Dispersion models of pesticides released from finfish aquaculture tarpaulin bath treatments part 2: Comparison of solutions

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125 Marine Science Drive
St Andrews, NB E5B 0E4

2024

Canadian Technical Report of Fisheries and Aquatic Sciences 3631

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Canadian Technical Report of Fisheries and Aquatic Sciences

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Cat. No. Fs97-6/3631E-PDF ISBN 978-0-660-72900-8 ISSN 1488-5379

Correct citation for this publication:

Haigh, S.P., Page, F.H., and O'Flaherty-Sproul, M.P.A. 2024. Dispersion models of pesticides released from finfish aquaculture tarpaulin bath treatments part 2: Comparison of solutions. Can. Tech. Rep. Fish. Aquat. Sci. 3631: x + 29 p.

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In the salmon aquaculture industry, bath pesticide treatments are used in the management of sea-lice infestations. Upon conclusion of the treatment, the pesticides are released into the environment. Haigh et al. (2024) presented models and their solutions for the growth and dilution of a released pesticide patch. The models have three components: horizontal diffusion parameterization (Fickian and Okubo), vertical extent (constant and vertical growth), and horizontal concentration distribution within the patch (mean and Gaussian). This report examines differences between model solutions using all combinations of the three components. Based on the calculated differences, recommendations of model use for calculating conservative estimates of the maximum toxic patch size and the total time that the patch contains toxic concentrations are given. The Okubo model for horizontal diffusion is recommended over the Fickian diffusion model. The combination of the vertical growth model with a mean concentration distribution is recommended for calculating the maximum toxic patch size. To estimate the total time that a patch contains harmful or toxic concentrations, the vertical growth model with a Gaussian radial concentration distribution is recommended. For a single release from a representative cage perimeter of 150 m, a treatment depth of 4 m, a maximum patch depth of 20 m and a dilution factor of 103 between the treatment concentration and an environmental quality standard, the recommended models result in a maximum estimated toxic patch size of approximately 320, 000 m2 (0.32 km2) and a total time that a patch contains toxic concentrations of approximately 11 h.

RÉSUMÉ

Haigh, S.P., Page, F.H., and O'Flaherty-Sproul, M.P.A. 2024. Dispersion models of pesticides released from finfish aquaculture tarpaulin bath treatments part 2: Comparison of solutions. Can. Tech. Rep. Fish. Aquat. Sci. 3631: x + 29 p.

Dans l'industrie de la salmoniculture, les traitements antiparasitaires par bain sont utilisés pour gérer les infestations de pou du poisson. Lorsque le traitement est terminé, les pesticides sont rejetés dans l'environnement. Haigh et ses collaborateurs (2024) ont présenté des modèles et leurs solutions pour la croissance et la dilution d'un panache de pesticide rejeté. Les modèles onttrois composantes : le paramétrage de la diffusion horizontale (Fickian et Okubo), l'étendue verticale (constante et croissance verticale) et la distribution horizontale de la concentration dans le panache (moyenne et gaussienne). Ce rapport examine les différences entre les solutions des modèles utilisant toutes les combinaisons des trois composantes. Sur la base des differences calculées, on fournit des recommandations d'utilisation des modèles pour le calcul d'estimations prudentes de la taille maximale du panache toxique et de la durée totale pendant laquelle le panache contient des concentrations toxiques. On recommande d'utiliser le modèle Okubo pour la diffusion horizontale au lieu du modèle de diffusion Fickian. On recommande une combinaison du modèle de croissance verticale avec une distribution de la concentration moyenne pour le calcul de la taille maximale du panache toxique. Pour estimer la durée totale pendant laquelle un panache contient des concentrations nocives ou toxiques, il est commandé d'utiliser le modèle de croissance verticale avec une distribution radiale aussienne des concentrations. Pour un rejet unique à partir d'un périmètre des cages représentatif de 150 m, une profondeur de traitement de 4 m, une profondeur maximale de panache de 20 m et un facteur de dilution de 103 entre la concentration de traitement et une norme de qualité environnementale, les modèles recommandés conduisent à une taille maximale estimée de panache toxique d'environ 320 000 m2 (0,32 km2) et à une durée totale pendant laquelle un panache contient des concentrations toxiques d'environ 11 heures.

1 INTRODUCTION

This is Part 2 of a two part report concerning simple models for the dispersal of pesticides released from open net pen aquaculture tarp treatments as they have been conducted in the southwest New Brunswick area of the Bay of Fundy, Canada. Part 1 contains descriptions and detailed derivations of the models and their equations (Haigh et al. 2024). In Part 2, this document, the outputs derived from the models developed in Part 1 are explored and compared for a range of input scenarios.

Parts 1 and 2 were produced to help contribute to the Government of Canada's effort to evolve their aquaculture environmental management in relation to the release of bath pesticides from commercial open net pen finfish operations. Pesticides are used by the commercial salmon farming industry in their efforts to manage sea-lice infestations at their farms. The pesticides are applied as bath treatments. Following a treatment, the bath water containing the pesticide is released into the environment, as described by Page et al. (2015) and is referred to as a pesticide patch. Due to local oceanographic conditions, the pesticide patch is advected away, i.e. carried by the local water currents, from the treatment site and may grow in the horizontal and vertical directions while decreasing in concentration, depending on the mixing and dispersion conditions. For a period of time, the concentration of the pesticide within the patch may be sufficiently high to be harmful to non-target organisms which may come into contact with the patch.

Haigh et al. (2024) presented equations, solution methods, and solutions to simple pesticide patch models that are of particular interest to Fisheries and Oceans Canada regulators of the aquaculture industry. The models are based on solutions to the standard horizontal diffusion equations. Solutions were given for Fickian and Okubo horizontal diffusion models, constant and vertical growth depth models, and mean and Gaussian concentration distributions. Specifically, the models predict the maximum toxic patch size, the time at which this maximum occurs, and the total duration over which the patch contains harmful concentrations. All combinations of the three model components yielded the same qualitative result: the maximum size of the toxic patch, the time required to achieve it, and the total time that the patch contains toxic concentrations increase with both the perimeter of the treatment cage and the ratio of the treatment concentration to a threshold concentration. The quantitative details of these solutions, however, varied with the combination of the components. These details are documented in this report and recommendations concerning the use of the models by aquaculture regulators are given.

2 MODEL REVIEW

2.1 MODEL DESCRIPTIONS

A brief summary of the models is given here. For more details see Haigh et al. (2024).

The models described below predict the vertical and horizontal growth of a pesticide patch containing toxic concentrations and the distribution of the pesticide concentration within the patch. A pesticide concentration is considered toxic if it is above a specified Environmental Quality Standard (EQS) concentration. The models described below assume that a toxic pesticide patch is represented by a cylinder with radius $r_e(t')$ and depth $H(t')$, where t' is the time post-release. The pesticide patch does not contain all the pesticide used during the treatment; non-toxic concentrations will lie outside the toxic patch. The models assume that the pesticide is a passive tracer. The models only consider the growth of a pesticide patch due to dispersion and do not take into account any shearing of the patch due to ambient currents and thus assume that the patch retains it cylindrical shape throughout its growth. Furthermore, it is assumed that the pesticide concentration is uniform in the vertical.

It is assumed that the pesticide decay rate is much smaller than the dilution rate. Hence the growth of the toxic pesticide patch is modelled using solutions from the diffusion equation. The distribution of the concentration within a patch can be modelled by (Page et al. 2015, 2023)

$$C(t', r, z) = \begin{cases} \dfrac{M}{\pi\sigma^2(t')H(t')} e^{-r^2/\sigma^2(t_0+t')} & if\ z \le H(t') \\ 0 & if\ z > H(t') \end{cases} \quad (2.1)$$

where r is the radial distance from the centre of the patch, M is the pesticide mass within the patch, σ^2 is the horizontal variance of the patch, and t_0 is the time at which the radius of the patch from the point source is equal to the initial radius of the treatment patch, as discussed below. Two horizontal diffusion models and two depth models are considered here.

1.1.1 HORIZONTAL DIFFUSION MODELS

1.1.1.1 FICKIAN MODEL

The Fickian model is the analytic solution of the two dimensional diffusion equation for an instantaneous source released at $(r, t) = (0,0)$ on a horizontal plane with constant and equal horizontal diffusion coefficients in the x and y directions, i.e., $K_x = K_y = K_h$ (Crank 1975). The horizontal variance of the patch is given by

$$\sigma_r^2(t) = 4K_h t \quad (2.2)$$

It should be noted that the time t differs from the time of post-release t' since (2.2) is the solution for a point source whereas the pesticide patch has an initial dimension. To account for this, we define t_0 as the time at which the radius of the patch from the point source is equal to the initial radius of the treatment patch. Thus, we write (2.2) as

$$\sigma_r^2(t') = 4K_h(t_0 + t') \quad (2.3)$$

The value of t_0 is dependent on the horizontal diffusion model, as discussed in section 1.1.3.

1.1.1.2 OKUBO MODEL

When using the Fickian horizontal diffusion model, the contours of constant concentrations are circles. In reality, the shapes of pesticide patches are more complicated and depend on ambient flow conditions (Lee et al. 2009). Using data from dye studies, Okubo (1968, 1971) defined the radius of the patch as that of a circular patch which has the same area as that contained within the dye contour of a given concentration. Okubo (1968, 1971) empirically determined the equivalent radius variance,

$$\sigma_{rc}^2(t) = \alpha\, t^{\beta} \quad (2.4)$$

where the values of the parameters α and β were initially estimated by visual inspection of dye patch data (Okubo 1968) and later estimated using additional data and a regression analysis (Lawrence et al. 1995). As with the Fickian case, we take into account the initial finite size of the pesticide patch

$$\sigma_{rc}^2(t') = \alpha\,(t_0 + t')^{\beta} \qquad (2.5)$$

In equation (2.1) we use σ^2 to represent σ_r^2 for the Fickian model and σ_{rc}^2 for the Okubo model.

1.1.2 VERTICAL MODELS

The patch depth (or thickness in the vertical) is given by a function $H(t')$, where t' is the time post-release of the patch. Two models are considered for the vertical behaviour of a pesticide patch. Both models assume the presence of a barrier that limits the vertical extent of the pesticide patch. The vertical barrier could be a pycnocline or the seabed and will depend on local oceanographic conditions.

1.1.2.1 CONSTANT DEPTH

The constant depth model assumes an instantaneous vertical mixing to the depth of the vertical barrier. Thus the vertical extent of a patch remains unchanged, i.e., constant, for the duration of its horizontal growth:

$$H(t') = \begin{cases} H_0 & \text{if } t' = 0 \\ H_{\max} & \text{if } t' > 0 \end{cases} \qquad (2.6)$$

where H_0 is the treatment depth and $H_{\max}$ is the depth of the vertical barrier. Here we have not prescribed a structure of the pesticide distribution in the vertical and are assuming that the pesticide is well mixed, i.e. uniformly distributed, in the vertical.

1.1.2.2 VERTICAL GROWTH

The vertical growth model was proposed by Page et al. (2023) and is given by equation (2.7). The model is based on dimensional analysis. The model assumes that the initial patch depth is equal to the treatment depth, H_0, and grows vertically until it reaches the vertical barrier at time t^*, at which point it remains a constant depth.

$$H(t') = \begin{cases} H_0 + \sqrt{K_z t'} & if\ t' < t^* \\ H_{\max} & if\ t' \geq t^* \end{cases} \qquad (2.7)$$

where K_z is the vertical coefficient of diffusivity, assumed to be constant through time and depth, and t^* is given by

$$t^* = \frac{(H_{\max} - H_0)^2}{K_z} \qquad (2.8)$$

As with the constant depth model, we have not prescribed a structure of the pesticide distribution in the vertical and are assuming that the pesticide is well mixed, i.e. uniformly distributed, in the vertical.

1.1.3 THREE DIMENSIONAL CONCENTRATION MODELS

Two models of concentration throughout the patch are considered. Both models assume that a pesticide patch is toxic if it contains concentrations above an EQS concentration, C_{eqs}. For both models we examine the maximum radius of the toxic patch, $r_{\max}$, the time at which this maximum occurs, $t_{\max}$, and the total time that the patch contains toxic concentrations, t_{tox}. The use of these models for the evolution of a released patch of pesticide was previously presented in Page et al. (2023).

