Engineering Mathematics

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Investigating Collisional Exchange as a Model for Pesticide Dispersal

Conor Cullen, Alessandro Scibetta, Louie Sellwood

Abstract

The use of chemical pesticides within the agricultural industry has been practised for millennia [1]. However, their use has recently been met with strong public opposition due to the multitude of negative effects that they impose on our environment. One of the most common methods of administering treatment is with the use of mechanical sprayers, which has become one of the main contributors to the problem termed as pesticide drift [2]. In this study we investigate the effectiveness of a collisional exchange model that employs local insect populations as carriers of the pesticide, which is administered to the crop population via pesticide-crop and insect-crop interactions. The movement of the insects and pesticide are characterised by Lévy Flight and Gaussian distributions respectively throughout the development of the model. Specialising our general model to simulate for Honeybees and Sunflower crops, our findings suggest that increasing the number of insects is roughly twice as effective in comparison to increasing the amount of pesticide used.

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1 Introduction

Agriculture can be described as the practice of farming, including the cultivation of land and breeding of animals for a wide range of uses such as production of food, wool or other products [3]. As the global demand for crop growth increases, the need for chemical pesticides has become a crucial requirement of the agricultural industry. Without this modern technology, the tripling of crop yields between 1962 and 1990 would have required the cultivation of an additional 25 to 30 million square kilometres of land [2]. It has further been shown that without adequate crop protection, UK farmers would see a 10-20% decline in yields of wheat, barley, sugar beet, potato and oil-seed rape [4].

Chemical pesticides is the umbrella term for substances that control the effects of pests on a crop. However, there are three types of pesticide that dominate this part of the chemical industry [5]:

- Herbicides: substances that kill or inhibit growth of unwanted plants (i.e. weeds, grasses, etc.), which account for 50-60% of pesticides applied worldwide.
- Insecticides: substances that kill arthropod pests (i.e. insects, mites, etc.), which account for 20-30% of pesticides applied worldwide.
- Fungicides: substances that destroy or prevent the growth of pathogenic fungi, which account for 10-20% of pesticides applied worldwide.

The use of pesticides within the agricultural industry has been widely adopted and is often touted as the future of agriculture and part of the solution to the ever-increasing global food demand. The United Nations Food and Agriculture Organisation has estimated that we currently lose 20-40% of our global crop yields due to plant pests (biological organisms that interfere with the production of crops, affecting quality and/or yield) and diseases [6]. However, despite being commonplace within the industry, there is growing public concern regarding its widespread use. Increasing public concern regarding the use of pesticides has placed a particular emphasis on the need to make this process as efficient as possible. Although large amounts of pesticides are applied, it has been estimated that less than 0.1% of the chemicals applied actually reach the target pests [7]. Due to the methods currently used to administer pesticides, their large-scale use can lead to damage to human health, environmental contamination and property damage [8].

The objective of pesticide applications is to apply the recommended amount of product uniformly onto the target, without contaminating other non-target areas [9]. One of the most common methods employed to apply pesticides is through the use of mechanical sprayers. Mechanical sprayers can be used in both pre-emergent and post-emergent (referring to the germination status of the crop) pesticide applications. One of the main problems with the use of mechanical sprayers is the vast range of droplet sizes that are outputted by traditional sprayers. The different droplet sizes exhibit dramatically different dispersal dynamics that generally leads to inconsistent and inefficient pesticide applications.

Due to the importance of pesticide use within the agricultural industry and the significance of their potential effects, it is imperative to understand the dynamics of the dispersal of these chemicals. This must be done in order to find the most efficient delivery of protection to a crop population being treated, whilst minimising the negative side effects caused by their use. Attempting to achieve the most efficient dispersal of these chemicals is a significant task. This is due to both the scale of the operation and the number of variables that govern results; variables including weather conditions, insect populations and species of crop.

By utilising the native insect populations, we aim to model a new method of chemical dispersal, which improves the efficiency through the implementation of a sustainable approach. We attempt to optimise

the reduction of the necessary quantity of chemical used. Estimating the movement of both chemical particles and insects through agent based modelling is a viable method to achieve this objective. The specific positions and concentrations can be determined by a series of well defined equations. The task at hand is to vary the parameters that define the initial concentration of the chemical and the number of agents in the model and observe its impact on the rate of dispersal and coverage of the pesticide.

2 Assumptions

In order to model the dynamics of pesticide dispersal, the following assumptions have to be made:

- The model considers a two-dimensional simulation space over a specified finite area referred to as the field.
- The field is contained within a circular reflective boundary that confines the movement of *insects* and *chemicals* to a circle that is slightly larger than the dimensions of the field.
- There are three agents considered to be present in the simulation space:
  - *Chemicals* represent particulates of the pesticide being dispersed.
  - *Insects* represent individuals of the insect population, employed to disperse *chemicals*.
  - *Crops* represent the pesticide targets.
- The transmission of *chemicals* follows a rate equation [10] that relates contacts to the probability of transmission.
- All members of the *insect* and *crop* populations are uniform in size and circular in shape. Our simulations use *insects* and *crops* with radius 7.5 mm and 75 mm respectively.
- Each member of the *insect* population follows the same type of random walk, characterised by the Lévy distribution [11]. Similarly, all *chemical* movement is characterised by the normal distribution in the form of Brownian Motion.
- Each instance of a *chemical* is defined as a body composed of distinct particles, each containing 0.01 mol of active pesticide.
- Time is considered in discrete steps. During the course of a time step, all *insects* and *chemicals* change position according to the probability distributions chosen to characterise their respective random walks.
- At time $t = 0$, *insects* are initialised in random positions across the area of the field.
- The transmission of the *chemical* from *insect* to *crop* follows the same rate equation as the transmission of the *chemical* from *insect* to *insect*. The transmission time is negligible.
- The transmission occurs at each discrete time step, where the *insect* or *chemical* is found to be close enough to its target. In other words, collisions are only considered at each time interval when the updated positions of the agents are calculated.

3 Characterising Insect Motion

The movement patterns of insects are dependent on a number of factors, including the insect species, the objective of their navigation and external conditions. A flying insect will perform path integration on its outward journey from its nest; the insect continuously integrates information about changes in distances and direction to compute the vector linking its current position to its starting point [12].

Here we define the movement trajectory of each moving entity as a collection of fixed locations observed over time, bounded within the confines of the field. We characterise the path of each individual agent using a stochastic process known as a random walk. A random walk consists of a succession of random steps over a defined space. Although the movement patterns of insects are not truly random, the distributions that govern displacement and turning angle provide an experimental representation of insect motion, which is suitable for modelling the number of collisions. There are a number of random walks that could be considered in this model, but we have considered the following to be the most relevant.

3.1 Brownian Motion

This is a simple random walk model that describes the seemingly 'random' motion of gas particles. This type of motion lends itself well to characterising the motion of an airborne *chemical* body since the position of a particle is considered completely random within continuous time.

Given a particle's 2-D coordinates in the x-y plane ($x(t)$, $y(t)$), the particle's position at the next step ($x(t+1)$, $y(t+1)$) given by its position at time t plus a normally distributed random scalar value multiplied by the step size,

$$x(t+1) = x(t) + h\epsilon, \tag{1}$$
$$y(t+1) = y(t) + h\phi,$$

where ϵ and ϕ are normally distributed random variables with mean 0 and variance 1, and h is the chosen step size. We choose a step size of 0.1 for agents moving with Brownian Motion as it gives a similar rate of motion to that of insects.

