

# **Dispersion models of pesticides released from finfish aquaculture tarpaulin bath treatments part 1: equations and solutions**

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## ABSTRACT

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 1: equations and solutions. Can. Tech. Rep. Fish. Aquat. Sci. 3619: iv + 24 p.

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. This report presents and expands upon the models from Page et al. (2015; 2023) for the growth and dilution of a released pesticide patch. Detailed mathematical descriptions of the models are given and the accompanying solutions are provided over a range of dilution ratios (treatment concentration divided by toxicity threshold) and treatment cage sizes. The models have three components: horizontal dispersion parameterization (Fickian and Okubo), vertical extent (constant and vertical growth), and concentration distribution with the patch (mean and Gaussian). Models with a constant depth are solved analytically whereas those with the vertical growth must be solved numerically. Solutions are presented for all combinations of the three components. For all models considered, the maximum size of the toxic patch, the time required to achieve the maximum size, and the total time that the patch contains toxic concentrations are calculated. The calculations indicate that both maximum size and total time of toxicity increase with both the perimeter of the treatment cage and dilution ratio.

## 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 1: equations and solutions. Can. Tech. Rep. Fish. Aquat. Sci. 3619: iv + 24 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. Le présent rapport explique en détail les modèles de Page et al. (2015, 2023) pour la croissance et la dilution des panaches de pesticide rejetés. Il contient des descriptions mathématiques détaillées des modèles et présente les solutions connexes pour une gamme de rapports de dilution (la concentration du traitement divisée par le seuil de toxicité) et de tailles de cages de traitement. Les modèles ont trois composantes : le paramétrage de la dispersion horizontale (Fickian et Okubo), l’étendue verticale (constante et croissance verticale) et la distribution de la concentration avec le panache (moyenne et gaussienne). Les modèles présentant une profondeur constante sont résolus de manière analytique, tandis que les modèles présentant une croissance verticale doivent être résolus de manière numérique. Les solutions sont fournies pour toutes les combinaisons des trois composantes. Pour chacun des modèles examinés, la taille maximale du panache toxique, le temps nécessaire pour atteindre la taille maximale et la durée totale pendant laquelle le panache contient des concentrations toxiques sont calculés. Les calculs indiquent que la taille maximale du panache et la durée totale de la toxicité augmentent toutes les deux avec le périmètre de la cage de traitement et avec le rapport de dilution.

# 1 INTRODUCTION

In the salmon aquaculture industry, one challenge associated with open net-pen aquaculture is the prevention and management of sea-lice infestations. Sea-lice infestations can directly impact the health and welfare of cultured fish. Also, sea-lice infestations may serve as reservoirs and amplifiers of sea lice abundance which may lead to impacts on the health and welfare of wild fish. These impacts have the potential to lead to economic consequences for the both the cultured and wild fishing industries as well as the potential for cultural impacts. Many methods are used to prevent and control these infestations including in-feed drug treatments, bath pesticide treatments, cleaner fish, pressure sprays, and warm water sprays. This document focuses on modelling the release and dispersal of pesticides into the environment after net-pen bath treatments.

Page et al. (2015) describe in detail the net-pen bath pesticide treatment method that has been used in the southwest New Brunswick area of the Bay of Fundy in eastern Canada. At the end of the treatment period, the pesticide is released into the environment. The pesticide patch grows due to turbulent dispersion and local current conditions and is transported (i.e. advected) away from the treatment site by the local water currents. The growth of the size of the patch results in a dilution of the pesticide concentration. 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. Page et al. (2015) showed that the growth of the pesticide patch is complicated and depends on multiple factors. The growth of the patch and its direction of movement is highly dependent on the location of the treatment in relation to other net pens on the site. Additionally, the growth and movement of the pesticide patch is dependent on the local hydrographic conditions at the site and the timing of the treatment since these determine the local currents which depend on, for example, the phase of the tide, vertical stratification, spatial variation in the currents, local weather conditions, and time of year. Finally, the pesticide patch growth and direction of movement also depend on the state of the farm infrastructure which includes, for example, the cage size, the mesh size, the amount of bio-fouling on the nets, and the cage array configuration and orientation. As a consequence the shapes of pesticide patches can be highly variable with the concentration of the pesticide within the patch being non-uniform and patchy.

Modelling the release, transport and dispersal of individual releases of pesticides from net-pen bath treatments requires hydrodynamic models that use spatially varying bathymetry and estimate the spatial and temporal variations in the local hydrographic characteristics (e.g. sea level, water velocity, turbulence, waves, water temperature, and salinity) for the time of treatment and for multiple hours afterwards Page et al. (2015). These modelling efforts require significant time and resources of both personnel and computing. In contrast, simpler models can be run quickly (order seconds to minutes) and can also provide useful, but less detailed, information for regulatory purposes. Page et al. (2015) showed that horizontal scale of pesticide patches agree reasonably well with the scaling curves established by the Okubo (1968; 1971) model. Page et al. (2023) further expanded on this, examining the temporal behaviour of a pesticide patch for a typical treatment scenario using two different concentration models.

This report gives a detailed mathematical description and derivation of the models presented in Page et al. (2015; 2023), the solution of the models for variables of potential interest to regulators,

and presents computed results over a range of parameters for all the models. Detailed comparisons of model solutions are presented in an accompanying report Haigh et al. (2024) as well as recommendations concerning model selection for calculating conservative estimates of the calculated variables.

## 2 DESCRIPTION OF MODELS

The models described below assume that a pesticide patch is represented by a cylinder with radius  $r_e(t')$  and depth  $H(t')$ , where  $t'$  is the time post-release. It is assumed that the horizontal and vertical growths are independent allowing for each direction to be modelled separately and then combined. This assumption is consistent with the relationships established by Okubo (1971) which were based on data from areas in which the dispersing patches did not interact with the seabed. There are three components to the models: the horizontal dispersion, the vertical extent, and the concentration distribution within the cylindrical patch. For each component two models are examined.

The horizontal dispersion models are solutions to the diffusion equation which are Gaussian distributions. One model assumes a constant dispersion coefficient (Fickian model) and the other model assumes the Okubo (1971) time-varying dispersion coefficient (Okubo Model). Models describing the vertical extent of the patch are given. One model assumes that the patch has a constant vertical depth throughout its growth. This model yields analytic solutions. The other model imposes a vertical growth structure up to a maximum depth and yields equations that must be solved numerically.

Models predicting the concentration distribution of released pesticide within the patch are given. The models assume that a pesticide patch is toxic if it contains concentrations above an Environmental Quality Standard (EQS) concentration,  $C_{eqs}$ . The mean concentration model has a uniform concentration in the horizontal. The Gaussian concentration model assumes a radial Gaussian distribution of concentration in the horizontal. Both the mean and Gaussian models assume a uniform concentration distribution in the vertical.

Details of the models are given below. The models predict quantities that may be of interest to regulators: the maximum horizontal radius of the toxic patch,  $r_{max}$  the time post-release at which this occurs,  $t_{max}$ , and the total time that the patch contains toxic concentrations,  $t_{tox}$ .

### 2.1 HORIZONTAL DISPERSION MODELS

#### 2.1.1 FICKIAN MODEL

Mathematically, the horizontal spread of a bath pesticide due to dispersion can be described by the diffusion equation (Crank, 1975)

$$\frac{\partial C}{\partial t} = K_x \frac{\partial^2 C}{\partial x^2} + K_y \frac{\partial^2 C}{\partial y^2} \quad (2.1)$$



where  $C(x, y, t)$  is the depth-averaged pesticide concentration at horizontal coordinates  $x$  and  $y$  at time  $t$  and  $K_x/K_y$  are the horizontal dispersion coefficients in the  $x / y$  directions . For an instantaneous source released at  $(x, y, t) = (0,0,0)$  on an infinite horizontal plane, the solution to (2.1) is given by Lee et al. (2009)

$$C(x, y, t) = \frac{M}{4\pi(K_x K_y)^{\frac{1}{2}} t} e^{-\left(\frac{x^2}{4K_x t} + \frac{y^2}{4K_y t}\right)} \quad (2.2)$$

where  $M$  is the total mass of the released bath pesticide. Equation (2.2) is a Gaussian relationship with the variances in  $x$  and  $y$  directions given by  $\sigma_x^2 = 2K_x t$  and  $\sigma_y^2 = 2K_y t$  , respectively, the mean variance defined as  $\sigma_x \sigma_y$  (Lee et al., 2009), and the standard deviation given by  $\sqrt{\sigma_x \sigma_y}$ . For a fixed time, the contours of constant concentrations are ellipses. For the case where the horizontal dispersion coefficient is independent of direction, i.e.,  $K_x = K_y = K_h$  the concentrations vary radially which can be observed by rewriting (2.2) as (Crank, 1975)

$$C(r, t) = \frac{M}{4\pi K_h t} e^{-r^2/4K_h t} \quad (2.3)$$

where  $r = \sqrt{x^2 + y^2}$  is the radial distance from the point source and the radial variance is given by (Lee et al., 2009)

$$\sigma_r^2 = \sigma_x^2 + \sigma_y^2 = 4K_h t \quad (2.4)$$

In this case, the contours of constant concentrations are circles.

