaculture releases. Although many current meters are capable of collecting vertical current velocities it is not common practice to do so. Three dimensional hydrodynamic models are able to calculate vertical current velocities, but frequently these are not well validated. Despite the fact that vertical velocities are generally small (<1 $cm \cdot s^{-1}$) relative to horizontal velocities (10 to 100 cm·s^{-1}), they are potentially large enough to alter the sinking rate of smaller salmon feces.

Commonly the values for the advective components of deposition modelling would be provided from a current meter record. Such records are normally collected over a 30 to 90 day period and only include the horizontal component. There is an inherent assumption that the collected records are representative of the current velocities experience by the farm site. Many areas can exhibit spatial and temporal variations that generate current velocities that could be several times than those of the data collected during an observation period. These variations introduce an addition source of uncertainty that could impact displacement distances on the order of a factor of two.

Dispersion

Dispersion is complex and the rates depend on many factors: water velocity shears (i.e., spatial variations in water velocities), turbulence (i.e., small scale variations in water velocities), net-pen infrastructure, and stratification. In terms of estimating the exposure to in-feed drugs, the above implies that models must at least sufficiently parameterize dispersion processes during the times of treatment, including the influence of the net-pens on the near-field flows. In the ocean, horizontal dispersion rates are typically one or two order of magnitude larger than vertical dispersion rates and often vertical dispersion rates are neglected when modelling the dispersion of released waste feed and feces particles.

Typically, simple models of dispersion are two-dimensional and assume a normal distribution of concentration with dispersion rates that are either constant, i.e., Fickian (Lewis 1997), or a function of the patch size, i.e., Okubo (1971). The Fickian model allows for different dispersion rates in the orthogonal directions but these do not vary spatially or temporally. On the other hand, the Okubo relationship includes temporal variation in the dispersion rate is based on an equivalent circular patch area. An assumption of these models is that the released substance behaves like a passive tracer. To our knowledge, this has not been confirmed for the dispersion of waste feed and feces though when modelling these particles, these relationships are assumed to apply and often used, for example in Cromey et al. (2002). For waste feed and feces there may be additional dispersion due to the shape the particle and the resulting motion as it sinks through the water column (Skøien et al. 2016).

The presence of the net-pens and farm infra-structure has an impact on the initial dispersion of a release but field studies have shown that once a patch has cleared the farm infrastructure, the patch size evolves according to the Okubo relationship (Page et al. 2015). The patch concentration representations from simple dispersion models assume a smooth distribution and may not represent the variability in distributions typically observed within a patch.

Treatment Details

Treatment details include aspects of the administration of the medicated feed. These aspects include the active ingredient, number of feedings and their timing, the locations (multiple net-pens), and the amount of active ingredient delivered per feeding. These details are important to predicting the deposition of feces and waste feed. Specifics of treatment timing and locations will impact the location of deposition on the seabed due to the spatio-temporal variations in the hydrography, for example particles released at different times will land in different places due to changes to currents. Similarly, the type and amount of active ingredient administered are required for the prediction of concentration of active ingredient on the seabed.

Although treatment details are probably the best characterized of all the components and can potentially be known a priori, modelling the exact location of deposition from a specific treatment scenario requires the ability to accurately forecast water currents, as they have a substantial impact on the fate of the deposition. Available forecast models for Canadian coastal waters provide 48 h predictions. Not only is this insufficient for the typical treatment regime of 7 – 10 days for drugs approved for use in Canada (Table 1) but the grid resolutions are typically not sufficient to adequately resolve currents in areas where aquaculture occurs.

Post-Deposit Processes

As with other processes and parameters, models of exposure should include processes affecting the degradation, resuspension, and redistribution of particulates after their initial deposit. For the models to be effective, included processes and their parameterizations must be adequate (Chamberlain and Stucchi 2007). The four post-deposit processes discussed are resuspension, leaching, decay, and consumption by wild organisms.

Resuspension and subsequent deposition are processes by which deposited substances are eroded from the bottom, are transported, and re-deposited in a different location. When the bottom shear stress reaches critical values, these processes can occur; the critical shear stress values depend on the bottom sediment texture and the characteristics of the deposit (Law et al. 2016) . These processes have been identified as having a very large impact on the concentration of deposited substances. For example, DEPOMOD predictions of carbon deposition rates are known to be very sensitive to resuspension; when the model's resuspension module is activated, the carbon deposits are often transported out of the model domain (Chamberlain and Stucchi 2007; Chang et al. 2012) and because of this sensitivity it is generally acknowledged that the resuspension module should not be activated until the module is updated and re-evaluated.

Leaching is a process that removes soluble constituents from a carrier substance into a liquid. The leaching of drug ingredients from feed and feces is not well documented. However, results from experiments estimating the leaching of carbon and nitrogen have shown that up to 22% of the carbon and 26% of the nitrogen in feces is leached out within 5 min after the feces are released into the environment and that leaching persists for about 4 h after release (Chen et al. 2003).

Decay is the in-situ reduction in concentration of a substance and the decay rate is expressed as a half-life. A half-life is the time that it takes for a quantity of a chemical to reduce to half of its initial amount. To reduce the initial amount of a substance to <1% of the initial amount will take seven half-lives. If the decay time is 30 d, then it will take 210 d to reduce the released amount to <1%. Decay times also depend on the surrounding environment and experimental lab studies may not be representative of the conditions for a deposited substance. Understanding of the different in-situ decay times for each released substance may alter long-term predictions of impacts.

The quantity of feed and feces eaten by wild organisms has been recognized as a potential process that contributes to the estimation of the amount of material that is deposited and remains on the seabed (Gowen and Bradbury 1987; Cromey and Black 2005). Unfortunately, the relative importance of this process is not well known and little to no information is available to quantify this loss rate (Hevia et al. 1996).

REVIEW OF MODELS

Relatively little literature exists concerning the modelling and prediction of benthic ecosystem or environmental exposures to in-feed drugs used by finfish aquaculture operations, since this field of modelling is in an early stage of development (Rico et al. 2019). DEPOMOD (SEPA 2005) has been widely used by the Scottish aquaculture industry for assessing benthic impact of in-feed drugs and ensuring compliance with environmental standards. In Canada a few efforts have been made to model the exposure of ecosystem components to bath pesticides (Page et al. 2015) and no efforts have been made to model the exposure to in-feed drugs. Gowen and Bradbury (1987) developed the first models for predicting the exposure to and impacts of benthic organic loading and is the basis of modern deposition models (Black et al. 2016; Falconer et al. 2016). Although benthic organic deposition models are not focused on veterinary medicines, they are of some relevance since they deal with the deposition of waste feed and feces which contain the active drug ingredient. The following review makes an effort to summarize the development of modelling capabilities related to benthic organic deposition models and to identify the assumptions that are made for each model.

The underlying assumption of all depositional models is the distance, d, travelled by the modelled agent, e.g., carbon or drug, can be estimated as

$$d = ut + R \tag{7}$$

where u is the water velocity and can include the effect of turbulent dispersion, t is the time needed for the drug to be deposited on the sea floor, and R is any subsequent remobilization. Remobilization includes processes that cause the deposed material to move once it has been deposited on the seabed, for example, resuspension and movement due to the ingestion by wild organisms. All models use some variant of (7). The complexity of depositional models has increased, as the availability of computer power has increased and knowledge of the processes and parameter values of relevance has expanded. The initial models were relatively simple and assumed parameters and variables were constant. More recent models include variation in many of the parameters and variables. For example, models may include spatial and temporal variation in the initial position of the particles and the advective and turbulence fields, and variations in the sinking rates due to specification of their frequency distributions. They may also include remobilization that is constant, spatially and temporally variable, or physically, chemically and biologically mediated. For drug deposition, models of exposure intensity may also include drug decay and leaching.

Models estimating the scale, i.e., the area covered and location of benthic exposure to the active ingredients, apply the above equation to the spatial and temporal domain defining the release. The intensity of the deposition is determined by scaling the spatial pattern of distribution by the quantity of drug active ingredient administered. The persistence of the deposited active ingredient is estimated by applying rates of degradation, resuspension and remobilization to the original deposit. Temporal variation in the exposures is estimated by repeating the above for multiply releases and summing the results over time for each area of deposition.