3.2 Lévy Flight

Lévy Flight is a type of random walk that is considered to share statistical similarities with human mobility [13]. A *flight* is defined to be the longest straight-line trip from one location to another that an agent makes without directional change or pause. This type of motion is frequently used to model foraging patterns in animals. There is considerable literature relating insects, including Honeybees and fruit flies, to probabilistic foraging movements characterised by Lévy Flight [14]. The principle is that each step made by an agent is governed by four variables: flight length (l), direction (θ, chosen uniformly from $[0, 2\pi]$), flight time (Δt_f), and pause time (Δt_p).

Flight lengths and pause times are selected randomly from their respective probability density functions $p(l)$ and $\psi(\Delta t_p)$, which are defined as Lévy distributions [15] with coefficients α and β respectively,

$$p(l) \propto |\Delta t_f|^{(1+\alpha)}, \tag{2}$$
$$\psi(\Delta t_p) \propto t^{-(1+\beta)},$$

where t is positive, $\alpha \in (1, 2]$ and $\beta \in [-1, 1]$. We allow the simulation parameters to be c, α and β, which represent the scale, stability and location parameters respectively. The positive constant c is a measure of the width of the distribution, α is the exponent of the distribution which describes the asymptotic behaviour, and β determines the shift of the distribution.

Given the current location of an *insect* in the x-y plane, $(x(t), y(t))$, its position at the next time step $(x(t+1), y(t+1))$ is

$$\begin{aligned} x(t+1) &= x(t) + h\cos\theta, \\ y(t+1) &= y(t) + h\sin\theta, \end{aligned} \tag{3}$$

where h is $c\epsilon^{-1/\alpha}$, and ϵ is again a normally distributed random variable. Through our simulations we use $c = 0.05$ as the scale parameter. This generates a suitable scale for insect collisions, as described in the agent based model in Section 5. We consider the midpoint of the possible stability values, setting parameters $\alpha = 1.5$. We also use $\beta = -1$ as this gives the same pause time at each step.

4 Collisional Exchange

Collisional exchange is a process in which two entities collide, transferring a property from one to another. Collisional exchange is most commonly referred to when describing the energy transfers associated with collisions between molecules. However, we will use a model based on collisional exchange to describe the interactions between the various agents in our system. The modelling of infection patterns between animals in a network is often a difficult process [10] as there is little knowledge of contact data. Observation of disease outbreaks can be measured with relative ease thanks to modern advances in data assembly, techniques for processing information, and technology enabling integrated analysis [16]. Conversely, finding how contact of the wildlife can affect the transmission takes a more difficult approach.

Given a crop population that requires pesticide treatment, confined within a region (the field), a pesticide is released in a specified localised area. As a result, insect populations living within the field may acquire some amount of the pesticide. Members of these local insect populations can be employed as carriers of these pesticides, delivering them to their targets (in this case, *crops*). The individuals can also transfer some amount of pesticide to other members of the insect population, should they happen to be close enough, allowing them to further disperse the pesticide around the field. We will show how the motion and collisions between insects - alongside the amount of the *chemical* acquired by each insect at a given time - affects the overall dispersal of the pesticide.

4.1 Transmission of Chemical

We assume that the pesticide is modelled as a pathogen (an *insect* or *crop* is 'infected' by a *chemical*), due to the way that the *chemical* disperses through the crop population being analogous to an epidemic. We use an SI (Susceptible-Infected) model - the simplest form of disease model [17] - to assign each agent in the system a state. This can be either susceptible (S) or infected (I), determined by whether or not the *crop* or *insect* has come into contact with the *chemical*. We assume that all *crops* and *insects* are susceptible to the transmission of a *chemical* at the initial stage of the simulation. Any given individual (*crop* or *insect*) can be 'infected' by the *chemical*, changing its state from 'susceptible' to 'infected' and may have a specified concentration of *chemical* at any given time. However, once an individual has left the 'susceptible' state, it is not possible to return to this state and it must remain

'infected' indefinitely.

The SI model describes the rate of increase of infected agents by the following ODE,

$$\frac{dI_{\mathrm{a}}}{dt} = \beta_{\mathrm{a}} I_{\mathrm{a}} \left(1 - \frac{1}{N_{\mathrm{a}}}\right), \tag{4}$$

where $N_{\mathrm{a}} = S_{\mathrm{a}} + I_{\mathrm{a}}$ is the total population of agent a ($\mathrm{a} \in \{insect, crop\}$) and β_{a} is the transmission rate of infection of agent a.

The probability of a *chemical* being passed on from an *insect* or *crop* must have a particular distribution once a collision has occurred. This relationship is used to give the transmission rate of infection [10],

$$\beta_{\mathrm{a}} = \gamma K_{\mathrm{a}}, \tag{5}$$

where γ is the probability of transmission given a contact and K_{a} is the contact rate for agent a.

5 Agent Based Model

In the model, we combine the random walk trajectories (see Fig. 1) that characterise *insect* movement with a bounded field containing 9 columns of 41 *crops* in each (see Fig. 2). This orientation of the field was chosen in consideration of common metrics used in agriculture [18]. The initial positions of the *insects* are randomly generated (within the confined bounds of the specified field area) and they move according to their random walk. The localised initial position of the *chemical* is chosen by the user of the program. The aim is to measure the Diffusion Coefficient (outlined later in section 5.2) of the *chemical* for the given input variables. These variables include number of *insects* (N_I), number of *chemical* bodies (N_P), the infected area ($IA_{threshold}$[%]) and the localised position of the released chemicals (P[m]).

5.1 Conditions of the Model

The *chemical* is sprayed in a localised position and disperses across the field via Brownian Motion. The *insects* move across the field via Lévy Flight and the *crops* are fixed in specified positions, as shown in Fig. 2. Collisions between the agents govern the spread of the pesticide, and the changes of state associated with these collisions follow a series of rules stated below:

- Each agent has an intrinsic infection metric, C, which represents the relative amount of *chemical* transmitted to it. All *crops* and *insects* begin with $C = 0$, whilst all *chemicals* are initialised with $C = 1$. Any agent that has $C{>}0$ is assigned state I (infected) and otherwise by default, the agent will be assigned state S (susceptible) if it has $C = 0$.

- During a collision between a susceptible *insect* or *crop* and a *chemical*, the *insect* or *crop* adopts the *chemical*, becomes infected and can continue to interact with other agents. The *chemical*, however, is used now used up and can participate in no further interactions.
  [*chemical* + *insect*/*crop* (state S) $\rightarrow$ *insect*/*crop* (state I)]

- An infected *insect* can infect a susceptible *insect* upon collision, the infected *insect* will transfer 10% of its current amount of *chemical*.
  [*insect* (state I) + *insect* (state S) $\rightarrow$ *insect* (state I) + *insect* (state I)].