### 2.1.2 OKUBO MODEL

In reality, as a result of the spatially varying flows in the ocean, pesticide patches do not evolve as simple ellipses or circles (Lee et al., 2009). To address this, one approach is to define the equivalent radius,  $r_e(c)$ , as the radius of a circular patch which has the same area as that contained within the pesticide contour of concentration  $c$  (Okubo, 1968; 1971; Lee et al. 2009). Thus, a given pesticide concentration distribution can be described by a radially symmetric function  $\hat{C}(t, r_e)$  where  $\hat{C}(t, r_e(c)) = c$  (Lee et al., 2009). It can be shown that the equivalent variance,  $\sigma_{rc}^2$ , is given by

$$\sigma_{rc}^2 = 2\sigma_x \sigma_y \quad (2.5)$$

i.e., twice the mean variance (Okubo, 1968). Lee et al. (2009) give the following interpretation of the equivalent variance: it is “the tracer-weighted average of the area enclosed by the tracer contours” where in our case the tracer is the pesticide being released. Here we will be using the

empirical time dependent relationship of the equivalent radial variance determined by Okubo (1968; 1971),

$$\sigma_{rc}^2 = \alpha t^\beta \quad (2.6)$$

As in Lee et al. (2009), we define the apparent diffusivity,  $K_a$ , as

$$K_a(t) = \frac{1}{4} \frac{\partial \sigma_{rc}^2}{\partial t} \quad (2.7)$$

Crank (1975) showed that the solution of the constant dispersion coefficient case, equation (2.3), can be used to find the solution using a time-dependent dispersion coefficient  $K_a(t)$ , as defined by equations (2.6) and (2.7). We outline the steps here. For the time-dependent dispersion coefficient case where the horizontal coefficient is independent of direction, the diffusion equation (2.1) becomes

$$\frac{\partial C}{\partial t} = K_a(t) \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) \quad (2.8)$$

To remove the time dependence of the dispersion coefficient in (2.8), Crank (1975) defined

$$T(t) = \int_0^t K_a(t') dt' \quad (2.9)$$

which gives

$$dT = K_a(t) dt \quad (2.10)$$

Substituting (2.10) into (2.8) gives

$$\frac{\partial C}{\partial T} = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \quad (2.11)$$

Noting that equation (2.11) is a special case of equation (2.1) with  $K_x = K_y = 1$  and  $t = T$ , the solution to (2.11) is given by equation (2.3) with  $K_h = 1$  and  $t = T$ , and is given by

$$C(T, r) = \frac{M}{4\pi T} e^{-r^2/4T} \quad (2.12)$$

Evaluating (2.9), using (2.7), gives

$$T(t) = \frac{1}{4} \sigma_{rc}^2 \quad (2.13)$$

Substituting (2.13) into (2.12) gives

$$C(t, r) = \frac{M}{\pi \sigma_{rc}^2} e^{-r^2 / \sigma_{rc}^2} \quad (2.14)$$

This is the solution given by Okubo (1968). Note that the solution for the constant horizontal coefficient of diffusivity case, i.e., equation (2.3), can be written in the same form as (2.14) using the radial variance defined in equation (2.4). From here forward, we will refer to the use of a constant horizontal coefficient of diffusivity as the Fickian horizontal dispersion model and the use of the time varying horizontal coefficient of diffusivity as defined by (2.6) and (2.7) as the Okubo horizontal dispersion model. Also we use  $\sigma^2$  to represent  $\sigma_r^2$  for the Fickian model and  $\sigma_{rc}^2$  for the Okubo model. Although Lee et al. (2009) recommend using the equivalent variance (i.e., the Okubo horizontal dispersion model) since it is independent of the actual shape of the patch, we will examine results from both models since the Fickian approach is often used.

## 2.2 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 assume there is a vertical barrier that limits the vertical extent of the pesticide patch. The vertical barrier could be a thermocline or the seabed and will depend on local hydrographic conditions.

### 2.2.1 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 growth:

$$H(t') = \begin{cases} H_0 & \text{if } t' = 0 \\ H_{\max} & \text{if } t' > 0 \end{cases} \quad (2.15)$$

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.

### 2.2.2 VERTICAL GROWTH

The vertical growth model was proposed by (Page et al., 2023) and is given by equation (2.16). 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 which point it remains a constant depth.

$$H(t') = \begin{cases} H_0 + \sqrt{K_z t'} & \text{if } H < H_{\max} \\ H_{\max} & \text{if } H \geq H_{\max} \end{cases} \quad (2.16)$$

$K_z$  is the vertical coefficient of diffusivity and it is assumed to be constant through time and depth. Equation (2.16) can be written as

$$H(t') = \begin{cases} H_0 + \sqrt{K_z t'} & \text{if } t' < t_{\text{growth}}^* \\ H_{\max} & \text{if } t' \geq t_{\text{growth}}^* \end{cases} \quad (2.17)$$

where  $t_{\text{growth}}^*$  is given by

$$t_{\text{growth}}^* = \frac{(H_{\max} - H_0)^2}{K_z} \quad (2.18)$$

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.

### 2.3 THREE DIMENSIONAL CONCENTRATION MODELS

Concentration solutions given for the horizontal dispersion model are the amount of pesticide per unit area. Since we are assuming that the growth of a pesticide patch in the horizontal direction is independent of its vertical growth, we can combine the horizontal and vertical models to determine the concentration per unit volume. The independence of pesticide patch growth in the horizontal and vertical directions suggest the impact of the vertical extent of the patch is seen in the concentration and not the horizontal spread (i.e. the horizontal scale of the patch), as suggested by Okubo (1971).

For both the constant depth and vertical growth models, we are assuming that the pesticide is uniformly distributed in the vertical. Thus the concentration per unit volume at a given depth can be determined by dividing the concentration per unit area in (2.14) by the depth  $H(t')$ :

$$C(t', r, z) = \begin{cases} \frac{M}{\pi \sigma^2 (t_0 + t') H(t')} e^{-r^2 / \sigma^2 (t_0 + t')} & \text{if } z \leq H(t') \\ 0 & \text{if } z > H(t') \end{cases} \quad (2.19)$$

where  $t_0$  takes into account the initial patch size and is dependent on the horizontal dispersion model, as discussed below in section 2.3.1. In (2.19)  $H(t')$  is given by either (2.15) or (2.17) for the constant depth or vertical growth model, respectively. It is assumed that at a given radius, the patch concentration is constant throughout its depth  $z$ ; note that there is no dependence on  $z$  in (2.19). The modelled maximum concentration within the patch at a given time,  $C_{\max}(t')$ , occurs at the centre of the patch, i.e., at  $r = 0$ , and is given by

$$C_{\max}(t') = \frac{M}{\pi\sigma^2(t_0 + t')H(t')} \quad (2.20)$$

The equations above were used previously in the Okubo horizontal dispersion model (Page et al., 2015; 2023).

Below, two models describing the concentration throughout the patch are discussed. Both models assume that a pesticide patch is toxic if it contains concentrations above an Environmental Quality Standard (EQS) concentration,  $C_{\text{eqs}}$ . For both models we define the patch radius and identify its maximum,  $r_{\max}$ , as well as examine the time at which this maximum occurs,  $t_{\max}$ , and the total time that the patch contains toxic concentrations,  $t_{\text{tox}}$ . The use of these models for the growth of aquaculture pesticide patch growth was previously presented in (Page et al., 2023).