The model of Hagino was one of the earliest models of waste discharge from fish farms operating in Japan. The original article (Hagino 1977, as cited in Gowen et al.1994) is in Japanese but a summary of his model is given in Gowen et al. (1994). This model used estimates of mean water current speed and direction and a normal probability distribution of measured sinking speeds for released waste particles. The model produced results that compared favourably to observed field observations (Gowen et al. 1994).

Another early effort by Gowen and Bradbury (1987) modelled the zone and intensity of environmental impact associated with the deposit of fish food pellets and fish feces from fish farming. The model, known as the Gowen model, is a variant of (7). Remobilization processes are ignored, i.e., $R = 0$, and the time, t, for the drug to be deposited to the seabed is a function of the sinking rate (W_s) of the particles being released and the depth of the water (H) in the vicinity of the release location

$$t = \frac{H}{W_s} \tag{8}$$

Using (8), equation (7) becomes

$$d = \frac{uH}{W_s} \tag{9}$$

Implementations of the Gowen model range from simple to complex. Simple models tend to use constant parameter values and limited, but potentially useful, output (Silvert and Sowles 1996; Chang et al. 2012). Comparisons between outputs from the simple models and measurements of benthic impact have shown reasonable agreement (Hevia et al. 1996). These relatively simple models are also sufficient to indicate that near field exposure is dominated by fluxes associated with feed pellets and far-field exposures are dominated by fluxes associated with feces (Gowen and Bradbury 1987). An example of a simple application of the Gowen model is the model for deriving circular zones of impact around net-pens in some southwestern New Brunswick salmon farms (Chang et al. 2012). Equation (9) was used to estimate horizontal dispersion with H equal to the average water depth at each site, u equal to the median and maximum current speeds at mid-depth during current meter deployments (minimum 35 d), and W_s equal to 11.0 and 3.2 cm s^{-1} for waste food and feces, respectively, (the default values in DEPOMOD; see below). Predicted zones of exposure were illustrated using GIS software. The combined zones for all net-pens at a farm produced the overall zone of impact for the farm.

Since their development, it has been recognized that the simple models make many assumptions that may or may not be reasonable in any particular circumstance. Hence, efforts have been made to enhance the simple models. Further development of the Gowen model has focused on improving the representation of input parameters, such as including multiple particle release locations; implementing spatial variation in water depth; using measured or inferred spatial (vertical and horizontal) and temporal variations in the water current; using ranges in particle sinking rates; and including resuspension dynamics (Gowen and Bradbury 1987; Silvert 1992; Gowen et al. 1994; Hevia et al. 1996; Gillibrand and Turrell 1997; Cromey et al. 2002; Stucchi et al. 2005; Black et al. 2016). These enhancements have been associated with the increased ability to record time series of water currents at one or more depths. The spatial variations in the currents have been inferred from relatively simple relationships.

Gowen et al. (1989) modified the Gowen model by incorporating temporal variability in currents using hourly mean current velocities from one current meter location at one depth. Hunter et al. (2006) used a simple waste spread model to predict the zones of impact of salmon farms in Scotland using current speeds and directions measured at regular time intervals. Hevia et al. (1996) included spatial variation in the water depth and current by assuming a power relationship which depended on depth for the vertical variation of the current. The Fox model (Gowen et al. 1994) was based on a USEPA sewage outfall model and used a time series of current speed and direction recorded from a single depth, spatial variation in water depth, multiple sizes and sinking rates of particles, and post-depositional decomposition of carbon. Gillibrand et al. (2002) modified the Gowen model for the purpose of assessing the cumulative impact of all farms within a Scottish loch, and to then assess all Scottish sea lochs where fish farming was occurring. Since current meter data were not available for all farm sites, this model estimated the average current speeds at each site, based on calculated tidal current amplitudes but included turbulent diffusion. Stucchi et al. (2005) used a similar concept to Gillibrand et al. (2002) but used measured current velocities. Silvert (1992, 1994) included estimates of feed and feces sinking rates and a model of fish growth to estimate releases of waste feed and feces.

Recently, more sophisticated models have emerged. These models are discussed below and use current meter data as the input velocity field and have additional features such as resuspension, i.e., $R \neq 0$ in (7), and the effects of net-pen movement.

DEPOMOD, a commercially available model originally developed for use at Scottish salmon farms (Cromey et al. 2002), has been the most published and widely used benthic deposition model for salmon aquaculture (Keeley et al. 2013). DEPOMOD includes modules for estimating waste production. Version 2 of this model has been in use since 2000. The model uses detailed water depths and farm net-pen dimensions and positions. Lagrangian particle tracking using current velocity from a single location is used to calculate the movement of the waste feed and feces before they settle on the seabed. The particle tracking module requires several data inputs: the food input rate per net-pen; food wastage rates; food digestibility, carbon content, and water content; carbon content of feces; sinking rates of waste particles (food and feces), as either single values or normal distributions; and current velocity data from a single location. The model also includes a resuspension module.

Variants of DEPOMOD have been developed for use with other species and geographic areas. CODMOD (Cromey et al. 2009) has been developed for cod farming and MERAMOD (Cromey et al. 2012) has been developed for sea bream and sea bass farming in the Mediterranean Sea. Cromey et al. (2002) noted some caveats with the use of DEPOMOD. The model is unsuitable for sites with steeply sloping water depths and sites with coarse sediments susceptible to wind-wave resuspension. The model does not include net-pen movement or spatial (horizontal) variability in currents.

DEPOMOD has been used by regulators to predict benthic impacts of proposed salmon farms in Scotland (SEPA 2005) and many other fish farming areas worldwide (DFO 2005). In Canada, this includes BC (Chamberlain et al. 2005) and Atlantic Canada (DFO 2009, 2011, 2012, 2013, 2014). It should be noted that the DFO (2014) report on impacts of salmon farming on the south coast of the Island of Newfoundland suggested that DEPOMOD may not be appropriate for hard bottom sites such as those in that region, as had been noted by the model developers (Cromey et al. 2002). DEPOMOD also forms the basis of the benthic module in the AquaModel software (O'Brien et al. 2011), which has been applied to various fish farming areas and species around the world. Another commercially available model is ORGANIX (Cubillo et al. 2016).

DEPOMOD also predicts concentrations of deposited in-feed drugs consented for use by the Scottish Environment Protection Agency (SEPA) and has been widely used in Scotland since 2005. At the time of development, two in-feed drugs were consented for use: emamectin benzoate and teflubenzuron. The predicted amount of drug deposited on the seabed is calculated using the predicted waste feed and feces depositions and the amount of drug contained in the deposited material. The predicted concentrations are compared against environmental standards set by SEPA. Since DEPOMOD provides predictions in mass per surface area and environmental standards are given in mass of chemical per mass of sediment, a conversion relationship is used that assumes the material is deposited over a sediment depth of 5 cm and the sediment density is constant. Results are used in SEPA's consenting process for in-feed drug use (SEPA 2005).

A new version of DEPOMOD, NewDEPOMOD (SAMS 2020), has recently been developed (version 1.1 was released in April 2018). NewDEPOMOD includes: an improved resuspension process; a redesigned user interface using new file formats for water depths, flow, and discharges; improved predictions at exposed sites; a simple user interface to generate models of farms using standard scenarios; and production of conservative estimates of holding capacity of proposed sites that can be tuned using data collected once a farm begins operating (Black et al. 2016). NewDEPOMOD can use water current data collected by a meter deployment, but also has the capacity to use spatially-variable water current data from a hydrodynamic model. Guidelines for the use of NewDEPOMOD in Scotland can be found in SEPA (2019); see also (Black et al. 2016).

While NewDEPOMOD has many improvements, it was stated in the final report of NewDEPOMOD by The Scottish Association for Marine Science (Black et al. 2016) that “there was no single configuration of parameters that could be considered to decisively provide good, spatially accurate fits, to the empirical data across all sites. These experiments did show that the model can produce approximately ‘correct’ (relative to the empirical data) magnitudes of impact, however, if not the precise seabed positions of these impacts.”