- Upon a collision between an infected *insect* and a susceptible *crop*, the *insect* will transfer 90% of its current amount of *chemical* to the *crop*. In this case the *crop* is now considered infected. Again, the *insect* is able to move freely and interact with other agents.
  [*insect* (state I) + *crop* (state S) $\rightarrow$ *insect* (state I) + *crop* (state I)].
- During a collision between an infected *crop* and a susceptible *insect*, the susceptible *insect* will become infected with 10% of the infected *crop's* concentration, the *crop* will remain unchanged.
  [*crop* (state I) + *insect* (state S) $\rightarrow$ *crop* (state I) + *insect* (state I)]

A collision occurs when two agents come within a specific threshold distance, unique to the specific agent being considered. For example, if the distance between *insect* i and *crop* c is 2 mm and the threshold distance of the *crop* is 5 mm, it holds true that a collision has taken place. The threshold distance is set by the user and can be defined as the diameter of the entity in question (the *chemical* particulates have negligible diameter and therefore no threshold distance). In other words, the user of the program has control over the type of *crop* and species of *insect* modelled in the system by varying the unique threshold distances, in addition to the parameter in the motion distributions that describes the maximum step taken by an agent. The distance between each agent and each *crop* is evaluated using the Euclidean distance measure. Using the Euclidean distance measure, the distance between two points, $p_1 = (x_1, y_1)$ and $p_2 = (x_2, y_2)$, in a 2-D plane is evaluated using

$$d(\mathbf{p_1}, \mathbf{p_2}) = d(\mathbf{p_2}, \mathbf{p_1}) = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}. \tag{6}$$

5.2 Diffusion Coefficient

One of the factors we must measure is the diffusion of substance per unit time. Fick's first law [19] relates the diffusive flux to the concentration under the assumption of a steady state. In our case, it postulates that the flux of the *chemical* goes from regions of higher concentration to regions of lower concentration, with a magnitude that is proportional to the concentration gradient of the *chemical* over the field area [m^2]. The diffusion flux J [$\mathrm{mol\,m^{-2}\,s^{-1}}$] in 2 dimensions is given by

$$J = -D\nabla\phi = -D\left(\frac{d\phi}{dx} + \frac{d\phi}{dy}\right), \tag{7}$$

where D [$\mathrm{m^2\,s^{-1}}$] is the Diffusion Coefficient, ϕ is the concentration of the *chemical* [$\mathrm{mol\,m^{-2}}$], x is the horizontal position and y is the vertical position, both given in metres. The Diffusion Coefficient is measured by the area of the infected regions of the field over the time taken to cover that area,

$$D = \frac{A}{t}. \tag{8}$$

The Diffusion Coefficient will form a metric which allows us to generate and understand observations from the model. The Diffusion Coefficient dimensions are $\mathrm{m^2\,t^{-1}}$ (i.e. the amount of area covered per unit time) and it is proportional to the squared velocity of the diffusing *chemical*.

5.3 Simulation Setup

The simulated random walks undertaken by the agents in the model are confined to a circular reflective boundary of radius of 2.5 m allowing which allows agents to travel up to 0.5 m outside of the field before returning. This design feature keeps *insects* from flying too far from their habitat, although the boundary could be easily altered to be penetrable (allowing agents to escape the system entirely) or periodic (allowing new agents to be generated to replace escapees). When a point is chosen outside of the boundary (call this *new point*), a line is drawn between this and the point at the previous time step

(*old point*). The intersection is found between the line and the circle (P), and *new point* is replaced by the reflection of vector $\mathbf{v}$ = *new point* - P with respect to the tangent line at the intersection point. A visualisation of the boundary conditions is shown in Fig. 3.

So far we have described the dynamics of one of the agents in the model, the *chemical*. In a more detailed description, each *chemical* that moves with Brownian Motion is a chemical body (composed of distinct particles) of the pesticide that has been released. This makes the model more manageable, as rather than modelling a very large number of singular microscopic particles that move randomly, we use chemical bodies that are on a similar scale to that of an insect. As all *chemicals* start the simulation with an infection rating of 1, this represents a relative amount of substance. In relativistic terms (and in no way accurate to real life, only for the purpose of simplifying the model), this amount is 0.01 mol of the gas. For example, if the gas is naphthalene, a common fumigant insecticide with a molar mass of 128 $\mathrm{g\,mol^{-1}}$, there would be 1.28 g of naphthalene in each particulate, corresponding to C=1. Concentration of the chemical is measured in $\mathrm{mol\,cm^{-2}}$, which is the amount of substance (C) over the area of the agent that contains the chemical.

Initially, the simulation begins by randomising the position of the *insects*, with the *chemicals* being positioned at one of the points highlighted in Fig. 2. Outputs of the program consist of D_{avg}, t_{avg} and IA_{avg}, which represent the average of the Diffusion Coefficient (D), the average number of time steps taken (t) and the average percentage of area (*crops*) infected respectively. The use of averages stems from the fluctuation in the results due to the modelling of completely random motion. For each simulation, we iterate the program five times and take the average for each output. Moreover, we have added an 80% threshold (cut-off percentage) to IA_{avg} in an attempt to reduce the fluctuation of the results further, meaning we only use outputs in the case where IA_{avg} reaches 80%. To counteract this key design decision, the area of the field is multiplied by IA_{avg} in an attempt to estimate the size of the infected area.

Due to the mechanics of the motions explained in Section 3, t_{avg} is a time step that cannot be expressed in seconds. As a result, we will adopt t as the units of t_{avg}, which is the unknown time taken for each time-step. Using this unit of measure, we are able to compare t_{avg}, and of course D_{avg}, for different starting states (e.g. number of starting *insects*) but cannot realistically quantify its magnitude in SI units (International System of Units).

6 Results

This section concentrates on the results of our model in the specific case of Honeybees pollinating Sunflower fields. Through research, we estimate that the extreme average length of Honeybees and Sunflowers (diameter of the face area) are 15 mm and 150 mm respectively. As a result, the threshold distances passed to the program were 7.5 mm and 75 mm. Our decisions on the *crop* and *insect* species were made with consideration to the sensitive dependence of the program on these threshold distances.

All of the results are observed on a particularly small scale area, with a horizontal distance of 4 m and a vertical distance of 4 m. Unfortunately, we were forced to experiment with this relatively small area due to software limitations. The running time of the simulation increases drastically with an increase in the field area due to the computational expense of the program. Our initial configuration uses a realistic crop spacing [18]; we initialised a field with 369 *crops* corresponding to 9 columns spaced 0.5 m apart with 41 rows of *crops* spaced 0.01 m apart as shown in Fig. 2. The size of field and orientation of the *crops* remains constant throughout each simulation.

Fig. 2 shows the initialisation of the grid, with the *crops* being represented by hollow circles and a possible subset of localised positions displayed in red. There is also an example of a series of colour maps displaying the concentration of the amount of *chemical* on the *crops* at different time steps. The area used in the calculation for concentration is πr^2, where r is the radius of a sunflower (75 mm).

6.1 Rate of Chemical Transmission Through Crops

Fig. 4 shows how the number of *crops* and *insects* in either state (susceptible or infected) change over time. Almost the entire *insect* population is infected within the first 10 seconds. However, the state of the *crops* have a more gradual change, with the graphs eventually levelling out at the point in time where 80% of *crops* have been infected. This is where the amount of *chemical* still available (which has not been absorbed by various *crops*) is diminishing. Therefore, this suggests that in some cases it is not possible to reach a point in the system whereby 100% of the crop population is in the infected state, since the system reaches this point exponentially slowly. This finding further reinstates our design decision of adding $IA_{threshold}$.