### 2.3.1 MEAN MODEL

The mean concentration model assumes that the chemical is uniformly distributed throughout the patch. The pesticide concentration solution given by (2.14) stretches out to infinity, with  $C \rightarrow 0$  as  $r \rightarrow \infty$ . This result is a mathematical construct. In reality, and for practical purposes, the pesticide patch has a finite size. Following Okubo (1968), we assumed that the radius of a circular patch,  $r_e$ , is defined as

$$r_e = n\sigma(t) \quad (2.21)$$

which contains  $(100 \gamma_n)\%$  of the pesticide mass where (see Okubo (1968) for derivation)

$$\gamma_n = 1 - e^{-n^2} \quad (2.22)$$

Computed values of  $\gamma_n$  for different values of  $n$  are given in Table 2.1.

**Table 2.1.** The fraction of pesticide mass  $\gamma_n$  contained within a radius of  $n\sigma_{rc}$  for several values of  $n$ . Note that values of  $\gamma_n$  for  $n = 1$  and  $n = 2$  are in agreement with those published by Okubo (1968). For  $n = 1.5$ , our value of  $\gamma_n$  differs from that of Okubo (1968) but is in agreement with the 0.90 value given by Lawrence et al. (1995).

$n$	$\gamma_n$
0.5	0.22
1	0.63
1.5	0.89
2	0.98
2.5	>0.99

In equation (2.21),  $t$  represents the time since the mass of pesticide was released from a point source. In reality the pesticide patch has an initial finite radius,  $r_0$ . We define  $t_0$  as the time required for a patch from a point source to grow to the initial patch size. From (2.21) we have

$$r_0 = n\sigma(t_0) \quad (2.23)$$

Using (2.4) for the Fickian model gives  $t_0 = r_0^2/(4n^2K_h)$  whereas for the Okubo model (2.6) gives  $t_0 = (r_0^2/n^2\alpha)^{1/\beta}$ . We set

$$t = t_0 + t' \quad (2.24)$$

in the horizontal concentration equations to account for the initial patch size.

The patch volume,  $V_{\text{patch}}$ , at a given time is given by the product of the patch horizontal area and the depth

$$V_{\text{patch}} = \pi n^2 \sigma^2(t_0 + t') H(t') \quad (2.25)$$

where  $H(t')$  depends on the vertical model. For a patch containing a uniformly distributed pesticide concentration, the concentration is simply the average concentration,  $C_{\text{avg}}$ , given by

$$C_{\text{avg}} = \frac{M_{\text{patch}}}{V_{\text{patch}}} \quad (2.26)$$

where  $M_{\text{patch}}$  is the mass of pesticide contained within the patch. Since we are using (2.21) to define the patch radius,  $M_{\text{patch}} = \gamma_n M$ . Thus, the mass within the patch is a proportion of the mass of quantity used in the treatment. The mass of the pesticide used in the treatment,  $M$ , is a function of the treatment concentration,  $C_0$ , and the treatment volume,  $V_0$ , i.e.,

$$M = V_0 C_0 \quad (2.27)$$

Thus we can express (2.26) as

$$C_{\text{avg}} = \frac{\gamma_n V_0 C_0}{\pi n^2 \sigma^2(t_0 + t') H(t')} \quad (2.28)$$

For a given treatment volume,  $V_0$ , and treatment concentration,  $C_0$ , the average concentration decreases with time since the total amount of mass in the patch remains constant and the volume increases. Assuming the patch is initially toxic, i.e.,  $C_0 > C_{\text{eqs}}$ , the patch is toxic until  $C_{\text{avg}} = C_{\text{eqs}}$ ,

after which it is no longer toxic. Since the patch size is always increasing, this also coincides with the time  $t'_{\max}$ , at which the maximum toxic patch size occurs, i.e., for the mean concentration model  $t'_{\max} = t'_{\text{tox}}$ , where  $t'_{\text{tox}}$  is the length of time that a patch is considered toxic. This behaviour was discussed in Page et al. (2023). We wish to know the time  $t'_{\max}$  at which  $C_{\text{avg}} = C_{\text{eqs}}$ , and the resulting patch radius,  $r_{\text{eqs}}$ . Defining the dilution factor,  $R$ , as

$$R = \frac{C_0}{C_{\text{eqs}}} \quad (2.29)$$

Substituting  $C_{\text{avg}} = C_{\text{eqs}}$  and using (2.29), we write (2.28) as

$$1 = \frac{\gamma_n V_0 R}{\pi n^2 \sigma^2 (t_0 + t'_{\max}) H(t'_{\max})} \quad (2.30)$$

which can be used to find  $t'_{\max}$ .

Using (2.21), the maximum size of the toxic patch,  $r_{\max}$ , can be calculated from (2.30) and is given by

$$r_{\max}^2 = \frac{\gamma_n V_0 R}{\pi H(t'_{\max})} \quad (2.31)$$

### 2.3.2 GAUSSIAN MODEL

An alternative to the mean concentration model, which assumes a spatially homogeneous distribution of the pesticide, is to use the Gaussian distribution of pesticide concentration to determine the patch size. At any given time post-release,  $t'$ , the size of the toxic patch can be defined as the radius at which the concentration equals the EQS concentration since only concentrations within this radius are greater than the EQS. We set  $C(t', r, z) = C_{\text{eqs}}$  in (2.19):

$$C_{\text{eqs}} = \frac{M}{\pi \sigma^2 (t_0 + t') H(t')} e^{-r_{\text{eqs}}^2 / \sigma^2 (t_0 + t')} \quad (2.32)$$

and solve for  $r_{\text{eqs}}^2$

$$r_{\text{eqs}}^2 = -\sigma^2 (t_0 + t') \cdot \ln \left[ \frac{\pi C_{\text{eqs}} \sigma^2 (t_0 + t') H(t')}{M} \right] \quad (2.33)$$

Expressing (2.33) as a function of the dilution ratio,  $R$ , gives

$$r_{\text{eqs}}^2 = -\sigma^2 (t_0 + t') \cdot \ln \left[ \frac{\pi \sigma^2 (t_0 + t') H(t')}{V_0 R} \right] \quad (2.34)$$

Equation (2.34) is only valid for the time period during which  $C_{\max} \geq C_{\text{eqs}}$ , or when  $V_0 R \geq \pi\sigma^2(t_0 + t')H(t')$ . Furthermore, depending on the value of  $n$  in equation (2.21) it is possible that  $r_{\text{eqs}}$  is initially larger than the patch size,  $r_e$ . If we define  $\sigma_0 = \sigma(t_0)$ , then setting  $t' = 0$  in (2.34) we get

$$r_{\text{eqs}}^2 = -\sigma_0^2 \cdot \ln \left[ \frac{1}{n^2 R} \right] \quad (2.35)$$

Whereas

$$r_0^2 = n^2 \sigma_0^2 \quad (2.36)$$

Comparing (2.35) and (2.36),  $r_{\text{eqs}}$  is initially larger than the patch size,  $r_0$  if

$$n^2 R > e^{n^2} \quad (2.37)$$

Recalling that  $r_0$  contains 100  $\gamma_n$ % of the pesticide mass (see equation (2.21) and accompanying text), the conditions in equation (2.37) will occur when the quantity of pesticide within the initial  $C_{\text{eqs}}$  concentration contour is greater than  $\gamma_n M$ . It should be noted that, for the Gaussian model, the quantity of pesticide within the toxic patch changes over time and eventually decreases to zero. In contrast, for the mean concentration model, the quantity of pesticide within the toxic patch is constant. In both models, the total quantity of pesticide within the environment is constant for all time. Thus the absence of concentrations above the EQS does not indicate a lack of pesticide in the environment and the spatial scale of the patch continues to grow with time.