1.1.3.1 MEAN MODEL

The mean concentration model assumes that the pesticide is uniformly distributed throughout the patch in both the horizontal and vertical directions. Following Okubo (1968), the radius of a circular patch, r_e, is defined as

$$r_e = n\sigma(t) \tag{2.9}$$

which contains $(100\,\gamma_n)$ % of the pesticide mass for some positive number n which defines the radius as a multiple of the standard deviation and where (see Okubo, 1968, for derivation)

$$\gamma_n = 1 - e^{-n^2} \tag{2.10}$$

In equation (2.9), t represents the time since the mass of pesticide was released from a point source. For an initial pesticide patch of radius r_0, t_0 is the time required for a patch to increase in size from a point source to the initial patch size. In (2.9) we set

$$t = t_0 + t' \tag{2.11}$$

where $t_0 = r_0^2/(4n^2K_h)$ for the Fickian horizontal diffusion model and $t_0 = (r_0^2/n^2\alpha)^{1/\beta}$ for the Okubo horizontal diffusion model. For a toxic patch with a radius defined by (2.9), the average concentration is given by

$$C_{\text{avg}} = \frac{\gamma_n V_0 C_0}{\pi n^2 \sigma^2 (t_0 + t')H(t')} \tag{2.12}$$

where V_0 is the treatment volume and C_0 is the treatment concentration. Note that the toxic patch ceases to exist once the average concentration fall below the EQS.

The dilution factor, R, is defined as

$$R = \frac{C_0}{C_{\text{eqs}}} \tag{2.13}$$

where C_{eqs} is the EQS concentration (assuming this is the threshold concentration of concern).

The time $t'_{\max}$, at which the maximum toxic patch size occurs can be found by solving the following equation.

$$1 = \frac{\gamma_n V_0 R}{\pi n^2 \sigma^2 (t_0 + t'_{\max})H(t'_{\max})} \tag{2.14}$$

The maximum size of the toxic patch, $r_{\max}$, is given by

$$r_{\max}^2 = \frac{\gamma_n V_0 R}{\pi H(t'_{\max})} \tag{2.15}$$

Note that $t'_{\max}$ depends on both the horizontal diffusion model and the depth model whereas $r_{\max}$ is independent of the horizontal diffusion model. For the mean concentration model, the patch is no longer considered toxic after $t'_{\max}$ since the average concentration will be less than C_{eqs} and thus $t'_{\max} = t'_{\text{tox}}$

1.1.3.2 GAUSSIAN MODEL

The Gaussian model assumes that the concentration within the patch is uniform in the vertical and varies in the horizontal according to (2.1). The radius of the toxic patch , r_{eqs}, is defined as the radius at which the concentration equals the EQS concentration. It was shown in Haigh et al. (2024) that

$$r_{\mathrm{eqs}}^2 = -\sigma^2(t_0 + t') \cdot \ln\left[\frac{\pi\sigma^2(t_0 + t')H(t')}{V_0 R}\right] \tag{2.16}$$

The solution to (2.16) produces a patch radius that increases with time to a maximum and then decreases until no concentrations within the patch are above C_{eqs} (Page et al. 2023). The precise details will depend on the patch depth function, $H(t')$. The time at which the maximum toxic patch size occurs, $t'_{\max}$, is given by the root of the following equation.

$$\frac{d}{dt}\left(\sigma^2(t)\right)\left(\ln\left[\frac{\pi\sigma^2(t)H_{\max}}{V_0 R}\right] + 1\right) = 0 \tag{2.17}$$

The method for determining the root of (2.17) depends on the selection of horizontal diffusion and vertical models. The methods for the various combinations are given in Haigh et al. (2024). Once $t'_{\max}$is found, the maximum radius of the toxic patch, $r_{\max}$, is determined by setting $t' = t'_{\max}$ in (2.16).

The length of time for which the patch contains concentrations above the EQS is given by solving for t'_{tox} in

$$R - \frac{\pi\sigma^2(t_0 + t'_{\mathrm{tox}})H(t'_{\mathrm{tox}})}{V_0} = 0 \tag{2.18}$$

Details of the solution methods for the different combinations of horizontal diffusion and vertical models are given in Haigh et al. (2024).

1.2 MODEL SOLUTIONS

Haigh et al. (2024) presented solutions for all combinations of horizontal diffusion, vertical, and concentration models. Solutions were calculated for a range of cage perimeters and dilution factors (Table 2.1). Parameter values used in the solutions are given in Table 2.1.

Table 2.1. Parameter values (or ranges) used in all solutions (both analytic and numeric) presented in this document.

Parameter	Description	Units	Value
α	Parameter used in equation (2.4)	-	5.6e-6
β	Parameter used in equation (2.4)	-	2.22
n	Parameter used in equation (2.9)	-	1.5
K_h	Horizontal coefficient of diffusivity	$m^2 \cdot s^{-1}$	1.0
K_Z	Vertical coefficient of diffusivity	$m^2 \cdot s^{-1}$	0.01
H_0	Treatment depth	m	4
$H_{\max}$	Maximum patch depth for all depth models	m	20
P_{cage}	Cage perimeter (assume circular cage)	m	[10,500]
R	C_0/C_{eqs}, dilution factor	-	$[10^2, 10^4]$

1.2.1 CONSTANT DEPTH MODEL

When the constant depth model is used, analytic solutions can be derived. A summary of the analytical solutions given in Haigh et al. (2024) are presented here as they are used in the analysis of model comparisons in section 2.

1.2.1.1 MEAN CONCENTRATION AND FICKIAN DIFFUSION

The solution to $t'_{\max}$ for the mean concentration model with constant depth and Fickian horizontal diffusion is given by

$$t'_{\max} = \frac{\gamma_n V_0 R}{4\pi n^2 K_h H_{\max}} - t_0 \tag{2.19}$$

and the solution for $r_{\max}$ is given by

$$r_{\max}^2 = \frac{\gamma_n V_0 R}{\pi H_{\max}} \tag{2.20}$$

1.2.1.2 MEAN CONCENTRATION AND OKUBO DIFFUSION

The solution to $t'_{\max}$ for the mean concentration model with constant depth and Okubo horizontal diffusion is given by

$$t'_{\max} = \left(\frac{\gamma_n V_0 R}{n^2 \pi \alpha H_{\max}}\right)^{1/\beta} - t_0 \tag{2.21}$$

The maximum size of the toxic patch, $r_{\max}$, is the same as for the Fickian model and given by (2.20).

1.2.1.3 GAUSSIAN CONCENTRATION AND FICKIAN DIFFUSION

The solution to $t'_{\max}$ for the Gaussian concentration model with constant depth and Fickian horizontal diffusion is given by

$$t'_{\max} = \frac{V_0 R}{4\pi e K_h H_{\max}} - t_0 \tag{2.22}$$

where e is Euler's number. The solution for $r_{\max}$ is given by

$$r^2_{\max} = \frac{V_0 R}{\pi e H_{\max}} \tag{2.23}$$

The solution to t'_{tox} for the Gaussian concentration model with constant depth and Fickian horizontal diffusion is given by

$$t'_{\text{tox}} = \frac{V_0 R}{4\pi K_h H_{\max}} - t_0 \tag{2.24}$$

1.2.1.4 GAUSSIAN CONCENTRATION AND OKUBO DIFFUSION

The solution to $t'_{\max}$ for the Gaussian concentration model with constant depth and Okubo horizontal diffusion is given by

$$t'_{\max} = \left(\frac{V_0 R}{e\pi\alpha H_{\max}}\right)^{\frac{1}{\beta}} - t_0 \tag{2.25}$$

The maximum size of the toxic patch, $r_{\max}$, is the same as for the Fickian model and given by (2.23).

The solution to t'_{tox} for the Gaussian concentration model with constant depth and Okubo horizontal diffusion is given by

$$t'_{\text{tox}} = \left(\frac{V_0 R}{\pi\alpha H_{\max}}\right)^{\frac{1}{\beta}} - t_0 \tag{2.26}$$

1.2.2 VERTICAL GROWTH MODEL

Numerical solutions were required when the vertical growth model is used and are presented in Haigh et al. (2024) for the parameter values given in Table 2.1.

2 MODEL COMPARISONS

Haigh et al. (2024) found that the maximum toxic patch size is independent of the horizontal diffusion model when a constant depth is used. It was also observed that solutions of the maximum toxic patch radius, the time post-release at which this occurs, and the total time post-release that a patch contains toxic concentrations all behave similarly with varying cage perimeter, P_{cage}, and the dilution factor, R, i.e., they all increase with increasing P_{cage} and R, regardless of the concentration, horizontal diffusion, and depth models. It was found, however, that the ranges of $r_{\max}$, $t'_{\max}$, and t'_{tox} vary significantly between models (Table 2.1). In order to better understand how the solutions are impacted by model choice, we explore in more detail differences in solutions to models.

Table 2.1. Intervals of minimum and maximum of calculated values r_{max}, t'_{max}, and t'_{tox}. for all the combinations of concentration, horizontal diffusion, and depth models. Model solutions were calculated over the P_{cage} and R ranges of [10,500] and [10^2,10^4], respectively. All other model parameters are given in Table 2.1.

Depth Model	Concentration Model	Horizontal Diffusion Model	$r_{\max}$ (m)	$t'_{\max}$ (h)	t'_{tox} (h)
Constant	Mean	Fickian	[7,3366]	[0.0,349.5]	[0.0,349.5]
Constant	Mean	Okubo	[7,3366]	[0.2,65.0]	[0.2,65.0]
Constant	Gaussian	Fickian	[4,2159]	[0.0,323.4]	[0.0,879.3]
Constant	Gaussian	Okubo	[4,2159]	[0.2,62.7]	[0.3,99.7]
Growth	Mean	Fickian	[14,3366]	[0.0,349.5]	[0.0,349.5]
Growth	Mean	Okubo	[11,3366]	[0.3,65.0]	[0.3,65.0]
Growth	Gaussian	Fickian	[9,2159]	[0.0,323.4]	[0.0,879.3]
Growth	Gaussian	Okubo	[7,2159]	[0.3,62.7]	[0.5,99.7]

2.1 CONSTANT DEPTH VS VERTICAL GROWTH MODELS

In this section we compare solutions from the two depth models for all combinations of horizontal diffusion and concentrations models.

2.1.1 MEAN CONCENTRATION AND FICKIAN DIFFUSION

Percent differences in $r_{\max}$ and $t'_{\max}$ for constant and vertical growth models using the mean concentration and Fickian horizontal diffusion models are shown in Figure 2.1. Blank areas indicate that the solutions are equal which occurs when $H(\, t'_{\max}) = H_{\max}$. The time at which this occurs, t^*, is given by equation (2.8). Equating $t'_{\max}$ in (2.19) to t^* in (2.8) and solving for R gives

$$R^*_{\text{mean}} = \frac{n^2 4\pi K_h H_{\max}\,(t^* + t_0)}{\gamma_n V_0} \tag{2.1}$$

The curve for R^*_{mean} is included in Figure 2.1 and marks the delineation between the two solutions. With the mean concentration model and Fickian horizontal diffusion, the growth of the patch radius is dependent only on the initial patch radius and the horizontal diffusion coefficient K_h, see equations (2.3) and (2.9). Thus when the toxic patch depth has reached its maximum value at $t'_{\max}$, the two solutions are equal. Before this occurs, i.e., when $t'_{\max} < t^*$, the maximum patch radius is larger when vertical growth is included; the depth is smaller when vertical growth is included and thus a larger radius is required to dilute to the threshold value. For the parameters used here, the maximum patch radius is up to 53% larger and takes up to 79% longer to be realized in the model with vertical growth when compared to the constant depth case (Figure 2.1 and Table 2.2). For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for $r_{\max}$ and $t'_{\max}$ are approximately 10% and 20%, respectively (Table 2.3).