Increasing the probability of transmission results in an increase in average transmission rate, as shown in Fig. 5. The transmission rate is found by counting the number of times the *chemical* is passed between agents (either those involving *crops* or *insects*) and dividing by the number of time steps taken (i.e. average total transmissions/average total time). This result is consistent with Eq. 5, which states that there is a linear relationship between β and γ. Using this result in conjunction with the rate equation, we calculate the average gradients of each plot and take this as an estimate of the contact rate, K. For *crops*, this is K=26.4 and for *insects* this is K=130.7.

6.2 Diffusion Rate of the Chemical

Here we test various states and observe the effect on D_{avg} of the *chemical*. To begin with, we tested how increasing N_P affects D_{avg} using the parameters noted in row 4 of Table. 2 as shown in Fig. 6. Observing this graph, there is no clear relationship between N_P and D_{avg}, which is a direct impact of the fluctuation in the results due to the modelling of random motion. Next we test how increasing N_I affects D_{avg} by using the parameters in row 2 of Table. 2. This provides a much clearer trend, as shown in Fig. 7. There is a strong positive correlation between N_I and D_{avg}.

In an attempt to understand the rate at which the relationship between N_P and D_{avg} increases in the long term, we evaluate D_{avg} when N_P is 5000. We estimate that D_{avg} is 0.553 at this value of N_P. Similarly, we estimated that D_{avg} is 1.308 when N_I is 5000. Therefore, a pattern is distinguished for both relationships. Comparing D_{avg} when N_P is 5000 with D_{avg} when N_P is 600, we see that there has only been a minimal 0.133 increase. Therefore, as N_P and N_I increase, the rate at which D_{avg} increases is exponentially lower.

6.3 Time Taken to Disperse Chemical Through Crops

In order to disperse the *chemical* in the most efficient way, the time taken for it to infect the majority of the field must be minimised. Here we test the impact that increasing N_P has on t_{avg} using simulation parameters noted in row 4 of Table. 2, as shown in Fig. 6 b). In addition, we measure t_{avg} as N_I increases, using the simulation parameters in row 2 of Table. 2, shown in Fig. 7 b).

Both figures follow a similar pattern. Generally, t_{avg} decreases, but notice that t_{avg} decreases at a lower rate as N_I/N_P is increased. This tells us that increasing N_I/N_P has a significant effect on the time steps for small increments, until a certain number is reached. Beyond this number the increase

no longer has the initial positive contribution. Similarly to Section 6.2, we evaluate that when N_I is 5000, t_{avg} is 18.3. Moreover, we evaluate that when N_P is 5000, t_{avg} is 40.8.

6.4 Stability Parameter

The stability parameter α (used in Eq. 3) also has an effect on the diffusion rate. This parameter ranges from 1 to 2 and defines the flight length of *insects* (see Eq. 2). Although this is kept at 1.5 for most of the simulations, increasing this parameter gives the graph shown in Fig. 8. These results show that α has a direct effect on D_{avg}, which stems from the relationship between α and the step size chosen for the next position of a given *insect*. The step size becomes smaller as α increases, hence the *insects* have a smaller flight length and thus will not cover as much distance across the field.

6.5 Initial Location of Chemical Dispersal

The *chemical* is released in localised positions across the field. As the *insects* are initialised in random positions, the *chemical* must be released in optimal positions in order to maximise D_{avg}. Here we show what localised position is considered optimal in this particular case.

By varying the initial placement of the released *chemical* (the localised position within the field), we used the inner rectangle of the top left side of the field. Due to the symmetrical nature of the field, we assume the results would be equivalent for the other segments of the field. Observing the results in Table. 1, the method that produces the highest values of D_{avg} and IA_{avg} is by initially releasing the *chemical* in the centre region of the field.

7 Discussion

The rate of infection is much faster for *insects* as it is for *crops*, as shown in Fig. 5. This comes as a result of there being more collisions that occur amongst *insects* than there are between *insects* and *crops*. In this instance of the model, *crops* are established to have 10 times the radius of transmission of *insects*, so one would assume that other agents would fall into this zone more often. However, this result shows that due to the *crops* being stationary agents and the *insects* dynamic ones, there are in fact more collisions with *insects* and *chemicals* per time step and thus the transmission rate is much faster.

In terms of decreasing t_{avg} and increasing D_{avg}, there are several possible ways of doing so. Increasing the N_I, adjusting the localised position where the *chemical* is released or increasing N_P (e.g. the area the *chemical* covers initially) are all possible solutions. In realistic applications of our model, constraints would be placed on N_I and N_P and the initial position of the *chemical* (i.e. the dimensions of the field constrains the initial position of the *chemical*). The optimal solution to minimising t_{avg} while obeying this real-life constraints, would be by combining all three methods using an optimisation method where the objective function would consist of a t_{avg} value for each variable, subjected to the constraints of the variables. A similar technique could be adopted for maximising D_{avg}.

As noted in Section 6.3, we see that t_{avg} is 40.8 when N_P is 5000 and t_{avg} is 18.3. This demonstrates that increasing N_I (Honeybees) is roughly twice as effective as increasing N_P (0.01 mol per particulate). However, it is required that an acceptable N_P is used (in this case there were $(1/50)N_I$ of N_P). It is notable how the particular *insect* species in question behaves in over populated circumstances, which will have a direct result on the constraint on N_I. More specifically, there is a threshold, that when crossed, the negative impacts of the addition of more *insects* out-weights the positive impacts. This is also true for the particular type of *chemical* in use. As a result, the objective function would

be scaled accordingly.

When using the method of spraying the chemical in a localised position, we found that the optimal area to spray the *chemical* was in a circle of radius 1 m centred at the origin of the field. Practically, it could be difficult to release the chemical in this position as opposed to outer regions. If using mechanical sprayers to disperse the chemical, it would be beneficial to spray a given amount of crop rows at once. Instead of using tractors, a recent method being used in El Salvador is to distribute pesticides using drones fitted with tanks [20]. This would be a more practical approach to disperse the chemical and could also be more efficient at the diffusion process than the insect method used in the Agent Based Model.

8 Conclusion

Our findings show that increasing N_I is roughly twice as effective at diffusing the *chemical* efficiently than increasing N_P. Also, the optimal area to release the *chemical* is a unit circle (circle of radius 1m) about the origin of the field. However, it should be noted that further analysis should be conducted on the desired species of *insects* to be used in an attempt to disperse the *chemical*. Examples of analysis required are how the species behaves in over-populated circumstances, how they travel (what type of motion), how they behave during mating seasons, lifespan and how they react after 'colliding' with the species of *crop* in question. All of these will have positive or negative effects on the how the *chemical* is dispersed.

To conclude, this report outlines the relevant steps to build an agent based model that uses an *insect* population to disperse of a particular pesticide to infect or treat a field of *crops*. Thus enabling the user to build an objective function for an optimisation problem with specific constraints, that can be used to find the optimal values of N_I, N_P, P.

8.1 Merits and Limitations

The distance function encoded defines a collision and determines if the distance is less than a specific threshold. This means that this is not a head-on collision between agents, which could result in some loss of accuracy. However, if the *chemical* is dispersed through the air in this small space it is reasonable to assume that this would result in transmission of the *chemical*.

A limitation is that the types of random walks have a small amount of reliability. The model uses different types of probability distribution to predict the movement of *insects* but it is unclear what type of movement might relate to them. This is to say that some trajectories are due to some form of search strategy [21] that may affect the way *insects* move. An improvement to make would be to include a link between the random walk type and the objective of the navigation (e.g. foraging, mating, etc.).