For a given time, the radius at which  $C_{\text{eqs}}$  occurs,  $r_{\text{eqs}}$ , can be found by taking the square root of  $r_{\text{eqs}}^2$  given in (2.34). Using the Okubo model, Page et al. (2023) illustrated that (2.34) produces a patch radius that increases with time to a maximum and then decreases until  $C_{\max}(t')$  attains  $C_{\text{eqs}}$  after which all concentrations within the patch are below  $C_{\text{eqs}}$ . The precise details will depend on the patch depth function,  $H(t')$ . To determine the length of time for which the patch contains concentrations above the EQS,  $t'_{\text{tox}}$ , we set  $C_{\max} = C_{\text{eqs}}$  in (2.20)

$$C_{\text{eqs}} = \frac{M}{\pi\sigma^2(t_0 + t'_{\text{tox}})H(t'_{\text{tox}})} \quad (2.38)$$

Which using (2.29) can be written as

$$R - \frac{\pi\sigma^2(t_0 + t'_{\text{tox}})H(t'_{\text{tox}})}{V_0} = 0 \quad (2.39)$$



and then solve for  $t'_{\text{tox}}$  in (2.39). Since the solution depends on the choice of depth and concentration models, they are presented for the different combinations in the next section.

### 3 MODEL SOLUTIONS

For a pesticide patch released from a single cage, we explore solutions to the different combinations of horizontal dispersion (Fickian or Okubo), depth (constant or vertical growth), and concentration (mean or Gaussian) models for a range of treatment cage sizes,  $10 \leq P_{\text{cage}} \leq 500$  (assuming a circular cage) and dilution ratios,  $10^2 \leq R \leq 10^4$ . As in Okubo (1968; 1971), we use  $n = 1.5$  (yielding  $\gamma_n = 0.89$ , see Table 2.1) with  $\alpha = 5.6 \times 10^{-6}$  and  $\beta = 2.22$  (Lawrence et al., 1995). We use typical values of 1.0 and 0.01  $\text{m}^2 \cdot \text{s}^{-1}$  for  $K_h$  and  $K_z$ , respectively (Lewis, 1997). A typical treatment depth,  $H_0$ , of 4 m (Page et al., 2015) and a maximum patch depth,  $H_{\text{const}} = H_{\text{max}}$  of 20 m are used. All parameter values are given in Table 3.1.

**Table 3.1.** Parameter values (or ranges) used in all solutions (both analytic and numeric) presented in this document.

Parameter	Description	Units	Value
$\alpha$	Parameter used in equation (2.6)	-	$5.6 \times 10^{-6}$
$\beta$	Parameter used in equation (2.6)	-	2.22
$n$	Parameter used in equation (2.21)	-	1.5
$K_h$	Horizontal coefficient of diffusivity	$\text{m}^2 \cdot \text{s}^{-1}$	1.0
$K_z$	Vertical coefficient of diffusivity	$\text{m}^2 \cdot \text{s}^{-1}$	0.01
$H_0$	Treatment depth	m	4
$H_{\text{max}}$	Maximum patch depth for all depth models	m	20
$P_{\text{cage}}$	Cage perimeter (assume circular cage)	m	[10,500]
$R$	$C_0/C_{\text{eqs}}$	-	[ $10^2, 10^4$ ]

#### 3.1 CONSTANT DEPTH

For an arbitrary depth function,  $H(t')$ , numerical solutions are likely required to determine the relationship between the maximum size of a toxic patch (where  $C \geq C_{\text{eqs}}$  implies toxicity) for both the Fickian and Okubo dispersion models and the Gaussian concentration and mean concentration models. However, for the simple case of a constant patch depth,  $H(t') = H_{\text{max}}$ , analytical solutions can be found.

### 3.1.1 MEAN CONCENTRATION MODEL

#### 3.1.1.1 FICKIAN DISPERSION MODEL

Using (2.4) in (2.30) we solve for  $t'_{\max}$  to determine the time post-release at which the maximum size of a toxic patch occurs

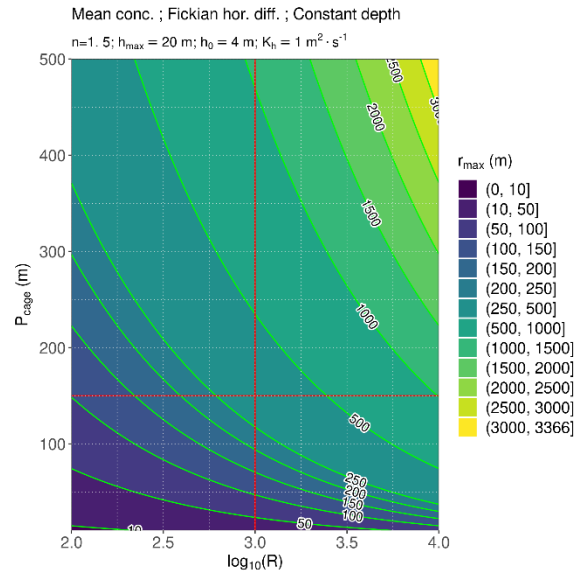
$$t'_{\max} = \frac{\gamma_n V_0 R}{4\pi n^2 K_h H_{\max}} - t_0 \quad (3.1)$$

The size of the patch having an average concentration equal to the EQS can be found from (2.31)

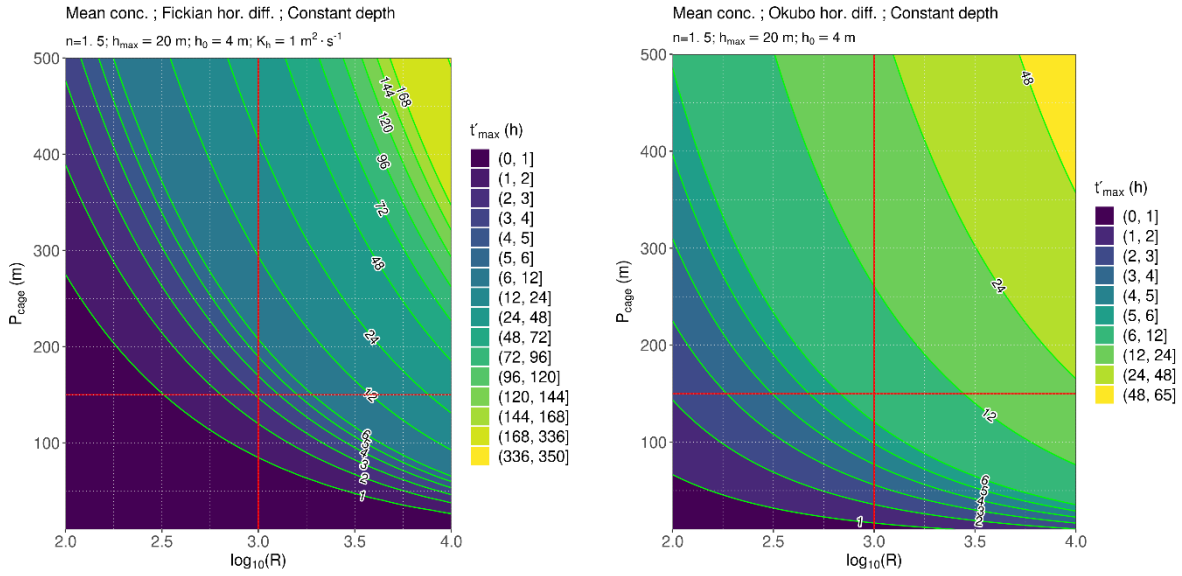
$$r_{\max}^2 = \frac{\gamma_n V_0 R}{\pi H_{\max}} \quad (3.2)$$

It should be noted that, for the mean concentration model with constant depth,  $r_{\max}^2$  is independent of the dispersion coefficient. This is unsurprising since the total volume required to dilute the pesticide concentration to the EQS depends only on the radius (and not the time required to get there) when the depth remains constant. Also recall that for the mean concentration model, the patch is no longer toxic when  $t' > t'_{\max}$ , i.e.,  $t'_{\max} = t'_{\text{tox}}$ .

Solutions to equations (3.1) and (3.2) are shown in Figure 3.1 and Figure 3.2. The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ . Ranges of the calculated values of  $r_{\max}$ ,  $t'_{\max}$ , and  $t'_{\text{tox}}$  are given in Table 3.2.