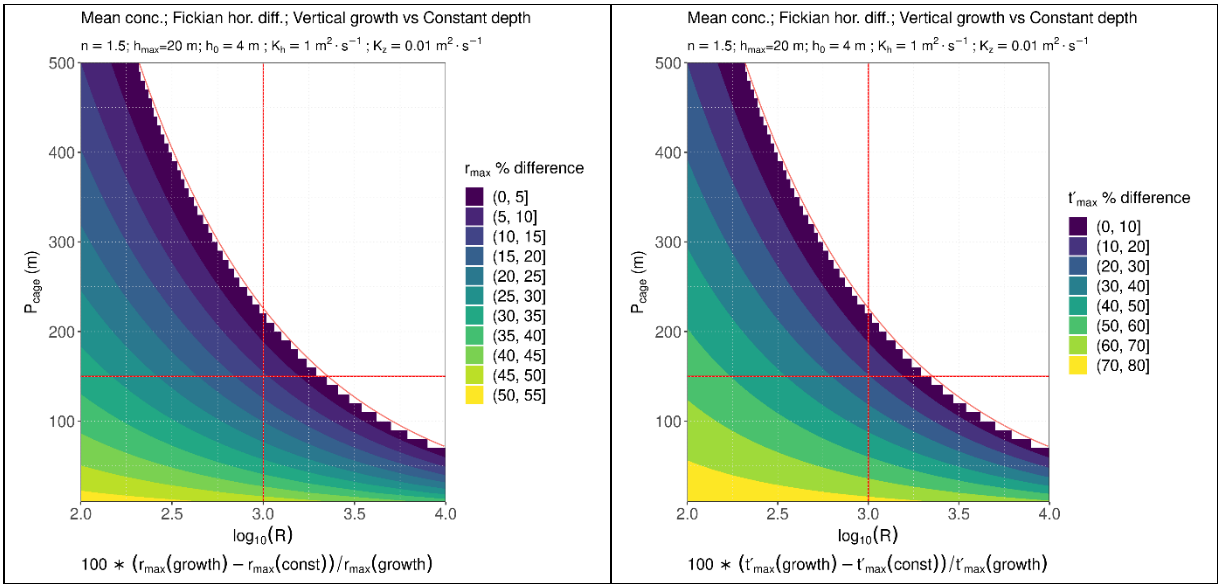

Figure 2.1. Percent differences between constant and vertical growth depth models using mean concentration and Fickian horizontal diffusion: r_{max} (left) and t'_{max} (right). Parameters used are given in Table 2.1. White areas indicate that the two solutions are equal. R^*_{mean}, as defined by equation (2.1), is the orange curve delineating the transition to the region where the two solutions are equal. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

Table 2.2. Intervals of minimum and maximum percent differences in model comparisons calculated as 100*(first model – second model)/(first model) over the P_{cage} and R ranges of [10,500] and [10^2,10^4], respectively. All other model parameters are given in Table 2.1.

Depth Model	Concentration Model	Horizontal Diffusion Model	% Δr_{max} (m)	% $\Delta t'_{\text{max}}$ (h)	% $\Delta t'_{\text{tox}}$ (h)
Growth-Constant	Mean	Fickian	[0.0,52.7]	[0.0,78.6]	[0.0,78.6]
Growth-Constant	Mean	Okubo	[0.0,39.2]	[0.0,43.7]	[0.0,43.7]
Growth-Constant	Gaussian	Fickian	[0.0,52.8]	[-41.7,77.7]	[0.0,76.8]
Growth-Constant	Gaussian	Okubo	[0.0,39.6]	[-13.6,40.8]	[0.0,37.5]
Constant	Gaussian-Mean	Fickian	[-56.0,-55.9]	[-8.6,-8.1]	[60.3,61.6]
Constant	Gaussian-Mean	Okubo	[-56.0,-55.9]	[-5.0,-3.7]	[34.8,41.5]
Growth	Gaussian-Mean	Fickian	[-55.9,-50.3]	[-53.4,-8.1]	[48.6,60.9]
Growth	Gaussian-Mean	Okubo	[-55.9,-53.0]	[-18.9,-3.7]	[30.4,40.5]
Constant	Mean	Okubo-Fickian	[0.0,0.0]	[-437.4,99.3]	[-437.4,99.3]
Constant	Gaussian	Okubo-Fickian	[0.0,0.0]	[-415.5,99.3]	[-781.7,98.9]
Growth	Mean	Okubo-Fickian	[-34.7,0.0]	[-437.4,98.1]	[-437.4,98.1]
Growth	Gaussian	Okubo-Fickian	[-34.7,0.0]	[-415.5,98.1]	[-781.7,97.0]

Table 2.3. Percent differences in model comparisons calculated as 100*(first model – second model)/(first model) for $P_{\text{cage}} = 150$ and $R = 10^3$. All other model parameters are given in Table 2.1.

Depth Model	Concentration Model	Horizontal Diffusion Model	% $\Delta r_{\max}$ (m)	% $\Delta t'_{\max}$ (h)	% $\Delta t'_{\text{tox}}$ (h)
Growth-Constant	Mean	Fickian	10.8	20.5	20.5
Growth-Constant	Mean	Okubo	0.0	0.0	0.0
Growth-Constant	Gaussian	Fickian	13.7	-1.4	0.0
Growth-Constant	Gaussian	Okubo	1.0	-8.5	0.0
Constant	Gaussian-Mean	Fickian	-55.9	-8.1	60.4
Constant	Gaussian-Mean	Okubo	-55.9	-4.0	36.3
Growth	Gaussian-Mean	Fickian	-50.9	-38.0	50.1
Growth	Gaussian-Mean	Okubo	-54.4	-12.8	36.3
Constant	Mean	Okubo-Fickian	0.0	57.1	57.1
Constant	Gaussian	Okubo-Fickian	0.0	58.7	31.0
Growth	Mean	Okubo-Fickian	-12.1	46.0	46.0
Growth	Gaussian	Okubo-Fickian	-14.7	55.8	31.0

2.1.2 MEAN CONCENTRATION AND OKUBO DIFFUSION

Percent differences in $r_{\max}$ and $t'_{\max}$ for constant and vertical growth models using the mean concentration and Okubo horizontal diffusion models are shown in Figure 2.2. Blank areas indicate that the solutions are equal which occurs when $H(t'_{\max}) = H_{\max}$. Similar to the Fickian case, setting $t'_{\max}$ given by (2.21) to t^*, we solve for R

$$R^*_{\text{mean}} = \frac{n^2 \pi \alpha H_{\max} (t^* + t_0)^\beta}{\gamma_n V_0} \tag{2.2}$$

The curve defined by (2.2) is included in Figure 2.2 and delineates the transition between the two solutions. With the mean concentration model and Okubo horizontal diffusion, the growth of the patch radius is only dependent on the initial patch radius and the Okubo parameters α and β, see equations (2.4) and (2.9). Thus when the patch depth has reached its maximum value at $t'_{\max}$, the two solutions are equal. Similar to the Fickian case, when $t'_{\max} < t^*$, the maximum patch radius is larger (up to 39%) and takes longer (up to 44%) to be realized in the model with vertical growth when compared to the constant depth case (Figure 2.2 and Table 2.2). For a representative net pen perimeter of 150 m and a concentration ratio of 10^3 (i.e., $R = 3$) the models predict the same values of $r_{\max}$ and $t'_{\max}$ (Table 2.3).

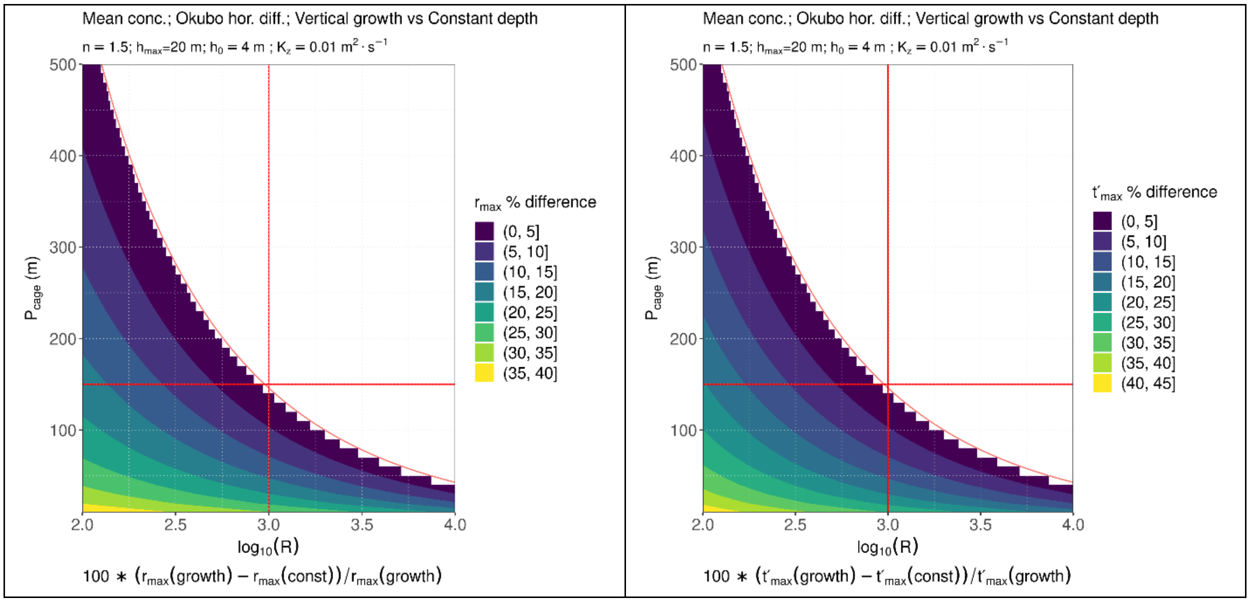

Figure 2.2. Percent differences between constant and vertical growth depth models using mean concentration and Okubo horizontal diffusion: $r_{\max}$ (left) and $t'_{\max}$ (right). Parameters used are given in Table 2.1. White areas indicate that the two solutions are equal. R^*_{mean}, as defined by equation (2.2) is the orange curve delineating the transition to the region where the two solutions are equal. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.1.3 GAUSSIAN CONCENTRATION AND FICKIAN DIFFUSION

Percent differences in $r_{\max}$, $t'_{\max}$, and t'_{tox} for constant and vertical growth depth models using the Gaussian concentration and Fickian horizontal diffusion models are shown in Figure 2.3 and Figure 2.4. As expected, when the two solutions are not equal, the maximum patch radius is larger (by up to 53%) for vertical growth depth model when compared to the constant depth case (Figure 2.3 and Table 2.2).