8.2 Further Steps

To improve the efficiency of the simulation and the model as a whole, a better approach could be used to observe collisions. It takes a long time to process the collisional exchange, since function that evaluates the distance between agents measures the distance for many *insects* at each time step. To improve this we could instead develop a discrete event simulation that models elastic collisions between *insects*, which would involve finding velocities of the *insects* and *chemicals* in the system.

The model could have some members of the *insect* population moving with Lévy flight characteristics and others via a correlated random walk; more information on this is provided in Appendix B. There may be other types of random walk that would change the diffusion rate, but a factor to consider would be the species of the *insect* and also the type of *chemical* being used. If provided with experimental field data, the model could be used to highlight any advantages or disadvantages associated with some existing pesticides. Examples of data that could be collected include *crop* residue levels, soil moisture measurements, and weather information such as temperature and rainfall. All metrics which would provide information on the health of the *crops* and any negative effects excessive pesticide application may have.

Relaxing some of the assumptions would result in a more accurate model. The agent species could be altered to have different population sizes, perhaps sampled from a distribution or a differential equation, to model the variety of *crop* sizes and also different types of *insects*. Another assumption to remove is the relative volume of *chemical* particulates, which assumes each particulate would have a specific molar mass. To optimise the number of agents required, we could use a linear programming method to make a polynomial that fits the Diffusion Coefficient curve in order to maximise the result.

References

[1] J. Unsworth, "History of pesticide use." https://agrochemicals.iupac.org/index.php?option=com_sobi2&sobi2Task=sobi2Details&catid=3&sobi2Id=31, (Accessed: 23/11/18).

[2] G. Matthews, "Pesticide application methods." International Pesticide Application Research Centre, Imperial College London, 2000.

[3] International Labour Organisation, "Safety and health in agriculture." p.77, 1999.

[4] E. Held, "What happens when you stop using crop protection?." http://www.foodinsight.org/crop-protection-importance-copa-cogeca-pesticides, (Accessed: 21/10/18).

[5] D. Pimentel, "Amounts of pesticides reaching target pests: Environmental impacts and ethics." Agric Environ Ethics 8(1):17-29, 1995.

[6] United Nations Food and Agriculture organization, "Food chain crisis." http://www.fao.org/food-chain-crisis/en/, (Accessed: 21/10/18).

[7] D. Pimentel and L. Levitan, "Pesticides: Amounts applied and amounts reaching pests." BioScience, 36(2):86-91, 01/02/1986.

[8] Montana State University, "Avoiding pesticide drift." http://www.pesticides.montana.edu/reference/drift.html, (Accessed: 26/11/2018).

[9] New Brunswick Canada, "Pesticide application." https://www2.gnb.ca/content/gnb/en/departments/10/agriculture/content/crops/potatoes/pesticide_application.html, (Accessed: 26/11/18).

[10] M. Craft, "Infectious disease transmission and contact networks in wildlife and livestock." Philosophical Transactions of the Royal Society Biological Sciences, 370(1669), 26/05/2015.

[11] G. Viswanathan, E. Raposo, and M. da Luz, "Lévy flights and superdiffusion in the context of biological encounters and random searches." Physics of Life Reviews, 5(3):133-150, 2008.

[12] R. Schick, S. Loarie, F. Colchero, B. Best, A. Boustany, D. Conde, P. Halpin, L. Joppa, C. McClellan, and J. Clark, "Understanding movement data and movement processes: current and emerging directions." Ecology Letters, 11(12):1338-1350, 2008.

[13] D. Raichlen, A. Wood, A. Gordon, A. Mabulla, F. Marlowe, and H. Pontzer, "Evidence of lévy walk foraging patterns in human hunter–gatherers." Proc Natl Acad Sci USA, 111(2):728-733, 14/01/2014.

[14] S. Wolf, E. Nicholls, A. Reynolds, P. Wells, K. Lim, R. Paxton, and J. Osborne, "Optimal search patterns in honeybee orientation flights are robust against emerging infectious diseases." Scientific Reports 6, Article 32612, 2016.

[15] N. Valler, A. Prakash, H. Tong, M. Faloutsos, and C. Faloutsos, "Epidemic spread in mobile ad hoc networks: Determining the tipping point." Lecture Notes in Computer Science, vol 6640. Springer, Berlin, Heidelberg, 2011.

[16] N. Fefferman and E. Naumova, "Innovation in observation: a vision for early outbreak detection." Emerging Health Threats Journal, 3(6), 2010.

[17] Institute for Disease Modeling, "Si and sis models." https://institutefordiseasemodeling.github.io/Documentation/general/model-si.html, (Accessed: 30/10/18).

[18] Grains Research and Development Corporation, "Crop placement and row spacing." https://grdc.com.au/__data/assets/pdf_file/0018/210294/crop-placement-and-row-spacing-northern-fact-sheet.pdf.pdf, (Accessed: 1/11/18).

[19] W. Smith, "Foundations of materials science and engineering (3rd ed.)." McGraw-Hill, 2004.

[20] C. Baraniuk, "The crop-spraying drones that go where tractors can't." https://www.bbc.co.uk/news/business-45020853, (Accessed: 30/11/18).

[21] L. Giuggioli and F. Bartumeus, "Animal movement, search strategies and behavioural ecology." Journal of Animal Ecology, 79(4):906-909, 22/03/2010.

[22] P. Kareiva and N. Shigesada, "Analysing insect movement as a correlated random walk." Oecologia (Berlin) 56:234-238, 1983.

Appendix A Graphs and Tables

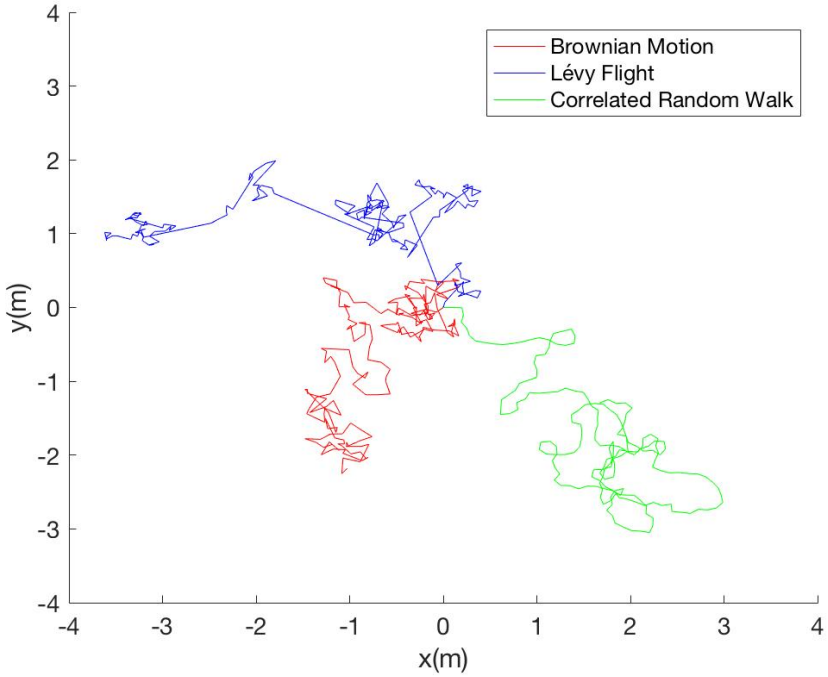

Figure 1: Examples of random trajectories, taken over a period of 200 steps. The characteristics of the different trajectories are quite varied. Brownian motion moves in a random pattern as it deviates from the origin, due to the fact that the turning angle at each step is generated randomly. However, Lévy flight has more obvious deviations as the turning angle is drawn from some distribution, but the direction still has an element of randomness and some large displacements. Finally, the correlated random walk (see Appendix B) shows directional movement (with some noise) due to the restriction of the turning angle choice.