**Figure 3.1.** Solutions of  $r_{\max}$  (m) for the mean concentration model with constant depth. Note that the solution is independent of the horizontal dispersion model used. Parameters used are given in Table 3.1. 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 3.2.** Solutions of  $t'_{max}$  (h) for the mean concentration model with constant depth using Fickian (left) and Okubo (right) horizontal dispersion models. Note for the mean concentration model  $t'_{max} = t'_{tox}$ . Parameters used are given in Table 3.1. Since  $R = C_0/C_{eqs}$ ,  $\log_{10} R$  gives the order of magnitude dilution factor, i.e.,  $\log_{10} R = 3$  is a factor of 1000 dilution.

**Table 3.2.** Intervals of minimum and maximum of calculated values  $r_{max}$ ,  $t'_{max}$ , and  $t'_{tox}$  for all the combinations of concentration, horizontal dispersion, 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 3.1.

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

### 3.1.1.2 OKUBO DISPERSION MODEL

For the mean depth model, the time at which the maximum size of a toxic patch occurs can be determined by substituting (2.6) into (2.30):

$$n^2 \alpha (t'_{\max} + t_0)^\beta = \frac{\gamma_n V_0 R}{\pi H_{\max}} \quad (3.3)$$

or

$$t'_{\max} = \left( \frac{\gamma_n V_0 R}{n^2 \pi \alpha H_{\max}} \right)^{1/\beta} - t_0 \quad (3.4)$$

From (2.31), the maximum size of the toxic patch is the same as for the Fickian model and given by (3.2). Thus, for the mean concentration model with constant depth, the maximum patch size is independent of the horizontal dispersion model and only the timing of when the maximum patch size occurs depends on the horizontal dispersion model.

Solutions to equations (3.4) and (3.2) are shown in Figure 3.1 and Figure 3.2 (parameter values used are given in Table 3.1). The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ .

### 3.1.2 GAUSSIAN CONCENTRATION MODEL

For the Gaussian concentration model, the time at which the maximum value of  $r_{\text{eqs}}$  occurs can be determined by setting  $\frac{dr_{\text{eqs}}}{dt} = 0$  and solving for  $t$ . From (2.34) we must solve for  $t$ :

$$\frac{d}{dt} \left( -\sigma^2(t) \cdot \ln \left[ \frac{\pi \sigma^2(t) H_{\max}}{R V_0} \right] \right) = 0 \quad (3.5)$$

$$-\frac{d}{dt} (\sigma^2(t)) \cdot \ln \left[ \frac{\pi \sigma^2(t) H_{\max}}{R V_0} \right] - \sigma^2(t) \frac{d}{dt} \left( \ln \left[ \frac{\pi \sigma^2(t) H_{\max}}{R V_0} \right] \right) = 0 \quad (3.6)$$

$$-\frac{d}{dt} (\sigma^2(t)) \cdot \ln \left[ \frac{\pi \sigma^2(t) H_{\max}}{R V_0} \right] - \sigma^2(t) \frac{R V_0}{\pi \sigma^2(t) H_{\max}} \frac{d}{dt} \left( \frac{\pi \sigma^2(t) H_{\max}}{R V_0} \right) = 0 \quad (3.7)$$

$$\frac{d}{dt} (\sigma^2(t)) \left( \ln \left[ \frac{\pi \sigma^2(t) H_{\max}}{R V_0} \right] + 1 \right) = 0 \quad (3.8)$$

The solution to (3.8) is dependent on the horizontal dispersion model used.

### 3.1.2.1 FICKIAN DISPERSION MODEL

Using the Fickian dispersion model (2.4), (3.8) becomes

$$4K_h \left( \ln \left[ \frac{\pi 4K_h (t'_{\max} + t_0) H_{\max}}{RV_0} \right] + 1 \right) = 0 \quad (3.9)$$

Solving for  $t'_{\max}$  gives the time post-release at which the maximum patch size occurs,  $t'_{\max}$  :

$$t'_{\max} = \frac{RV_0}{4e\pi K_h H_{\max}} - t_0 \quad (3.10)$$

To find the maximum patch size,  $r_{\max}$ , we substitute (3.10) into (2.34) and simplify, giving

$$r_{\max}^2 = \frac{RV_0}{e\pi H_{\max}} \quad (3.11)$$

It should be noted that, for the Gaussian concentration model with constant depth,  $r_{\max}^2$  is independent of the dispersion coefficient.

In contrast to the mean model, the size of the toxic patch for the Gaussian model is non-zero after it has reached its maximum size. The patch will contain no concentrations above the EQS after the time at which the peak concentration equals the EQS, i.e.,  $C_{\text{eqs}} = C_{\text{max}}$ . From (2.20)

$$C_{\text{eqs}} = \frac{M}{\pi \sigma^2 (t_0 + t') H_{\max}} \quad (3.12)$$

Recalling that  $\sigma^2$  is given by (2.4) for the Fickian case and  $M$  is given by (2.27), we can use equation (3.12) to solve for the time post-deposit  $t'_{\text{tox}}$ :

$$t'_{\text{tox}} = \frac{V_0 R}{4\pi K_h H_{\max}} - t_0 \quad (3.13)$$

When  $t' \geq t'_{\text{tox}}$ , the pesticide patch contains no concentrations above the EQS and occurs at a time  $\Delta t$  after  $t'_{\max}$  where

$$\Delta t = \frac{V_0 R}{4\pi K_h H_{\max}} \left( 1 - \frac{1}{e} \right) \quad (3.14)$$

Solutions to  $r_{\max}$ ,  $t'_{\max}$ ,  $t'_{\text{tox}}$ , given by equations (3.11), (3.10), and (3.13), respectively, are shown in Figure I.1, Figure I.2, and Figure I.3. The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ . Also, the total time during which a patch contains toxic concentrations increases with both the perimeter of the treatment cage and  $R$ .

### 3.1.2.2 OKUBO DISPERSION MODEL

Using the Okubo dispersion model (2.6), (3.8) becomes

$$\alpha \beta (t'_{\max} + t_0)^{\beta-1} \left( \ln \left[ \frac{\pi \alpha (t'_{\max} + t_0)^\beta H_{\max}}{RV_0} \right] + 1 \right) = 0 \quad (3.15)$$

There are two solutions to (3.15):  $t'_{\max} = -t_0$ , which is not physically realistic, and

$$\ln \left[ \frac{\pi \alpha (t'_{\max} + t_0)^\beta H_{\max}}{RV_0} \right] + 1 = 0 \quad (3.16)$$

Solving for  $t'_{\max}$  gives the time post-release at which the maximum patch size occurs,  $t'_{\max}$  :

$$t'_{\max} = \left( \frac{RV_0}{e\pi\alpha H_{\max}} \right)^{\frac{1}{\beta}} - t_0 \quad (3.17)$$

To find the maximum patch size,  $r_{\max}$ , substitute (3.17) into (2.34):

$$r_{\max}^2 = -\alpha \left( \frac{RV_0}{e\pi\alpha H_{\max}} \right) \cdot \ln \left[ \frac{\pi \alpha \left( \frac{RV_0}{e\pi\alpha H_{\max}} \right) H_{\max}}{RV_0} \right] \quad (3.18)$$

Simplifying (3.18) gives

$$r_{\max}^2 = \frac{RV_0}{e\pi H_{\max}} \quad (3.19)$$

which is identical to the solution of  $r_{\max}^2$  for the Fickian case with constant depth and a Gaussian concentration distribution. (see equation (3.11)). To find the time after which the patch contains no concentrations above the EQS, we use (2.6) in (3.12)

$$t'_{\text{tox}} = \left( \frac{RV_0}{\pi\alpha H_{\max}} \right)^{\frac{1}{\beta}} - t_0 \quad (3.20)$$

When  $t' \geq t'_{\text{tox}}$ , pesticide patch contains no concentrations above the EQS and occurs at a time  $\Delta t$  after  $t'_{\max}$  where

$$\Delta t = \left( \frac{RV_0}{\pi\alpha H_{\max}} \right)^{\frac{1}{\beta}} \left[ 1 - \frac{1}{e^{1/\beta}} \right] \quad (3.21)$$

Solutions to  $r_{\max}$ ,  $t'_{\max}$ ,  $t'_{\text{tox}}$ , given by equations (3.19), (3.17), and (3.20), are shown in Figure I.1, Figure I.2, and Figure I.3, respectively. The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ . Also, the total time during which a patch contains toxic concentrations increases with both the perimeter of the treatment cage and  $R$ .