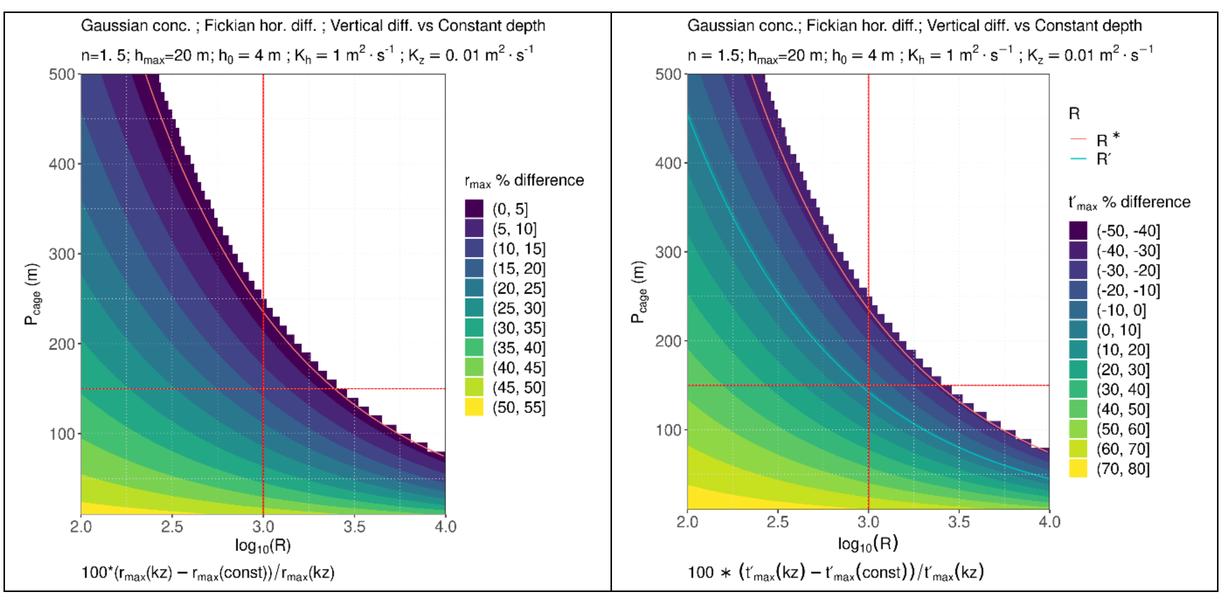

Figure 2.3. Percent differences between constant and vertical growth depth models using Gaussian concentration and Fickian horizontal diffusion: $r_{\max}$ (left) and $t'_{\max}$ (right). Parameters used are given in Table

2.1. White areas indicate that the two solutions are equal. The curve for R^*_{gauss}, as defined by equation (2.3) is shown in orange in both plots. The curve for R', as defined by equation (2.4) is shown in blue on the $t'_{\max}$ plot. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

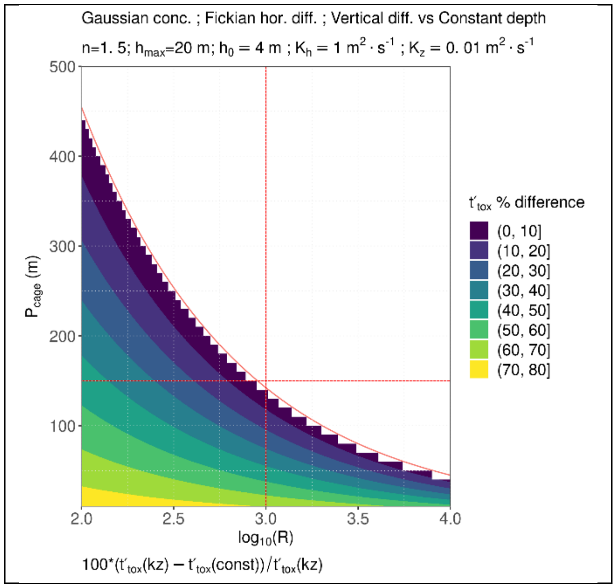

Figure 2.4. Percent differences in t'_{tox} between constant and vertical growth depth models using Gaussian concentration and Fickian horizontal diffusion. Parameters used are given in Table 2.1. White areas indicate that the two solutions are equal. The curve for R', as defined by equation (2.4) is shown in orange and delineates the transition to the region where the two solutions are equal. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

As with the mean concentration model, we can define the curve along which $t^* = t'_{\max}$. Setting $t'_{\max}$ given by (2.22) to t^*, we solve for R

$$R^*_{\text{gauss}} = \frac{4e\pi K_h H_{\max}\,(t^* + t_0)}{V_0} \tag{2.3}$$

The curve defined by equation (2.3) is included in Figure 2.3. Although it gives a close approximation to the transition to the region where the two solutions are equal, unlike the mean concentration model, it does not exactly delineate the transition. When $R > R^*_{\text{gauss}}$ for a given initial patch size, it is possible that the two depth representations have different maximum radius values at different times. This is illustrated in Figure 2.5 which shows the temporal evolution of the patch radius for the Gaussian concentration and Fickian diffusion models using the constant and vertical growth depth models when $R = 10^3$ and $P_{\text{cage}} = 100,\ 230,\ 240,$ and 300 m. The corresponding values for R^*_{gauss} are respectively $5500,\ 1045,\ 960,$ and 617. When $P_{\text{cage}} = 100$ and 230 (Figure 2.5a and b), the maximum solutions are both achieved before $t = t^*$ (Table 2.4). In both cases $R < R^*_{\text{gauss}}$ and the radius is larger when vertical growth is included but the maximum radius with vertical growth is achieved later when $P_{\text{cage}} = 100$m and earlier when $P_{\text{cage}} = 230$ m. When $P_{\text{cage}} = 240$ m (Figure 2.5c), the maximum radius is achieved after/before $t = t^*$ when the constant/vertical growth depth model is used. Here $R > R^*_{\text{gauss}}$ but the two solutions are not equal. Finally, when $P_{\text{cage}} = 300$ m (Figure 2.5d), the maximum radius is the same for both depth models.

In contrast to the mean concentration model, the time at which the maximum radius occurs varies from being shorter by 42% to longer by 78% (Figure 2.3 and Table 2.2).

Similar to R^*_{gauss}, we define the curve along which $t^* = t'_{\mathrm{tox}}$ by setting t'_{tox} in (2.24) to t^* and solving for R

$$R' = \frac{4\pi K_h H_{\mathrm{max}}\,(t^* + t_0)}{V_0} \tag{2.4}$$

Comparing equations (2.3) and (2.4), we see that $R^*_{\mathrm{gauss}} = eR'$. We observe that the curve defined by equation (2.4) approximately delineates the transition between the behaviour of t'_{max} (right panel of Figure 2.3). Below R' curve the maximum patch size occurs sooner for the constant depth case whereas above the curve, the maximum patch size occurs later for the constant case. For t'_{tox} , the R'curve delineates the transition to the region where the two solutions are equal (Figure 2.4). When $t'_{\mathrm{tox}} < t^*$, the time for which the patch contains toxic concentration is up to 77% longer in the model with vertical growth when compared to the constant depth case (Figure 2.4 and Table 2.2). For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for r_{max}, t'_{max}, and t'_{tox} are approximately 15%, approximately equal, and exactly equal, respectively (Table 2.3).

Table 2.4. Values of R^*_{gauss}, r_{max}, and t'_{max} for the constant and vertical growth depth models with Gaussian concentration and Fickian horizontal diffusion using $R = 10^3$and the cage perimeters corresponding to those used in Figure 2.5. All other model parameters are given in Table 2.1.

P_{cage} (m)	R^*_{gauss}	r_{max} (m)		t'_{max} (h)		t^* (h)
		Constant	Diffusion	Constant	Diffusion	
100	5500	137	175	1.3	1.6	7.1
230	1045	314	324	6.8	5.2	7.1
240	960	328	334	7.4	5.5	7.1
300	617	410	410	11.6	11.6	7.1

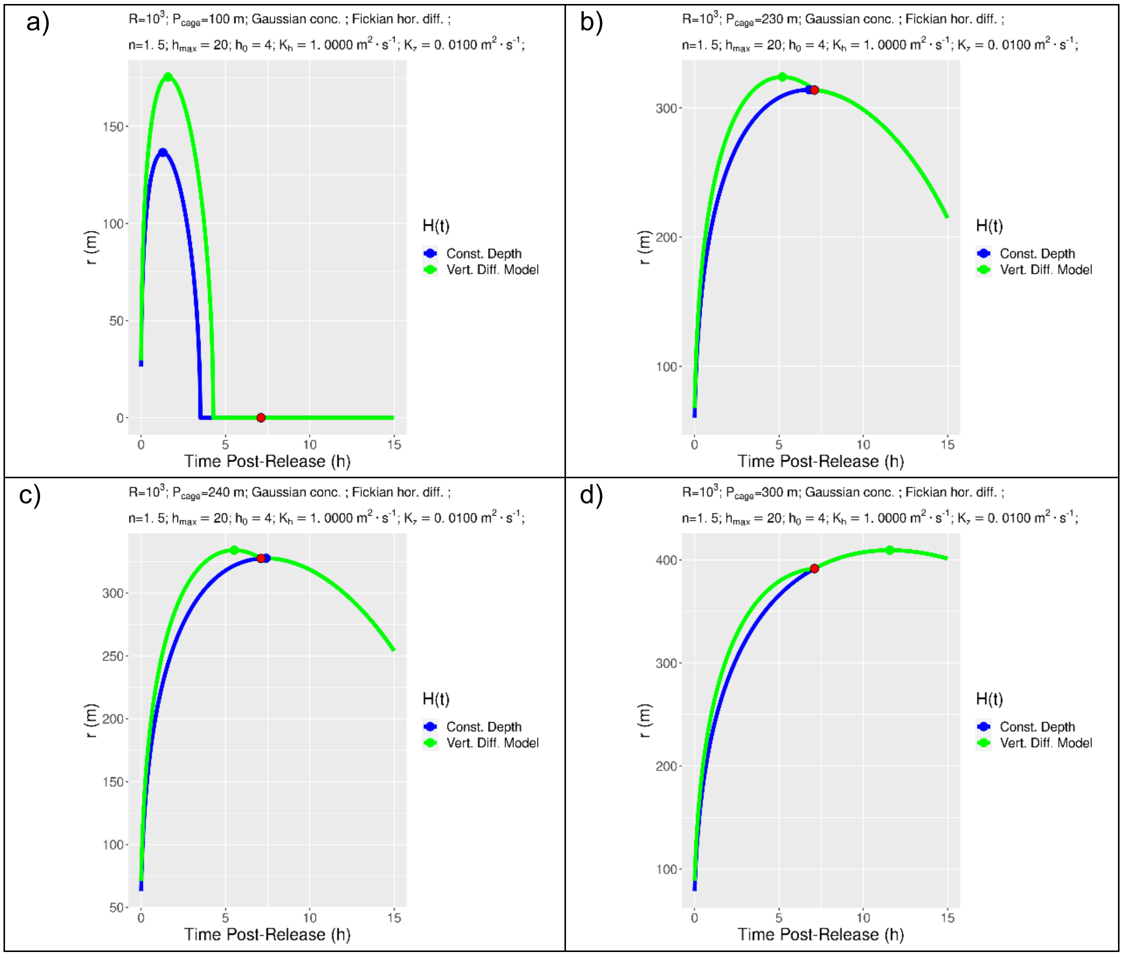

Figure 2.5. Time series solution of the patch radius using the Gaussian concentration and Fickian horizontal diffusion models with constant (blue) and vertical growth (green) depth models for $R = 10^3$ and $P_{\text{cage}} = 100$(a), 230 (b), 240 (c), and 300 (d) m. All other model parameters are given in Table 2.1. The time at which $t' = t^*$ is shown in red. The blue (green) circle indicates the maximum radius and the time it occurs for the constant (vertical growth) depth model.

2.1.4 GAUSSIAN CONCENTRATION AND OKUBO DIFFUSION

Percent differences in r_{max}, t'_{max}, and t'_{tox} for constant and vertical growth depth models using the Gaussian concentration and Okubo horizontal diffusion models are shown in Figure 2.6 and Figure 2.7. Blank areas indicate that the solutions are equal. When the two solutions are not equal, the maximum patch radius is up to 40% larger for vertical growth depth model when compared to the constant depth case (Figure 2.6 and Table 2.2).

We define the curve along which $t^* = t'_{\text{max}}$. Setting t'_{max} given by (2.25) to t^*, we solve for R

$$R^*_{\text{gauss}} = \frac{e\pi\alpha H_{\text{max}}\,(t^* + t_0)^{\beta}}{V_0} \tag{2.5}$$

The curve defined by (2.5) is shown in Figure 2.6. As with the Fickian case, it gives a close approximation to the transition to the region where the two solutions are equal but does not exactly delineate the transition. When $R > R^*_{\text{gauss}}$ for a given initial patch size, it is possible that the two depth representations have different maximum radius values at different times. In contrast to the mean concentration model, the time at which the maximum radius occurs varies from being shorter by 14% to larger by 41% (Figure 2.7 and Table 2.2).