Two other models that use current meter data as input are a GIS-based model by Corner et al. (2006) and the KK3D model (Jusup et al. 2007). Although not as widely used as DEPOMOD, they have some interesting features. Corner et al. (2006) developed a model that included a dispersion module developed in the IDRISI32 GIS environment. Model input is similar to that of DEPOMOD: detailed water depths (from nautical charts); net-pen dimensions and locations; feeding rate per net-pen; carbon and water content of food; food wastage rate; and food and fecal sinking rates. For food and feces, sinking rates were selected randomly from an assumed normal distribution with specified mean and standard deviation. This model also included the effects of net-pen movement. This GIS-based model has further evolved into the Cage Aquaculture Particulate Output Transport (CAPOT) model (Falconer et al. 2016).

The KK3D model (Jusup et al. 2007) couples current velocity data with a Lagrangian particle tracking model to predict benthic carbon loading from fish farms. The model is based on stochastic differential equations for particle transport consistent with the semi-empirical advection/diffusion equation, applied to measured current velocity data. The model does not include resuspension, but does determine the probability of whether a settled particle will remain motionless on the seabed or will move again. The model can also be used to examine the effects of variable depth. The KK3D model has been used for environmental impact assessments of fish farms in Croatia (Jusup et al. 2007).

A major concern with models using measured current data is that data from just one location are usually used and hence do not account for horizontal spatial variability in current velocities. Using data from different current meter records obtained from the same farm site, Chang et al. (2012) found the exposure area was relatively insensitive to the dataset used and that detailed estimates of the deposition areas were consistent with the simple estimates, although the distribution of organic carbon deposition varied with the use of different current meter records. This indicates that models based on current data from a single location can give useful order of magnitude estimates but if more details are required then the model may need to take into account spatial variability of currents. Vertical variability can be measured using an acoustic Doppler current profiler or by deploying current meters at various depths at the same location. However, to measure horizontal variability adequately would usually require deployment of meters at several locations simultaneously, which is often not feasible. A way of overcoming this, especially where available current velocity data are limited, is to use results of a hydrodynamic model, which can predict variations in velocity over the entire area where particles are expected to spread.

Several modelling efforts have incorporated the outputs from hydrodynamic water circulation models in an effort to improve the spatial and temporal resolution of the water current information used in estimating exposure zones. These efforts have benefitted greatly from the improvements in the availability and affordability of computer power that have been made in the past decade or so. Circulation models, especially fully baroclinic models forced with spatially and temporally varying atmospheric, oceanographic, and river runoff inputs, are now able to estimate water currents on spatial and temporal scales appropriate for the task of estimating the transport, dispersal, spread, and deposition of discharges from fish farms, i.e., horizontal resolutions of order 10 m, vertical resolutions of order 1 m and temporal resolutions of order minutes (Nudds et al. 2020) but implementation at these scales are not yet readily available.

Many circulation models have been used to predict benthic deposition from a fish farm. The typical strategy is to use a hydrodynamic model to predict the temporally and spatially varying current field and a particle tracking model that uses the currents to predict the movement of waste feed and feces being released from the fish farm. There have been several models developed specifically for aquaculture: a model for tuna farming in Japan (Kishi et al. 1994), AWATS (Aquaculture Waste Transport Simulator) developed by Dudley et al. (2000), and MAMS (Modular Aquaculture Modelling System) developed by Carswell and Chandler (2001). There have also been several studies that have used existing models that are not necessarily specific to aquaculture. The coupled POM (Princeton Ocean Model)-LAMP3D (a particle tracking model) model was used by Doglioli et al. (2004). Tironi et al. (2010) used the hydrodynamics and particle tracking modules within the open-source MOHID Water Modelling System to predict waste deposition from salmon farming in Chile. Ali et al. (2011) developed a benthic deposition model using the Bergen Ocean Model (BOM) with a particle tracking model. A far-field model (for a loch or bay) was developed by Symonds (2011) using Delft3D. Bannister et al. (2016) coupled the Regional Ocean Model System (ROMS), a 3D circulation model, with a Lagrangian diffusion model to predict waste particle spread from a salmon farm in a Norwegian fjord. Broch et al. (2017) used SINMOD, a 3D hydrodynamic-ecological model system, to simulate current velocities and DREAM (Dose-related Risk and Effects Assessment Model), a 3D Lagrangian particle tracking model based on a model originally developed for predicting impacts of drilling mud, to simulate waste particle distributions from fish farms in Norway. NewDEPOMOD has the ability to input and use current fields generated from a hydrodynamic model (SAMS 2021).

Although it is generally believed that these models provide more representative estimates of spatial variation in water currents than current meter records, care must be made to ensure that model results are validated in the area of interest. To accurately model the circulation near fish farms, hydrodynamic models will need a high-resolution grid due to the small scales associated with the farms. Additionally, the effects of the fish farm may need to be incorporated into the model as both field studies (Fredriksson et al. 2006) and modelling studies (Helsley and Kim 2005; Venayagamoorthy et al. 2011; Wu et al. 2014) have shown that the presence of fish net-pens impacts the direction and speed of local currents. Accurately modelling the impact of the fish net-pens on the surrounding flow is challenging: very small scale model grid resolution is required; there is variability in farm layouts; there are variations in the drag associated with net mesh size, bio-fouling, stocking density, and net-pen size. Also, there are technical challenges associated with measuring currents in close proximity to farms, which makes collecting validation data difficult.

Additionally, even with good predictions of the current field, it remains challenging to simulate the trajectories of particles, i.e., the transport and dispersal of particles, for long durations since even small errors can quickly accumulate to give inaccurate particle trajectory predictions. These errors are perhaps less likely to be problematic for the dispersion of waste feed which settles relatively quickly, but, depending on local current conditions and water depths, the dispersion of feces may be sensitive to this error accumulation.

Finally, even if the models are technically sufficient for the task of estimating exposure from a physical perspective, the outputs from the models are only as good as the inputs. The input needs for accurately modelling the deposition and exposure to drug active ingredients include sufficiently resolved inputs that force the water circulation for times and locations of relevance to the scenario being modelling, accurate specification of release characteristics such as drug treatment times, locations, amounts and treatment frequencies, and sufficient knowledge of the chemical properties of the active ingredients of relevance to their environmental behaviour in marine coastal systems.

MODEL SENSITIVITIES

Few models to date have thoroughly evaluated the sensitivity of their outputs to the required inputs. Most models have focused on the incorporation of additional processes and higher resolutions of processes in an effort to improve model estimates of the exposure and impact of aquaculture releases. However, although inclusion of more processes does help make the models more credible, the results are, at best, within an order of magnitude of observations (Black et al. 2016).

Ultimately model evaluations require comparison between model results and empirical data. Unfortunately, data gathering is relatively expensive and hence these evaluations are not conducted as often as perhaps they should be. Hence, the accuracy of model outputs is often unknown, and users can be left uncertain as to how to interpret and what weight to assign to the outputs. The allocation of significant resources and expertise may be required to improve precision of model output, especially in the case of a hydrodynamic model. For example, to double the spatial resolution and precision (i.e., 100 m grid reduced to 50 m) of an FVCOM model results in a factor of 8 increase in the required computation and hence an eight-fold increase in computing cost to run the model. Therefore, it would seem prudent to initially triage whether this investment is likely to provide significantly better predictions.

A first principle consideration may help indicate if the improvement to displacement estimates would be sufficient to warrant the effort. The time spent by medicated feed and feces in the water column ranges from minutes to hours (Table 3) and the displacement is a linear function of the current speed (see equation (7)). Hence, the percent change in the displacement will be the same as the percent change in the velocity estimate, for example a 50% change in the current will result in a 50% change in the displacement estimate. If the changes are not sufficient to change the advice, management decision, or action that the exposure estimates were supporting, then perhaps developing models with more detail or precision is not necessary.

There are many parameters and processes important to estimating the exposure of ecosystem components to released in-feed pesticides and drugs: water depths, feed wastage rate, post-depositional resuspension, currents, sinking rates, chemical partitioning, and chemical decay. Simple models may only include a subset of these processes. For example, resuspension and decay are typically not included in simple models (Gowen and Bradbury 1987; Gowen et al. 1994; Hevia et al. 1996; Gillibrand and Turrell 1997). Even when included, many of these processes and parameterizations remain ill defined and as a result models continue to have a high degree of uncertainty associated with them (Gillibrand et al. 2002).