## 3.2 VERTICAL GROWTH

Here we explore the behaviour of the patch radius size when vertical growth model, see equation (2.16), is used. Since there are no simple analytical solutions for  $t'_{\max}$ ,  $t'_{\text{tox}}$ , and  $r_{\max}$  for this case, numerical solutions are calculated to explore the behaviour for a range of  $R$  and  $P_{\text{cage}}$  values. All calculations were done using the statistical software R version 4.2.0. Parameter values used are given in Table 3.1.

### 3.2.1 MEAN CONCENTRATION MODEL

#### 3.2.1.1 FICKIAN DISPERSION MODEL

Using the function *uniroot* from the R software package version 4.2.0, the root to (2.30) with  $H(t')$  given by (2.16) and  $\sigma^2$  given by (2.4),  $t'_{\max}$ , was estimated. The maximum radius,  $r_{\max}$ , was found by substituting the estimated value of  $t'_{\max}$ , into (2.31). Solutions are shown in Figure I.4 and Figure I.5 (parameter values used are given in Table 3.1). The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ .

#### 3.2.1.2 OKUBO DISPERSION MODEL

The time at which the largest toxic patch occurs,  $t'_{\max}$ , is found using the same method as for the mean model with Fickian horizontal dispersion and vertical growth. In this case, the root to (2.30) is found using  $\sigma^2$  given by (2.6). The maximum radius,  $r_{\max}$ , was found by substituting the estimated value of  $t'_{\max}$ , into (2.31). Solutions are shown in Figure I.4 and Figure I.5 (parameter values used are given in Table 3.1). The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ .

### 3.2.2 GAUSSIAN CONCENTRATION MODEL

#### 3.2.2.1 FICKIAN DISPERSION MODEL

For the Gaussian concentration model with Fickian horizontal dispersion and vertical growth, the maximum toxic patch size,  $r_{\max}$ , and the time at which it occurs,  $t'_{\max}$ , are found by finding the maximum of equation (2.34) using (2.4) for  $\sigma^2(t_0 + t')$  and (2.16) for  $H(t')$ . This is estimated numerically using the function *optimize* from the R software package version 4.2.0. The total length of time during which a patch contains concentrations above the EQS,  $t'_{\text{tox}}$ , is given by the root to equation (2.39) which is found using the function *uniroot* from the R software package version 4.2.0 using (2.4) for  $\sigma^2(t_0 + t')$  and (2.16) for  $H(t')$ .

Solutions for  $r_{\max}$ ,  $t'_{\max}$ , and  $t'_{\text{tox}}$  are shown in Figure I.6, Figure I.7, and Figure I.8, respectively. The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ . Also, the total time during which a patch contains toxic concentrations increases with both the perimeter of the treatment cage and  $R$ .

### 3.2.2.2 OKUBO DISPERSION MODEL

The radius of the largest toxic patch,  $r_{\max}$ , that time at which it occurs,  $t'_{\max}$ , and the total time that the patch contains toxic concentrations,  $t'_{\text{tox}}$ , are found using the same methods as for the Gaussian model with Fickian horizontal dispersion and vertical growth (see above). In this case,  $\sigma^2(t_0 + t')$  is given by (2.6).

Solutions for  $r_{\max}$ ,  $t'_{\max}$ , and  $t'_{\text{tox}}$  are shown in Figure I.6, Figure I.7, and Figure I.8, respectively. The maximum size of the toxic patch and the time required to achieve it increase with both the perimeter of the treatment cage and  $R$ . Also, the total time during which a patch contains toxic concentrations increases with both the perimeter of the treatment cage and  $R$ .



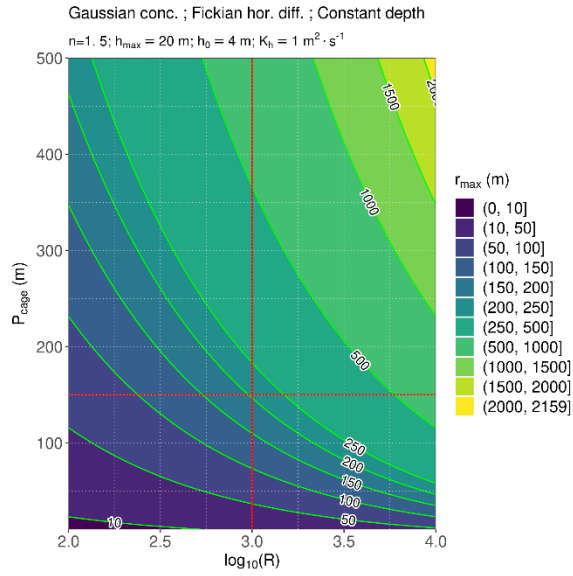
## 4 SUMMARY

- Other than the Okubo horizontal dispersion model, all the models require choices of parameters. The model solutions are sensitive to the value of these parameters. In this document, the impact of the dilution ratio and the cage size were explored, all other parameters were fixed.
- Analytical solutions of the maximum size of the toxic patch, the time at which this occurs, and the total time patch contains toxic concentrations are easily derived when a constant patch depth is assumed. Analytical solutions can be used to give insight on how parameters impact solutions.
- When the constant depth solution is used, maximum patch size is independent of the horizontal dispersion model.
- For all combinations of horizontal dispersion, depth, and concentration models, 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  $R$ . The details of the solution, however, vary with the combination of horizontal dispersion, depth, and concentration models.
- An accompanying report (Haigh et al., 2024) compares solutions of the models, examines sensitivity of some of the parameters, and recommends model selection for regulatory use.
- For a net pen perimeter of 150 m and a dilution ratio of 3, the toxic patch achieves a maximum size between 205 m and 358 m which occurs between 2.9 h and 7.3 h post-release, and no toxic concentrations are present after 3.1 h to 11.4 h post-release