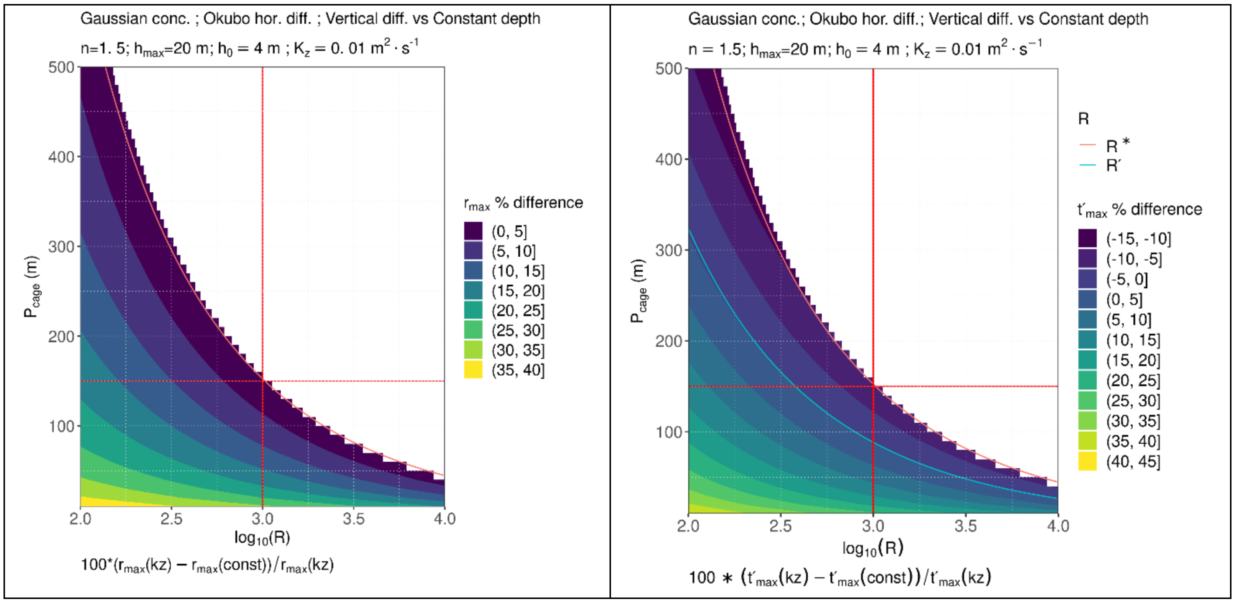

Figure 2.6. Percent differences between constant and vertical growth depth models using Gaussian concentration and Okubo horizontal diffusion: $r_{\max}$ (left) and $t'_{\max}$ (right). Parameters used are given in Table 2.1. The curve for R^{*}_{gauss}, as defined by equation (2.5) is shown in orange in both plots. The curve for R', as defined by equation (2.6) is shown in blue on the t'_{max} plot. Blank areas indicate that the two solutions are equal. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

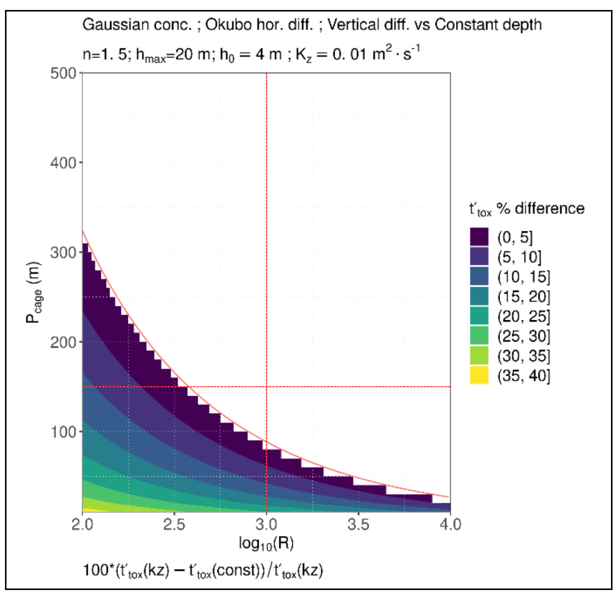

Figure 2.7. Percent differences in t'_{tox} between constant and vertical growth depth models using Gaussian concentration and Okubo horizontal diffusion. Parameters used are given in Table 2.1. The curve for R', as defined by equation (2.6) is shown in orange. Blank areas indicate that the two solutions are equal. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

Using the same method as the Fickian case, we define the curve along which $t^* = t'_{\text{tox}}$ by setting t'_{tox} in (2.26) to t^* and solving for R

$$R' = \frac{\pi\alpha H_{\max}\,(t^* + t_0)^\beta}{V_0} \tag{2.6}$$

Comparing equations (2.5) and (2.6), we see that $R^*_{\text{gauss}} = eR'$. Again, we observe that the curve defined by equation (2.6) approximately delineates the transition between the behaviour of $t'_{\max}$ (right panel of Figure 2.6). Furthermore, R' delineates the transition to the region where the two solutions for t'_{tox} are equal (Figure 2.7). When $t'_{\text{tox}} < t^*$, the time for which the patch contains toxic concentration is up to 38% longer in the model with vertical growth when compared to the constant depth case (Figure 2.7 and Table 2.2). For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for $r_{\max}$, $t'_{\max}$, and t'_{tox} are approximately equal, approximately -10%, and exactly equal, respectively (Table 2.3).

2.2 MEAN VS GAUSSIAN CONCENTRATION MODELS

In this section we compare solutions from the two concentration models for all combinations of horizontal diffusion and vertical models.

2.2.1 CONSTANT DEPTH AND FICKIAN DIFFUSION

For the constant depth case with Fickian horizontal diffusion, comparing (2.20) with (2.23), we see that the radius at which the mean concentration is C_{eqs} is a factor of $\sqrt{\gamma_n e} \approx 1.56$ larger, or 56% larger, than the maximum radius of the patch using a Gaussian distribution of concentration and a boundary of C_{eqs}. Also, comparing (2.19) with (2.22), since $\gamma_n e > n^2$(at least for the value of n used here, if we were to use $n = 2$ then the opposite is true) it takes longer for the mean concentration to reach the EQS concentration than it does to reach the maximum radius using a Gaussian distribution of concentration and a boundary of C_{eqs}. Figure 2.8 shows the percent difference of time at which the maximum occurs between the two models. Using equations (2.19) and (2.22), assuming $t'_{\max} \gg t_0$, it can be shown that the approximate value of $(t'_{\max}(\text{Gaussian}) - t'_{\max}(\text{Mean})/t'_{\max}(\text{Gaussian}))$ depends on the initial treatment depth but not the initial treatment radius. Since we used a constant initial treatment depth, the percent time difference is approximately constant for a given value of R (as seen in Figure 2.8), furthermore it decreases with increasing R and, for the explored values, ranges from -8.6% to -8.1% (Table 2.2).

For t'_{tox} we compare equations (2.19) (recall $t'_{\text{tox}} = t'_{\max}$ for the mean concentration model) and (2.24). It can be shown that the difference between the two solutions is always positive since $n^2 - \gamma_n = n^2 + \exp(-n^2) - 1 > 0$ when $n > 0$. Thus the patch remains toxic longer when considering the Gaussian concentration model in comparison with the mean concentration model. For the parameter values examined here, the Gaussian concentration model predicts toxic patches for 60% to 62% longer when compared with the mean concentration model (see Table 2.2) and the difference decreases with increasing R (Figure 2.8). As with $t'_{\max}$, it can be shown that, assuming $t'_{\text{tox}} \gg t_0$, the approximate value of $(t'_{\text{tox}}(\text{Gaussian}) - t'_{\text{tox}}(\text{Mean})/t'_{\text{tox}}(\text{Gaussian}))$ depends on the initial treatment depth but not the initial treatment radius and so percent differences are approximately constant for a given value of R. For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for $r_{\max}$, $t'_{\max}$, and t'_{tox} are approximately -56%, -10%, and 60%, respectively (Table 2.3).

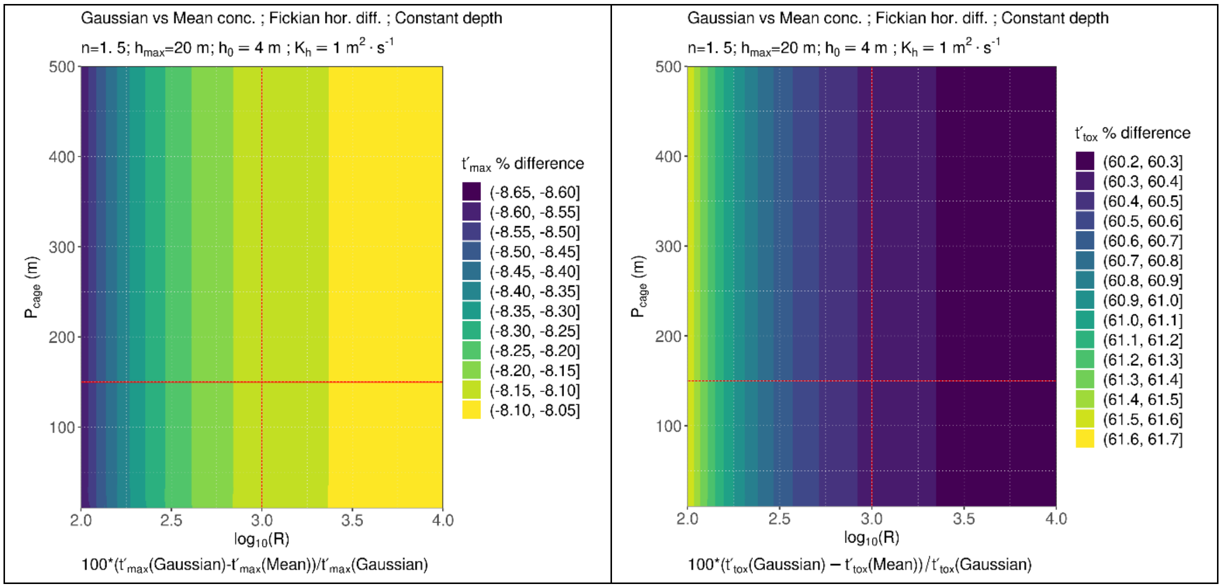

Figure 2.8. Percent differences between Gaussian and mean concentration models with the constant depth and Fickian horizontal diffusion models: t'_{max} (left) and t'_{tox} (right). Parameters used are given in Table 2.1. Since $R = C_0/C_{\mathrm{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.2.2 CONSTANT DEPTH AND OKUBO DIFFUSION

For the constant depth model, the predicted maximum radius is independent of the horizontal diffusion model for both the mean and Gaussian concentration models. Therefore, differences in the predicted maximum radius are the same as those discussed above for the Fickian horizontal diffusion model. Also, comparing (2.21) with (2.25), it can be shown that the sign of $(t'_{\mathrm{max}}(\mathrm{Gaussian}) - t'_{\mathrm{max}}(\mathrm{Mean})$ is always negative since $n^2 - e\gamma_n < 0$ when $n > 0$. Thus it takes longer for the mean concentration to reach the EQS concentration than it does to reach the maximum radius using a Gaussian distribution of concentration and a boundary of C_{eqs}. Similar to the Fickian case, using equations (2.21) and (2.25), it can be shown that, assuming $t'_{\mathrm{max}} \gg t_0$, the approximate value of $(t'_{\mathrm{max}}(\mathrm{Gaussian}) - t'_{\mathrm{max}}(\mathrm{Mean})/t'_{\mathrm{max}}(\mathrm{Gaussian}))$ depends on the treatment depth but not the treatment radius. Thus the percent time difference is approximately constant for a given value of R (as seen in Figure 2.9), furthermore it decreases with increasing R and, for the explored values, ranges from -5.0% to -3.7% (Table 2.2).

For t'_{tox} we compare equations (2.21) (recall $t'_{\mathrm{tox}} = t'_{\mathrm{max}}$ for the mean concentration model) and (2.26). Similar to the Fickian case, it can be shown that the difference between the two solutions is always positive. Thus the patch remains toxic longer when considering the Gaussian concentration model in comparison with the mean concentration model. For the parameter values examined here, the Gaussian concentration model predicts toxic patches for 35% to 42% longer when compared with the mean concentration model (see Table 2.2) and the difference decreases with increasing R (Figure 2.9). As with t'_{max}, it can be shown that, approximately, $(t'_{\mathrm{tox}}(\mathrm{Gaussian}) - t'_{\mathrm{tox}}(\mathrm{Mean})/t'_{\mathrm{tox}}(\mathrm{Gaussian}))$ depends on the treatment depth but not the treatment radius and so percent differences are approximately constant for a given value of R. For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for r_{max}, t'_{max}, and t'_{tox} are approximately -56%, -5%, and 40%, respectively (Table 2.3).