Estimates of water depths in fish farming areas are often required on horizontal scales of order 10 m. Modern bathymetric technology such as multibeam acoustic sounding systems is able to resolve the horizontal scales at the desired resolutions. However, the currently available data may not fully cover all areas of interest.

Estimates of particle sinking rates are still relatively sparse and exposure models are known to be sensitive to assumptions and parameterizations concerning these rates (Bannister et al. 2016).

Model results are sensitive to assumptions made about resuspension (Cromey et al. 2002; Chang et al. 2012; Chang et al. 2014). Resuspension depends on many factors including current speeds, bottom type, and properties of the deposited material. Critical shear stress values are dependent on bottom type and properties of the deposited material and thus model results are sensitive to how well these are parameterized. Furthermore, resuspension processes operate on time scales of minutes. Thus, models that include resuspension processes must consider using currents estimated on short time scales since currents averaged over many days, weeks and months lack the short-term variability required for estimating resuspension (Findlay and Watling 1994). In addition, in some areas, resuspension might be dominated by waves and current dynamics associated with storm events. These events may not be captured by measurements.

Accuracy of depositional model results rely on accurate input of local currents. Simple models often use measured currents from a single location. Currents can vary significantly in time and space. Although the vertical variation in the current field is usually included, the horizontal variation is not often taken into account, which can significantly impact the precision of the predictions. Furthermore, the duration of current meter records used are often short, containing approximately a one-month record, and do not take into account the seasonal variability of the current field. These simplifications may miss events and structures that have strong influences on the exposure estimates (Gowen et al. 1994).

Estimates of the uncertainty associated with outputs from simple models can be made if the input values are considered as mean values or typical values for a specific scenario. An estimate of upper or lower limits bracketing a displacement prediction can be made using lower and upper limits of the water velocity (U_{min} and U_{max}) and sinking time (T_{min} and T_{max}), which depends on upper and lower values of water depth and sinking rate. These upper and lower values can be represented as multipliers of the mean values (i.e., $U_{min} = \alpha_l \overline{U}$, $U_{max} = \alpha_u \overline{U}$, $T_{min} = \beta_l \overline{T}$, and $T_{max} = \beta_l \overline{T}$) so that the lower limit is estimated as $D_l = U_{min} T_{min} = \alpha_l \overline{U} \beta_l \overline{T} = \alpha_l \beta_l \overline{U}\overline{T}$ and the upper limit is estimated as $D_u = U_{max} T_{max} = \alpha_u \overline{U} \beta_u \overline{T} = \alpha_u \beta_u \overline{U}\overline{T}$. The estimate of the displacement range is $D_u - D_l$ and the estimate of the displacement limits is $D_l < \overline{D} < D_u$.

As an example, if $\overline{U} = 0.1$ m·s^{-1}, $\alpha_l = 0.1$ and $\alpha_u = 10$, then U_{min} is 0.01 m·s^{-1} and U_{max} is 1 m·s^{-1}; values that are not unreasonable for water current in a macrotidal area. Furthermore if $\overline{T} = 1\,000$ s, $\beta_l = 0.3$, $\beta_l = 5$, then $T_{min} = 300$ s and $T_{max} = 5\,000$ s. The mean displacement, $\overline{D}$, is 100 m with the lower and upper limits being $D_l = 3$ m and $D_u = 5\,000$ m, respectively, and the displacement range is approximately 5 000 m. The above extremes in sinking time can arise from different combinations of depths and sinking rates, for example a water depth of 50 m which is typical for coastal fish farms, an intermediate sinking rate of 5 cm·s^{-1}, a relatively high particle sinking rate of 15 cm·s^{-1} (relevant to waste feed), and a relatively low sinking rate of 1 cm·s^{-1} (relevant to feces).

The above calculations indicate that the variability around an estimate of displacement is potentially very large and that displacement estimates based on mean or typical values can underestimate the potential maximum displacement by an order of magnitude.

More precise estimates can potentially be obtained using results from a calibrated and validated hydrodynamic model. Advantages of using currents predicted from a hydrodynamic model are that they vary spatially and temporally and can be run over time-periods that take into account seasonal variations. The use of hydrodynamic models for predicting deposition can provide detailed estimates of the footprint and the concentrations (see REVIEW OF MODELS Section for references). When circulation models are used to determine local current fields, evaluation of the accuracy of model estimates of spatial variation in current magnitude, direction and phasing is important (Page et al. 2015). It is critical that both temporal and spatial variations are accurately simulated if the modelled transport, dispersal, and resulting trajectories of released substances are to be accurate. Unfortunately, it is difficult to evaluate the accuracy of the spatial variations. Deployment of current meters at many locations within the spatial and temporal domain of interest is still expensive and largely impractical. The gathering of vertical current profiles along strategically placed horizontal transects by mounting acoustic current meters and GPS recording systems on vessels or remotely controlled vehicles is one approach to improving the evaluation of circulation models on the scales of relevance to fish farms. The use of GPS tracked drifters is also becoming more cost effective and is beginning to be used to help evaluate trajectory models (Page et al. 2015; Nudds et al. 2020). Although dye is still an effective tracer, it is not often used due to the difficulty in tracking and measuring the dye concentrations over the spatial and temporal scales of interest. Both drifters and dye suffer from the practical challenges of collecting data from numerous release scenarios and the impractically of tracking patches over long time periods. Comparisons between drifter tracks and dye dispersal patterns indicate that well calibrated models can perform reasonably well over short time periods, but deviations from observations increase rapidly beyond a few hours (Page et al. 2015; Nudds et al. 2020).

Even with a well-calibrated hydrodynamic model, care must be taken in interpreting results as model output accuracies are not always known. Furthermore, as with simple models, neglecting processes can impact how well the model results represent reality. It is known that the presence of net-pens and net-pen arrays affects current speeds and directions in and around the fish farm (Fredriksson et al. 2006; Venayagamoorthy et al. 2011; Wu et al. 2014). These effects can persist for distances of several multiples (2 – 10) of the net-pen and net-pen array length scale (Helsley and Kim 2005). As an example of an estimate of the affected length scales, a net-pen with a diameter of 30 m impacts the water velocity (current speed and direction) for distances of 60 to 300 m downstream of the net-pen. A net-pen array that has a length scale of 200 m perpendicular to the flow influences the water current velocity for distances of 400 m or greater downstream from the farm. Most hydrodynamic models do not include these effects. Also, hydrodynamic models evaluated against current measurements made before the presence of the fish farm and within several length scales of the net-pens may not provide a good evaluation of the model performance for the situation of interest. This consideration could be important in situations where the particles spend the majority of their sinking time in the three-dimensional envelope of the water influenced by the presence of the net-pens.

In summary, the uncertainty (or accuracy) of exposure estimates can be reduced (or increased) by improving the estimates of water current, water depths, resuspension, and sinking rates. Progress in this direction has focused on the incorporation of spatial and temporal variation in these three variables into models. An equally important component of the improvement of the projected trajectory involves the acquisition of observations of sufficient resolution (spatially and temporally) and accuracy since these are the basis for model calibrations and evaluations. A perspective that may help determine the suitability of exposure models is to define the resolution and accuracy needs of regulators, determine what modelling approaches can satisfy these needs and determine whether it is presently cost effective to improve models beyond the foreseeable needs of the regulators.

MODELS FOR POTENTIAL PRACTICAL APPLICATION

Potential Exposure Zone (PEZ)

A simple variant of the Gowen model can be used to estimate the potential exposure zone (PEZ) associated with the release of drugs in net-pen aquaculture. The PEZ model is used to provide upper bounds on the expected exposure area. To this end, estimates of the maximum current speed, the maximum depth, and minimum sinking rates are used in equation (9). The model indicates that the displacement associated with the release of medicated feed has a length scale of order 1 – 1000 m for a range of water depths and current speeds typical of fish farming locations (Table 3). The displacement length scales associated with feces are larger and of order 1 – 10000 m (Table 3). These displacement length scales can be combined with the dimensions of net-pens or net-pen arrays to give an order of magnitude estimate of the size of a benthic zone of exposure to medicated feed. Similar calculations have been to set the dimensions of model grids used to provide more detailed estimates of waste deposition (Hevia et al. 1996).