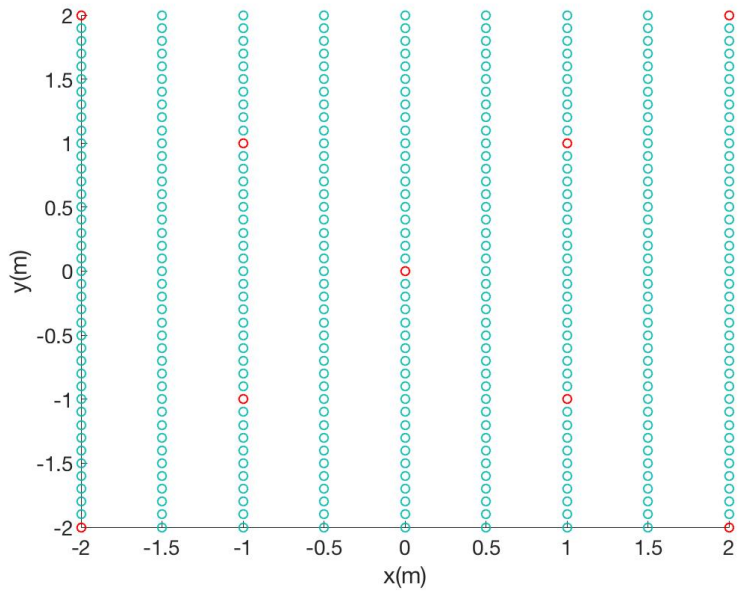

Figure 2: *Crops* initialised in nine columns that are spaced 0.5 metres apart [18] with 41 rows. The *crops* circled in red indicate some of localised positions we have experimented with in which the *chemical* is initially released.

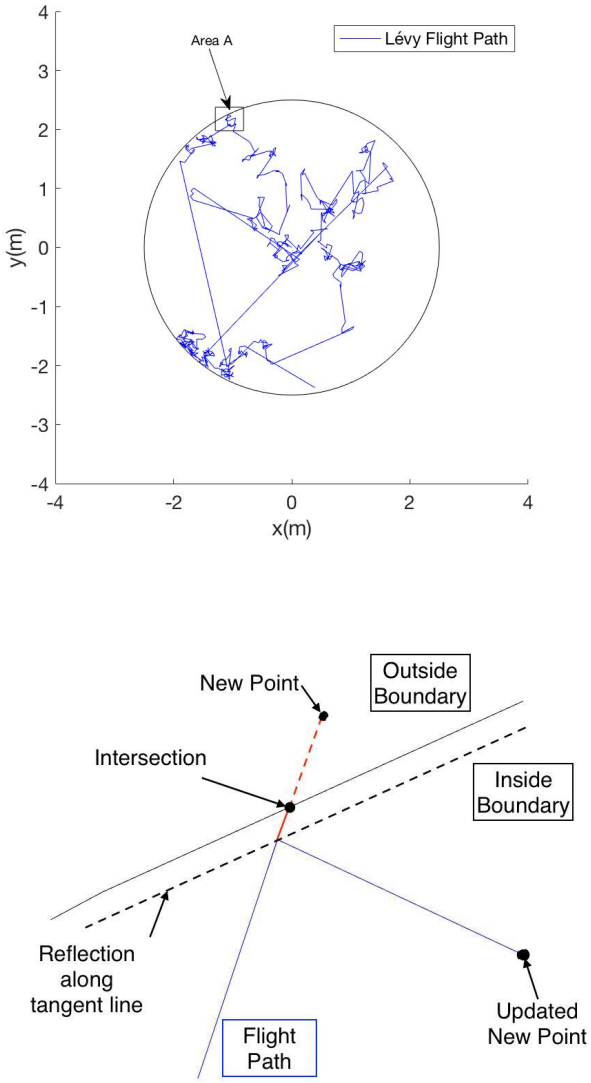

Figure 3: Figure depicting the reflective boundary placed on the field. This shows a single *insect* moving with Lévy flight that is constrained to move within a theoretical circle of radius 2.5 metres. The top image shows the *insect's* path over 500 time steps, and the below image shows a zoomed in version of Area A. The New Point is outside of the boundary, so the vector from the Intersection to the New Point is reflected along the tangent line as shown. Hence, the flight path is corrected to follow this reflected vector and the Updated New Point is chosen as the next position for this *insect*.

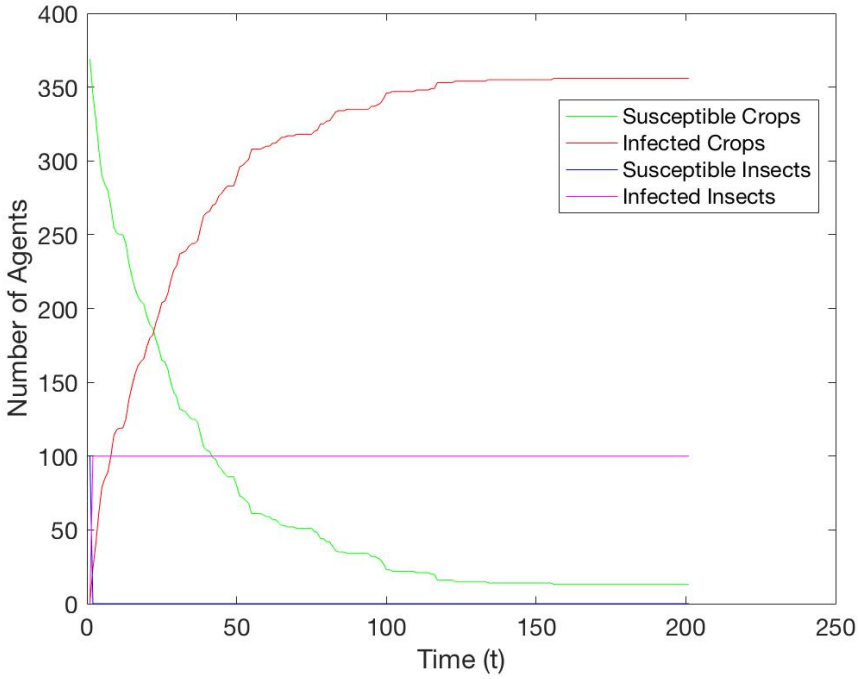

Figure 4: Population change of susceptible agents vs. infected agents over the number of time steps, t. The conditions of this simulation are noted in row 1 of Table 2