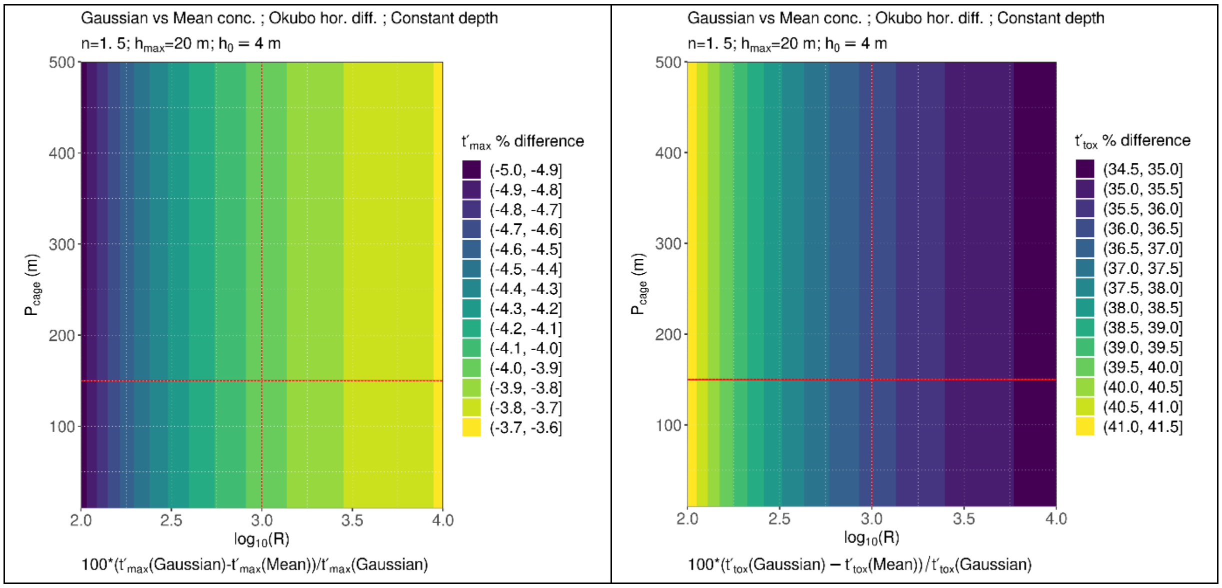

Figure 2.9. Percent differences between Gaussian and mean concentration models with the constant depth and Okubo horizontal diffusion models: $t'_{\max}$ (left) and t'_{tox} (right). Parameters used are given in Table 2.1. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.2.3 VERTICAL GROWTH AND FICKIAN DIFFUSION

Percent differences in $r_{\max}$ and $t'_{\max}$ between the Gaussian and mean concentration models with vertical growth and Fickian horizontal diffusion models are shown in Figure 2.10. The curves for R^*_{mean} and R^*_{gauss}, given by equations (2.1) and (2.3), are also shown and indicate that there is a transition after which the differences in the solutions are the same as the constant depth case. We observe that the transition between the solutions starts at the curve for R^*_{mean} and ends roughly beyond the curve for R^*_{gauss}. The reason that R^*_{gauss} is not a firm delimiter for this transition period is discussed above. The maximum radius with the mean concentration model is 50 to 56% larger than the maximum radius of the patch using a Gaussian distribution of concentration and a boundary of C_{eqs} and occurs 8 to 53% later (Table 2.2).

Percent differences in t'_{tox} between the Gaussian and mean concentrations models with vertical growth and Fickian horizontal diffusion models are shown in Figure 2.11. The curves for $R'_{\text{mean}} = R^*_{\text{mean}}$ and $R'_{\text{gauss}} = R'$, given by equations (2.1) and (2.4), are also shown and indicate that there is a transition between the two curves after which the differences in the solutions are the same as the constant depth case. The duration that a patch contains toxic concentrations is longer when the Gaussian concentration model is used by 49 to 61 % (Table 2.2). For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for $r_{\max}$, $t'_{\max}$, and t'_{tox} are approximately -50%, -40%, and 50%, respectively (Table 2.3).

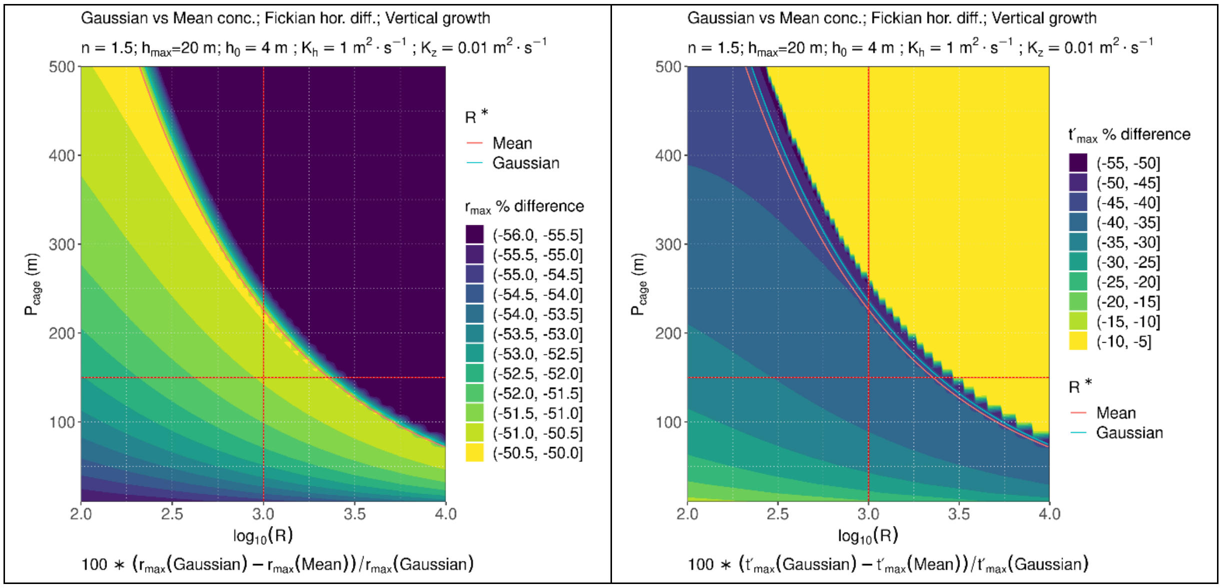

Figure 2.10. Percent differences between Gaussian and mean concentration models with the vertical growth and Fickian horizontal diffusion models: r_{max} (left) and t'_{max} (right). The curves for R^{*}, given by equations (2.1) and (2.3) for the mean and Gaussian concentration models, respectively, are included. Parameters used are given in Table 2.1. Since $R = C_0/C_{\mathrm{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

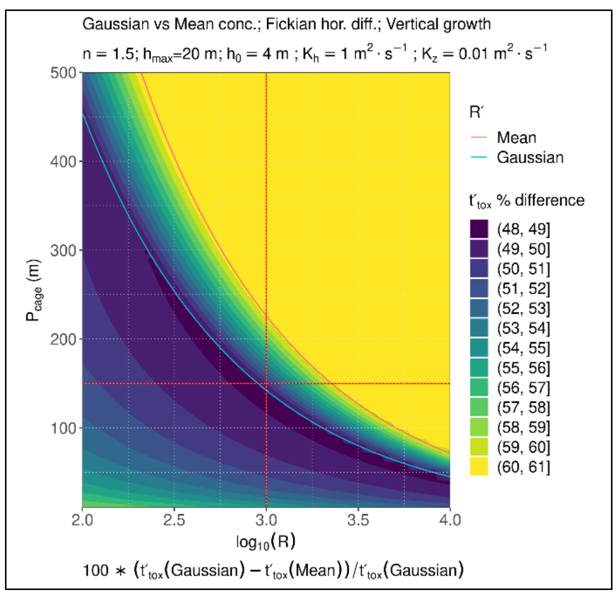

Figure 2.11. Percent differences in t'_{tox} between Gaussian and mean concentration models with the vertical growth and Fickian horizontal diffusion models. Parameters used are given in Table 2.1. The curves for R', given by equations (2.1) and (2.4) for the mean and Gaussian concentration models, respectively, are included.. Since $R = C_0/C_{\mathrm{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.2.4 VERTICAL GROWTH AND OKUBO DIFFUSION

Percent differences in $r_{\max}$ and $t'_{\max}$ between the Gaussian and mean concentrations models with vertical growth and Okubo horizontal diffusion models are shown in Figure 2.12. The curves for R^*_{mean} and R^*_{gauss}, given by equations (2.2) and (2.5), are also shown and indicate that there is a transition after which the differences in the solutions are the same as the constant depth case. We observe that the transition between the solutions starts at the curve for R^*_{mean} and ends roughly beyond the curve for R^*_{gauss}. The reason that R^*_{gauss} is not a firm delimiter for this transition period is discussed above. The maximum radius with the Gaussian concentration model is 53 to 56% smaller than the maximum radius of the patch using a mean distribution of concentration and a boundary of C_{eqs} and occurs 4 to 19% earlier (Table 2.2).

Percent differences in t'_{tox} between the Gaussian and mean concentration models with vertical growth and Fickian horizontal diffusion models are shown in Figure 2.13. The curves for $R'_{\text{mean}} = R^*_{\text{mean}}$ and R'_{gauss}, given by equations (2.2) and (2.6), are also shown and indicate that there is a clear transition between the two curves after which the differences in the solutions are the same as the constant depth case. The duration that a patch contains toxic concentrations is longer when the Gaussian concentration model is used by 30 to 41 % (Table 2.2). For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for $r_{\max}$, $t'_{\max}$, and t'_{tox} are approximately -55%, -10%, and 40%, respectively (Table 2.3).

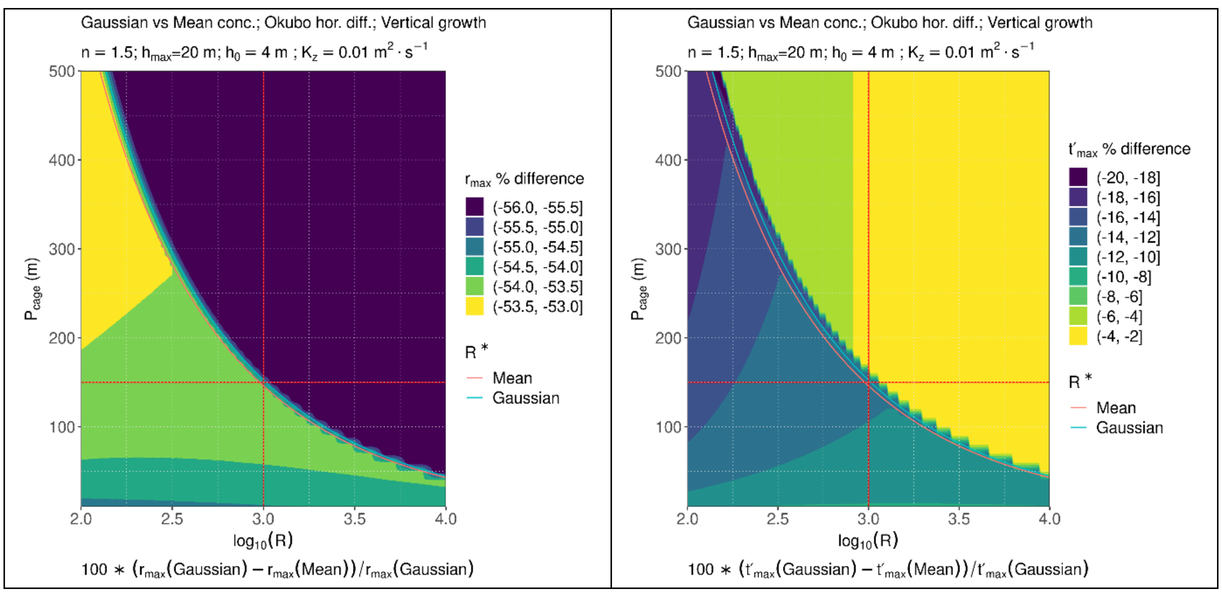

Figure 2.12. Percent differences between Gaussian and mean concentration models with the vertical growth and Okubo horizontal diffusion models: $r_{\max}$ (left) and t'_{max} (right). The curves for R^*, given by equations (2.2) and (2.5) for the mean and Gaussian concentration models, respectively, are included. Parameters used are given in Table 2.1. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

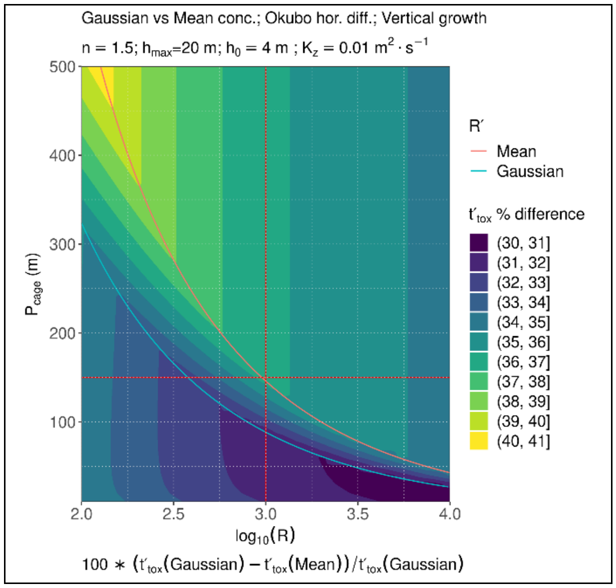

Figure 2.13. Percent differences in t'_{tox} between Gaussian and mean concentration models with the vertical growth and Okubo horizontal diffusion models. Parameters used are given in Table 2.1. The curves for R', given by equations (2.2) and (2.6) for the mean and Gaussian concentration models, respectively, are included.. Since $R = C_0/C_{\mathrm{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.3 FICKIAN VS OKUBO HORIZONTAL DIFFUSION MODEL

In this section we compare solutions from the two horizontal diffusion models for all combinations of concentration and vertical models.