The PEZ model is a useful tool in the screening process for site assessments. It should be emphasized, however, that a footprint delineated by a PEZ encompasses the actual benthic exposure regions to in-feed drugs. This does not imply that all areas within the PEZ will be exposed. If there are areas of potential concern within a calculated PEZ, then a more sophisticated model might be needed to assess the potential impact.

The potential area of exposure represents the precautionary spatial domain within which the deposition of discharged drug will occur. The PEZ boundary is calculated as the maximum horizontal water velocity times the maximum time needed for the discharged particle type to settle to the seabed. The PEZ does not take current direction into consideration and does not consider the frequency distributions of current speeds or particle sinking rates. The PEZ will not provide an accurate estimate of the actual deposition area and hence should not be used to estimate deposition concentration.

Okubo-Based Deposition Model

One of the limitations of the benthic PEZ model is that it does not predict concentration. The Okubo relationship (Okubo 1971, 1974) can be used to develop a simple screening model that complements the PEZ and helps illustrate the advection, dispersal, deposition locations on the seafloor, and concentration within the deposit of an in-feed drug discharge. The model estimates a mean concentration associated with an individual discharge event from a single net-pen. The model assumes the discharged particles are dispersed horizontally according to the Okubo relationship, are displaced horizontally by a representation of the ambient current and are moved vertically by the particle sinking rate. The model estimates the quantity of active ingredient in the waste feed and feces discharged in association with each feeding event. The quantity of active ingredient in the waste feed is estimated as the product of the quantity of feed added to the net-pen, the concentration of the active ingredient in the feed, and the proportion of feed not ingested (i.e., wasted). The amount of active ingredient in the feces is divided into two pathways: the quantity of active ingredient ingested times the proportion not absorbed; and the remainder of the active ingredient that is assumed to be absorbed and egested or excreted over time as it is processed by the fish. The model allows specification of multiple discharge times corresponding to the assumed time of day when the fish are fed. The timing of fecal discharges is assumed to be the feeding time(s) plus a delay that represents the time for the food to be processed through the fish's digestive system (Figure 2). The model estimates a separate deposition location and area for each discharge event. The model can be used to generate a precautionary estimate of deposition by assuming most or all of the ingested active ingredient is not absorbed and hence is egested in a single fecal discharge event.

The model assumes:

- a spatially and temporally constant water depth,

- an ambient horizontal water current, (U, V), composed of a spatially and temporally constant mean current, $(U_{\text{mean}}, V_{\text{mean}})$, and a spatially constant and temporally varying tidal current, $(U_{\text{amp}}, V_{\text{amp}})$, (Figure 2),
- a horizontal dispersal rate that is given by the Lawrence et al. (1995) parameterization of the Okubo (1971, 1974) dispersion relationship,
- a constant sinking rate for each discharged particle type,
- an instantaneous discharge of particles containing the drug active ingredient, and
- an area over which the medicated feed is initially distributed (usually assumed to be the area of the net-pen).

The horizontal displacement of discharges is the integral of the current velocity during the time period between discharge and deposition on the seabed. The model is run separately for waste feed and fish feces.

This simple model illustrates (Figure 3) that discharges from individual feeding events are transported to different locations on the seabed due to being released into a current regime that varies over time (Figure 2), that some degree of overlap between the releases may occur, and that deposition might not be under the net-pen when the displacement associated with the mean current speed exceeds that associated with the tidal current. It also illustrates that the individual deposition areas are smaller than the PEZ area.

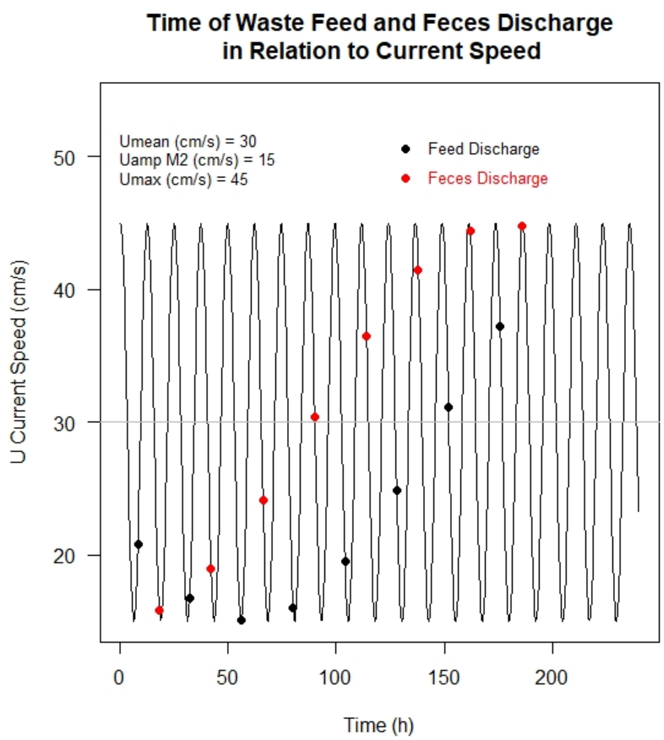
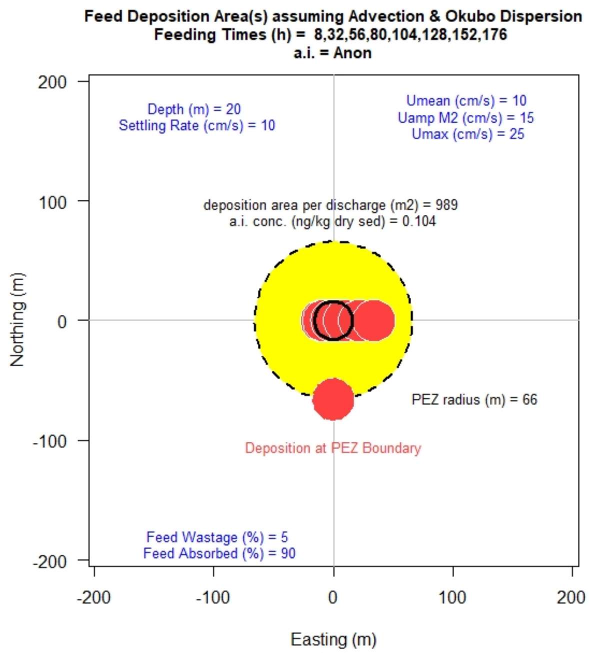


Figure 2. Time series of the U component of water current (V component assumed to be 0) and times when waste feed and fish feces are released in association with seven in-feed medicine treatment events. $U = U_{mean}, + U_{amp}\cos(2\pi t/T_{M2})$) where T_{M2} is the M2 tidal period. For illustrative purposes, feeding events are 24 hours apart and the fecal discharge is assumed to be 10 hours after each feeding event.

The concentration of active ingredient in the deposition areas will vary with sinking time, which is determined by the water depth and the particle sinking rate, and the Okubo relationship.

Screening estimates of maximum concentrations could be approximated as the concentration within each deposition area times the number of overlaps. A precautionary worst-case scenario can be estimated by assuming all discharges occur at the same time; this is equivalent to assuming all discharges are deposited in the same location and over the same area and that all active ingredient is discharged at once. In effect the concentration can be estimated as the deposit concentration associated with one discharge event times the number of discharge events. This is similar to the approach used by Health Canada in their bath pesticide assessments (Health Canada 2017).

In principle the model can be expanded to include multiple net-pens, a radially symmetrical normal distribution of concentration, spatially varying water currents, net-pen specific discharge quantities, and discharge times. Estimates for multiple net-pens can be obtained by combining the outputs from single net-pen calculations. Perhaps a preferred approach is to use a fully integrated model and use the simple model to help understand, check and interpret the output from the more integrated model.