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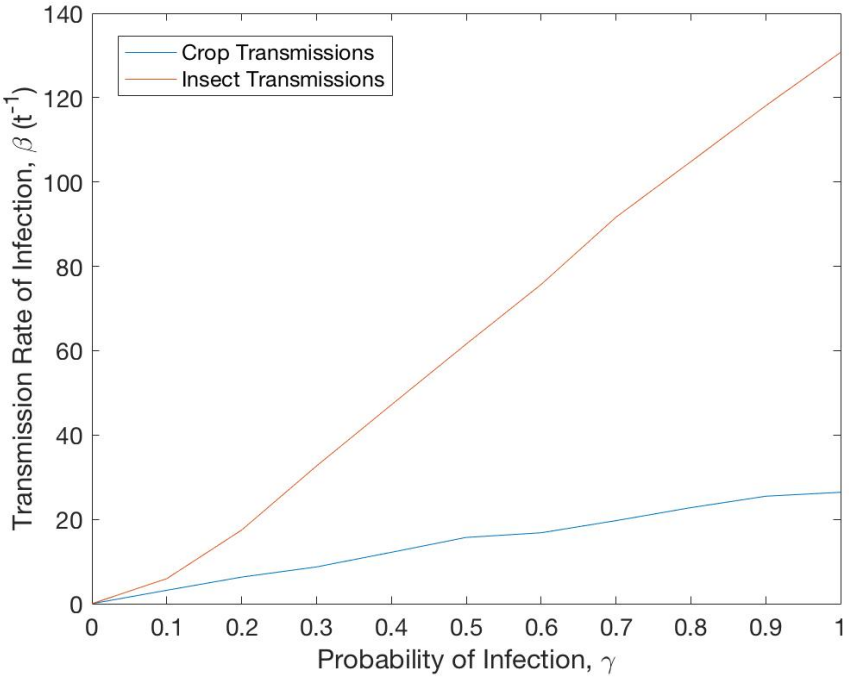
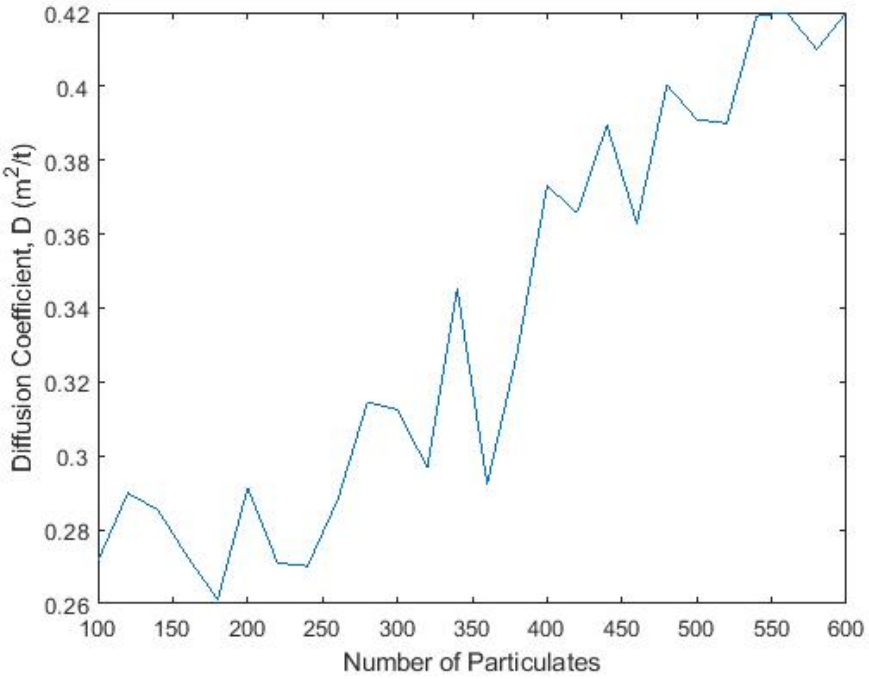
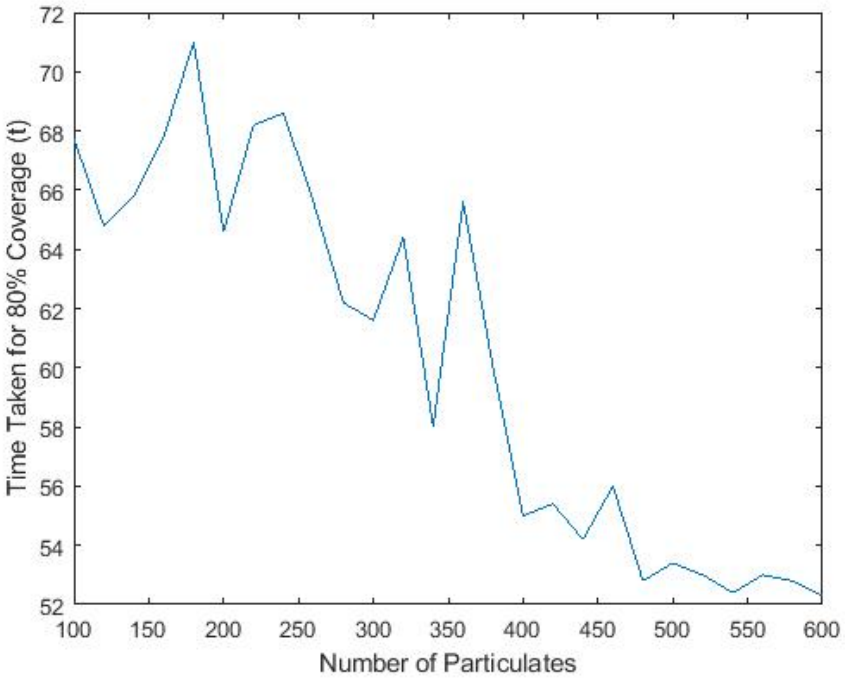


Figure 5: This shows the difference between transmission rates for *insects* and *crops*. One transmission occurs whenever the *chemical* is passed between agents with probability γ. *Crop* transmissions are those involving *crops* and *insects* transmissions are those involving *insects*. Results were obtained using simulation 1 in Table 2