2.3.1 CONSTANT DEPTH AND MEAN CONCENTRATION

For the mean concentration model with the constant depth model, r_{max} is independent of the horizontal diffusion model. Percent differences in t'_{max} between the Fickian and Okubo horizontal diffusion models with constant depth and mean concentration models are shown in Figure 2.14. We note that the differences in t'_{max} depend on the parameters R and P_{cage}. For small values of these two parameters, the time at which the maximum toxic patch occurs is greater by up to 99% (Table 2.2) when the Okubo horizontal diffusion model is used. As the values of these parameters increase, the Fickian horizontal diffusion model takes longer to achieve the maximum size, by up to 437%. Recall that for the mean concentration model $t'_{\mathrm{tox}} = t'_{\mathrm{max}}$. For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for r_{max}, t'_{max}, and t'_{tox} are exactly equal, approximately 60%, and approximately 60%, respectively (Table 2.3).

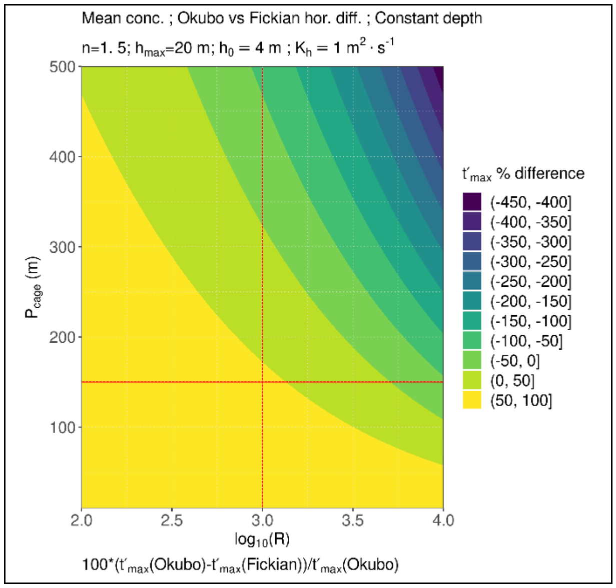

Figure 2.14. Percent differences in $t'_{\max}$ between Okubo and Fickian horizontal diffusion models with the constant depth and the mean concentration models. Parameters used are given in Table 2.1. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.3.2 CONSTANT DEPTH AND GAUSSIAN CONCENTRATION

For the Gaussian concentration model with the constant depth model, $r_{\max}$ is independent of the horizontal diffusion model. Percent differences in $t'_{\max}$ between the Fickian and Okubo horizontal diffusion models with constant depth and Gaussian concentration models are shown in Figure 2.15. Percent differences in $t'_{\max}$ follow a similar pattern as the mean concentration case. The time at which the maximum toxic patch occurs is greater by up to 99% (Table 2.2) for smaller values of R and P_{cage} when the Okubo horizontal diffusion model is used. As the value of these parameters increase, the Fickian horizontal diffusion model takes longer to achieve the maximum size, by up to 416%. Percent differences for t'_{tox} are also shown in Figure 2.15. The pattern is the same as for $t'_{\max}$ but the patch can remain toxic for up to 782% times longer with the Fickian diffusion model compared to the Okubo diffusion model. For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for $r_{\max}$, $t'_{\max}$, and t'_{tox} are exactly equal, approximately 60%, and approximately 30%, respectively (Table 2.3).

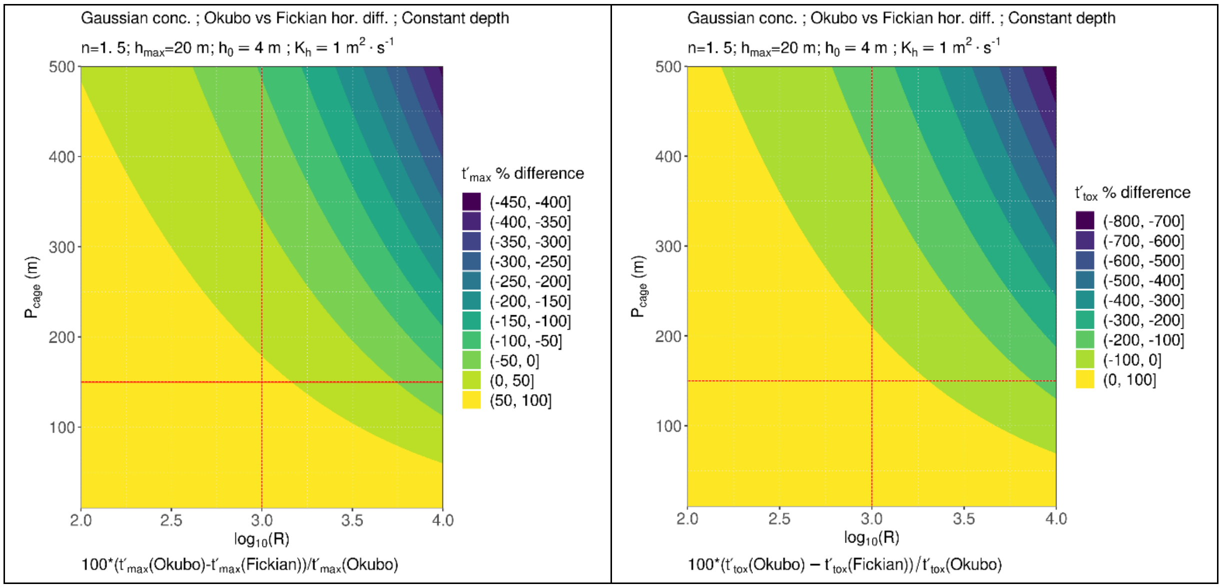

Figure 2.15. Percent differences in t'_{max} (left) and t'_{tox} (right) between Okubo and Fickian horizontal diffusion models with the constant depth and the Gaussian concentration models. Parameters used are given in Table 2.1. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.3.3 VERTICAL GROWTH AND MEAN CONCENTRATION

Percent differences in r_{max} and t'_{max} between the Fickian and Okubo horizontal diffusion models with vertical growth and mean concentration models are shown in Figure 2.16. The curves for R^*_{mean}, as defined by equations (2.1) and (2.2) for the Fickian and Okubo horizontal diffusion models, respectively, are included. These curves delineate a transition to the constant depth case (though not apparent in the plot for t'_{max}). The transition between the solutions starts at the R^*_{mean} curve for the Okubo case and ends at the R^*_{mean} curve for the Fickian case. When the two solutions are not equal, the maximum radius with the Fickian diffusion model is up to 35% larger than the maximum radius of the patch using the Okubo diffusion model (Table 2.2). Percent differences in t'_{max} have a similar behaviour to those of the constant depth model (compare Figure 2.16 with Figure 2.14) with similar ranges (Table 2.2) though the details differ when $R < R^*_{\text{mean}}$, where R^*_{mean} is given by equation (2.1). Since the mean concentration model is being considered $t'_{\text{tox}} = t'_{\text{max}}$. For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for r_{max}, t'_{max}, and t'_{tox} are approximately -10%, 50%, and 50%, respectively (Table 2.3).

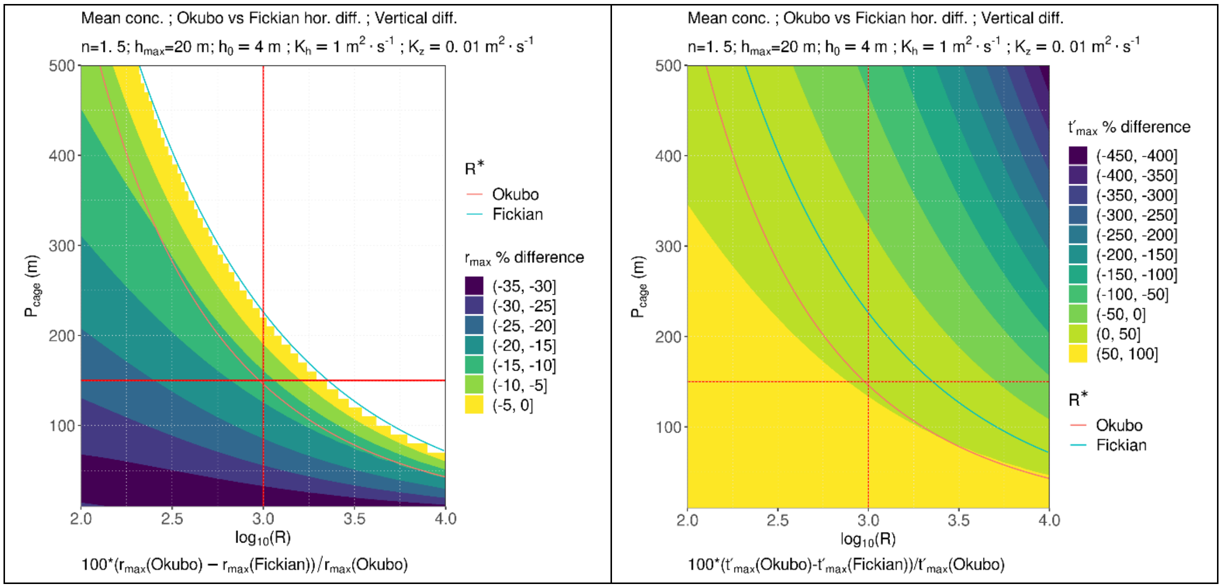

Figure 2.16. Percent differences between Okubo and Fickian horizontal diffusion models with the vertical growth depth and the mean concentration models: $r_{\max}$ (left) and $t'_{\max}$ (right). Parameters used are given in Table 2.1. The curves for R^*_{mean}, as defined by equations (2.1) and (2.2) for the Fickian and Okubo horizontal diffusion models, respectively, are included. Blank areas indicate that the two solutions are equal. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.3.4 VERTICAL GROWTH AND GAUSSIAN CONCENTRATION

Percent differences in $r_{\max}$ and $t'_{\max}$ between the Fickian and Okubo horizontal diffusion models with vertical growth and Gaussian concentration models are shown in Figure 2.17. The curves for R^*_{gauss}, as defined by equations (2.3) and (2.5) for the Fickian and Okubo horizontal diffusion models, respectively, are included. These curves delineate an approximate transition to the constant depth case, similar to the comparisons made using the Gaussian concentration model in sections 2.1.3 and 1.2.1.4. When the two solutions are not equal, the maximum radius with the Fickian diffusion model is up to 35% larger than the maximum radius of the patch using the Okubo diffusion model (Table 2.2). Percent differences in $t'_{\max}$ have a similar behaviour to those of the constant depth model (compare Figure 2.15 with Figure 2.17) with similar ranges (Table 2.2) though the details differ when $R < R^*_{\text{gauss}}$, where R^*_{gauss} is given by equation (2.3).