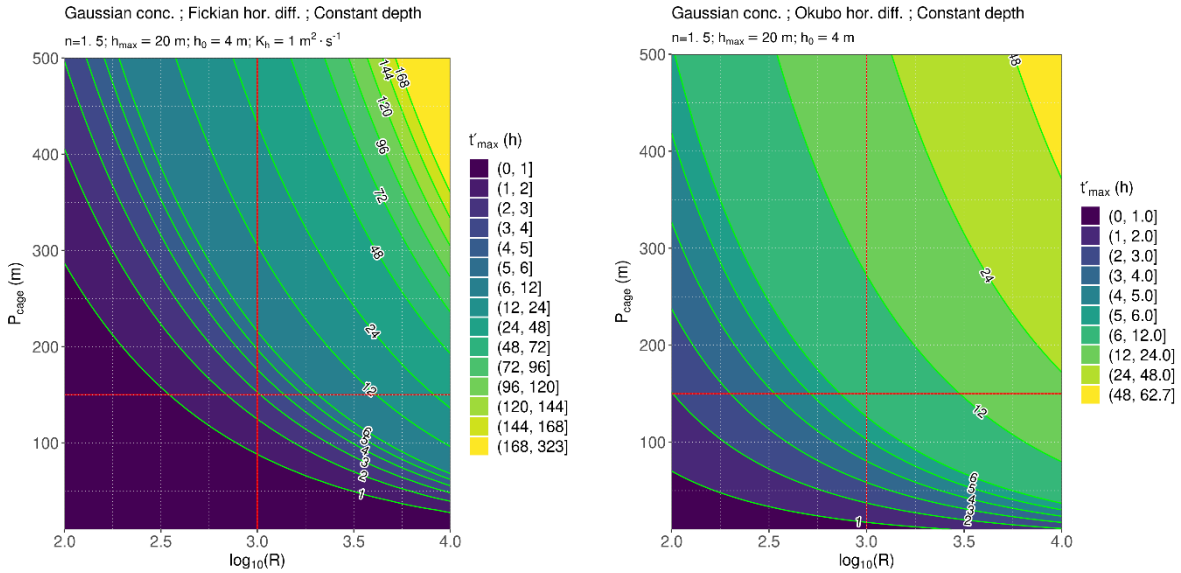
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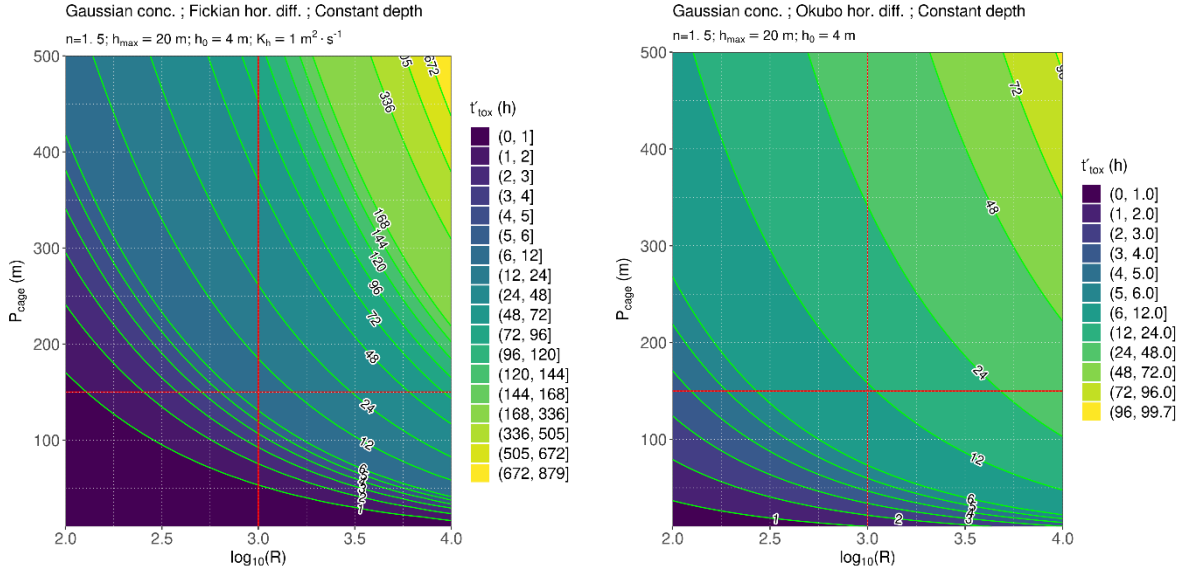
# APPENDIX I: MODEL SOLUTION FIGURES



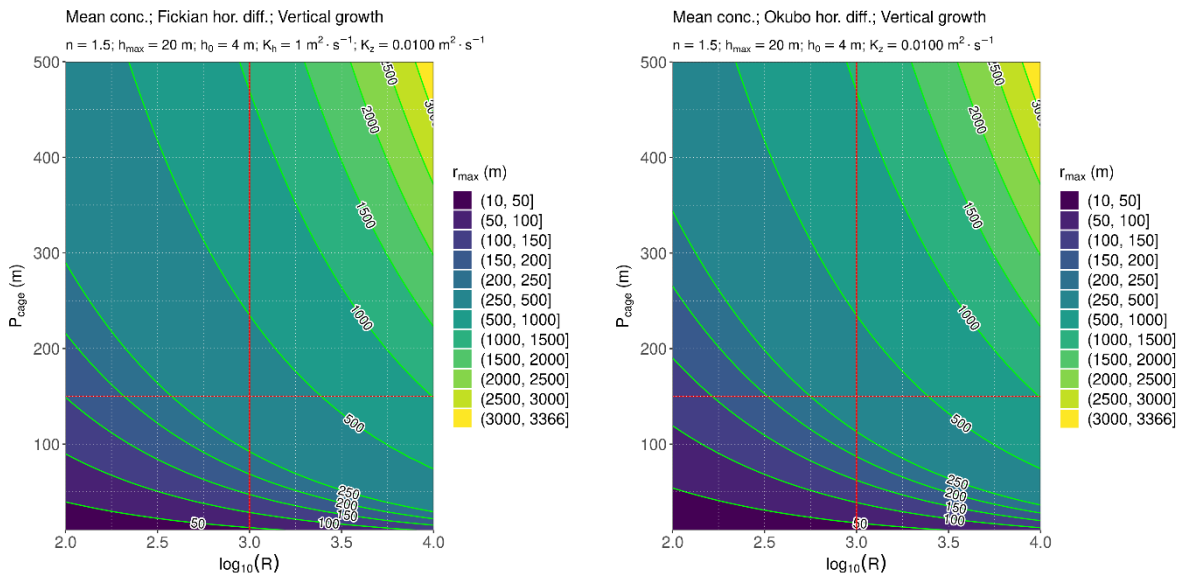
**Figure I.1.** Solutions of  $r_{max}$  (m) for the Gaussian concentration model with constant depth. Note that the solution is independent of the horizontal dispersion model used. Parameters used are given in Table 3.1. Since  $R = C_0/C_{eqs}$ ,  $\log_{10} R$  gives the order of magnitude dilution factor, i.e.,  $\log_{10} R = 3$  is a factor of 1000 dilution.



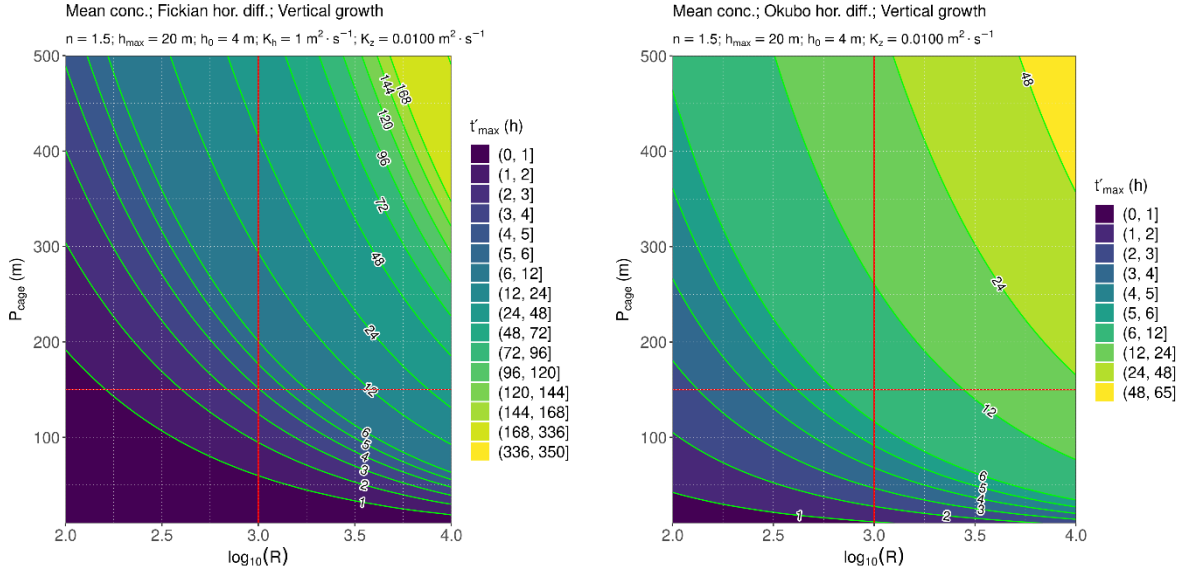
**Figure I.2.** Solutions of  $t'_{max}$  (h) for the Gaussian concentration model with constant depth using Fickian (left) and Okubo (right) horizontal dispersion models. Parameters used are given in Table 3.1. Since  $R = C_0/C_{eqs}$ ,  $\log_{10} R$  gives the order of magnitude dilution factor, i.e.,  $\log_{10} R = 3$  is a factor of 1000 dilution.