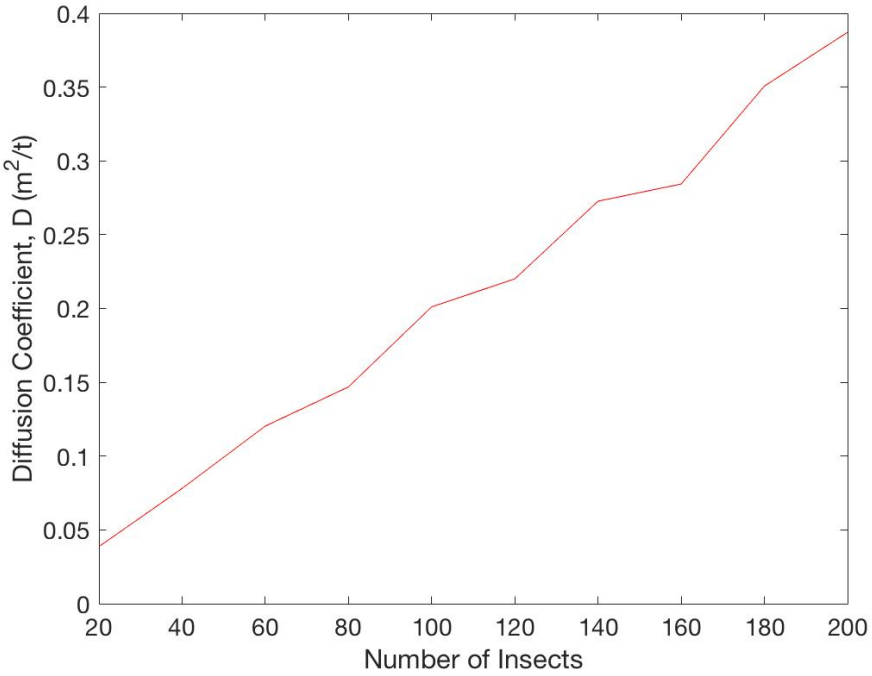


(a) T_{avg} for 80% of the *crops* to become infected Vs. N_P

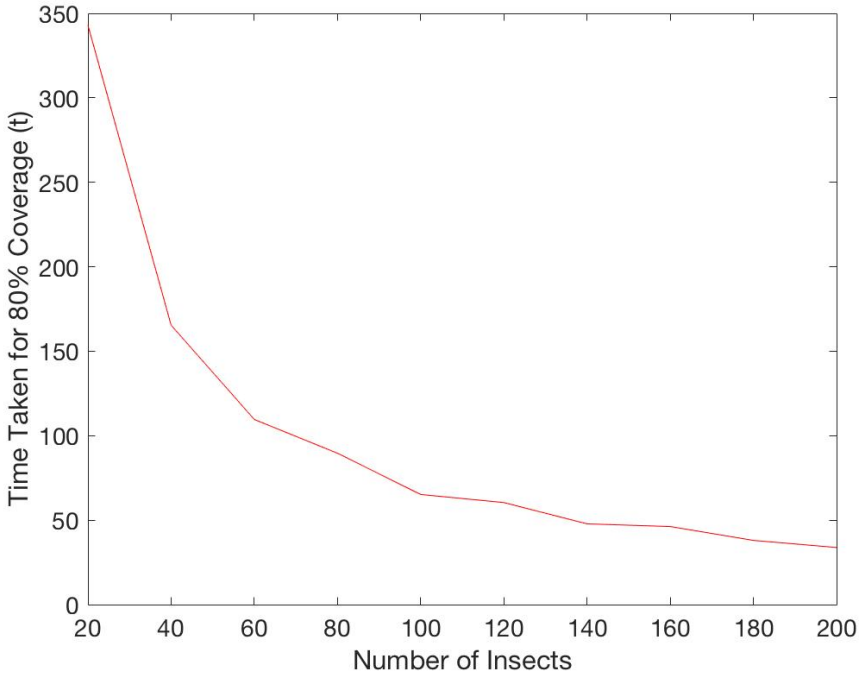


(b) T_{avg} for 80% of the *crops* to become infected Vs. N_P

Figure 6: The effect on the measured T_{avg} for 80% of the *crops* to become infected and the Diffusion coefficient, D_{avg}, when the number of particulates is increased and the number of *insects* is constant. The parameters of the simulation are noted in row 4 of Table. 2



(a) T_{avg} for 80% of the *crops* to become infected Vs. the N_I.



(b) T_{avg} for 80% of the *crops* to become infected Vs. the N_I.

Figure 7: The effect on the measured t_{avg} for 80% of the *crops* to become infected and the Diffusion coefficient, D_{avg}, when the number of *insects* is increased as the number of particulates is constant. The parameters of the simulation are noted in row 2 of Table. 2

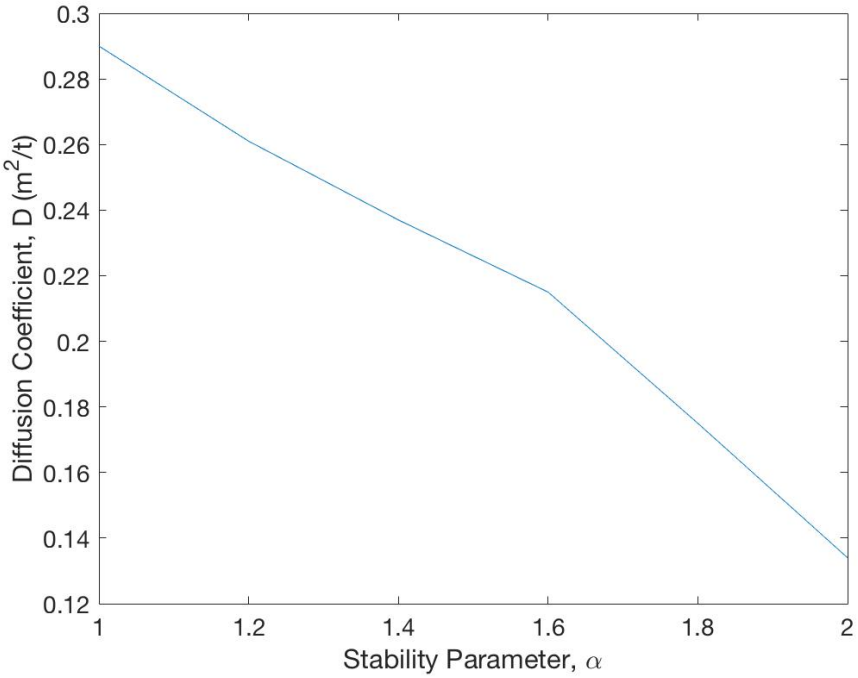


Figure 8: How varying the stability parameter effects the Diffusion coefficient, D.

Initial Placement	D_{avg} (m^2/t)	IA_{avg} (%)
(-2,2)	0.163	74.9
(-1,2)	0.171	77.6
(0,2)	0.151	68.6
(-2,1)	0.176	78.8
(-1,1)	0.188	79.4
(0,1)	0.203	80.8
(-2,0)	0.148	68.2
(-1,0)	0.227	82.7
(0,0)	0.215	81.6

Table 1: How varying the localised positions of the sprayed *chemical* impacts the values of D_{avg} and the IA_{avg}. Only the top-left section of the field has been considered due to the symmetry of the field. This simulation used the parameters noted in row 3 of Table. 2

Simulation	N_I	N_P	$IA_{threshold}(\%)$	P(m)
1	100	100	80	(0,0)
2	20-200	100	80	(0,0)
3	100	100	none	(0,0)-(-2,2)
4	100	100-600	80	(0,0)
5	0	100	80	(0,0)

Table 2: The values for each parameter in the different simulations of the program. N_I is the number of *insects*, N_P is the number of particulates, $IA_{threshold}$ is threshold coverage (the cut-off percentage of infected *crops*), and P is the localised position of the spray.

Appendix B Further Information

Correlated Random Walk

In this type of random walk the direction of movement at one time is correlated with the direction of movement at the next time. In other words, this type of random walk is different due to directional persistence. This type of motion best applies to *insects* that typically move in a generalised direction [22]. The turning angles between steps are not uniformly distributed as in our other random walk models. Instead, they are chosen so that the most probable turning angle is zero, meaning the walker tends to continue in the same direction. This gives the comparison of an *insect* flying in a more controlled path with fewer deviations, as opposed to Lévy flight (see Fig. 1).

The step made by each *insect* is similar to Brownian motion, except the angle at each time step is dependent on the previous angle. There is a max value that the angle can vary between, θ_{max}. The turning angle and position are given by

$$\theta(t+1) = \theta(t) + \theta_{max}\epsilon - \frac{\theta_{max}}{2}, \tag{9}$$

$$x(t+1) = x(t) + r\cos\theta,$$

$$y(t+1) = y(t) + r\sin\theta,$$

where we choose $\theta_{max} = \pi/4$ to be a suitable maximum angle, as this would allow a fair range of motion whilst moving in the same general direction.