Percent differences in t'_{tox} between the Fickian and Okubo horizontal diffusion models with vertical growth and Gaussian concentration models are shown in Figure 2.18. The curves for R'_{gauss}, given by equations(2.4) and (2.6) for the Fickian and Okubo horizontal diffusion models, respectively, are also shown and indicate that there is a transition between the two curves after which the differences in the solutions are the same as the constant depth case. The behaviour of differences in t'_{tox} is similar to the constant depth case (compare Figure 2.18 with Figure 2.15) with the Okubo concentration model being toxic for up to 97% longer for smaller values of R and P_{cage} and the Fickian concentration model being toxic for up to 782% long for larger values of R and P_{cage} (see Figure 2.18 and Table 2.2). For a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$), the differences between models for $r_{\max}$, $t'_{\max}$, and t'_{tox} are approximately -15%, 60%, and 30%, respectively (Table 2.3).

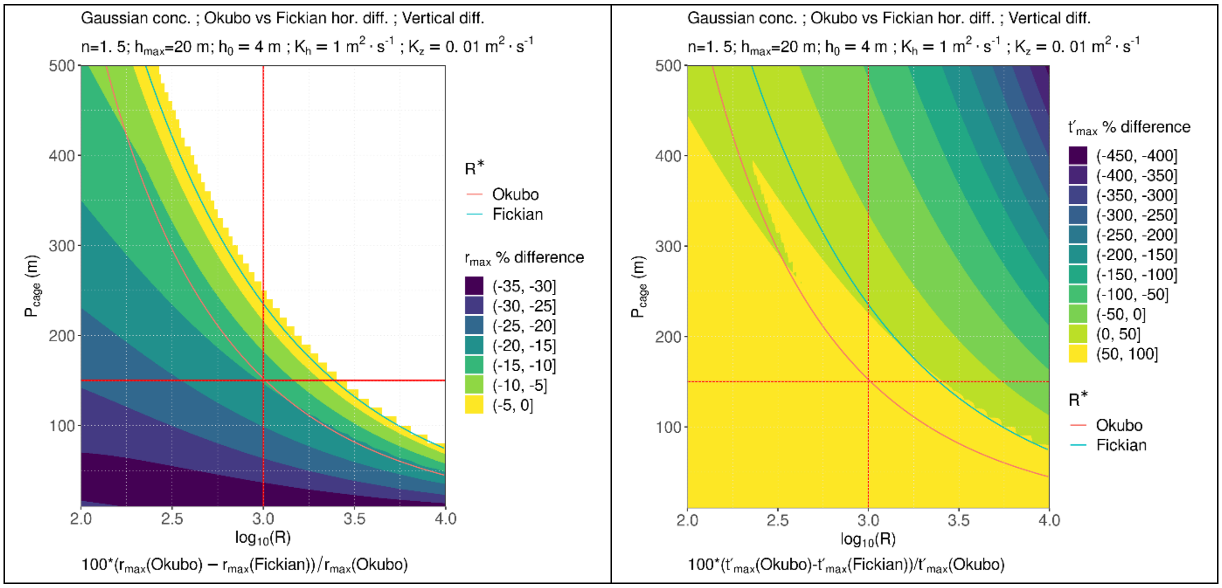

Figure 2.17. Percent differences between Okubo and Fickian horizontal diffusion models with the vertical growth depth and the Gaussian concentration models: $r_{\max}$ (left) and $t'_{\max}$ (right). Parameters used are given in Table 2.1. The curves for R^*_{gauss}, as defined by equations (2.3) and (2.5) for the Fickian and Okubo horizontal diffusion models, respectively, are included. Blank areas indicate that the two solutions are equal. Since $R = C_0/C_{\text{eqs}}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

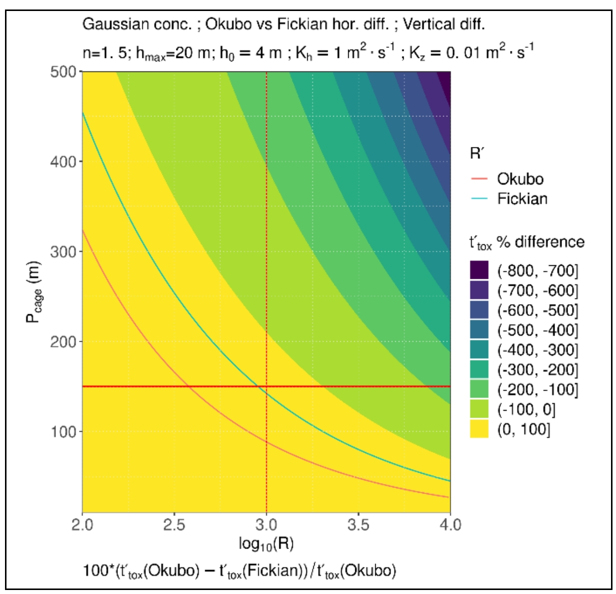

Figure 2.18. Percent differences in t'_{tox} between Okubo and Fickian horizontal diffusion models with the vertical growth depth and the Gaussian concentration models. Parameters used are given in Table 2.1. The curves for R', as defined by equations (2.4) and (2.6) for the Fickian and Okubo horizontal diffusion models, respectively, are included. Since $R = C_{treat}/C_{eqs}$, $\log_{10} R$ gives the order of magnitude dilution factor, i.e., $\log_{10} R = 3$ is a factor of 1000 dilution.

2.4 SUMMARY

- For the two depth models (constant and vertical growth) considered:

- When vertical growth is included, the maximum patch radius is the same as or larger than that predicted from the constant depth model solution.
- When vertical growth is included, the patch contains concentrations above the EQS for the same amount of time or longer than that predicted from the constant depth model solution.
- For the mean concentration model, the time to reach the maximum patch size is either the same or longer when vertical growth is used when compared to the predictions using the constant depth model.
- For the Gaussian horizontal concentration model, the time to reach the maximum patch size is sometimes longer and sometimes shorter when vertical growth is included when compared to the results using the constant depth model. The curve defining R' gives a reasonable approximation to the transition with the time to reach maximum longer/shorter when vertical growth is included when $R < R'$ / $R > R'$.
- When the vertical growth model is used, the total time that the patch is considered toxic is always greater than or equal to the time predicted when a constant depth is assumed.

* For the two concentration models (mean and Gaussian) considered:
    - Compared to the mean concentration model, the maximum patch radius is smaller when the Gaussian horizontal concentration model is used.
    - Compared to the mean concentration model, the time to reach the maximum patch size is shorter when the Gaussian horizontal concentration model is used.
    - Compared to the mean concentration model, the total time that the patch is considered toxic is longer when the Gaussian horizontal concentration is used.
* For the two horizontal diffusion models (Fickian and Okubo) considered:
    - When a constant depth is assumed, the maximum patch size is independent of the horizontal diffusion model for both the mean and Gaussian concentration models.
    - When vertical growth is included, the predicted maximum patch size using the Fickian model is either equal to or larger than that predicted using the Okubo model. This result is likely dependent on the choice of the horizontal diffusion coefficient used in the Fickian model.
    - No mathematical expression was determined to delineate the transition. There is no clear pattern in the differences between the time at which the maximum patch size occurs or the duration of toxicity between the two horizontal diffusion models.

3 DISCUSSION

The pesticide patch concentration models presented in this document have three components: horizontal diffusion parameterization (Fickian and Okubo), vertical extent (constant and vertical growth), and concentration distribution within the patch (mean and Gaussian). The impacts of these components on the predicted values of variables of potential interest to aquaculture regulators were examined. In some cases, clear patterns in the differences between models were established whereas in others, no patterns were identified. This leads the reader to question which model combination is most appropriate.

Comparisons of model solutions indicate that model choices impact predictions of maximum patch size, the time at which this maximum occurs, and the total time that a patch contains toxic concentrations. That being said, the differences are all less than a factor of 2, with the exception of the comparison between Fickian and Okubo horizontal diffusion models. In this case, the Fickian model can give much longer times to both reach the maximum patch size and to dilute completely below the EQS. Although we presented solutions for the Fickian model, limited data (Page et al. 2015) indicates that Okubo horizontal diffusion better represents the growth of a pesticide patch. This is unsurprising since the Okubo relationship is an empirical derivation from multiple dye studies at different scales (Okubo 1968, 1971, Lawrence et al. 1995). Furthermore, the Fickian model requires selecting a value of the horizontal diffusion coefficient, the value of which can vary over several orders of magnitude depending on the location and hydrographic conditions (Lewis 1997). We have used a representative value but the results will change if a different value is used. Thus, it is our recommendation that the Okubo horizontal diffusion model should be selected over the Fickian diffusion model.

Selecting the appropriate depth model is more difficult. The use of a constant depth model has the advantage of giving analytic solutions but other than providing insight as to how the patch growth depends on input variables, this is of little advantage as the solutions using the vertical growth model can easily be solved numerically on a modern computer. The solutions using the vertical growth model always gave larger (or equal) maximum patch sizes and the total time that a patch contains toxic concentrations was always longer (or the same). Thus, use of the vertical growth model holds merit for calculating these two variables as it yields the most conservative result. The behaviour of the timing at which the maximum patch size occurs was more variable, at least for the Gaussian concentration model. A range of time at which the maximum patch size occurs could be given to account for solution differences between the two depth models. One of the challenges in using the vertical growth model is the selection of the rate of vertical dispersion. Furthermore, the solutions of both models are particularly sensitive to the treatment depth and the maximum depth of the patch. A treatment depth of 4 m and maximum depth of 20 m were used in these comparisons. These values are representative of aquaculture sites in southwest New Brunswick. The values of these parameters should be chosen to reflect the treatment protocol of interest and local vertical barriers, i.e. the depth of the pycnocline or the total depth in the location of treatment. If the patch is released in an area with much deeper depths that does not have a pycnocline, differences in the two solutions may be larger and a sensitivity study should be conducted to determine the impact of changing the maximum depth.

Results of the comparisons between the mean and Gaussian concentrations models were consistent for all combinations of the other model components. The mean concentration model always gave a larger maximum radius by 50% to 56%. The maximum patch size always occurred sooner with the mean concentration model and the patch remained toxic longer for the Gaussian concentration model. A conservative approach may be to use the Gaussian model to determine the time to dilute below the EQS and the mean model to predict the maximum patch size. Differences in the time at which the maximum occurs was always less than 20% except when the Fickian diffusion model was used with the vertical growth model. As we do not recommend using the Fickian diffusion model, this is of little concern. A range of time at which the maximum patch size occurs could be given to account for differences between the two concentration models.

In summary, several models estimating the dispersion of pesticide released from tarped fish net pens have been explored. Although a discharge of pesticide released from a net pen evolves horizontally into an elongated and meandering plume, the models have assumed a horizontal circular patch with a radius that results in an area that is equivalent to the area of the dispersing patch. Three variable of interest have been investigated; the maximum patch equivalent radius, the time post release at which this maximum occurs, and the total time needed to dilute the pesticide to below an environmental quality standard. The area of the maximum patch size can be calculated from the maximum radius. We recommend that the Okubo horizontal diffusion model be used. For conservative estimates, the recommended combination of the depth model and the horizontal concentration distribution depends on the variable of interest. For the maximum patch size, it is recommended that the vertical growth model with the mean concentration distribution be used. For the total time that a patch contains toxic concentrations, the vertical growth model with the Gaussian concentration distribution should be used. Since the comparison of the results for the time at which the maximum patch size occurs were variable, it is recommended that a range of times at which the maximum patch size occurs should be calculated using the four combination achieved by using the two vertical depth models and the two concentration distributions. Based on the chosen values and recommendations the following model outputs are estimated for a representative cage perimeter of 150 m and a dilution factor of 10^3 (i.e., $R = 10^3$); the maximum patch radius is 319 m (equivalent area of 320, 000 m^2) , the time at which the maximum patch size occurs is between 6.5 h and 7.3 h post-release, and the total time that a patch contains toxic concentrations is 11.4 h.

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