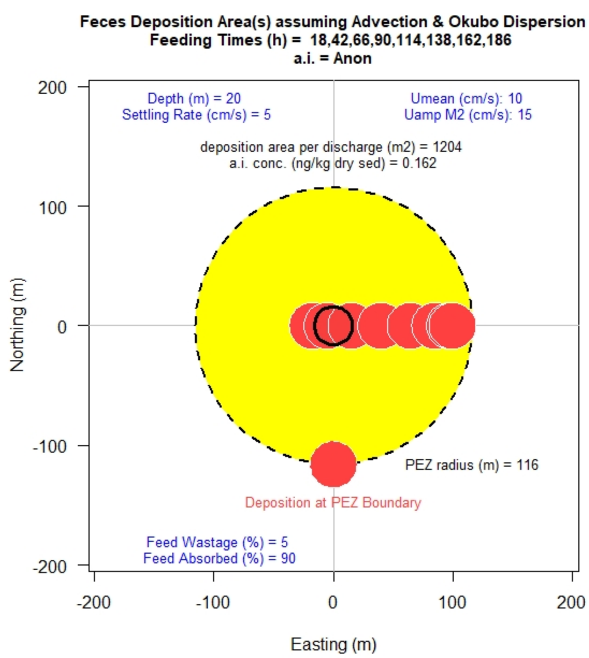


Figure 3. Illustrations showing locations and sizes of seabed deposition areas for an anonymous active ingredient (i.e. a.i.= Anon) in waste feed (top) and un-absorbed feces (bottom) discharged from seven feeding events administered at the single net-pen (central black circle) at hourly intervals in a tidal environment. The potential exposure zones (PEZ) for each discharge type are shown (dashed black circle). The deposition circle straddling the PEZ boundary (at the bottom of the figure) illustrates a deposition area that would be associated with a discharge that was translated horizontally at the maximum current speed; this circle is not associated with the seven other circles. The location of the circle is not representative of the direction of the deposition, it is only meant to illustrate that the center of the deposit would be somewhere on the PEZ outline. For the cases shown in the top and bottom panels, the concentrations of a.i. in all the red circles within a given panel are the same and are not representative of any particular a.i. Overlapping circles suggest the potential for higher concentrations.

Partitioning

Proper calculation of discharge concentrations requires knowledge of the partitioning pathways of the treatment drug. The partitioning concepts are discussed in the Partitioning of Active Ingredient section. The total amount of drug in the environment varies with time after treatment due to several factors: the egestion, excretion, and metabolic transformation of the absorbed drug and the continuous time decay of the drug and its metabolites once in the environment. Here the temporal variation of the amount of drug in each partition is examined for a treatment scenario using emamectin benzoate. The amount of drug in each partition is calculated using equations (1) through (6). Since the absorbed emamectin benzoate is released over time primarily in the feces (Benson et al. 2017), contributions through urine are ignored. Also, it is assumed that the absorbed emamectin benzoate is excreted continuously in the feces with an excretion half-life of t_e; in reality this excretion would likely occur sporadically in time. Once on the seabed, the emamectin benzoate is assumed to decay exponentially with a half-life of t_d. A schematic of the partitioning model is shown in Figure 1 and the values used are given in Table 4. The results were calculated using a stocking density of 20 kg·m^{-3}, a circular fish net-pen with a 100 m perimeter and 10 m depth, a total biomass of fish of 159155 kg, a feeding rate of 0.5%, and a concentration of emamectin benzoate in the feed of 10 mg·kg^{-1}. In addition, an excretion half-life of 36 d (SEPA 2005) was used. Once in the environment, the drug was assumed to decay exponentially with a half-life of 250 d (SEPA 2019).

Results of the partitioning model for both a single treatment and a seven-day treatment regime are shown in Figure 4. Waste feed is immediately deposited on the seabed and starts to decay. The largest portion of the released drug comes from the slow release of the absorbed drug through the feces. The amount of drug in the environment from this partition reaches a maximum 118 days post-release (SEPA 2005). The concentrations associated with this pathway are small since the amount released at any given time is small. However, the released drug can accumulate in the seabed over time and could result in concentrations of concern. Proper assessment of the impact of the drug partitioning requires a link with a deposition concentration model which includes dispersion and sinking rates.

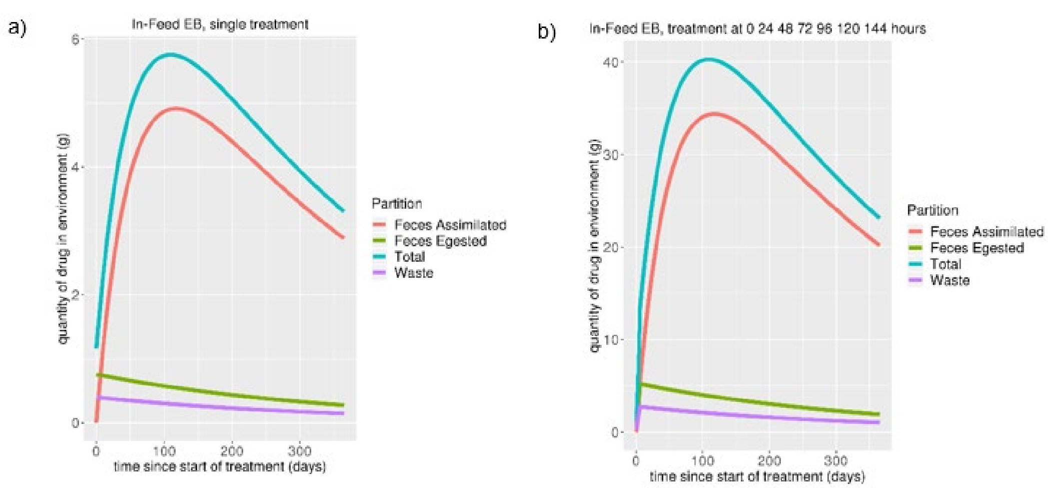


Figure 4. Cumulative quantity of emamectin benzoate in the environment in each partition for a) a single treatment dose and b) seven daily treatments doses using values given in Table 4 with $t_e = 36$ d and $t_d = 250$ d.

APPLICABILITY OF 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 among regions, the particulars of the differences may alter model suitability when considered against the priorities of a region.

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, climates, and purposes across Canada it becomes clear there is not a “one size fits all” solution. 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.

A region that requires a detailed prediction of exposure, might consider a full hydrodynamic model. Although hydrodynamic models can provide detailed information for input into a depositional model, implementing such a model in a new area can be time consuming and expensive. As a result, a hydrodynamic-based depositional model may 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. Furthermore, at the time of writing, hydrodynamic models have not yet been implemented at suitable scales for all areas in Canada where marine finfish aquaculture occurs.

DISCUSSION

The release of chemicals from in-feed drug treatments into the environment follows several pathways. The chemical enters the environment through waste feed, feces, and urine. Both waste feed and feces are eventually deposited on the seabed whereas urine remains in the water and will result in a pelagic impact. This document has only focused on reviewing the state of models for predicting the benthic impact of chemicals released from in-feed drugs, i.e., the chemical contained in the waste feed or feces. Typically, the largest portion of the treatment chemical enters the environment through feces.

Few models have been developed specifically to predict the benthic deposition of in-feed drugs and these range in complexity. Scotland has used the drug deposition model DEPOMOD (SEPA 2005) for regulatory purposes and has recently released new regulations requiring the use of NewDEPOMOD (SAMS 2020) in the licensing of in-feed drug use (SEPA 2019). In Atlantic Canada, the PEZ model is being used in screening of site applications.

In contrast, many models for predicting the deposition of organic waste produced by net-pen fish farms (from waste feed and feces) have been developed. In Canada, a number of organic deposition models have been used but not all models have been assessed for all regions and applications. Many of the underlying assumptions of these models are applicable to models for in-feed drugs. One of the fundamental differences is the concentration of the drug in the feces changes over time. Thus, the ratio of drug to carbon in the feces is not constant and it is not appropriate to simply use a conversion factor to convert carbon deposition amounts to drug deposition amounts. The models of benthic deposition of organic waste must therefore be modified to include the time varying quantity of the drug in the feces as they are released.