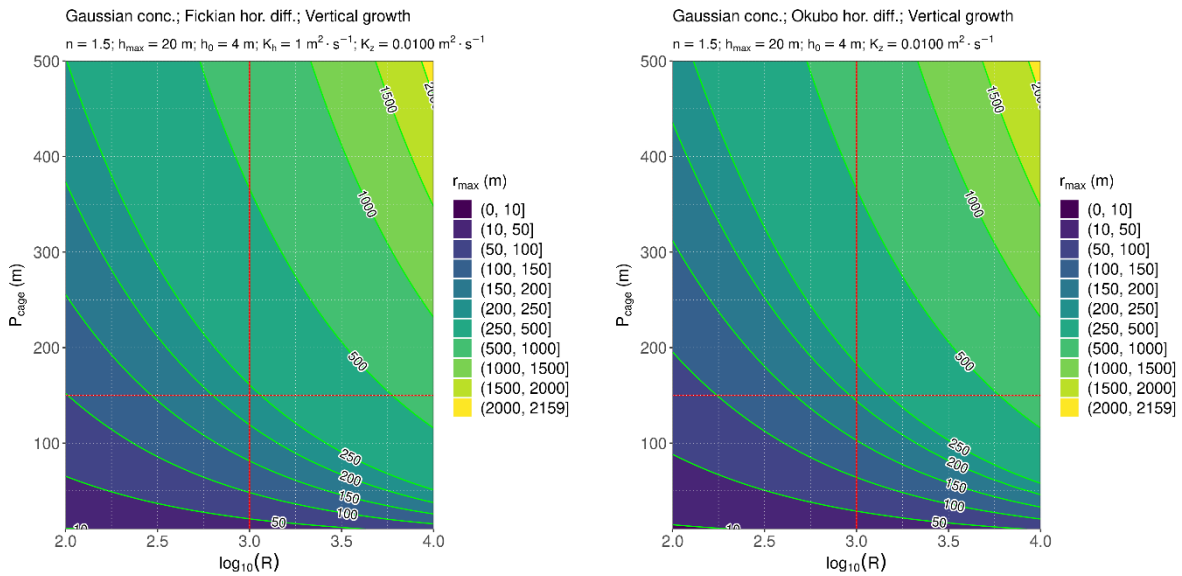
**Figure I.3.** Solutions of  $t'_{tox}$  (h) for the Gaussian concentration model with constant depth using Fickian (left) and Okubo (right) horizontal dispersion models. Parameters used are given in Table 3.1. Since  $R = C_0/C_{eqs}$ ,  $\log_{10} R$  gives the order of magnitude dilution factor, i.e.  $\log_{10} R = 3$  is a factor of 1000 dilution.



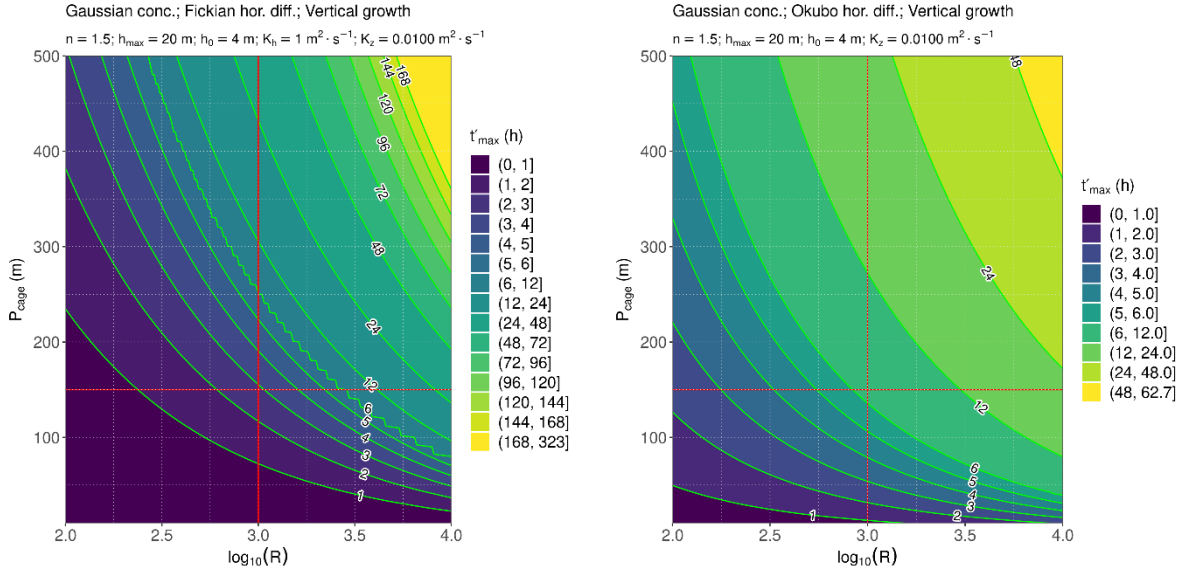
**Figure I.4.** Solutions of  $r_{max}$  (m) for the mean concentration model with vertical growth using Fickian (left) and Okubo (right) horizontal dispersion models. Parameters used are given in Table 3.1. Since  $R = C_0/C_{eqs}$ ,  $\log_{10} R$  gives the order of magnitude dilution factor, i.e.,  $\log_{10} R = 3$  is a factor of 1000 dilution.



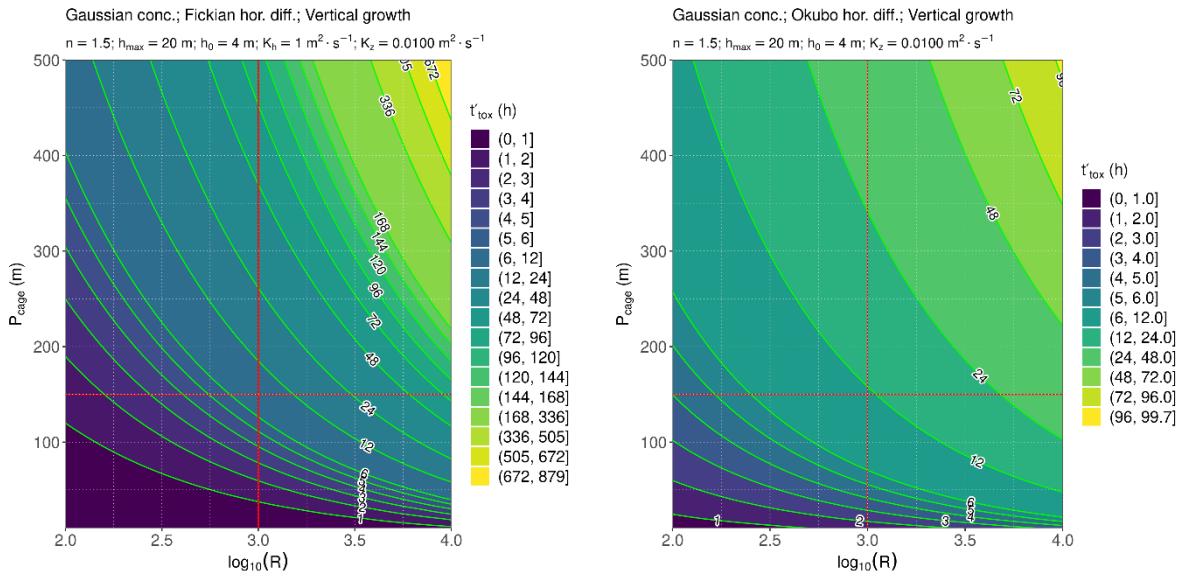
**Figure I.5.** Solutions of  $t'_{\max}$  (h) for the mean concentration model with vertical growth using Fickian (left) and Okubo (right) horizontal dispersion models. Note for the mean concentration model  $t'_{\max} = t'_{\text{tox}}$ . Parameters used are given in Table 3.1. Since  $R = C_0/C_{\text{eqs}}$ ,  $\log_{10} R$  gives the order of magnitude dilution factor, i.e.,  $\log_{10} R = 3$  is a factor of 1000 dilution.



**Figure I.6.** Solutions of  $r_{\max}$  (m) for the Gaussian concentration model with vertical growth using Fickian (left) and Okubo (right) horizontal dispersion models. Parameters used are given in Table 3.1. 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 I.7.** Solutions of  $t'_{\max}$  (h) for the Gaussian concentration model with vertical growth using Fickian (left) and Okubo (right) horizontal dispersion models. Parameters used are given in Table 3.1. 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 I.8.** Solutions of  $t'_{\text{tox}}$  (h) for the Gaussian concentration model with vertical growth using Fickian (left) and Okubo (right) horizontal dispersion models. Parameters used are given in Table 3.1. 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.