The pathways associated with the deposition of chemicals from in-feed drug treatments and their parametrization are often complex and uncertain. Model results are sensitive to the representation of processes and the parameter values used. Furthermore, exact values for the parameterization are unknown and estimates from the literature can vary significantly and be contradictory. For specific applications the required outputs and precision should be known, the precision of the desired model outputs should be estimated, the criteria for assessing the suitability of a model for the application should be established, an assessment of the suitability of available models should be made for each scenario under consideration, and a decision as to which model or models will be used is needed. Unfortunately, the sensitivity of models to variations of their input parameters and variables and the accuracy of model outputs are often not estimated or assessed. Furthermore, the outputs and precision desired by the users of the model results are often not specified. A recent review that focused on models concerning the exposure to, and impacts associated with, veterinary medicines stated that " … it is unclear whether present scientific knowledge … is sufficiently developed and rigorous to represent environmentally relevant conditions in different aquaculture production systems and environments within Europe" (Rico et al. 2019). Additionally, Symonds (2011) and Bannister et al. (2016) have demonstrated that model outputs are sensitive to input parameters such as discharge sinking rates and water currents.

A model should not be used until it has been validated for the application of interest. This requires the collection of empirical data with which to compare model results. For circulation models used to drive the transport, validation of current fields is required. Since currents vary spatially and temporally, it is challenging and expensive to collect sufficient data, both from current meters and Lagrangian drifters, for model comparison. The final output of these models is the amount of drug that settles to the seabed; however, few reported field measurements of drug concentrations in sediments exist, though some monitoring has been conducted for emamectin benzoate in sediments in the vicinity of salmon farms in Canada, Scotland, Norway, and Chile, summarized in Table 5. The results of these studies are sensitive to methods used to collect and analyze the samples and should be interpreted in light of the levels of detection (LODs) and levels of quantification (LOQ) (Table 5). Additionally, observations are collected on spatial scales of 0.1 m and at discrete points in time. Model output is frequently a spatial and temporal average. Averages are calculated over spatial scales of 10s to 100s of meters (the horizontal resolution of the model) and temporal scales of hours, days, or weeks. Matching of model outputs to observations is therefore challenging (SAMS 2005). At best the comparisons between model outputs and observations should be based on averages taken over similar scales. In most cases this means the spatial data needs to be averaged over the spatial scale of the model resolution, although this is not always possible. Of the few validations that have been done (SAMS 2005; Black et al. 2016; Rico et al. 2019) results suggest that the models, at best, give an order of magnitude estimate of seabed drug concentrations, even when input parameters are considered to be representative of the studied scenario.

Models of the environmental deposition of in-feed drugs typically predict benthic concentrations of the chemical. In order to properly infer ecological implications from model results, the predicted concentration must be compared to a specified EQS. One strategy is to allow an impact zone and specify two maximum allowable concentrations, one within and one outside this zone. This is the approach that Scotland has adapted (SEPA 2005, 2019). A 'mixing zone' is applied to each site which defines the area over which certain impacts are considered acceptable. The recently revised SEPA guidelines have new definitions of the mixing zone and new concentration limits, but the concept has not changed. The SEPA 2019 guidelines define the mixing zone as an area equivalent to the area lying within 100 meters of the pens in all directions. Although the area is the same as the previously defined mixing zone (SEPA 2005), the definition is more general and allows for zones that are not symmetrical, allowing the effects of local currents to be taken into account. Two concentration limits are applied: one inside the mixing zone and one at and beyond the mixing zone limit. Applicants for licenses under "The Water Environment (Controlled Activities) (Scotland) Regulations 2011" are expected to use modelling (newDEPOMOD) to demonstrate that potential treatments are likely to be in compliance with the environmental standards (SEPA 2019). In Canada, the zone regulated by the Federal Aquaculture Activity Regulations is the area encompassed by the facility which is defined as the area inside the boundary marked by the net-pen grid anchors. At this time, Canada has not set concentration limits within this zone for in-feed drugs.

How models will be used by decision makers depends on the regulatory goals and the accuracy and precision of the available models. For sufficiently precise models, decision makers could use modelled exposure scenarios to determine if treatments are acceptable. When models are not sufficiently accurate and precise, either because highly accurate precise validated models are not available, or it is deemed they would be neither practical nor cost effective to develop and run, simpler less precise models will need to be used. Less precise models can take many different forms but should have the commonality of being conservative estimates of the exposure. Empirical sampling should be conducted to validate the model predictions and to establish actual exposure characteristics. When precise models are available, the sampling domain should be guided by the predictions. When precise predictions are not available, a more extensive sampling program will be needed to detect the exposure domains and intensities, or decision makers will need to decide if the risk of some degree and extent of potential exposure within the full exposure domain is acceptable.

Our current level of knowledge of the input variables and parameters for in-feed drug models varies considerably. Some variables are well quantified, for example water depths, whereas others are poorly characterized, for example feces sinking rates. Thus, even the simplest models can have a high degree of uncertainty associated with their results. Hence, at present, the main use of models should be to help develop understanding of the dynamics and sensitivity of model outputs to various inputs, parameterizations and assumptions, to help guide environmental sampling designs that will enable evaluation of model outputs and the establishment of model accuracies, and help establish regulatory regimes that are consistent with predictive, environmental, and practical realities.

Table 5. Monitoring data for emamectin benzoate in sediments near marine salmon farms. Values are for emamectin benzoate, except DM = desmethyl metabolite. LOD= Limit of detection; LOQ = Limit of quantification; ND = not detected; n/a = not available; trace = detected, but <LOQ.

Source	Location	Sampling stations	Sampling dates	Sampling time relative to treatment time	LOD ($ng \cdot g^{-1}$)	LOQ ($ng \cdot g^{-1}$)	Max. concentration detected ($ng \cdot g^{-1}$)	Max. distance (from cages) detected
Packer & Mallory (2003)	SWNB	1 farm & 3 control areas	Jun & Dec-02	Pre & 10 weeks post	400*	n/a	ND	ND
Packer & Mallory (2004)	SWNB	1 farm & 3 control areas	Jul-Sep-03	Pre & 1-8 weeks post	50*	n/a	ND	ND
SAMS (2005)	Scotland	1 farm (0-60m) & reference (400 m)**	Apr-02 to Jan-03	Pre & 1-9 months post	0.03 dry wt	1 dry wt	7.38 dry wt	Trace at 60 m & reference stations (400 m)
Telfer et al. (2006)	Scotland	1 farm: 10-100 m from cages & reference (1 km)	Sep-97 to Sep-98	Pre & 1-52 weeks post	0.25 wet wt	0.50 wet wt	2.7 wet wt DM: 2.8 wet wt	mostly ≤ 25m, except at one 100 m station (0.62 $ng \cdot g^{-1}$ wet wt); trace in floc at 1000 m DM: 0.52 $ng \cdot g^{-1}$ wet wt at 100m
Benson et al. (2017): SEPA monitoring data	Scotland	All licensed farms : 0, 25, 100 & 150 m from cages	2001-2016	n/a	n/a	n/a	50.2 dry wt	Mean 1.38 $ng \cdot g^{-1}$ dry wt at 150 m
SEPA (2011)	Scotland	5 farms (0 m) & 4 reference (>500 m)	2009	n/a	0.08 wet wt	0.08 wet wt	1.9-44.0 wet wt	Means ND to 12.5 $ng \cdot g^{-1}$ at reference stations (>500 m)
Bloodworth et al. (2019); SEPA (2018)	Scotland	8 farms: 0 m, far-field (>100 m) & reference (≥500 m)	May-Jun-17	n/a	0.0034 dry wt 0.002 wet wt	n/a	<LOD to 7.58 dry wt	Mean ~0.05 $ng \cdot g^{-1}$ at reference stations (≥500 m)
Langford et al. (2014)	Norway	In the vicinity of 2 farms	2008	2 months post	2 dry wt	n/a	2.4 & 6.5 dry wt	n/a
Tucca et al. (2017)	Chile	1 farm: 0-100 m from cages	Dec-10	5-d post	0.1 dry wt	n/a	14.6 dry wt	9.97 $ng \cdot g^{-1}$ ± 1.7 SE dry wt at 100 m
Ikonomou & Surridge (2013)	BC	1 farm: 0-200 m from cages	n/a	0-4 months post	0.04 wet wt	0.132 wet wt	35 wet wt	n/a

Source	Location	Sampling stations	Sampling dates	Sampling time relative to treatment time	LOD (ng·g^{-1})	LOQ (ng·g^{-1})	Max. concentration detected (ng·g^{-1})	Max. distance (from cages) detected
					DM 0.031 wet wt	DM: 0.083 wet wt		
Hamoutene et al. (2018): flocculent matter	NL	1 fallow farm: 0-160 m from cages 1 active farm: 0-20 m from cages	Sep-Oct-16	n/a	0.00068 dry wt	n/a	0.058 dry wt (fallow) 41.8 dry wt (active)	n/a
DFO (unpublished data)	SWNB	3 farms: 0-~1 km from cages	Nov-17 to Jan-18	Various	n/a	0.21 wet wt DM: 0.17 wet wt	2.2-212.9 wet wt DM: 0.56-69.9 wet wt	Trace or low (0.22-0.61 ng·g^{-1} wet wt) at up to ~1000 m DM: trace at ~500-1000 m

* not clear if these values are for wet weight or dry weight.

** another farm that treated with EB was also sampled in this report, but trace or low levels of EB were detected in most of the pre-treatment and reference samples; the authors concluded that there may have been some contamination of these samples, so the results from that farm have been excluded.

SUMMARY AND CONCLUSIONS

- The pathway of environmental exposure to in-feed drugs includes waste feed, feces, and urine. Details of the distribution of a drug's active ingredient among the different pathways are dependent on the in-feed drug used.
- Environmental deposits and impacts of released waste feed and feces are primarily considered to be benthic, whereas urine impacts are primarily considered to be pelagic. This paper only reviewed models for benthic deposits.
- There are few models for depositions of in-feed drugs from fish farms.
- Models of carbon deposition seem to give reasonable order of magnitude estimates of the scale of near-field deposition. It is unknown how well models estimate far-field deposition. Whether the same perspective holds for drugs is unknown at this time.
- Although models of in-feed drug deposition share many similarities with carbon deposition models, their application to modelling in-feed drug deposition requires the inclusion of drug partitioning dynamics.
- Models range in complexity from predictions based on simple assumptions such as a mean current, a constant water depth, and constant sinking rates for waste feed and feces to detailed predictions based on spatially and temporally varying water depths, spatially and temporally varying current fields, and a range of sinking rates.
- Complex models usually require more inputs and more assumptions than less complex models and therefore, in order to gain confidence in the model outputs, more extensive evaluation and validation for each application should be considered.
- The objectives for model outputs must be specified before the adequacy or sufficiency of model outputs can be assessed.
  - Simple models can give useful results when the objectives only require a bounding of the potential exposure zones or an order of magnitude estimate of exposure extent and intensity.
  - More complex models are needed to give higher spatial and temporal resolution outputs. Care must be taken in the interpretation of the solutions as they do not necessarily result in better estimates than simple models.
- Model estimates of exposure domain and intensity are sensitive to many of the assumptions made in the development of the models. These assumptions include:
  - the choice of distribution and parameterization of fish feed and feces sinking rates,
  - the specification of the partitioning of chemicals between waste feed, feces, urine and gill exchange,
  - the type of flow field used, i.e., a single current meter record or model generated spatially and temporally varying flow field, and
  - the implemented resuspension formulations.
- Models help to develop understanding of the dynamics of exposure processes.
- Models of drug deposition are subject to many sources of uncertainty; for example, the relative proportion of drugs that are released as waste feed, feces, or urine is not well known and sinking rates are poorly characterized. These uncertainties influence the details of outputs from models and hence the output should be interpreted cautiously. Perhaps the best use of their results is as a guide to the scale of intensity and area of depositions.

- All models should be compared to data from the location of interest.
- Maximum estimates of exposure distances and areas can be calculated using minimum sinking rates, maximum current speeds, and maximum water depths. This approach indicates drugs have the potential to be spread over very large distances (order kilometers to 10s of kilometers) and areas (order 10s of square kilometers) in some locations.
- Complex models require additional inputs relative to those for simple models, such as spatially varying water depths and current fields. When this information is not available, simple models should be considered. The outputs should be interpreted in ways that are appropriate for the uncertainty of the provided predictions, i.e., predicted exposure zones are orders of magnitude estimates.
- State-of-the-art models are only able to resolve the details of exposure to an accuracy that is dependent upon the accuracy of the input variables and parameters. Exact values for the parameterization are often unknown and estimates from the literature can vary significantly and be contradictory. As a result, existing models are of uncertain precision although the limited evidence indicates that they, at best, have an order of magnitude accuracy.
- Management decisions should recognize the accuracy limitations of the models and make decisions commensurate with these limitations.
- The first step in the development of any model is to first establish the goal of the modelling exercise. In the case of a model to be used for management guidance, these goals should be identified through a series of interactive and iterative communications between management and science. Subsequent steps in modelling efforts will depend on the outcomes of these meetings.
- Once modelling goals have been established and models have been selected and/or developed, models must be first validated before being implemented.
- In summary, due the uncertainties in the model inputs and parameterizations and lack of model validations, current complex models are only able to provide order of magnitude estimates of deposition. Simple models are also able to give order of magnitude estimates. Thus, at this time, simple models may be sufficient for decision support. This sentiment may change as science better characterizes model inputs and processes, and conducts more validation studies.

KNOWLEDGE GAPS

MANAGEMENT

- There is a lack of clarity in the management needs for models.
- There is uncertainty regarding the required level of accuracy and precision of model output.
- In general, environmental thresholds (for example, thresholds regarding area, location, duration, and concentration) have not been clearly articulated.

RESEARCH

- Chemical dependent partitioning rates of absorption, egestion, and excretion are poorly understood and quantified.
- The statistics of fecal sinking rates are poorly quantified.

- There is a lack of detailed characterization on how the spatial and temporal variability of currents varies among the different regions in which Canadian aquaculture is present.
- It is largely unknown how sensitive model outputs are to variations in the inputs, especially for more complex models.
- There are sparse data of current variability on seasonal and annual time scales.
- In-situ decay of deposited drugs is not well known.
- Knowledge of treatment plans, for example frequency, timing, and consistency between net-pens, is limited.
- Existing in-feed drug deposition models have not been thoroughly validated world-wide and, furthermore, these models have not been used or validated for regions in which Canadian marine net-pen aquaculture occurs.

RECOMMENDATIONS

MANAGEMENT

- Fill the management knowledge gaps identified above.
- There needs to be a reconciliation of model output accuracy and precision with management goals and delivery timelines.
- Science needs to better understand the modelling requirements for management considerations.
- Management and science should understand the importance of having calibrated and validated models.
- Management should understand the assumptions and precisions of models so that they may properly incorporate the results into their decision processes.
- Due to the uncertainties associated with model outputs, managers will need to continue to rely on well-designed sampling strategies and use model outputs cautiously and in a well-informed manner.
- Regular efforts should be made to update and communicate evaluations of models and management needs so the appropriate balance between needs and use can be attained and maintained.

RESEARCH

- Fill the research knowledge gaps identified above.
- Conduct a full research program which includes surveying, monitoring, and modelling at an initially uncontaminated, isolated aquaculture site for the entire duration of a production cycle. The goals of the research program should include understanding the sensitivities of model formulations and the sensitivities of model outputs to input values.
- Science should work with management to select, refine, and/or develop a subset of operational models that support management needs. This effort should include model evaluation and procedures for calibration.
- Evaluate the applicability of the Okubo relationship for modelling in-feed dispersion.

- Obtain more measurements of the initial treatment doses of drugs.
- Assess the sensitivity of vertical variations in water current on the estimate of the horizontal displacement of particles containing medicines. Many simple models assume a vertically and horizontally constant water velocity. It may be useful to estimate the variability or error associated with this assumption, since most of the current in the vicinity of many finfish aquaculture farms is probably not spatially homogeneous.
- Generate hydrodynamic models with seasonal and inter-annual forcing to better understand the current variability.

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